Full wwPDB NMR Structure Validation Report (i)

Mar 23, 2026 – 07:49 PM UTC

PDB ID	:	6CM1 / pdb_00006cm1
BMRB ID	:	30426
Title	:	MT1-MMP HPX Domain with Blade 2 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:

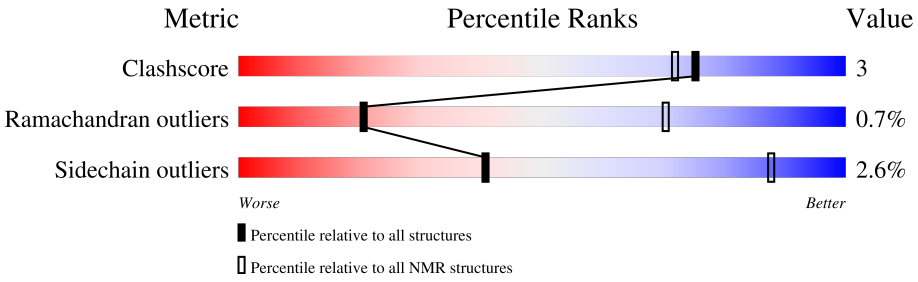
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	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	40% 59% .
2	B	211	33% 66% .
2	C	211	31% 67% .

2 Ensemble composition and analysis

This entry contains 15 models. Model 10 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:262 (615)	1.54	10

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

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:

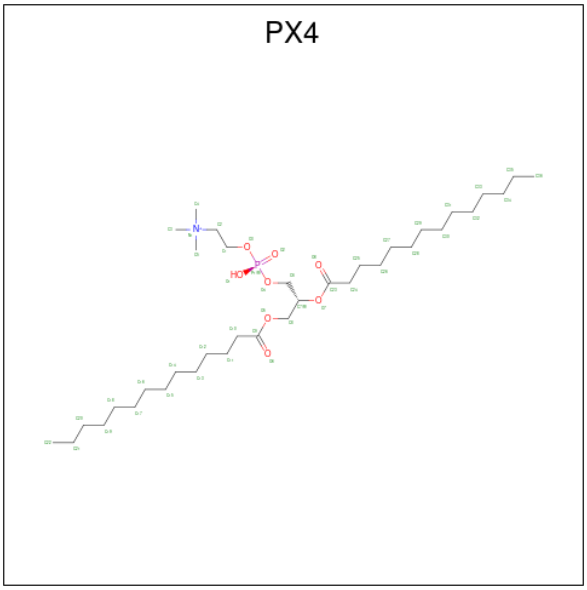
Chain	Residue	Modelled	Actual	Comment	Reference
B	99	PRO	-	insertion	UNP P02647
B	100	TYR	-	insertion	UNP P02647
B	101	LEU	-	insertion	UNP P02647
B	102	ASP	-	insertion	UNP P02647
B	103	ASP	-	insertion	UNP P02647
B	104	PHE	-	insertion	UNP P02647
B	105	GLN	-	insertion	UNP P02647
B	106	LYS	-	insertion	UNP 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
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			118	36	72	1	8	1
3	C	1	Total	C	H	N	O	P
			118	36	72	1	8	1
3	C	1	Total	C	H	N	O	P
			118	36	72	1	8	1
3	C	1	Total	C	H	N	O	P
			118	36	72	1	8	1
3	C	1	Total	C	H	N	O	P
			118	36	72	1	8	1
3	C	1	Total	C	H	N	O	P
			118	36	72	1	8	1
3	C	1	Total	C	H	N	O	P
			118	36	72	1	8	1
3	C	1	Total	C	H	N	O	P
			118	36	72	1	8	1
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
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

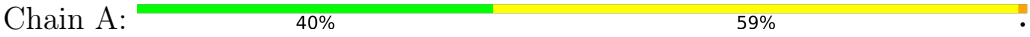
4 Residue-property plots

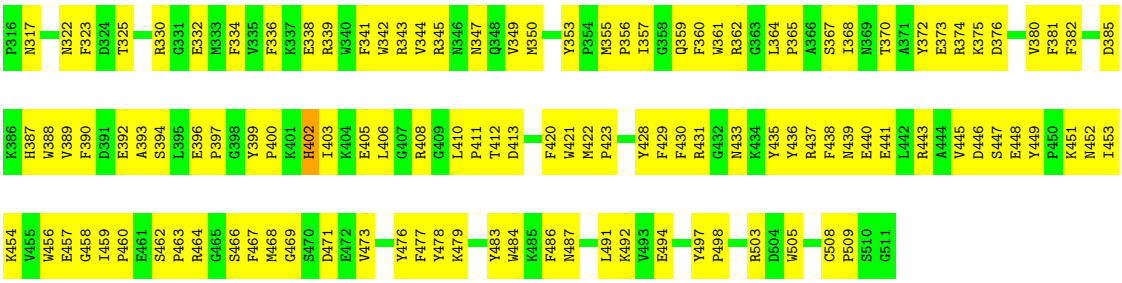
4.1 Average score per residue in the NMR ensemble

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

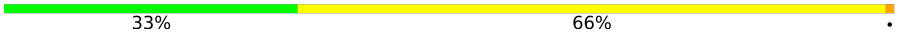
Chain A:





• Molecule 2: Apolipoprotein A-I

Chain B:

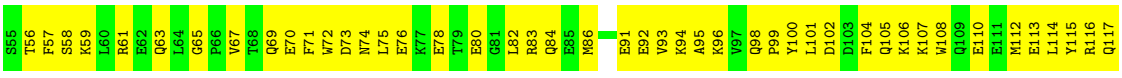


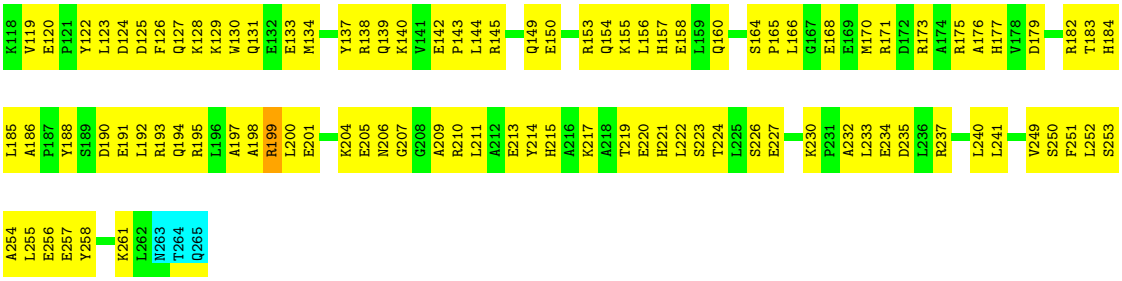


• Molecule 2: Apolipoprotein A-I

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:

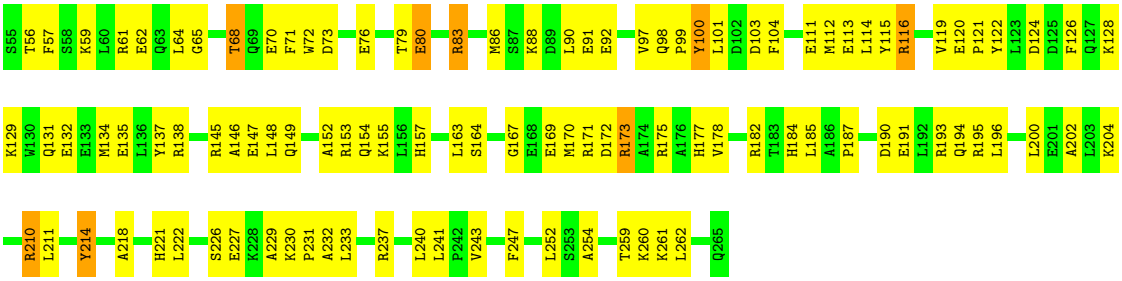




• Molecule 2: Apolipoprotein A-I

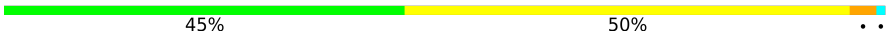
Chain B:

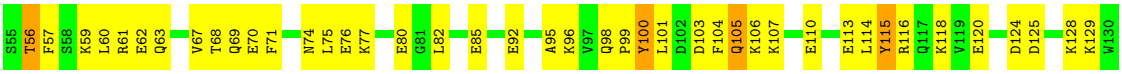


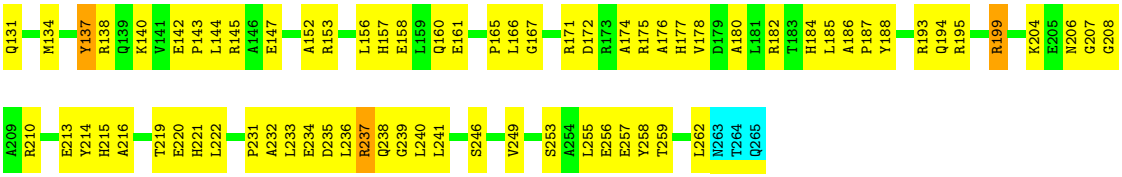


• Molecule 2: Apolipoprotein A-I

Chain C:





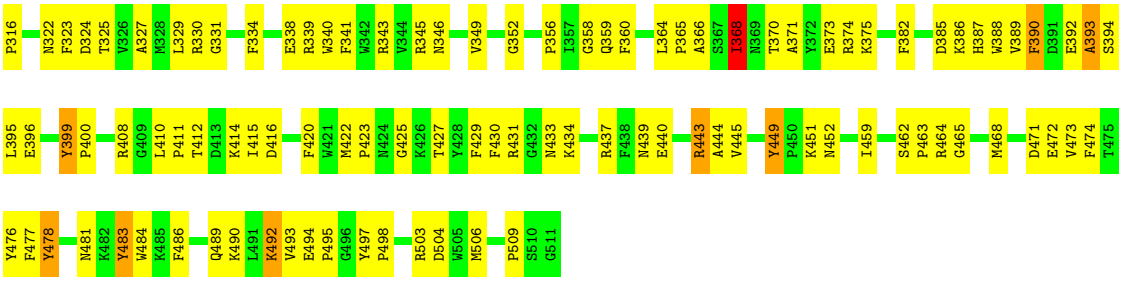


4.2.2 Score per residue for model 2

• Molecule 1: Matrix metalloproteinase-14

Chain A:

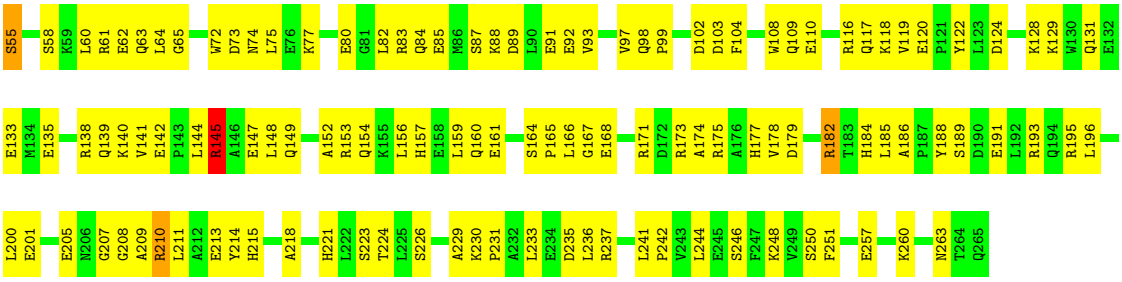




• Molecule 2: Apolipoprotein A-I

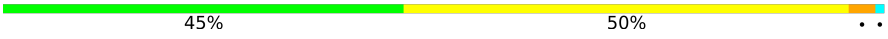
Chain B:

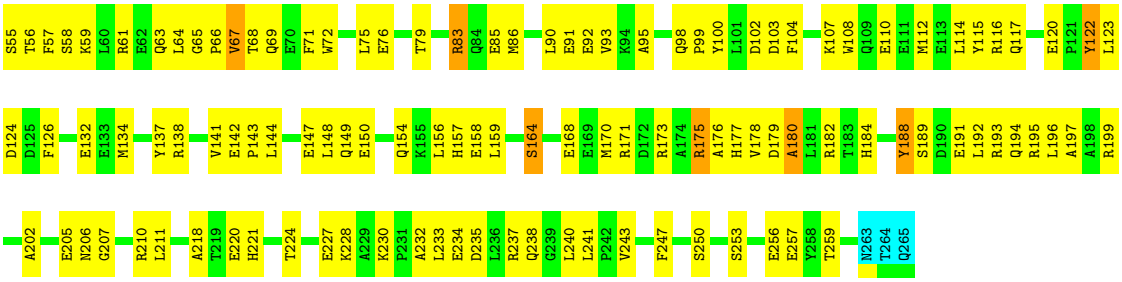




• Molecule 2: Apolipoprotein A-I

Chain C:

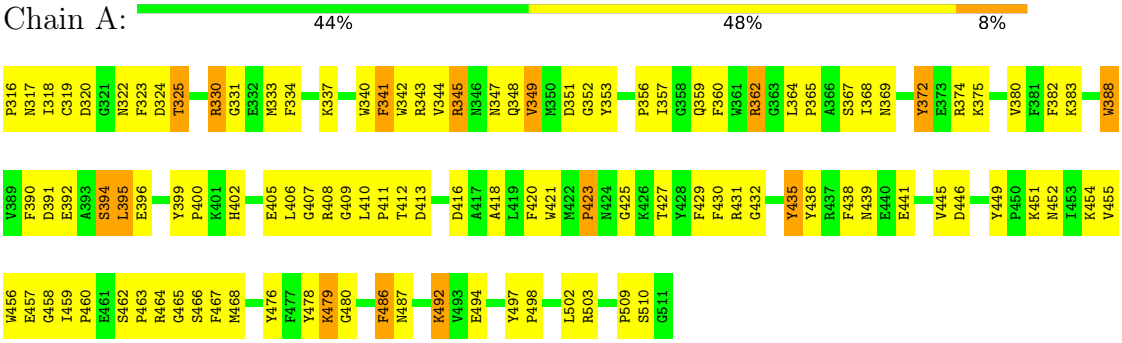




4.2.3 Score per residue for model 3

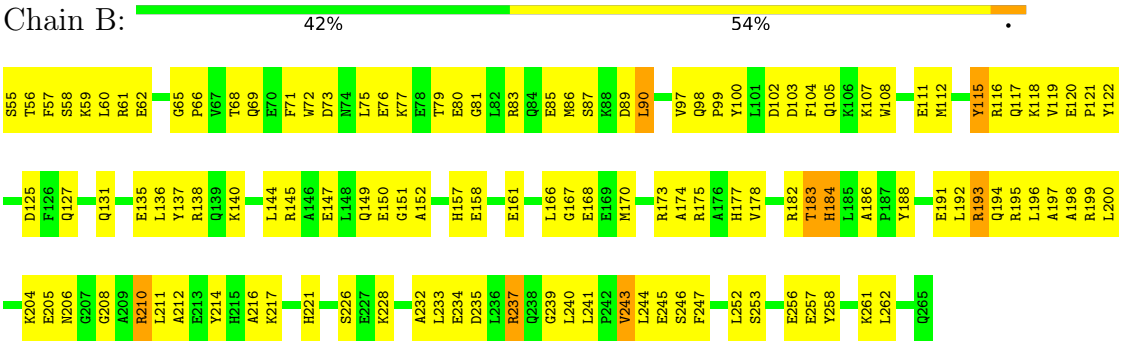
• Molecule 1: Matrix metalloproteinase-14

Chain A:



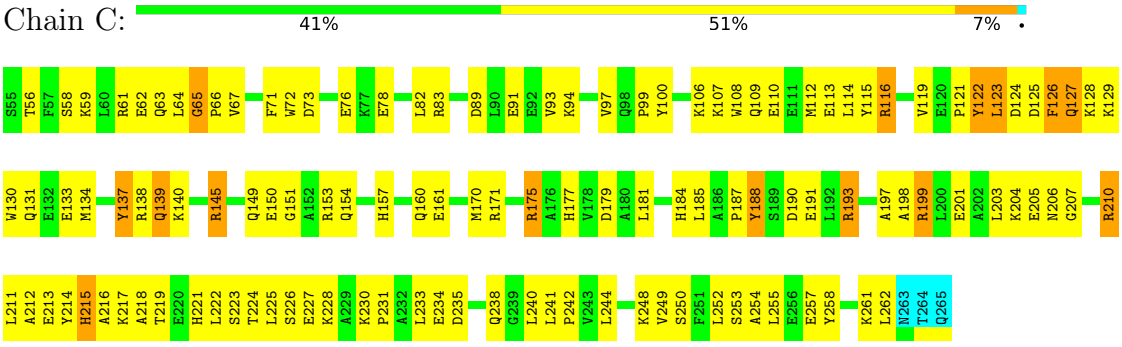
• Molecule 2: Apolipoprotein A-I

Chain B:



• Molecule 2: Apolipoprotein A-I

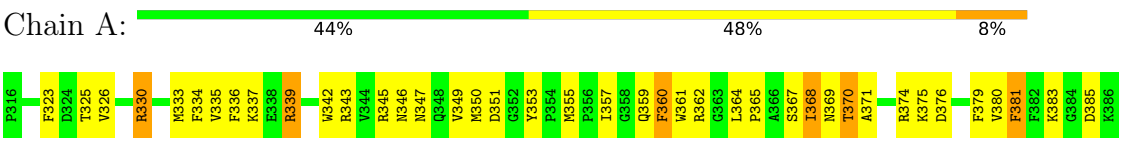
Chain C:

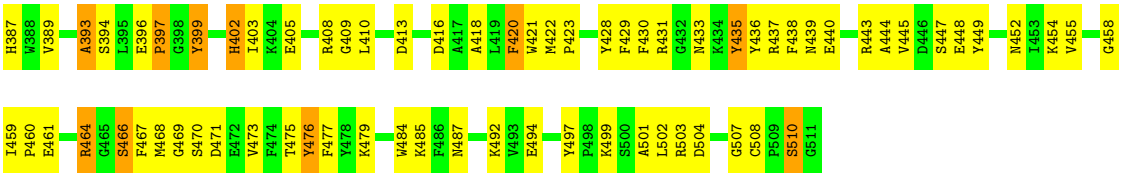


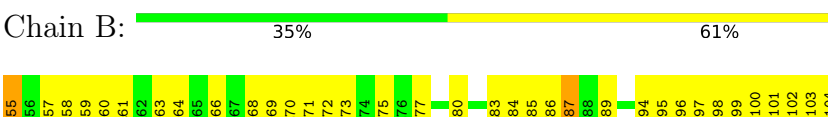
4.2.4 Score per residue for model 4

• Molecule 1: Matrix metalloproteinase-14

Chain A:

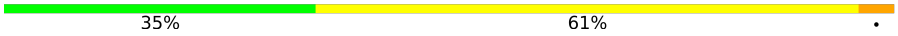


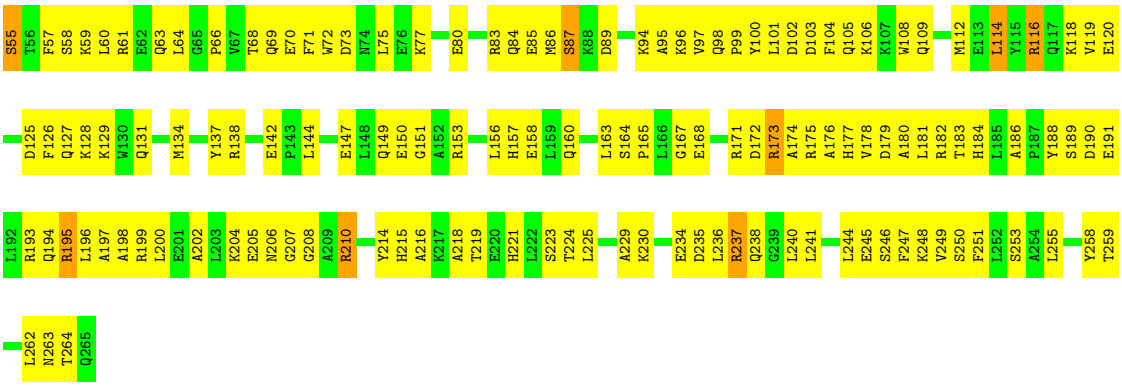




• Molecule 2: Apolipoprotein A-I

Chain B:

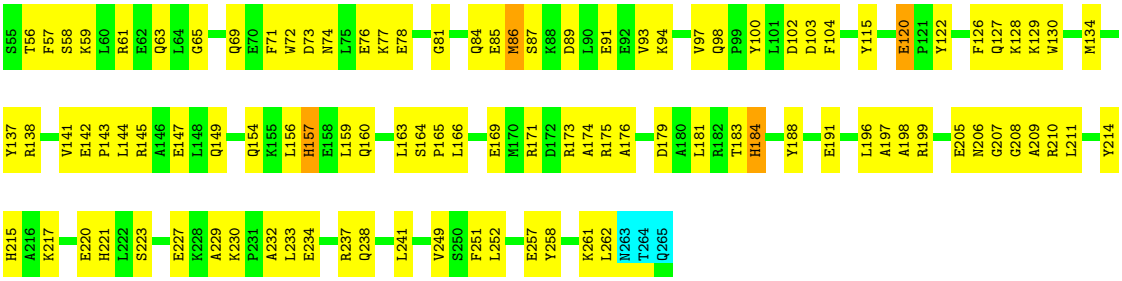




• Molecule 2: Apolipoprotein A-I

Chain C:



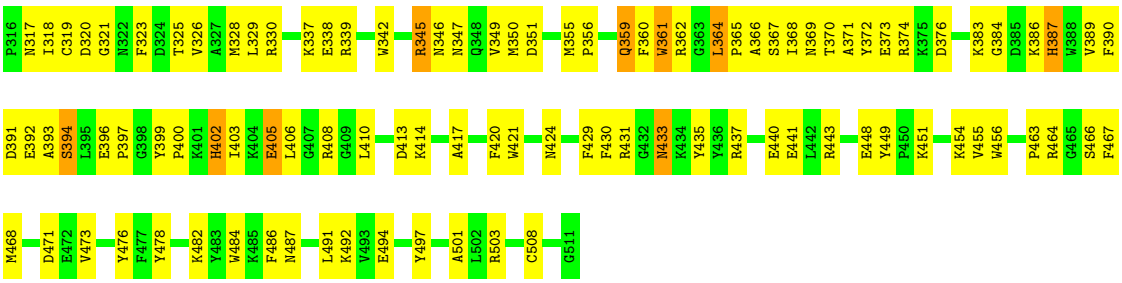


4.2.5 Score per residue for model 5

• Molecule 1: Matrix metalloproteinase-14

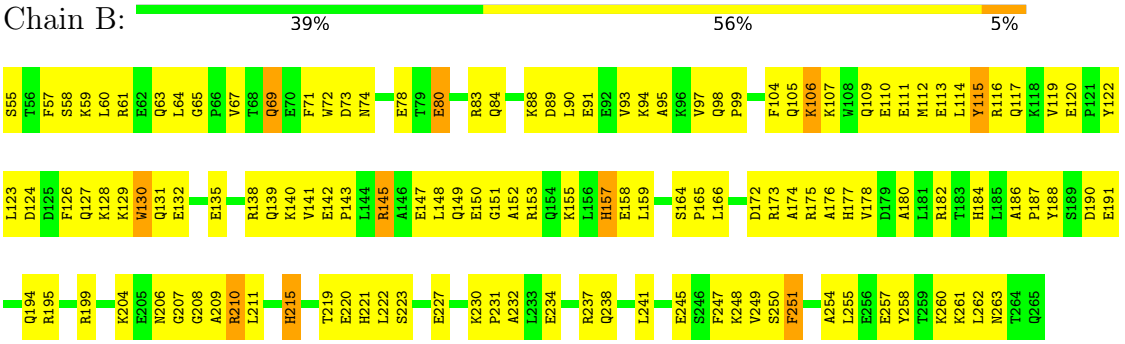
Chain A:





• Molecule 2: Apolipoprotein A-I

Chain B:



• Molecule 2: Apolipoprotein A-I

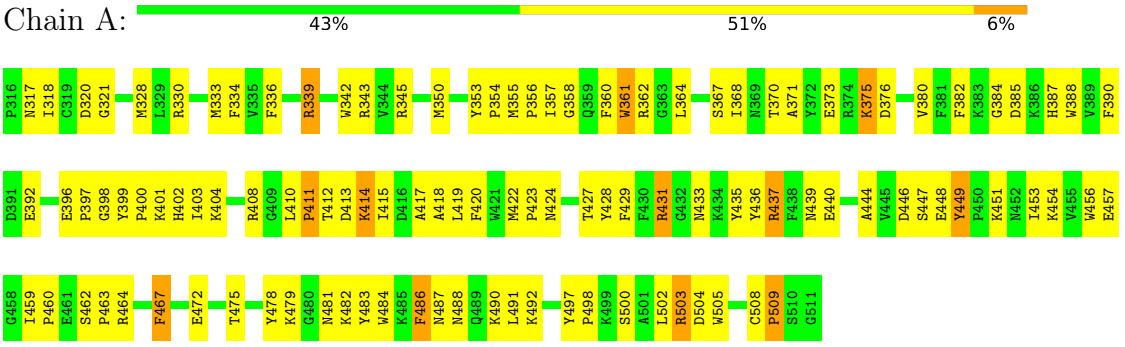
Chain C:



4.2.6 Score per residue for model 6

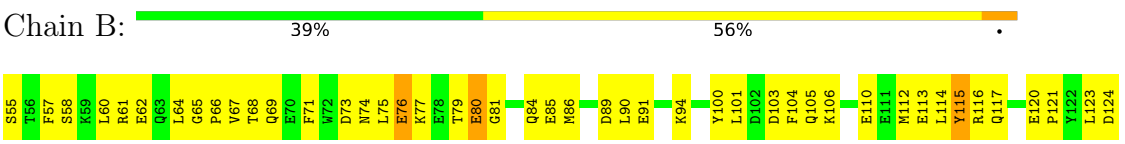
• Molecule 1: Matrix metalloproteinase-14

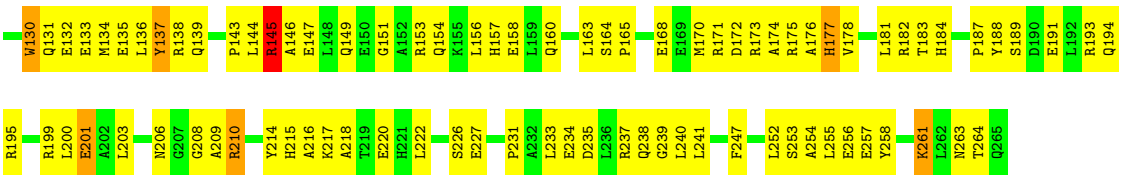
Chain A:



• Molecule 2: Apolipoprotein A-I

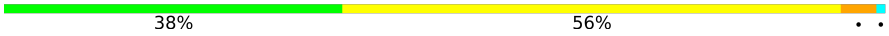
Chain B:





• Molecule 2: Apolipoprotein A-I

Chain C:



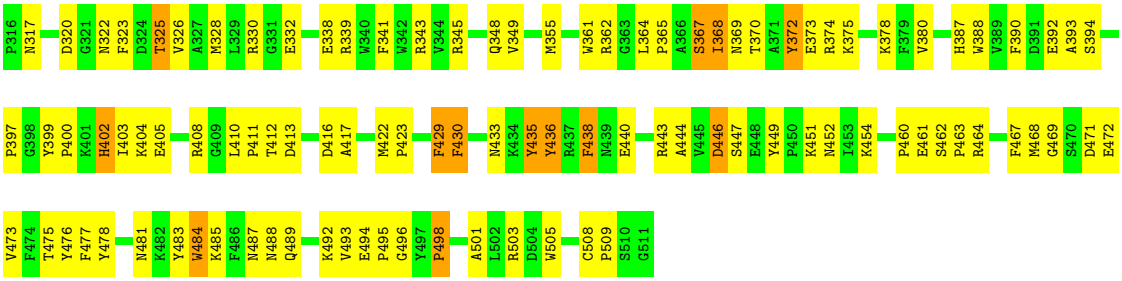


4.2.7 Score per residue for model 7

• Molecule 1: Matrix metalloproteinase-14

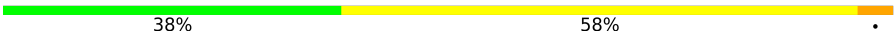
Chain A:

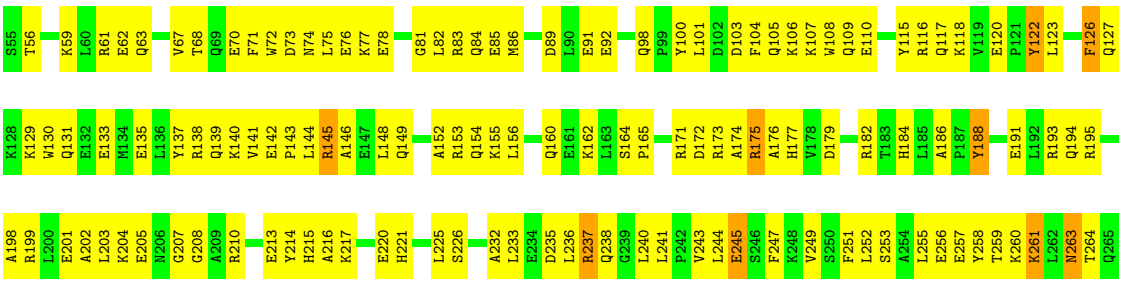




• Molecule 2: Apolipoprotein A-I

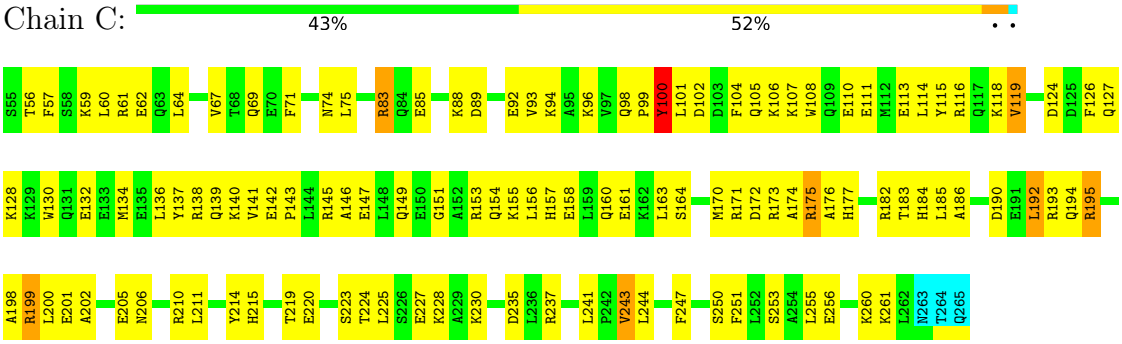
Chain B:





• Molecule 2: Apolipoprotein A-I

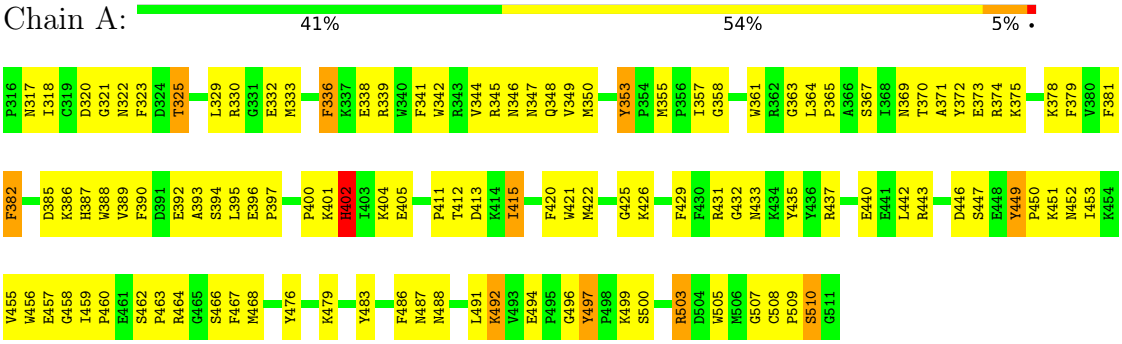
Chain C:



4.2.8 Score per residue for model 8

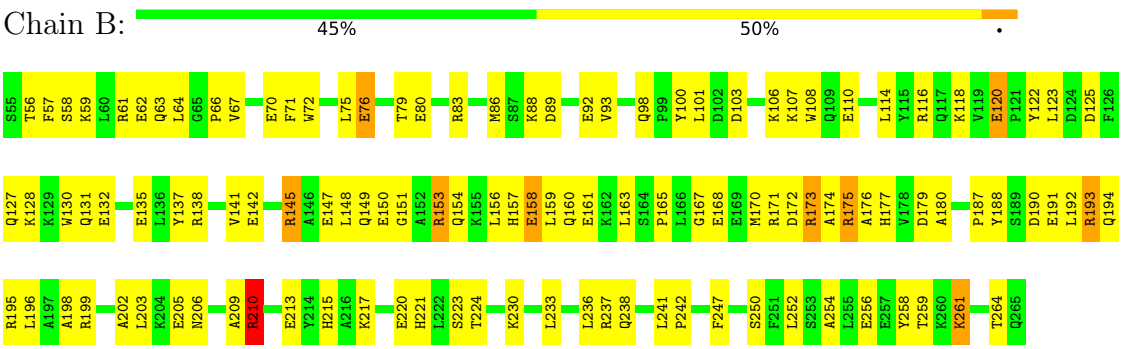
• Molecule 1: Matrix metalloproteinase-14

Chain A:



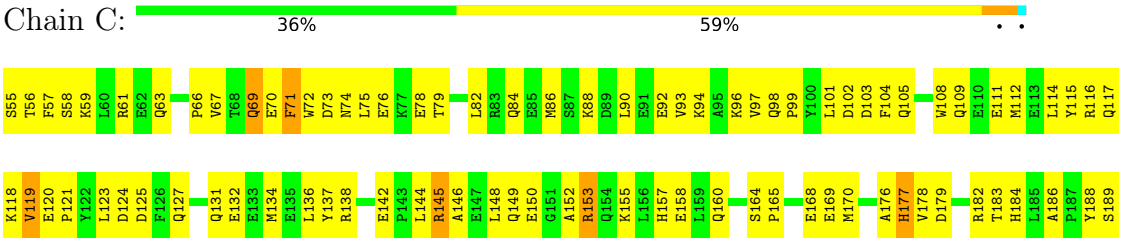
• Molecule 2: Apolipoprotein A-I

Chain B:



• Molecule 2: Apolipoprotein A-I

Chain C:

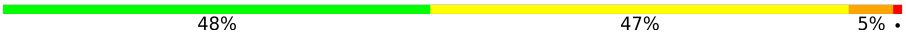


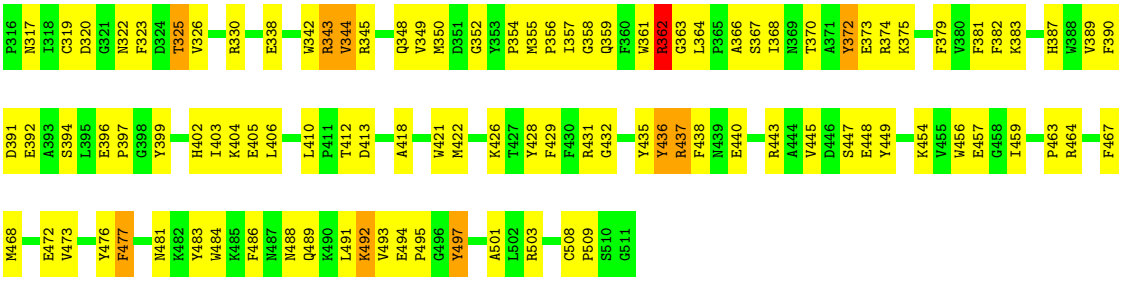


4.2.9 Score per residue for model 9

• Molecule 1: Matrix metalloproteinase-14

Chain A:

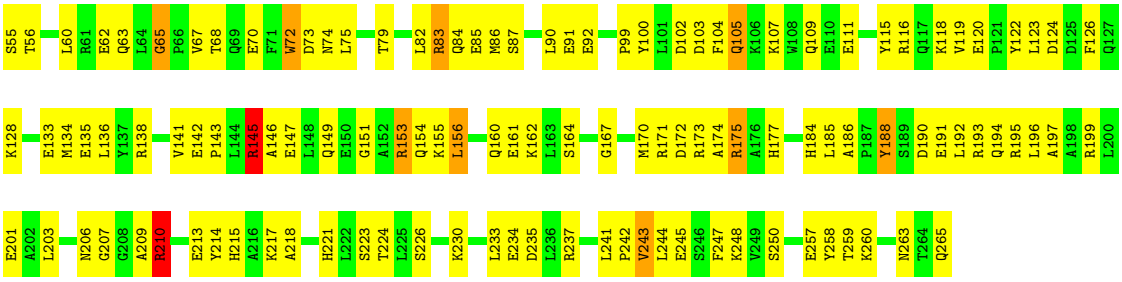




• Molecule 2: Apolipoprotein A-I

Chain B:

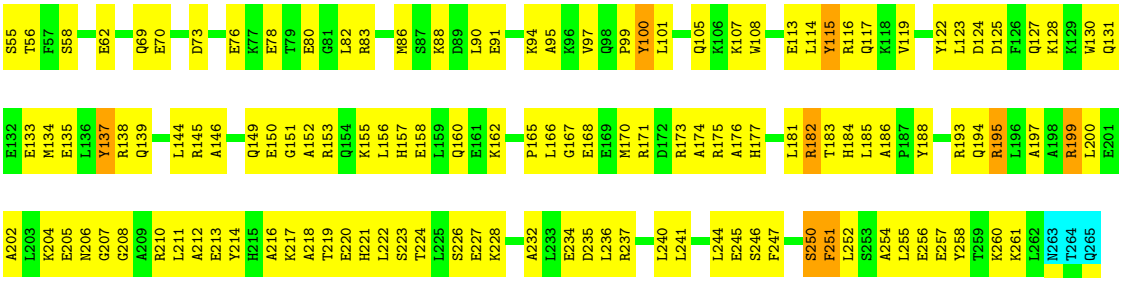




• Molecule 2: Apolipoprotein A-I

Chain C:

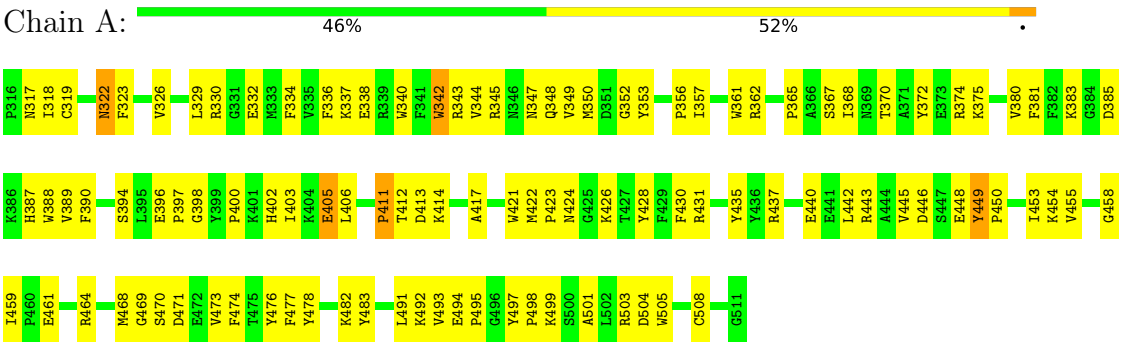




4.2.10 Score per residue for model 10 (medoid)

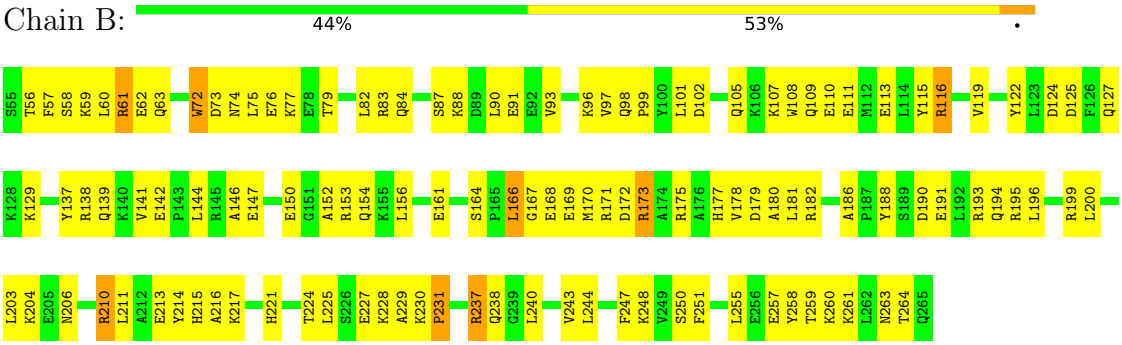
• Molecule 1: Matrix metalloproteinase-14

Chain A:



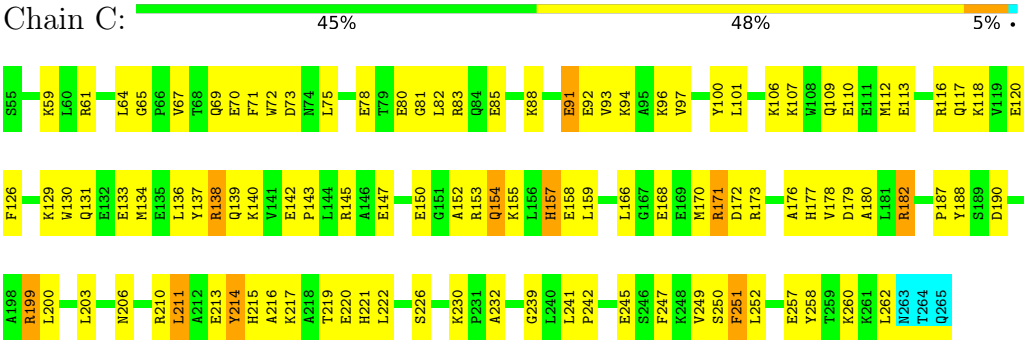
• Molecule 2: Apolipoprotein A-I

Chain B:



• Molecule 2: Apolipoprotein A-I

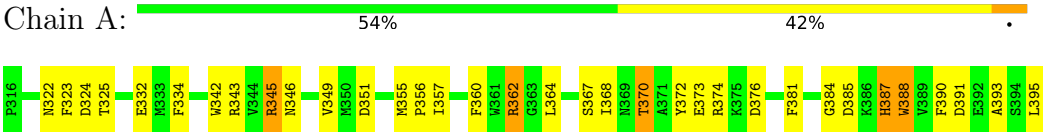
Chain C:

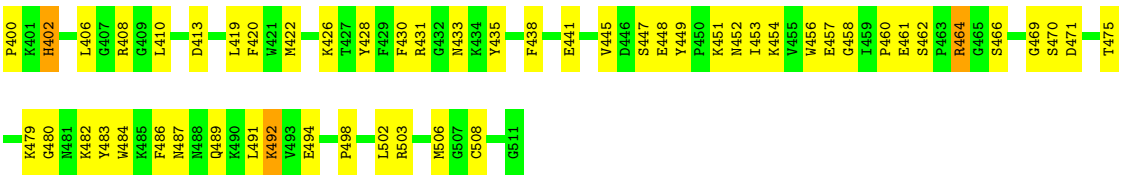


4.2.11 Score per residue for model 11

• Molecule 1: Matrix metalloproteinase-14

Chain A:





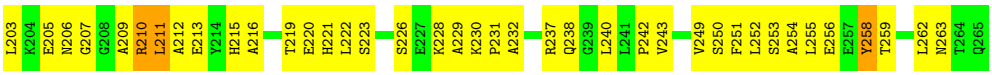
• Molecule 2: Apolipoprotein A-I

Chain B:









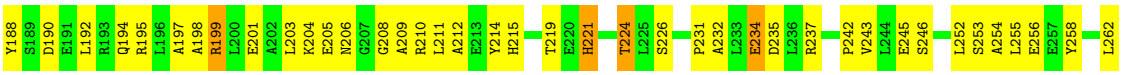
• Molecule 2: Apolipoprotein A-I

Chain C:







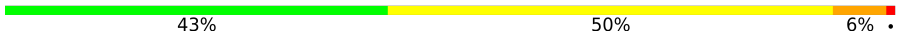




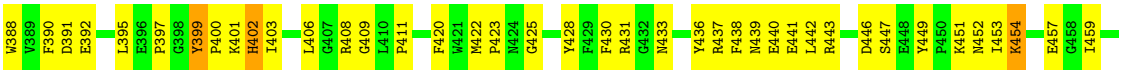
4.2.12 Score per residue for model 12

• Molecule 1: Matrix metalloproteinase-14

Chain A:



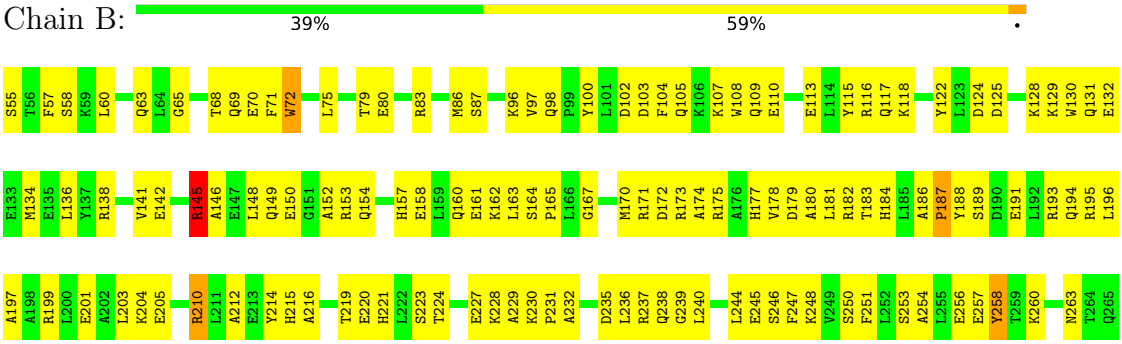






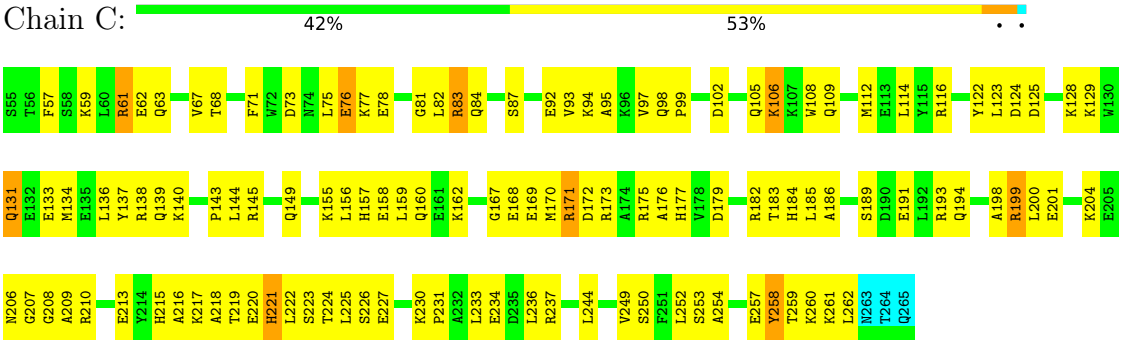
• Molecule 2: Apolipoprotein A-I

Chain B:



• Molecule 2: Apolipoprotein A-I

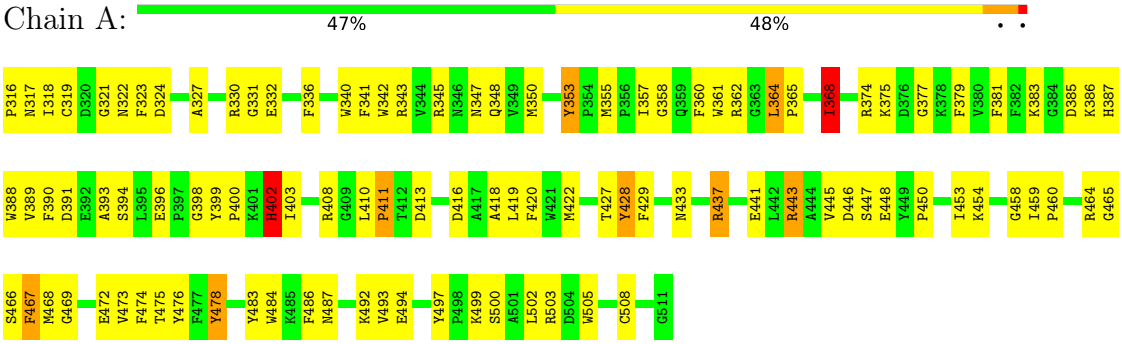
Chain C:



4.2.13 Score per residue for model 13

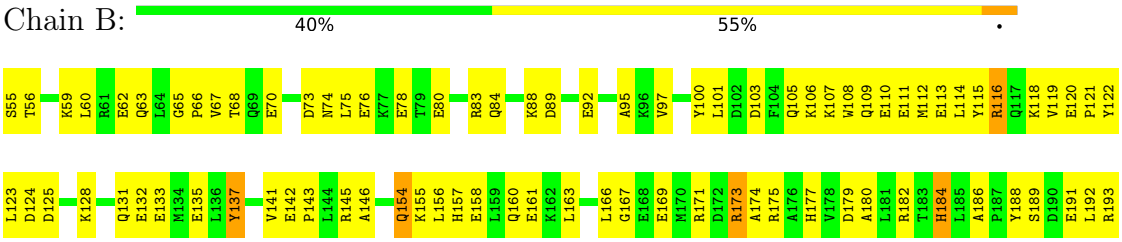
• Molecule 1: Matrix metalloproteinase-14

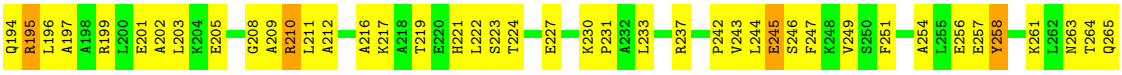
Chain A:



• Molecule 2: Apolipoprotein A-I

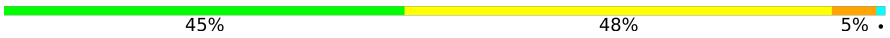
Chain B:

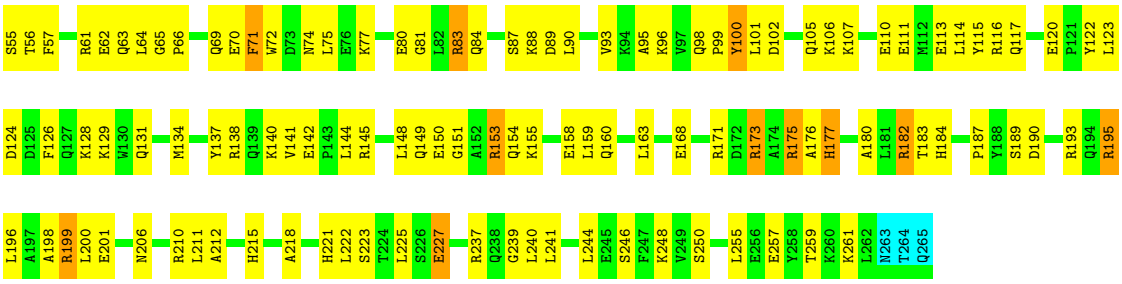




• Molecule 2: Apolipoprotein A-I

Chain C:





4.2.14 Score per residue for model 14

• Molecule 1: Matrix metalloproteinase-14

Chain A:

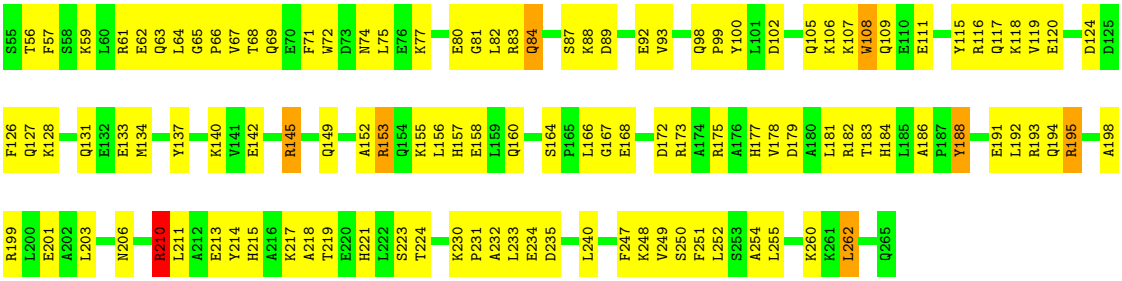




• Molecule 2: Apolipoprotein A-I

Chain B:

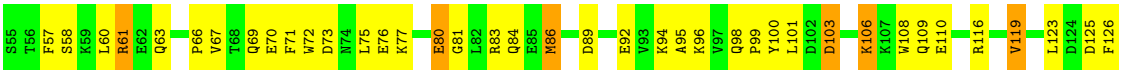


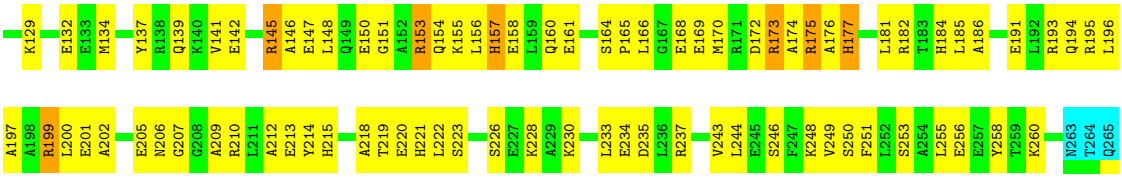


• Molecule 2: Apolipoprotein A-I

Chain C:



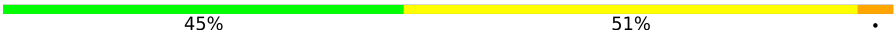


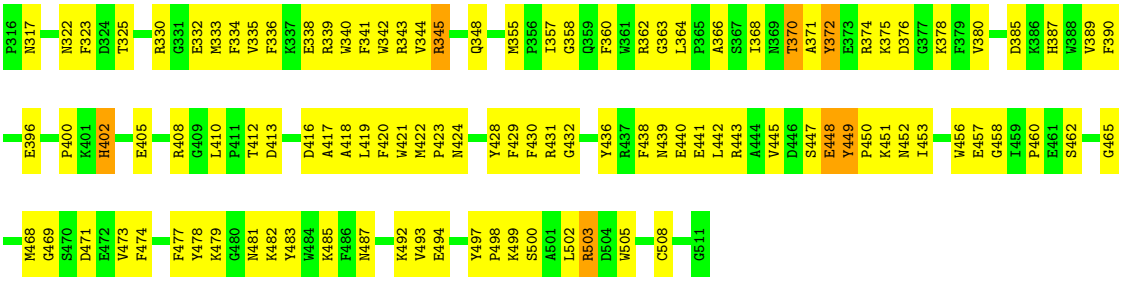


4.2.15 Score per residue for model 15

• Molecule 1: Matrix metalloproteinase-14

Chain A:

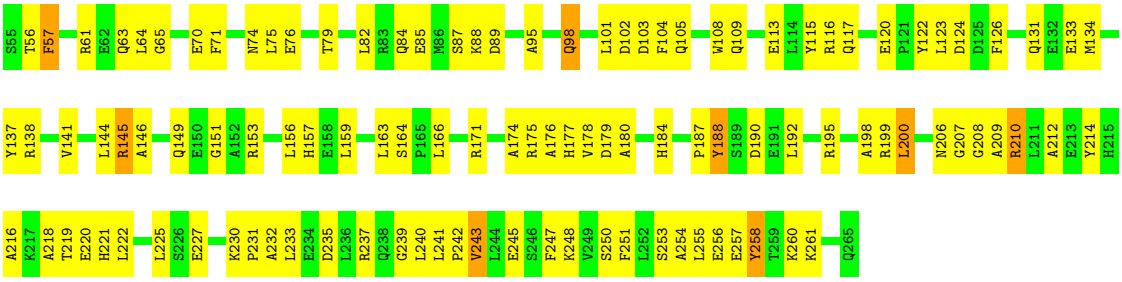




• Molecule 2: Apolipoprotein A-I

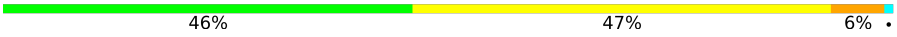
Chain B:

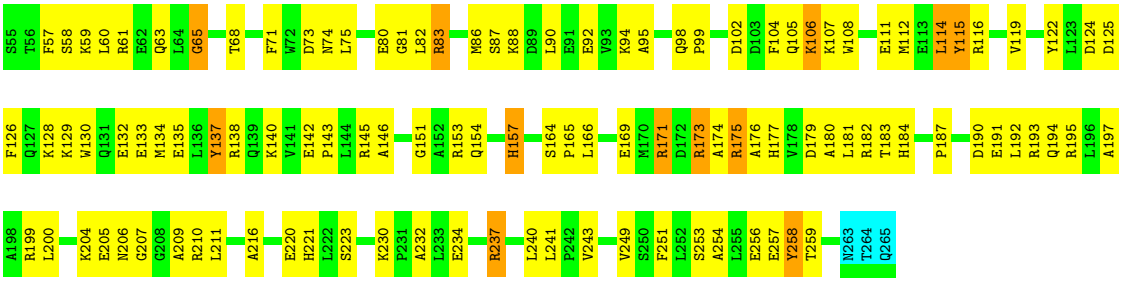




• Molecule 2: Apolipoprotein A-I

Chain C:





5 Refinement protocol and experimental data overview

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

Of the 15 calculated structures, 15 were deposited, based on the following criterion: *all calculated structures submitted*.

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

Software name	Classification	Version
HADDOCK	structure calculation	HADDOCK2.1
NAMD	refinement	NAMD2.1 with CUDA GPU processing
NAMD	structure calculation	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: CL, NA, 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	2.09±0.05	44±7/1696 (2.6± 0.4%)	2.38±0.04	102±10/2286 (4.4± 0.4%)
2	B	2.18±0.04	55±8/1784 (3.1± 0.4%)	2.63±0.05	155±12/2394 (6.5± 0.5%)
2	C	2.17±0.04	53±8/1760 (3.0± 0.5%)	2.63±0.04	150±10/2364 (6.4± 0.4%)
All	All	2.15	2290/78600 (2.9%)	2.55	6114/105660 (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	8.9±2.3
2	B	0.0±0.0	5.9±1.6
2	C	0.0±0.0	7.5±1.6
All	All	0	335

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	152	ALA	N-CA	-11.49	1.32	1.46	12	3
2	B	172	ASP	CA-C	-10.13	1.42	1.53	12	1
2	C	95	ALA	N-CA	-10.01	1.34	1.46	15	1
1	A	477	PHE	CA-C	-10.00	1.39	1.52	15	2
2	C	221	HIS	ND1-CE1	9.78	1.42	1.32	14	4
2	B	157	HIS	ND1-CE1	9.76	1.42	1.32	2	5
2	B	232	ALA	C-N	9.58	1.46	1.33	5	2
2	B	63	GLN	CA-C	-9.54	1.39	1.52	12	1
2	C	106	LYS	CA-C	9.43	1.65	1.52	12	2
1	A	456	TRP	CA-C	-9.37	1.40	1.52	9	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	65	GLY	CA-C	9.35	1.58	1.51	1	3
1	A	368	ILE	CA-CB	-9.35	1.41	1.54	9	2
2	C	143	PRO	N-CD	9.24	1.60	1.47	12	1
1	A	462	SER	CA-C	9.23	1.60	1.53	12	3
2	B	148	LEU	CA-CB	9.22	1.68	1.53	8	2
2	C	142	GLU	N-CA	9.16	1.55	1.46	2	1
2	C	261	LYS	N-CA	-9.16	1.33	1.46	9	2
2	C	151	GLY	CA-C	-9.07	1.42	1.52	3	2
2	C	186	ALA	CA-C	8.96	1.63	1.52	7	2
1	A	361	TRP	NE1-CE2	-8.94	1.27	1.37	12	3
2	B	214	TYR	CA-C	-8.91	1.41	1.52	6	1
2	C	235	ASP	C-N	8.88	1.45	1.33	5	1
1	A	484	TRP	NE1-CE2	-8.86	1.27	1.37	12	3
2	C	207	GLY	C-N	8.84	1.43	1.33	2	3
2	C	78	GLU	CA-CB	8.83	1.67	1.53	9	2
2	C	167	GLY	CA-C	8.81	1.61	1.52	1	1
2	B	67	VAL	CA-C	8.79	1.63	1.52	6	2
1	A	439	ASN	CA-CB	8.71	1.64	1.52	15	3
2	B	171	ARG	CA-C	8.70	1.64	1.52	1	2
1	A	418	ALA	N-CA	-8.68	1.35	1.46	4	1
2	C	157	HIS	ND1-CE1	8.65	1.41	1.32	4	4
2	C	233	LEU	CA-CB	8.64	1.66	1.53	4	1
2	C	253	SER	CA-CB	8.56	1.66	1.53	14	2
1	A	353	TYR	CA-CB	8.54	1.64	1.54	10	3
2	C	130	TRP	NE1-CE2	-8.51	1.28	1.37	10	2
2	C	103	ASP	CA-CB	8.49	1.66	1.53	4	1
1	A	372	TYR	CA-C	8.47	1.62	1.52	12	4
2	B	59	LYS	CA-CB	8.47	1.66	1.53	8	2
2	C	65	GLY	N-CA	8.45	1.56	1.44	2	1
2	C	221	HIS	CG-CD2	8.44	1.45	1.35	1	1
2	B	79	THR	CA-CB	-8.40	1.40	1.53	1	1
2	B	176	ALA	CA-C	8.38	1.63	1.52	4	2
1	A	386	LYS	N-CA	-8.37	1.35	1.45	1	2
1	A	353	TYR	N-CA	8.36	1.51	1.46	1	2
2	C	164	SER	CA-CB	8.36	1.65	1.53	7	3
1	A	459	ILE	CA-CB	8.35	1.65	1.54	1	2
1	A	469	GLY	N-CA	8.33	1.55	1.45	7	2
2	B	189	SER	C-N	8.32	1.43	1.33	4	2
2	C	94	LYS	C-N	8.31	1.45	1.34	9	2
1	A	500	SER	CA-CB	8.29	1.64	1.53	13	1
2	B	196	LEU	CA-C	8.29	1.63	1.52	9	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	231	PRO	CA-C	-8.29	1.40	1.52	14	1
2	C	105	GLN	CA-C	-8.28	1.42	1.52	12	2
2	B	108	TRP	NE1-CE2	-8.27	1.28	1.37	8	1
2	B	177	HIS	ND1-CE1	8.25	1.40	1.32	1	4
2	B	72	TRP	CA-C	8.24	1.63	1.52	2	1
1	A	349	VAL	CA-CB	-8.24	1.45	1.54	10	3
2	B	230	LYS	CA-C	8.20	1.62	1.52	15	1
2	B	67	VAL	N-CA	8.20	1.56	1.46	13	1
2	B	231	PRO	N-CD	8.18	1.59	1.47	2	2
2	B	237	ARG	N-CA	8.15	1.56	1.46	11	1
2	C	230	LYS	CA-C	8.14	1.62	1.52	12	2
1	A	449	TYR	CA-CB	8.14	1.63	1.53	9	3
2	B	203	LEU	C-N	8.14	1.44	1.33	8	1
2	B	237	ARG	CD-NE	8.13	1.57	1.46	6	1
2	C	149	GLN	CA-C	8.12	1.63	1.52	8	2
1	A	490	LYS	CA-CB	8.11	1.66	1.53	6	1
2	B	150	GLU	N-CA	8.10	1.56	1.46	11	1
2	B	67	VAL	CA-CB	-8.10	1.44	1.54	9	2
1	A	417	ALA	CA-C	8.09	1.62	1.52	6	3
2	B	184	HIS	ND1-CE1	8.08	1.40	1.32	4	5
1	A	450	PRO	C-N	8.07	1.44	1.33	8	1
2	C	145	ARG	CD-NE	8.04	1.57	1.46	5	3
2	B	204	LYS	CA-C	-8.04	1.42	1.52	12	2
2	C	96	LYS	CA-C	-8.03	1.42	1.52	10	2
2	B	91	GLU	N-CA	-8.03	1.36	1.46	9	3
1	A	394	SER	N-CA	7.99	1.56	1.46	5	1
2	C	240	LEU	N-CA	-7.99	1.36	1.46	1	2
2	C	241	LEU	CA-C	7.98	1.62	1.52	15	4
2	C	133	GLU	N-CA	7.98	1.56	1.46	10	3
2	B	246	SER	N-CA	7.97	1.56	1.46	12	1
2	B	167	GLY	CA-C	-7.97	1.43	1.52	9	2
2	C	256	GLU	CA-C	7.95	1.62	1.52	6	2
2	C	95	ALA	CA-C	-7.94	1.42	1.52	15	2
2	B	233	LEU	CA-C	7.94	1.63	1.52	9	3
2	B	187	PRO	CA-C	7.93	1.63	1.52	5	1
2	C	214	TYR	CA-CB	7.92	1.65	1.53	10	2
2	C	168	GLU	N-CA	-7.92	1.36	1.46	8	2
1	A	494	GLU	CA-C	7.88	1.62	1.53	1	3
2	C	235	ASP	CA-C	7.87	1.64	1.52	9	1
2	B	146	ALA	N-CA	7.86	1.55	1.46	13	2
2	C	132	GLU	N-CA	7.86	1.56	1.46	8	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	483	TYR	CA-C	7.86	1.62	1.52	15	4
2	B	159	LEU	N-CA	-7.86	1.37	1.46	5	1
2	B	56	THR	CA-C	-7.85	1.42	1.52	13	3
2	C	98	GLN	CA-C	7.84	1.62	1.52	6	1
1	A	347	ASN	CA-CB	7.84	1.64	1.53	13	2
2	B	243	VAL	CA-C	7.83	1.62	1.52	7	2
2	B	123	LEU	C-N	7.83	1.44	1.33	6	1
2	C	91	GLU	N-CA	7.82	1.55	1.46	5	1
2	C	216	ALA	CA-C	-7.82	1.42	1.52	12	1
1	A	373	GLU	N-CA	-7.82	1.36	1.46	7	2
1	A	357	ILE	CA-C	-7.81	1.42	1.52	3	2
1	A	396	GLU	N-CA	-7.81	1.36	1.45	15	2
2	B	228	LYS	CA-C	7.81	1.63	1.52	3	1
2	B	120	GLU	CA-CB	7.79	1.63	1.53	7	5
2	C	132	GLU	C-N	7.79	1.43	1.33	15	1
2	B	187	PRO	C-N	7.77	1.44	1.33	8	2
2	B	98	GLN	CA-C	7.77	1.62	1.52	14	2
2	C	244	LEU	N-CA	-7.77	1.37	1.46	7	2
1	A	370	THR	N-CA	-7.75	1.36	1.46	9	1
1	A	370	THR	CA-C	-7.73	1.43	1.52	15	2
2	B	215	HIS	CE1-NE2	-7.73	1.24	1.32	2	3
1	A	403	ILE	CA-C	-7.71	1.42	1.52	13	3
2	C	237	ARG	CA-C	7.71	1.62	1.52	4	2
1	A	497	TYR	CA-C	7.70	1.60	1.52	3	2
1	A	476	TYR	CA-C	7.70	1.62	1.52	9	1
1	A	402	HIS	CE1-NE2	7.70	1.40	1.32	3	1
2	B	245	GLU	C-N	7.70	1.44	1.34	5	1
1	A	317	ASN	CA-C	7.69	1.61	1.52	3	2
2	B	137	TYR	CA-C	7.69	1.62	1.52	4	2
2	B	151	GLY	C-N	7.68	1.44	1.33	9	2
2	B	221	HIS	ND1-CE1	7.67	1.40	1.32	13	5
2	C	156	LEU	N-CA	7.65	1.55	1.46	1	1
2	B	242	PRO	C-N	7.65	1.43	1.33	11	2
2	B	60	LEU	CA-C	7.65	1.62	1.52	5	2
1	A	364	LEU	CA-C	7.63	1.61	1.52	13	3
2	B	264	THR	N-CA	7.63	1.54	1.46	8	2
2	C	156	LEU	C-N	7.61	1.43	1.33	4	1
1	A	388	TRP	C-N	7.60	1.44	1.33	12	2
1	A	387	HIS	ND1-CE1	7.60	1.40	1.32	10	5
2	B	155	LYS	CA-C	7.60	1.62	1.52	11	2
2	B	141	VAL	CA-CB	7.60	1.64	1.54	8	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	C	103	ASP	CA-C	7.59	1.62	1.52	2	1
2	C	138	ARG	CZ-NH2	-7.59	1.23	1.33	11	1
1	A	348	GLN	CA-CB	7.58	1.66	1.53	3	1
1	A	359	GLN	CA-C	7.58	1.63	1.52	5	1
2	C	257	GLU	CA-C	7.57	1.62	1.52	1	1
2	C	187	PRO	N-CD	-7.57	1.37	1.47	15	1
2	C	72	TRP	CA-C	7.56	1.62	1.52	11	1
2	B	147	GLU	CA-C	-7.55	1.43	1.52	9	2
2	B	254	ALA	C-N	7.54	1.43	1.33	1	1
1	A	334	PHE	CA-CB	7.53	1.63	1.53	6	3
1	A	442	LEU	C-N	7.53	1.43	1.33	10	1
1	A	457	GLU	N-CA	-7.53	1.36	1.46	12	1
1	A	461	GLU	CA-C	7.53	1.62	1.52	11	1
2	C	191	GLU	C-N	7.52	1.43	1.33	15	2
2	C	125	ASP	N-CA	-7.52	1.37	1.46	6	1
2	C	217	LYS	CA-C	-7.51	1.43	1.52	4	2
2	B	180	ALA	CA-C	7.50	1.62	1.52	15	3
2	B	114	LEU	CA-C	-7.48	1.42	1.52	4	1
2	C	173	ARG	N-CA	-7.47	1.37	1.46	5	1
2	B	164	SER	N-CA	7.47	1.54	1.46	14	3
2	C	200	LEU	C-N	7.47	1.43	1.33	7	1
2	B	70	GLU	N-CA	7.46	1.55	1.46	8	1
1	A	495	PRO	CA-CB	7.46	1.64	1.53	14	1
2	C	257	GLU	N-CA	-7.46	1.37	1.46	15	2
1	A	389	VAL	CA-C	-7.46	1.43	1.52	1	2
2	B	182	ARG	CD-NE	7.46	1.56	1.46	12	1
1	A	402	HIS	ND1-CE1	7.45	1.40	1.32	8	4
2	B	113	GLU	CA-C	-7.44	1.43	1.52	12	1
1	A	501	ALA	CA-C	-7.44	1.43	1.52	7	2
1	A	366	ALA	N-CA	-7.43	1.36	1.46	2	1
2	C	161	GLU	CA-CB	7.43	1.64	1.53	1	1
2	C	132	GLU	CA-C	-7.43	1.42	1.52	8	1
2	C	184	HIS	CA-CB	7.42	1.65	1.53	5	1
2	B	108	TRP	CA-C	7.42	1.62	1.52	13	2
2	B	261	LYS	CA-C	-7.42	1.43	1.52	15	2
2	B	164	SER	CA-CB	7.40	1.64	1.53	10	3
2	B	105	GLN	N-CA	7.39	1.55	1.46	4	2
2	C	137	TYR	C-N	7.39	1.43	1.33	8	3
2	C	141	VAL	C-N	7.39	1.43	1.33	4	1
2	B	195	ARG	N-CA	7.39	1.55	1.46	15	2
2	B	87	SER	C-O	-7.39	1.15	1.24	9	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	75	LEU	CA-C	7.37	1.62	1.52	9	2
2	B	145	ARG	CA-CB	7.36	1.64	1.53	2	2
1	A	391	ASP	CA-CB	7.36	1.62	1.53	9	1
2	B	122	TYR	CA-C	7.35	1.62	1.52	9	2
2	C	131	GLN	CA-C	-7.35	1.43	1.52	12	1
2	B	164	SER	CA-C	7.34	1.61	1.52	12	4
2	C	117	GLN	CA-C	7.34	1.62	1.52	11	1
2	C	179	ASP	C-N	7.34	1.43	1.33	11	2
1	A	464	ARG	N-CA	-7.34	1.36	1.46	6	1
2	C	207	GLY	CA-C	-7.34	1.43	1.52	4	5
2	C	142	GLU	CA-CB	7.34	1.62	1.53	2	2
1	A	418	ALA	CA-C	7.33	1.61	1.52	15	1
2	C	144	LEU	CA-CB	-7.33	1.42	1.53	2	3
2	C	197	ALA	N-CA	-7.33	1.37	1.46	14	3
2	C	136	LEU	CA-CB	7.33	1.64	1.53	10	1
1	A	458	GLY	C-N	7.32	1.39	1.33	4	5
2	C	173	ARG	C-N	7.32	1.43	1.33	9	2
2	C	79	THR	CA-C	-7.32	1.43	1.52	5	1
1	A	505	TRP	N-CA	-7.32	1.38	1.46	12	1
2	B	221	HIS	CG-CD2	7.32	1.43	1.35	15	1
1	A	373	GLU	CA-C	-7.32	1.43	1.52	5	3
1	A	365	PRO	C-N	7.31	1.43	1.33	4	1
2	C	259	THR	N-CA	7.31	1.55	1.46	8	2
2	B	108	TRP	N-CA	7.31	1.55	1.46	11	2
2	C	184	HIS	ND1-CE1	7.30	1.39	1.32	12	6
2	B	123	LEU	CA-CB	7.30	1.64	1.53	7	2
2	C	259	THR	CA-C	7.29	1.62	1.53	12	2
2	C	218	ALA	N-CA	-7.29	1.37	1.46	6	2
2	C	177	HIS	CB-CG	7.29	1.60	1.50	5	2
1	A	380	VAL	N-CA	-7.29	1.37	1.46	14	2
2	B	103	ASP	C-N	7.28	1.43	1.33	1	1
2	B	121	PRO	CA-CB	7.28	1.64	1.53	3	1
1	A	355	MET	N-CA	7.28	1.57	1.46	7	1
2	B	116	ARG	CD-NE	7.28	1.56	1.46	8	3
1	A	431	ARG	CD-NE	7.28	1.56	1.46	2	1
2	B	199	ARG	CA-CB	7.27	1.64	1.53	6	2
1	A	436	TYR	C-O	7.27	1.33	1.23	1	1
1	A	416	ASP	C-N	7.27	1.42	1.33	4	1
2	C	64	LEU	N-CA	7.27	1.55	1.46	2	2
2	B	215	HIS	CA-CB	7.27	1.64	1.53	4	2
2	B	149	GLN	CA-C	-7.25	1.43	1.52	6	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	244	LEU	CA-C	7.25	1.61	1.52	3	2
1	A	419	LEU	CA-C	-7.24	1.43	1.52	11	2
1	A	424	ASN	CA-CB	7.24	1.64	1.54	10	1
2	C	129	LYS	C-O	-7.24	1.15	1.24	3	3
2	B	191	GLU	CA-C	7.24	1.62	1.52	8	2
2	B	108	TRP	CA-CB	7.23	1.64	1.53	14	3
2	C	66	PRO	C-N	7.23	1.43	1.33	13	2
2	B	251	PHE	CA-CB	7.22	1.64	1.53	15	3
2	B	207	GLY	CA-C	7.22	1.60	1.52	7	1
2	B	168	GLU	CA-CB	7.22	1.64	1.53	14	2
2	C	157	HIS	CA-CB	7.22	1.64	1.53	9	3
2	C	110	GLU	CA-CB	7.21	1.64	1.53	5	2
1	A	455	VAL	CA-CB	-7.21	1.45	1.54	5	1
1	A	435	TYR	CA-C	7.21	1.61	1.52	10	3
2	B	115	TYR	N-CA	-7.21	1.38	1.46	6	2
2	B	193	ARG	N-CA	7.20	1.54	1.46	12	1
1	A	325	THR	CA-C	-7.19	1.43	1.52	3	1
2	B	211	LEU	CA-CB	7.18	1.64	1.53	13	2
2	B	95	ALA	CA-C	-7.17	1.43	1.52	4	2
2	C	255	LEU	CA-C	-7.17	1.43	1.52	11	1
2	C	139	GLN	CA-C	7.17	1.62	1.52	6	2
1	A	332	GLU	C-N	7.16	1.43	1.33	1	2
2	C	76	GLU	C-N	7.16	1.43	1.33	12	1
2	C	122	TYR	C-N	7.15	1.43	1.33	6	3
2	C	220	GLU	CA-CB	7.15	1.64	1.53	7	3
1	A	462	SER	CA-CB	7.15	1.57	1.52	12	1
1	A	459	ILE	CA-C	7.14	1.58	1.53	12	3
2	B	73	ASP	C-N	7.14	1.43	1.33	7	3
2	C	131	GLN	CA-CB	7.14	1.64	1.53	9	3
1	A	352	GLY	CA-C	-7.14	1.41	1.51	3	1
1	A	449	TYR	CA-C	7.13	1.59	1.52	9	2
2	B	156	LEU	CA-C	7.13	1.62	1.52	14	3
1	A	346	ASN	CA-C	7.12	1.62	1.53	5	1
2	C	230	LYS	N-CA	-7.10	1.39	1.46	15	2
2	C	192	LEU	CA-CB	7.09	1.64	1.53	6	2
2	B	195	ARG	CD-NE	7.09	1.56	1.46	14	4
2	B	72	TRP	N-CA	-7.08	1.37	1.46	1	3
2	B	137	TYR	N-CA	-7.07	1.37	1.46	6	1
2	B	59	LYS	N-CA	7.07	1.54	1.46	4	1
1	A	420	PHE	CA-CB	7.07	1.62	1.53	6	3
1	A	470	SER	CA-C	7.07	1.62	1.52	11	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	C	76	GLU	CA-C	7.06	1.61	1.52	8	1
2	C	191	GLU	CA-CB	7.05	1.64	1.53	5	2
2	B	168	GLU	CA-C	7.03	1.62	1.52	3	3
1	A	360	PHE	CA-C	7.03	1.62	1.52	1	1
1	A	436	TYR	CA-C	7.03	1.60	1.52	9	2
2	C	180	ALA	CA-C	7.02	1.61	1.52	13	3
2	B	184	HIS	CA-CB	7.02	1.65	1.53	11	3
1	A	445	VAL	CA-C	-7.01	1.44	1.52	10	3
2	C	129	LYS	CA-CB	7.01	1.64	1.53	12	1
2	C	233	LEU	N-CA	-7.00	1.37	1.46	2	3
2	B	210	ARG	CA-CB	7.00	1.64	1.53	15	2
2	B	64	LEU	C-N	7.00	1.39	1.34	1	2
2	B	194	GLN	N-CA	-7.00	1.38	1.46	7	2
1	A	473	VAL	CA-CB	7.00	1.63	1.54	5	1
1	A	380	VAL	CA-CB	-7.00	1.45	1.54	10	1
1	A	471	ASP	CA-CB	6.99	1.65	1.53	10	2
2	B	197	ALA	N-CA	6.99	1.54	1.46	11	1
2	B	120	GLU	CA-C	6.99	1.59	1.52	14	2
2	C	221	HIS	CA-CB	6.99	1.64	1.53	14	1
1	A	318	ILE	CA-C	6.98	1.62	1.52	6	1
2	B	252	LEU	C-N	6.98	1.43	1.33	14	2
1	A	421	TRP	CA-CB	6.97	1.63	1.53	10	1
2	C	82	LEU	CA-CB	6.97	1.64	1.53	1	2
2	C	161	GLU	C-O	-6.97	1.16	1.24	14	2
2	C	182	ARG	CA-CB	6.96	1.64	1.53	7	1
2	B	241	LEU	N-CA	6.95	1.52	1.46	5	3
2	C	166	LEU	N-CA	-6.95	1.38	1.46	9	1
2	C	145	ARG	NE-CZ	6.95	1.40	1.33	13	1
2	B	157	HIS	CG-ND1	6.95	1.45	1.38	1	1
1	A	374	ARG	CD-NE	6.95	1.55	1.46	9	3
2	B	182	ARG	CA-C	6.95	1.61	1.52	4	1
2	B	170	MET	C-N	6.94	1.42	1.33	9	1
2	C	97	VAL	C-N	6.94	1.42	1.33	3	2
1	A	428	TYR	CA-CB	6.92	1.64	1.53	1	1
2	C	153	ARG	CA-CB	6.91	1.64	1.53	3	2
2	C	61	ARG	CA-C	-6.90	1.43	1.52	3	1
2	B	77	LYS	CA-C	-6.90	1.43	1.52	10	1
2	C	194	GLN	CA-C	6.90	1.61	1.52	10	1
1	A	487	ASN	CA-CB	6.90	1.63	1.53	7	3
2	B	74	ASN	N-CA	-6.89	1.38	1.46	10	2
1	A	397	PRO	CA-C	6.89	1.60	1.52	9	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	264	THR	CA-C	-6.88	1.43	1.52	7	1
2	B	124	ASP	C-N	6.88	1.43	1.33	10	2
1	A	387	HIS	CD2-NE2	6.88	1.45	1.37	8	2
2	B	260	LYS	C-O	-6.87	1.16	1.24	2	2
2	B	115	TYR	CA-C	6.87	1.61	1.52	15	2
2	B	261	LYS	CA-CB	6.87	1.64	1.53	5	3
2	B	130	TRP	N-CA	-6.86	1.38	1.46	12	1
2	B	201	GLU	N-CA	-6.86	1.38	1.46	7	1
2	B	79	THR	C-N	6.86	1.42	1.33	12	1
1	A	394	SER	CA-C	6.86	1.60	1.52	8	1
2	C	84	GLN	C-O	-6.84	1.16	1.24	6	1
1	A	453	ILE	CA-CB	-6.84	1.44	1.54	10	1
2	B	179	ASP	CA-C	-6.84	1.43	1.52	7	2
1	A	334	PHE	CA-C	6.84	1.60	1.52	14	1
2	C	213	GLU	N-CA	-6.84	1.38	1.46	10	2
2	B	132	GLU	CA-CB	6.83	1.64	1.53	5	1
2	B	253	SER	N-CA	-6.83	1.38	1.46	6	2
2	C	262	LEU	CB-CG	6.83	1.67	1.53	12	1
2	C	150	GLU	CA-C	-6.83	1.43	1.52	6	1
1	A	380	VAL	CA-C	6.82	1.60	1.52	3	2
2	B	97	VAL	N-CA	6.82	1.53	1.45	4	1
2	B	126	PHE	N-CA	-6.82	1.38	1.46	4	1
2	C	153	ARG	CD-NE	6.82	1.55	1.46	8	2
2	C	166	LEU	CA-CB	6.82	1.64	1.53	5	1
2	C	199	ARG	N-CA	6.82	1.54	1.46	7	2
2	C	162	LYS	CA-CB	6.81	1.64	1.53	6	1
2	B	263	ASN	CA-C	-6.80	1.43	1.52	11	4
2	C	157	HIS	CB-CG	6.80	1.59	1.50	14	1
2	B	194	GLN	CA-CB	6.79	1.63	1.53	14	2
2	B	105	GLN	CA-C	-6.79	1.43	1.52	5	3
2	C	215	HIS	CA-C	-6.79	1.44	1.52	10	1
2	C	244	LEU	CA-C	6.78	1.61	1.52	12	2
1	A	371	ALA	CA-C	6.78	1.60	1.52	15	1
2	C	155	LYS	CA-C	-6.77	1.43	1.52	13	1
1	A	488	ASN	CA-CB	6.77	1.64	1.53	6	2
2	C	114	LEU	CA-C	-6.77	1.44	1.52	8	2
1	A	381	PHE	CA-C	6.76	1.61	1.52	10	3
1	A	355	MET	CA-C	-6.76	1.45	1.52	9	3
2	B	160	GLN	C-N	6.76	1.42	1.33	8	3
1	A	464	ARG	CZ-NH2	-6.75	1.24	1.33	11	1
1	A	502	LEU	N-CA	6.75	1.54	1.46	4	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	C	186	ALA	N-CA	-6.75	1.40	1.46	1	4
1	A	484	TRP	C-N	6.75	1.43	1.33	13	1
2	B	104	PHE	CA-C	6.75	1.61	1.52	11	2
1	A	385	ASP	CA-CB	6.73	1.62	1.53	12	3
2	B	244	LEU	C-N	6.73	1.42	1.33	2	1
2	B	93	VAL	CA-C	6.72	1.63	1.52	8	1
2	C	175	ARG	CD-NE	6.72	1.55	1.46	11	1
1	A	492	LYS	CA-C	6.72	1.60	1.52	3	1
2	B	251	PHE	CA-C	6.72	1.61	1.52	14	1
2	B	208	GLY	C-N	6.71	1.43	1.34	5	1
2	C	73	ASP	CA-C	6.70	1.61	1.52	3	3
2	C	227	GLU	C-N	6.70	1.42	1.33	9	2
2	B	156	LEU	N-CA	-6.70	1.38	1.46	8	2
1	A	398	GLY	CA-C	6.70	1.60	1.51	10	1
1	A	406	LEU	C-N	6.70	1.43	1.33	5	2
2	B	106	LYS	CA-CB	6.70	1.64	1.53	7	1
2	B	145	ARG	CD-NE	6.70	1.55	1.46	12	1
2	B	144	LEU	CA-C	6.70	1.61	1.52	7	2
1	A	342	TRP	CD2-CE3	-6.69	1.29	1.40	9	1
2	C	107	LYS	CA-C	6.69	1.61	1.52	1	2
1	A	475	THR	N-CA	6.69	1.54	1.46	4	1
2	C	126	PHE	CA-C	6.69	1.61	1.52	14	2
2	C	88	LYS	CA-CB	6.69	1.63	1.53	9	1
2	B	120	GLU	C-N	-6.69	1.26	1.34	2	1
2	B	261	LYS	N-CA	-6.68	1.38	1.46	6	3
1	A	422	MET	C-N	6.68	1.42	1.34	6	1
2	C	96	LYS	N-CA	6.68	1.54	1.46	8	2
2	C	210	ARG	N-CA	-6.67	1.38	1.46	13	3
2	C	136	LEU	N-CA	-6.67	1.38	1.46	7	2
1	A	497	TYR	CA-CB	6.67	1.62	1.53	1	2
1	A	447	SER	C-O	6.66	1.31	1.23	1	3
1	A	433	ASN	N-CA	6.66	1.54	1.46	5	1
1	A	447	SER	C-N	6.66	1.42	1.33	1	3
2	B	129	LYS	CA-C	6.66	1.61	1.52	7	2
2	B	260	LYS	CA-C	-6.66	1.43	1.52	5	1
2	B	247	PHE	CA-C	6.66	1.61	1.52	13	2
2	B	101	LEU	C-N	6.65	1.42	1.33	15	1
2	C	69	GLN	CA-C	-6.65	1.44	1.52	7	2
2	B	235	ASP	C-N	6.65	1.42	1.33	3	1
2	C	177	HIS	ND1-CE1	6.65	1.39	1.32	9	3
2	B	255	LEU	N-CA	6.65	1.54	1.46	6	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	96	LYS	N-CA	-6.65	1.38	1.46	12	1
2	B	209	ALA	CA-C	6.64	1.61	1.52	6	2
2	B	90	LEU	C-N	6.64	1.42	1.33	11	2
2	C	163	LEU	CA-C	6.64	1.61	1.52	7	1
2	B	246	SER	CA-C	-6.63	1.44	1.52	4	1
2	C	205	GLU	N-CA	6.63	1.54	1.46	5	1
1	A	443	ARG	CA-C	6.62	1.62	1.53	4	2
1	A	491	LEU	C-N	6.62	1.41	1.33	12	1
1	A	437	ARG	CD-NE	6.62	1.55	1.46	1	2
1	A	338	GLU	N-CA	-6.62	1.37	1.46	15	2
1	A	509	PRO	N-CA	6.62	1.55	1.47	3	2
2	C	206	ASN	CA-CB	6.62	1.63	1.53	15	3
2	B	258	TYR	CA-CB	6.62	1.63	1.53	9	5
2	B	167	GLY	N-CA	6.61	1.54	1.45	10	3
2	B	152	ALA	C-N	6.61	1.42	1.33	14	1
1	A	376	ASP	CA-CB	6.61	1.64	1.53	15	1
2	C	67	VAL	N-CA	-6.61	1.38	1.46	3	1
1	A	318	ILE	N-CA	-6.61	1.38	1.46	13	3
2	B	216	ALA	CA-C	6.60	1.61	1.52	10	1
1	A	433	ASN	CA-CB	6.60	1.64	1.53	13	2
1	A	344	VAL	CA-CB	-6.60	1.46	1.54	3	2
2	C	149	GLN	C-N	6.60	1.42	1.33	5	1
1	A	483	TYR	C-N	6.60	1.42	1.33	13	1
2	B	77	LYS	C-N	6.60	1.42	1.33	3	1
2	B	106	LYS	CA-C	6.59	1.61	1.52	4	1
2	B	186	ALA	CA-C	6.59	1.60	1.52	13	1
2	C	70	GLU	N-CA	-6.59	1.38	1.46	14	4
1	A	430	PHE	CA-C	6.59	1.60	1.52	4	2
2	B	255	LEU	CA-CB	6.59	1.64	1.53	5	1
1	A	340	TRP	CA-C	-6.58	1.44	1.52	12	2
1	A	464	ARG	NE-CZ	6.58	1.40	1.33	6	2
2	C	223	SER	CA-CB	6.58	1.63	1.53	4	3
1	A	461	GLU	N-CA	6.58	1.54	1.46	1	2
1	A	464	ARG	CD-NE	6.58	1.55	1.46	8	3
2	B	80	GLU	CA-C	6.58	1.61	1.52	5	1
2	C	116	ARG	C-N	6.58	1.43	1.34	10	1
2	B	215	HIS	C-N	6.58	1.42	1.33	8	1
2	C	98	GLN	N-CA	6.57	1.55	1.46	4	2
1	A	344	VAL	N-CA	-6.57	1.38	1.46	12	1
2	C	221	HIS	N-CA	6.57	1.54	1.46	8	1
2	B	85	GLU	C-N	6.57	1.42	1.33	3	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	C	212	ALA	CA-C	-6.57	1.44	1.52	14	1
1	A	487	ASN	CA-C	-6.57	1.44	1.52	15	3
2	B	160	GLN	CA-CB	6.57	1.63	1.53	2	2
2	C	130	TRP	CA-CB	6.56	1.63	1.53	3	1
2	B	188	TYR	CA-CB	6.56	1.63	1.53	14	2
2	B	249	VAL	CA-CB	6.55	1.62	1.54	14	2
2	C	125	ASP	CA-C	-6.55	1.44	1.52	15	3
1	A	369	ASN	CA-C	-6.55	1.43	1.52	5	2
1	A	361	TRP	N-CA	-6.55	1.38	1.46	7	1
2	B	261	LYS	C-N	6.55	1.42	1.33	3	1
1	A	492	LYS	CA-CB	6.55	1.64	1.53	3	1
2	C	57	PHE	CA-C	6.54	1.61	1.52	6	3
2	B	235	ASP	CA-C	-6.54	1.44	1.52	12	2
2	B	160	GLN	N-CA	6.54	1.53	1.46	13	1
2	B	192	LEU	CA-C	6.54	1.61	1.52	13	1
2	B	157	HIS	CA-CB	6.54	1.63	1.53	11	1
2	B	73	ASP	N-CA	-6.54	1.38	1.46	1	2
1	A	347	ASN	N-CA	-6.54	1.36	1.46	4	1
2	C	101	LEU	CA-C	-6.53	1.44	1.52	9	1
2	B	241	LEU	CA-CB	6.53	1.62	1.53	15	2
2	B	66	PRO	C-N	6.53	1.41	1.33	4	1
1	A	330	ARG	CD-NE	6.52	1.55	1.46	5	1
2	C	185	LEU	C-N	6.52	1.42	1.33	9	1
2	B	81	GLY	CA-C	-6.52	1.45	1.52	14	1
2	B	126	PHE	CA-C	6.51	1.61	1.52	7	1
2	B	204	LYS	N-CA	6.51	1.54	1.46	12	1
2	B	173	ARG	CD-NE	6.51	1.55	1.46	9	3
2	B	194	GLN	C-N	6.50	1.42	1.33	1	2
2	C	63	GLN	C-N	6.50	1.43	1.33	4	2
2	C	92	GLU	N-CA	-6.50	1.38	1.46	11	2
2	B	213	GLU	C-N	6.50	1.42	1.33	8	3
2	C	124	ASP	CA-CB	6.50	1.63	1.53	12	1
2	C	222	LEU	N-CA	-6.50	1.38	1.46	5	1
2	B	229	ALA	CA-CB	6.50	1.63	1.53	12	1
2	C	173	ARG	CA-C	6.50	1.61	1.52	7	1
2	B	126	PHE	CA-CB	6.49	1.63	1.53	15	2
2	B	204	LYS	CA-CB	6.49	1.63	1.53	3	3
2	C	68	THR	C-N	6.49	1.42	1.33	12	1
2	C	134	MET	C-N	6.49	1.42	1.33	9	2
2	C	224	THR	C-N	6.49	1.42	1.33	9	2
1	A	364	LEU	CA-CB	6.49	1.63	1.52	5	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	C	239	GLY	CA-C	-6.48	1.44	1.52	1	2
2	B	111	GLU	CA-CB	6.48	1.63	1.53	13	2
2	B	186	ALA	C-O	-6.48	1.18	1.24	12	1
2	B	111	GLU	CA-C	6.47	1.61	1.52	14	2
2	B	100	TYR	C-N	6.47	1.42	1.33	13	1
1	A	502	LEU	CA-CB	6.47	1.63	1.53	15	1
1	A	468	MET	CA-CB	6.47	1.63	1.53	2	4
2	B	118	LYS	C-N	6.46	1.42	1.33	7	1
1	A	405	GLU	CA-C	6.46	1.61	1.52	10	2
1	A	356	PRO	C-N	6.45	1.42	1.33	6	2
2	C	70	GLU	CA-CB	6.45	1.63	1.53	5	2
2	C	152	ALA	CA-C	6.45	1.61	1.52	10	1
2	B	220	GLU	CA-C	6.44	1.61	1.52	8	1
2	B	124	ASP	CA-C	6.44	1.61	1.52	5	1
1	A	390	PHE	C-N	6.44	1.40	1.33	9	1
1	A	343	ARG	N-CA	-6.44	1.38	1.46	3	1
2	C	226	SER	N-CA	6.43	1.54	1.46	6	1
1	A	331	GLY	C-N	-6.43	1.24	1.33	3	1
2	B	226	SER	CA-CB	6.43	1.63	1.53	7	2
2	C	185	LEU	CA-C	-6.43	1.44	1.52	7	1
2	B	198	ALA	C-N	6.43	1.42	1.33	11	1
2	C	213	GLU	CA-CB	6.42	1.63	1.53	3	1
1	A	337	LYS	CA-CB	6.42	1.63	1.53	3	3
2	C	199	ARG	CD-NE	6.42	1.55	1.46	9	1
2	B	76	GLU	C-N	6.42	1.42	1.33	15	1
2	C	251	PHE	CA-C	6.41	1.61	1.52	15	3
2	B	250	SER	N-CA	6.41	1.54	1.46	14	1
2	C	258	TYR	CA-C	6.41	1.60	1.52	15	1
1	A	419	LEU	N-CA	-6.41	1.38	1.46	13	1
2	C	175	ARG	CA-C	-6.40	1.44	1.52	4	3
2	C	233	LEU	CA-C	-6.40	1.44	1.52	3	2
2	B	208	GLY	CA-C	-6.40	1.44	1.51	6	2
2	B	69	GLN	CA-C	6.40	1.61	1.52	6	2
2	B	206	ASN	CA-CB	6.40	1.64	1.53	6	2
2	B	172	ASP	CA-CB	6.39	1.62	1.54	1	1
2	C	93	VAL	C-N	6.39	1.42	1.33	12	2
2	B	234	GLU	C-N	6.38	1.42	1.33	9	3
1	A	429	PHE	CA-CB	6.38	1.63	1.53	6	2
1	A	365	PRO	CA-C	6.38	1.60	1.52	7	1
1	A	387	HIS	N-CA	-6.38	1.38	1.46	2	1
2	C	126	PHE	CA-CB	6.38	1.63	1.53	2	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	240	LEU	CA-C	-6.38	1.44	1.52	6	1
2	C	145	ARG	C-N	6.38	1.42	1.33	7	1
1	A	481	ASN	CA-C	6.38	1.60	1.52	2	1
1	A	479	LYS	CA-CB	6.38	1.64	1.53	3	1
2	C	119	VAL	C-N	6.38	1.43	1.33	14	1
1	A	340	TRP	N-CA	-6.37	1.37	1.45	3	1
1	A	411	PRO	CA-C	6.37	1.61	1.52	13	1
2	C	74	ASN	C-N	6.37	1.42	1.33	11	2
1	A	384	GLY	N-CA	6.37	1.55	1.45	5	1
2	C	76	GLU	CA-CB	6.37	1.63	1.53	9	2
2	C	133	GLU	CA-CB	6.36	1.63	1.53	3	1
2	C	133	GLU	CA-C	6.36	1.61	1.52	10	2
1	A	325	THR	N-CA	6.36	1.54	1.46	11	1
2	C	176	ALA	CA-C	6.36	1.61	1.52	14	1
1	A	460	PRO	CA-C	-6.36	1.45	1.52	3	2
2	B	137	TYR	CZ-OH	6.36	1.51	1.38	6	1
2	B	260	LYS	CA-CB	6.36	1.63	1.53	12	1
2	C	258	TYR	CA-CB	6.35	1.63	1.53	3	3
2	B	55	SER	CA-CB	6.35	1.66	1.53	6	1
2	B	182	ARG	NE-CZ	6.35	1.40	1.33	2	2
2	B	57	PHE	N-CA	6.35	1.54	1.46	14	3
2	B	244	LEU	N-CA	-6.35	1.38	1.46	10	1
1	A	390	PHE	CA-CB	6.35	1.63	1.53	12	1
2	C	182	ARG	CD-NE	6.34	1.55	1.46	10	3
1	A	389	VAL	N-CA	6.34	1.54	1.46	14	2
2	C	226	SER	C-N	6.34	1.42	1.33	9	2
2	B	62	GLU	CA-CB	6.34	1.63	1.53	14	3
1	A	383	LYS	CA-C	6.34	1.59	1.52	10	1
2	B	65	GLY	N-CA	6.34	1.53	1.44	3	2
2	B	62	GLU	C-N	6.34	1.43	1.33	11	1
1	A	429	PHE	N-CA	-6.33	1.38	1.46	5	1
2	C	69	GLN	CA-CB	6.33	1.63	1.53	1	2
2	B	125	ASP	CA-C	-6.33	1.44	1.52	10	2
2	C	81	GLY	CA-C	-6.33	1.45	1.52	14	1
2	B	233	LEU	CA-CB	6.33	1.63	1.53	6	2
2	C	174	ALA	CA-CB	6.33	1.63	1.53	4	1
2	C	101	LEU	N-CA	-6.33	1.39	1.46	10	1
2	C	173	ARG	NE-CZ	-6.33	1.26	1.33	15	2
2	C	115	TYR	N-CA	-6.32	1.38	1.46	7	2
2	C	171	ARG	CA-C	6.32	1.60	1.52	1	1
2	C	215	HIS	ND1-CE1	6.32	1.38	1.32	1	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	137	TYR	C-N	6.31	1.42	1.33	15	1
2	B	133	GLU	N-CA	-6.31	1.38	1.46	13	1
2	C	160	GLN	CA-C	6.31	1.61	1.52	5	3
1	A	478	TYR	CA-CB	6.30	1.62	1.53	14	2
2	C	240	LEU	C-N	6.29	1.41	1.33	3	1
2	B	248	LYS	CA-C	-6.29	1.44	1.52	10	1
2	B	113	GLU	C-N	6.28	1.42	1.33	5	2
2	B	107	LYS	CA-C	6.28	1.61	1.52	5	3
2	B	165	PRO	CA-CB	-6.28	1.45	1.53	6	1
2	B	148	LEU	N-CA	6.28	1.53	1.46	5	1
2	B	73	ASP	CA-C	6.27	1.60	1.52	9	1
2	C	251	PHE	CG-CD2	6.27	1.52	1.38	8	1
2	C	171	ARG	N-CA	-6.27	1.38	1.46	15	1
1	A	437	ARG	CA-C	6.27	1.60	1.52	6	1
1	A	457	GLU	CA-CB	6.27	1.64	1.53	15	2
2	B	151	GLY	C-O	-6.27	1.16	1.23	6	2
2	C	73	ASP	C-N	6.26	1.41	1.33	3	2
2	B	149	GLN	C-O	-6.26	1.16	1.24	6	1
2	B	82	LEU	C-N	6.26	1.41	1.33	14	2
2	C	256	GLU	CA-CB	6.26	1.63	1.53	9	1
2	C	114	LEU	C-N	6.26	1.42	1.33	13	2
1	A	399	TYR	CA-CB	6.26	1.63	1.53	2	1
1	A	451	LYS	CA-C	6.26	1.60	1.52	2	1
2	C	210	ARG	CD-NE	6.26	1.55	1.46	14	3
1	A	406	LEU	N-CA	6.26	1.54	1.46	3	1
2	C	112	MET	N-CA	-6.26	1.38	1.46	2	2
2	B	185	LEU	CA-CB	6.25	1.64	1.53	1	1
2	B	158	GLU	CA-C	6.24	1.60	1.52	8	1
2	C	135	GLU	CA-C	-6.24	1.44	1.52	9	1
2	C	236	LEU	C-N	6.24	1.43	1.33	12	1
1	A	453	ILE	CA-C	-6.24	1.43	1.52	15	1
2	C	247	PHE	CA-CB	6.24	1.63	1.53	8	3
2	C	59	LYS	CA-C	-6.24	1.44	1.52	15	2
1	A	388	TRP	CA-C	-6.24	1.44	1.52	7	1
2	B	239	GLY	CA-C	-6.24	1.45	1.52	12	1
1	A	408	ARG	CA-CB	6.23	1.61	1.53	15	1
2	C	246	SER	CA-C	6.23	1.61	1.52	8	2
2	C	177	HIS	CD2-NE2	6.23	1.44	1.37	12	1
2	B	225	LEU	C-N	6.23	1.42	1.33	15	1
2	C	68	THR	N-CA	6.22	1.54	1.46	5	2
2	B	71	PHE	CA-C	-6.22	1.44	1.52	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	C	188	TYR	C-N	6.22	1.42	1.33	3	1
2	C	149	GLN	N-CA	-6.22	1.38	1.46	9	1
2	C	253	SER	N-CA	-6.22	1.39	1.46	11	1
2	C	99	PRO	N-CA	6.21	1.54	1.47	7	2
2	C	232	ALA	N-CA	6.21	1.53	1.46	11	1
2	C	100	TYR	CA-CB	6.21	1.64	1.53	6	2
2	B	166	LEU	CA-CB	6.21	1.62	1.53	10	2
1	A	389	VAL	CA-CB	-6.21	1.46	1.53	2	1
2	B	153	ARG	CA-C	6.20	1.60	1.52	14	2
2	B	198	ALA	N-CA	6.20	1.53	1.46	8	2
2	B	104	PHE	C-N	6.20	1.42	1.33	4	1
2	C	70	GLU	CA-C	-6.20	1.44	1.52	11	3
1	A	431	ARG	CA-C	-6.20	1.44	1.52	6	1
2	C	124	ASP	N-CA	6.19	1.53	1.46	10	2
2	C	67	VAL	CA-C	6.19	1.60	1.52	1	2
1	A	404	LYS	N-CA	6.19	1.54	1.46	9	1
2	C	235	ASP	N-CA	-6.19	1.38	1.46	6	1
1	A	402	HIS	CD2-NE2	6.19	1.44	1.37	14	1
2	B	211	LEU	N-CA	6.19	1.53	1.46	3	1
1	A	439	ASN	N-CA	-6.18	1.38	1.46	4	1
1	A	413	ASP	CA-C	6.18	1.61	1.52	6	3
1	A	388	TRP	CA-CB	6.18	1.63	1.53	13	1
1	A	326	VAL	C-N	6.17	1.41	1.33	4	1
2	C	150	GLU	N-CA	-6.17	1.38	1.46	9	1
2	B	259	THR	CA-C	6.17	1.60	1.52	7	1
1	A	403	ILE	N-CA	6.17	1.53	1.46	1	1
2	B	92	GLU	C-N	6.17	1.41	1.33	8	2
2	C	142	GLU	CA-C	6.17	1.60	1.52	8	3
2	C	134	MET	CA-C	6.17	1.60	1.52	7	4
2	C	118	LYS	CA-C	6.17	1.61	1.52	10	2
1	A	437	ARG	NE-CZ	-6.17	1.26	1.33	8	1
2	B	98	GLN	CA-CB	6.17	1.61	1.53	5	2
2	C	89	ASP	C-N	6.17	1.42	1.33	13	2
2	C	240	LEU	CA-C	6.17	1.60	1.52	9	2
2	B	195	ARG	NE-CZ	6.16	1.39	1.33	10	2
2	B	175	ARG	N-CA	-6.16	1.39	1.46	9	2
2	B	194	GLN	CA-C	-6.16	1.44	1.52	6	1
2	C	250	SER	CA-C	6.15	1.60	1.52	5	1
2	C	234	GLU	N-CA	-6.15	1.39	1.46	14	2
2	C	254	ALA	N-CA	-6.15	1.38	1.46	3	1
2	B	72	TRP	CA-CB	6.15	1.63	1.53	5	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	C	195	ARG	NE-CZ	6.14	1.39	1.33	14	1
2	B	155	LYS	CA-CB	6.14	1.62	1.53	14	2
2	B	59	LYS	CA-C	-6.14	1.45	1.52	14	1
1	A	458	GLY	CA-C	-6.14	1.43	1.51	14	1
2	C	169	GLU	CA-CB	6.14	1.63	1.53	15	1
1	A	421	TRP	CA-C	-6.13	1.45	1.53	3	1
1	A	445	VAL	C-N	6.13	1.41	1.33	9	2
1	A	362	ARG	C-N	6.13	1.42	1.33	6	2
2	B	112	MET	CA-C	6.12	1.60	1.52	11	1
1	A	457	GLU	CA-C	6.12	1.60	1.52	3	2
2	C	205	GLU	CA-C	6.12	1.60	1.52	7	2
1	A	402	HIS	CA-C	6.12	1.60	1.52	13	1
2	C	223	SER	CA-C	-6.12	1.44	1.52	13	1
2	C	77	LYS	N-CA	-6.12	1.39	1.46	13	2
2	C	158	GLU	CA-C	-6.12	1.45	1.52	7	3
2	C	83	ARG	CA-C	-6.12	1.45	1.52	5	1
2	C	145	ARG	CA-CB	6.12	1.62	1.53	14	1
2	C	65	GLY	CA-C	6.11	1.60	1.51	15	1
2	C	187	PRO	CA-CB	6.11	1.62	1.53	15	1
2	C	221	HIS	CE1-NE2	-6.11	1.26	1.32	3	2
1	A	456	TRP	CA-CB	6.11	1.60	1.53	11	2
2	B	170	MET	CA-C	-6.10	1.44	1.52	10	2
2	C	256	GLU	C-N	6.10	1.42	1.33	7	3
2	B	96	LYS	CA-CB	6.10	1.62	1.53	12	1
2	C	249	VAL	N-CA	6.10	1.53	1.46	14	1
2	B	173	ARG	C-N	6.10	1.42	1.34	14	1
2	B	199	ARG	CA-C	-6.10	1.44	1.52	14	2
2	C	240	LEU	CA-CB	6.09	1.62	1.53	9	2
2	C	100	TYR	N-CA	-6.09	1.38	1.46	9	2
2	C	94	LYS	CA-CB	6.09	1.62	1.53	3	1
1	A	456	TRP	N-CA	6.09	1.54	1.46	8	1
2	B	135	GLU	C-O	-6.09	1.17	1.24	13	1
2	C	127	GLN	CA-C	6.09	1.60	1.52	5	1
2	C	57	PHE	N-CA	-6.09	1.39	1.46	14	1
2	C	172	ASP	CA-CB	6.09	1.62	1.53	7	1
2	B	102	ASP	CA-CB	6.09	1.62	1.53	11	2
1	A	446	ASP	N-CA	-6.09	1.38	1.46	10	2
2	C	86	MET	CA-C	-6.08	1.45	1.52	4	1
1	A	421	TRP	C-O	-6.08	1.17	1.24	10	2
2	C	123	LEU	CA-CB	6.08	1.62	1.53	5	1
2	C	212	ALA	CA-CB	-6.08	1.43	1.53	3	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	C	262	LEU	CA-CB	6.08	1.63	1.53	4	1
2	B	171	ARG	CD-NE	6.08	1.54	1.46	12	2
1	A	445	VAL	CA-CB	-6.07	1.48	1.54	4	2
1	A	322	ASN	C-N	6.07	1.41	1.33	15	1
2	C	123	LEU	C-O	-6.07	1.17	1.24	6	1
2	C	184	HIS	N-CA	-6.07	1.38	1.46	15	1
2	B	153	ARG	N-CA	-6.06	1.39	1.46	12	1
2	C	159	LEU	C-N	6.06	1.41	1.33	10	3
2	B	219	THR	CA-CB	-6.06	1.43	1.53	13	1
1	A	454	LYS	CA-C	6.05	1.61	1.52	3	1
2	C	189	SER	C-O	-6.05	1.17	1.24	13	2
1	A	472	GLU	CA-C	6.05	1.61	1.52	9	1
2	C	253	SER	C-O	-6.05	1.17	1.24	11	1
2	C	238	GLN	N-CA	-6.05	1.38	1.46	3	1
2	C	105	GLN	CA-CB	6.04	1.63	1.53	1	3
1	A	451	LYS	N-CA	6.04	1.53	1.45	3	2
2	B	83	ARG	N-CA	-6.04	1.39	1.46	7	1
2	B	215	HIS	ND1-CE1	6.04	1.38	1.32	10	2
2	B	66	PRO	CA-C	6.03	1.60	1.52	3	1
2	C	146	ALA	N-CA	-6.03	1.39	1.46	7	1
2	C	251	PHE	CA-CB	6.03	1.62	1.53	8	1
2	B	178	VAL	CA-CB	-6.03	1.47	1.54	12	2
2	C	140	LYS	N-CA	-6.03	1.39	1.46	12	2
2	B	90	LEU	N-CA	6.02	1.53	1.46	3	1
2	C	182	ARG	C-N	6.02	1.42	1.33	5	2
2	C	87	SER	CA-CB	6.02	1.62	1.53	13	2
2	C	136	LEU	C-N	6.02	1.42	1.34	5	1
2	B	98	GLN	N-CA	-6.01	1.40	1.46	2	2
2	B	251	PHE	C-O	-6.01	1.17	1.24	2	2
2	C	123	LEU	N-CA	-6.01	1.39	1.46	2	1
1	A	328	MET	C-N	6.01	1.41	1.33	5	1
1	A	397	PRO	CA-CB	-6.01	1.45	1.53	12	1
2	B	80	GLU	C-O	-6.01	1.17	1.24	12	1
1	A	466	SER	C-N	6.01	1.40	1.33	11	3
2	B	209	ALA	N-CA	-6.00	1.38	1.46	5	2
1	A	350	MET	CA-CB	6.00	1.63	1.53	9	2
1	A	491	LEU	CA-CB	6.00	1.62	1.53	8	1
1	A	495	PRO	N-CA	-6.00	1.39	1.47	2	1
2	B	72	TRP	C-O	-6.00	1.17	1.24	2	1
2	B	103	ASP	N-CA	6.00	1.54	1.46	6	2
2	C	228	LYS	N-CA	-6.00	1.38	1.46	14	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	161	GLU	N-CA	6.00	1.53	1.46	8	2
2	B	61	ARG	CD-NE	5.99	1.54	1.46	11	3
2	B	121	PRO	C-N	5.99	1.41	1.33	3	1
2	B	138	ARG	CA-C	-5.99	1.44	1.52	12	1
1	A	493	VAL	CA-C	5.99	1.60	1.52	13	1
2	C	114	LEU	N-CA	5.99	1.53	1.46	12	1
2	C	137	TYR	CA-C	5.99	1.60	1.52	15	3
2	C	215	HIS	CG-ND1	-5.99	1.31	1.38	11	2
2	B	61	ARG	CA-CB	5.98	1.62	1.53	3	2
1	A	379	PHE	CA-CB	5.98	1.61	1.53	12	3
2	B	61	ARG	CA-C	5.98	1.60	1.52	11	1
2	C	115	TYR	C-N	5.98	1.41	1.33	4	1
1	A	418	ALA	C-N	5.98	1.42	1.33	13	1
2	C	253	SER	CA-C	5.97	1.60	1.52	7	1
2	B	194	GLN	C-O	-5.97	1.17	1.24	12	3
1	A	438	PHE	N-CA	-5.97	1.38	1.46	15	3
1	A	340	TRP	CA-CB	5.97	1.63	1.53	12	1
2	C	253	SER	C-N	5.97	1.42	1.33	6	1
1	A	462	SER	C-N	5.97	1.41	1.33	12	2
2	B	143	PRO	CA-CB	-5.97	1.45	1.53	7	1
1	A	316	PRO	N-CD	5.97	1.56	1.47	13	1
1	A	499	LYS	N-CA	-5.96	1.38	1.45	15	1
2	C	219	THR	C-N	5.96	1.41	1.33	8	3
2	B	64	LEU	CA-CB	5.96	1.63	1.53	8	1
2	B	108	TRP	C-N	5.96	1.41	1.33	10	1
2	B	227	GLU	CA-CB	5.96	1.62	1.53	6	2
2	C	158	GLU	C-O	-5.96	1.17	1.24	6	1
2	B	193	ARG	CD-NE	5.96	1.54	1.46	3	3
2	B	149	GLN	N-CA	-5.96	1.39	1.46	1	2
2	C	117	GLN	C-O	-5.96	1.16	1.24	6	1
2	C	237	ARG	NE-CZ	5.96	1.39	1.33	14	1
1	A	387	HIS	CG-ND1	5.96	1.44	1.38	6	1
2	C	100	TYR	CA-C	5.95	1.60	1.52	2	3
2	B	158	GLU	CA-CB	5.95	1.62	1.53	6	1
2	B	76	GLU	N-CA	-5.95	1.39	1.46	1	1
2	B	97	VAL	C-N	5.95	1.41	1.33	2	1
2	C	117	GLN	CA-CB	5.95	1.63	1.53	13	1
1	A	375	LYS	CA-C	-5.95	1.45	1.52	3	1
1	A	420	PHE	CA-C	-5.95	1.45	1.52	6	4
1	A	474	PHE	N-CA	-5.95	1.38	1.46	13	1
1	A	317	ASN	CA-CB	5.95	1.66	1.53	12	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	230	LYS	C-N	-5.94	1.26	1.34	10	1
2	B	190	ASP	N-CA	-5.94	1.39	1.46	1	2
2	C	80	GLU	CA-CB	5.94	1.63	1.53	1	1
2	B	211	LEU	C-O	-5.94	1.17	1.24	5	3
2	C	195	ARG	CZ-NH2	-5.93	1.25	1.33	14	1
1	A	487	ASN	N-CA	-5.93	1.38	1.46	8	1
2	B	249	VAL	CA-C	5.93	1.60	1.52	11	1
2	C	219	THR	CA-CB	5.92	1.62	1.53	10	1
2	C	258	TYR	C-N	5.92	1.41	1.33	12	1
2	B	107	LYS	C-N	5.92	1.42	1.33	7	1
2	C	183	THR	CA-CB	-5.92	1.44	1.53	15	1
1	A	441	GLU	C-N	5.92	1.42	1.33	3	1
1	A	493	VAL	CA-CB	-5.91	1.48	1.54	9	1
2	C	113	GLU	N-CA	-5.91	1.39	1.46	1	1
2	B	84	GLN	C-N	5.91	1.41	1.33	7	1
2	B	223	SER	C-N	5.91	1.41	1.33	13	1
1	A	324	ASP	N-CA	-5.91	1.38	1.46	2	2
1	A	357	ILE	CA-CB	-5.91	1.47	1.54	4	1
2	B	193	ARG	NE-CZ	5.91	1.39	1.33	8	1
1	A	388	TRP	NE1-CE2	5.91	1.44	1.37	13	1
1	A	413	ASP	C-N	5.90	1.40	1.33	11	1
2	C	58	SER	C-O	-5.90	1.17	1.24	2	1
2	C	85	GLU	CA-CB	5.90	1.62	1.53	4	1
1	A	463	PRO	C-O	-5.90	1.17	1.23	8	1
2	C	190	ASP	CA-CB	5.90	1.62	1.53	13	2
1	A	348	GLN	C-N	5.90	1.41	1.33	13	1
2	C	170	MET	N-CA	5.90	1.53	1.46	9	2
2	B	180	ALA	CA-CB	5.90	1.62	1.53	13	1
1	A	482	LYS	CA-C	5.90	1.59	1.52	15	2
1	A	327	ALA	C-N	5.89	1.41	1.33	14	2
2	B	105	GLN	C-N	5.89	1.41	1.33	9	3
1	A	345	ARG	CA-CB	5.89	1.64	1.53	13	1
2	B	198	ALA	CA-CB	5.89	1.62	1.53	3	2
2	C	100	TYR	CZ-OH	5.88	1.50	1.38	2	1
1	A	421	TRP	NE1-CE2	-5.88	1.30	1.37	8	3
2	C	170	MET	CA-CB	5.88	1.62	1.53	6	1
1	A	366	ALA	CA-C	-5.88	1.45	1.52	5	1
2	B	57	PHE	CA-CB	5.88	1.62	1.53	6	1
2	C	210	ARG	C-N	5.88	1.41	1.33	1	2
2	C	84	GLN	C-N	5.88	1.41	1.33	5	1
2	B	189	SER	CA-CB	5.87	1.62	1.53	12	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	C	83	ARG	CA-CB	5.87	1.62	1.53	13	2
1	A	474	PHE	C-O	-5.87	1.17	1.24	15	1
2	C	108	TRP	CA-CB	5.86	1.63	1.53	3	2
2	B	219	THR	CA-C	5.86	1.60	1.52	11	1
2	B	240	LEU	N-CA	-5.86	1.38	1.46	14	1
1	A	494	GLU	CA-CB	5.86	1.63	1.53	3	1
2	B	247	PHE	C-N	5.85	1.41	1.33	10	3
1	A	463	PRO	C-N	5.85	1.41	1.33	14	1
2	C	110	GLU	CA-C	5.85	1.60	1.52	7	1
1	A	332	GLU	N-CA	-5.85	1.38	1.45	11	2
2	C	124	ASP	C-N	5.84	1.41	1.33	7	1
2	B	227	GLU	CA-C	-5.84	1.44	1.52	13	2
2	C	246	SER	C-O	-5.84	1.17	1.24	9	1
1	A	345	ARG	C-O	5.84	1.30	1.23	10	2
2	C	198	ALA	CA-C	-5.84	1.45	1.52	12	2
2	B	99	PRO	CA-C	5.84	1.60	1.52	2	1
2	B	247	PHE	CA-CB	5.84	1.62	1.53	6	2
1	A	348	GLN	N-CA	5.84	1.53	1.45	7	2
1	A	399	TYR	CA-C	-5.83	1.44	1.52	1	2
2	C	108	TRP	CD2-CE3	-5.83	1.30	1.40	9	1
1	A	342	TRP	NE1-CE2	-5.83	1.31	1.37	14	2
1	A	370	THR	CB-OG1	-5.83	1.34	1.43	12	1
1	A	403	ILE	CA-CB	5.83	1.61	1.54	6	1
1	A	374	ARG	CZ-NH2	-5.83	1.25	1.33	8	1
2	C	148	LEU	N-CA	-5.83	1.39	1.46	14	1
2	C	206	ASN	C-N	5.82	1.40	1.33	7	1
1	A	330	ARG	N-CA	-5.82	1.37	1.46	5	1
2	C	98	GLN	CA-CB	5.82	1.60	1.53	8	2
1	A	358	GLY	CA-C	-5.82	1.45	1.52	9	1
2	C	71	PHE	CA-C	-5.82	1.45	1.52	10	1
2	C	92	GLU	CA-C	5.82	1.60	1.52	8	2
2	B	241	LEU	CA-C	5.82	1.59	1.52	1	1
1	A	370	THR	C-N	5.82	1.42	1.33	12	1
1	A	414	LYS	N-CA	-5.81	1.38	1.46	5	1
2	C	108	TRP	N-CA	-5.81	1.39	1.46	14	1
2	B	201	GLU	C-N	5.81	1.41	1.33	13	2
2	B	63	GLN	CA-CB	5.80	1.62	1.53	14	3
2	C	240	LEU	C-O	-5.80	1.16	1.24	5	1
2	B	57	PHE	CA-C	-5.80	1.45	1.52	14	1
2	B	55	SER	N-CA	5.80	1.57	1.46	9	2
2	C	232	ALA	CA-C	5.80	1.60	1.52	2	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	470	SER	N-CA	5.79	1.53	1.46	12	1
2	C	58	SER	N-CA	5.79	1.53	1.46	9	1
2	B	125	ASP	N-CA	-5.79	1.39	1.46	3	1
2	C	143	PRO	N-CA	-5.78	1.39	1.47	1	2
2	B	191	GLU	C-N	5.78	1.41	1.33	10	2
2	C	137	TYR	CA-CB	5.78	1.62	1.53	14	2
2	C	260	LYS	N-CA	5.78	1.53	1.46	5	1
2	B	253	SER	CB-OG	5.78	1.53	1.42	6	1
2	C	118	LYS	CA-CB	5.78	1.62	1.53	8	1
2	C	194	GLN	CA-CB	5.78	1.62	1.53	2	2
2	B	144	LEU	CA-CB	5.78	1.62	1.53	4	2
2	B	184	HIS	CB-CG	5.78	1.58	1.50	5	2
2	C	139	GLN	N-CA	-5.78	1.39	1.46	6	1
2	C	112	MET	CA-C	5.78	1.60	1.52	5	1
2	C	145	ARG	N-CA	-5.78	1.39	1.46	14	2
2	B	88	LYS	N-CA	-5.78	1.39	1.46	15	1
2	B	213	GLU	N-CA	-5.77	1.39	1.46	11	1
2	C	208	GLY	N-CA	5.77	1.52	1.45	12	1
2	B	72	TRP	C-N	5.77	1.41	1.33	7	1
2	C	214	TYR	C-O	-5.77	1.17	1.24	14	1
2	C	90	LEU	CA-CB	5.77	1.62	1.53	8	2
2	B	174	ALA	CA-CB	5.77	1.62	1.53	13	1
2	B	74	ASN	C-N	5.76	1.41	1.33	2	1
2	B	240	LEU	CA-CB	5.76	1.62	1.53	14	3
2	C	125	ASP	CA-CB	5.76	1.62	1.53	10	1
2	C	116	ARG	CA-C	5.76	1.60	1.52	9	1
2	B	144	LEU	C-N	5.76	1.41	1.33	2	1
1	A	320	ASP	CA-CB	5.76	1.63	1.53	5	1
2	B	171	ARG	CA-CB	5.76	1.62	1.53	2	2
1	A	369	ASN	C-N	5.76	1.40	1.33	4	1
2	B	101	LEU	CA-C	-5.76	1.45	1.52	4	2
2	B	128	LYS	CA-CB	5.75	1.62	1.53	5	3
2	C	237	ARG	CZ-NH2	-5.75	1.25	1.33	4	1
2	B	218	ALA	N-CA	-5.75	1.39	1.46	6	1
2	C	58	SER	CA-CB	5.75	1.62	1.53	8	1
1	A	368	ILE	N-CA	-5.75	1.39	1.46	9	1
2	C	255	LEU	N-CA	5.75	1.53	1.46	14	1
2	B	193	ARG	C-N	5.75	1.41	1.33	3	1
1	A	463	PRO	N-CA	-5.75	1.40	1.47	5	1
1	A	431	ARG	NE-CZ	-5.74	1.26	1.33	1	1
2	B	239	GLY	C-N	5.74	1.42	1.33	3	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	C	163	LEU	N-CA	-5.74	1.39	1.46	6	1
1	A	415	ILE	CA-C	5.74	1.60	1.52	1	1
2	C	209	ALA	N-CA	-5.74	1.39	1.46	11	1
1	A	336	PHE	CA-C	5.73	1.59	1.52	13	1
2	B	243	VAL	CA-CB	-5.73	1.47	1.54	10	1
2	C	61	ARG	CA-CB	-5.73	1.44	1.53	1	5
2	B	223	SER	CA-CB	5.73	1.62	1.53	9	2
2	B	181	LEU	C-N	5.73	1.41	1.33	14	1
2	C	157	HIS	CA-C	-5.73	1.45	1.52	7	1
1	A	503	ARG	C-N	5.73	1.41	1.33	3	1
1	A	350	MET	N-CA	-5.72	1.39	1.46	6	1
1	A	373	GLU	CA-CB	5.72	1.60	1.53	6	2
2	B	124	ASP	N-CA	-5.72	1.39	1.46	9	2
1	A	346	ASN	CA-CB	5.72	1.63	1.53	11	1
1	A	390	PHE	CA-C	5.72	1.59	1.52	13	1
1	A	383	LYS	N-CA	-5.72	1.39	1.46	3	1
2	B	234	GLU	N-CA	-5.72	1.39	1.46	14	1
2	B	83	ARG	CA-C	5.72	1.60	1.52	4	2
2	B	134	MET	N-CA	-5.72	1.39	1.46	12	2
2	B	248	LYS	C-N	5.71	1.41	1.33	12	1
2	B	230	LYS	CA-CB	5.71	1.59	1.54	1	2
1	A	443	ARG	NE-CZ	-5.71	1.26	1.33	7	1
2	B	197	ALA	C-N	5.71	1.41	1.33	13	1
2	B	245	GLU	N-CA	5.71	1.53	1.46	12	3
1	A	505	TRP	NE1-CE2	-5.71	1.31	1.37	8	1
2	B	76	GLU	CA-C	5.71	1.60	1.52	1	1
2	C	72	TRP	NE1-CE2	-5.71	1.31	1.37	8	1
1	A	330	ARG	C-N	5.71	1.42	1.33	7	2
1	A	437	ARG	N-CA	-5.71	1.39	1.46	2	1
1	A	508	CYS	CA-CB	5.70	1.62	1.52	4	2
1	A	429	PHE	CA-C	-5.70	1.45	1.52	8	2
2	B	57	PHE	CB-CG	5.70	1.63	1.50	14	1
1	A	440	GLU	C-N	5.70	1.41	1.33	10	2
1	A	447	SER	CA-CB	5.70	1.62	1.53	13	2
2	B	175	ARG	CA-CB	5.70	1.62	1.53	5	1
1	A	460	PRO	C-O	-5.70	1.16	1.24	15	1
2	B	69	GLN	C-N	5.69	1.41	1.33	3	1
2	C	78	GLU	C-N	5.69	1.40	1.33	3	3
2	C	83	ARG	C-N	5.69	1.41	1.33	3	1
1	A	476	TYR	CZ-OH	5.69	1.50	1.38	13	1
1	A	410	LEU	CA-CB	5.69	1.61	1.53	1	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	188	TYR	CA-C	5.69	1.60	1.52	4	4
2	B	174	ALA	C-N	5.69	1.41	1.33	3	1
2	C	205	GLU	CA-CB	5.68	1.62	1.53	6	1
2	B	110	GLU	C-N	5.68	1.41	1.33	2	1
2	B	206	ASN	CA-C	5.68	1.60	1.52	3	1
2	C	166	LEU	C-O	-5.68	1.17	1.24	6	1
2	C	136	LEU	C-O	5.68	1.30	1.24	12	2
1	A	395	LEU	CA-CB	5.68	1.62	1.53	2	1
1	A	392	GLU	CA-C	5.68	1.60	1.52	6	1
2	B	210	ARG	CD-NE	5.68	1.54	1.46	14	1
1	A	341	PHE	CA-C	5.67	1.59	1.52	14	3
1	A	353	TYR	CA-C	-5.67	1.46	1.52	1	2
1	A	449	TYR	N-CA	5.67	1.54	1.45	4	1
2	B	131	GLN	C-N	5.67	1.41	1.33	7	1
2	B	110	GLU	CA-CB	5.67	1.62	1.53	13	1
2	C	75	LEU	C-N	5.67	1.41	1.33	15	1
2	B	71	PHE	C-O	5.67	1.30	1.24	4	1
2	C	165	PRO	CA-CB	-5.67	1.46	1.53	8	1
2	C	102	ASP	CA-CB	5.67	1.62	1.53	2	2
2	C	67	VAL	C-N	5.67	1.41	1.33	14	1
2	B	179	ASP	CA-CB	5.67	1.62	1.53	13	2
2	C	82	LEU	N-CA	5.66	1.53	1.46	5	2
1	A	509	PRO	CA-C	-5.66	1.44	1.52	8	2
1	A	419	LEU	C-N	5.66	1.41	1.33	6	2
1	A	486	PHE	C-N	5.66	1.41	1.33	11	1
2	B	84	GLN	N-CA	5.66	1.53	1.46	2	1
2	B	75	LEU	CA-CB	5.66	1.62	1.53	6	3
1	A	330	ARG	CZ-NH2	-5.66	1.26	1.33	2	1
2	B	87	SER	CA-C	-5.66	1.45	1.52	12	1
2	B	219	THR	N-CA	5.66	1.53	1.46	15	1
2	C	130	TRP	CA-C	5.65	1.59	1.52	3	2
2	B	87	SER	CA-CB	5.65	1.62	1.53	4	1
2	B	129	LYS	C-O	-5.65	1.17	1.24	1	2
2	B	99	PRO	CA-CB	-5.65	1.45	1.53	10	1
2	C	148	LEU	CA-CB	5.65	1.62	1.53	2	1
2	B	136	LEU	CA-CB	5.65	1.62	1.53	6	1
2	B	182	ARG	CA-CB	-5.64	1.44	1.53	13	1
2	B	199	ARG	CZ-NH2	5.64	1.40	1.33	13	3
1	A	426	LYS	CA-CB	5.64	1.61	1.53	11	1
2	B	263	ASN	C-N	5.64	1.41	1.33	11	1
2	C	171	ARG	CD-NE	5.64	1.54	1.46	6	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	C	194	GLN	N-CA	-5.64	1.39	1.46	14	1
2	B	184	HIS	CG-ND1	-5.63	1.32	1.38	13	2
2	C	144	LEU	C-N	5.63	1.41	1.33	5	1
2	C	152	ALA	N-CA	-5.63	1.39	1.46	8	1
2	B	196	LEU	N-CA	-5.63	1.39	1.46	3	1
2	B	153	ARG	CD-NE	5.63	1.54	1.46	4	3
1	A	498	PRO	C-N	5.63	1.41	1.33	7	2
2	B	215	HIS	CG-CD2	5.63	1.42	1.35	10	1
1	A	378	LYS	CA-C	-5.63	1.45	1.52	15	1
2	B	154	GLN	N-CA	-5.62	1.39	1.46	7	1
1	A	338	GLU	CA-C	5.62	1.58	1.52	2	2
2	C	177	HIS	CE1-NE2	-5.62	1.26	1.32	11	1
1	A	385	ASP	CA-C	5.62	1.60	1.52	12	1
2	C	95	ALA	CA-CB	5.62	1.62	1.53	13	1
1	A	423	PRO	CA-C	5.62	1.60	1.52	2	3
2	C	149	GLN	CA-CB	5.62	1.62	1.53	4	2
2	B	210	ARG	CA-C	5.62	1.60	1.52	8	2
1	A	356	PRO	CA-CB	-5.62	1.46	1.53	1	1
1	A	434	LYS	CA-C	-5.62	1.46	1.52	2	1
2	C	200	LEU	CA-C	-5.62	1.45	1.52	15	2
2	B	146	ALA	CA-C	5.61	1.60	1.52	15	1
2	B	172	ASP	N-CA	5.61	1.53	1.46	5	2
2	C	143	PRO	CA-CB	5.61	1.61	1.53	7	2
2	C	155	LYS	N-CA	-5.61	1.39	1.46	13	1
2	C	189	SER	N-CA	5.61	1.53	1.46	12	1
2	C	217	LYS	CA-CB	5.61	1.62	1.53	9	1
1	A	445	VAL	N-CA	-5.61	1.39	1.46	10	1
1	A	503	ARG	CD-NE	5.61	1.54	1.46	14	1
2	C	104	PHE	CA-C	5.60	1.60	1.52	1	2
2	C	203	LEU	N-CA	-5.60	1.39	1.46	10	1
2	B	119	VAL	N-CA	5.60	1.53	1.46	13	2
1	A	443	ARG	CD-NE	5.60	1.54	1.46	10	1
2	C	243	VAL	N-CA	5.60	1.53	1.46	14	1
1	A	408	ARG	CZ-NH2	-5.60	1.26	1.33	4	2
2	B	209	ALA	C-N	5.60	1.41	1.33	11	2
1	A	319	CYS	CA-C	-5.60	1.45	1.52	3	1
2	B	221	HIS	CB-CG	5.60	1.57	1.50	10	1
2	B	72	TRP	CZ2-CH2	5.59	1.47	1.37	4	2
1	A	318	ILE	CA-CB	-5.59	1.47	1.54	5	1
2	B	201	GLU	CA-C	5.59	1.59	1.52	12	1
1	A	399	TYR	C-O	-5.59	1.18	1.24	4	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	C	166	LEU	CA-C	-5.59	1.45	1.52	1	1
2	C	99	PRO	C-N	5.59	1.41	1.33	3	1
2	B	56	THR	N-CA	-5.59	1.39	1.46	15	1
2	B	147	GLU	C-O	-5.59	1.17	1.24	2	1
2	C	94	LYS	N-CA	5.59	1.53	1.46	6	1
2	C	121	PRO	CA-C	5.59	1.60	1.52	8	1
2	B	116	ARG	C-N	5.59	1.41	1.34	10	1
1	A	427	THR	CA-CB	-5.59	1.45	1.53	2	1
2	C	110	GLU	C-N	5.59	1.41	1.34	3	1
1	A	429	PHE	C-N	5.58	1.41	1.33	7	2
2	B	157	HIS	C-N	5.58	1.41	1.33	1	1
2	C	197	ALA	CA-C	-5.58	1.45	1.52	3	1
2	B	106	LYS	N-CA	-5.58	1.39	1.46	5	1
1	A	360	PHE	CA-CB	5.58	1.62	1.53	11	1
2	B	258	TYR	N-CA	5.58	1.53	1.46	15	1
1	A	345	ARG	CD-NE	5.58	1.54	1.46	2	2
2	B	175	ARG	CD-NE	5.58	1.54	1.46	3	3
2	C	166	LEU	C-N	5.58	1.41	1.33	9	2
1	A	409	GLY	N-CA	5.58	1.52	1.45	1	2
2	B	141	VAL	N-CA	5.57	1.53	1.46	7	1
1	A	468	MET	CG-SD	5.57	1.94	1.80	5	1
2	C	215	HIS	CE1-NE2	5.57	1.38	1.32	13	1
2	C	89	ASP	N-CA	-5.57	1.39	1.46	14	1
2	C	157	HIS	N-CA	-5.57	1.39	1.46	1	1
1	A	463	PRO	CA-CB	5.57	1.61	1.53	14	1
2	C	119	VAL	CA-CB	-5.57	1.48	1.54	7	1
1	A	406	LEU	CA-CB	5.57	1.62	1.53	14	2
1	A	387	HIS	C-N	5.57	1.41	1.33	13	1
1	A	504	ASP	CA-CB	5.56	1.62	1.53	4	1
2	B	219	THR	C-N	5.56	1.41	1.33	15	1
2	B	222	LEU	CA-CB	5.56	1.61	1.53	15	1
2	C	209	ALA	CA-CB	5.56	1.61	1.53	15	1
2	B	235	ASP	N-CA	-5.56	1.39	1.46	4	1
1	A	408	ARG	N-CA	-5.56	1.39	1.46	2	2
2	B	234	GLU	CA-C	-5.56	1.45	1.52	5	1
2	C	110	GLU	CD-OE1	5.56	1.35	1.25	13	1
2	C	110	GLU	N-CA	5.55	1.53	1.46	13	1
1	A	508	CYS	CA-C	-5.55	1.46	1.53	5	1
2	C	115	TYR	CA-CB	5.55	1.61	1.53	7	1
2	C	250	SER	C-N	5.55	1.41	1.33	13	1
2	C	138	ARG	N-CA	-5.55	1.39	1.46	10	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	195	ARG	C-N	5.55	1.41	1.33	14	1
2	B	147	GLU	C-N	5.55	1.41	1.33	8	2
1	A	361	TRP	CA-CB	5.55	1.62	1.53	8	1
2	B	80	GLU	CA-CB	5.54	1.61	1.53	12	2
1	A	357	ILE	C-N	5.54	1.41	1.33	4	1
2	C	224	THR	N-CA	-5.54	1.39	1.46	9	2
1	A	387	HIS	CB-CG	5.54	1.57	1.50	10	2
2	B	128	LYS	CA-C	-5.54	1.45	1.52	9	1
1	A	391	ASP	C-O	-5.54	1.17	1.23	14	1
2	C	66	PRO	CA-CB	5.54	1.61	1.53	14	1
2	C	241	LEU	CA-CB	5.54	1.60	1.53	15	1
2	B	66	PRO	CA-CB	5.54	1.61	1.53	4	1
1	A	386	LYS	C-N	5.54	1.41	1.33	2	1
2	C	95	ALA	C-O	-5.53	1.17	1.24	14	1
1	A	474	PHE	CA-C	-5.53	1.46	1.52	15	1
2	C	91	GLU	CA-C	-5.53	1.45	1.52	2	1
2	B	225	LEU	CA-CB	5.53	1.61	1.53	4	1
2	B	250	SER	C-N	5.53	1.41	1.33	8	1
2	C	255	LEU	C-N	5.53	1.41	1.33	8	1
1	A	320	ASP	C-N	5.53	1.41	1.33	9	2
1	A	343	ARG	CD-NE	5.53	1.53	1.46	10	1
1	A	468	MET	CA-C	5.53	1.60	1.52	14	1
2	B	181	LEU	CA-C	-5.53	1.45	1.52	4	1
2	C	134	MET	N-CA	5.53	1.52	1.46	10	2
2	B	178	VAL	C-N	5.52	1.41	1.33	12	2
1	A	324	ASP	C-N	5.52	1.40	1.33	1	1
2	C	56	THR	CA-CB	5.52	1.62	1.53	1	1
1	A	404	LYS	C-N	5.52	1.41	1.33	8	2
1	A	510	SER	N-CA	5.52	1.52	1.46	12	1
2	B	89	ASP	N-CA	-5.52	1.39	1.46	14	1
2	C	170	MET	C-O	-5.52	1.17	1.24	3	1
2	C	249	VAL	CA-CB	-5.52	1.47	1.54	4	1
1	A	318	ILE	C-N	5.52	1.41	1.33	8	1
2	C	219	THR	CA-C	5.52	1.59	1.52	9	1
2	B	177	HIS	CB-CG	5.52	1.57	1.50	2	1
2	C	62	GLU	N-CA	5.51	1.52	1.46	1	1
2	B	220	GLU	N-CA	5.51	1.52	1.46	7	2
2	C	113	GLU	C-N	5.51	1.41	1.33	10	1
2	C	223	SER	N-CA	5.51	1.53	1.46	3	1
2	B	80	GLU	C-N	5.51	1.40	1.33	11	2
2	C	56	THR	C-N	5.51	1.41	1.33	6	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	175	ARG	CZ-NH1	5.51	1.40	1.32	9	1
1	A	480	GLY	C-O	-5.51	1.16	1.24	3	1
2	C	154	GLN	CA-C	5.51	1.59	1.52	7	1
2	B	146	ALA	CA-CB	5.51	1.61	1.53	15	1
2	B	182	ARG	N-CA	5.51	1.53	1.46	6	1
2	B	108	TRP	C-O	-5.51	1.17	1.24	10	1
1	A	323	PHE	CA-C	-5.51	1.45	1.52	3	3
2	B	237	ARG	CA-CB	5.51	1.62	1.53	5	2
1	A	501	ALA	N-CA	-5.51	1.39	1.46	4	2
2	B	158	GLU	C-N	5.50	1.41	1.33	13	1
2	B	88	LYS	CA-C	5.50	1.59	1.52	1	1
1	A	323	PHE	CA-CB	5.50	1.62	1.53	11	2
2	B	78	GLU	CA-CB	5.50	1.62	1.53	5	1
2	B	176	ALA	CA-CB	5.50	1.61	1.53	6	1
2	C	231	PRO	CA-C	-5.50	1.44	1.52	11	1
1	A	351	ASP	CA-CB	5.50	1.62	1.53	4	1
1	A	436	TYR	N-CA	5.50	1.52	1.46	3	1
1	A	361	TRP	CA-C	-5.50	1.46	1.52	5	1
2	C	177	HIS	CG-CD2	5.50	1.41	1.35	8	1
1	A	372	TYR	CZ-OH	5.50	1.49	1.38	10	1
2	B	222	LEU	N-CA	5.49	1.53	1.46	6	1
1	A	332	GLU	CA-C	5.49	1.59	1.52	8	2
2	C	164	SER	C-O	-5.49	1.19	1.24	7	2
2	C	190	ASP	CA-C	5.49	1.59	1.52	5	2
1	A	485	LYS	N-CA	5.49	1.54	1.46	4	1
2	C	225	LEU	N-CA	5.49	1.53	1.46	7	1
1	A	482	LYS	C-N	5.49	1.41	1.33	10	1
2	C	197	ALA	C-N	5.49	1.41	1.33	11	1
2	B	156	LEU	C-O	5.49	1.30	1.24	8	1
2	C	123	LEU	C-N	5.49	1.40	1.33	9	1
1	A	449	TYR	C-O	5.49	1.28	1.24	10	1
2	B	158	GLU	N-CA	-5.49	1.39	1.46	6	1
1	A	423	PRO	C-N	5.48	1.42	1.33	12	1
2	B	114	LEU	C-N	5.48	1.41	1.33	4	1
2	B	123	LEU	N-CA	-5.48	1.39	1.46	9	1
2	B	173	ARG	CA-C	-5.48	1.45	1.52	11	1
2	C	79	THR	C-N	5.48	1.41	1.33	8	2
1	A	470	SER	CA-CB	5.48	1.61	1.53	11	2
2	B	101	LEU	CA-CB	5.47	1.61	1.53	1	1
2	B	199	ARG	C-N	-5.47	1.26	1.33	3	1
2	B	190	ASP	C-N	5.47	1.41	1.33	4	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	C	165	PRO	C-O	-5.47	1.17	1.24	5	1
2	C	220	GLU	C-N	5.47	1.41	1.33	7	1
2	C	156	LEU	CA-CB	5.47	1.61	1.53	1	1
1	A	393	ALA	CA-C	5.47	1.59	1.52	13	2
2	C	61	ARG	CD-NE	5.47	1.53	1.46	10	2
2	B	83	ARG	CD-NE	5.47	1.53	1.46	14	1
1	A	327	ALA	N-CA	5.47	1.52	1.46	2	1
2	B	71	PHE	C-N	5.47	1.41	1.33	5	1
2	B	109	GLN	N-CA	-5.47	1.39	1.46	5	1
2	B	177	HIS	CE1-NE2	5.47	1.38	1.32	15	1
2	B	104	PHE	CA-CB	5.46	1.61	1.53	2	2
2	C	171	ARG	CA-CB	5.46	1.61	1.53	12	2
2	C	248	LYS	CA-C	5.46	1.59	1.52	3	1
1	A	415	ILE	C-O	5.46	1.30	1.24	2	1
2	B	216	ALA	CA-CB	5.46	1.62	1.53	7	2
2	C	97	VAL	CA-CB	-5.46	1.47	1.54	12	1
1	A	456	TRP	NE1-CE2	-5.46	1.31	1.37	6	1
1	A	485	LYS	CA-C	-5.45	1.46	1.52	12	1
1	A	502	LEU	C-N	5.45	1.40	1.33	3	1
2	C	155	LYS	CA-CB	5.45	1.61	1.53	12	2
1	A	495	PRO	CA-C	5.45	1.60	1.52	14	1
2	C	75	LEU	CA-CB	5.45	1.61	1.53	10	1
2	C	217	LYS	C-N	5.45	1.41	1.33	12	1
2	C	103	ASP	C-N	5.45	1.41	1.33	11	1
2	C	232	ALA	C-N	5.45	1.40	1.33	15	1
2	B	215	HIS	CG-ND1	5.44	1.44	1.38	6	1
2	C	211	LEU	CA-C	5.44	1.59	1.52	13	1
2	C	183	THR	CA-C	-5.44	1.46	1.52	7	2
2	C	116	ARG	CD-NE	5.43	1.53	1.46	2	3
1	A	452	ASN	CA-C	5.43	1.59	1.52	2	1
1	A	413	ASP	CA-CB	5.43	1.61	1.53	7	2
2	C	178	VAL	CA-C	5.43	1.59	1.52	6	1
1	A	483	TYR	CA-CB	5.43	1.65	1.54	10	1
2	B	83	ARG	C-N	5.43	1.41	1.33	13	3
2	C	114	LEU	CA-CB	5.43	1.62	1.53	15	2
1	A	510	SER	CA-CB	5.43	1.62	1.53	3	2
2	C	68	THR	CA-CB	5.42	1.61	1.53	1	1
2	B	165	PRO	N-CD	-5.42	1.40	1.47	2	1
2	C	114	LEU	C-O	-5.42	1.17	1.24	8	1
1	A	455	VAL	CA-C	-5.42	1.46	1.52	4	1
2	C	195	ARG	N-CA	-5.42	1.39	1.46	11	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	411	PRO	C-N	5.42	1.40	1.33	14	1
2	B	61	ARG	CZ-NH2	-5.42	1.26	1.33	14	1
2	B	116	ARG	CA-C	5.42	1.60	1.52	2	1
2	C	83	ARG	CD-NE	5.42	1.53	1.46	10	1
2	C	87	SER	C-O	-5.42	1.17	1.24	11	1
1	A	495	PRO	C-N	5.42	1.40	1.33	2	1
2	C	193	ARG	CD-NE	5.42	1.53	1.46	6	1
1	A	372	TYR	N-CA	-5.41	1.39	1.45	3	1
2	C	237	ARG	N-CA	5.41	1.52	1.46	13	2
2	B	112	MET	CA-CB	5.41	1.61	1.53	1	1
1	A	329	LEU	C-N	5.41	1.41	1.33	2	2
2	C	116	ARG	CZ-NH2	-5.41	1.26	1.33	7	1
2	C	158	GLU	CA-CB	5.41	1.62	1.53	10	1
1	A	453	ILE	C-N	5.41	1.41	1.33	11	2
2	B	85	GLU	N-CA	5.41	1.52	1.46	7	1
2	C	112	MET	CA-CB	5.40	1.61	1.53	6	2
2	C	75	LEU	CA-C	5.40	1.59	1.52	11	1
2	B	182	ARG	C-O	-5.40	1.17	1.24	5	1
1	A	472	GLU	CA-CB	5.40	1.61	1.53	7	1
2	C	179	ASP	CA-CB	5.40	1.61	1.53	2	1
2	B	109	GLN	CA-C	-5.40	1.45	1.52	15	2
1	A	421	TRP	C-N	5.39	1.40	1.33	14	1
2	C	164	SER	CA-C	5.39	1.59	1.52	5	2
2	C	146	ALA	CA-CB	5.39	1.63	1.53	14	1
2	C	201	GLU	CA-CB	5.39	1.61	1.53	7	1
1	A	330	ARG	CA-C	5.39	1.59	1.52	2	1
1	A	444	ALA	N-CA	-5.38	1.39	1.46	4	1
2	B	238	GLN	N-CA	-5.38	1.39	1.46	8	1
1	A	365	PRO	N-CA	-5.38	1.40	1.47	1	1
2	B	191	GLU	N-CA	-5.38	1.39	1.46	5	1
1	A	339	ARG	CD-NE	5.38	1.53	1.46	12	2
1	A	472	GLU	N-CA	-5.38	1.39	1.46	12	1
2	B	155	LYS	C-N	5.38	1.41	1.33	5	1
1	A	358	GLY	N-CA	5.38	1.53	1.45	2	1
2	C	150	GLU	C-N	5.38	1.40	1.33	3	1
2	B	163	LEU	CA-C	5.38	1.60	1.52	4	2
1	A	475	THR	C-O	-5.38	1.17	1.24	13	1
2	B	100	TYR	N-CA	5.38	1.52	1.46	9	1
1	A	503	ARG	N-CA	-5.38	1.40	1.46	6	1
2	B	96	LYS	C-N	5.37	1.39	1.33	4	1
2	B	184	HIS	CD2-NE2	5.37	1.43	1.37	7	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	381	PHE	N-CA	-5.37	1.39	1.46	14	1
1	A	484	TRP	CA-CB	5.37	1.61	1.53	6	2
2	B	111	GLU	C-O	-5.37	1.18	1.24	10	1
2	C	140	LYS	CA-CB	5.37	1.61	1.53	10	1
2	C	167	GLY	C-N	5.37	1.40	1.33	12	1
1	A	427	THR	N-CA	5.37	1.52	1.46	13	1
2	B	161	GLU	C-N	5.37	1.41	1.33	13	1
2	C	257	GLU	C-N	5.37	1.41	1.33	4	1
1	A	401	LYS	CA-C	-5.37	1.45	1.52	8	1
2	C	75	LEU	C-O	5.36	1.30	1.24	1	1
1	A	473	VAL	C-N	5.36	1.41	1.33	5	1
1	A	402	HIS	C-N	5.36	1.40	1.33	4	1
1	A	364	LEU	C-N	-5.36	1.26	1.33	5	1
2	B	135	GLU	N-CA	-5.36	1.40	1.46	6	1
2	C	60	LEU	C-N	5.36	1.41	1.33	7	1
2	C	122	TYR	N-CA	-5.36	1.40	1.46	12	1
2	C	131	GLN	C-O	-5.36	1.17	1.24	1	1
2	C	260	LYS	C-O	-5.36	1.17	1.24	7	1
2	B	65	GLY	C-N	5.36	1.40	1.34	12	1
2	B	145	ARG	CA-C	-5.35	1.45	1.52	5	1
1	A	479	LYS	CA-C	-5.35	1.46	1.52	4	1
1	A	485	LYS	CA-CB	5.35	1.59	1.53	15	1
1	A	320	ASP	N-CA	-5.35	1.39	1.46	3	1
2	C	231	PRO	C-N	5.35	1.41	1.33	3	1
1	A	491	LEU	N-CA	5.35	1.53	1.46	10	1
2	B	175	ARG	CZ-NH2	-5.35	1.26	1.33	13	1
2	B	173	ARG	CA-CB	5.35	1.61	1.53	10	2
1	A	379	PHE	N-CA	5.35	1.52	1.46	13	1
2	C	234	GLU	C-N	-5.35	1.26	1.33	1	2
1	A	328	MET	CA-CB	5.34	1.61	1.53	6	1
2	B	186	ALA	C-N	5.34	1.46	1.33	7	1
2	B	250	SER	C-O	5.34	1.30	1.24	9	1
1	A	342	TRP	C-O	-5.34	1.17	1.23	15	1
2	C	59	LYS	N-CA	-5.34	1.39	1.46	4	1
2	B	173	ARG	NE-CZ	-5.34	1.27	1.33	2	1
2	B	131	GLN	CA-CB	5.34	1.61	1.53	6	1
2	B	248	LYS	N-CA	-5.34	1.40	1.46	9	1
2	C	168	GLU	C-N	5.33	1.40	1.33	11	1
1	A	391	ASP	N-CA	5.33	1.52	1.45	3	1
2	C	252	LEU	CA-CB	5.33	1.61	1.53	8	2
2	C	78	GLU	N-CA	5.33	1.52	1.46	12	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	138	ARG	CZ-NH2	-5.33	1.26	1.33	15	1
2	C	57	PHE	CG-CD1	5.33	1.50	1.38	1	1
1	A	440	GLU	CA-CB	5.33	1.62	1.53	4	1
2	B	104	PHE	N-CA	5.33	1.52	1.46	12	1
2	C	238	GLN	C-N	5.33	1.40	1.33	4	1
1	A	454	LYS	N-CA	5.33	1.53	1.46	10	1
1	A	511	GLY	N-CA	5.33	1.54	1.45	12	1
2	B	200	LEU	CA-CB	5.32	1.61	1.53	4	1
2	B	203	LEU	CB-CG	5.32	1.64	1.53	11	1
1	A	382	PHE	CG-CD1	5.32	1.50	1.38	2	1
2	B	175	ARG	NE-CZ	5.32	1.39	1.33	13	1
1	A	371	ALA	C-O	-5.32	1.18	1.24	5	1
2	C	168	GLU	CA-CB	5.32	1.61	1.53	5	1
1	A	367	SER	CA-C	5.32	1.59	1.52	6	3
2	C	127	GLN	N-CA	5.32	1.52	1.46	9	1
2	C	104	PHE	CA-CB	5.32	1.62	1.53	7	1
2	C	71	PHE	CA-CB	5.31	1.61	1.53	2	1
1	A	494	GLU	C-N	-5.31	1.26	1.33	8	1
1	A	317	ASN	C-N	5.31	1.40	1.33	13	1
2	C	249	VAL	CA-C	5.31	1.59	1.52	15	1
2	B	257	GLU	C-O	-5.31	1.18	1.24	3	1
2	C	181	LEU	CB-CG	5.31	1.64	1.53	9	1
2	C	55	SER	N-CA	5.31	1.56	1.46	8	3
1	A	455	VAL	C-N	5.31	1.40	1.33	8	2
2	C	185	LEU	CB-CG	5.31	1.64	1.53	11	1
2	B	217	LYS	N-CA	-5.31	1.39	1.46	14	1
2	B	159	LEU	C-N	5.31	1.40	1.33	15	1
1	A	408	ARG	CD-NE	5.31	1.53	1.46	5	1
1	A	454	LYS	C-N	5.31	1.40	1.34	6	2
1	A	351	ASP	CA-C	5.30	1.59	1.52	3	1
2	B	183	THR	CA-C	-5.30	1.45	1.52	12	1
2	C	104	PHE	N-CA	-5.30	1.40	1.46	15	1
2	C	208	GLY	CA-C	-5.30	1.46	1.52	5	2
2	C	179	ASP	N-CA	-5.30	1.39	1.46	10	1
1	A	376	ASP	CA-C	5.30	1.59	1.52	1	1
1	A	505	TRP	CA-CB	5.30	1.61	1.54	7	3
1	A	467	PHE	C-O	-5.30	1.17	1.23	5	1
1	A	394	SER	CA-CB	5.30	1.63	1.53	9	1
1	A	384	GLY	C-N	5.30	1.40	1.33	11	1
2	C	195	ARG	CD-NE	5.29	1.53	1.46	1	2
2	B	138	ARG	CA-CB	5.29	1.62	1.53	8	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	216	ALA	N-CA	-5.29	1.39	1.46	15	1
2	C	210	ARG	NE-CZ	5.29	1.38	1.33	15	1
2	B	177	HIS	N-CA	-5.29	1.40	1.46	3	3
1	A	473	VAL	C-O	-5.29	1.19	1.24	15	1
1	A	391	ASP	C-N	5.29	1.41	1.33	5	1
2	B	58	SER	CA-CB	5.29	1.61	1.53	5	1
2	B	136	LEU	C-N	5.29	1.40	1.33	6	1
1	A	443	ARG	CZ-NH2	-5.29	1.26	1.33	8	1
1	A	411	PRO	CA-CB	-5.29	1.46	1.53	7	1
2	C	168	GLU	CA-C	-5.29	1.46	1.52	10	1
2	C	220	GLU	N-CA	-5.29	1.40	1.46	10	3
2	B	138	ARG	CZ-NH1	-5.28	1.25	1.32	8	1
2	C	61	ARG	NE-CZ	5.28	1.38	1.33	10	2
2	C	171	ARG	CZ-NH2	-5.28	1.26	1.33	10	1
2	B	188	TYR	CZ-OH	5.28	1.49	1.38	15	1
2	B	139	GLN	C-N	5.28	1.40	1.33	5	1
2	B	217	LYS	CA-C	5.28	1.59	1.52	13	1
2	C	243	VAL	CA-C	-5.28	1.46	1.52	15	1
2	B	186	ALA	N-CA	5.28	1.51	1.46	7	1
1	A	391	ASP	CA-C	-5.28	1.45	1.52	11	1
1	A	425	GLY	CA-C	5.28	1.57	1.51	2	1
2	C	247	PHE	C-N	5.27	1.41	1.33	10	1
2	B	259	THR	C-N	5.27	1.40	1.33	1	1
1	A	443	ARG	N-CA	-5.27	1.39	1.46	5	1
1	A	380	VAL	C-N	5.27	1.41	1.33	10	1
2	C	117	GLN	C-N	5.27	1.41	1.34	2	1
2	B	255	LEU	CA-C	-5.27	1.46	1.52	11	1
2	B	178	VAL	CA-C	-5.27	1.46	1.52	2	3
2	B	121	PRO	CA-C	5.27	1.61	1.52	13	1
2	B	192	LEU	CA-CB	5.27	1.61	1.53	15	1
1	A	486	PHE	N-CA	5.27	1.52	1.46	14	1
2	B	119	VAL	CA-C	5.26	1.59	1.52	2	1
2	C	57	PHE	C-N	5.26	1.40	1.33	15	1
2	B	203	LEU	CA-CB	5.26	1.61	1.53	7	2
2	C	250	SER	CA-CB	5.26	1.61	1.53	10	1
1	A	482	LYS	N-CA	5.26	1.52	1.45	6	1
1	A	467	PHE	CA-C	-5.26	1.45	1.52	13	2
2	B	174	ALA	N-CA	5.26	1.52	1.46	11	1
2	C	71	PHE	CG-CD2	5.26	1.49	1.38	4	1
1	A	466	SER	CA-C	-5.26	1.45	1.52	8	1
2	C	211	LEU	C-N	5.25	1.40	1.33	8	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	124	ASP	CA-CB	5.25	1.62	1.53	5	1
2	C	232	ALA	CA-CB	5.25	1.61	1.53	9	1
2	C	126	PHE	C-N	5.25	1.40	1.33	10	1
2	C	125	ASP	C-N	5.25	1.41	1.33	14	1
1	A	381	PHE	C-N	5.25	1.40	1.33	4	1
2	C	59	LYS	C-N	5.25	1.40	1.33	8	1
2	B	145	ARG	CZ-NH2	-5.25	1.26	1.33	14	1
2	C	184	HIS	CD2-NE2	5.24	1.43	1.37	1	1
2	C	149	GLN	C-O	-5.24	1.18	1.24	2	1
2	C	82	LEU	C-N	5.24	1.40	1.33	3	2
2	B	222	LEU	CA-C	5.24	1.59	1.52	11	1
2	C	249	VAL	C-O	-5.24	1.18	1.24	4	1
2	B	141	VAL	C-N	5.24	1.40	1.33	13	1
2	B	192	LEU	C-N	5.24	1.40	1.33	9	1
2	B	214	TYR	CZ-OH	5.23	1.49	1.38	2	1
1	A	396	GLU	C-N	5.23	1.39	1.33	13	1
1	A	510	SER	C-N	5.23	1.40	1.33	12	2
1	A	410	LEU	N-CA	5.23	1.53	1.45	1	1
2	B	63	GLN	N-CA	-5.23	1.40	1.46	9	1
2	C	237	ARG	C-O	-5.23	1.18	1.24	14	1
2	B	61	ARG	N-CA	-5.22	1.40	1.46	15	1
2	C	254	ALA	CA-C	-5.22	1.46	1.52	12	1
2	C	113	GLU	CA-C	-5.22	1.46	1.52	3	1
2	B	254	ALA	CA-CB	5.22	1.61	1.53	6	1
2	C	255	LEU	C-O	5.22	1.30	1.24	7	1
1	A	393	ALA	N-CA	-5.22	1.40	1.46	2	1
1	A	330	ARG	CA-CB	5.22	1.61	1.53	3	1
2	B	127	GLN	CA-CB	5.22	1.61	1.53	5	1
1	A	503	ARG	CA-C	-5.22	1.46	1.52	12	2
2	B	192	LEU	N-CA	-5.21	1.40	1.46	14	1
2	B	127	GLN	C-N	5.21	1.41	1.34	11	1
1	A	460	PRO	C-N	5.21	1.40	1.33	13	1
2	C	140	LYS	CA-C	-5.21	1.45	1.52	5	1
2	C	212	ALA	N-CA	-5.21	1.40	1.46	9	1
2	B	125	ASP	C-N	5.21	1.40	1.33	12	1
2	B	133	GLU	C-N	5.20	1.40	1.33	6	1
1	A	396	GLU	CA-C	5.20	1.58	1.53	11	1
1	A	462	SER	N-CA	-5.20	1.38	1.46	2	1
1	A	345	ARG	CA-C	5.20	1.58	1.52	5	1
2	C	180	ALA	CA-CB	-5.20	1.45	1.53	5	1
1	A	453	ILE	N-CA	5.20	1.53	1.46	13	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	C	147	GLU	CA-C	5.20	1.59	1.52	14	1
2	C	176	ALA	N-CA	-5.19	1.40	1.46	13	3
1	A	319	CYS	C-N	5.19	1.41	1.33	13	1
1	A	440	GLU	CA-C	-5.19	1.45	1.52	7	2
1	A	480	GLY	CA-C	-5.19	1.44	1.51	1	1
2	B	233	LEU	N-CA	5.19	1.52	1.46	7	1
2	C	99	PRO	CA-C	-5.19	1.46	1.52	1	1
2	C	195	ARG	C-N	5.19	1.40	1.33	10	1
2	C	102	ASP	N-CA	5.18	1.52	1.46	13	1
1	A	316	PRO	N-CA	5.18	1.54	1.47	3	1
1	A	326	VAL	CA-CB	-5.18	1.48	1.54	7	1
2	B	130	TRP	NE1-CE2	5.18	1.43	1.37	7	1
2	C	221	HIS	CA-C	5.18	1.59	1.52	9	1
2	C	234	GLU	CA-C	-5.18	1.46	1.52	11	1
2	B	164	SER	C-N	5.18	1.40	1.34	6	1
2	C	245	GLU	CA-C	5.18	1.59	1.52	6	1
2	C	108	TRP	C-O	-5.18	1.18	1.24	15	1
2	B	246	SER	CA-CB	5.18	1.61	1.53	4	1
2	B	227	GLU	N-CA	-5.18	1.40	1.46	5	1
2	B	166	LEU	C-N	5.18	1.40	1.34	15	1
2	C	83	ARG	N-CA	5.18	1.52	1.46	15	1
2	B	221	HIS	N-CA	-5.17	1.40	1.46	1	1
1	A	356	PRO	CA-C	5.17	1.58	1.52	14	1
2	B	240	LEU	C-N	5.17	1.40	1.33	15	1
1	A	385	ASP	N-CA	-5.17	1.40	1.46	6	1
1	A	416	ASP	CA-CB	5.17	1.61	1.53	13	1
1	A	509	PRO	CA-CB	5.17	1.60	1.53	2	1
2	C	106	LYS	CA-CB	5.16	1.64	1.54	7	1
2	C	242	PRO	CA-CB	-5.16	1.46	1.53	10	1
1	A	365	PRO	C-O	5.16	1.30	1.23	12	1
1	A	367	SER	CA-CB	5.16	1.62	1.53	14	1
2	B	84	GLN	CA-C	-5.16	1.46	1.52	2	1
2	C	212	ALA	C-N	5.16	1.40	1.33	13	1
2	C	93	VAL	N-CA	5.16	1.52	1.46	2	1
2	C	198	ALA	C-N	5.16	1.40	1.33	3	1
1	A	468	MET	C-N	5.16	1.39	1.33	5	1
2	B	151	GLY	CA-C	-5.16	1.46	1.52	9	1
2	C	188	TYR	CA-CB	5.16	1.61	1.53	11	1
2	B	117	GLN	CA-CB	5.16	1.61	1.53	14	1
2	C	193	ARG	CA-CB	5.16	1.61	1.53	15	1
2	B	83	ARG	CA-CB	5.16	1.61	1.53	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	238	GLN	C-O	-5.16	1.18	1.24	6	1
2	C	214	TYR	CA-C	5.15	1.59	1.52	14	1
1	A	476	TYR	C-O	-5.15	1.18	1.24	1	1
2	B	103	ASP	CA-CB	5.15	1.61	1.53	13	1
2	B	60	LEU	N-CA	-5.14	1.40	1.46	3	1
2	C	107	LYS	C-N	5.14	1.41	1.33	11	1
1	A	466	SER	N-CA	5.14	1.52	1.46	13	1
2	B	140	LYS	C-N	5.14	1.40	1.33	2	1
2	B	177	HIS	CG-CD2	-5.14	1.30	1.35	6	1
2	C	243	VAL	CA-CB	5.14	1.60	1.54	2	1
2	B	109	GLN	CA-CB	5.14	1.61	1.53	12	1
2	B	165	PRO	N-CA	-5.14	1.40	1.47	12	1
2	B	217	LYS	CA-CB	5.13	1.61	1.53	6	1
2	C	62	GLU	CA-CB	5.13	1.61	1.53	13	1
2	C	193	ARG	N-CA	5.13	1.52	1.46	12	1
2	B	74	ASN	CA-CB	5.13	1.61	1.53	5	1
1	A	326	VAL	N-CA	-5.13	1.39	1.46	10	1
1	A	465	GLY	CA-C	-5.13	1.46	1.51	12	1
1	A	353	TYR	CZ-OH	5.13	1.48	1.38	8	1
2	B	153	ARG	CZ-NH2	-5.13	1.26	1.33	9	1
2	C	111	GLU	CD-OE2	5.13	1.35	1.25	13	1
2	B	162	LYS	CA-CB	5.12	1.62	1.53	7	1
2	C	207	GLY	C-O	5.12	1.30	1.23	15	1
2	B	110	GLU	C-O	-5.12	1.18	1.24	7	1
2	C	214	TYR	C-N	5.12	1.40	1.33	7	1
1	A	484	TRP	N-CA	-5.12	1.40	1.46	9	1
2	C	105	GLN	CD-NE2	5.12	1.44	1.33	7	1
1	A	350	MET	C-N	5.12	1.40	1.33	8	1
2	B	253	SER	C-N	5.12	1.40	1.33	11	1
2	B	150	GLU	C-N	5.12	1.41	1.33	4	1
2	C	98	GLN	C-O	-5.12	1.17	1.24	4	1
2	B	257	GLU	CA-C	-5.12	1.46	1.52	7	1
2	B	69	GLN	CA-CB	5.12	1.61	1.53	4	1
2	C	118	LYS	N-CA	-5.12	1.39	1.46	1	1
2	C	102	ASP	C-N	5.12	1.40	1.33	12	1
1	A	402	HIS	CG-CD2	5.11	1.41	1.35	5	1
1	A	473	VAL	N-CA	-5.11	1.39	1.46	4	1
2	B	241	LEU	C-O	-5.11	1.19	1.24	4	1
2	B	127	GLN	N-CA	5.11	1.52	1.46	7	1
2	C	246	SER	CA-CB	5.11	1.61	1.53	9	1
2	C	147	GLU	N-CA	-5.11	1.40	1.46	7	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	90	LEU	CA-CB	5.11	1.61	1.53	10	1
2	C	60	LEU	N-CA	5.11	1.52	1.46	14	1
2	B	224	THR	CA-CB	5.11	1.61	1.53	4	1
2	C	172	ASP	N-CA	-5.11	1.40	1.46	7	1
2	B	99	PRO	N-CD	5.11	1.54	1.47	10	1
1	A	394	SER	C-N	5.10	1.40	1.33	8	1
2	B	60	LEU	CA-CB	5.10	1.61	1.53	10	1
1	A	478	TYR	N-CA	5.10	1.52	1.46	13	1
1	A	451	LYS	C-N	5.10	1.40	1.33	15	1
2	C	119	VAL	CA-C	5.10	1.60	1.52	3	1
2	B	216	ALA	C-N	5.10	1.40	1.33	3	1
2	B	205	GLU	C-N	5.09	1.40	1.33	4	1
1	A	349	VAL	C-N	5.09	1.40	1.33	5	1
1	A	401	LYS	N-CA	5.09	1.52	1.45	6	1
2	B	251	PHE	C-N	5.09	1.40	1.33	15	1
1	A	382	PHE	CA-C	5.09	1.58	1.52	6	1
1	A	483	TYR	CZ-OH	5.09	1.48	1.38	11	1
2	B	142	GLU	C-O	-5.08	1.19	1.24	4	1
1	A	397	PRO	C-N	5.08	1.40	1.33	5	1
2	C	98	GLN	CG-CD	5.08	1.64	1.52	7	1
2	B	253	SER	CA-CB	5.08	1.61	1.53	11	1
2	C	242	PRO	N-CD	-5.08	1.40	1.47	10	1
1	A	432	GLY	CA-C	-5.08	1.44	1.51	15	1
2	B	249	VAL	N-CA	5.08	1.52	1.46	5	1
2	C	257	GLU	CA-CB	5.08	1.61	1.53	5	1
2	B	154	GLN	CA-C	5.08	1.59	1.52	7	1
2	C	142	GLU	C-O	5.08	1.29	1.24	7	1
1	A	359	GLN	CA-CB	5.08	1.61	1.53	9	1
1	A	366	ALA	C-N	5.07	1.40	1.33	2	1
1	A	352	GLY	C-O	-5.07	1.17	1.24	9	1
1	A	317	ASN	C-O	-5.07	1.17	1.23	10	1
1	A	431	ARG	C-N	5.07	1.41	1.33	6	1
2	B	252	LEU	CB-CG	5.07	1.63	1.53	6	1
2	B	190	ASP	CA-CB	5.07	1.61	1.53	8	1
2	B	230	LYS	N-CA	5.07	1.51	1.46	13	1
1	A	442	LEU	CA-C	-5.07	1.45	1.52	10	1
1	A	399	TYR	CG-CD1	5.07	1.50	1.39	4	1
1	A	443	ARG	CA-CB	5.07	1.60	1.53	13	1
1	A	505	TRP	CZ2-CH2	5.07	1.46	1.37	14	1
2	B	70	GLU	CA-C	5.07	1.59	1.52	4	1
2	C	223	SER	C-N	5.07	1.40	1.33	6	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	468	MET	N-CA	-5.07	1.39	1.45	9	1
2	B	135	GLU	C-N	5.07	1.40	1.33	9	1
2	C	179	ASP	CA-C	5.07	1.59	1.52	12	1
1	A	499	LYS	CA-C	-5.07	1.46	1.52	13	1
1	A	438	PHE	C-O	-5.07	1.18	1.24	15	1
1	A	477	PHE	CA-CB	5.06	1.60	1.53	14	1
1	A	392	GLU	CA-CB	5.06	1.61	1.53	6	1
2	C	143	PRO	CA-C	5.06	1.59	1.52	10	1
2	C	112	MET	C-O	-5.06	1.17	1.24	3	2
2	C	196	LEU	C-O	-5.06	1.18	1.24	10	1
2	C	109	GLN	CA-CB	5.06	1.61	1.53	12	1
2	B	90	LEU	CA-C	5.06	1.59	1.52	5	1
2	B	199	ARG	CD-NE	5.06	1.53	1.46	15	1
1	A	482	LYS	CA-CB	5.06	1.61	1.53	11	1
2	B	127	GLN	CA-C	-5.06	1.46	1.52	14	1
2	B	157	HIS	CA-C	-5.05	1.46	1.52	6	1
2	C	165	PRO	C-N	5.05	1.40	1.33	9	1
2	C	75	LEU	N-CA	5.05	1.52	1.46	12	1
1	A	486	PHE	CA-C	5.05	1.58	1.52	13	1
2	B	221	HIS	C-N	5.05	1.40	1.33	9	1
2	B	262	LEU	C-N	5.05	1.41	1.34	1	1
1	A	474	PHE	C-N	5.05	1.40	1.33	2	1
2	B	233	LEU	C-N	5.05	1.40	1.33	3	1
2	B	221	HIS	CA-CB	5.05	1.61	1.53	5	1
2	B	116	ARG	CA-CB	5.05	1.61	1.53	6	1
2	B	100	TYR	CA-CB	5.04	1.61	1.53	4	1
1	A	432	GLY	C-N	5.04	1.40	1.33	3	1
1	A	481	ASN	CA-CB	5.04	1.60	1.53	15	1
2	B	176	ALA	C-O	-5.04	1.18	1.24	4	1
2	B	206	ASN	C-N	5.04	1.40	1.33	3	1
1	A	334	PHE	C-O	-5.04	1.17	1.24	10	1
2	C	72	TRP	N-CA	-5.04	1.40	1.46	3	1
2	C	176	ALA	C-O	5.04	1.30	1.24	5	1
2	C	120	GLU	N-CA	-5.04	1.39	1.46	10	1
2	C	64	LEU	CA-CB	5.04	1.61	1.53	7	1
2	C	184	HIS	CB-CG	5.04	1.57	1.50	5	2
2	B	94	LYS	C-N	5.04	1.40	1.34	11	1
2	B	64	LEU	N-CA	-5.04	1.39	1.46	15	1
2	B	196	LEU	CA-CB	5.03	1.61	1.53	8	1
1	A	333	MET	CA-C	5.03	1.59	1.52	3	1
2	B	237	ARG	CA-C	5.03	1.59	1.52	12	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	375	LYS	N-CA	-5.02	1.40	1.46	4	1
2	B	252	LEU	CA-C	-5.02	1.46	1.52	1	1
2	B	256	GLU	N-CA	5.02	1.52	1.46	7	1
2	B	118	LYS	CA-C	5.02	1.59	1.52	8	1
1	A	504	ASP	N-CA	-5.02	1.39	1.46	1	1
2	C	204	LYS	C-N	-5.02	1.27	1.34	6	1
2	B	238	GLN	CA-C	-5.02	1.45	1.52	7	1
2	C	226	SER	CA-CB	5.02	1.61	1.53	12	1
2	C	186	ALA	C-O	-5.02	1.19	1.24	11	1
1	A	342	TRP	CA-C	-5.01	1.46	1.52	14	1
1	A	438	PHE	CA-CB	5.01	1.61	1.53	14	1
1	A	344	VAL	C-N	-5.01	1.27	1.33	9	1
2	C	177	HIS	N-CA	5.01	1.52	1.46	13	1
2	B	197	ALA	CA-C	-5.01	1.46	1.52	9	1
2	C	261	LYS	CA-CB	-5.01	1.45	1.53	9	1
1	A	422	MET	CA-C	-5.01	1.46	1.52	15	1
2	C	66	PRO	C-O	-5.01	1.17	1.24	8	1
2	B	205	GLU	C-O	5.01	1.29	1.24	4	1
2	C	216	ALA	C-N	5.01	1.41	1.33	9	1
2	B	161	GLU	CA-C	5.01	1.59	1.52	10	1
2	B	236	LEU	CA-C	5.00	1.59	1.52	2	1
2	B	119	VAL	CA-CB	5.00	1.60	1.54	3	1
2	C	227	GLU	CA-C	-5.00	1.45	1.52	3	1
2	B	69	GLN	N-CA	5.00	1.52	1.46	5	1
2	C	237	ARG	CA-CB	5.00	1.61	1.53	1	1
2	C	247	PHE	CA-C	-5.00	1.46	1.52	7	1
2	B	220	GLU	C-O	-5.00	1.18	1.24	11	1
1	A	333	MET	C-N	5.00	1.40	1.33	15	1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	65	GLY	O-C-N	-21.37	113.38	121.07	15	5
1	A	503	ARG	NE-CZ-NH2	16.84	134.36	119.20	6	10
2	B	210	ARG	NE-CZ-NH2	15.39	133.06	119.20	11	9
2	B	153	ARG	NE-CZ-NH2	15.34	133.01	119.20	1	6
2	B	173	ARG	NE-CZ-NH2	15.17	132.85	119.20	12	8
1	A	330	ARG	NE-CZ-NH2	14.66	132.39	119.20	10	8
2	C	171	ARG	NE-CZ-NH2	14.56	132.30	119.20	15	10
2	B	138	ARG	NE-CZ-NH2	14.32	132.09	119.20	2	9

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	C	153	ARG	NE-CZ-NH2	13.85	131.66	119.20	10	10
1	A	413	ASP	CA-CB-CG	13.77	126.37	112.60	10	7
2	C	61	ARG	NE-CZ-NH2	13.69	131.52	119.20	4	8
2	C	251	PHE	CA-CB-CG	13.35	127.14	113.80	4	4
2	C	138	ARG	NE-CZ-NH2	13.34	131.21	119.20	2	10
1	A	343	ARG	NE-CZ-NH2	13.20	131.08	119.20	2	7
2	C	199	ARG	NE-CZ-NH2	13.15	131.04	119.20	12	9
2	C	193	ARG	NE-CZ-NH2	12.89	130.81	119.20	8	10
2	C	164	SER	O-C-N	-12.86	109.03	120.48	4	4
2	C	206	ASN	CA-CB-CG	12.75	125.35	112.60	8	6
1	A	343	ARG	NE-CZ-NH1	-12.70	108.80	121.50	11	4
2	C	175	ARG	NE-CZ-NH2	12.64	130.58	119.20	2	11
2	B	193	ARG	NE-CZ-NH2	12.63	130.56	119.20	1	10
2	C	195	ARG	NE-CZ-NH2	12.29	130.26	119.20	8	7
2	B	57	PHE	CA-CB-CG	-12.24	101.56	113.80	8	3
1	A	376	ASP	CA-CB-CG	12.20	124.80	112.60	1	5
2	C	145	ARG	NE-CZ-NH2	12.10	130.09	119.20	4	11
2	C	237	ARG	NE-CZ-NH2	12.02	130.02	119.20	11	8
2	C	98	GLN	O-C-N	-11.90	109.89	120.48	11	2
2	B	195	ARG	NE-CZ-NH2	11.86	129.88	119.20	5	12
1	A	345	ARG	NE-CZ-NH2	11.83	129.84	119.20	6	9
2	B	92	GLU	N-CA-C	11.76	124.10	111.28	2	4
1	A	474	PHE	CA-CB-CG	-11.76	102.05	113.80	10	3
2	C	138	ARG	NE-CZ-NH1	-11.69	109.81	121.50	2	5
2	B	116	ARG	NE-CZ-NH1	-11.69	109.81	121.50	1	4
1	A	464	ARG	NE-CZ-NH2	11.61	129.65	119.20	14	6
2	C	173	ARG	NE-CZ-NH2	11.60	129.64	119.20	5	8
1	A	429	PHE	CA-CB-CG	-11.59	102.21	113.80	7	8
1	A	469	GLY	CA-C-N	11.56	136.22	120.38	1	5
1	A	469	GLY	C-N-CA	11.56	136.22	120.38	1	5
1	A	317	ASN	OD1-CG-ND2	-11.53	111.08	122.60	6	5
2	C	116	ARG	NE-CZ-NH2	11.45	129.51	119.20	5	8
2	B	125	ASP	N-CA-C	11.45	123.76	111.28	3	2
2	C	153	ARG	NE-CZ-NH1	-11.39	110.11	121.50	6	5
1	A	437	ARG	NE-CZ-NH2	-11.38	108.96	119.20	4	5
1	A	443	ARG	NE-CZ-NH2	11.37	129.44	119.20	1	7
2	C	262	LEU	N-CA-C	11.37	124.75	111.11	10	4
2	B	61	ARG	NE-CZ-NH2	11.34	129.41	119.20	8	4
2	C	210	ARG	NE-CZ-NH2	11.24	129.32	119.20	14	11
2	B	153	ARG	NE-CZ-NH1	-11.21	110.29	121.50	5	6
2	B	232	ALA	CA-C-N	11.21	135.30	120.28	11	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	232	ALA	C-N-CA	11.21	135.30	120.28	11	4
2	C	107	LYS	N-CA-C	11.16	123.01	111.07	10	7
1	A	449	TYR	O-C-N	-11.09	112.90	121.55	11	5
1	A	446	ASP	N-CA-C	11.06	124.60	110.33	1	5
1	A	408	ARG	NE-CZ-NH1	-11.03	110.47	121.50	4	1
1	A	408	ARG	NE-CZ-NH2	11.01	129.11	119.20	4	6
1	A	364	LEU	CA-C-O	-11.00	111.18	119.32	4	5
2	C	150	GLU	N-CA-C	10.96	122.98	111.14	10	1
2	C	252	LEU	N-CA-C	10.95	123.22	111.28	3	4
2	B	258	TYR	N-CA-C	10.93	123.19	111.28	13	4
2	B	210	ARG	NE-CZ-NH1	-10.90	110.60	121.50	13	5
2	B	119	VAL	N-CA-C	10.77	121.27	110.82	1	8
2	C	116	ARG	CA-C-N	10.72	134.65	120.28	1	4
2	C	116	ARG	C-N-CA	10.72	134.65	120.28	1	4
2	B	254	ALA	CA-C-O	10.72	131.91	120.55	11	2
2	B	98	GLN	CA-C-O	-10.70	108.79	118.63	10	3
2	C	122	TYR	CA-C-N	10.68	134.32	120.44	5	3
2	C	122	TYR	C-N-CA	10.68	134.32	120.44	5	3
2	B	136	LEU	O-C-N	-10.67	110.56	122.09	12	1
2	B	171	ARG	N-CA-C	10.67	122.91	111.28	7	3
2	B	69	GLN	OE1-CD-NE2	-10.66	111.94	122.60	4	3
1	A	387	HIS	CA-CB-CG	10.63	124.43	113.80	6	5
2	B	190	ASP	CA-CB-CG	10.63	123.23	112.60	10	2
2	B	195	ARG	NE-CZ-NH1	-10.62	110.88	121.50	15	9
2	B	108	TRP	CA-C-N	10.60	134.85	120.54	15	2
2	B	108	TRP	C-N-CA	10.60	134.85	120.54	15	2
2	C	158	GLU	N-CA-C	10.59	122.82	111.28	8	5
2	C	173	ARG	NE-CZ-NH1	-10.47	111.03	121.50	5	5
1	A	333	MET	CA-C-O	10.46	131.56	120.36	6	1
2	C	89	ASP	CA-CB-CG	-10.45	102.15	112.60	11	3
2	B	63	GLN	OE1-CD-NE2	10.43	133.03	122.60	4	1
1	A	389	VAL	O-C-N	-10.43	112.23	123.18	9	3
2	C	172	ASP	CA-CB-CG	10.41	123.01	112.60	6	3
2	C	83	ARG	NE-CZ-NH1	-10.38	111.12	121.50	7	4
1	A	393	ALA	N-CA-C	10.27	123.55	111.02	2	3
2	B	127	GLN	N-CA-C	10.26	122.05	111.07	5	2
2	B	193	ARG	NE-CZ-NH1	-10.24	111.26	121.50	1	8
2	B	264	THR	N-CA-C	10.19	122.14	111.14	4	1
2	C	186	ALA	O-C-N	-10.17	110.89	120.55	9	4
2	B	220	GLU	N-CA-C	10.12	123.35	111.71	8	3
2	B	184	HIS	N-CA-C	10.12	121.90	111.07	3	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	C	199	ARG	NE-CZ-NH1	-10.09	111.41	121.50	8	7
2	C	204	LYS	N-CA-C	10.04	121.81	111.07	3	5
2	B	194	GLN	CA-C-N	10.01	133.45	120.44	3	4
2	B	194	GLN	C-N-CA	10.01	133.45	120.44	3	4
2	C	171	ARG	NE-CZ-NH1	-9.98	111.52	121.50	9	7
1	A	487	ASN	CB-CA-C	9.97	126.87	110.22	3	1
2	C	224	THR	CA-C-N	9.95	133.37	120.44	6	4
2	C	224	THR	C-N-CA	9.95	133.37	120.44	6	4
2	B	227	GLU	N-CA-C	9.93	121.70	111.07	10	3
2	B	143	PRO	CA-C-N	9.92	133.93	120.54	5	4
2	B	143	PRO	C-N-CA	9.92	133.93	120.54	5	4
1	A	433	ASN	OD1-CG-ND2	-9.90	112.70	122.60	11	2
2	C	151	GLY	CA-C-N	9.88	133.92	120.38	9	1
2	C	151	GLY	C-N-CA	9.88	133.92	120.38	9	1
2	B	61	ARG	NE-CZ-NH1	-9.88	111.62	121.50	8	4
2	B	206	ASN	CA-CB-CG	9.88	122.48	112.60	14	2
2	B	173	ARG	N-CA-C	9.88	122.12	111.36	4	8
1	A	459	ILE	CA-C-N	9.87	129.96	119.89	6	6
1	A	459	ILE	C-N-CA	9.87	129.96	119.89	6	6
2	C	57	PHE	CA-CB-CG	-9.83	103.97	113.80	5	3
2	C	83	ARG	NE-CZ-NH2	9.82	128.04	119.20	5	8
2	C	127	GLN	N-CA-C	9.81	121.98	111.28	3	2
1	A	404	LYS	O-C-N	-9.80	109.58	122.33	14	1
1	A	467	PHE	O-C-N	-9.80	112.51	123.48	6	3
2	C	80	GLU	O-C-N	-9.79	111.75	122.12	10	1
2	C	98	GLN	N-CA-C	9.77	126.67	113.77	12	8
2	C	86	MET	N-CA-C	9.72	122.78	111.11	15	2
1	A	431	ARG	NE-CZ-NH2	9.69	127.92	119.20	5	7
2	C	194	GLN	CA-C-N	9.69	134.24	120.28	2	1
2	C	194	GLN	C-N-CA	9.69	134.24	120.28	2	1
1	A	396	GLU	N-CA-C	9.68	121.94	109.64	11	6
2	B	230	LYS	N-CA-C	9.66	126.88	113.45	5	4
2	B	116	ARG	NE-CZ-NH2	9.65	127.89	119.20	1	5
1	A	374	ARG	NE-CZ-NH2	9.65	127.89	119.20	3	5
2	C	180	ALA	N-CA-C	9.65	122.69	111.11	2	2
2	B	114	LEU	O-C-N	-9.59	112.19	122.07	13	2
2	B	89	ASP	CA-C-N	9.59	133.12	120.28	6	4
2	B	89	ASP	C-N-CA	9.59	133.12	120.28	6	4
1	A	503	ARG	NH1-CZ-NH2	-9.57	106.86	119.30	6	3
1	A	390	PHE	CA-CB-CG	9.57	123.37	113.80	15	8
2	B	192	LEU	N-CA-C	9.55	121.78	111.36	8	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	120	GLU	O-C-N	-9.55	111.74	120.71	1	5
1	A	443	ARG	NE-CZ-NH1	-9.52	111.98	121.50	1	5
2	C	257	GLU	CA-C-N	9.50	133.01	120.28	5	4
2	C	257	GLU	C-N-CA	9.50	133.01	120.28	5	4
2	B	209	ALA	N-CA-C	9.50	121.63	111.28	8	2
2	C	165	PRO	CA-C-N	9.48	132.77	120.44	1	5
2	C	165	PRO	C-N-CA	9.48	132.77	120.44	1	5
2	B	138	ARG	NE-CZ-NH1	-9.44	112.06	121.50	4	2
1	A	430	PHE	CA-CB-CG	-9.43	104.37	113.80	2	7
2	B	145	ARG	NE-CZ-NH1	-9.43	112.07	121.50	13	5
1	A	421	TRP	CA-C-O	9.41	130.28	120.40	10	3
2	C	155	LYS	N-CA-C	9.40	122.71	111.33	9	1
2	B	91	GLU	CA-C-N	9.39	132.87	120.28	7	2
2	B	91	GLU	C-N-CA	9.39	132.87	120.28	7	2
2	C	62	GLU	O-C-N	-9.39	111.45	122.15	3	2
2	C	148	LEU	N-CA-C	9.39	121.12	111.07	2	1
1	A	323	PHE	CA-CB-CG	-9.39	104.41	113.80	13	5
2	C	98	GLN	CA-C-O	-9.38	109.63	118.44	12	3
2	B	68	THR	CA-C-N	9.36	133.17	120.54	1	3
2	B	68	THR	C-N-CA	9.36	133.17	120.54	1	3
2	B	87	SER	O-C-N	-9.35	112.44	122.07	12	2
1	A	465	GLY	CA-C-O	-9.35	112.52	121.49	12	2
2	B	199	ARG	NE-CZ-NH2	9.35	127.61	119.20	5	7
2	B	145	ARG	NE-CZ-NH2	9.34	127.60	119.20	13	6
1	A	341	PHE	CA-CB-CG	9.33	123.13	113.80	2	5
1	A	487	ASN	CA-CB-CG	9.31	121.92	112.60	5	4
2	C	260	LYS	N-CA-C	9.30	122.58	111.33	12	3
2	C	177	HIS	CE1-NE2-CD2	-9.29	99.71	109.00	7	8
2	C	207	GLY	CA-C-N	9.28	130.05	119.94	1	2
2	C	207	GLY	C-N-CA	9.28	130.05	119.94	1	2
2	B	179	ASP	CA-CB-CG	9.28	121.88	112.60	15	2
2	B	255	LEU	CA-C-N	9.27	132.49	120.44	14	3
2	B	255	LEU	C-N-CA	9.27	132.49	120.44	14	3
2	C	56	THR	N-CA-C	9.27	125.77	113.72	6	3
2	B	171	ARG	NE-CZ-NH2	9.26	127.53	119.20	2	7
1	A	422	MET	CA-C-O	-9.26	110.11	118.63	1	2
2	B	139	GLN	N-CA-C	9.24	120.95	111.07	11	1
2	B	173	ARG	NE-CZ-NH1	-9.23	112.27	121.50	8	7
2	C	170	MET	O-C-N	9.21	131.56	122.07	6	2
2	C	221	HIS	CA-CB-CG	-9.20	104.60	113.80	14	3
2	C	221	HIS	N-CA-C	9.20	120.91	111.07	2	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	C	73	ASP	N-CA-C	9.19	122.14	111.11	14	1
1	A	424	ASN	CA-CB-CG	9.18	121.78	112.60	5	2
2	B	262	LEU	CA-C-N	9.18	132.37	120.44	4	1
2	B	262	LEU	C-N-CA	9.18	132.37	120.44	4	1
2	C	138	ARG	N-CA-C	9.15	121.26	111.28	8	5
1	A	375	LYS	O-C-N	-9.15	111.72	122.15	3	3
2	C	232	ALA	N-CA-C	9.15	120.86	111.07	9	5
2	B	87	SER	N-CA-C	9.14	120.85	111.07	3	3
2	B	251	PHE	CA-CB-CG	9.14	122.94	113.80	4	5
2	B	65	GLY	CA-C-O	-9.13	113.53	119.65	14	2
2	C	63	GLN	CA-C-N	9.11	132.49	120.28	6	3
2	C	63	GLN	C-N-CA	9.11	132.49	120.28	6	3
2	C	185	LEU	CA-C-O	-9.11	110.90	120.55	12	2
2	C	142	GLU	O-C-N	-9.11	110.85	121.32	5	3
1	A	350	MET	N-CA-C	9.10	123.43	110.23	13	3
1	A	317	ASN	CA-CB-CG	9.10	121.70	112.60	15	6
2	B	172	ASP	CA-C-N	9.09	133.20	120.29	6	4
2	B	172	ASP	C-N-CA	9.09	133.20	120.29	6	4
2	C	57	PHE	N-CA-C	9.08	121.18	111.28	8	6
1	A	426	LYS	O-C-N	-9.08	111.39	123.19	14	2
2	B	182	ARG	NE-CZ-NH1	-9.06	112.44	121.50	14	2
2	B	234	GLU	N-CA-C	9.06	120.77	111.07	3	3
2	C	223	SER	N-CA-C	9.06	120.92	111.14	14	4
1	A	349	VAL	CA-C-O	9.05	131.32	121.36	9	2
2	C	117	GLN	N-CA-C	9.04	121.14	111.28	8	1
2	C	120	GLU	O-C-N	-9.02	111.77	120.70	1	4
2	B	74	ASN	OD1-CG-ND2	-9.02	113.58	122.60	15	2
2	C	235	ASP	CA-CB-CG	9.01	121.61	112.60	9	5
2	C	84	GLN	N-CA-C	9.01	120.71	111.07	13	5
2	C	128	LYS	N-CA-C	9.00	120.70	111.07	15	4
2	B	229	ALA	N-CA-C	8.99	120.69	111.07	12	4
1	A	353	TYR	O-C-N	-8.99	112.85	121.57	3	4
1	A	347	ASN	OD1-CG-ND2	-8.99	113.61	122.60	8	2
1	A	350	MET	O-C-N	-8.98	112.27	122.86	5	2
2	C	210	ARG	NE-CZ-NH1	-8.97	112.53	121.50	4	4
2	B	141	VAL	N-CA-C	8.96	119.76	110.62	9	1
2	B	191	GLU	N-CA-C	8.92	120.62	111.07	3	4
2	B	59	LYS	N-CA-C	8.91	120.99	111.28	5	4
2	B	136	LEU	CA-C-N	8.90	132.58	120.38	12	2
2	B	136	LEU	C-N-CA	8.90	132.58	120.38	12	2
2	B	244	LEU	N-CA-C	8.89	120.98	111.28	12	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	260	LYS	O-C-N	-8.89	112.85	122.09	2	2
2	B	175	ARG	NE-CZ-NH2	8.88	127.19	119.20	6	11
2	C	92	GLU	N-CA-C	8.87	120.56	111.07	7	5
1	A	477	PHE	CA-CB-CG	-8.85	104.95	113.80	2	3
1	A	369	ASN	CA-CB-CG	8.85	121.45	112.60	8	2
2	B	56	THR	N-CA-C	8.85	121.89	111.71	9	5
2	C	206	ASN	CA-C-N	8.84	129.73	120.00	14	8
2	C	206	ASN	C-N-CA	8.84	129.73	120.00	14	8
2	B	118	LYS	N-CA-C	8.82	120.51	111.07	7	4
2	C	200	LEU	CA-C-N	8.80	131.88	120.44	8	4
2	C	200	LEU	C-N-CA	8.80	131.88	120.44	8	4
2	B	61	ARG	N-CA-C	8.80	120.87	111.28	11	3
2	C	178	VAL	O-C-N	-8.78	112.79	121.83	11	2
2	B	114	LEU	CA-C-O	8.77	130.02	120.82	13	1
2	C	202	ALA	N-CA-C	8.76	120.83	111.28	7	1
2	C	219	THR	N-CA-C	8.75	120.44	111.07	11	4
2	B	124	ASP	CA-C-N	8.75	132.00	120.28	12	2
2	B	124	ASP	C-N-CA	8.75	132.00	120.28	12	2
2	C	81	GLY	CA-C-N	8.75	131.81	120.44	12	3
2	C	81	GLY	C-N-CA	8.75	131.81	120.44	12	3
2	B	235	ASP	CA-C-N	8.74	131.80	120.44	7	2
2	B	235	ASP	C-N-CA	8.74	131.80	120.44	7	2
2	C	182	ARG	N-CA-C	8.72	121.74	111.71	1	3
1	A	412	THR	O-C-N	-8.72	112.86	122.10	7	2
2	B	134	MET	CA-C-O	8.72	129.68	120.70	6	1
2	B	119	VAL	O-C-N	-8.71	112.86	121.83	11	3
2	C	189	SER	N-CA-C	8.71	120.77	111.28	6	2
2	B	183	THR	CA-C-N	8.70	132.65	120.29	12	1
2	B	183	THR	C-N-CA	8.70	132.65	120.29	12	1
2	C	215	HIS	CA-CB-CG	8.69	122.49	113.80	1	5
2	B	221	HIS	CA-CB-CG	-8.68	105.12	113.80	15	4
1	A	431	ARG	NE-CZ-NH1	-8.68	112.83	121.50	12	7
2	C	87	SER	O-C-N	-8.68	112.26	122.15	12	2
1	A	381	PHE	CA-CB-CG	-8.67	105.13	113.80	8	2
1	A	462	SER	CA-C-O	-8.66	108.29	120.16	7	3
2	B	113	GLU	N-CA-C	8.66	120.33	111.07	6	3
2	C	67	VAL	CA-C-N	8.65	131.69	120.44	2	4
2	C	67	VAL	C-N-CA	8.65	131.69	120.44	2	4
2	B	177	HIS	CA-CB-CG	-8.64	105.16	113.80	13	6
2	B	172	ASP	CA-CB-CG	8.63	121.23	112.60	14	2
2	B	118	LYS	CA-C-N	8.63	131.44	120.56	14	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	118	LYS	C-N-CA	8.63	131.44	120.56	14	3
2	C	177	HIS	ND1-CE1-NE2	8.63	117.03	108.40	10	5
2	B	62	GLU	N-CA-C	8.62	120.67	111.28	13	7
2	B	110	GLU	CA-C-N	8.61	132.18	120.38	2	4
2	B	110	GLU	C-N-CA	8.61	132.18	120.38	2	4
1	A	324	ASP	CA-CB-CG	-8.59	104.01	112.60	3	1
2	B	167	GLY	CA-C-N	8.56	132.10	120.54	8	6
2	B	167	GLY	C-N-CA	8.56	132.10	120.54	8	6
2	B	69	GLN	CA-C-N	8.56	131.75	120.28	14	2
2	B	69	GLN	C-N-CA	8.56	131.75	120.28	14	2
1	A	375	LYS	N-CA-C	8.55	121.55	111.71	2	8
2	C	246	SER	O-C-N	-8.56	113.05	122.12	1	2
2	B	83	ARG	NE-CZ-NH2	8.55	126.90	119.20	1	5
1	A	420	PHE	CB-CA-C	8.55	123.08	110.26	13	3
2	B	177	HIS	CE1-NE2-CD2	-8.54	100.46	109.00	10	4
2	B	236	LEU	CA-C-N	8.53	131.53	120.44	7	3
2	B	236	LEU	C-N-CA	8.53	131.53	120.44	7	3
2	B	65	GLY	CA-C-N	8.53	128.15	118.85	2	1
2	B	65	GLY	C-N-CA	8.53	128.15	118.85	2	1
1	A	403	ILE	N-CA-C	8.53	119.31	110.36	4	4
2	B	240	LEU	N-CA-C	-8.52	103.02	113.50	3	1
2	C	103	ASP	CA-CB-CG	8.52	121.12	112.60	14	1
2	C	193	ARG	N-CA-C	8.50	121.49	111.71	6	7
2	B	79	THR	N-CA-CB	8.50	122.33	110.01	3	2
2	C	137	TYR	CA-C-N	8.50	132.01	120.54	7	3
2	C	137	TYR	C-N-CA	8.50	132.01	120.54	7	3
2	B	237	ARG	NE-CZ-NH2	8.49	126.85	119.20	11	9
2	B	86	MET	CA-C-N	8.49	131.66	120.28	6	3
2	B	86	MET	C-N-CA	8.49	131.66	120.28	6	3
2	C	175	ARG	NE-CZ-NH1	-8.49	113.01	121.50	2	5
1	A	464	ARG	NE-CZ-NH1	-8.49	113.01	121.50	11	3
2	B	68	THR	CA-CB-OG1	8.49	122.33	109.60	7	1
2	C	81	GLY	O-C-N	-8.48	113.73	122.13	10	2
2	B	85	GLU	N-CA-C	8.48	121.59	111.33	4	4
2	B	96	LYS	CA-C-N	8.48	131.25	120.56	11	2
2	B	96	LYS	C-N-CA	8.48	131.25	120.56	11	2
2	B	257	GLU	CA-C-N	8.47	131.45	120.44	3	7
2	B	257	GLU	C-N-CA	8.47	131.45	120.44	3	7
2	B	77	LYS	N-CA-C	8.47	120.13	111.07	3	6
2	B	102	ASP	CA-CB-CG	8.46	121.06	112.60	2	3
2	C	218	ALA	CA-C-O	-8.46	111.94	120.82	6	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	410	LEU	N-CA-C	8.45	121.58	109.84	3	1
2	C	80	GLU	N-CA-C	8.45	120.11	111.07	13	2
2	C	59	LYS	CA-C-O	8.44	129.69	120.82	1	1
1	A	358	GLY	N-CA-C	8.44	124.29	113.24	13	3
2	C	177	HIS	N-CA-C	8.43	120.47	111.28	1	4
1	A	318	ILE	O-C-N	-8.43	113.36	121.87	3	2
2	C	218	ALA	N-CA-C	8.43	124.14	112.93	13	3
2	B	166	LEU	N-CA-C	8.42	120.08	111.07	2	4
2	B	160	GLN	O-C-N	-8.42	113.19	122.12	11	2
2	B	170	MET	CA-C-N	8.42	131.56	120.28	10	4
2	B	170	MET	C-N-CA	8.42	131.56	120.28	10	4
2	C	237	ARG	N-CA-C	8.42	120.08	111.07	13	3
2	B	207	GLY	O-C-N	8.41	130.35	122.19	9	3
2	C	145	ARG	O-C-N	-8.40	113.42	122.07	13	1
2	B	161	GLU	N-CA-C	8.40	120.43	111.28	3	4
2	B	138	ARG	NH1-CZ-NH2	-8.39	108.39	119.30	2	2
2	B	92	GLU	O-C-N	-8.39	113.23	122.12	8	3
2	C	134	MET	N-CA-C	8.39	120.04	111.07	12	4
2	B	116	ARG	N-CA-C	8.38	121.34	111.71	6	4
2	B	202	ALA	N-CA-C	8.38	121.47	111.33	8	4
2	C	234	GLU	N-CA-C	8.38	121.47	111.33	9	1
1	A	402	HIS	CA-CB-CG	8.37	122.17	113.80	7	6
1	A	440	GLU	N-CA-C	8.36	120.47	111.36	10	6
2	C	249	VAL	N-CA-C	8.36	119.14	110.62	8	3
2	C	257	GLU	N-CA-C	8.36	121.44	111.33	3	3
1	A	449	TYR	CA-C-O	-8.34	112.83	120.50	10	4
2	B	201	GLU	N-CA-C	8.34	121.42	111.33	6	1
2	B	260	LYS	N-CA-C	8.33	121.30	111.71	5	2
2	C	73	ASP	O-C-N	-8.33	112.65	122.15	10	3
2	C	125	ASP	N-CA-C	8.33	120.36	111.28	3	4
1	A	463	PRO	O-C-N	-8.32	112.33	122.89	3	1
2	B	74	ASN	CA-CB-CG	-8.31	104.29	112.60	10	3
1	A	344	VAL	O-C-N	-8.31	114.45	123.18	10	2
2	B	145	ARG	CA-C-N	8.31	131.41	120.28	13	2
2	B	145	ARG	C-N-CA	8.31	131.41	120.28	13	2
2	C	164	SER	CA-C-O	-8.30	110.28	118.34	5	4
2	C	175	ARG	NH1-CZ-NH2	-8.30	108.52	119.30	1	5
2	B	247	PHE	N-CA-C	8.29	120.32	111.28	12	2
2	C	201	GLU	O-C-N	-8.29	113.47	122.09	13	3
2	B	186	ALA	O-C-N	-8.29	113.10	120.48	9	3
2	C	205	GLU	N-CA-C	8.29	120.39	111.36	11	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	123	LEU	N-CA-C	8.29	119.94	111.07	6	2
2	C	255	LEU	CA-C-N	8.28	131.21	120.44	13	4
2	C	255	LEU	C-N-CA	8.28	131.21	120.44	13	4
1	A	341	PHE	O-C-N	-8.28	113.67	123.27	15	2
2	C	94	LYS	CA-C-N	8.27	131.19	120.44	11	2
2	C	94	LYS	C-N-CA	8.27	131.19	120.44	11	2
1	A	500	SER	N-CA-CB	8.27	123.16	109.60	15	1
2	B	71	PHE	CA-CB-CG	-8.27	105.53	113.80	14	3
2	C	116	ARG	NE-CZ-NH1	-8.26	113.24	121.50	5	4
2	C	97	VAL	N-CA-C	8.25	118.34	110.42	8	4
2	C	130	TRP	CA-C-N	8.25	131.68	120.54	5	1
2	C	130	TRP	C-N-CA	8.25	131.68	120.54	5	1
2	C	123	LEU	CA-C-N	8.25	132.26	120.79	8	4
2	C	123	LEU	C-N-CA	8.25	132.26	120.79	8	4
2	B	132	GLU	N-CA-C	8.25	120.27	111.28	5	4
1	A	508	CYS	CA-C-N	8.25	128.28	119.78	10	4
1	A	508	CYS	C-N-CA	8.25	128.28	119.78	10	4
2	C	156	LEU	CA-C-O	8.24	129.28	120.55	12	2
2	C	243	VAL	CA-CB-CG1	8.24	124.40	110.40	5	3
2	C	195	ARG	NH1-CZ-NH2	-8.23	108.59	119.30	11	3
2	B	256	GLU	CA-C-N	8.23	131.31	120.28	11	2
2	B	256	GLU	C-N-CA	8.23	131.31	120.28	11	2
2	C	82	LEU	N-CA-C	8.22	119.86	111.07	12	3
2	C	78	GLU	N-CA-C	8.21	120.31	111.36	9	2
2	B	247	PHE	CA-CB-CG	-8.21	105.59	113.80	5	3
2	C	244	LEU	N-CA-C	8.21	120.96	111.11	7	5
2	C	106	LYS	N-CA-C	8.21	123.97	113.88	11	2
2	C	151	GLY	N-CA-C	8.21	123.27	112.77	7	2
2	C	185	LEU	N-CA-C	8.20	121.34	111.82	5	2
2	B	102	ASP	N-CA-C	8.20	119.84	111.07	12	4
2	B	108	TRP	CB-CA-C	8.20	123.75	110.88	11	1
2	C	210	ARG	CA-C-N	8.20	131.10	120.44	8	1
2	C	210	ARG	C-N-CA	8.20	131.10	120.44	8	1
2	C	109	GLN	N-CA-C	8.19	119.84	111.07	11	3
2	B	195	ARG	CA-C-N	8.19	131.25	120.28	14	2
2	B	195	ARG	C-N-CA	8.19	131.25	120.28	14	2
2	B	150	GLU	CA-C-N	8.17	129.01	119.94	3	5
2	B	150	GLU	C-N-CA	8.17	129.01	119.94	3	5
2	C	185	LEU	O-C-N	8.17	130.78	122.12	12	1
1	A	382	PHE	CA-CB-CG	8.16	121.96	113.80	9	3
2	C	179	ASP	N-CA-C	8.15	120.25	111.36	8	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	C	226	SER	CA-C-N	8.14	131.85	120.29	9	2
2	C	226	SER	C-N-CA	8.14	131.85	120.29	9	2
2	C	74	ASN	CA-CB-CG	-8.14	104.46	112.60	15	3
2	C	141	VAL	O-C-N	-8.13	114.76	122.16	14	1
2	B	152	ALA	N-CA-C	8.12	120.13	111.28	10	2
2	B	127	GLN	OE1-CD-NE2	-8.12	114.48	122.60	5	2
2	B	72	TRP	CA-C-N	8.12	130.99	120.44	4	3
2	B	72	TRP	C-N-CA	8.12	130.99	120.44	4	3
2	C	216	ALA	N-CA-C	8.11	119.75	111.07	10	1
1	A	433	ASN	CA-CB-CG	8.11	120.71	112.60	1	5
1	A	374	ARG	NE-CZ-NH1	-8.11	113.39	121.50	4	3
2	B	256	GLU	N-CA-C	8.11	119.74	111.07	7	5
2	B	237	ARG	NE-CZ-NH1	-8.10	113.40	121.50	8	6
1	A	349	VAL	N-CA-C	8.10	119.53	108.84	12	3
2	C	115	TYR	CA-C-N	8.09	130.96	120.44	13	5
2	C	115	TYR	C-N-CA	8.09	130.96	120.44	13	5
2	C	104	PHE	CA-CB-CG	8.08	121.88	113.80	2	2
2	B	100	TYR	CA-C-N	8.07	131.10	120.28	1	3
2	B	100	TYR	C-N-CA	8.07	131.10	120.28	1	3
2	B	187	PRO	CA-C-N	8.07	131.44	120.38	12	3
2	B	187	PRO	C-N-CA	8.07	131.44	120.38	12	3
2	C	241	LEU	CA-C-O	-8.07	110.83	118.73	2	3
1	A	454	LYS	CA-C-N	8.06	131.50	120.46	7	4
1	A	454	LYS	C-N-CA	8.06	131.50	120.46	7	4
2	B	88	LYS	N-CA-C	8.06	120.07	111.28	10	4
1	A	364	LEU	CA-C-N	8.05	128.07	119.78	11	10
1	A	364	LEU	C-N-CA	8.05	128.07	119.78	11	10
1	A	325	THR	CA-CB-CG2	8.05	124.18	110.50	3	2
2	B	127	GLN	CA-C-N	8.04	131.06	120.28	3	3
2	B	127	GLN	C-N-CA	8.04	131.06	120.28	3	3
1	A	351	ASP	O-C-N	-8.04	113.37	122.86	11	1
2	C	138	ARG	CA-C-N	8.04	131.05	120.28	5	3
2	C	138	ARG	C-N-CA	8.04	131.05	120.28	5	3
2	B	101	LEU	N-CA-C	8.04	120.05	111.28	11	3
2	C	215	HIS	CA-C-N	8.04	131.05	120.28	12	3
2	C	215	HIS	C-N-CA	8.04	131.05	120.28	12	3
2	C	143	PRO	CA-C-N	8.04	132.88	120.82	5	3
2	C	143	PRO	C-N-CA	8.04	132.88	120.82	5	3
2	C	184	HIS	CA-CB-CG	-8.03	105.77	113.80	4	2
2	B	122	TYR	CB-CA-C	8.04	123.50	110.88	11	3
2	B	206	ASN	CA-C-N	8.02	128.88	119.98	3	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	206	ASN	C-N-CA	8.02	128.88	119.98	3	6
2	C	230	LYS	N-CA-C	8.02	124.59	113.45	3	5
1	A	360	PHE	CA-CB-CG	8.01	121.81	113.80	15	3
1	A	425	GLY	O-C-N	-8.01	113.17	122.31	8	1
2	B	215	HIS	CA-CB-CG	8.01	121.81	113.80	12	3
2	C	71	PHE	N-CA-C	8.01	120.01	111.28	12	2
2	C	176	ALA	N-CA-C	8.00	120.00	111.28	10	5
1	A	329	LEU	O-C-N	-8.00	113.95	123.31	8	3
1	A	410	LEU	CA-C-N	8.00	128.05	119.89	15	6
1	A	410	LEU	C-N-CA	8.00	128.05	119.89	15	6
2	C	215	HIS	CE1-NE2-CD2	-7.99	101.01	109.00	8	4
2	C	222	LEU	N-CA-C	7.99	119.62	111.07	13	5
1	A	493	VAL	N-CA-C	7.99	119.88	109.58	15	1
2	B	98	GLN	CA-C-N	7.98	127.55	118.85	1	1
2	B	98	GLN	C-N-CA	7.98	127.55	118.85	1	1
2	C	156	LEU	N-CA-C	7.98	119.98	111.28	7	3
1	A	453	ILE	CA-C-N	7.98	132.02	120.38	1	3
1	A	453	ILE	C-N-CA	7.98	132.02	120.38	1	3
2	C	61	ARG	NE-CZ-NH1	-7.97	113.53	121.50	12	7
2	C	59	LYS	CA-C-N	7.97	131.60	120.29	12	3
2	C	59	LYS	C-N-CA	7.97	131.60	120.29	12	3
2	C	61	ARG	O-C-N	-7.96	113.68	122.12	5	2
2	B	83	ARG	NE-CZ-NH1	-7.96	113.54	121.50	5	2
2	B	109	GLN	OE1-CD-NE2	-7.96	114.64	122.60	2	2
2	B	191	GLU	CA-C-N	7.96	131.59	120.29	8	6
2	B	191	GLU	C-N-CA	7.96	131.59	120.29	8	6
1	A	350	MET	CA-C-N	7.95	132.03	120.82	13	1
1	A	350	MET	C-N-CA	7.95	132.03	120.82	13	1
2	C	94	LYS	N-CA-C	7.94	119.56	111.07	8	5
1	A	415	ILE	O-C-N	-7.94	114.84	123.18	6	1
1	A	388	TRP	CB-CG-CD2	7.93	137.91	126.80	11	5
2	B	199	ARG	NE-CZ-NH1	-7.93	113.57	121.50	11	2
2	C	73	ASP	CA-C-O	7.92	128.82	120.42	10	2
2	C	56	THR	CA-C-N	7.92	130.74	120.44	7	4
2	C	56	THR	C-N-CA	7.92	130.74	120.44	7	4
2	C	215	HIS	N-CA-C	7.92	119.54	111.07	11	2
2	B	141	VAL	CA-C-N	7.91	129.98	120.09	15	1
2	B	141	VAL	C-N-CA	7.91	129.98	120.09	15	1
2	B	138	ARG	N-CA-C	7.90	119.52	111.07	5	3
1	A	345	ARG	O-C-N	-7.90	114.17	123.41	13	3
2	C	71	PHE	CA-C-O	7.89	128.92	120.55	8	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	355	MET	O-C-N	-7.89	113.92	121.57	5	3
2	C	69	GLN	OE1-CD-NE2	-7.89	114.71	122.60	8	4
2	B	247	PHE	CA-C-N	7.89	130.69	120.44	1	2
2	B	247	PHE	C-N-CA	7.89	130.69	120.44	1	2
2	B	228	LYS	N-CA-C	7.89	121.39	111.69	3	3
2	B	226	SER	N-CA-C	7.88	120.78	111.71	3	3
2	C	85	GLU	N-CA-C	7.88	120.96	111.82	1	5
2	C	142	GLU	CA-C-O	-7.88	109.37	120.16	5	5
2	B	58	SER	N-CA-CB	7.87	121.80	110.16	6	2
2	C	100	TYR	CA-C-N	7.86	131.72	120.79	10	3
2	C	100	TYR	C-N-CA	7.86	131.72	120.79	10	3
2	C	88	LYS	O-C-N	-7.86	113.79	122.12	10	2
1	A	495	PRO	O-C-N	-7.85	113.43	123.00	7	2
1	A	333	MET	O-C-N	-7.83	114.29	123.22	6	2
2	C	124	ASP	O-C-N	-7.83	113.82	122.12	11	1
2	C	90	LEU	N-CA-C	7.83	119.44	111.07	8	1
2	B	149	GLN	O-C-N	7.82	130.13	122.07	1	3
1	A	343	ARG	NH1-CZ-NH2	-7.82	109.13	119.30	1	4
2	C	230	LYS	O-C-N	-7.82	113.52	120.48	7	2
1	A	489	GLN	N-CA-C	7.82	119.44	111.07	9	2
2	C	182	ARG	N-CA-CB	7.81	121.58	109.94	13	2
2	C	134	MET	O-C-N	-7.81	113.24	122.15	3	2
2	C	173	ARG	N-CA-C	7.81	119.43	111.07	7	4
2	B	223	SER	N-CA-C	7.81	119.87	111.36	9	4
1	A	435	TYR	O-C-N	-7.81	114.35	123.25	6	1
2	B	258	TYR	CA-C-N	7.80	130.58	120.44	8	4
2	B	258	TYR	C-N-CA	7.80	130.58	120.44	8	4
2	C	63	GLN	OE1-CD-NE2	-7.80	114.80	122.60	3	2
2	B	208	GLY	N-CA-C	7.79	122.08	112.73	3	2
1	A	481	ASN	CA-CB-CG	-7.79	104.81	112.60	2	3
2	C	252	LEU	CA-C-N	7.78	130.56	120.44	10	3
2	C	252	LEU	C-N-CA	7.78	130.56	120.44	10	3
2	C	132	GLU	N-CA-C	7.78	119.54	111.14	7	3
2	C	206	ASN	OD1-CG-ND2	7.78	130.38	122.60	11	3
2	B	203	LEU	N-CA-CB	-7.78	98.69	110.12	11	1
2	C	100	TYR	CA-C-O	7.77	126.77	119.00	4	1
2	C	197	ALA	CA-C-O	7.77	128.87	120.24	15	2
2	C	142	GLU	N-CA-C	7.77	124.25	113.45	8	5
2	B	86	MET	O-C-N	-7.77	113.88	122.12	3	2
2	C	111	GLU	N-CA-C	7.76	119.82	111.36	15	3
1	A	385	ASP	CA-CB-CG	7.76	120.36	112.60	13	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	236	LEU	O-C-N	-7.76	113.71	122.09	8	1
2	B	241	LEU	O-C-N	-7.76	113.02	120.70	15	2
1	A	446	ASP	CA-CB-CG	7.75	120.36	112.60	6	2
1	A	365	PRO	N-CA-C	7.75	123.54	111.21	1	1
2	B	72	TRP	O-C-N	-7.75	113.90	122.12	12	1
2	B	182	ARG	NE-CZ-NH2	7.75	126.17	119.20	14	5
2	B	105	GLN	N-CA-C	7.75	119.72	111.28	13	3
2	C	187	PRO	CA-C-N	7.74	130.65	120.28	3	5
2	C	187	PRO	C-N-CA	7.74	130.65	120.28	3	5
2	B	58	SER	CA-C-O	7.74	128.62	120.42	3	1
2	B	72	TRP	N-CA-C	7.73	119.79	111.36	9	3
2	B	56	THR	O-C-N	-7.73	114.05	122.09	8	1
1	A	505	TRP	CB-CG-CD2	-7.73	115.98	126.80	13	1
2	C	122	TYR	N-CA-C	7.73	119.70	111.28	15	4
2	C	202	ALA	CA-C-N	7.73	132.05	120.31	6	3
2	C	202	ALA	C-N-CA	7.73	132.05	120.31	6	3
2	B	258	TYR	O-C-N	-7.72	114.11	122.07	9	3
2	B	184	HIS	O-C-N	-7.72	113.75	122.09	2	2
2	B	85	GLU	CA-C-N	7.72	130.48	120.44	2	3
2	B	85	GLU	C-N-CA	7.72	130.48	120.44	2	3
1	A	459	ILE	N-CA-C	7.72	115.27	108.63	2	2
2	B	106	LYS	N-CA-C	7.71	119.69	111.28	14	1
1	A	421	TRP	CB-CG-CD1	-7.71	115.33	126.90	3	1
2	C	91	GLU	N-CA-C	7.71	119.77	111.36	11	2
2	C	160	GLN	N-CA-C	7.71	120.66	111.33	8	5
2	B	259	THR	CA-C-N	7.71	131.24	120.29	11	3
2	B	259	THR	C-N-CA	7.71	131.24	120.29	11	3
2	C	85	GLU	CA-C-N	7.71	130.95	120.54	2	3
2	C	85	GLU	C-N-CA	7.71	130.95	120.54	2	3
2	C	150	GLU	CA-C-N	7.71	128.48	120.00	2	4
2	C	150	GLU	C-N-CA	7.71	128.48	120.00	2	4
2	C	256	GLU	CA-C-N	7.71	130.61	120.28	1	2
2	C	256	GLU	C-N-CA	7.71	130.61	120.28	1	2
2	B	130	TRP	CA-C-N	7.71	130.94	120.38	12	2
2	B	130	TRP	C-N-CA	7.71	130.94	120.38	12	2
2	B	79	THR	CA-C-N	7.70	130.45	120.44	3	4
2	B	79	THR	C-N-CA	7.70	130.45	120.44	3	4
2	B	119	VAL	CA-C-O	7.70	128.96	120.95	9	2
2	B	231	PRO	CA-C-N	7.70	130.60	120.28	11	5
2	B	231	PRO	C-N-CA	7.70	130.60	120.28	11	5
2	C	166	LEU	CA-C-N	7.70	128.47	120.00	14	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	C	166	LEU	C-N-CA	7.70	128.47	120.00	14	2
2	B	177	HIS	N-CA-C	7.70	119.31	111.07	12	4
2	C	229	ALA	CA-C-O	7.70	128.36	119.35	8	1
2	C	215	HIS	CG-CD2-NE2	7.69	114.89	107.20	6	3
2	B	59	LYS	O-C-N	-7.69	113.39	122.15	7	3
2	B	228	LYS	CA-C-N	7.69	130.92	120.54	11	1
2	B	228	LYS	C-N-CA	7.69	130.92	120.54	11	1
2	C	208	GLY	N-CA-C	-7.69	102.93	112.77	11	1
2	C	153	ARG	CD-NE-CZ	7.68	135.15	124.40	3	1
2	B	205	GLU	CA-C-O	-7.68	112.75	120.82	12	3
2	B	208	GLY	CA-C-N	7.68	130.42	120.44	6	4
2	B	208	GLY	C-N-CA	7.68	130.42	120.44	6	4
2	C	105	GLN	OE1-CD-NE2	-7.68	114.92	122.60	15	1
2	B	214	TYR	N-CA-C	7.67	120.32	111.11	1	2
1	A	458	GLY	CA-C-N	-7.67	117.38	122.60	11	1
1	A	458	GLY	C-N-CA	-7.67	117.38	122.60	11	1
2	B	174	ALA	N-CA-C	7.67	119.64	111.28	7	4
2	C	153	ARG	NH1-CZ-NH2	-7.67	109.33	119.30	7	4
2	B	149	GLN	N-CA-C	7.66	119.27	111.07	14	5
1	A	464	ARG	NH1-CZ-NH2	-7.66	109.34	119.30	5	2
2	B	66	PRO	CA-C-N	7.66	130.21	120.56	6	2
2	B	66	PRO	C-N-CA	7.66	130.21	120.56	6	2
1	A	486	PHE	N-CA-CB	-7.66	98.54	110.57	13	1
1	A	451	LYS	CA-C-N	7.66	132.00	121.05	7	4
1	A	451	LYS	C-N-CA	7.66	132.00	121.05	7	4
2	B	248	LYS	N-CA-C	7.65	119.62	111.28	5	3
2	B	241	LEU	CA-C-O	-7.64	111.24	118.73	6	2
2	B	177	HIS	N-CA-CB	7.64	121.47	110.16	10	1
1	A	471	ASP	CA-CB-CG	7.64	120.24	112.60	12	6
2	C	105	GLN	N-CA-C	7.64	120.28	111.11	15	3
2	B	180	ALA	N-CA-C	7.63	119.60	111.28	12	3
1	A	472	GLU	CB-CG-CD	7.63	125.57	112.60	1	1
2	B	84	GLN	OE1-CD-NE2	-7.63	114.97	122.60	4	1
2	C	190	ASP	O-C-N	-7.62	114.04	122.12	7	2
1	A	460	PRO	N-CA-C	7.62	123.19	111.15	7	4
2	C	244	LEU	O-C-N	-7.62	113.47	122.15	3	1
2	B	175	ARG	NE-CZ-NH1	-7.62	113.88	121.50	15	4
2	B	111	GLU	O-C-N	-7.61	113.47	122.15	11	3
2	B	198	ALA	O-C-N	-7.61	113.47	122.15	4	1
2	B	154	GLN	CA-C-O	7.61	128.81	120.82	9	1
2	B	121	PRO	CA-C-N	7.61	130.80	120.38	6	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	121	PRO	C-N-CA	7.61	130.80	120.38	6	3
1	A	422	MET	N-CA-C	7.61	123.14	113.25	10	7
2	C	125	ASP	CA-CB-CG	7.60	120.20	112.60	9	1
1	A	367	SER	N-CA-C	7.60	121.54	111.28	8	3
1	A	345	ARG	NE-CZ-NH1	-7.59	113.91	121.50	7	4
2	C	245	GLU	N-CA-CB	7.59	121.02	110.01	11	2
2	B	109	GLN	O-C-N	7.59	130.17	122.12	13	2
2	B	236	LEU	N-CA-C	7.59	119.56	111.28	12	1
2	B	221	HIS	CB-CG-CD2	-7.59	121.33	131.20	5	2
2	C	217	LYS	N-CA-C	7.58	119.33	111.14	4	5
2	B	189	SER	O-C-N	-7.58	114.08	122.12	12	1
2	C	181	LEU	CA-C-N	7.58	130.76	120.38	4	1
2	C	181	LEU	C-N-CA	7.58	130.76	120.38	4	1
1	A	332	GLU	CA-C-O	-7.58	111.94	120.66	13	2
2	C	202	ALA	CA-C-O	7.58	128.58	120.55	7	1
2	C	123	LEU	N-CA-C	7.58	119.54	111.28	6	1
2	B	186	ALA	CA-C-O	-7.58	110.99	118.34	10	1
1	A	505	TRP	CE2-CD2-CE3	7.57	126.37	118.80	6	2
1	A	492	LYS	CA-C-N	7.57	130.65	120.50	8	2
1	A	492	LYS	C-N-CA	7.57	130.65	120.50	8	2
2	C	81	GLY	N-CA-C	7.57	121.28	112.50	4	2
2	C	219	THR	CA-CB-OG1	7.56	120.94	109.60	1	3
1	A	330	ARG	NE-CZ-NH1	-7.56	113.94	121.50	5	4
2	B	259	THR	N-CA-CB	7.55	121.23	110.12	4	2
2	C	182	ARG	NE-CZ-NH2	-7.55	112.41	119.20	6	5
2	B	109	GLN	CA-C-N	7.54	130.72	120.54	4	3
2	B	109	GLN	C-N-CA	7.54	130.72	120.54	4	3
2	C	250	SER	CA-C-N	7.54	130.24	120.44	12	3
2	C	250	SER	C-N-CA	7.54	130.24	120.44	12	3
2	C	158	GLU	CA-C-N	7.54	130.38	120.28	5	3
2	C	158	GLU	C-N-CA	7.54	130.38	120.28	5	3
2	B	164	SER	CA-C-N	7.54	127.18	119.19	6	5
2	B	164	SER	C-N-CA	7.54	127.18	119.19	6	5
2	C	225	LEU	N-CA-C	7.53	120.56	111.82	8	5
2	B	167	GLY	O-C-N	7.53	129.42	122.19	10	1
2	C	237	ARG	NE-CZ-NH1	-7.53	113.97	121.50	1	5
2	C	170	MET	N-CA-C	7.52	119.12	111.07	6	1
1	A	484	TRP	CA-C-O	7.52	128.21	120.24	7	2
2	C	177	HIS	CA-C-N	7.52	130.03	120.56	9	3
2	C	177	HIS	C-N-CA	7.52	130.03	120.56	9	3
2	B	223	SER	CA-C-N	7.51	130.21	120.44	14	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	223	SER	C-N-CA	7.51	130.21	120.44	14	4
1	A	321	GLY	CA-C-N	7.51	133.45	122.63	5	2
1	A	321	GLY	C-N-CA	7.51	133.45	122.63	5	2
1	A	338	GLU	CB-CA-C	-7.51	107.92	116.63	10	2
2	B	73	ASP	CA-CB-CG	7.51	120.11	112.60	3	4
2	C	210	ARG	NH1-CZ-NH2	-7.50	109.55	119.30	9	5
2	C	239	GLY	N-CA-C	7.50	121.73	112.73	13	4
1	A	368	ILE	O-C-N	-7.50	114.72	123.04	7	3
2	C	69	GLN	CA-C-N	7.50	130.66	120.54	2	2
2	C	69	GLN	C-N-CA	7.50	130.66	120.54	2	2
1	A	353	TYR	CA-C-O	-7.49	113.61	120.50	8	4
2	C	71	PHE	CA-C-N	7.49	130.32	120.28	12	3
2	C	71	PHE	C-N-CA	7.49	130.32	120.28	12	3
2	C	72	TRP	CB-CA-C	7.49	122.63	110.88	2	1
2	C	232	ALA	CA-C-N	7.48	130.31	120.28	5	1
2	C	232	ALA	C-N-CA	7.48	130.31	120.28	5	1
2	B	190	ASP	CA-C-N	7.48	130.30	120.28	4	1
2	B	190	ASP	C-N-CA	7.48	130.30	120.28	4	1
1	A	346	ASN	CA-CB-CG	-7.47	105.13	112.60	2	3
2	B	116	ARG	CD-NE-CZ	-7.47	113.94	124.40	13	2
2	B	80	GLU	CA-C-N	7.47	128.08	119.94	3	4
2	B	80	GLU	C-N-CA	7.47	128.08	119.94	3	4
2	B	93	VAL	N-CA-C	7.46	118.23	110.62	10	4
2	B	237	ARG	N-CA-C	7.46	120.07	111.11	4	3
1	A	322	ASN	CA-CB-CG	-7.46	105.14	112.60	1	4
2	C	182	ARG	CA-C-O	7.46	128.32	120.42	8	1
2	B	184	HIS	CE1-NE2-CD2	-7.45	101.55	109.00	7	8
2	C	177	HIS	CB-CG-CD2	-7.45	121.51	131.20	7	1
2	C	100	TYR	O-C-N	-7.45	114.48	121.56	4	1
2	B	177	HIS	ND1-CE1-NE2	7.45	115.85	108.40	10	3
2	C	208	GLY	CA-C-N	7.45	130.13	120.44	4	2
2	C	208	GLY	C-N-CA	7.45	130.13	120.44	4	2
2	B	203	LEU	CA-C-N	7.45	130.12	120.44	10	4
2	B	203	LEU	C-N-CA	7.45	130.12	120.44	10	4
2	B	196	LEU	CA-C-N	7.45	130.59	120.54	4	1
2	B	196	LEU	C-N-CA	7.45	130.59	120.54	4	1
1	A	348	GLN	O-C-N	-7.44	114.32	123.33	8	3
2	B	102	ASP	CA-C-O	7.44	128.44	120.55	9	1
2	C	250	SER	CA-C-O	7.44	128.44	120.55	14	3
2	C	181	LEU	N-CA-CB	-7.44	99.28	110.07	3	1
1	A	380	VAL	O-C-N	-7.44	114.47	122.95	4	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	351	ASP	CA-CB-CG	7.44	120.04	112.60	14	2
2	B	224	THR	N-CA-CB	7.44	120.80	110.01	4	1
2	C	176	ALA	CA-C-N	7.44	130.25	120.28	13	4
2	C	176	ALA	C-N-CA	7.44	130.25	120.28	13	4
2	B	172	ASP	N-CA-CB	7.44	121.34	110.26	10	2
2	C	188	TYR	CA-C-N	7.43	130.57	120.54	2	5
2	C	188	TYR	C-N-CA	7.43	130.57	120.54	2	5
2	B	131	GLN	OE1-CD-NE2	-7.42	115.18	122.60	2	4
1	A	319	CYS	CA-C-N	7.42	130.55	120.38	10	2
1	A	319	CYS	C-N-CA	7.42	130.55	120.38	10	2
2	B	105	GLN	OE1-CD-NE2	-7.42	115.18	122.60	6	2
2	C	86	MET	O-C-N	-7.42	114.43	122.07	9	2
2	B	193	ARG	N-CA-C	7.42	120.24	111.71	11	3
2	C	96	LYS	N-CA-C	7.42	119.44	111.36	14	3
2	C	254	ALA	N-CA-C	7.42	119.36	111.28	8	3
2	C	103	ASP	CA-C-O	7.41	128.28	120.42	14	1
2	B	206	ASN	OD1-CG-ND2	-7.41	115.19	122.60	10	3
2	C	205	GLU	O-C-N	-7.41	114.44	122.07	14	3
2	C	102	ASP	CA-CB-CG	7.41	120.01	112.60	8	4
1	A	404	LYS	N-CA-C	7.41	121.97	112.34	6	1
2	B	233	LEU	N-CA-CB	-7.41	99.20	110.16	2	2
2	C	59	LYS	N-CA-C	7.41	120.23	111.71	12	4
1	A	483	TYR	CA-C-O	7.41	129.77	121.40	11	2
2	B	227	GLU	CA-C-O	-7.40	112.70	120.55	12	1
1	A	441	GLU	O-C-N	-7.39	113.82	122.32	1	3
2	C	261	LYS	N-CA-C	7.39	121.20	112.93	4	3
2	B	82	LEU	O-C-N	-7.38	114.30	122.12	10	3
2	B	63	GLN	N-CA-C	7.38	119.41	111.36	8	4
2	B	215	HIS	CA-C-O	7.38	128.60	120.63	5	2
2	C	65	GLY	O-C-N	-7.38	114.39	121.77	15	2
2	C	183	THR	O-C-N	-7.38	113.74	122.15	11	1
2	B	83	ARG	N-CA-C	7.37	119.95	111.11	14	1
2	B	86	MET	CG-SD-CE	-7.37	84.69	100.90	4	3
2	B	129	LYS	CA-C-N	7.36	130.00	120.44	12	1
2	B	129	LYS	C-N-CA	7.36	130.00	120.44	12	1
2	B	168	GLU	N-CA-C	7.35	119.30	111.28	4	7
2	B	88	LYS	CA-C-N	7.35	130.13	120.28	14	3
2	B	88	LYS	C-N-CA	7.35	130.13	120.28	14	3
2	C	77	LYS	CA-C-O	7.35	128.34	120.55	1	2
1	A	476	TYR	CA-CB-CG	-7.35	100.67	113.90	10	3
2	C	175	ARG	CD-NE-CZ	7.35	134.69	124.40	5	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	447	SER	CB-CA-C	-7.35	97.52	109.72	8	2
2	C	60	LEU	CA-C-N	7.35	130.12	120.28	6	1
2	C	60	LEU	C-N-CA	7.35	130.12	120.28	6	1
2	C	74	ASN	CA-C-O	-7.34	113.11	120.82	6	1
2	C	76	GLU	N-CA-C	7.34	118.93	111.07	6	5
2	B	154	GLN	N-CA-C	7.34	118.92	111.07	6	4
2	C	213	GLU	N-CA-CB	7.33	120.70	110.07	9	1
2	C	112	MET	CA-C-N	7.33	129.97	120.44	8	1
2	C	112	MET	C-N-CA	7.33	129.97	120.44	8	1
2	B	238	GLN	N-CA-CB	7.33	121.05	110.06	12	2
2	B	230	LYS	O-C-N	-7.33	113.96	120.48	12	4
1	A	331	GLY	CA-C-O	7.33	127.08	119.10	2	1
2	C	227	GLU	CA-C-N	7.32	130.82	120.28	12	1
2	C	227	GLU	C-N-CA	7.32	130.82	120.28	12	1
1	A	408	ARG	N-CA-C	7.32	120.94	109.96	14	1
1	A	459	ILE	CB-CA-C	7.32	117.74	110.94	2	3
1	A	357	ILE	CA-C-N	7.32	128.10	119.98	9	3
1	A	357	ILE	C-N-CA	7.32	128.10	119.98	9	3
1	A	367	SER	CA-C-N	7.31	130.30	120.50	11	2
1	A	367	SER	C-N-CA	7.31	130.30	120.50	11	2
2	C	124	ASP	CA-CB-CG	7.31	119.91	112.60	1	5
2	B	211	LEU	CA-C-O	7.31	128.72	120.90	10	1
2	B	205	GLU	N-CA-C	7.31	119.24	111.28	3	1
1	A	345	ARG	CA-C-N	7.30	135.49	121.54	3	2
1	A	345	ARG	C-N-CA	7.30	135.49	121.54	3	2
2	C	108	TRP	O-C-N	-7.30	114.38	122.12	5	2
2	C	126	PHE	CA-C-O	-7.30	112.81	120.55	6	2
2	B	99	PRO	CA-C-N	7.30	130.66	120.29	5	6
2	B	99	PRO	C-N-CA	7.30	130.66	120.29	5	6
1	A	374	ARG	NH1-CZ-NH2	-7.30	109.81	119.30	3	1
2	B	105	GLN	CB-CG-CD	7.30	125.00	112.60	10	1
2	B	222	LEU	N-CA-C	7.29	119.23	111.28	1	3
2	B	202	ALA	CA-C-N	7.29	129.92	120.44	8	2
2	B	202	ALA	C-N-CA	7.29	129.92	120.44	8	2
2	C	171	ARG	CA-C-N	7.29	129.92	120.44	2	3
2	C	171	ARG	C-N-CA	7.29	129.92	120.44	2	3
1	A	388	TRP	CB-CG-CD1	-7.29	115.96	126.90	11	4
2	B	97	VAL	CA-C-N	7.29	129.20	120.09	4	2
2	B	97	VAL	C-N-CA	7.29	129.20	120.09	4	2
2	C	168	GLU	CA-C-N	7.28	130.03	120.28	9	3
2	C	168	GLU	C-N-CA	7.28	130.03	120.28	9	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	C	167	GLY	N-CA-C	7.28	121.46	112.73	6	2
2	B	165	PRO	N-CA-C	-7.27	104.04	113.57	6	2
2	C	229	ALA	CA-C-N	7.27	130.18	120.58	6	1
2	C	229	ALA	C-N-CA	7.27	130.18	120.58	6	1
2	B	119	VAL	N-CA-CB	7.27	121.48	110.58	11	1
2	C	116	ARG	N-CA-C	7.27	119.20	111.28	2	4
1	A	489	GLN	OE1-CD-NE2	-7.27	115.33	122.60	2	2
2	B	173	ARG	NH1-CZ-NH2	-7.27	109.85	119.30	7	3
1	A	416	ASP	CA-CB-CG	-7.26	105.33	112.60	15	3
1	A	387	HIS	CA-C-N	7.26	134.87	122.37	7	4
1	A	387	HIS	C-N-CA	7.26	134.87	122.37	7	4
2	C	93	VAL	N-CA-CB	7.26	120.42	110.54	8	3
2	C	166	LEU	CA-C-O	7.26	128.24	120.55	15	1
2	C	75	LEU	CA-C-N	7.25	130.33	120.54	11	3
2	C	75	LEU	C-N-CA	7.25	130.33	120.54	11	3
2	C	177	HIS	CB-CG-ND1	7.25	133.58	122.70	7	2
1	A	317	ASN	O-C-N	-7.25	114.67	123.30	8	1
2	C	70	GLU	N-CA-C	7.25	119.18	111.28	8	1
2	B	120	GLU	CA-C-N	7.25	127.25	119.28	9	3
2	B	120	GLU	C-N-CA	7.25	127.25	119.28	9	3
1	A	458	GLY	O-C-N	-7.24	113.34	122.32	13	3
1	A	365	PRO	O-C-N	7.24	132.26	123.13	13	1
2	B	147	GLU	N-CA-C	7.24	119.17	111.28	1	4
2	B	221	HIS	CA-C-O	-7.24	113.22	120.82	7	2
2	C	223	SER	O-C-N	7.24	129.79	122.12	8	3
2	B	107	LYS	CA-C-N	7.24	129.84	120.44	12	4
2	B	107	LYS	C-N-CA	7.24	129.84	120.44	12	4
2	B	70	GLU	CA-C-N	7.24	130.28	120.44	15	4
2	B	70	GLU	C-N-CA	7.24	130.28	120.44	15	4
2	C	83	ARG	CA-C-N	7.23	129.84	120.44	2	1
2	C	83	ARG	C-N-CA	7.23	129.84	120.44	2	1
1	A	370	THR	CA-CB-CG2	7.23	122.79	110.50	4	3
2	C	120	GLU	CA-C-O	-7.23	111.33	118.34	11	1
2	B	224	THR	CB-CA-C	-7.22	98.80	110.79	10	2
2	B	131	GLN	N-CA-C	7.22	119.15	111.28	4	4
2	B	188	TYR	CA-C-N	7.22	130.26	120.44	9	2
2	B	188	TYR	C-N-CA	7.22	130.26	120.44	9	2
2	C	130	TRP	CA-C-O	-7.22	113.24	120.82	3	1
2	C	80	GLU	CA-C-O	7.22	128.20	120.55	10	2
2	B	107	LYS	N-CA-C	7.22	119.23	111.36	3	3
2	C	120	GLU	N-CA-C	7.22	123.30	113.77	6	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	170	MET	CG-SD-CE	-7.22	85.02	100.90	8	2
2	C	246	SER	CA-C-N	7.21	130.53	120.29	11	1
2	C	246	SER	C-N-CA	7.21	130.53	120.29	11	1
1	A	408	ARG	NH1-CZ-NH2	-7.21	109.92	119.30	13	1
2	C	213	GLU	CA-C-N	7.21	129.81	120.44	14	1
2	C	213	GLU	C-N-CA	7.21	129.81	120.44	14	1
2	C	149	GLN	N-CA-CB	7.21	120.46	110.01	12	2
1	A	437	ARG	NE-CZ-NH1	7.20	128.70	121.50	5	4
1	A	334	PHE	CA-CB-CG	-7.19	106.61	113.80	2	5
2	C	131	GLN	CA-C-O	-7.19	112.93	120.55	9	1
2	B	241	LEU	N-CA-C	7.19	122.60	113.25	8	2
2	C	168	GLU	N-CA-C	7.19	119.98	111.71	8	2
2	B	98	GLN	N-CA-C	7.18	123.44	113.45	8	4
2	C	195	ARG	NE-CZ-NH1	-7.18	114.32	121.50	8	4
2	C	199	ARG	CA-C-N	7.18	129.77	120.44	12	2
2	C	199	ARG	C-N-CA	7.18	129.77	120.44	12	2
2	B	126	PHE	O-C-N	-7.18	114.51	122.12	9	2
1	A	510	SER	O-C-N	-7.18	115.44	123.48	12	1
2	B	149	GLN	OE1-CD-NE2	-7.17	115.42	122.60	4	3
2	C	145	ARG	N-CA-C	7.17	119.77	111.02	7	1
1	A	349	VAL	O-C-N	-7.16	115.04	122.63	9	3
2	C	205	GLU	CA-C-N	7.16	130.20	120.54	7	4
2	C	205	GLU	C-N-CA	7.16	130.20	120.54	7	4
1	A	339	ARG	NE-CZ-NH1	7.16	128.66	121.50	15	3
2	C	107	LYS	CA-C-N	7.16	129.87	120.28	6	2
2	C	107	LYS	C-N-CA	7.16	129.87	120.28	6	2
2	B	265	GLN	OE1-CD-NE2	-7.16	115.44	122.60	9	2
2	B	150	GLU	O-C-N	-7.16	114.70	122.07	11	1
1	A	402	HIS	CE1-NE2-CD2	-7.15	101.85	109.00	1	6
2	B	64	LEU	N-CA-C	7.15	119.16	111.36	14	2
2	B	139	GLN	O-C-N	7.15	129.70	122.12	7	1
1	A	493	VAL	CA-C-N	7.15	131.54	120.60	7	4
1	A	493	VAL	C-N-CA	7.15	131.54	120.60	7	4
2	B	55	SER	CA-C-N	7.15	130.19	120.54	11	6
2	B	55	SER	C-N-CA	7.15	130.19	120.54	11	6
2	C	117	GLN	CA-C-N	7.15	132.66	120.72	9	1
2	C	117	GLN	C-N-CA	7.15	132.66	120.72	9	1
2	B	75	LEU	O-C-N	-7.14	114.55	122.12	12	3
2	C	154	GLN	CA-C-N	7.14	129.72	120.44	7	6
2	C	154	GLN	C-N-CA	7.14	129.72	120.44	7	6
2	C	87	SER	CA-C-N	7.14	130.43	120.29	4	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	C	87	SER	C-N-CA	7.14	130.43	120.29	4	3
2	B	195	ARG	N-CA-C	7.14	119.97	111.33	15	2
2	C	183	THR	N-CA-C	7.13	119.05	111.28	13	1
2	C	261	LYS	CA-C-N	7.13	130.16	120.54	12	1
2	C	261	LYS	C-N-CA	7.13	130.16	120.54	12	1
2	C	186	ALA	CA-C-N	7.12	126.74	119.19	7	3
2	C	186	ALA	C-N-CA	7.12	126.74	119.19	7	3
1	A	413	ASP	CB-CA-C	7.12	121.90	111.65	5	2
2	C	194	GLN	CA-C-O	7.11	127.96	120.42	9	1
2	B	219	THR	O-C-N	-7.11	114.58	122.12	13	2
2	C	65	GLY	CA-C-N	7.11	126.60	118.85	3	1
2	C	65	GLY	C-N-CA	7.11	126.60	118.85	3	1
2	B	84	GLN	CA-C-N	7.11	129.80	120.28	15	3
2	B	84	GLN	C-N-CA	7.11	129.80	120.28	15	3
2	C	119	VAL	N-CA-C	-7.11	105.68	113.43	5	1
1	A	397	PRO	N-CA-C	7.11	122.46	110.95	8	2
1	A	367	SER	N-CA-CB	7.10	122.49	110.49	7	2
2	B	158	GLU	O-C-N	-7.10	114.59	122.12	4	3
1	A	330	ARG	NH1-CZ-NH2	-7.10	110.07	119.30	9	4
2	C	182	ARG	NE-CZ-NH1	7.09	128.59	121.50	8	4
2	C	166	LEU	N-CA-C	7.09	121.52	113.01	10	1
2	C	58	SER	N-CA-C	7.09	119.09	111.36	11	1
2	C	116	ARG	NH1-CZ-NH2	-7.08	110.10	119.30	13	2
1	A	399	TYR	O-C-N	-7.08	112.57	121.70	12	3
2	C	67	VAL	CA-C-O	7.07	127.89	120.25	10	5
2	B	72	TRP	N-CA-CB	-7.07	99.75	110.01	4	2
2	B	164	SER	CA-C-O	-7.07	111.48	118.34	4	3
1	A	430	PHE	O-C-N	-7.07	115.07	123.27	7	3
1	A	326	VAL	CB-CA-C	-7.05	100.75	110.77	10	1
1	A	414	LYS	CA-C-N	-7.05	114.44	123.19	6	1
1	A	414	LYS	C-N-CA	-7.05	114.44	123.19	6	1
2	B	65	GLY	N-CA-C	7.05	126.72	112.34	9	2
2	B	254	ALA	CA-C-N	7.05	129.72	120.28	14	5
2	B	254	ALA	C-N-CA	7.05	129.72	120.28	14	5
2	C	109	GLN	CA-C-N	7.05	130.03	120.44	10	3
2	C	109	GLN	C-N-CA	7.05	130.03	120.44	10	3
2	B	201	GLU	CA-C-O	-7.05	113.42	120.82	12	2
2	C	163	LEU	O-C-N	-7.05	113.60	122.27	4	1
2	B	151	GLY	N-CA-C	7.04	121.16	112.64	15	2
2	C	238	GLN	OE1-CD-NE2	7.04	129.64	122.60	2	1
1	A	466	SER	N-CA-CB	7.04	122.39	110.49	4	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	172	ASP	N-CA-C	-7.04	105.22	113.88	5	3
1	A	318	ILE	CA-C-O	7.04	127.67	119.36	14	3
2	C	89	ASP	O-C-N	-7.04	114.77	122.09	6	1
1	A	473	VAL	CA-C-O	7.04	127.85	120.25	9	2
2	C	157	HIS	N-CA-C	7.03	118.94	111.28	14	2
2	C	250	SER	N-CA-C	7.03	118.94	111.28	9	3
1	A	322	ASN	OD1-CG-ND2	-7.03	115.57	122.60	8	2
2	B	144	LEU	O-C-N	7.03	129.57	122.12	4	2
2	B	170	MET	N-CA-C	7.03	121.44	113.01	6	1
2	B	235	ASP	O-C-N	-7.03	114.83	122.07	14	1
1	A	356	PRO	CA-C-N	7.02	131.82	120.30	11	4
1	A	356	PRO	C-N-CA	7.02	131.82	120.30	11	4
2	B	128	LYS	CA-C-N	7.02	130.39	120.28	14	2
2	B	128	LYS	C-N-CA	7.02	130.39	120.28	14	2
1	A	378	LYS	N-CA-CB	7.01	120.29	110.26	1	1
2	C	57	PHE	N-CA-CB	7.01	120.18	110.01	2	1
1	A	433	ASN	N-CA-C	-7.01	104.30	112.92	2	3
2	C	144	LEU	N-CA-C	7.01	119.00	111.36	8	2
2	C	71	PHE	O-C-N	-7.00	114.69	122.12	12	3
2	B	184	HIS	ND1-CE1-NE2	7.00	115.40	108.40	9	3
1	A	445	VAL	N-CA-C	7.00	117.50	108.12	3	3
2	B	238	GLN	N-CA-C	7.00	119.76	111.71	10	2
2	B	206	ASN	N-CA-C	7.00	118.90	111.28	15	2
2	B	260	LYS	CA-C-N	7.00	129.53	120.44	7	2
2	B	260	LYS	C-N-CA	7.00	129.53	120.44	7	2
2	B	175	ARG	N-CA-CB	-6.99	99.81	110.16	4	1
2	B	216	ALA	CA-C-N	6.99	129.65	120.28	6	2
2	B	216	ALA	C-N-CA	6.99	129.65	120.28	6	2
2	B	183	THR	O-C-N	-6.99	114.71	122.12	6	2
2	B	114	LEU	CA-C-N	6.99	129.88	120.65	6	4
2	B	114	LEU	C-N-CA	6.99	129.88	120.65	6	4
2	B	133	GLU	O-C-N	-6.99	114.71	122.12	2	2
2	B	73	ASP	CA-C-N	6.99	129.97	120.54	4	4
2	B	73	ASP	C-N-CA	6.99	129.97	120.54	4	4
1	A	397	PRO	O-C-N	-6.99	115.37	122.98	8	2
1	A	487	ASN	OD1-CG-ND2	-6.99	115.61	122.60	11	2
1	A	412	THR	CA-C-N	6.98	130.75	122.44	1	2
1	A	412	THR	C-N-CA	6.98	130.75	122.44	1	2
2	B	76	GLU	O-C-N	-6.98	114.88	122.07	8	1
2	C	113	GLU	CA-C-N	6.98	129.51	120.44	9	3
2	C	113	GLU	C-N-CA	6.98	129.51	120.44	9	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	190	ASP	CA-C-O	6.98	128.15	120.82	8	1
2	C	92	GLU	O-C-N	-6.98	114.72	122.12	11	2
2	C	201	GLU	N-CA-C	6.98	118.54	111.07	11	4
2	B	175	ARG	N-CA-C	6.98	118.88	111.28	6	1
2	B	154	GLN	O-C-N	-6.97	114.89	122.07	9	2
2	B	176	ALA	N-CA-C	6.97	122.87	111.37	5	2
2	B	137	TYR	N-CA-C	6.97	118.53	111.07	4	4
2	C	253	SER	CA-C-N	6.97	129.50	120.44	7	3
2	C	253	SER	C-N-CA	6.97	129.50	120.44	7	3
2	B	76	GLU	CA-C-N	6.97	129.95	120.54	10	1
2	B	76	GLU	C-N-CA	6.97	129.95	120.54	10	1
2	B	179	ASP	O-C-N	-6.97	114.73	122.12	14	2
2	B	110	GLU	CB-CG-CD	-6.97	100.75	112.60	10	1
1	A	503	ARG	N-CA-C	6.97	118.56	110.97	7	2
2	B	219	THR	CA-C-O	6.97	127.93	120.55	5	1
2	C	160	GLN	O-C-N	-6.96	113.70	122.27	4	1
2	C	236	LEU	N-CA-C	6.96	118.52	111.07	8	1
1	A	477	PHE	CA-C-O	-6.96	113.11	121.05	15	1
2	C	201	GLU	CA-C-N	6.96	130.89	120.31	13	2
2	C	201	GLU	C-N-CA	6.96	130.89	120.31	13	2
1	A	495	PRO	CA-C-N	6.96	131.15	121.26	7	2
1	A	495	PRO	C-N-CA	6.96	131.15	121.26	7	2
2	C	158	GLU	CA-C-O	6.96	128.13	120.82	7	2
1	A	390	PHE	N-CA-C	6.96	120.79	109.59	8	2
1	A	380	VAL	CA-C-N	6.95	132.02	122.77	10	2
1	A	380	VAL	C-N-CA	6.95	132.02	122.77	10	2
2	B	218	ALA	N-CA-C	6.95	118.51	111.07	6	4
2	C	243	VAL	N-CA-C	6.95	117.71	110.62	7	1
2	B	120	GLU	N-CA-CB	6.95	118.62	110.42	9	1
2	B	146	ALA	N-CA-C	6.95	118.51	111.07	12	3
1	A	406	LEU	CA-C-O	6.95	127.96	119.97	5	2
1	A	332	GLU	O-C-N	-6.95	114.79	123.27	7	1
2	C	212	ALA	CA-C-N	6.95	129.47	120.44	13	2
2	C	212	ALA	C-N-CA	6.95	129.47	120.44	13	2
2	B	238	GLN	CA-C-N	6.95	127.51	119.94	12	1
2	B	238	GLN	C-N-CA	6.95	127.51	119.94	12	1
1	A	503	ARG	CA-C-N	6.94	134.80	121.54	2	1
1	A	503	ARG	C-N-CA	6.94	134.80	121.54	2	1
2	C	105	GLN	CA-C-O	-6.94	112.26	120.10	1	2
1	A	340	TRP	O-C-N	-6.94	114.13	123.15	10	2
2	B	207	GLY	CA-C-N	6.94	127.80	120.03	2	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	207	GLY	C-N-CA	6.94	127.80	120.03	2	4
2	C	159	LEU	CA-C-N	6.94	130.14	120.29	12	4
2	C	159	LEU	C-N-CA	6.94	130.14	120.29	12	4
2	B	83	ARG	O-C-N	6.94	129.47	122.12	12	1
2	B	157	HIS	CA-C-O	6.94	127.90	120.55	12	1
2	B	80	GLU	N-CA-C	6.93	118.63	111.14	4	3
2	C	184	HIS	CE1-NE2-CD2	-6.93	102.07	109.00	6	5
1	A	389	VAL	N-CA-CB	6.93	118.27	110.72	5	2
2	C	124	ASP	N-CA-C	6.93	118.48	111.07	13	3
2	C	195	ARG	CA-C-N	6.92	130.12	120.29	13	2
2	C	195	ARG	C-N-CA	6.92	130.12	120.29	13	2
1	A	425	GLY	CA-C-O	6.92	128.17	119.72	12	1
2	B	122	TYR	O-C-N	-6.92	114.94	122.07	5	1
2	C	221	HIS	ND1-CE1-NE2	6.92	115.32	108.40	8	3
2	C	73	ASP	CA-CB-CG	-6.92	105.68	112.60	9	3
1	A	351	ASP	CA-C-O	6.92	129.10	121.56	11	1
2	B	117	GLN	N-CA-C	6.92	118.82	111.28	7	4
2	C	191	GLU	O-C-N	-6.92	114.95	122.07	3	2
2	B	189	SER	N-CA-C	6.91	119.41	111.11	4	3
2	B	158	GLU	N-CA-C	6.91	118.82	111.28	14	3
2	C	99	PRO	CA-C-O	-6.91	113.46	121.34	15	1
2	B	257	GLU	CA-C-O	6.91	127.88	120.55	2	2
1	A	364	LEU	O-C-N	6.90	129.59	121.10	1	4
2	C	189	SER	CA-C-N	6.90	129.53	120.28	8	2
2	C	189	SER	C-N-CA	6.90	129.53	120.28	8	2
2	B	113	GLU	CA-C-N	6.90	129.41	120.44	10	6
2	B	113	GLU	C-N-CA	6.90	129.41	120.44	10	6
1	A	467	PHE	CA-CB-CG	6.90	120.70	113.80	8	2
2	B	152	ALA	CA-C-N	6.90	129.53	120.28	7	2
2	B	152	ALA	C-N-CA	6.90	129.53	120.28	7	2
2	C	123	LEU	O-C-N	-6.90	114.81	122.12	14	1
1	A	365	PRO	N-CD-CG	6.89	113.54	103.20	5	1
2	B	215	HIS	ND1-CE1-NE2	6.89	115.29	108.40	10	4
2	C	59	LYS	O-C-N	-6.89	114.97	122.07	1	1
2	B	147	GLU	O-C-N	-6.89	113.79	122.27	8	1
2	B	157	HIS	O-C-N	-6.89	114.81	122.12	12	1
1	A	323	PHE	N-CA-C	6.88	119.95	110.24	7	1
2	C	246	SER	N-CA-C	6.88	119.66	111.33	11	2
2	B	262	LEU	N-CA-C	6.88	118.43	111.07	3	1
2	C	61	ARG	CA-CB-CG	6.88	127.86	114.10	3	1
1	A	402	HIS	CA-C-N	6.88	129.88	120.46	10	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	402	HIS	C-N-CA	6.88	129.88	120.46	10	3
2	B	91	GLU	CA-C-O	-6.88	113.26	120.55	11	1
1	A	317	ASN	CA-C-N	6.88	129.88	120.46	9	4
1	A	317	ASN	C-N-CA	6.88	129.88	120.46	9	4
2	C	88	LYS	CA-C-N	6.88	129.82	120.54	6	2
2	C	88	LYS	C-N-CA	6.88	129.82	120.54	6	2
2	B	137	TYR	CA-C-N	6.88	129.49	120.28	3	3
2	B	137	TYR	C-N-CA	6.88	129.49	120.28	3	3
1	A	452	ASN	N-CA-C	6.87	120.20	110.23	14	2
1	A	414	LYS	CA-C-O	-6.87	113.64	121.40	6	1
2	C	83	ARG	CA-C-O	-6.87	113.27	120.55	11	2
2	C	174	ALA	CA-C-N	6.87	129.37	120.44	15	2
2	C	174	ALA	C-N-CA	6.87	129.37	120.44	15	2
2	B	256	GLU	CA-C-O	6.87	128.25	120.90	3	1
2	C	198	ALA	CA-C-N	6.87	129.81	120.54	7	5
2	C	198	ALA	C-N-CA	6.87	129.81	120.54	7	5
1	A	396	GLU	CA-C-N	6.86	127.28	119.93	10	4
1	A	396	GLU	C-N-CA	6.86	127.28	119.93	10	4
1	A	370	THR	O-C-N	-6.86	115.58	123.33	12	1
1	A	468	MET	CA-C-N	6.85	128.28	120.53	13	3
1	A	468	MET	C-N-CA	6.85	128.28	120.53	13	3
1	A	499	LYS	O-C-N	-6.85	114.28	123.19	10	2
2	C	211	LEU	CA-C-O	6.85	127.81	120.55	13	2
1	A	374	ARG	CA-C-N	6.85	129.46	120.28	1	5
1	A	374	ARG	C-N-CA	6.85	129.46	120.28	1	5
2	B	74	ASN	O-C-N	-6.85	114.86	122.12	6	3
2	C	108	TRP	CD2-CE2-CZ2	-6.85	115.55	122.40	12	1
2	C	233	LEU	CA-C-N	6.85	129.46	120.28	5	1
2	C	233	LEU	C-N-CA	6.85	129.46	120.28	5	1
1	A	392	GLU	O-C-N	-6.84	114.86	122.12	2	1
2	B	200	LEU	CA-C-N	6.84	129.45	120.28	10	1
2	B	200	LEU	C-N-CA	6.84	129.45	120.28	10	1
1	A	442	LEU	CA-C-O	6.84	127.35	119.35	15	1
2	C	200	LEU	N-CA-C	6.83	118.73	111.28	10	3
2	C	235	ASP	CA-C-N	6.83	129.99	120.29	11	2
2	C	235	ASP	C-N-CA	6.83	129.99	120.29	11	2
2	B	171	ARG	NE-CZ-NH1	-6.83	114.67	121.50	7	2
2	B	122	TYR	N-CA-CB	-6.83	100.08	110.12	8	1
2	C	124	ASP	CA-C-O	-6.83	113.31	120.55	10	2
1	A	440	GLU	CA-C-N	6.83	129.31	120.44	2	2
1	A	440	GLU	C-N-CA	6.83	129.31	120.44	2	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	184	HIS	CG-CD2-NE2	6.83	114.03	107.20	4	1
1	A	394	SER	CA-C-O	6.83	128.61	121.31	7	1
2	C	69	GLN	N-CA-C	6.82	118.72	111.28	1	4
2	B	221	HIS	N-CA-CB	6.82	119.90	110.01	10	3
2	B	94	LYS	O-C-N	-6.82	115.00	122.09	5	1
2	B	184	HIS	CA-CB-CG	-6.82	106.98	113.80	5	3
2	C	220	GLU	CA-C-N	6.82	129.42	120.28	12	2
2	C	220	GLU	C-N-CA	6.82	129.42	120.28	12	2
2	C	72	TRP	CB-CG-CD2	-6.82	117.26	126.80	5	1
2	B	251	PHE	N-CA-C	6.81	118.36	111.07	5	4
2	B	255	LEU	N-CA-CB	6.81	120.13	110.12	6	1
2	C	119	VAL	O-C-N	-6.81	115.39	122.20	11	1
1	A	343	ARG	CA-C-O	6.81	127.58	120.30	3	1
2	C	113	GLU	O-C-N	-6.81	115.06	122.07	7	1
1	A	436	TYR	N-CA-C	-6.80	98.97	109.24	7	2
2	B	145	ARG	CA-C-O	6.80	127.56	119.60	12	1
1	A	438	PHE	CA-C-O	6.80	127.71	120.36	3	1
2	B	204	LYS	N-CA-C	6.80	118.35	111.07	7	3
2	C	184	HIS	N-CA-C	6.80	119.71	111.82	15	1
2	B	257	GLU	N-CA-C	6.80	118.77	111.36	7	1
2	B	100	TYR	N-CA-C	6.80	118.69	111.28	3	3
2	C	119	VAL	N-CA-CB	-6.80	103.49	112.26	15	1
1	A	351	ASP	N-CA-C	6.79	119.59	110.35	4	1
2	C	254	ALA	CA-C-N	6.79	129.38	120.28	11	1
2	C	254	ALA	C-N-CA	6.79	129.38	120.28	11	1
2	C	74	ASN	CA-C-N	6.79	129.38	120.28	4	2
2	C	74	ASN	C-N-CA	6.79	129.38	120.28	4	2
2	B	224	THR	N-CA-C	6.79	118.68	111.28	2	3
2	B	122	TYR	N-CA-C	6.79	118.76	111.36	15	3
2	B	237	ARG	CA-C-N	6.79	129.38	120.28	9	4
2	B	237	ARG	C-N-CA	6.79	129.38	120.28	9	4
2	C	234	GLU	CA-C-N	6.79	131.00	120.82	2	3
2	C	234	GLU	C-N-CA	6.79	131.00	120.82	2	3
2	B	106	LYS	O-C-N	-6.79	114.76	122.09	7	1
2	B	178	VAL	O-C-N	-6.79	114.84	121.90	6	1
1	A	397	PRO	CA-C-N	6.79	134.71	121.41	9	3
1	A	397	PRO	C-N-CA	6.79	134.71	121.41	9	3
2	B	250	SER	N-CA-C	6.78	118.67	111.28	10	3
1	A	468	MET	CG-SD-CE	-6.78	85.98	100.90	14	2
2	C	84	GLN	CA-C-N	6.78	129.69	120.54	12	2
2	C	84	GLN	C-N-CA	6.78	129.69	120.54	12	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	142	GLU	N-CA-C	6.78	122.72	113.77	14	2
2	C	163	LEU	N-CA-C	6.78	118.75	111.36	11	2
2	C	193	ARG	NH1-CZ-NH2	-6.78	110.49	119.30	14	3
2	B	185	LEU	N-CA-C	6.78	118.74	111.36	2	1
2	B	144	LEU	N-CA-C	6.78	118.67	111.28	4	2
2	C	150	GLU	O-C-N	-6.78	113.42	122.23	6	3
2	B	104	PHE	O-C-N	-6.77	115.09	122.07	3	2
2	B	180	ALA	CA-C-O	-6.77	113.71	120.82	8	2
2	B	96	LYS	N-CA-C	6.77	119.52	111.33	10	2
2	B	213	GLU	CB-CG-CD	6.77	124.11	112.60	2	3
2	C	70	GLU	CB-CG-CD	6.77	124.11	112.60	5	1
1	A	421	TRP	CA-C-N	6.77	128.55	120.09	5	1
1	A	421	TRP	C-N-CA	6.77	128.55	120.09	5	1
2	B	218	ALA	CA-C-N	6.76	130.97	120.82	14	3
2	B	218	ALA	C-N-CA	6.76	130.97	120.82	14	3
1	A	497	TYR	O-C-N	-6.76	115.57	121.32	8	2
2	B	163	LEU	CA-C-N	6.76	130.98	120.97	1	4
2	B	163	LEU	C-N-CA	6.76	130.98	120.97	1	4
2	B	62	GLU	CA-C-N	6.76	129.34	120.28	6	2
2	B	62	GLU	C-N-CA	6.76	129.34	120.28	6	2
2	C	162	LYS	CA-C-N	6.76	129.88	120.29	11	4
2	C	162	LYS	C-N-CA	6.76	129.88	120.29	11	4
2	B	90	LEU	CA-C-N	6.76	129.64	120.38	9	2
2	B	90	LEU	C-N-CA	6.76	129.64	120.38	9	2
2	B	245	GLU	CA-C-N	6.75	129.33	120.28	4	1
2	B	245	GLU	C-N-CA	6.75	129.33	120.28	4	1
1	A	411	PRO	N-CA-CB	-6.75	96.16	103.25	10	2
1	A	360	PHE	N-CA-C	-6.75	105.04	113.55	11	1
2	C	72	TRP	O-C-N	-6.75	114.97	122.12	4	3
2	B	132	GLU	CA-C-N	6.75	133.93	121.52	11	3
2	B	132	GLU	C-N-CA	6.75	133.93	121.52	11	3
2	C	255	LEU	N-CA-C	6.75	118.29	111.07	9	1
2	B	76	GLU	N-CA-C	6.74	118.42	111.14	11	5
1	A	438	PHE	CA-CB-CG	6.74	120.54	113.80	4	2
2	C	103	ASP	CA-C-N	6.74	129.63	120.54	8	2
2	C	103	ASP	C-N-CA	6.74	129.63	120.54	8	2
2	B	230	LYS	CA-C-O	-6.73	112.13	118.73	4	2
2	C	235	ASP	O-C-N	-6.73	114.48	122.15	6	2
2	B	70	GLU	N-CA-C	6.72	118.26	111.07	1	2
2	B	152	ALA	CA-C-O	-6.72	113.76	120.82	2	3
2	B	177	HIS	CA-C-N	6.72	129.03	120.56	11	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	177	HIS	C-N-CA	6.72	129.03	120.56	11	3
2	C	188	TYR	CA-C-O	6.72	127.67	120.55	9	2
2	C	215	HIS	ND1-CE1-NE2	6.71	115.11	108.40	1	4
1	A	408	ARG	CA-C-N	6.71	130.59	123.08	1	1
1	A	408	ARG	C-N-CA	6.71	130.59	123.08	1	1
2	B	243	VAL	CA-C-N	6.71	129.59	120.54	9	2
2	B	243	VAL	C-N-CA	6.71	129.59	120.54	9	2
2	B	75	LEU	N-CA-C	6.71	118.67	111.36	13	3
2	B	160	GLN	N-CA-C	6.71	119.42	111.71	7	3
2	C	241	LEU	O-C-N	-6.71	114.51	120.48	9	1
2	C	236	LEU	O-C-N	6.70	129.79	122.15	6	2
2	C	223	SER	CA-C-O	6.70	127.60	120.70	14	2
2	B	134	MET	N-CA-C	6.70	118.38	111.14	4	3
1	A	326	VAL	O-C-N	-6.70	116.10	123.20	10	1
2	C	262	LEU	CB-CA-C	-6.70	100.10	110.81	10	1
2	C	119	VAL	CA-C-O	6.69	126.38	119.35	15	2
1	A	422	MET	CA-C-N	6.69	126.14	118.85	9	3
1	A	422	MET	C-N-CA	6.69	126.14	118.85	9	3
2	B	98	GLN	N-CA-CB	6.69	120.79	110.43	4	1
2	C	93	VAL	N-CA-C	6.68	117.47	110.72	13	3
1	A	473	VAL	CB-CA-C	-6.68	105.18	111.06	13	2
1	A	438	PHE	O-C-N	-6.68	115.22	123.44	11	2
2	B	165	PRO	N-CA-CB	6.68	109.92	103.51	12	1
2	C	197	ALA	CA-C-N	6.68	129.23	120.28	2	3
2	C	197	ALA	C-N-CA	6.68	129.23	120.28	2	3
2	B	245	GLU	N-CA-C	6.67	118.55	111.28	13	3
1	A	424	ASN	CA-C-O	6.67	126.39	119.05	6	2
1	A	325	THR	O-C-N	-6.67	115.24	123.44	12	2
2	C	235	ASP	N-CA-CB	-6.67	100.32	110.12	1	2
2	B	243	VAL	CB-CA-C	-6.67	103.02	112.22	9	1
1	A	494	GLU	O-C-N	-6.67	113.96	121.43	5	4
1	A	504	ASP	CA-C-O	6.67	126.38	119.05	6	1
1	A	357	ILE	N-CA-C	6.67	118.22	110.62	10	3
1	A	497	TYR	CA-C-O	-6.67	113.77	120.63	9	1
2	B	126	PHE	CA-CB-CG	6.66	120.46	113.80	7	3
2	C	116	ARG	N-CA-CB	-6.66	99.97	110.22	14	1
2	B	79	THR	N-CA-C	6.66	119.38	111.33	15	3
2	B	217	LYS	N-CA-C	6.65	118.19	111.07	8	2
2	C	151	GLY	CA-C-O	-6.65	113.90	120.75	13	3
1	A	320	ASP	CA-CB-CG	-6.65	105.95	112.60	5	2
1	A	347	ASN	CA-CB-CG	-6.65	105.95	112.60	14	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	C	211	LEU	N-CA-CB	6.65	119.84	109.94	3	1
2	C	96	LYS	CA-C-N	6.65	131.18	120.55	13	3
2	C	96	LYS	C-N-CA	6.65	131.18	120.55	13	3
1	A	389	VAL	CA-C-O	6.65	127.52	120.48	9	1
2	C	195	ARG	N-CA-C	6.64	118.52	111.28	1	3
2	C	230	LYS	CA-C-N	6.64	128.15	119.84	15	4
2	C	230	LYS	C-N-CA	6.64	128.15	119.84	15	4
2	C	190	ASP	CA-CB-CG	6.64	119.24	112.60	15	1
2	C	112	MET	N-CA-C	6.63	118.51	111.28	12	4
2	B	117	GLN	CA-C-N	6.63	129.70	120.29	12	3
2	B	117	GLN	C-N-CA	6.63	129.70	120.29	12	3
2	C	199	ARG	NH1-CZ-NH2	-6.63	110.68	119.30	12	1
2	C	77	LYS	O-C-N	-6.62	115.10	122.12	13	3
2	C	192	LEU	O-C-N	-6.62	115.10	122.12	5	2
2	C	259	THR	N-CA-C	6.62	119.10	111.02	15	3
2	C	260	LYS	N-CA-CB	6.62	119.86	110.12	14	1
1	A	399	TYR	N-CA-C	6.62	120.56	110.50	4	1
1	A	447	SER	N-CA-C	6.62	119.36	110.35	15	3
2	C	72	TRP	CA-C-N	6.62	129.04	120.44	8	3
2	C	72	TRP	C-N-CA	6.62	129.04	120.44	8	3
2	C	92	GLU	CA-C-O	6.62	127.57	120.55	15	2
1	A	444	ALA	O-C-N	-6.62	116.07	123.48	6	3
2	B	115	TYR	CB-CA-C	6.62	121.27	110.88	3	1
2	C	126	PHE	N-CA-C	6.62	118.49	111.28	5	2
2	B	98	GLN	OE1-CD-NE2	-6.61	115.99	122.60	15	2
2	C	88	LYS	N-CA-C	6.61	119.33	111.33	7	4
2	C	74	ASN	O-C-N	6.61	128.88	122.07	6	1
2	C	149	GLN	N-CA-C	6.61	118.14	111.07	6	2
2	C	130	TRP	CA-CB-CG	6.61	126.15	113.60	5	3
1	A	483	TYR	N-CA-C	6.61	119.47	109.23	8	1
2	B	72	TRP	CB-CG-CD1	6.61	136.81	126.90	8	1
2	C	83	ARG	N-CA-C	6.60	118.48	111.28	7	3
2	B	69	GLN	N-CA-CB	-6.60	100.39	110.16	4	1
1	A	446	ASP	CA-C-N	6.60	130.09	120.71	12	1
1	A	446	ASP	C-N-CA	6.60	130.09	120.71	12	1
1	A	492	LYS	N-CA-CB	6.60	121.62	111.46	2	1
2	C	198	ALA	N-CA-C	6.60	118.47	111.28	12	2
2	C	120	GLU	CB-CG-CD	-6.60	101.39	112.60	4	1
2	C	158	GLU	O-C-N	-6.59	115.13	122.12	9	2
2	B	122	TYR	CA-C-O	-6.59	113.56	120.55	7	4
2	C	131	GLN	CA-C-N	6.59	129.41	120.38	8	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	C	131	GLN	C-N-CA	6.59	129.41	120.38	8	2
2	C	177	HIS	CG-CD2-NE2	6.59	113.79	107.20	9	5
2	B	240	LEU	CA-C-O	6.59	126.66	119.15	12	1
2	C	124	ASP	CA-C-N	6.58	129.00	120.44	7	4
2	C	124	ASP	C-N-CA	6.58	129.00	120.44	7	4
2	B	146	ALA	O-C-N	-6.58	115.14	122.12	1	2
2	C	127	GLN	OE1-CD-NE2	6.58	129.18	122.60	7	3
2	C	157	HIS	CE1-NE2-CD2	-6.58	102.42	109.00	9	3
2	C	80	GLU	CA-C-N	6.58	127.42	119.99	10	3
2	C	80	GLU	C-N-CA	6.58	127.42	119.99	10	3
2	C	220	GLU	N-CA-C	6.58	118.11	111.07	14	5
1	A	421	TRP	CB-CG-CD2	6.58	136.00	126.80	3	1
2	C	77	LYS	N-CA-C	6.58	118.45	111.28	5	1
2	B	120	GLU	N-CA-C	6.57	121.69	112.75	2	3
2	B	167	GLY	CA-C-O	-6.57	113.54	120.90	10	1
1	A	339	ARG	NE-CZ-NH2	-6.57	113.29	119.20	6	2
2	C	104	PHE	N-CA-C	6.57	118.10	111.07	6	3
2	C	186	ALA	N-CA-C	6.57	121.79	113.25	9	2
2	C	253	SER	O-C-N	-6.57	115.31	122.07	2	2
2	C	245	GLU	CA-C-N	6.57	130.29	120.31	8	3
2	C	245	GLU	C-N-CA	6.57	130.29	120.31	8	3
1	A	433	ASN	N-CA-CB	6.56	119.99	110.47	13	2
2	B	70	GLU	O-C-N	-6.56	115.31	122.07	13	2
2	B	118	LYS	O-C-N	6.56	128.83	122.07	14	2
2	C	84	GLN	O-C-N	-6.56	114.67	122.15	8	2
1	A	387	HIS	CE1-NE2-CD2	-6.56	102.44	109.00	13	3
2	B	241	LEU	CA-C-N	6.56	126.14	119.19	3	2
2	B	241	LEU	C-N-CA	6.56	126.14	119.19	3	2
2	B	89	ASP	N-CA-C	6.56	118.43	111.28	3	3
2	C	190	ASP	CB-CA-C	-6.56	99.70	110.85	5	1
1	A	505	TRP	CA-C-N	6.55	129.06	120.28	12	1
1	A	505	TRP	C-N-CA	6.55	129.06	120.28	12	1
2	C	108	TRP	CB-CG-CD2	6.55	135.97	126.80	14	2
2	C	225	LEU	CA-C-O	6.55	127.51	120.24	7	2
2	B	212	ALA	O-C-N	6.55	128.81	122.07	13	1
2	C	129	LYS	CA-C-N	6.55	129.38	120.54	1	5
2	C	129	LYS	C-N-CA	6.55	129.38	120.54	1	5
1	A	466	SER	O-C-N	-6.55	116.02	123.48	5	1
2	C	248	LYS	N-CA-C	6.55	118.42	111.28	8	2
2	C	205	GLU	CA-C-O	6.54	127.44	120.70	15	1
2	B	186	ALA	N-CA-C	6.54	122.55	113.45	3	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	437	ARG	N-CA-C	6.54	120.06	109.40	12	1
2	C	61	ARG	CD-NE-CZ	6.54	133.56	124.40	3	1
1	A	330	ARG	N-CA-C	6.54	120.44	111.54	5	3
2	B	162	LYS	O-C-N	-6.54	113.50	122.46	9	1
2	C	220	GLU	N-CA-CB	6.54	119.83	110.16	2	1
2	B	205	GLU	CA-C-N	6.54	129.57	120.29	13	1
2	B	205	GLU	C-N-CA	6.54	129.57	120.29	13	1
2	B	108	TRP	CA-C-O	6.53	127.34	120.42	7	2
2	C	160	GLN	CA-C-N	6.53	129.02	120.28	12	3
2	C	160	GLN	C-N-CA	6.53	129.02	120.28	12	3
2	C	156	LEU	N-CA-CB	6.52	119.71	110.12	14	1
2	C	173	ARG	NH1-CZ-NH2	-6.52	110.82	119.30	15	1
2	B	229	ALA	CA-C-O	6.52	127.33	120.42	4	2
1	A	479	LYS	N-CA-C	6.52	119.08	108.26	15	1
1	A	409	GLY	N-CA-C	-6.52	105.76	114.95	12	2
2	B	263	ASN	CA-CB-CG	-6.52	106.08	112.60	4	3
2	B	130	TRP	CB-CG-CD2	6.52	135.92	126.80	5	1
1	A	450	PRO	CA-C-N	6.52	133.04	122.81	13	1
1	A	450	PRO	C-N-CA	6.52	133.04	122.81	13	1
2	C	239	GLY	CA-C-N	6.51	129.01	120.28	1	3
2	C	239	GLY	C-N-CA	6.51	129.01	120.28	1	3
1	A	320	ASP	CA-C-N	6.51	129.81	119.98	5	2
1	A	320	ASP	C-N-CA	6.51	129.81	119.98	5	2
2	C	181	LEU	N-CA-C	6.51	118.17	111.14	3	4
2	B	128	LYS	N-CA-C	6.51	118.37	111.28	13	3
2	B	135	GLU	CA-C-N	6.51	129.00	120.28	1	4
2	B	135	GLU	C-N-CA	6.51	129.00	120.28	1	4
2	B	86	MET	N-CA-C	6.50	118.37	111.28	11	4
2	C	175	ARG	O-C-N	-6.50	115.37	122.07	4	3
2	C	242	PRO	CA-C-N	6.50	129.37	120.46	3	4
2	C	242	PRO	C-N-CA	6.50	129.37	120.46	3	4
2	C	203	LEU	N-CA-C	6.50	118.37	111.28	5	2
1	A	360	PHE	CB-CA-C	6.50	119.41	109.34	4	1
2	B	194	GLN	N-CA-C	6.50	118.36	111.28	8	4
1	A	361	TRP	CG-CD2-CE3	-6.50	127.40	133.90	14	1
1	A	330	ARG	CA-C-N	6.50	131.94	122.46	9	1
1	A	330	ARG	C-N-CA	6.50	131.94	122.46	9	1
2	C	197	ALA	O-C-N	-6.49	113.79	122.23	15	1
2	C	101	LEU	CA-C-O	6.49	127.47	120.20	1	1
1	A	468	MET	N-CA-C	6.49	119.65	110.50	13	2
2	C	230	LYS	CA-C-O	-6.49	112.05	118.34	12	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	462	SER	O-C-N	-6.49	118.55	121.53	8	4
1	A	425	GLY	CA-C-N	6.49	131.06	122.30	3	1
1	A	425	GLY	C-N-CA	6.49	131.06	122.30	3	1
2	B	144	LEU	CA-C-N	6.49	128.97	120.28	7	1
2	B	144	LEU	C-N-CA	6.49	128.97	120.28	7	1
2	C	84	GLN	CA-C-O	6.49	127.30	120.42	8	1
2	B	147	GLU	CB-CG-CD	-6.48	101.58	112.60	10	1
2	C	128	LYS	CA-C-O	-6.48	113.97	120.90	3	1
1	A	342	TRP	CE2-CD2-CE3	-6.48	112.32	118.80	13	2
2	C	131	GLN	N-CA-C	6.48	119.16	111.71	8	3
1	A	407	GLY	O-C-N	-6.48	114.28	122.70	3	1
1	A	402	HIS	CB-CG-CD2	6.48	139.62	131.20	15	2
1	A	335	VAL	O-C-N	-6.48	116.44	123.18	15	2
2	C	175	ARG	N-CA-C	6.47	118.00	111.07	4	2
2	C	191	GLU	CA-C-N	6.47	129.48	120.29	12	3
2	C	191	GLU	C-N-CA	6.47	129.48	120.29	12	3
2	B	221	HIS	CE1-NE2-CD2	-6.46	102.54	109.00	8	2
2	C	149	GLN	CA-C-N	6.46	128.94	120.28	4	1
2	C	149	GLN	C-N-CA	6.46	128.94	120.28	4	1
2	B	124	ASP	CA-C-O	6.46	127.27	120.42	14	2
2	C	258	TYR	CA-C-N	6.46	129.46	120.29	10	3
2	C	258	TYR	C-N-CA	6.46	129.46	120.29	10	3
2	B	213	GLU	O-C-N	-6.45	115.12	122.09	10	1
2	C	220	GLU	O-C-N	6.45	128.80	122.09	6	2
2	B	250	SER	CA-C-O	-6.45	114.05	120.82	11	1
2	C	141	VAL	CA-C-N	6.45	128.90	120.26	7	2
2	C	141	VAL	C-N-CA	6.45	128.90	120.26	7	2
2	B	251	PHE	CB-CA-C	6.45	121.12	110.81	2	1
1	A	372	TYR	CA-CB-CG	6.45	125.50	113.90	10	2
2	C	111	GLU	CA-C-N	6.45	128.92	120.28	7	1
2	C	111	GLU	C-N-CA	6.45	128.92	120.28	7	1
1	A	440	GLU	N-CA-CB	-6.45	100.62	110.16	10	1
2	B	74	ASN	N-CA-C	6.44	118.30	111.28	13	1
2	C	212	ALA	CB-CA-C	6.44	121.16	110.92	8	1
1	A	487	ASN	N-CA-CB	6.44	119.93	109.95	12	2
2	B	61	ARG	O-C-N	-6.44	115.30	122.12	10	2
1	A	385	ASP	N-CA-C	6.44	120.14	112.93	10	2
2	C	197	ALA	N-CA-CB	-6.43	100.66	110.12	3	3
1	A	494	GLU	CA-C-N	6.43	126.40	119.78	4	6
1	A	494	GLU	C-N-CA	6.43	126.40	119.78	4	6
1	A	423	PRO	N-CA-CB	-6.43	97.34	103.51	3	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	157	HIS	CB-CG-CD2	-6.43	122.84	131.20	6	2
2	B	192	LEU	O-C-N	-6.43	115.31	122.12	14	2
2	B	135	GLU	N-CA-C	6.43	118.82	111.11	8	3
2	C	241	LEU	N-CA-C	6.43	122.25	113.77	3	2
2	C	214	TYR	O-C-N	-6.42	115.15	122.09	8	1
2	B	157	HIS	CA-CB-CG	-6.42	107.38	113.80	5	5
2	C	160	GLN	CA-C-O	-6.42	114.08	120.82	7	1
2	C	100	TYR	CB-CA-C	6.42	119.73	110.04	13	2
2	B	254	ALA	N-CA-C	6.41	118.27	111.28	15	2
2	C	150	GLU	CA-C-O	6.41	126.81	119.18	8	2
2	C	159	LEU	N-CA-C	6.41	118.27	111.28	12	1
1	A	494	GLU	N-CA-C	6.41	118.74	109.84	1	3
2	B	71	PHE	N-CA-CB	6.41	119.54	110.12	3	2
1	A	503	ARG	NE-CZ-NH1	-6.41	115.09	121.50	15	2
2	C	139	GLN	CB-CG-CD	6.40	123.49	112.60	3	2
2	C	183	THR	CA-C-N	6.40	128.86	120.28	9	2
2	C	183	THR	C-N-CA	6.40	128.86	120.28	9	2
1	A	467	PHE	CA-C-O	6.40	128.28	120.60	12	1
2	B	59	LYS	CA-C-N	6.39	128.85	120.28	8	3
2	B	59	LYS	C-N-CA	6.39	128.85	120.28	8	3
2	C	64	LEU	O-C-N	-6.39	114.67	122.34	13	2
1	A	441	GLU	CA-C-O	6.39	127.71	121.00	5	3
2	C	82	LEU	CA-C-N	6.39	128.75	120.44	3	2
2	C	82	LEU	C-N-CA	6.39	128.75	120.44	3	2
1	A	340	TRP	CA-C-O	6.39	128.92	121.44	10	2
2	C	100	TYR	N-CA-C	6.38	123.31	113.28	4	1
1	A	322	ASN	CA-C-N	6.38	131.52	121.56	10	2
1	A	322	ASN	C-N-CA	6.38	131.52	121.56	10	2
2	C	250	SER	O-C-N	-6.38	115.35	122.12	2	2
1	A	491	LEU	N-CA-C	6.38	120.22	111.54	6	2
2	B	203	LEU	CA-C-O	-6.38	113.78	120.55	6	1
2	C	99	PRO	O-C-N	6.38	131.26	122.64	14	2
2	B	81	GLY	CA-C-N	6.38	128.74	120.44	7	3
2	B	81	GLY	C-N-CA	6.38	128.74	120.44	7	3
2	C	221	HIS	N-CA-CB	6.38	120.04	110.22	4	1
2	C	251	PHE	CA-C-N	6.38	129.12	120.44	9	1
2	C	251	PHE	C-N-CA	6.38	129.12	120.44	9	1
2	B	126	PHE	CB-CG-CD1	6.38	131.54	120.70	14	2
1	A	508	CYS	O-C-N	-6.38	114.29	121.43	11	1
2	B	89	ASP	CA-CB-CG	6.37	118.97	112.60	8	2
2	C	69	GLN	CB-CA-C	-6.37	100.83	110.90	7	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	C	207	GLY	O-C-N	6.37	128.31	122.19	2	2
2	B	115	TYR	N-CA-C	6.37	118.02	111.14	15	3
2	B	73	ASP	O-C-N	-6.37	115.37	122.12	10	1
2	C	107	LYS	N-CA-CB	6.37	119.50	109.82	2	3
1	A	487	ASN	CB-CG-ND2	6.37	125.95	116.40	11	1
2	B	153	ARG	NH1-CZ-NH2	-6.37	111.03	119.30	1	2
2	C	215	HIS	O-C-N	-6.37	113.80	122.33	3	1
1	A	349	VAL	CA-C-N	6.37	133.70	121.54	12	2
1	A	349	VAL	C-N-CA	6.37	133.70	121.54	12	2
2	B	263	ASN	N-CA-C	6.37	118.22	111.28	13	1
1	A	459	ILE	O-C-N	-6.36	115.20	121.12	6	3
2	B	63	GLN	CA-C-N	6.36	128.81	120.28	2	1
2	B	63	GLN	C-N-CA	6.36	128.81	120.28	2	1
1	A	489	GLN	O-C-N	-6.36	115.22	122.09	7	1
1	A	402	HIS	CG-CD2-NE2	6.36	113.56	107.20	8	2
2	C	228	LYS	N-CA-C	6.36	119.03	111.71	14	4
2	C	237	ARG	CB-CG-CD	6.36	125.93	111.30	7	1
2	B	146	ALA	CA-C-O	6.36	127.16	120.42	9	2
2	B	201	GLU	CA-C-N	6.36	128.71	120.44	2	4
2	B	201	GLU	C-N-CA	6.36	128.71	120.44	2	4
2	B	199	ARG	NH1-CZ-NH2	-6.36	111.03	119.30	8	2
2	C	172	ASP	CA-C-N	6.36	129.12	120.54	14	1
2	C	172	ASP	C-N-CA	6.36	129.12	120.54	14	1
2	C	140	LYS	N-CA-C	6.36	118.21	111.28	6	2
2	C	101	LEU	N-CA-C	6.35	117.87	111.07	7	5
2	C	120	GLU	CA-C-N	6.35	125.77	118.85	10	2
2	C	120	GLU	C-N-CA	6.35	125.77	118.85	10	2
1	A	391	ASP	O-C-N	-6.35	114.96	122.96	13	1
2	B	152	ALA	O-C-N	6.34	129.64	122.22	5	1
2	C	178	VAL	CB-CA-C	-6.34	103.47	112.22	11	1
1	A	500	SER	CA-C-N	6.34	129.41	120.28	1	1
1	A	500	SER	C-N-CA	6.34	129.41	120.28	1	1
2	C	221	HIS	CE1-NE2-CD2	-6.34	102.66	109.00	14	4
2	B	128	LYS	CB-CA-C	6.34	121.63	110.85	2	1
2	B	248	LYS	CA-C-O	6.34	127.26	120.10	14	1
2	C	221	HIS	CA-C-N	6.34	128.68	120.44	12	1
2	C	221	HIS	C-N-CA	6.34	128.68	120.44	12	1
2	B	117	GLN	N-CA-CB	6.33	119.43	110.12	14	1
2	C	176	ALA	CB-CA-C	-6.33	100.28	110.79	10	2
2	B	123	LEU	N-CA-CB	6.33	119.19	110.01	15	2
2	C	247	PHE	N-CA-C	6.33	118.26	111.36	9	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	118	LYS	CA-C-O	6.33	127.25	119.97	3	2
1	A	422	MET	CG-SD-CE	-6.33	86.97	100.90	4	2
2	C	62	GLU	CA-C-O	6.33	127.13	120.42	3	1
2	C	184	HIS	ND1-CE1-NE2	6.33	114.73	108.40	6	2
1	A	391	ASP	CA-CB-CG	6.33	118.92	112.60	3	2
1	A	484	TRP	CD2-CE2-CZ2	-6.33	116.07	122.40	5	1
2	B	174	ALA	O-C-N	-6.33	115.42	122.12	5	3
1	A	476	TYR	CA-C-O	6.32	127.11	120.54	7	2
2	B	150	GLU	CA-C-O	6.32	127.46	120.82	11	1
2	B	148	LEU	O-C-N	-6.32	115.42	122.12	7	2
2	C	173	ARG	N-CA-CB	6.32	119.51	110.16	5	2
1	A	372	TYR	O-C-N	-6.32	116.63	123.26	9	1
1	A	494	GLU	CA-C-O	-6.32	113.55	120.69	1	2
2	B	215	HIS	N-CA-CB	6.32	119.51	110.16	9	1
1	A	372	TYR	CA-C-N	6.31	130.88	121.72	7	1
1	A	372	TYR	C-N-CA	6.31	130.88	121.72	7	1
2	C	226	SER	O-C-N	-6.31	115.43	122.12	3	1
1	A	359	GLN	CA-C-N	6.31	130.36	120.89	12	3
1	A	359	GLN	C-N-CA	6.31	130.36	120.89	12	3
1	A	361	TRP	N-CA-CB	6.31	121.17	111.46	5	1
2	B	171	ARG	NH1-CZ-NH2	-6.31	111.10	119.30	15	3
1	A	444	ALA	CA-C-O	6.31	127.32	120.32	2	2
1	A	428	TYR	CB-CA-C	-6.31	98.72	109.51	13	1
2	B	133	GLU	N-CA-CB	6.31	119.49	110.16	6	1
2	B	215	HIS	CE1-NE2-CD2	-6.30	102.70	109.00	7	4
2	B	221	HIS	N-CA-C	6.30	117.81	111.07	1	1
2	B	147	GLU	CA-C-N	6.30	128.72	120.28	4	3
2	B	147	GLU	C-N-CA	6.30	128.72	120.28	4	3
1	A	376	ASP	N-CA-C	-6.30	105.23	113.17	6	2
1	A	459	ILE	CA-C-O	-6.30	115.09	119.19	10	1
2	C	148	LEU	CA-C-N	6.30	128.63	120.44	13	1
2	C	148	LEU	C-N-CA	6.30	128.63	120.44	13	1
1	A	387	HIS	CA-C-O	6.30	128.04	120.99	5	2
2	B	58	SER	O-C-N	6.30	130.01	122.27	12	2
2	C	253	SER	CA-CB-OG	6.30	123.69	111.10	3	1
1	A	495	PRO	N-CD-CG	6.30	112.64	103.20	10	1
2	B	91	GLU	O-C-N	-6.29	115.45	122.12	10	2
2	B	163	LEU	N-CA-CB	6.29	120.26	110.44	13	1
2	C	256	GLU	N-CA-C	6.29	118.14	111.28	1	1
2	B	252	LEU	N-CA-C	-6.29	104.50	111.36	3	2
2	B	242	PRO	CA-C-O	6.29	128.86	119.74	15	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	C	94	LYS	O-C-N	-6.29	115.45	122.12	15	1
2	B	251	PHE	O-C-N	-6.29	115.45	122.12	13	1
2	B	237	ARG	NH1-CZ-NH2	-6.28	111.14	119.30	4	1
1	A	336	PHE	CA-C-N	6.28	131.55	122.44	10	1
1	A	336	PHE	C-N-CA	6.28	131.55	122.44	10	1
1	A	340	TRP	CE2-CD2-CE3	6.28	125.08	118.80	2	1
1	A	472	GLU	N-CA-CB	6.27	121.09	110.49	13	1
1	A	441	GLU	N-CA-C	6.27	117.91	111.14	11	4
2	C	114	LEU	CA-C-N	6.26	129.83	120.31	9	1
2	C	114	LEU	C-N-CA	6.26	129.83	120.31	9	1
1	A	505	TRP	CE2-CD2-CG	-6.26	99.69	107.20	6	1
2	C	247	PHE	CA-CB-CG	6.26	120.06	113.80	9	2
2	C	110	GLU	O-C-N	-6.26	115.33	122.09	11	1
2	B	83	ARG	N-CA-CB	6.26	119.32	110.12	9	2
2	B	212	ALA	CA-C-N	6.26	128.58	120.44	12	2
2	B	212	ALA	C-N-CA	6.26	128.58	120.44	12	2
2	C	129	LYS	CA-C-O	6.26	127.14	120.70	1	2
1	A	507	GLY	N-CA-C	6.26	122.61	113.48	4	1
1	A	443	ARG	N-CA-C	6.26	119.87	111.24	10	1
2	C	112	MET	O-C-N	6.25	128.75	122.12	11	1
1	A	431	ARG	NH1-CZ-NH2	-6.25	111.17	119.30	15	1
2	B	253	SER	N-CA-CB	6.25	119.44	110.06	4	2
2	B	156	LEU	N-CA-CB	-6.25	100.88	110.20	10	3
1	A	325	THR	CA-C-O	6.25	128.23	120.54	7	1
2	B	210	ARG	N-CA-C	6.25	117.76	111.07	13	2
2	B	258	TYR	CA-C-O	6.25	127.18	120.55	13	1
2	B	240	LEU	O-C-N	-6.25	113.53	122.41	4	1
2	B	109	GLN	N-CA-CB	6.25	119.08	110.01	5	1
2	C	192	LEU	N-CA-C	6.25	118.09	111.28	7	1
2	B	182	ARG	N-CA-C	6.25	118.17	111.36	3	1
2	C	148	LEU	O-C-N	6.25	128.74	122.12	11	2
1	A	381	PHE	CA-C-O	6.25	126.98	120.30	14	1
2	B	204	LYS	CA-C-N	6.25	128.56	120.44	1	2
2	B	204	LYS	C-N-CA	6.25	128.56	120.44	1	2
2	C	63	GLN	N-CA-C	6.25	118.09	111.28	12	3
2	C	102	ASP	CB-CA-C	6.25	120.81	110.81	7	1
1	A	317	ASN	CB-CG-ND2	6.25	125.77	116.40	10	1
2	C	79	THR	N-CA-CB	6.24	119.12	110.07	6	3
2	B	120	GLU	CA-C-O	-6.24	112.28	118.34	6	2
2	B	254	ALA	N-CA-CB	-6.24	100.69	110.30	13	1
1	A	410	LEU	O-C-N	-6.24	114.99	121.60	4	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	134	MET	CB-CA-C	6.24	121.15	110.79	9	1
2	B	117	GLN	CB-CA-C	-6.24	100.44	110.79	12	2
2	C	216	ALA	O-C-N	-6.24	115.51	122.12	1	2
2	C	261	LYS	CA-C-O	6.24	126.74	119.32	13	2
2	B	137	TYR	O-C-N	-6.23	115.04	122.15	3	1
1	A	326	VAL	N-CA-CB	-6.23	103.62	111.41	9	2
2	B	224	THR	CA-C-N	6.23	128.95	120.54	13	2
2	B	224	THR	C-N-CA	6.23	128.95	120.54	13	2
2	B	61	ARG	CA-C-N	6.23	128.63	120.28	10	1
2	B	61	ARG	C-N-CA	6.23	128.63	120.28	10	1
2	C	67	VAL	O-C-N	-6.23	115.83	121.87	12	2
1	A	382	PHE	CA-C-O	-6.23	113.93	121.28	14	1
1	A	359	GLN	CA-C-O	6.23	127.14	119.79	2	1
2	B	223	SER	N-CA-CB	6.23	119.28	110.12	2	1
2	B	182	ARG	N-CA-CB	6.23	119.04	110.01	4	1
2	B	133	GLU	CA-C-N	6.22	128.53	120.44	2	2
2	B	133	GLU	C-N-CA	6.22	128.53	120.44	2	2
1	A	343	ARG	CA-C-N	6.22	130.91	123.19	3	1
1	A	343	ARG	C-N-CA	6.22	130.91	123.19	3	1
2	B	77	LYS	CA-C-N	6.22	128.53	120.44	2	3
2	B	77	LYS	C-N-CA	6.22	128.53	120.44	2	3
2	B	175	ARG	CA-C-N	6.22	129.24	120.28	3	3
2	B	175	ARG	C-N-CA	6.22	129.24	120.28	3	3
2	C	114	LEU	N-CA-CB	6.22	119.03	110.01	13	1
1	A	362	ARG	NE-CZ-NH1	6.22	127.72	121.50	5	4
2	B	104	PHE	CA-C-N	6.21	128.61	120.28	6	1
2	B	104	PHE	C-N-CA	6.21	128.61	120.28	6	1
2	B	95	ALA	N-CA-C	6.21	118.85	111.71	5	2
2	C	131	GLN	N-CA-CB	6.21	119.20	109.94	5	2
1	A	328	MET	N-CA-CB	-6.21	99.96	110.46	7	1
1	A	378	LYS	N-CA-C	6.21	118.73	110.53	7	1
2	C	75	LEU	O-C-N	-6.21	115.54	122.12	11	3
1	A	343	ARG	O-C-N	-6.21	116.07	123.27	3	1
2	B	117	GLN	OE1-CD-NE2	-6.21	116.39	122.60	2	1
2	C	97	VAL	O-C-N	-6.21	115.83	121.91	8	1
1	A	460	PRO	CB-CA-C	6.21	121.80	111.56	13	2
2	C	70	GLU	CA-C-N	6.21	128.88	120.38	9	2
2	C	70	GLU	C-N-CA	6.21	128.88	120.38	9	2
2	C	248	LYS	O-C-N	-6.21	115.39	122.09	14	1
2	C	67	VAL	CB-CA-C	-6.21	103.92	112.24	8	1
2	B	243	VAL	O-C-N	-6.20	115.44	121.83	11	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	115	TYR	CB-CG-CD2	6.20	130.10	120.80	9	1
2	B	63	GLN	O-C-N	-6.20	113.91	122.46	2	2
1	A	497	TYR	CA-CB-CG	-6.20	102.74	113.90	4	2
2	C	115	TYR	N-CA-C	6.20	118.04	111.28	2	2
2	B	157	HIS	N-CA-C	6.20	118.03	111.28	3	1
2	C	193	ARG	NE-CZ-NH1	-6.20	115.30	121.50	10	5
2	B	215	HIS	CG-CD2-NE2	6.20	113.40	107.20	7	1
2	C	186	ALA	CA-C-O	-6.20	111.67	120.16	14	1
1	A	362	ARG	NE-CZ-NH2	-6.19	113.63	119.20	3	3
2	C	255	LEU	CB-CA-C	6.19	120.61	110.88	5	1
2	C	86	MET	CA-C-O	6.19	127.32	120.82	9	1
2	C	181	LEU	O-C-N	-6.19	115.56	122.12	15	3
1	A	418	ALA	O-C-N	-6.19	116.09	123.27	3	2
2	B	89	ASP	CB-CA-C	-6.19	101.12	110.90	2	1
2	B	178	VAL	N-CA-C	6.19	116.93	110.62	10	2
1	A	457	GLU	N-CA-C	6.19	118.26	108.67	11	2
1	A	477	PHE	O-C-N	-6.19	116.17	123.22	7	1
2	B	101	LEU	O-C-N	-6.19	115.56	122.12	1	1
1	A	502	LEU	CA-C-N	6.19	128.57	120.28	11	1
1	A	502	LEU	C-N-CA	6.19	128.57	120.28	11	1
2	B	108	TRP	N-CA-CB	6.19	118.98	110.01	15	1
2	B	177	HIS	O-C-N	-6.18	115.66	122.09	5	4
2	C	170	MET	CA-C-N	6.18	128.48	120.44	12	2
2	C	170	MET	C-N-CA	6.18	128.48	120.44	12	2
1	A	469	GLY	N-CA-C	6.18	120.45	112.54	13	2
1	A	433	ASN	CA-C-O	6.18	126.88	119.59	8	1
2	B	98	GLN	O-C-N	-6.18	114.22	121.32	1	1
2	B	114	LEU	N-CA-C	6.18	117.68	111.07	8	3
2	B	198	ALA	N-CA-CB	6.18	118.97	110.01	3	1
2	C	242	PRO	N-CA-CB	6.18	109.20	103.46	6	1
2	C	210	ARG	CD-NE-CZ	6.17	133.04	124.40	11	2
2	C	94	LYS	CA-C-O	-6.17	114.01	120.55	14	1
1	A	358	GLY	CA-C-O	6.17	126.75	120.45	8	2
1	A	396	GLU	CA-C-O	-6.17	113.97	120.70	4	3
2	B	197	ALA	CA-C-N	6.17	128.46	120.44	12	3
2	B	197	ALA	C-N-CA	6.17	128.46	120.44	12	3
1	A	400	PRO	N-CA-CB	6.17	109.39	102.60	14	1
2	B	211	LEU	CB-CA-C	6.17	121.03	110.79	2	1
1	A	415	ILE	CA-C-O	6.17	127.02	120.48	8	1
2	C	212	ALA	O-C-N	6.16	128.75	122.09	5	1
1	A	345	ARG	N-CA-C	-6.16	98.21	108.75	12	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	499	LYS	CG-CD-CE	6.16	125.47	111.30	8	1
1	A	452	ASN	CA-C-N	6.16	130.20	120.47	12	3
1	A	452	ASN	C-N-CA	6.16	130.20	120.47	12	3
2	B	153	ARG	O-C-N	6.16	128.42	122.07	8	2
2	C	260	LYS	O-C-N	6.16	130.40	122.39	7	1
2	C	169	GLU	O-C-N	-6.16	115.59	122.12	12	2
2	B	162	LYS	CA-C-O	6.16	126.48	119.27	9	2
2	B	217	LYS	O-C-N	-6.16	115.59	122.12	9	1
2	B	110	GLU	N-CA-C	6.16	118.00	111.28	12	1
2	B	161	GLU	CA-C-N	6.16	129.67	120.31	3	2
2	B	161	GLU	C-N-CA	6.16	129.67	120.31	3	2
1	A	321	GLY	N-CA-C	6.16	122.38	111.73	13	2
2	B	221	HIS	CG-CD2-NE2	6.15	113.35	107.20	8	1
1	A	447	SER	N-CA-CB	6.15	119.80	110.45	11	1
2	C	144	LEU	CA-C-N	6.15	128.84	120.54	4	6
2	C	144	LEU	C-N-CA	6.15	128.84	120.54	4	6
2	B	118	LYS	CB-CA-C	6.15	121.31	110.85	12	1
2	C	109	GLN	OE1-CD-NE2	-6.15	116.45	122.60	6	1
1	A	493	VAL	O-C-N	-6.15	116.11	122.63	14	1
2	B	134	MET	O-C-N	-6.15	115.45	122.09	6	1
2	B	88	LYS	CB-CA-C	6.14	120.53	110.88	5	1
2	C	147	GLU	N-CA-C	6.14	118.48	111.11	7	2
2	C	59	LYS	CB-CG-CD	6.14	125.43	111.30	7	1
1	A	479	LYS	O-C-N	-6.14	116.48	123.48	6	1
2	B	235	ASP	CA-CB-CG	-6.14	106.46	112.60	15	3
2	C	69	GLN	CA-CB-CG	6.14	126.38	114.10	5	1
2	B	151	GLY	O-C-N	-6.14	116.24	122.19	8	3
2	B	71	PHE	N-CA-C	6.14	118.05	111.36	11	4
2	C	159	LEU	O-C-N	-6.13	115.46	122.09	6	2
1	A	492	LYS	O-C-N	-6.13	116.86	123.42	11	2
2	B	195	ARG	NH1-CZ-NH2	-6.13	111.33	119.30	11	2
1	A	459	ILE	CA-CB-CG2	6.13	120.92	110.50	9	1
2	B	116	ARG	CA-C-O	6.13	127.05	120.55	15	2
2	B	178	VAL	CB-CA-C	-6.13	103.86	112.14	10	1
2	C	193	ARG	CA-C-N	6.13	128.40	120.44	8	4
2	C	193	ARG	C-N-CA	6.13	128.40	120.44	8	4
2	B	139	GLN	CA-C-O	6.13	127.04	120.24	6	2
2	C	174	ALA	N-CA-CB	6.12	119.12	110.12	14	2
2	B	190	ASP	N-CA-C	6.12	117.95	111.28	9	3
2	C	194	GLN	CG-CD-OE1	6.12	133.04	120.80	12	1
2	B	90	LEU	CA-C-O	6.12	128.18	121.02	3	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	C	243	VAL	N-CA-CB	6.12	117.71	110.55	11	1
1	A	392	GLU	N-CA-C	6.12	118.73	111.33	8	4
2	C	153	ARG	O-C-N	-6.11	115.77	122.07	6	1
2	B	240	LEU	CA-C-N	6.11	127.73	120.09	7	5
2	B	240	LEU	C-N-CA	6.11	127.73	120.09	7	5
2	B	173	ARG	CA-C-O	6.11	127.03	120.55	9	1
1	A	443	ARG	CA-C-O	6.11	128.67	121.40	9	1
2	B	169	GLU	O-C-N	6.11	129.67	122.34	10	1
2	C	141	VAL	N-CA-C	-6.11	104.70	113.07	11	1
2	B	204	LYS	O-C-N	-6.11	115.68	122.03	5	1
1	A	435	TYR	CA-C-O	6.11	128.61	121.46	7	2
2	B	163	LEU	O-C-N	-6.11	114.70	122.34	6	1
1	A	348	GLN	CA-C-O	6.11	127.93	120.60	8	2
2	B	261	LYS	CA-C-N	6.11	129.29	120.38	5	3
2	B	261	LYS	C-N-CA	6.11	129.29	120.38	5	3
1	A	357	ILE	O-C-N	-6.10	115.70	121.87	12	2
2	C	110	GLU	CA-C-N	6.10	128.46	120.28	6	2
2	C	110	GLU	C-N-CA	6.10	128.46	120.28	6	2
2	C	240	LEU	CA-C-N	6.10	128.43	120.26	13	3
2	C	240	LEU	C-N-CA	6.10	128.43	120.26	13	3
1	A	453	ILE	N-CA-C	6.10	117.57	110.62	6	3
1	A	435	TYR	CB-CA-C	6.09	122.12	109.38	5	1
2	C	227	GLU	N-CA-CB	6.09	119.34	110.26	2	1
2	C	65	GLY	CA-C-O	-6.09	112.81	121.52	4	2
2	B	221	HIS	CA-C-N	6.09	128.44	120.28	4	3
2	B	221	HIS	C-N-CA	6.09	128.44	120.28	4	3
2	B	102	ASP	CB-CA-C	6.09	120.34	110.96	15	2
1	A	446	ASP	CB-CA-C	6.09	120.07	109.65	12	1
1	A	507	GLY	CA-C-O	6.09	125.44	118.98	12	1
1	A	350	MET	CB-CA-C	6.09	119.82	109.53	10	1
1	A	372	TYR	N-CA-C	6.09	118.54	108.99	3	2
2	C	117	GLN	OE1-CD-NE2	-6.09	116.51	122.60	5	3
2	B	62	GLU	CA-C-O	-6.09	114.10	120.55	7	1
2	C	149	GLN	OE1-CD-NE2	6.09	128.69	122.60	8	1
1	A	371	ALA	O-C-N	-6.08	116.45	123.33	8	2
2	C	199	ARG	N-CA-C	6.08	117.91	111.28	10	4
2	B	195	ARG	CG-CD-NE	-6.08	98.61	112.00	7	2
2	C	140	LYS	CA-C-O	-6.08	114.10	120.55	7	2
2	B	116	ARG	O-C-N	-6.08	115.67	122.12	14	1
2	B	233	LEU	O-C-N	-6.08	115.67	122.12	3	1
2	C	133	GLU	CA-C-N	6.08	128.43	120.28	11	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	C	133	GLU	C-N-CA	6.08	128.43	120.28	11	1
2	B	97	VAL	N-CA-C	6.08	116.86	110.72	5	4
2	B	157	HIS	CE1-NE2-CD2	-6.08	102.92	109.00	8	4
2	B	181	LEU	CA-C-N	6.08	128.34	120.44	12	3
2	B	181	LEU	C-N-CA	6.08	128.34	120.44	12	3
1	A	355	MET	CA-C-N	6.08	127.44	119.84	13	2
1	A	355	MET	C-N-CA	6.08	127.44	119.84	13	2
2	B	239	GLY	N-CA-C	6.08	120.02	112.73	15	1
2	B	153	ARG	N-CA-C	6.08	117.70	111.14	9	3
2	B	174	ALA	CA-C-N	6.07	128.42	120.28	2	2
2	B	174	ALA	C-N-CA	6.07	128.42	120.28	2	2
2	B	264	THR	N-CA-CB	6.07	119.78	110.61	6	1
2	C	128	LYS	CA-C-N	6.07	128.70	120.44	13	4
2	C	128	LYS	C-N-CA	6.07	128.70	120.44	13	4
2	B	129	LYS	N-CA-C	6.07	117.90	111.28	10	3
2	B	161	GLU	O-C-N	-6.07	115.78	122.09	9	1
2	B	141	VAL	O-C-N	-6.07	115.98	121.87	2	1
2	C	210	ARG	CG-CD-NE	-6.07	98.65	112.00	9	1
2	C	96	LYS	CA-C-O	6.07	126.70	119.60	13	2
1	A	385	ASP	N-CA-CB	-6.07	101.77	110.57	2	1
1	A	475	THR	N-CA-CB	6.07	120.71	110.46	14	2
2	C	75	LEU	CB-CA-C	-6.07	100.72	110.79	7	1
2	B	179	ASP	CB-CA-C	6.07	120.86	110.79	8	1
1	A	387	HIS	ND1-CE1-NE2	6.06	114.46	108.40	10	4
1	A	449	TYR	N-CA-C	6.06	117.10	110.13	1	1
2	C	64	LEU	CB-CA-C	-6.06	100.32	110.56	7	1
1	A	365	PRO	N-CA-CB	6.06	108.70	103.31	4	2
2	C	227	GLU	N-CA-C	6.06	120.28	113.01	7	3
1	A	336	PHE	N-CA-C	6.06	119.35	109.24	12	1
1	A	325	THR	CA-C-N	6.05	130.86	122.93	9	1
1	A	325	THR	C-N-CA	6.05	130.86	122.93	9	1
2	C	234	GLU	CA-C-O	6.05	126.93	119.97	12	1
1	A	465	GLY	O-C-N	-6.05	118.33	123.23	15	2
2	C	103	ASP	N-CA-C	6.05	117.54	111.07	4	2
2	C	73	ASP	CB-CA-C	6.05	120.83	110.79	3	1
1	A	402	HIS	N-CA-C	6.05	118.51	110.53	8	2
2	B	191	GLU	O-C-N	-6.05	114.37	122.23	9	1
2	B	116	ARG	NH1-CZ-NH2	-6.05	111.44	119.30	11	1
2	C	148	LEU	N-CA-CB	6.05	119.01	110.12	11	1
2	C	69	GLN	CA-C-O	-6.04	114.47	120.70	7	1
2	B	71	PHE	O-C-N	-6.04	114.37	122.23	7	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	219	THR	N-CA-C	6.04	118.66	111.71	12	1
2	B	68	THR	CA-C-O	6.04	126.95	120.55	9	2
1	A	391	ASP	CA-C-N	6.04	128.70	120.54	12	2
1	A	391	ASP	C-N-CA	6.04	128.70	120.54	12	2
2	C	157	HIS	ND1-CE1-NE2	6.04	114.44	108.40	14	2
2	B	226	SER	CA-C-N	6.04	130.91	120.58	7	2
2	B	226	SER	C-N-CA	6.04	130.91	120.58	7	2
2	C	163	LEU	CA-C-N	6.04	128.35	120.26	4	1
2	C	163	LEU	C-N-CA	6.04	128.35	120.26	4	1
2	B	240	LEU	CB-CA-C	-6.04	99.15	109.65	12	1
2	C	135	GLU	N-CA-CB	6.03	118.76	110.01	6	1
2	C	56	THR	O-C-N	-6.03	114.94	122.24	8	1
2	B	119	VAL	CB-CA-C	-6.03	103.90	112.22	11	1
1	A	336	PHE	CA-CB-CG	6.03	119.83	113.80	8	3
2	C	145	ARG	CA-C-O	6.03	126.81	120.42	8	1
1	A	395	LEU	O-C-N	-6.03	115.91	123.27	14	2
2	C	66	PRO	CA-C-N	6.03	128.72	120.46	3	2
2	C	66	PRO	C-N-CA	6.03	128.72	120.46	3	2
2	C	119	VAL	CA-CB-CG1	6.03	120.65	110.40	9	1
1	A	493	VAL	CA-C-O	6.03	127.99	121.36	14	1
2	C	184	HIS	N-CA-CB	6.03	118.98	110.12	13	1
2	B	212	ALA	N-CA-C	6.02	118.64	111.71	3	1
2	B	252	LEU	N-CA-CB	6.02	118.97	110.12	11	1
1	A	481	ASN	CA-C-O	6.02	130.58	119.32	6	1
2	C	180	ALA	CA-C-N	6.01	128.66	120.54	1	1
2	C	180	ALA	C-N-CA	6.01	128.66	120.54	1	1
2	B	250	SER	CA-C-N	6.01	128.26	120.44	4	3
2	B	250	SER	C-N-CA	6.01	128.26	120.44	4	3
2	B	197	ALA	O-C-N	6.01	128.34	122.09	4	1
2	C	178	VAL	CA-C-N	6.01	128.33	120.28	11	3
2	C	178	VAL	C-N-CA	6.01	128.33	120.28	11	3
1	A	379	PHE	CA-CB-CG	-6.01	107.79	113.80	1	1
2	B	179	ASP	CA-C-N	6.01	128.25	120.44	2	1
2	B	179	ASP	C-N-CA	6.01	128.25	120.44	2	1
2	B	248	LYS	O-C-N	-6.01	115.75	122.12	5	2
2	B	94	LYS	N-CA-C	6.00	117.82	111.28	6	1
2	B	153	ARG	N-CA-CB	6.00	118.77	110.07	15	1
2	C	117	GLN	O-C-N	-6.00	115.89	122.07	9	1
2	C	144	LEU	CA-C-O	6.00	126.86	119.79	12	1
2	C	83	ARG	O-C-N	5.99	128.47	122.12	11	1
2	C	152	ALA	O-C-N	-5.99	114.90	122.27	1	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	357	ILE	CA-C-O	5.99	126.94	120.47	11	2
2	B	154	GLN	N-CA-CB	-5.99	101.32	110.01	2	1
2	B	57	PHE	N-CA-C	5.99	117.81	111.28	15	2
2	B	67	VAL	CA-C-O	-5.99	114.82	121.17	6	1
2	B	141	VAL	N-CA-CB	-5.99	102.39	110.54	9	2
1	A	383	LYS	O-C-N	-5.99	116.31	123.31	9	2
2	C	90	LEU	O-C-N	-5.99	115.78	122.12	13	1
2	C	137	TYR	N-CA-C	5.98	117.80	111.28	1	1
1	A	402	HIS	O-C-N	-5.98	115.80	122.86	14	5
2	B	94	LYS	CA-C-N	5.98	128.89	120.28	5	3
2	B	94	LYS	C-N-CA	5.98	128.89	120.28	5	3
2	C	146	ALA	CA-C-N	5.98	128.57	120.44	6	2
2	C	146	ALA	C-N-CA	5.98	128.57	120.44	6	2
1	A	381	PHE	N-CA-C	5.98	118.69	109.07	1	1
2	B	133	GLU	CA-C-O	5.98	126.73	119.38	7	1
2	B	104	PHE	N-CA-CB	5.98	118.67	110.01	3	1
1	A	505	TRP	CD2-CE3-CZ3	-5.97	110.83	118.60	6	1
1	A	399	TYR	CA-C-O	-5.97	114.45	120.96	7	2
2	C	235	ASP	N-CA-C	5.97	118.28	111.11	14	1
1	A	486	PHE	O-C-N	-5.97	116.42	123.22	6	2
1	A	486	PHE	CA-C-N	5.96	131.18	122.41	6	1
1	A	486	PHE	C-N-CA	5.96	131.18	122.41	6	1
2	B	84	GLN	N-CA-C	5.96	117.45	111.07	10	5
1	A	380	VAL	N-CA-CB	5.96	118.19	111.21	15	3
2	C	160	GLN	OE1-CD-NE2	-5.96	116.64	122.60	9	1
2	B	200	LEU	CA-C-O	5.96	127.28	120.90	15	1
2	B	154	GLN	CB-CA-C	5.96	120.24	110.88	1	1
2	C	125	ASP	CA-C-N	5.96	128.19	120.44	9	1
2	C	125	ASP	C-N-CA	5.96	128.19	120.44	9	1
2	B	101	LEU	CA-C-N	5.96	128.76	120.29	11	2
2	B	101	LEU	C-N-CA	5.96	128.76	120.29	11	2
2	B	214	TYR	CA-C-N	5.96	128.26	120.28	2	3
2	B	214	TYR	C-N-CA	5.96	128.26	120.28	2	3
2	C	100	TYR	N-CA-CB	5.96	120.56	110.49	7	1
1	A	385	ASP	CB-CA-C	5.96	120.77	110.94	1	1
2	B	217	LYS	N-CA-CB	5.96	118.97	110.16	10	1
2	C	170	MET	CB-CA-C	-5.96	98.23	110.38	7	1
1	A	330	ARG	CB-CA-C	5.95	120.18	111.73	8	3
1	A	496	GLY	N-CA-C	-5.95	106.73	115.72	8	1
2	B	229	ALA	O-C-N	-5.95	114.95	122.27	10	1
2	C	194	GLN	OE1-CD-NE2	-5.95	116.65	122.60	7	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	C	174	ALA	N-CA-C	5.95	117.77	111.28	9	2
1	A	463	PRO	N-CA-CB	5.95	108.48	103.25	6	1
2	B	214	TYR	O-C-N	-5.95	115.82	122.12	7	2
2	C	86	MET	CA-C-N	5.95	128.52	120.38	11	2
2	C	86	MET	C-N-CA	5.95	128.52	120.38	11	2
2	C	91	GLU	N-CA-CB	5.95	118.63	110.01	10	1
1	A	374	ARG	CG-CD-NE	-5.94	98.92	112.00	2	2
2	B	69	GLN	N-CA-C	5.94	117.84	111.36	11	3
1	A	439	ASN	N-CA-CB	-5.94	100.76	110.21	6	1
1	A	488	ASN	OD1-CG-ND2	-5.94	116.66	122.60	6	1
1	A	408	ARG	O-C-N	-5.94	115.51	122.81	6	3
2	C	236	LEU	CA-C-N	5.94	128.24	120.28	9	1
2	C	236	LEU	C-N-CA	5.94	128.24	120.28	9	1
2	C	204	LYS	O-C-N	-5.94	115.83	122.12	12	1
2	B	91	GLU	N-CA-C	5.93	118.23	111.11	5	2
2	B	179	ASP	CA-C-O	5.93	127.05	120.82	15	1
2	B	103	ASP	CA-C-O	5.93	126.84	120.55	8	2
2	B	215	HIS	O-C-N	5.93	128.41	122.12	2	2
2	C	216	ALA	CB-CA-C	-5.93	101.32	110.81	15	1
1	A	384	GLY	CA-C-N	5.93	132.27	122.73	1	1
1	A	384	GLY	C-N-CA	5.93	132.27	122.73	1	1
2	B	103	ASP	CA-C-N	5.93	128.71	120.29	15	4
2	B	103	ASP	C-N-CA	5.93	128.71	120.29	15	4
2	B	214	TYR	N-CA-CB	-5.92	101.11	109.94	1	1
1	A	478	TYR	CA-C-O	-5.92	113.96	120.36	13	1
2	B	210	ARG	O-C-N	5.92	128.17	122.07	15	3
2	C	187	PRO	CB-CA-C	5.92	120.75	112.11	10	1
2	C	63	GLN	CA-C-O	5.92	126.78	119.97	1	1
2	C	131	GLN	OE1-CD-NE2	-5.92	116.69	122.60	10	2
1	A	335	VAL	N-CA-C	-5.91	99.83	108.11	4	1
2	C	138	ARG	O-C-N	-5.91	115.85	122.12	9	2
2	B	199	ARG	N-CA-C	5.91	117.72	111.28	8	3
1	A	501	ALA	CB-CA-C	-5.91	99.33	110.67	10	1
2	B	255	LEU	O-C-N	-5.91	115.86	122.12	11	2
2	B	177	HIS	CB-CG-CD2	-5.90	123.53	131.20	14	2
2	B	72	TRP	CA-C-O	5.90	127.01	120.82	11	2
2	C	146	ALA	CA-C-O	5.90	126.77	120.70	15	1
2	B	221	HIS	CB-CG-ND1	5.89	131.54	122.70	5	3
2	C	58	SER	O-C-N	-5.89	114.57	122.23	4	1
2	C	128	LYS	O-C-N	5.89	128.22	122.09	3	3
2	C	206	ASN	CB-CG-ND2	5.89	125.24	116.40	6	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	C	237	ARG	NH1-CZ-NH2	-5.89	111.64	119.30	6	1
2	C	156	LEU	O-C-N	-5.89	115.88	122.12	2	3
2	C	211	LEU	CA-C-N	5.89	128.45	120.44	11	5
2	C	211	LEU	C-N-CA	5.89	128.45	120.44	11	5
1	A	427	THR	O-C-N	-5.89	116.06	123.01	3	1
1	A	488	ASN	CA-CB-CG	-5.88	106.72	112.60	7	1
2	C	143	PRO	N-CA-CB	5.88	109.75	103.52	10	1
2	C	108	TRP	CB-CG-CD1	-5.88	118.08	126.90	14	1
2	C	216	ALA	N-CA-CB	5.88	118.59	110.07	3	1
1	A	476	TYR	O-C-N	-5.88	116.06	123.05	7	1
1	A	423	PRO	N-CA-C	5.87	122.50	113.75	10	3
2	B	144	LEU	CB-CA-C	-5.87	100.87	110.85	3	1
2	B	131	GLN	O-C-N	-5.87	115.98	122.09	5	2
2	B	253	SER	CA-C-N	5.87	128.15	120.28	7	1
2	B	253	SER	C-N-CA	5.87	128.15	120.28	7	1
2	B	228	LYS	CB-CA-C	-5.87	101.05	110.79	10	1
2	B	113	GLU	O-C-N	-5.87	115.90	122.12	12	1
2	C	70	GLU	CB-CA-C	5.87	120.09	110.88	6	1
2	B	234	GLU	CA-C-N	5.87	128.06	120.44	14	1
2	B	234	GLU	C-N-CA	5.87	128.06	120.44	14	1
2	B	157	HIS	CG-CD2-NE2	5.86	113.06	107.20	2	3
1	A	405	GLU	N-CA-CB	5.86	119.66	110.46	7	1
1	A	333	MET	CB-CA-C	5.86	120.44	109.71	8	1
1	A	399	TYR	CA-CB-CG	-5.86	103.35	113.90	13	1
2	B	209	ALA	CA-C-N	5.86	128.06	120.44	15	1
2	B	209	ALA	C-N-CA	5.86	128.06	120.44	15	1
2	C	62	GLU	CA-C-N	5.86	128.13	120.28	5	1
2	C	62	GLU	C-N-CA	5.86	128.13	120.28	5	1
2	B	198	ALA	CA-C-O	-5.86	114.67	120.82	14	1
2	B	182	ARG	CA-C-N	5.86	128.13	120.28	11	4
2	B	182	ARG	C-N-CA	5.86	128.13	120.28	11	4
2	B	164	SER	N-CA-C	5.86	120.72	112.75	2	1
1	A	471	ASP	CA-C-N	5.86	132.73	121.54	4	1
1	A	471	ASP	C-N-CA	5.86	132.73	121.54	4	1
2	C	209	ALA	N-CA-C	5.86	117.74	111.36	8	1
2	C	168	GLU	O-C-N	-5.85	114.48	122.33	14	2
2	C	245	GLU	N-CA-C	5.85	118.14	111.11	9	1
2	B	63	GLN	CB-CG-CD	-5.85	102.65	112.60	10	1
1	A	488	ASN	N-CA-C	-5.85	105.64	112.89	1	1
2	B	249	VAL	CA-C-N	5.85	128.92	120.79	7	2
2	B	249	VAL	C-N-CA	5.85	128.92	120.79	7	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	154	GLN	OE1-CD-NE2	-5.85	116.75	122.60	7	2
2	C	138	ARG	NH1-CZ-NH2	-5.85	111.70	119.30	10	2
1	A	448	GLU	N-CA-C	5.85	119.18	111.28	11	1
2	B	244	LEU	CA-C-N	5.85	128.04	120.44	4	1
2	B	244	LEU	C-N-CA	5.85	128.04	120.44	4	1
1	A	427	THR	N-CA-CB	5.85	119.99	110.17	6	1
1	A	394	SER	O-C-N	-5.84	117.44	123.29	2	2
2	B	78	GLU	CA-C-N	5.84	128.04	120.44	7	1
2	B	78	GLU	C-N-CA	5.84	128.04	120.44	7	1
2	B	243	VAL	CA-C-O	5.84	127.03	120.95	3	1
1	A	484	TRP	CD2-CE3-CZ3	5.84	126.19	118.60	4	1
2	B	178	VAL	CA-C-N	5.84	128.04	120.44	15	2
2	B	178	VAL	C-N-CA	5.84	128.04	120.44	15	2
2	C	169	GLU	N-CA-CB	5.84	118.81	110.16	14	1
2	C	121	PRO	N-CA-CB	5.84	109.38	103.25	6	1
2	C	139	GLN	N-CA-C	5.84	117.64	111.28	6	2
2	B	70	GLU	CA-C-O	5.84	126.61	120.42	12	3
2	B	245	GLU	N-CA-CB	-5.84	101.54	110.12	7	1
2	B	210	ARG	CB-CG-CD	5.84	124.73	111.30	14	1
1	A	374	ARG	CD-NE-CZ	5.83	132.57	124.40	15	1
2	C	136	LEU	O-C-N	-5.83	115.40	122.22	7	1
1	A	498	PRO	CA-C-N	5.83	131.71	122.62	2	3
1	A	498	PRO	C-N-CA	5.83	131.71	122.62	2	3
2	C	196	LEU	N-CA-CB	-5.83	101.53	110.16	2	1
2	C	222	LEU	CA-C-N	5.83	129.92	120.60	9	2
2	C	222	LEU	C-N-CA	5.83	129.92	120.60	9	2
1	A	361	TRP	CA-C-N	5.83	130.76	122.72	14	2
1	A	361	TRP	C-N-CA	5.83	130.76	122.72	14	2
1	A	414	LYS	N-CA-CB	5.83	120.59	111.56	2	2
2	B	194	GLN	OE1-CD-NE2	-5.82	116.78	122.60	9	2
2	B	111	GLU	CB-CG-CD	5.82	122.50	112.60	13	1
2	B	60	LEU	N-CA-CB	-5.82	101.57	110.01	4	2
2	B	72	TRP	CB-CG-CD2	-5.82	118.65	126.80	8	1
2	B	230	LYS	CA-C-N	5.82	125.36	119.19	2	4
2	B	230	LYS	C-N-CA	5.82	125.36	119.19	2	4
1	A	341	PHE	CA-C-O	-5.82	114.82	121.40	12	2
2	C	118	LYS	N-CA-C	-5.82	105.44	112.54	10	1
2	C	93	VAL	CA-C-N	5.82	128.00	120.44	5	2
2	C	93	VAL	C-N-CA	5.82	128.00	120.44	5	2
2	C	222	LEU	N-CA-CB	5.82	118.50	110.07	3	2
2	B	231	PRO	O-C-N	5.82	129.50	122.23	10	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	C	117	GLN	CA-C-O	5.82	126.71	120.55	11	2
2	C	188	TYR	O-C-N	-5.82	115.96	122.12	10	1
2	C	84	GLN	OE1-CD-NE2	-5.82	116.78	122.60	14	1
1	A	327	ALA	O-C-N	-5.81	117.71	123.46	12	1
2	C	57	PHE	O-C-N	-5.81	115.96	122.12	15	2
1	A	366	ALA	N-CA-C	5.81	118.25	110.35	15	1
2	C	209	ALA	CA-C-N	5.81	128.38	120.54	14	4
2	C	209	ALA	C-N-CA	5.81	128.38	120.54	14	4
2	B	102	ASP	N-CA-CB	-5.80	101.57	110.16	3	1
2	B	93	VAL	CA-C-N	5.80	128.06	120.28	8	2
2	B	93	VAL	C-N-CA	5.80	128.06	120.28	8	2
2	C	212	ALA	N-CA-C	-5.80	104.87	111.14	11	1
2	B	187	PRO	CB-CA-C	-5.80	103.84	112.55	15	1
2	C	232	ALA	CA-C-O	-5.80	113.55	120.10	8	2
2	B	231	PRO	N-CA-CB	5.80	109.94	103.44	5	1
2	B	63	GLN	CA-C-O	-5.80	112.95	119.79	11	3
1	A	361	TRP	CD2-CE3-CZ3	-5.80	111.06	118.60	14	1
1	A	329	LEU	CA-C-N	5.80	130.37	122.19	8	1
1	A	329	LEU	C-N-CA	5.80	130.37	122.19	8	1
2	C	232	ALA	N-CA-CB	-5.80	101.56	110.20	4	1
2	B	131	GLN	CA-C-N	5.79	128.32	120.38	1	4
2	B	131	GLN	C-N-CA	5.79	128.32	120.38	1	4
2	C	132	GLU	CA-C-O	5.79	126.69	120.55	2	1
2	B	192	LEU	CA-C-O	5.79	126.69	120.55	14	1
2	C	246	SER	CB-CA-C	-5.79	101.75	110.90	14	1
1	A	445	VAL	O-C-N	-5.79	117.10	123.18	15	1
2	B	177	HIS	CG-CD2-NE2	5.79	112.99	107.20	7	5
1	A	509	PRO	CB-CA-C	5.79	121.12	111.56	3	2
2	C	137	TYR	O-C-N	-5.79	116.07	122.09	9	1
2	C	175	ARG	CB-CG-CD	5.79	124.62	111.30	9	1
2	B	195	ARG	CB-CG-CD	5.79	124.62	111.30	13	1
2	B	188	TYR	O-C-N	-5.79	115.15	122.27	5	3
2	B	123	LEU	CA-C-N	5.79	128.04	120.28	13	2
2	B	123	LEU	C-N-CA	5.79	128.04	120.28	13	2
2	B	210	ARG	CA-C-N	5.79	128.50	120.29	14	3
2	B	210	ARG	C-N-CA	5.79	128.50	120.29	14	3
2	C	184	HIS	CG-CD2-NE2	5.79	112.99	107.20	6	2
2	B	172	ASP	CA-C-O	5.78	126.61	119.79	4	4
2	B	199	ARG	CD-NE-CZ	5.78	132.50	124.40	11	1
2	C	211	LEU	N-CA-C	5.78	117.58	111.28	15	2
1	A	376	ASP	CA-C-O	5.78	126.48	119.31	14	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	208	GLY	O-C-N	-5.78	116.41	122.13	15	1
2	C	111	GLU	N-CA-CB	5.78	118.39	110.01	5	3
2	C	249	VAL	CA-CB-CG2	-5.77	100.59	110.40	1	1
2	B	233	LEU	CA-C-N	5.77	128.02	120.28	8	2
2	B	233	LEU	C-N-CA	5.77	128.02	120.28	8	2
1	A	496	GLY	CA-C-O	5.77	125.44	118.86	8	2
1	A	475	THR	CA-C-O	5.77	126.59	120.36	11	1
2	C	194	GLN	N-CA-C	5.77	117.24	111.07	1	2
1	A	393	ALA	N-CA-CB	-5.76	102.92	110.88	8	1
2	B	261	LYS	CA-C-O	5.76	126.66	120.55	10	1
1	A	388	TRP	N-CA-CB	5.76	120.93	111.08	3	1
2	C	55	SER	CA-C-N	5.76	131.42	122.26	6	1
2	C	55	SER	C-N-CA	5.76	131.42	122.26	6	1
2	B	146	ALA	CA-C-N	5.76	128.27	120.38	10	2
2	B	146	ALA	C-N-CA	5.76	128.27	120.38	10	2
1	A	324	ASP	N-CA-C	5.76	117.23	111.07	3	1
2	C	122	TYR	CA-C-O	5.76	126.53	120.42	5	1
2	C	219	THR	OG1-CB-CG2	-5.76	97.78	109.30	9	1
2	C	214	TYR	CA-C-N	5.76	127.92	120.44	1	2
2	C	214	TYR	C-N-CA	5.76	127.92	120.44	1	2
2	B	220	GLU	CB-CA-C	-5.76	101.84	110.88	7	1
1	A	379	PHE	CA-C-N	5.76	130.76	123.10	8	1
1	A	379	PHE	C-N-CA	5.76	130.76	123.10	8	1
1	A	455	VAL	CA-C-N	5.76	130.80	122.16	10	1
1	A	455	VAL	C-N-CA	5.76	130.80	122.16	10	1
2	B	175	ARG	CD-NE-CZ	5.76	132.46	124.40	14	1
2	C	161	GLU	N-CA-CB	-5.75	101.67	110.01	14	1
2	B	246	SER	CA-C-N	5.75	127.92	120.44	2	2
2	B	246	SER	C-N-CA	5.75	127.92	120.44	2	2
2	C	252	LEU	CA-C-O	5.75	126.65	120.55	6	3
2	C	241	LEU	CA-C-N	5.75	125.12	118.85	10	2
2	C	241	LEU	C-N-CA	5.75	125.12	118.85	10	2
2	B	109	GLN	CA-CB-CG	5.75	125.60	114.10	5	1
1	A	482	LYS	N-CA-CB	5.75	120.05	110.85	6	1
1	A	490	LYS	O-C-N	5.75	128.94	122.27	1	1
2	B	75	LEU	CA-C-N	5.75	128.30	120.54	12	3
2	B	75	LEU	C-N-CA	5.75	128.30	120.54	12	3
2	B	236	LEU	CA-C-O	5.75	126.64	120.55	2	2
2	B	103	ASP	CA-CB-CG	5.75	118.35	112.60	9	2
1	A	342	TRP	N-CA-CB	5.74	120.50	111.20	6	3
2	B	168	GLU	CA-C-N	-5.74	113.46	122.65	10	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	168	GLU	C-N-CA	-5.74	113.46	122.65	10	1
2	B	85	GLU	O-C-N	-5.74	116.03	122.12	11	1
2	C	198	ALA	N-CA-CB	-5.74	101.44	110.46	13	1
1	A	443	ARG	N-CA-CB	5.74	120.19	110.49	1	1
2	B	263	ASN	O-C-N	-5.74	116.03	122.12	2	1
2	C	93	VAL	CB-CA-C	-5.74	104.30	112.22	4	1
2	C	74	ASN	OD1-CG-ND2	-5.74	116.86	122.60	8	1
1	A	417	ALA	O-C-N	-5.74	116.85	122.99	1	2
2	C	147	GLU	CA-C-N	5.74	127.90	120.44	14	3
2	C	147	GLU	C-N-CA	5.74	127.90	120.44	14	3
1	A	452	ASN	CA-CB-CG	-5.73	106.87	112.60	15	5
1	A	361	TRP	O-C-N	-5.73	117.79	123.46	6	1
1	A	352	GLY	CA-C-O	5.73	125.65	119.06	10	1
1	A	487	ASN	O-C-N	-5.73	115.40	122.68	6	1
2	B	255	LEU	CA-C-O	5.73	126.62	120.55	7	2
2	B	244	LEU	N-CA-CB	-5.73	101.70	110.12	10	1
2	C	72	TRP	N-CA-CB	-5.73	101.70	110.01	14	1
2	B	142	GLU	CA-C-O	-5.73	112.78	118.34	7	2
2	B	242	PRO	N-CA-C	-5.73	106.06	113.57	8	2
2	C	164	SER	N-CA-C	5.73	121.29	113.16	2	1
2	C	108	TRP	CA-C-O	-5.73	114.48	120.55	8	4
2	B	216	ALA	CA-C-O	5.73	126.60	120.70	12	2
2	B	156	LEU	O-C-N	-5.73	116.05	122.12	7	1
2	C	213	GLU	N-CA-C	5.73	117.20	111.07	10	1
2	B	112	MET	CG-SD-CE	-5.73	88.30	100.90	4	1
2	C	156	LEU	CA-C-N	5.72	127.95	120.28	9	1
2	C	156	LEU	C-N-CA	5.72	127.95	120.28	9	1
1	A	354	PRO	N-CD-CG	5.72	110.66	103.80	1	2
2	B	113	GLU	N-CA-CB	-5.72	101.41	110.22	5	1
2	C	97	VAL	CA-C-O	5.72	127.23	121.17	8	1
2	B	194	GLN	CG-CD-NE2	-5.72	107.82	116.40	11	1
2	C	73	ASP	CA-C-N	5.72	127.94	120.28	15	2
2	C	73	ASP	C-N-CA	5.72	127.94	120.28	15	2
2	B	105	GLN	CA-C-N	5.72	128.22	120.44	5	1
2	B	105	GLN	C-N-CA	5.72	128.22	120.44	5	1
2	B	158	GLU	CA-C-N	5.72	127.87	120.44	14	1
2	B	158	GLU	C-N-CA	5.72	127.87	120.44	14	1
2	C	252	LEU	O-C-N	-5.71	115.92	122.09	9	2
2	B	89	ASP	CA-C-O	5.71	126.61	120.55	14	1
2	C	216	ALA	CA-C-O	5.71	126.82	120.82	10	3
1	A	500	SER	O-C-N	-5.71	115.41	123.01	6	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	C	210	ARG	CA-CB-CG	5.71	125.52	114.10	2	1
2	B	116	ARG	CB-CA-C	5.71	120.27	110.79	5	1
1	A	386	LYS	N-CA-C	5.71	118.97	110.52	8	1
1	A	342	TRP	N-CA-C	-5.71	100.83	109.85	6	2
1	A	457	GLU	CA-C-N	5.71	131.90	121.85	14	2
1	A	457	GLU	C-N-CA	5.71	131.90	121.85	14	2
2	B	97	VAL	N-CA-CB	-5.71	102.29	111.82	13	1
2	C	220	GLU	CB-CA-C	-5.71	101.15	110.85	2	1
2	C	114	LEU	O-C-N	-5.71	116.19	122.07	9	1
2	C	192	LEU	CA-C-N	5.71	127.92	120.28	15	1
2	C	192	LEU	C-N-CA	5.71	127.92	120.28	15	1
1	A	410	LEU	CA-C-O	-5.70	114.25	120.69	3	4
2	B	68	THR	N-CA-CB	5.70	118.50	110.12	9	2
2	C	102	ASP	CA-C-N	5.70	127.85	120.44	13	1
2	C	102	ASP	C-N-CA	5.70	127.85	120.44	13	1
1	A	419	LEU	N-CA-C	-5.70	97.52	107.20	1	1
2	C	261	LYS	O-C-N	-5.70	115.22	122.34	9	1
2	B	60	LEU	O-C-N	-5.70	116.17	122.09	13	2
2	C	96	LYS	O-C-N	-5.70	114.27	122.36	13	3
1	A	438	PHE	CA-C-N	5.70	130.78	122.41	7	1
1	A	438	PHE	C-N-CA	5.70	130.78	122.41	7	1
2	B	142	GLU	O-C-N	-5.69	115.22	120.51	8	3
2	B	224	THR	O-C-N	-5.69	115.66	122.15	9	2
2	B	108	TRP	CB-CG-CD2	5.69	134.77	126.80	2	1
2	C	259	THR	O-C-N	5.69	128.15	122.12	8	1
2	C	95	ALA	O-C-N	-5.69	115.67	122.15	1	1
1	A	456	TRP	N-CA-C	-5.69	101.69	109.71	3	2
2	B	142	GLU	CA-C-N	5.69	126.95	119.84	4	1
2	B	142	GLU	C-N-CA	5.69	126.95	119.84	4	1
1	A	326	VAL	N-CA-C	-5.69	99.99	108.46	12	1
2	C	206	ASN	O-C-N	-5.68	116.09	122.12	4	1
1	A	361	TRP	CB-CG-CD2	-5.68	118.84	126.80	8	1
1	A	461	GLU	N-CA-C	5.68	118.25	110.24	10	1
2	B	77	LYS	N-CA-CB	5.68	118.41	109.94	14	1
2	C	185	LEU	CA-C-N	5.68	127.88	120.26	1	1
2	C	185	LEU	C-N-CA	5.68	127.88	120.26	1	1
2	C	76	GLU	CB-CG-CD	5.68	122.26	112.60	3	1
2	C	219	THR	N-CA-CB	5.68	120.09	110.49	14	3
1	A	346	ASN	N-CA-C	5.68	119.40	111.90	12	1
2	C	239	GLY	O-C-N	-5.68	116.68	122.19	1	1
2	C	235	ASP	CB-CA-C	5.68	119.79	110.88	7	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	371	ALA	N-CA-C	5.67	117.47	108.79	6	2
2	C	76	GLU	CA-C-N	5.67	128.20	120.54	8	2
2	C	76	GLU	C-N-CA	5.67	128.20	120.54	8	2
2	B	97	VAL	CA-CB-CG1	5.67	120.05	110.40	10	2
1	A	401	LYS	CA-CB-CG	5.67	125.45	114.10	14	1
2	B	127	GLN	CG-CD-OE1	5.67	132.15	120.80	4	1
2	B	73	ASP	N-CA-CB	-5.67	101.79	110.01	7	2
2	C	60	LEU	N-CA-C	5.67	117.46	111.28	1	1
2	B	159	LEU	CA-C-N	5.67	127.88	120.28	2	1
2	B	159	LEU	C-N-CA	5.67	127.88	120.28	2	1
2	C	192	LEU	CA-C-O	5.67	126.56	120.55	5	1
1	A	507	GLY	O-C-N	-5.67	117.42	122.57	8	1
2	B	258	TYR	CB-CA-C	5.66	119.77	110.88	3	1
2	B	193	ARG	CA-CB-CG	5.66	125.42	114.10	12	1
2	B	87	SER	CA-C-N	5.66	128.14	120.44	15	1
2	B	87	SER	C-N-CA	5.66	128.14	120.44	15	1
1	A	361	TRP	CH2-CZ2-CE2	5.66	124.86	117.50	7	1
2	C	126	PHE	CA-CB-CG	-5.66	108.14	113.80	7	1
2	C	212	ALA	N-CA-CB	-5.66	101.79	110.16	14	1
2	C	134	MET	CA-C-N	5.66	128.42	120.28	14	3
2	C	134	MET	C-N-CA	5.66	128.42	120.28	14	3
1	A	504	ASP	CA-CB-CG	-5.66	106.94	112.60	10	1
2	B	232	ALA	CA-C-O	-5.66	114.56	120.55	14	1
1	A	362	ARG	NH1-CZ-NH2	-5.65	111.95	119.30	5	2
1	A	457	GLU	O-C-N	-5.65	115.50	123.01	14	1
2	B	150	GLU	N-CA-C	5.65	117.11	111.07	3	1
2	B	125	ASP	CA-CB-CG	5.65	118.25	112.60	4	1
2	C	134	MET	CG-SD-CE	-5.65	88.48	100.90	1	1
2	C	224	THR	CA-C-O	5.65	126.78	119.95	12	1
1	A	334	PHE	O-C-N	-5.64	116.58	123.19	4	1
2	C	58	SER	CB-CA-C	-5.64	101.43	110.79	15	1
2	C	55	SER	CA-CB-OG	5.64	122.37	111.10	8	1
2	B	148	LEU	CB-CA-C	5.63	120.14	110.79	1	1
1	A	432	GLY	N-CA-C	5.63	121.65	110.77	8	1
2	C	204	LYS	CA-C-N	5.63	127.83	120.28	1	1
2	C	204	LYS	C-N-CA	5.63	127.83	120.28	1	1
2	C	90	LEU	CA-C-O	-5.63	114.58	120.55	2	1
2	B	139	GLN	CA-C-N	5.63	127.76	120.44	10	1
2	B	139	GLN	C-N-CA	5.63	127.76	120.44	10	1
2	C	62	GLU	N-CA-C	5.63	118.35	111.82	7	1
1	A	355	MET	N-CA-C	-5.63	101.49	110.10	15	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	350	MET	CA-C-O	5.63	127.70	121.56	5	1
1	A	508	CYS	CB-CA-C	5.63	116.96	108.86	8	1
2	B	88	LYS	CA-C-O	-5.63	114.58	120.55	10	1
2	C	145	ARG	NH1-CZ-NH2	-5.63	111.98	119.30	14	3
2	B	57	PHE	CB-CG-CD2	5.63	130.26	120.70	5	1
2	B	155	LYS	N-CA-CB	5.63	118.23	110.07	7	1
2	B	195	ARG	N-CA-CB	5.63	118.89	110.22	11	1
1	A	397	PRO	N-CA-CB	-5.62	98.13	103.19	4	1
2	B	151	GLY	CA-C-N	5.62	128.08	120.38	9	1
2	B	151	GLY	C-N-CA	5.62	128.08	120.38	9	1
1	A	445	VAL	CA-C-O	-5.62	114.42	121.11	11	1
2	C	177	HIS	CA-CB-CG	5.62	119.42	113.80	13	1
2	B	60	LEU	CA-C-O	5.62	126.51	120.55	3	1
1	A	360	PHE	CA-C-O	5.62	126.13	119.67	4	2
2	C	182	ARG	O-C-N	-5.62	115.74	122.15	8	1
2	B	220	GLU	N-CA-CB	5.62	118.76	110.33	12	1
1	A	341	PHE	CD1-CG-CD2	-5.62	110.17	118.60	13	1
1	A	323	PHE	CA-C-N	5.62	128.26	120.29	10	2
1	A	323	PHE	C-N-CA	5.62	128.26	120.29	10	2
1	A	452	ASN	OD1-CG-ND2	-5.61	116.99	122.60	14	2
2	C	145	ARG	NE-CZ-NH1	-5.61	115.89	121.50	12	3
2	B	159	LEU	N-CA-CB	-5.61	101.87	110.12	8	1
1	A	385	ASP	CA-C-N	5.61	131.01	122.65	14	1
1	A	385	ASP	C-N-CA	5.61	131.01	122.65	14	1
2	B	245	GLU	O-C-N	-5.61	116.17	122.12	5	1
2	B	108	TRP	CG-CD1-NE1	-5.61	102.91	110.20	11	1
2	B	140	LYS	N-CA-CB	5.61	118.14	110.01	5	1
1	A	363	GLY	CA-C-N	-5.61	113.90	122.42	9	1
1	A	363	GLY	C-N-CA	-5.61	113.90	122.42	9	1
2	B	154	GLN	CA-C-N	5.61	127.79	120.28	13	1
2	B	154	GLN	C-N-CA	5.61	127.79	120.28	13	1
1	A	380	VAL	CB-CA-C	-5.61	103.30	110.98	14	1
2	C	247	PHE	CB-CG-CD2	5.60	130.23	120.70	2	1
1	A	337	LYS	CA-C-N	5.60	132.24	121.54	5	1
1	A	337	LYS	C-N-CA	5.60	132.24	121.54	5	1
1	A	439	ASN	CB-CA-C	5.60	120.52	111.05	12	1
2	C	76	GLU	N-CA-CB	-5.60	101.87	110.16	4	1
1	A	331	GLY	O-C-N	-5.60	115.51	122.34	1	2
2	B	80	GLU	O-C-N	-5.60	116.30	122.07	1	1
1	A	501	ALA	CA-C-O	5.60	126.27	119.38	9	1
2	C	100	TYR	CB-CG-CD1	5.60	129.20	120.80	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	C	157	HIS	CA-C-N	5.60	128.05	120.38	4	1
2	C	157	HIS	C-N-CA	5.60	128.05	120.38	4	1
2	C	91	GLU	CA-C-N	5.59	128.04	120.38	4	1
2	C	91	GLU	C-N-CA	5.59	128.04	120.38	4	1
1	A	411	PRO	CB-CA-C	5.59	120.79	111.56	6	1
1	A	498	PRO	O-C-N	5.59	131.73	121.10	15	1
2	B	202	ALA	CA-C-O	5.59	126.48	120.55	4	2
1	A	442	LEU	N-CA-CB	-5.59	102.90	110.67	8	1
2	C	227	GLU	CA-C-O	5.59	126.05	119.28	13	1
1	A	416	ASP	CA-C-O	-5.59	114.94	120.70	2	1
2	B	258	TYR	CB-CG-CD1	5.59	129.19	120.80	3	1
1	A	505	TRP	CA-CB-CG	5.59	124.22	113.60	7	3
2	B	57	PHE	N-CA-CB	5.59	118.53	110.20	8	2
2	C	246	SER	CA-C-O	-5.59	114.95	120.82	13	1
2	C	203	LEU	CA-C-O	5.58	126.13	119.60	3	1
1	A	423	PRO	CA-C-N	-5.58	111.83	121.66	4	1
1	A	423	PRO	C-N-CA	-5.58	111.83	121.66	4	1
2	B	220	GLU	CA-CB-CG	-5.58	102.93	114.10	7	1
2	B	232	ALA	N-CA-C	5.58	118.08	111.33	5	2
2	C	196	LEU	CA-C-N	5.58	127.70	120.44	14	2
2	C	196	LEU	C-N-CA	5.58	127.70	120.44	14	2
2	B	126	PHE	CA-C-O	5.58	126.87	120.90	14	1
2	C	114	LEU	N-CA-C	5.58	117.36	111.28	7	1
2	C	228	LYS	O-C-N	5.58	128.75	122.22	14	2
1	A	426	LYS	N-CA-CB	5.57	119.72	110.52	9	1
2	C	238	GLN	CA-C-N	5.57	126.13	120.00	1	1
2	C	238	GLN	C-N-CA	5.57	126.13	120.00	1	1
2	C	184	HIS	CA-C-N	5.57	128.30	120.28	13	1
2	C	184	HIS	C-N-CA	5.57	128.30	120.28	13	1
2	B	89	ASP	N-CA-CB	5.57	118.14	110.07	2	1
2	B	80	GLU	N-CA-CB	5.57	118.40	110.16	6	2
1	A	374	ARG	N-CA-CB	5.57	118.92	110.45	8	1
2	B	208	GLY	CA-C-O	-5.57	115.34	120.80	2	2
2	C	176	ALA	CA-C-O	-5.57	113.57	119.97	4	1
2	B	217	LYS	CA-C-N	5.57	128.77	120.31	7	2
2	B	217	LYS	C-N-CA	5.57	128.77	120.31	7	2
2	B	244	LEU	CA-C-O	-5.57	114.97	120.82	13	1
2	B	57	PHE	CB-CA-C	-5.57	101.39	110.85	1	1
1	A	486	PHE	CA-CB-CG	-5.57	108.23	113.80	6	4
1	A	463	PRO	CA-C-O	-5.57	114.99	121.34	9	3
2	B	140	LYS	CA-C-O	-5.57	114.65	120.55	7	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	C	251	PHE	CA-C-O	-5.57	114.98	120.82	10	1
1	A	368	ILE	N-CA-C	5.56	118.44	110.09	4	3
2	C	164	SER	CA-C-N	5.56	125.08	119.19	8	1
2	C	164	SER	C-N-CA	5.56	125.08	119.19	8	1
2	B	59	LYS	CA-C-O	5.56	126.31	120.42	3	1
2	C	143	PRO	O-C-N	-5.56	115.28	122.23	2	1
2	B	198	ALA	CA-C-N	5.56	127.73	120.28	4	1
2	B	198	ALA	C-N-CA	5.56	127.73	120.28	4	1
2	C	157	HIS	CA-CB-CG	5.56	119.36	113.80	4	2
2	C	84	GLN	CG-CD-NE2	5.56	124.74	116.40	13	1
2	B	137	TYR	CB-CA-C	5.56	120.01	110.79	6	1
1	A	453	ILE	CA-CB-CG2	5.56	119.94	110.50	10	1
2	B	175	ARG	CA-C-O	5.56	126.31	120.42	14	1
1	A	447	SER	CA-C-O	-5.56	115.66	121.55	15	1
2	B	234	GLU	CB-CG-CD	5.55	122.04	112.60	9	1
2	C	140	LYS	CA-C-N	5.55	128.06	120.46	7	1
2	C	140	LYS	C-N-CA	5.55	128.06	120.46	7	1
2	B	79	THR	CA-CB-CG2	5.55	119.94	110.50	9	1
2	C	110	GLU	CA-C-O	5.55	126.42	120.70	10	1
1	A	369	ASN	OD1-CG-ND2	-5.55	117.05	122.60	7	1
2	C	140	LYS	O-C-N	5.55	128.00	122.12	7	2
1	A	413	ASP	CA-C-N	5.54	131.77	121.62	3	1
1	A	413	ASP	C-N-CA	5.54	131.77	121.62	3	1
2	B	92	GLU	CA-C-O	-5.54	115.00	120.82	11	1
2	C	147	GLU	O-C-N	-5.54	116.24	122.12	4	1
1	A	395	LEU	CA-C-O	5.54	126.23	120.30	11	2
2	B	159	LEU	N-CA-C	5.54	118.03	111.33	15	1
2	C	258	TYR	CB-CG-CD1	-5.54	112.49	120.80	15	1
2	B	155	LYS	CA-C-N	5.54	127.64	120.44	1	1
2	B	155	LYS	C-N-CA	5.54	127.64	120.44	1	1
1	A	369	ASN	CB-CA-C	-5.54	99.76	109.07	7	1
1	A	379	PHE	O-C-N	-5.54	116.74	123.27	1	1
1	A	356	PRO	N-CA-C	5.54	120.18	111.38	10	2
1	A	383	LYS	CA-C-N	5.53	129.02	120.00	4	1
1	A	383	LYS	C-N-CA	5.53	129.02	120.00	4	1
2	C	133	GLU	O-C-N	-5.53	116.26	122.12	9	2
2	B	124	ASP	N-CA-C	5.53	117.31	111.28	1	1
2	C	179	ASP	CA-CB-CG	5.53	118.13	112.60	4	2
1	A	475	THR	O-C-N	-5.53	116.80	123.27	7	2
2	C	154	GLN	OE1-CD-NE2	-5.53	117.07	122.60	4	2
2	C	188	TYR	N-CA-C	-5.53	105.25	111.28	10	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	355	MET	CB-CA-C	5.53	118.31	110.02	11	1
2	B	67	VAL	CA-CB-CG1	-5.53	101.01	110.40	8	1
2	B	155	LYS	O-C-N	-5.52	116.26	122.12	13	1
1	A	319	CYS	CB-CA-C	5.52	119.95	110.01	5	1
2	C	61	ARG	CB-CA-C	5.52	120.24	110.85	14	1
1	A	341	PHE	N-CA-C	5.52	117.57	109.24	8	1
2	C	71	PHE	CG-CD1-CE1	5.52	130.08	120.70	15	1
1	A	455	VAL	CB-CA-C	-5.52	103.61	112.16	1	1
1	A	470	SER	N-CA-CB	5.52	118.20	109.82	12	1
2	B	129	LYS	CA-C-O	-5.51	115.03	120.82	4	1
1	A	487	ASN	CA-C-N	5.51	127.67	120.28	7	2
1	A	487	ASN	C-N-CA	5.51	127.67	120.28	7	2
2	B	252	LEU	CA-C-N	5.51	127.67	120.28	14	2
2	B	252	LEU	C-N-CA	5.51	127.67	120.28	14	2
2	C	96	LYS	CB-CA-C	-5.51	100.61	110.70	7	1
2	C	254	ALA	O-C-N	-5.51	114.94	122.33	6	1
1	A	456	TRP	N-CA-CB	5.51	118.23	110.24	9	1
1	A	320	ASP	N-CA-CB	-5.51	102.52	110.56	3	2
1	A	477	PHE	N-CA-C	-5.51	100.72	109.59	12	1
1	A	390	PHE	CA-C-N	5.51	131.18	122.36	13	1
1	A	390	PHE	C-N-CA	5.51	131.18	122.36	13	1
1	A	338	GLU	CB-CG-CD	5.51	121.96	112.60	1	1
2	B	249	VAL	CB-CA-C	5.51	119.62	112.24	4	1
2	C	151	GLY	O-C-N	-5.51	116.85	122.19	14	1
2	C	130	TRP	O-C-N	-5.51	116.28	122.12	4	2
2	B	133	GLU	N-CA-C	5.51	119.26	112.54	7	2
2	C	78	GLU	CB-CG-CD	5.51	121.96	112.60	11	1
1	A	362	ARG	O-C-N	-5.50	116.80	123.29	10	2
2	C	108	TRP	N-CA-CB	5.50	118.21	110.12	6	1
2	C	180	ALA	N-CA-CB	5.50	117.99	110.01	13	1
2	B	206	ASN	O-C-N	-5.50	116.37	122.09	14	1
2	C	176	ALA	O-C-N	-5.50	116.29	122.12	15	1
1	A	352	GLY	CA-C-N	5.50	132.70	121.48	2	1
1	A	352	GLY	C-N-CA	5.50	132.70	121.48	2	1
2	B	104	PHE	CA-CB-CG	5.50	119.30	113.80	3	1
1	A	473	VAL	N-CA-C	5.50	118.81	111.44	14	3
2	C	117	GLN	CB-CG-CD	-5.50	103.25	112.60	9	2
2	C	174	ALA	O-C-N	5.50	127.73	122.07	15	1
2	B	196	LEU	CA-C-O	-5.50	114.60	120.42	2	1
2	B	163	LEU	N-CA-C	-5.50	106.42	113.23	13	1
2	B	250	SER	O-C-N	-5.49	115.89	122.15	12	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	74	ASN	N-CA-CB	5.49	118.29	110.16	14	1
1	A	464	ARG	CG-CD-NE	-5.49	99.92	112.00	12	1
2	C	194	GLN	CG-CD-NE2	-5.49	108.16	116.40	12	1
2	B	58	SER	CA-C-N	5.49	127.64	120.28	10	3
2	B	58	SER	C-N-CA	5.49	127.64	120.28	10	3
1	A	323	PHE	CA-C-O	5.49	127.37	121.55	12	1
1	A	483	TYR	CA-C-N	5.49	130.51	122.77	7	1
1	A	483	TYR	C-N-CA	5.49	130.51	122.77	7	1
2	C	170	MET	CG-SD-CE	-5.49	88.82	100.90	10	1
2	C	56	THR	N-CA-CB	5.49	118.71	110.53	13	1
1	A	353	TYR	CB-CA-C	5.49	117.08	108.63	13	1
1	A	429	PHE	O-C-N	-5.49	116.69	123.33	5	1
2	C	203	LEU	O-C-N	-5.48	116.31	122.12	5	1
1	A	373	GLU	O-C-N	-5.48	116.97	123.22	14	2
2	B	214	TYR	CA-C-O	-5.48	115.03	120.90	1	1
2	B	111	GLU	N-CA-CB	-5.48	102.06	110.01	3	1
2	B	112	MET	N-CA-C	5.48	117.69	111.11	5	2
2	B	117	GLN	CA-C-O	5.48	126.36	120.55	7	1
2	C	161	GLU	O-C-N	5.48	127.93	122.12	7	1
2	C	221	HIS	CB-CG-CD2	-5.48	124.08	131.20	9	2
2	C	72	TRP	CD2-CE2-CZ2	-5.48	116.92	122.40	10	1
2	B	216	ALA	N-CA-CB	-5.48	102.07	110.12	11	1
2	B	104	PHE	CA-C-O	5.47	126.57	120.82	12	2
2	C	249	VAL	CA-C-N	5.47	128.63	120.31	1	1
2	C	249	VAL	C-N-CA	5.47	128.63	120.31	1	1
2	B	145	ARG	CD-NE-CZ	-5.47	116.74	124.40	6	1
2	C	61	ARG	CA-C-N	5.47	127.55	120.44	12	1
2	C	61	ARG	C-N-CA	5.47	127.55	120.44	12	1
2	C	154	GLN	N-CA-C	5.47	117.95	111.33	13	2
2	C	63	GLN	CG-CD-OE1	5.47	131.74	120.80	3	1
2	B	128	LYS	O-C-N	-5.47	116.40	122.09	5	1
1	A	475	THR	N-CA-C	-5.47	99.99	108.90	11	1
2	C	75	LEU	CA-C-O	5.47	126.25	119.79	14	1
2	C	255	LEU	N-CA-CB	5.47	118.16	110.12	14	1
1	A	378	LYS	O-C-N	-5.47	116.56	122.79	8	1
2	C	253	SER	CB-CA-C	-5.47	101.56	110.85	7	1
2	B	71	PHE	CA-C-N	5.47	127.61	120.28	15	1
2	B	71	PHE	C-N-CA	5.47	127.61	120.28	15	1
2	B	64	LEU	N-CA-CB	5.46	118.15	110.12	2	1
2	C	71	PHE	CA-CB-CG	5.46	119.27	113.80	6	2
2	B	181	LEU	N-CA-C	5.46	117.24	111.28	10	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	478	TYR	N-CA-C	5.46	117.80	108.90	6	1
2	B	124	ASP	O-C-N	5.46	127.91	122.12	6	1
2	C	256	GLU	CB-CG-CD	5.46	121.89	112.60	8	1
1	A	509	PRO	N-CA-CB	-5.46	97.52	103.25	3	2
2	B	223	SER	CA-C-O	-5.46	115.09	120.82	12	1
2	C	139	GLN	O-C-N	-5.46	116.34	122.12	5	2
2	B	226	SER	O-C-N	-5.46	116.45	122.07	6	2
2	B	106	LYS	CA-C-N	5.45	127.53	120.44	13	1
2	B	106	LYS	C-N-CA	5.45	127.53	120.44	13	1
2	B	176	ALA	CA-C-N	5.45	127.53	120.44	15	1
2	B	176	ALA	C-N-CA	5.45	127.53	120.44	15	1
1	A	413	ASP	N-CA-C	5.45	119.60	112.13	4	1
2	B	221	HIS	ND1-CE1-NE2	5.45	113.85	108.40	5	1
2	C	207	GLY	CA-C-O	5.45	126.30	120.30	12	1
2	B	257	GLU	CB-CA-C	-5.45	101.42	110.68	15	1
2	C	254	ALA	N-CA-CB	-5.45	102.10	110.16	9	2
1	A	431	ARG	CA-C-O	5.45	127.56	120.21	2	3
2	C	157	HIS	N-CA-CB	5.45	118.12	110.12	10	1
2	C	217	LYS	O-C-N	-5.45	115.85	122.22	10	1
2	C	258	TYR	N-CA-C	5.45	117.64	111.11	11	1
2	C	229	ALA	O-C-N	-5.44	115.00	122.46	4	1
2	C	261	LYS	CB-CA-C	5.44	119.18	110.09	9	1
1	A	373	GLU	CA-C-O	5.44	126.31	120.32	2	2
1	A	488	ASN	CA-C-N	5.44	127.84	120.44	7	2
1	A	488	ASN	C-N-CA	5.44	127.84	120.44	7	2
2	B	164	SER	O-C-N	-5.44	115.60	120.71	10	2
1	A	414	LYS	O-C-N	-5.44	117.28	123.48	10	1
2	C	192	LEU	CB-CA-C	5.43	120.09	110.85	8	1
1	A	316	PRO	N-CD-CG	5.43	111.35	103.20	2	1
2	C	209	ALA	CA-C-O	5.43	126.30	120.70	12	1
2	C	243	VAL	CA-C-N	5.43	127.50	120.44	2	1
2	C	243	VAL	C-N-CA	5.43	127.50	120.44	2	1
2	B	232	ALA	O-C-N	-5.43	116.36	122.12	15	1
2	B	225	LEU	O-C-N	-5.43	116.37	122.12	7	1
2	B	122	TYR	CA-C-N	5.43	127.55	120.28	9	3
2	B	122	TYR	C-N-CA	5.43	127.55	120.28	9	3
2	B	235	ASP	N-CA-C	5.43	116.88	111.07	2	2
1	A	418	ALA	CA-C-O	5.42	127.79	120.47	9	1
2	B	183	THR	CA-CB-OG1	5.42	117.74	109.60	14	1
1	A	403	ILE	CA-CB-CG1	5.42	119.62	110.40	5	1
1	A	448	GLU	CA-C-N	5.42	129.88	122.07	6	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	448	GLU	C-N-CA	5.42	129.88	122.07	6	1
2	C	195	ARG	CD-NE-CZ	5.42	131.99	124.40	6	1
2	C	165	PRO	CA-C-O	-5.42	111.88	119.74	15	1
2	C	214	TYR	CA-C-O	5.42	126.51	120.82	3	1
1	A	394	SER	N-CA-C	5.42	117.46	108.13	13	2
2	B	75	LEU	N-CA-CB	-5.42	102.14	110.16	13	1
2	B	175	ARG	CB-CG-CD	5.42	123.76	111.30	1	2
1	A	323	PHE	O-C-N	-5.42	116.28	122.89	3	2
2	B	107	LYS	O-C-N	-5.42	116.49	122.07	14	1
1	A	342	TRP	CD2-CE2-CZ2	-5.42	116.98	122.40	11	1
2	B	157	HIS	CB-CG-ND1	5.41	130.82	122.70	6	1
2	C	77	LYS	CA-C-N	5.41	127.53	120.28	14	1
2	C	77	LYS	C-N-CA	5.41	127.53	120.28	14	1
1	A	360	PHE	N-CA-CB	-5.41	101.80	110.19	2	2
2	C	193	ARG	CD-NE-CZ	-5.41	116.82	124.40	6	1
1	A	416	ASP	N-CA-C	5.41	117.26	111.36	7	1
1	A	456	TRP	CB-CG-CD2	5.41	134.38	126.80	5	1
2	C	76	GLU	O-C-N	5.41	127.64	122.07	6	1
2	C	224	THR	N-CA-CB	5.41	118.76	110.70	7	1
2	C	82	LEU	CA-C-O	5.41	126.19	119.97	15	1
2	B	253	SER	O-C-N	-5.41	115.98	122.15	3	1
2	C	183	THR	N-CA-CB	5.41	117.85	110.01	15	1
2	C	109	GLN	CG-CD-NE2	5.41	124.51	116.40	3	1
1	A	358	GLY	CA-C-N	5.40	130.85	122.26	8	2
1	A	358	GLY	C-N-CA	5.40	130.85	122.26	8	2
2	C	175	ARG	CA-C-N	5.40	127.52	120.28	15	2
2	C	175	ARG	C-N-CA	5.40	127.52	120.28	15	2
2	C	206	ASN	CA-C-O	5.40	126.28	120.55	15	1
2	B	199	ARG	N-CA-CB	5.40	118.06	110.12	4	1
2	B	188	TYR	CB-CG-CD2	-5.40	112.70	120.80	3	1
1	A	468	MET	O-C-N	-5.40	116.90	123.16	15	1
2	C	259	THR	CA-C-O	5.40	127.01	121.07	15	1
2	B	126	PHE	N-CA-C	-5.40	105.48	111.36	15	2
2	C	184	HIS	CB-CG-CD2	5.40	138.22	131.20	5	1
2	B	188	TYR	N-CA-CB	-5.40	102.19	110.12	7	1
1	A	354	PRO	CA-N-CD	-5.40	103.94	111.50	12	1
2	B	130	TRP	CE3-CZ3-CH2	5.40	128.12	121.10	7	1
1	A	429	PHE	CA-C-O	5.40	126.53	120.70	8	1
1	A	492	LYS	CA-C-O	5.40	127.00	121.23	9	1
2	C	202	ALA	O-C-N	5.40	128.53	122.22	14	1
2	C	63	GLN	CG-CD-NE2	5.39	124.49	116.40	2	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	C	98	GLN	CA-C-N	5.39	126.58	119.84	11	2
2	C	98	GLN	C-N-CA	5.39	126.58	119.84	11	2
1	A	445	VAL	N-CA-CB	-5.39	104.83	110.82	9	2
2	B	141	VAL	CA-CB-CG1	5.39	119.57	110.40	7	1
2	B	92	GLU	CB-CA-C	-5.39	101.84	110.79	14	1
2	C	99	PRO	N-CA-C	5.39	120.05	111.26	8	1
2	C	157	HIS	CG-CD2-NE2	5.39	112.59	107.20	15	2
1	A	486	PHE	CB-CG-CD2	-5.39	111.54	120.70	9	1
2	B	253	SER	N-CA-C	5.39	116.84	111.07	12	2
2	C	150	GLU	CB-CA-C	-5.39	102.19	110.81	11	1
2	C	233	LEU	CA-C-O	5.39	126.13	120.42	12	1
2	C	78	GLU	CA-C-N	5.39	128.28	120.79	4	2
2	C	78	GLU	C-N-CA	5.39	128.28	120.79	4	2
1	A	482	LYS	O-C-N	-5.39	116.65	123.17	5	1
2	C	155	LYS	O-C-N	-5.39	116.52	122.07	7	2
1	A	379	PHE	CB-CA-C	-5.38	101.47	110.19	4	1
2	B	56	THR	CA-C-O	-5.38	115.17	120.82	15	1
1	A	449	TYR	CA-CB-CG	-5.38	104.21	113.90	12	2
2	C	261	LYS	CG-CD-CE	5.38	123.68	111.30	6	1
1	A	451	LYS	CB-CG-CD	5.38	123.68	111.30	8	1
2	C	201	GLU	CB-CG-CD	5.38	121.75	112.60	8	1
2	B	97	VAL	O-C-N	-5.38	116.29	121.83	12	1
1	A	508	CYS	CA-C-O	-5.38	114.61	120.69	9	1
2	B	261	LYS	O-C-N	5.38	127.61	122.07	7	1
1	A	364	LEU	N-CA-C	5.38	118.37	108.69	12	1
2	C	123	LEU	CA-C-O	5.38	126.25	120.55	14	1
2	B	216	ALA	N-CA-C	5.38	117.56	111.11	6	1
2	B	157	HIS	ND1-CE1-NE2	5.38	113.78	108.40	4	3
2	B	198	ALA	CB-CA-C	-5.37	101.72	110.85	7	2
2	B	175	ARG	NH1-CZ-NH2	-5.37	112.31	119.30	14	1
2	C	128	LYS	CG-CD-CE	5.37	123.66	111.30	9	1
1	A	403	ILE	N-CA-CB	5.37	117.19	110.47	14	1
2	C	72	TRP	CB-CG-CD1	5.37	134.96	126.90	5	1
2	B	148	LEU	CA-C-O	5.37	126.24	120.55	2	1
2	C	158	GLU	N-CA-CB	5.37	118.01	110.12	2	1
1	A	392	GLU	CA-C-N	5.37	128.25	120.79	7	1
1	A	392	GLU	C-N-CA	5.37	128.25	120.79	7	1
2	C	148	LEU	CB-CA-C	5.37	119.31	110.88	14	1
2	B	148	LEU	N-CA-CB	-5.37	102.23	110.12	1	1
1	A	420	PHE	CA-CB-CG	-5.37	108.43	113.80	2	2
2	B	202	ALA	O-C-N	-5.37	116.03	122.15	7	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	460	PRO	CA-C-N	5.36	128.32	120.71	6	1
1	A	460	PRO	C-N-CA	5.36	128.32	120.71	6	1
2	C	204	LYS	CB-CA-C	-5.36	102.23	110.81	11	1
1	A	444	ALA	N-CA-CB	-5.36	102.01	111.39	1	1
2	B	194	GLN	CB-CG-CD	5.36	121.71	112.60	3	1
2	C	116	ARG	O-C-N	-5.36	116.55	122.07	13	1
1	A	370	THR	CA-C-O	5.36	126.99	120.99	12	1
2	B	64	LEU	CA-C-N	5.36	130.28	121.87	4	3
2	B	64	LEU	C-N-CA	5.36	130.28	121.87	4	3
1	A	345	ARG	CB-CG-CD	5.36	123.62	111.30	9	2
2	C	133	GLU	CB-CG-CD	5.36	121.71	112.60	15	1
2	C	213	GLU	O-C-N	5.36	127.59	122.07	3	2
2	C	100	TYR	CB-CG-CD2	-5.35	112.77	120.80	1	1
2	B	112	MET	CA-C-N	5.35	127.45	120.28	3	1
2	B	112	MET	C-N-CA	5.35	127.45	120.28	3	1
2	C	196	LEU	N-CA-C	5.35	116.80	111.07	4	1
2	B	192	LEU	CA-C-N	5.35	127.40	120.44	3	1
2	B	192	LEU	C-N-CA	5.35	127.40	120.44	3	1
1	A	502	LEU	N-CA-CB	5.35	117.77	110.01	13	1
2	C	115	TYR	O-C-N	-5.35	116.45	122.12	7	1
2	C	226	SER	N-CA-CB	5.35	119.27	110.39	10	1
2	C	223	SER	N-CA-CB	-5.35	102.31	110.07	14	1
1	A	363	GLY	CA-C-O	5.35	124.30	118.95	15	1
2	B	136	LEU	N-CA-CB	5.35	118.08	110.06	3	1
2	B	155	LYS	CA-C-O	5.35	126.09	120.42	5	1
2	B	165	PRO	CA-C-N	5.35	127.88	120.29	5	2
2	B	165	PRO	C-N-CA	5.35	127.88	120.29	5	2
1	A	346	ASN	CA-C-O	-5.35	115.34	121.54	1	1
2	C	106	LYS	O-C-N	-5.35	115.52	122.09	1	1
2	B	88	LYS	O-C-N	-5.35	116.45	122.12	13	1
2	C	203	LEU	CA-C-N	5.34	128.84	120.82	5	1
2	C	203	LEU	C-N-CA	5.34	128.84	120.82	5	1
2	B	112	MET	O-C-N	-5.34	116.06	122.15	13	1
1	A	384	GLY	CA-C-O	5.34	128.41	121.68	6	1
2	C	97	VAL	CA-C-N	5.34	127.63	120.58	3	1
2	C	97	VAL	C-N-CA	5.34	127.63	120.58	3	1
1	A	457	GLU	CA-C-O	5.34	126.98	120.62	8	2
1	A	455	VAL	N-CA-C	-5.34	105.81	113.07	3	1
2	C	99	PRO	CA-C-N	5.34	132.77	123.91	3	2
2	C	99	PRO	C-N-CA	5.34	132.77	123.91	3	2
2	C	149	GLN	CB-CG-CD	5.34	121.68	112.60	3	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	C	157	HIS	CA-C-O	5.34	126.21	120.55	3	1
2	C	93	VAL	CA-C-O	-5.34	115.19	120.85	4	1
1	A	396	GLU	O-C-N	-5.34	117.00	121.38	5	1
1	A	414	LYS	N-CA-C	5.34	117.30	109.24	6	1
2	B	206	ASN	CB-CA-C	5.34	119.35	110.81	14	1
1	A	415	ILE	N-CA-C	5.34	115.64	108.17	6	1
2	B	86	MET	CA-C-O	5.34	126.09	119.79	8	1
2	B	67	VAL	CA-C-N	5.34	128.42	120.31	6	1
2	B	67	VAL	C-N-CA	5.34	128.42	120.31	6	1
2	B	173	ARG	N-CA-CB	-5.34	102.26	110.16	6	1
1	A	501	ALA	N-CA-C	5.34	118.01	111.82	10	1
2	B	130	TRP	N-CA-C	5.33	116.78	111.07	5	1
2	C	60	LEU	CB-CA-C	5.33	119.64	110.79	15	1
2	C	140	LYS	CB-CA-C	-5.33	101.78	110.85	15	1
1	A	364	LEU	CB-CA-C	-5.33	102.98	110.13	1	1
1	A	447	SER	O-C-N	-5.33	116.25	122.81	6	1
2	B	56	THR	CA-C-N	5.33	129.62	120.71	11	1
2	B	56	THR	C-N-CA	5.33	129.62	120.71	11	1
2	C	222	LEU	CB-CA-C	-5.33	102.48	110.90	1	1
2	C	126	PHE	CA-C-N	5.33	127.73	120.54	11	1
2	C	126	PHE	C-N-CA	5.33	127.73	120.54	11	1
2	B	80	GLU	CB-CG-CD	-5.33	103.54	112.60	13	1
2	B	189	SER	CA-C-N	5.33	128.19	120.79	2	1
2	B	189	SER	C-N-CA	5.33	128.19	120.79	2	1
1	A	410	LEU	CB-CA-C	5.33	117.84	109.37	5	1
2	B	254	ALA	O-C-N	-5.33	115.19	122.33	5	1
1	A	461	GLU	CB-CG-CD	5.33	121.65	112.60	7	1
1	A	506	MET	CA-C-N	5.33	130.03	120.77	11	1
1	A	506	MET	C-N-CA	5.33	130.03	120.77	11	1
1	A	405	GLU	CG-CD-OE1	-5.33	106.15	118.40	15	1
2	C	113	GLU	N-CA-CB	5.32	117.87	109.94	13	1
2	C	250	SER	CB-CA-C	-5.32	101.96	110.79	2	1
1	A	409	GLY	CA-C-N	5.32	128.74	120.60	3	1
1	A	409	GLY	C-N-CA	5.32	128.74	120.60	3	1
2	C	127	GLN	CA-C-O	-5.32	114.91	120.55	8	1
2	C	146	ALA	N-CA-C	5.32	116.76	111.07	8	2
2	C	62	GLU	CB-CA-C	-5.32	102.53	110.88	12	1
1	A	461	GLU	CA-C-O	-5.32	115.34	121.19	1	1
1	A	375	LYS	CG-CD-CE	5.32	123.52	111.30	7	1
2	B	259	THR	CA-CB-OG1	5.32	117.57	109.60	9	1
2	C	154	GLN	CA-C-O	-5.32	114.89	120.63	10	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	260	LYS	CG-CD-CE	5.32	123.52	111.30	15	1
1	A	411	PRO	N-CA-C	5.31	123.42	112.47	8	1
2	B	213	GLU	CA-C-O	5.31	126.17	120.70	10	1
2	B	238	GLN	CA-C-O	5.31	125.91	119.38	4	1
2	C	169	GLU	CB-CG-CD	5.31	121.63	112.60	11	1
2	B	202	ALA	N-CA-CB	-5.31	102.31	110.16	7	1
2	C	102	ASP	N-CA-CB	5.31	118.47	110.30	15	1
2	C	254	ALA	CA-C-O	5.31	126.58	120.90	15	1
1	A	509	PRO	N-CA-C	5.30	123.40	112.47	14	2
1	A	346	ASN	OD1-CG-ND2	-5.30	117.30	122.60	4	1
2	C	243	VAL	CA-CB-CG2	-5.30	101.39	110.40	2	1
2	B	149	GLN	CB-CA-C	5.30	119.29	110.81	3	1
2	C	246	SER	N-CA-CB	5.30	117.76	110.07	14	1
2	C	171	ARG	N-CA-C	5.30	117.05	111.28	13	3
2	C	132	GLU	CA-CB-CG	5.30	124.69	114.10	5	1
1	A	441	GLU	CB-CA-C	5.29	119.11	110.96	5	1
2	B	170	MET	CA-C-O	5.29	125.54	119.35	10	1
2	C	64	LEU	CA-C-N	5.29	130.18	121.87	10	1
2	C	64	LEU	C-N-CA	5.29	130.18	121.87	10	1
2	C	205	GLU	CA-CB-CG	5.29	124.68	114.10	9	1
2	C	177	HIS	O-C-N	5.29	127.73	122.12	13	1
2	B	250	SER	CB-CA-C	-5.29	101.86	110.85	2	1
1	A	395	LEU	N-CA-C	5.29	122.07	110.80	3	1
2	B	57	PHE	O-C-N	-5.29	115.34	122.43	3	1
2	B	169	GLU	CA-C-N	5.29	131.11	122.65	13	1
2	B	169	GLU	C-N-CA	5.29	131.11	122.65	13	1
2	B	242	PRO	CA-C-N	5.29	128.97	120.30	15	1
2	B	242	PRO	C-N-CA	5.29	128.97	120.30	15	1
2	C	155	LYS	CA-CB-CG	-5.29	103.53	114.10	14	1
2	C	83	ARG	NH1-CZ-NH2	-5.29	112.43	119.30	5	1
1	A	448	GLU	N-CA-CB	5.29	119.42	110.49	9	2
1	A	405	GLU	CA-C-O	5.28	125.67	119.28	4	1
2	C	221	HIS	CG-CD2-NE2	5.28	112.48	107.20	14	1
2	C	253	SER	CA-C-O	5.28	126.04	119.97	3	1
2	C	174	ALA	CA-C-O	-5.28	115.27	120.82	15	1
2	B	130	TRP	CB-CG-CD1	-5.28	118.98	126.90	5	1
2	C	152	ALA	CA-C-N	5.28	127.30	120.44	6	2
2	C	152	ALA	C-N-CA	5.28	127.30	120.44	6	2
2	C	155	LYS	CA-C-N	5.28	127.66	120.54	6	1
2	C	155	LYS	C-N-CA	5.28	127.66	120.54	6	1
2	B	237	ARG	CB-CA-C	-5.28	102.37	110.81	9	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	508	CYS	N-CA-C	5.28	117.95	110.24	13	1
1	A	500	SER	N-CA-C	5.28	117.82	109.96	6	2
2	B	104	PHE	N-CA-C	-5.28	105.53	111.28	7	1
2	B	200	LEU	N-CA-C	5.27	116.71	111.07	3	3
1	A	342	TRP	CB-CA-C	-5.27	98.94	109.33	4	1
2	B	262	LEU	N-CA-CB	5.27	118.99	110.40	14	1
2	C	240	LEU	CB-CA-C	5.27	119.15	110.88	13	1
1	A	356	PRO	O-C-N	-5.27	116.58	123.06	10	1
1	A	464	ARG	N-CA-C	-5.27	106.24	113.30	11	1
2	B	200	LEU	N-CA-CB	5.26	117.64	110.01	6	1
1	A	389	VAL	CA-CB-CG1	-5.26	101.45	110.40	10	1
1	A	486	PHE	CA-C-O	-5.26	114.73	120.36	12	1
2	C	249	VAL	O-C-N	-5.26	116.77	121.87	3	1
1	A	439	ASN	CA-C-N	5.26	128.10	120.79	14	3
1	A	439	ASN	C-N-CA	5.26	128.10	120.79	14	3
2	B	227	GLU	CB-CA-C	-5.26	100.90	110.63	1	1
2	B	205	GLU	O-C-N	-5.26	116.41	122.09	2	1
1	A	406	LEU	N-CA-C	-5.26	105.72	111.82	3	2
2	B	145	ARG	N-CA-C	-5.25	106.37	112.89	8	1
2	B	92	GLU	N-CA-CB	5.25	117.84	110.12	14	1
2	C	92	GLU	CA-C-N	5.25	127.66	120.46	14	1
2	C	92	GLU	C-N-CA	5.25	127.66	120.46	14	1
2	B	199	ARG	CA-C-N	5.25	127.63	120.54	15	1
2	B	199	ARG	C-N-CA	5.25	127.63	120.54	15	1
1	A	451	LYS	O-C-N	-5.25	116.78	123.24	14	2
2	C	147	GLU	N-CA-CB	5.25	118.39	110.30	2	1
2	B	57	PHE	CA-C-N	5.25	127.75	120.29	3	1
2	B	57	PHE	C-N-CA	5.25	127.75	120.29	3	1
1	A	346	ASN	CB-CG-ND2	-5.25	108.52	116.40	8	1
2	B	242	PRO	CB-CA-C	5.25	119.78	112.11	8	1
1	A	354	PRO	N-CA-CB	5.25	108.38	102.60	12	1
1	A	344	VAL	N-CA-C	5.25	115.52	108.17	3	1
1	A	392	GLU	CB-CA-C	5.25	119.61	110.68	3	1
2	B	217	LYS	CA-C-O	5.25	126.33	120.82	3	1
2	B	224	THR	CA-CB-OG1	5.25	117.47	109.60	4	1
1	A	355	MET	CA-C-O	-5.25	115.31	120.19	7	3
2	C	69	GLN	O-C-N	-5.25	116.63	122.09	11	1
1	A	503	ARG	CD-NE-CZ	5.25	131.75	124.40	13	1
2	C	193	ARG	O-C-N	-5.25	116.63	122.09	14	1
1	A	456	TRP	CA-C-N	5.25	129.84	121.66	1	2
1	A	456	TRP	C-N-CA	5.25	129.84	121.66	1	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	C	224	THR	N-CA-C	-5.25	106.88	113.28	5	1
2	C	257	GLU	O-C-N	-5.25	116.56	122.12	13	1
2	B	247	PHE	O-C-N	-5.25	116.56	122.12	14	1
1	A	426	LYS	CA-C-O	5.24	126.02	120.36	8	3
2	B	166	LEU	CB-CA-C	-5.24	99.35	110.31	14	1
2	C	101	LEU	CA-C-N	5.24	127.83	120.28	14	1
2	C	101	LEU	C-N-CA	5.24	127.83	120.28	14	1
2	B	57	PHE	CA-C-O	5.24	126.11	120.55	15	1
1	A	454	LYS	O-C-N	-5.24	115.62	122.59	12	1
2	C	204	LYS	CA-C-O	-5.24	114.86	120.42	15	1
2	C	221	HIS	CB-CG-ND1	5.24	130.56	122.70	9	1
1	A	502	LEU	CA-C-O	-5.24	115.00	120.55	6	1
2	C	215	HIS	N-CA-CB	-5.24	102.41	110.01	6	1
2	B	101	LEU	N-CA-CB	-5.24	102.41	110.01	10	1
2	B	85	GLU	CB-CA-C	5.24	119.48	110.79	6	1
2	C	212	ALA	CA-C-O	5.24	126.83	121.07	8	1
1	A	467	PHE	CB-CA-C	5.23	119.73	110.16	3	1
1	A	431	ARG	O-C-N	-5.23	116.34	123.24	15	2
2	B	211	LEU	CA-C-N	5.23	127.24	120.44	13	2
2	B	211	LEU	C-N-CA	5.23	127.24	120.44	13	2
2	B	252	LEU	CA-C-O	5.23	126.28	120.63	1	1
2	C	170	MET	CA-C-O	-5.23	115.01	120.55	14	2
2	C	170	MET	N-CA-CB	5.23	117.59	110.01	9	1
2	B	132	GLU	O-C-N	-5.23	116.58	122.12	1	1
2	B	237	ARG	CD-NE-CZ	-5.23	117.08	124.40	9	1
2	B	248	LYS	N-CA-CB	5.22	117.80	110.12	4	1
1	A	480	GLY	CA-C-N	5.22	135.32	125.66	11	2
1	A	480	GLY	C-N-CA	5.22	135.32	125.66	11	2
2	C	134	MET	CA-C-O	5.22	126.30	120.82	4	1
2	B	78	GLU	CB-CA-C	-5.22	101.97	110.85	5	1
2	B	210	ARG	CD-NE-CZ	-5.22	117.09	124.40	11	2
2	C	114	LEU	CA-C-O	5.22	126.08	120.70	3	1
2	C	169	GLU	N-CA-C	5.22	116.97	111.28	4	1
2	C	229	ALA	N-CA-CB	-5.22	102.46	110.44	6	1
2	C	207	GLY	N-CA-C	5.22	120.47	114.16	8	1
2	C	224	THR	O-C-N	-5.22	115.82	122.34	11	1
2	B	220	GLU	CA-C-N	5.22	127.22	120.44	12	1
2	B	220	GLU	C-N-CA	5.22	127.22	120.44	12	1
1	A	332	GLU	CA-C-N	-5.21	115.26	122.30	10	1
1	A	332	GLU	C-N-CA	-5.21	115.26	122.30	10	1
2	C	106	LYS	CA-C-N	5.21	127.69	120.29	14	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	C	106	LYS	C-N-CA	5.21	127.69	120.29	14	1
1	A	381	PHE	N-CA-CB	-5.21	102.39	110.57	1	1
1	A	324	ASP	O-C-N	5.21	127.44	122.07	3	1
2	C	76	GLU	CA-C-O	-5.21	114.90	120.42	2	1
2	C	59	LYS	N-CA-CB	5.21	117.78	110.12	8	1
2	C	139	GLN	CA-C-N	5.21	127.26	120.28	7	1
2	C	139	GLN	C-N-CA	5.21	127.26	120.28	7	1
2	C	74	ASN	N-CA-CB	5.21	117.87	110.16	13	1
2	C	178	VAL	N-CA-C	5.20	115.93	110.62	10	2
2	C	210	ARG	N-CA-CB	-5.20	102.47	110.12	2	1
1	A	410	LEU	N-CA-CB	-5.20	103.70	109.74	5	1
1	A	381	PHE	O-C-N	-5.20	117.23	123.27	9	1
1	A	432	GLY	O-C-N	-5.20	116.08	122.58	9	1
1	A	421	TRP	CZ3-CH2-CZ2	-5.20	114.74	121.50	14	1
2	B	193	ARG	CA-C-N	5.20	127.25	120.28	14	1
2	B	193	ARG	C-N-CA	5.20	127.25	120.28	14	1
2	C	256	GLU	N-CA-CB	5.20	117.55	110.01	14	1
2	C	108	TRP	CZ3-CH2-CZ2	-5.20	114.74	121.50	11	1
2	C	165	PRO	O-C-N	5.20	128.73	122.23	15	1
1	A	392	GLU	CA-C-O	5.20	126.06	120.55	2	1
2	B	82	LEU	N-CA-CB	5.20	117.76	110.12	2	2
1	A	451	LYS	CA-C-O	-5.20	115.36	121.44	3	1
2	B	133	GLU	CB-CA-C	5.20	119.69	110.85	13	1
1	A	435	TYR	CA-CB-CG	5.20	123.25	113.90	4	1
2	B	178	VAL	CA-C-O	-5.20	115.86	121.27	5	2
2	B	134	MET	CA-C-N	5.20	127.67	120.29	1	1
2	B	134	MET	C-N-CA	5.20	127.67	120.29	1	1
2	C	86	MET	CG-SD-CE	-5.20	89.47	100.90	2	1
1	A	485	LYS	CA-C-N	5.20	129.31	122.30	7	1
1	A	485	LYS	C-N-CA	5.20	129.31	122.30	7	1
1	A	353	TYR	CA-CB-CG	-5.20	104.55	113.90	10	2
1	A	422	MET	O-C-N	-5.20	115.61	120.55	11	1
2	C	132	GLU	CA-C-N	5.20	127.55	120.54	11	1
2	C	132	GLU	C-N-CA	5.20	127.55	120.54	11	1
1	A	343	ARG	CD-NE-CZ	-5.20	117.13	124.40	14	1
1	A	348	GLN	N-CA-CB	-5.20	103.51	111.56	15	1
2	C	143	PRO	CA-C-O	5.20	125.77	118.86	15	1
2	B	199	ARG	CA-C-O	5.19	126.06	120.55	4	1
2	B	73	ASP	CA-C-O	5.19	126.05	120.55	2	1
2	C	169	GLU	CA-C-N	-5.19	113.69	120.44	6	1
2	C	169	GLU	C-N-CA	-5.19	113.69	120.44	6	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	189	SER	CA-C-O	-5.19	115.37	120.82	6	1
1	A	417	ALA	N-CA-C	5.19	116.73	108.79	7	1
2	B	245	GLU	CA-C-O	-5.19	115.05	120.55	9	1
1	A	370	THR	CA-C-N	5.19	130.71	122.62	12	1
1	A	370	THR	C-N-CA	5.19	130.71	122.62	12	1
2	B	192	LEU	N-CA-CB	-5.19	102.48	110.16	8	1
2	B	161	GLU	CB-CA-C	5.19	119.11	110.81	12	1
2	B	67	VAL	N-CA-C	5.19	115.40	110.42	7	1
2	C	58	SER	N-CA-CB	5.18	117.93	110.20	3	1
2	B	184	HIS	CB-CG-CD2	-5.18	124.46	131.20	7	1
2	B	153	ARG	CA-C-O	5.18	126.05	120.55	14	1
2	B	90	LEU	O-C-N	-5.18	115.93	122.20	3	1
1	A	350	MET	CA-CB-CG	-5.18	103.73	114.10	12	1
1	A	442	LEU	CA-C-N	5.18	129.77	122.46	12	1
1	A	442	LEU	C-N-CA	5.18	129.77	122.46	12	1
2	C	198	ALA	O-C-N	5.18	127.61	122.12	5	1
2	C	244	LEU	CA-C-N	5.18	127.17	120.44	7	1
2	C	244	LEU	C-N-CA	5.18	127.17	120.44	7	1
2	B	116	ARG	N-CA-CB	5.18	118.31	110.28	11	1
1	A	396	GLU	N-CA-CB	5.18	117.28	110.29	3	1
2	C	56	THR	CA-CB-OG1	5.18	117.37	109.60	4	1
2	C	249	VAL	N-CA-CB	5.18	117.58	110.54	10	1
2	C	71	PHE	CD1-CG-CD2	-5.18	110.83	118.60	15	1
1	A	362	ARG	CB-CA-C	5.18	118.70	109.38	13	2
2	C	72	TRP	N-CA-C	5.17	116.61	111.07	8	1
2	C	95	ALA	N-CA-C	5.17	116.92	111.28	12	3
1	A	495	PRO	N-CA-CB	5.17	108.68	103.25	2	2
1	A	405	GLU	O-C-N	5.17	128.63	122.27	9	1
1	A	383	LYS	N-CA-CB	5.17	119.20	110.77	10	2
2	C	173	ARG	CA-C-N	5.17	127.21	120.28	4	1
2	C	173	ARG	C-N-CA	5.17	127.21	120.28	4	1
1	A	420	PHE	CA-C-O	5.17	126.58	120.69	5	1
2	B	132	GLU	CA-C-O	5.17	126.21	120.63	8	1
2	B	102	ASP	CA-C-N	5.17	127.16	120.44	12	2
2	B	102	ASP	C-N-CA	5.17	127.16	120.44	12	2
2	B	179	ASP	N-CA-C	-5.17	105.33	111.69	10	1
2	B	244	LEU	CD1-CG-CD2	-5.17	99.43	110.80	13	1
2	B	124	ASP	N-CA-CB	5.17	117.72	110.12	15	1
2	B	198	ALA	N-CA-C	5.17	117.31	111.11	15	1
2	B	149	GLN	CA-C-N	5.17	129.40	121.19	14	1
2	B	149	GLN	C-N-CA	5.17	129.40	121.19	14	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	C	83	ARG	CG-CD-NE	-5.17	100.64	112.00	13	1
1	A	388	TRP	CD2-CE2-CZ2	5.16	127.56	122.40	1	1
2	B	64	LEU	CA-C-O	5.16	125.89	120.42	4	1
2	B	263	ASN	OD1-CG-ND2	5.16	127.76	122.60	10	1
2	B	108	TRP	CD2-CE2-CZ2	-5.16	117.24	122.40	11	1
2	B	116	ARG	CA-CB-CG	5.16	124.42	114.10	1	1
1	A	361	TRP	CB-CG-CD1	5.16	134.64	126.90	8	1
2	C	119	VAL	CA-C-N	5.16	128.61	120.97	8	1
2	C	119	VAL	C-N-CA	5.16	128.61	120.97	8	1
1	A	377	GLY	N-CA-C	-5.16	107.67	114.95	13	1
1	A	502	LEU	N-CA-C	5.16	116.59	111.07	15	1
2	C	68	THR	O-C-N	-5.16	116.76	122.07	2	1
2	B	239	GLY	O-C-N	5.16	128.51	122.68	6	1
1	A	464	ARG	O-C-N	-5.16	115.66	122.42	8	1
1	A	403	ILE	O-C-N	5.16	127.08	121.87	12	1
2	B	96	LYS	O-C-N	-5.16	116.65	122.12	4	1
2	C	90	LEU	CA-C-N	5.16	127.61	120.29	9	1
2	C	90	LEU	C-N-CA	5.16	127.61	120.29	9	1
1	A	337	LYS	O-C-N	-5.16	117.07	123.36	4	1
2	C	234	GLU	CB-CG-CD	5.16	121.36	112.60	4	1
1	A	351	ASP	CA-C-N	5.16	131.52	121.41	14	1
1	A	351	ASP	C-N-CA	5.16	131.52	121.41	14	1
2	B	210	ARG	CA-C-O	-5.15	114.04	119.97	14	2
2	B	180	ALA	CA-C-N	5.15	127.45	120.44	4	1
2	B	180	ALA	C-N-CA	5.15	127.45	120.44	4	1
2	B	141	VAL	CG1-CB-CG2	-5.15	99.46	110.80	9	1
2	B	117	GLN	CB-CG-CD	5.15	121.36	112.60	11	2
2	B	161	GLU	CA-C-O	5.15	126.41	120.90	9	1
2	B	84	GLN	CB-CG-CD	5.15	121.36	112.60	11	1
1	A	491	LEU	CA-C-O	-5.15	114.20	120.12	1	2
2	C	58	SER	CA-C-N	5.15	127.18	120.28	8	1
2	C	58	SER	C-N-CA	5.15	127.18	120.28	8	1
2	C	91	GLU	CB-CG-CD	5.15	121.35	112.60	9	1
2	C	157	HIS	CB-CG-CD2	-5.15	124.51	131.20	11	1
1	A	505	TRP	CH2-CZ2-CE2	5.15	124.19	117.50	13	1
2	B	156	LEU	CB-CA-C	5.15	119.33	110.79	14	1
2	B	173	ARG	O-C-N	-5.14	116.67	122.12	9	2
2	B	184	HIS	CA-C-O	5.14	126.22	120.82	1	1
2	C	55	SER	O-C-N	-5.14	114.77	123.00	2	1
2	B	219	THR	CA-CB-CG2	5.14	119.25	110.50	4	1
2	C	147	GLU	CB-CG-CD	5.14	121.35	112.60	4	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	C	116	ARG	CD-NE-CZ	5.14	131.60	124.40	3	1
1	A	494	GLU	CB-CA-C	5.14	117.89	109.46	10	1
2	C	188	TYR	N-CA-CB	-5.14	102.31	110.28	8	1
1	A	505	TRP	CB-CG-CD1	5.14	134.61	126.90	13	1
2	C	247	PHE	CB-CG-CD1	-5.14	111.96	120.70	2	1
2	C	175	ARG	CB-CA-C	-5.14	102.11	110.85	14	2
2	C	89	ASP	CA-C-O	5.14	125.94	120.24	13	1
2	C	218	ALA	O-C-N	-5.14	116.78	122.07	3	1
1	A	421	TRP	CA-CB-CG	5.14	123.36	113.60	4	1
2	B	134	MET	CG-SD-CE	-5.14	89.60	100.90	15	2
2	B	175	ARG	O-C-N	-5.14	116.29	122.15	14	1
2	C	236	LEU	N-CA-CB	-5.13	102.39	110.30	1	1
2	B	122	TYR	CA-CB-CG	5.13	123.14	113.90	3	1
2	C	78	GLU	CB-CA-C	-5.13	102.82	110.88	4	1
2	B	166	LEU	N-CA-CB	5.13	117.76	110.16	5	1
2	C	137	TYR	CB-CA-C	-5.13	102.27	110.79	8	1
1	A	338	GLU	O-C-N	-5.13	115.76	122.59	9	1
1	A	348	GLN	CA-C-N	5.13	127.38	120.50	9	1
1	A	348	GLN	C-N-CA	5.13	127.38	120.50	9	1
1	A	324	ASP	CA-C-N	-5.13	113.26	121.58	11	1
1	A	324	ASP	C-N-CA	-5.13	113.26	121.58	11	1
2	B	226	SER	CA-C-O	5.13	126.21	120.82	6	2
1	A	394	SER	CA-C-N	5.13	128.00	120.71	4	2
1	A	394	SER	C-N-CA	5.13	128.00	120.71	4	2
1	A	454	LYS	N-CA-C	-5.13	106.97	113.18	5	1
2	B	209	ALA	N-CA-CB	-5.13	102.58	110.12	8	1
2	C	231	PRO	CA-C-N	5.13	127.11	120.44	12	1
2	C	231	PRO	C-N-CA	5.13	127.11	120.44	12	1
1	A	412	THR	N-CA-CB	5.13	118.06	110.53	2	1
1	A	347	ASN	CA-C-O	5.13	127.44	119.96	5	1
2	B	186	ALA	CA-C-N	5.12	124.44	118.85	4	2
2	B	186	ALA	C-N-CA	5.12	124.44	118.85	4	2
2	B	233	LEU	N-CA-C	5.12	116.87	111.28	8	1
1	A	460	PRO	N-CD-CG	5.12	110.89	103.20	11	1
2	B	139	GLN	CB-CG-CD	5.12	121.31	112.60	2	1
2	C	177	HIS	ND1-CG-CD2	-5.12	100.98	106.10	8	1
1	A	325	THR	N-CA-CB	5.12	119.23	110.57	9	1
2	B	261	LYS	N-CA-C	5.12	116.86	111.28	1	2
2	B	215	HIS	N-CA-C	5.12	116.86	111.28	2	2
2	B	130	TRP	CZ3-CH2-CZ2	5.12	128.15	121.50	12	1
2	C	206	ASN	CB-CA-C	-5.12	102.29	110.79	14	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	C	257	GLU	CB-CA-C	-5.12	102.85	110.88	9	1
2	C	160	GLN	CB-CG-CD	-5.12	103.90	112.60	14	1
2	B	218	ALA	CA-C-O	-5.12	115.13	120.55	15	1
2	B	110	GLU	N-CA-CB	5.11	117.64	110.12	12	1
1	A	474	PHE	CA-C-O	5.11	126.54	120.66	12	1
2	C	56	THR	CB-CA-C	-5.11	101.53	110.17	3	1
2	C	200	LEU	O-C-N	-5.11	116.70	122.12	14	1
2	B	140	LYS	N-CA-C	5.11	117.58	111.71	3	1
1	A	433	ASN	O-C-N	-5.11	116.07	122.35	14	2
2	C	179	ASP	CA-C-N	5.11	127.08	120.44	10	1
2	C	179	ASP	C-N-CA	5.11	127.08	120.44	10	1
2	C	248	LYS	CA-C-O	5.11	125.96	120.70	14	1
2	B	70	GLU	CB-CG-CD	5.11	121.28	112.60	7	1
2	C	211	LEU	CB-CA-C	5.11	118.89	110.88	10	1
2	B	60	LEU	CA-C-N	5.11	127.12	120.28	12	1
2	B	60	LEU	C-N-CA	5.11	127.12	120.28	12	1
2	B	205	GLU	CB-CG-CD	5.11	121.28	112.60	12	1
2	B	83	ARG	CA-C-N	5.10	127.12	120.28	3	1
2	B	83	ARG	C-N-CA	5.10	127.12	120.28	3	1
2	B	89	ASP	O-C-N	-5.10	116.71	122.12	14	1
2	B	140	LYS	O-C-N	-5.10	116.81	122.07	14	1
1	A	419	LEU	CB-CA-C	5.10	117.76	111.43	1	1
2	C	175	ARG	CA-C-O	-5.10	115.46	120.82	2	1
1	A	443	ARG	CA-C-N	5.10	130.48	122.21	15	1
1	A	443	ARG	C-N-CA	5.10	130.48	122.21	15	1
2	B	238	GLN	OE1-CD-NE2	-5.10	117.50	122.60	5	1
2	B	209	ALA	CA-C-O	5.10	126.17	120.82	11	1
1	A	334	PHE	CA-C-O	5.10	125.99	120.43	3	1
2	B	156	LEU	CA-C-N	5.10	127.53	120.29	4	1
2	B	156	LEU	C-N-CA	5.10	127.53	120.29	4	1
2	B	125	ASP	N-CA-CB	-5.10	102.62	110.01	13	2
2	B	180	ALA	N-CA-CB	-5.10	102.63	110.12	12	1
2	C	130	TRP	N-CA-C	5.09	117.24	111.02	5	3
2	C	206	ASN	N-CA-C	5.09	116.52	111.07	10	2
1	A	392	GLU	N-CA-CB	5.09	117.53	109.94	12	1
2	B	127	GLN	CG-CD-NE2	5.09	124.04	116.40	5	1
1	A	325	THR	N-CA-C	5.09	117.64	108.48	8	1
1	A	479	LYS	CA-C-N	5.09	131.39	121.41	12	1
1	A	479	LYS	C-N-CA	5.09	131.39	121.41	12	1
2	C	165	PRO	N-CA-C	5.09	120.24	113.57	1	1
2	B	75	LEU	CA-C-O	-5.09	115.48	120.82	8	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	450	PRO	N-CA-C	5.09	125.33	112.10	10	1
1	A	427	THR	CA-CB-OG1	-5.09	101.97	109.60	13	1
1	A	380	VAL	CA-C-O	-5.09	115.04	120.59	14	1
1	A	342	TRP	CG-CD2-CE3	-5.09	128.81	133.90	5	1
2	B	247	PHE	CB-CA-C	5.08	118.93	110.90	5	1
2	B	246	SER	N-CA-C	5.08	117.55	111.71	3	1
1	A	387	HIS	O-C-N	-5.08	117.07	123.27	9	1
2	C	57	PHE	CA-C-N	5.08	127.04	120.44	5	1
2	C	57	PHE	C-N-CA	5.08	127.04	120.44	5	1
2	C	122	TYR	CA-CB-CG	5.08	123.04	113.90	13	2
1	A	385	ASP	CA-C-O	5.08	125.82	119.78	4	1
2	C	68	THR	CA-CB-OG1	5.08	117.22	109.60	12	1
2	C	111	GLU	CB-CG-CD	5.08	121.23	112.60	8	1
1	A	372	TYR	N-CA-CB	5.08	119.43	111.56	12	1
2	C	153	ARG	CA-C-N	5.08	127.39	120.54	1	1
2	C	153	ARG	C-N-CA	5.08	127.39	120.54	1	1
2	C	201	GLU	CA-C-O	-5.08	115.49	120.82	5	1
1	A	330	ARG	N-CA-CB	5.08	120.02	112.30	7	1
1	A	489	GLN	CG-CD-OE1	5.08	130.95	120.80	9	1
1	A	403	ILE	CA-C-N	5.08	127.59	120.28	10	1
1	A	403	ILE	C-N-CA	5.08	127.59	120.28	10	1
1	A	397	PRO	N-CD-CG	5.08	110.81	103.20	11	1
2	B	144	LEU	CA-C-O	5.07	125.93	120.55	10	2
2	B	207	GLY	CA-C-O	5.07	126.28	121.05	4	1
2	B	142	GLU	CB-CA-C	5.07	120.16	110.17	5	1
2	C	219	THR	CA-C-O	5.07	126.15	120.82	12	1
1	A	437	ARG	CA-C-O	5.07	126.46	120.69	9	1
2	C	131	GLN	CG-CD-NE2	5.07	124.00	116.40	10	1
2	B	78	GLU	CA-C-O	5.07	125.79	120.42	13	1
2	C	184	HIS	CA-C-O	-5.07	115.18	120.55	14	1
2	C	145	ARG	N-CA-CB	5.06	117.52	109.82	7	1
2	C	194	GLN	O-C-N	-5.06	116.38	122.15	9	2
1	A	458	GLY	CA-C-O	5.06	123.96	119.56	3	1
2	B	141	VAL	CA-C-O	5.06	125.70	119.58	10	1
1	A	504	ASP	N-CA-CB	5.06	119.04	110.49	2	2
2	B	185	LEU	CA-C-O	-5.06	115.19	120.55	9	1
2	B	203	LEU	N-CA-C	5.06	116.48	111.07	9	1
1	A	486	PHE	CB-CA-C	5.06	118.39	110.19	12	1
2	C	129	LYS	CB-CG-CD	5.06	122.94	111.30	15	1
2	C	178	VAL	N-CA-CB	5.06	118.17	110.58	11	1
2	C	149	GLN	CA-C-O	-5.06	115.51	120.82	12	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	490	LYS	CA-C-N	5.06	131.20	121.54	14	1
1	A	490	LYS	C-N-CA	5.06	131.20	121.54	14	1
2	B	101	LEU	CB-CA-C	-5.06	101.28	110.63	6	1
1	A	365	PRO	CA-C-N	5.06	128.25	120.82	10	1
1	A	365	PRO	C-N-CA	5.06	128.25	120.82	10	1
2	C	103	ASP	N-CA-CB	5.06	117.55	110.12	11	1
1	A	405	GLU	CA-C-N	5.06	127.32	120.44	14	1
1	A	405	GLU	C-N-CA	5.06	127.32	120.44	14	1
1	A	462	SER	CA-C-N	5.06	124.96	119.85	15	1
1	A	462	SER	C-N-CA	5.06	124.96	119.85	15	1
2	C	191	GLU	N-CA-CB	5.05	117.34	110.01	2	1
2	B	78	GLU	N-CA-CB	5.05	117.50	109.82	11	1
1	A	408	ARG	N-CA-CB	5.05	119.03	110.49	4	1
1	A	345	ARG	NH1-CZ-NH2	-5.05	112.73	119.30	8	1
2	C	123	LEU	CB-CA-C	5.05	118.81	110.88	13	1
1	A	387	HIS	CB-CG-CD2	-5.05	124.64	131.20	11	1
2	B	111	GLU	CA-C-O	-5.05	115.70	121.00	5	1
1	A	363	GLY	O-C-N	-5.05	116.14	122.70	8	1
1	A	346	ASN	CA-C-N	5.05	129.53	122.36	2	1
1	A	346	ASN	C-N-CA	5.05	129.53	122.36	2	1
2	C	72	TRP	CA-C-O	5.05	126.08	120.63	5	1
2	C	126	PHE	O-C-N	-5.05	116.40	122.15	13	1
2	B	183	THR	CA-CB-CG2	5.04	119.07	110.50	3	1
2	C	216	ALA	CA-C-N	5.04	127.54	120.28	10	1
2	C	216	ALA	C-N-CA	5.04	127.54	120.28	10	1
2	B	176	ALA	O-C-N	5.04	127.47	122.12	11	1
1	A	387	HIS	CG-CD2-NE2	5.04	112.24	107.20	1	1
2	C	210	ARG	O-C-N	-5.04	116.78	122.12	7	1
1	A	509	PRO	CA-C-N	5.04	131.17	121.54	2	1
1	A	509	PRO	C-N-CA	5.04	131.17	121.54	2	1
2	C	135	GLU	CA-CB-CG	-5.04	104.02	114.10	15	1
2	C	237	ARG	CA-C-N	5.04	127.03	120.28	4	1
2	C	237	ARG	C-N-CA	5.04	127.03	120.28	4	1
2	C	172	ASP	CA-C-O	-5.04	115.51	120.90	10	1
2	B	191	GLU	CA-C-O	-5.04	115.21	120.55	1	1
2	B	166	LEU	CA-C-N	5.04	125.53	119.94	2	1
2	B	166	LEU	C-N-CA	5.04	125.53	119.94	2	1
2	B	196	LEU	N-CA-C	-5.03	105.79	111.28	1	1
2	B	68	THR	N-CA-C	5.03	116.77	111.28	14	1
2	B	225	LEU	CA-C-O	-5.03	115.22	120.55	15	1
2	B	95	ALA	CB-CA-C	5.03	118.78	110.88	4	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	B	167	GLY	N-CA-C	5.03	119.21	112.77	9	1
1	A	490	LYS	N-CA-C	5.03	120.26	113.72	2	1
1	A	361	TRP	CA-CB-CG	5.03	123.16	113.60	9	1
2	C	122	TYR	CB-CA-C	5.03	118.71	110.96	11	1
2	B	131	GLN	CA-C-O	-5.03	115.22	120.55	14	1
1	A	390	PHE	O-C-N	-5.03	117.85	123.48	7	1
2	B	260	LYS	N-CA-CB	5.03	117.51	110.12	10	1
2	B	264	THR	CA-CB-OG1	5.03	117.14	109.60	10	1
2	C	169	GLU	CA-C-O	5.03	125.88	120.55	12	1
2	B	109	GLN	CA-C-O	-5.02	115.22	120.55	13	1
2	C	173	ARG	CD-NE-CZ	5.02	131.43	124.40	5	1
2	B	243	VAL	N-CA-C	-5.02	105.81	110.53	10	1
1	A	467	PHE	CA-C-N	5.02	127.84	120.71	4	1
1	A	467	PHE	C-N-CA	5.02	127.84	120.71	4	1
2	B	138	ARG	CD-NE-CZ	-5.02	117.37	124.40	5	1
2	B	171	ARG	CD-NE-CZ	5.02	131.43	124.40	9	1
2	B	114	LEU	CB-CA-C	5.02	118.83	110.90	5	1
1	A	389	VAL	CA-C-N	5.02	130.20	122.93	8	1
1	A	389	VAL	C-N-CA	5.02	130.20	122.93	8	1
1	A	436	TYR	CA-C-N	-5.02	115.92	122.99	6	1
1	A	436	TYR	C-N-CA	-5.02	115.92	122.99	6	1
2	B	84	GLN	O-C-N	-5.01	116.43	122.15	2	1
2	C	251	PHE	N-CA-C	-5.01	105.70	111.07	10	1
2	B	204	LYS	N-CA-CB	5.01	117.28	110.01	12	1
1	A	438	PHE	CB-CA-C	5.01	118.48	110.16	12	1
1	A	336	PHE	O-C-N	-5.01	116.68	123.19	1	1
2	C	110	GLU	N-CA-C	5.01	117.12	111.11	2	1
2	B	66	PRO	N-CD-CG	5.01	110.71	103.20	14	1
2	B	169	GLU	CA-C-O	5.01	125.56	119.05	1	1
2	C	247	PHE	CA-C-N	5.01	127.75	120.79	2	1
2	C	247	PHE	C-N-CA	5.01	127.75	120.79	2	1
2	C	99	PRO	N-CA-CB	5.01	107.77	103.31	12	1
2	B	61	ARG	N-CA-CB	5.00	117.48	110.12	7	1
1	A	479	LYS	N-CA-CB	5.00	119.03	110.57	8	1
1	A	412	THR	N-CA-C	5.00	116.81	111.36	1	1
2	B	126	PHE	CB-CG-CD2	-5.00	112.19	120.70	5	1
2	B	111	GLU	N-CA-C	5.00	116.42	111.07	9	1
2	B	193	ARG	NH1-CZ-NH2	-5.00	112.80	119.30	12	1
1	A	402	HIS	ND1-CE1-NE2	5.00	113.40	108.40	1	1
2	B	55	SER	O-C-N	-5.00	115.00	123.00	3	1
2	B	108	TRP	CB-CG-CD1	-5.00	119.40	126.90	3	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	C	179	ASP	CA-C-O	5.00	125.85	120.55	5	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
2	C	199	ARG	Sidechain	11
1	A	478	TYR	Sidechain	9
2	B	188	TYR	Sidechain	9
1	A	449	TYR	Sidechain	8
1	A	428	TYR	Sidechain	8
1	A	497	TYR	Sidechain	7
1	A	503	ARG	Sidechain	7
2	B	214	TYR	Sidechain	7
2	C	137	TYR	Sidechain	7
1	A	464	ARG	Sidechain	6
2	C	175	ARG	Sidechain	6
2	C	195	ARG	Sidechain	6
2	B	115	TYR	Sidechain	6
1	A	372	TYR	Sidechain	6
1	A	343	ARG	Sidechain	5
2	B	100	TYR	Sidechain	5
2	B	173	ARG	Sidechain	5
2	B	237	ARG	Sidechain	5
2	C	115	TYR	Sidechain	5
2	C	258	TYR	Sidechain	5
1	A	435	TYR	Sidechain	5
1	A	339	ARG	Sidechain	5
1	A	399	TYR	Sidechain	5
2	C	157	HIS	Sidechain	5
2	C	61	ARG	Sidechain	5
2	C	138	ARG	Sidechain	5
2	C	171	ARG	Sidechain	5
2	B	210	ARG	Sidechain	5
1	A	436	TYR	Sidechain	4
2	C	100	TYR	Sidechain	4
2	B	145	ARG	Sidechain	4
2	C	83	ARG	Sidechain	4
2	C	122	TYR	Sidechain	4
1	A	345	ARG	Sidechain	4

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	476	TYR	Sidechain	4
2	C	214	TYR	Sidechain	4
1	A	437	ARG	Sidechain	4
2	B	137	TYR	Sidechain	4
2	B	258	TYR	Sidechain	4
1	A	336	PHE	Sidechain	3
1	A	362	ARG	Sidechain	3
2	B	116	ARG	Sidechain	3
2	B	122	TYR	Sidechain	3
2	C	188	TYR	Sidechain	3
1	A	330	ARG	Sidechain	3
2	C	145	ARG	Sidechain	3
2	C	193	ARG	Sidechain	3
2	B	195	ARG	Sidechain	3
1	A	467	PHE	Sidechain	3
2	C	173	ARG	Sidechain	3
1	A	353	TYR	Sidechain	3
2	B	153	ARG	Sidechain	3
2	B	175	ARG	Sidechain	3
2	C	153	ARG	Sidechain	3
1	A	477	PHE	Sidechain	3
2	C	182	ARG	Sidechain	3
1	A	402	HIS	Sidechain	2
2	B	83	ARG	Sidechain	2
2	C	237	ARG	Sidechain	2
1	A	443	ARG	Sidechain	2
1	A	486	PHE	Sidechain	2
2	B	193	ARG	Sidechain	2
2	B	171	ARG	Sidechain	2
2	B	177	HIS	Sidechain	2
1	A	387	HIS	Sidechain	2
1	A	431	ARG	Sidechain	2
2	C	210	ARG	Sidechain	2
1	A	374	ARG	Sidechain	2
1	A	334	PHE	Sidechain	2
2	C	126	PHE	Sidechain	2
2	C	71	PHE	Sidechain	2
1	A	483	TYR	Sidechain	1
2	B	182	ARG	Sidechain	1
1	A	341	PHE	Sidechain	1
1	A	394	SER	Peptide	1
1	A	465	GLY	Peptide	1

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Mol	Chain	Res	Type	Group	Models (Total)
2	C	116	ARG	Sidechain	1
2	C	215	HIS	Sidechain	1
1	A	420	PHE	Sidechain	1
2	B	247	PHE	Sidechain	1
2	C	104	PHE	Sidechain	1
2	C	184	HIS	Sidechain	1
2	B	157	HIS	Sidechain	1
2	B	251	PHE	Sidechain	1
2	C	60	LEU	Mainchain	1
2	C	94	LYS	Mainchain	1
2	C	177	HIS	Sidechain	1
1	A	414	LYS	Peptide	1
1	A	429	PHE	Sidechain	1
1	A	430	PHE	Sidechain	1
1	A	438	PHE	Sidechain	1
2	B	126	PHE	Sidechain	1
2	B	138	ARG	Sidechain	1
2	C	251	PHE	Mainchain	1
1	A	342	TRP	Peptide	1
2	B	61	ARG	Sidechain	1
2	B	211	LEU	Mainchain	1
2	C	190	ASP	Mainchain	1
2	C	221	HIS	Sidechain	1
1	A	408	ARG	Sidechain	1
1	A	474	PHE	Sidechain	1
2	C	218	ALA	Peptide	1
2	B	184	HIS	Sidechain	1
1	A	381	PHE	Sidechain	1
1	A	471	ASP	Sidechain	1
1	A	508	CYS	Peptide	1
2	B	57	PHE	Sidechain	1
2	B	104	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	1562	4±2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes
2	B	1753	1745	1742	4±2
2	C	1728	1724	1721	2±2
3	A	2484	3888	3888	35±5
3	B	4600	7200	7200	53±8
3	C	2944	4608	4608	29±5
All	All	227220	310950	310821	1651

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
1:A:402:HIS:CE1	3:A:649:PX4:H12	0.90	2.00	7	5
3:B:338:PX4:H4	3:B:343:PX4:O3	0.74	1.82	2	1
3:C:358:PX4:H9	3:C:361:PX4:O3	0.72	1.85	6	1
3:B:326:PX4:O3	3:B:355:PX4:H3	0.71	1.84	5	3
3:C:351:PX4:O4	3:C:351:PX4:H4	0.70	1.86	13	2
3:B:334:PX4:O1	3:B:348:PX4:H4	0.69	1.87	15	2
3:B:322:PX4:O4	3:B:350:PX4:H11	0.69	1.86	1	1
3:A:636:PX4:O4	3:A:645:PX4:H11	0.68	1.88	1	1
3:B:373:PX4:H6	3:B:380:PX4:O4	0.68	1.89	5	1
3:B:375:PX4:O4	3:B:376:PX4:H5	0.68	1.88	3	1
3:B:361:PX4:H4	3:B:368:PX4:O3	0.68	1.89	10	2
3:B:325:PX4:O2	3:B:357:PX4:H3	0.67	1.88	13	1
3:A:640:PX4:H3	3:B:398:PX4:O6	0.67	1.88	13	1
3:B:351:PX4:H4	3:B:354:PX4:O4	0.67	1.90	15	2
3:B:374:PX4:O2	3:B:384:PX4:H6	0.67	1.89	1	3
3:A:614:PX4:H4	3:C:336:PX4:O4	0.67	1.88	6	5
3:A:625:PX4:O7	3:A:625:PX4:H3	0.67	1.90	2	2
3:B:333:PX4:O3	3:B:361:PX4:H12	0.66	1.89	14	1
3:B:320:PX4:H4	3:B:340:PX4:O4	0.66	1.90	5	1
3:B:312:PX4:O1	3:B:317:PX4:H4	0.66	1.90	10	2
3:B:373:PX4:H4	3:B:373:PX4:O4	0.66	1.90	1	3
3:C:312:PX4:O3	3:C:312:PX4:H6	0.66	1.91	1	2
3:B:361:PX4:O3	3:B:368:PX4:H3	0.66	1.90	11	3
3:B:391:PX4:H9	3:C:303:PX4:O5	0.66	1.91	2	1
3:B:383:PX4:O4	3:B:383:PX4:H3	0.66	1.90	2	2
3:A:613:PX4:O4	3:A:628:PX4:H4	0.65	1.92	9	2
3:A:607:PX4:H10	3:A:607:PX4:O2	0.65	1.92	1	1
3:C:338:PX4:O4	3:C:345:PX4:H9	0.65	1.92	12	1
1:A:405:GLU:OE1	3:A:641:PX4:H4	0.65	1.90	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:361:PX4:H3	3:B:368:PX4:O3	0.65	1.90	11	5
3:A:642:PX4:O4	3:A:642:PX4:H4	0.65	1.92	10	7
3:B:362:PX4:O1	3:B:366:PX4:H3	0.65	1.92	11	1
3:B:380:PX4:O2	3:B:387:PX4:H3	0.64	1.92	8	1
3:A:628:PX4:O6	3:A:642:PX4:H8	0.64	1.92	10	1
3:A:622:PX4:O1	3:A:635:PX4:H4	0.64	1.93	7	2
3:C:307:PX4:H10	3:C:307:PX4:O2	0.64	1.93	12	2
3:B:333:PX4:O4	3:B:333:PX4:H13	0.64	1.93	12	2
3:B:310:PX4:O1	3:B:310:PX4:H9	0.64	1.92	12	2
3:C:309:PX4:H4	3:C:315:PX4:O1	0.64	1.92	2	2
3:B:323:PX4:O1	3:B:346:PX4:H3	0.64	1.93	5	2
1:A:402:HIS:CE1	3:A:649:PX4:H6	0.64	2.28	15	2
3:A:632:PX4:H4	3:A:647:PX4:O2	0.64	1.93	14	5
3:A:614:PX4:O1	3:A:625:PX4:H9	0.64	1.93	3	2
3:A:641:PX4:H15	3:A:641:PX4:H10	0.64	1.69	12	1
3:A:625:PX4:O4	3:A:625:PX4:H3	0.63	1.93	7	8
1:A:359:GLN:OE1	3:A:640:PX4:H10	0.63	1.93	5	2
3:C:358:PX4:H10	3:C:358:PX4:H16	0.63	1.68	11	1
3:B:360:PX4:O2	3:B:362:PX4:H9	0.63	1.93	2	1
3:C:316:PX4:H3	3:C:342:PX4:O1	0.63	1.92	6	2
3:B:349:PX4:O1	3:B:357:PX4:H11	0.63	1.94	5	1
3:C:333:PX4:H9	3:C:352:PX4:O2	0.63	1.94	13	1
3:A:632:PX4:H9	3:A:647:PX4:O4	0.63	1.94	13	3
3:B:301:PX4:O1	3:B:301:PX4:H3	0.63	1.92	6	2
3:A:631:PX4:O1	3:A:642:PX4:H3	0.63	1.94	13	1
3:A:647:PX4:H13	3:A:652:PX4:O1	0.63	1.93	15	1
3:A:627:PX4:O4	3:A:643:PX4:H6	0.63	1.94	1	1
3:B:380:PX4:O3	3:B:380:PX4:H6	0.63	1.94	13	1
3:B:335:PX4:H3	3:B:353:PX4:O2	0.62	1.94	8	1
3:B:380:PX4:O2	3:B:387:PX4:H4	0.62	1.94	2	2
3:B:360:PX4:O4	3:B:360:PX4:H3	0.62	1.93	13	7
3:C:350:PX4:O1	3:C:350:PX4:H4	0.62	1.95	4	1
3:C:330:PX4:O2	3:C:330:PX4:H3	0.62	1.94	13	3
3:C:359:PX4:H9	3:C:359:PX4:O1	0.62	1.94	10	1
3:C:318:PX4:H8	3:C:321:PX4:C1	0.62	2.24	14	1
3:B:337:PX4:O1	3:B:352:PX4:H7	0.62	1.93	12	2
3:A:626:PX4:O2	3:A:626:PX4:H12	0.62	1.95	15	1
3:B:363:PX4:H3	3:B:363:PX4:O1	0.62	1.94	3	4
3:B:368:PX4:O2	3:B:368:PX4:H7	0.62	1.93	10	2
3:A:606:PX4:O2	3:A:606:PX4:H4	0.62	1.95	9	3
3:A:607:PX4:O1	3:A:612:PX4:H3	0.62	1.95	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:325:PX4:O4	3:C:325:PX4:H7	0.62	1.94	11	1
3:A:619:PX4:H69	3:A:632:PX4:H5	0.61	1.71	4	1
3:B:400:PX4:H11	3:C:347:PX4:O4	0.61	1.95	9	1
3:B:348:PX4:O1	3:B:348:PX4:H3	0.61	1.95	5	3
3:C:343:PX4:H4	3:C:353:PX4:O2	0.61	1.95	6	1
3:C:307:PX4:O4	3:C:310:PX4:H5	0.61	1.95	14	1
3:A:617:PX4:H4	3:A:617:PX4:O4	0.61	1.96	14	1
3:B:363:PX4:H8	3:C:302:PX4:O2	0.61	1.95	15	1
3:B:311:PX4:O2	3:B:345:PX4:H3	0.61	1.96	1	1
3:A:641:PX4:H9	3:A:641:PX4:O3	0.61	1.96	14	3
3:C:340:PX4:H11	3:C:360:PX4:O4	0.61	1.95	14	1
3:B:368:PX4:H9	3:B:368:PX4:O3	0.61	1.96	7	1
3:A:613:PX4:O7	3:A:613:PX4:H9	0.61	1.95	11	1
3:A:618:PX4:O3	3:A:633:PX4:H6	0.61	1.94	15	1
3:A:611:PX4:H5	3:B:394:PX4:O4	0.61	1.95	2	2
3:B:397:PX4:H7	3:B:397:PX4:O4	0.61	1.96	1	2
3:A:614:PX4:O4	3:A:614:PX4:H3	0.61	1.96	2	3
3:A:633:PX4:O2	3:A:638:PX4:H6	0.61	1.96	4	1
3:C:307:PX4:O1	3:C:310:PX4:H9	0.61	1.96	7	1
3:B:329:PX4:O3	3:B:329:PX4:H6	0.61	1.96	2	5
3:B:383:PX4:H9	3:B:383:PX4:O3	0.60	1.96	5	4
3:A:610:PX4:H4	3:B:389:PX4:O1	0.60	1.96	6	3
3:A:645:PX4:H3	3:A:646:PX4:O2	0.60	1.96	4	1
3:A:632:PX4:O4	3:A:632:PX4:H12	0.60	1.95	7	2
3:A:628:PX4:O8	3:A:642:PX4:H5	0.60	1.95	6	1
1:A:400:PRO:O	3:A:652:PX4:H11	0.60	1.96	6	7
3:A:609:PX4:H8	3:B:384:PX4:O4	0.60	1.96	7	4
3:C:350:PX4:O3	3:C:355:PX4:H4	0.60	1.97	5	1
3:B:386:PX4:H16	3:B:386:PX4:H10	0.60	1.71	7	1
3:A:645:PX4:O1	3:A:648:PX4:H11	0.60	1.96	4	1
3:B:327:PX4:O1	3:B:351:PX4:H4	0.60	1.96	6	2
3:C:332:PX4:O1	3:C:332:PX4:H3	0.60	1.97	8	3
3:C:337:PX4:O2	3:C:337:PX4:H4	0.60	1.97	11	1
3:B:353:PX4:H6	3:B:353:PX4:O2	0.60	1.97	15	1
3:A:614:PX4:O3	3:A:614:PX4:H12	0.59	1.97	11	2
3:B:353:PX4:H3	3:B:369:PX4:O3	0.59	1.97	4	5
3:C:307:PX4:H4	3:C:340:PX4:O2	0.59	1.97	14	3
3:A:605:PX4:O2	3:A:609:PX4:H4	0.59	1.97	8	2
3:B:327:PX4:O1	3:B:351:PX4:H7	0.59	1.97	7	1
3:B:362:PX4:H4	3:B:362:PX4:O2	0.59	1.97	7	1
2:B:76:GLU:OE2	3:B:305:PX4:H4	0.59	1.96	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:389:PX4:H10	3:B:389:PX4:O3	0.59	1.96	8	1
3:C:323:PX4:H4	3:C:323:PX4:O4	0.59	1.97	10	2
3:A:647:PX4:H10	3:A:652:PX4:O1	0.59	1.97	3	4
3:C:349:PX4:O4	3:C:358:PX4:H5	0.59	1.97	7	1
3:A:631:PX4:H10	3:A:646:PX4:O5	0.59	1.98	13	4
3:A:640:PX4:O2	3:A:650:PX4:H8	0.59	1.97	6	1
3:B:320:PX4:H13	3:B:340:PX4:O4	0.59	1.98	6	1
3:B:376:PX4:O6	3:B:390:PX4:H3	0.59	1.97	12	1
3:B:305:PX4:H3	3:B:305:PX4:O1	0.59	1.97	15	2
1:A:400:PRO:O	3:A:652:PX4:H5	0.59	1.97	8	3
3:B:362:PX4:H4	3:B:366:PX4:O4	0.59	1.97	14	1
3:C:317:PX4:O4	3:C:344:PX4:H10	0.59	1.97	12	2
3:C:323:PX4:O8	3:C:323:PX4:H6	0.59	1.98	12	1
3:A:648:PX4:O2	3:A:654:PX4:H4	0.59	1.98	15	1
3:A:605:PX4:O6	3:A:609:PX4:H9	0.59	1.98	3	4
3:B:392:PX4:C6	3:B:392:PX4:H3	0.59	2.26	4	3
3:A:612:PX4:H9	3:A:612:PX4:O3	0.59	1.97	11	4
3:B:393:PX4:O2	3:B:393:PX4:H4	0.58	1.99	4	1
3:A:613:PX4:O2	3:A:628:PX4:H12	0.58	1.98	11	2
3:B:309:PX4:O1	3:B:309:PX4:H3	0.58	1.97	2	2
3:B:338:PX4:H48	3:B:343:PX4:H8	0.58	1.74	8	1
3:B:365:PX4:O6	3:B:378:PX4:H4	0.58	1.99	2	1
3:A:606:PX4:O2	3:B:381:PX4:H10	0.58	1.99	6	1
3:B:320:PX4:H6	3:B:340:PX4:O4	0.58	1.98	7	1
3:A:632:PX4:H7	3:A:647:PX4:O4	0.58	1.99	15	3
3:B:363:PX4:H9	3:C:302:PX4:O1	0.58	1.98	6	2
3:C:353:PX4:H3	3:C:353:PX4:O1	0.58	1.97	4	1
3:B:363:PX4:H13	3:B:363:PX4:O8	0.58	1.98	14	1
3:B:360:PX4:H3	3:B:360:PX4:O7	0.58	1.99	2	2
3:C:305:PX4:C3	3:C:324:PX4:H6	0.58	2.29	3	1
3:A:618:PX4:H67	3:A:633:PX4:H45	0.58	1.76	8	1
1:A:402:HIS:CE1	3:A:649:PX4:H10	0.58	2.33	8	1
3:C:336:PX4:H15	3:C:355:PX4:H13	0.58	1.75	3	1
3:A:601:PX4:O1	3:B:377:PX4:H4	0.58	1.99	4	1
3:B:398:PX4:H3	3:C:357:PX4:O3	0.58	1.98	8	2
3:A:647:PX4:H3	3:A:652:PX4:O2	0.58	1.99	11	5
3:B:327:PX4:O2	3:B:351:PX4:H7	0.58	1.99	4	2
3:B:354:PX4:O4	3:B:354:PX4:H3	0.58	1.98	6	2
2:C:71:PHE:CE1	2:C:75:LEU:HD11	0.58	2.34	8	1
3:B:369:PX4:O1	3:B:386:PX4:H4	0.58	1.98	13	2
3:C:323:PX4:O6	3:C:323:PX4:H13	0.57	1.99	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:611:PX4:H11	3:B:394:PX4:O3	0.57	1.98	3	2
3:A:611:PX4:H5	3:B:394:PX4:O6	0.57	1.98	6	2
3:C:361:PX4:H10	3:C:361:PX4:O3	0.57	1.99	12	2
3:A:633:PX4:O2	3:A:638:PX4:H9	0.57	1.99	14	1
3:C:322:PX4:H4	3:C:325:PX4:O6	0.57	1.99	15	1
3:C:320:PX4:H9	3:C:341:PX4:O1	0.57	1.99	3	1
3:B:306:PX4:H13	3:B:348:PX4:O2	0.57	1.99	1	1
3:A:630:PX4:O1	3:A:630:PX4:H3	0.57	1.99	7	1
2:B:201:GLU:OE2	3:B:313:PX4:H6	0.57	2.00	6	1
3:A:613:PX4:O8	3:A:628:PX4:H6	0.57	1.99	13	1
3:C:313:PX4:H9	3:C:337:PX4:O2	0.57	2.00	15	1
2:B:120:GLU:OE2	3:B:311:PX4:H4	0.57	1.98	8	1
2:B:72:TRP:CD2	3:B:341:PX4:H13	0.57	2.34	12	1
3:C:347:PX4:O3	3:C:347:PX4:H13	0.57	2.00	14	1
3:A:609:PX4:H11	3:B:384:PX4:O2	0.57	1.99	7	4
3:A:623:PX4:O1	3:A:640:PX4:H3	0.57	1.99	15	2
3:B:374:PX4:O1	3:B:384:PX4:H6	0.57	2.00	5	1
3:B:301:PX4:O2	3:B:304:PX4:H3	0.57	2.00	1	1
3:A:604:PX4:O2	3:A:607:PX4:H9	0.57	2.00	10	1
3:A:607:PX4:O1	3:A:612:PX4:H12	0.56	2.00	3	1
3:A:633:PX4:H44	3:C:303:PX4:H71	0.56	1.77	7	1
3:B:306:PX4:O3	3:B:306:PX4:H7	0.56	1.99	13	2
3:C:352:PX4:O3	3:C:352:PX4:H6	0.56	1.98	4	1
3:A:610:PX4:H3	3:B:389:PX4:O2	0.56	2.01	11	2
3:B:335:PX4:H10	3:B:353:PX4:O1	0.56	2.01	7	1
3:C:339:PX4:H7	3:C:339:PX4:O1	0.56	2.00	7	1
3:A:618:PX4:O2	3:A:630:PX4:H10	0.56	2.01	5	1
3:A:626:PX4:H13	3:C:362:PX4:O4	0.56	1.99	11	2
3:B:316:PX4:H3	3:B:316:PX4:O1	0.56	2.01	11	2
3:A:605:PX4:O2	3:B:379:PX4:H12	0.56	2.00	1	1
3:A:604:PX4:H7	3:B:392:PX4:H2	0.56	1.77	2	1
3:B:375:PX4:H7	3:B:375:PX4:O3	0.56	2.00	2	3
3:B:390:PX4:H9	3:B:390:PX4:O1	0.56	1.99	8	1
2:B:142:GLU:OE2	3:B:328:PX4:H8	0.56	2.00	10	3
3:A:601:PX4:H12	3:A:601:PX4:O4	0.56	2.01	12	4
3:A:647:PX4:O3	3:A:647:PX4:H7	0.56	2.01	5	1
3:B:375:PX4:H9	3:B:375:PX4:O1	0.56	2.00	12	1
3:A:602:PX4:O4	3:A:602:PX4:H3	0.56	1.99	1	2
3:B:380:PX4:O8	3:B:387:PX4:H4	0.56	2.00	9	2
3:A:605:PX4:H13	3:B:379:PX4:O4	0.56	2.00	10	1
3:A:636:PX4:O2	3:A:645:PX4:H8	0.56	2.00	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:318:PX4:O3	3:B:318:PX4:H6	0.56	2.00	1	3
3:A:607:PX4:H3	3:B:392:PX4:O2	0.56	2.01	3	1
3:A:605:PX4:O3	3:B:379:PX4:H10	0.56	2.00	10	1
3:C:321:PX4:O1	3:C:350:PX4:H6	0.56	2.01	13	1
2:B:76:GLU:HB3	3:B:305:PX4:H13	0.56	1.77	6	1
2:B:130:TRP:CD1	2:C:177:HIS:CE1	0.56	2.93	6	2
3:A:608:PX4:H4	3:A:608:PX4:O4	0.56	2.01	11	1
3:B:323:PX4:H4	3:B:323:PX4:O2	0.56	1.99	15	1
3:A:624:PX4:H34	3:A:639:PX4:H48	0.56	1.76	3	1
3:B:363:PX4:O3	3:B:363:PX4:H12	0.55	2.01	4	2
3:A:633:PX4:H12	3:A:633:PX4:O1	0.55	2.02	13	1
1:A:443:ARG:CD	3:A:651:PX4:H7	0.55	2.31	14	1
3:C:305:PX4:O4	3:C:311:PX4:H3	0.55	2.01	6	2
2:B:184:HIS:CD2	2:C:126:PHE:CD2	0.55	2.94	3	1
3:B:323:PX4:O3	3:B:323:PX4:H13	0.55	2.01	11	2
3:B:364:PX4:H3	3:C:301:PX4:O2	0.55	2.01	5	2
3:B:304:PX4:O2	3:B:345:PX4:H12	0.55	2.02	9	1
3:B:307:PX4:H7	3:B:318:PX4:O1	0.55	2.01	9	1
3:A:620:PX4:H1	3:A:636:PX4:H11	0.55	1.77	11	1
3:B:305:PX4:H32	3:B:356:PX4:H43	0.55	1.78	12	1
3:B:374:PX4:O4	3:B:384:PX4:H3	0.55	2.02	1	5
3:A:604:PX4:H4	3:B:376:PX4:O2	0.55	2.01	4	3
3:B:387:PX4:O1	3:B:390:PX4:H6	0.55	2.02	5	2
3:B:316:PX4:H5	3:B:321:PX4:O4	0.55	2.01	6	1
3:B:396:PX4:O2	3:B:396:PX4:H3	0.55	2.02	13	1
3:C:321:PX4:H4	3:C:321:PX4:O2	0.55	2.01	1	1
3:B:353:PX4:O3	3:B:353:PX4:H13	0.55	2.01	9	1
3:A:626:PX4:O1	3:A:626:PX4:H4	0.55	2.02	10	1
3:B:301:PX4:O3	3:B:301:PX4:H13	0.55	2.01	10	1
3:A:617:PX4:H5	3:A:625:PX4:O1	0.55	2.02	1	1
3:A:613:PX4:O2	3:A:628:PX4:H4	0.55	2.01	5	2
3:C:358:PX4:H14	3:C:361:PX4:H7	0.55	1.79	6	1
3:A:632:PX4:H7	3:A:647:PX4:O2	0.55	2.02	11	1
3:A:645:PX4:O1	3:A:648:PX4:H9	0.55	2.02	3	1
3:B:306:PX4:H12	3:B:348:PX4:O4	0.55	2.02	13	1
3:B:301:PX4:O1	3:B:303:PX4:H10	0.55	2.02	6	1
3:C:315:PX4:H7	3:C:315:PX4:O3	0.55	2.02	13	4
3:B:374:PX4:C6	3:B:384:PX4:H3	0.55	2.32	9	1
3:C:360:PX4:O2	3:C:360:PX4:H12	0.55	2.01	5	2
3:A:645:PX4:O1	3:A:653:PX4:H5	0.55	2.02	6	1
3:B:345:PX4:O8	3:B:369:PX4:H7	0.55	2.02	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:306:PX4:H4	3:B:339:PX4:O1	0.55	2.02	10	3
3:B:393:PX4:H10	3:B:393:PX4:O3	0.55	2.02	12	3
3:B:364:PX4:H13	3:C:301:PX4:O2	0.55	2.02	2	2
3:A:605:PX4:H3	3:B:379:PX4:O4	0.55	2.02	12	1
3:C:314:PX4:O2	3:C:314:PX4:H4	0.55	2.01	12	2
3:C:349:PX4:O8	3:C:349:PX4:H4	0.55	2.01	12	1
3:B:363:PX4:H4	3:B:381:PX4:O1	0.55	2.01	15	1
3:A:644:PX4:H12	3:A:650:PX4:H13	0.54	1.78	1	1
3:A:624:PX4:O1	3:A:639:PX4:H7	0.54	2.02	5	1
3:B:334:PX4:H7	3:B:352:PX4:O1	0.54	2.02	6	1
3:B:395:PX4:H3	3:C:358:PX4:O2	0.54	2.02	14	2
3:A:621:PX4:O3	3:A:621:PX4:H12	0.54	2.02	12	2
3:C:349:PX4:O8	3:C:349:PX4:H10	0.54	2.02	12	1
3:B:310:PX4:O8	3:B:358:PX4:H5	0.54	2.02	2	1
3:B:343:PX4:O4	3:B:343:PX4:H4	0.54	2.01	6	1
3:B:392:PX4:O1	3:B:394:PX4:H12	0.54	2.03	7	1
3:B:346:PX4:O4	3:B:346:PX4:H4	0.54	2.02	12	2
3:B:397:PX4:H9	3:C:312:PX4:O2	0.54	2.01	15	1
3:B:338:PX4:H10	3:B:338:PX4:O2	0.54	2.02	7	1
3:A:616:PX4:O2	3:A:634:PX4:H11	0.54	2.02	14	3
3:C:358:PX4:H10	3:C:358:PX4:O4	0.54	2.03	7	2
3:C:340:PX4:H4	3:C:360:PX4:H12	0.54	1.78	8	1
3:A:622:PX4:H10	3:A:622:PX4:O4	0.54	2.02	10	1
3:A:642:PX4:O1	3:A:651:PX4:H5	0.54	2.02	10	1
3:B:363:PX4:H8	3:B:381:PX4:O4	0.54	2.01	10	1
3:B:399:PX4:O4	3:B:399:PX4:H12	0.54	2.02	11	1
3:B:399:PX4:H13	3:C:357:PX4:O3	0.54	2.03	13	1
3:C:312:PX4:H7	3:C:312:PX4:H15	0.54	1.80	5	1
3:B:342:PX4:H4	3:B:342:PX4:O2	0.54	2.03	6	1
3:A:602:PX4:H6	3:B:372:PX4:O1	0.54	2.02	13	1
2:B:76:GLU:OE1	3:B:305:PX4:H9	0.54	2.03	8	1
3:B:369:PX4:O6	3:B:386:PX4:H13	0.54	2.02	5	1
3:B:379:PX4:H9	3:B:379:PX4:O3	0.54	2.03	5	2
3:B:380:PX4:H15	3:B:380:PX4:H3	0.54	1.79	15	1
3:A:649:PX4:O3	3:A:649:PX4:H13	0.54	2.02	2	2
3:B:311:PX4:O4	3:B:311:PX4:H4	0.54	2.01	4	2
3:B:380:PX4:O8	3:B:387:PX4:H10	0.54	2.03	10	3
3:B:369:PX4:O1	3:B:386:PX4:H7	0.54	2.03	11	1
3:A:618:PX4:H3	3:A:620:PX4:O1	0.54	2.02	5	3
3:A:649:PX4:O7	3:A:652:PX4:H7	0.54	2.03	5	1
3:B:400:PX4:O8	3:B:400:PX4:H7	0.54	2.02	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:329:PX4:O4	3:B:355:PX4:H3	0.54	2.03	12	2
3:B:342:PX4:O2	3:B:367:PX4:H3	0.54	2.02	13	1
3:B:356:PX4:H4	3:B:373:PX4:O1	0.54	2.03	14	1
3:A:649:PX4:O4	3:A:652:PX4:H8	0.54	2.02	1	1
3:C:307:PX4:O6	3:C:310:PX4:H8	0.54	2.03	1	2
3:B:307:PX4:O1	3:B:307:PX4:H3	0.54	2.03	4	2
2:C:91:GLU:OE1	3:C:314:PX4:H5	0.54	2.03	5	1
3:C:327:PX4:H5	3:C:334:PX4:O1	0.54	2.03	8	1
3:A:630:PX4:O8	3:A:648:PX4:H7	0.53	2.02	2	1
1:A:443:ARG:HD2	3:A:651:PX4:H6	0.53	1.80	1	1
3:C:352:PX4:H3	3:C:352:PX4:O1	0.53	2.03	6	1
2:B:72:TRP:CE2	3:B:341:PX4:H6	0.53	2.38	9	2
3:B:342:PX4:O4	3:B:350:PX4:H6	0.53	2.04	9	1
3:C:325:PX4:O3	3:C:325:PX4:H9	0.53	2.03	11	2
3:B:382:PX4:H13	3:B:382:PX4:C6	0.53	2.33	11	1
3:A:605:PX4:H6	3:B:379:PX4:O2	0.53	2.02	11	3
3:A:602:PX4:O1	3:B:375:PX4:H4	0.53	2.03	12	1
3:C:303:PX4:H10	3:C:303:PX4:O2	0.53	2.03	12	1
3:C:364:PX4:H3	3:C:364:PX4:O2	0.53	2.03	4	1
3:A:617:PX4:H3	3:A:617:PX4:O4	0.53	2.03	7	1
3:A:652:PX4:O2	3:A:652:PX4:H12	0.53	2.04	7	1
3:A:653:PX4:O4	3:A:653:PX4:H3	0.53	2.03	10	1
3:C:328:PX4:H3	3:C:337:PX4:O1	0.53	2.03	15	1
3:B:370:PX4:H4	3:B:370:PX4:O2	0.53	2.03	10	3
3:B:392:PX4:O3	3:B:392:PX4:H12	0.53	2.03	4	4
3:C:323:PX4:H4	3:C:323:PX4:C6	0.53	2.34	4	1
1:A:405:GLU:O	3:A:641:PX4:H6	0.53	2.03	5	1
3:C:358:PX4:O8	3:C:361:PX4:H4	0.53	2.04	8	1
3:C:358:PX4:O1	3:C:361:PX4:H4	0.53	2.03	10	1
3:C:320:PX4:H3	3:C:330:PX4:O8	0.53	2.04	15	2
3:B:345:PX4:O4	3:B:345:PX4:H4	0.53	2.03	1	1
3:C:313:PX4:H3	3:C:313:PX4:O1	0.53	2.03	9	2
3:A:620:PX4:O3	3:A:620:PX4:H6	0.53	2.03	3	1
3:C:357:PX4:O1	3:C:357:PX4:H3	0.53	2.02	14	1
3:B:376:PX4:O1	3:B:390:PX4:H9	0.53	2.03	5	1
3:C:306:PX4:H12	3:C:306:PX4:O2	0.53	2.04	5	1
3:B:333:PX4:O1	3:B:361:PX4:H10	0.53	2.04	6	1
3:A:616:PX4:H4	3:A:616:PX4:O2	0.53	2.04	12	1
3:C:344:PX4:H7	3:C:364:PX4:O1	0.53	2.04	14	1
3:B:304:PX4:O1	3:B:304:PX4:H3	0.53	2.03	2	2
3:C:318:PX4:H5	3:C:321:PX4:O4	0.53	2.03	4	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:301:PX4:H4	3:B:303:PX4:O3	0.53	2.04	3	2
3:A:643:PX4:H12	3:A:643:PX4:O1	0.53	2.04	12	2
3:A:623:PX4:H3	3:B:398:PX4:O1	0.53	2.03	14	1
3:B:381:PX4:H4	3:B:381:PX4:O2	0.53	2.04	14	1
3:C:333:PX4:O4	3:C:333:PX4:H3	0.53	2.03	3	2
3:B:398:PX4:O2	3:B:398:PX4:H4	0.52	2.02	5	1
3:A:611:PX4:O4	3:A:611:PX4:H6	0.52	2.04	7	1
3:A:602:PX4:O2	3:A:604:PX4:H9	0.52	2.04	9	1
3:A:606:PX4:H3	3:B:383:PX4:O2	0.52	2.04	9	1
3:A:630:PX4:O3	3:A:648:PX4:H7	0.52	2.04	12	1
3:B:373:PX4:H3	3:B:380:PX4:O2	0.52	2.03	12	1
3:C:347:PX4:O2	3:C:347:PX4:H4	0.52	2.04	12	2
3:B:351:PX4:H7	3:B:354:PX4:O3	0.52	2.03	13	1
3:C:325:PX4:O1	3:C:325:PX4:H3	0.52	2.04	2	1
3:B:392:PX4:O6	3:B:392:PX4:H6	0.52	2.04	4	1
3:B:320:PX4:H6	3:B:340:PX4:O2	0.52	2.04	5	1
3:B:329:PX4:O3	3:B:355:PX4:H5	0.52	2.04	6	1
3:B:334:PX4:H12	3:B:334:PX4:O1	0.52	2.05	6	1
3:B:338:PX4:O2	3:B:358:PX4:H6	0.52	2.04	6	1
3:B:342:PX4:O2	3:B:350:PX4:H4	0.52	2.03	8	3
3:C:339:PX4:O1	3:C:339:PX4:H9	0.52	2.03	9	1
3:A:614:PX4:H4	3:A:628:PX4:O2	0.52	2.05	11	1
2:B:229:ALA:HB2	3:B:332:PX4:H61	0.52	1.80	11	1
3:A:636:PX4:O3	3:A:645:PX4:H5	0.52	2.04	1	1
3:A:646:PX4:H8	3:A:653:PX4:O2	0.52	2.05	1	1
3:B:396:PX4:O3	3:B:396:PX4:H6	0.52	2.03	4	1
3:B:356:PX4:H7	3:B:356:PX4:O3	0.52	2.05	13	1
3:B:332:PX4:O1	3:B:332:PX4:H3	0.52	2.04	12	2
3:B:352:PX4:O1	3:B:352:PX4:H3	0.52	2.05	6	1
3:A:644:PX4:O2	3:A:650:PX4:H3	0.52	2.04	7	1
3:B:353:PX4:H11	3:B:382:PX4:O2	0.52	2.04	10	1
3:B:400:PX4:H10	3:B:400:PX4:O8	0.52	2.05	10	1
3:A:648:PX4:H10	3:A:648:PX4:O4	0.52	2.05	11	1
3:B:312:PX4:O3	3:B:317:PX4:H13	0.52	2.04	12	1
3:C:312:PX4:O3	3:C:312:PX4:C3	0.52	2.58	14	1
3:C:313:PX4:O1	3:C:328:PX4:H11	0.52	2.04	15	2
3:C:346:PX4:H5	3:C:362:PX4:O1	0.52	2.04	1	1
3:A:611:PX4:O1	3:A:611:PX4:H13	0.52	2.05	2	2
3:A:614:PX4:H7	3:C:336:PX4:O1	0.52	2.05	2	1
3:A:625:PX4:H3	3:A:625:PX4:C6	0.52	2.35	13	2
3:B:378:PX4:O2	3:C:302:PX4:H12	0.52	2.05	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:642:PX4:O2	3:A:651:PX4:H8	0.52	2.05	5	1
2:B:80:GLU:OE1	3:B:305:PX4:H7	0.52	2.04	5	1
3:A:612:PX4:O2	3:A:612:PX4:H7	0.52	2.03	6	1
3:C:332:PX4:H6	3:C:335:PX4:O3	0.52	2.05	7	1
3:C:351:PX4:O2	3:C:359:PX4:H4	0.52	2.04	9	1
3:B:306:PX4:O1	3:B:306:PX4:H9	0.52	2.04	10	1
3:C:323:PX4:O2	3:C:342:PX4:H12	0.52	2.04	10	1
3:B:399:PX4:O2	3:C:326:PX4:H13	0.52	2.04	14	1
3:B:321:PX4:O2	3:B:321:PX4:H4	0.52	2.05	15	1
3:A:614:PX4:H9	3:C:336:PX4:O2	0.52	2.05	4	1
3:B:311:PX4:H71	3:C:309:PX4:H44	0.52	1.81	4	1
3:C:328:PX4:O4	3:C:356:PX4:H3	0.52	2.05	6	1
3:A:624:PX4:O3	3:A:624:PX4:H9	0.52	2.04	10	1
3:A:631:PX4:O1	3:A:631:PX4:H9	0.52	2.04	12	1
3:A:611:PX4:P1	3:A:611:PX4:H13	0.52	2.45	13	1
3:A:651:PX4:O1	3:A:651:PX4:H4	0.52	2.05	13	1
3:B:363:PX4:H11	3:B:381:PX4:O4	0.52	2.05	5	2
3:B:339:PX4:H3	3:B:339:PX4:O1	0.52	2.04	5	1
3:C:328:PX4:O4	3:C:356:PX4:H6	0.52	2.05	5	1
3:A:636:PX4:O2	3:A:636:PX4:H7	0.52	2.05	6	2
3:B:380:PX4:O1	3:B:380:PX4:H3	0.52	2.05	6	1
3:A:644:PX4:H3	3:A:650:PX4:O2	0.52	2.04	14	2
3:B:399:PX4:O1	3:C:326:PX4:H13	0.52	2.05	8	1
3:A:607:PX4:P1	3:A:612:PX4:H3	0.52	2.44	9	1
3:B:320:PX4:O4	3:B:320:PX4:H3	0.52	2.05	11	1
3:A:629:PX4:O2	3:A:629:PX4:H4	0.52	2.03	12	1
3:A:613:PX4:O2	3:A:628:PX4:H6	0.52	2.05	14	1
3:B:356:PX4:H3	3:B:373:PX4:O2	0.52	2.05	15	1
3:B:366:PX4:H13	3:B:383:PX4:O1	0.52	2.05	3	1
3:B:319:PX4:O1	3:B:319:PX4:H3	0.52	2.04	10	2
3:A:614:PX4:O1	3:A:625:PX4:H4	0.52	2.04	6	3
3:C:338:PX4:O2	3:C:345:PX4:H9	0.52	2.05	11	1
3:B:359:PX4:O2	3:B:373:PX4:H13	0.52	2.04	14	1
3:B:374:PX4:O1	3:B:384:PX4:H11	0.52	2.05	14	1
3:B:382:PX4:H5	3:B:391:PX4:O1	0.52	2.04	15	1
3:B:392:PX4:O1	3:B:394:PX4:H10	0.52	2.05	10	1
3:A:629:PX4:O6	3:A:631:PX4:H12	0.52	2.05	9	3
3:B:312:PX4:H5	3:B:356:PX4:O1	0.52	2.05	3	1
3:A:635:PX4:O6	3:A:637:PX4:H8	0.52	2.05	5	1
3:B:361:PX4:H3	3:B:368:PX4:O1	0.52	2.04	7	1
3:C:348:PX4:O2	3:C:348:PX4:H10	0.52	2.04	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:350:PX4:O2	3:C:355:PX4:H4	0.51	2.04	1	1
3:B:369:PX4:O1	3:B:369:PX4:H13	0.51	2.06	9	2
3:B:328:PX4:H4	3:B:328:PX4:O2	0.51	2.04	11	1
3:B:346:PX4:H4	3:B:346:PX4:O2	0.51	2.05	13	1
3:C:313:PX4:H7	3:C:337:PX4:O3	0.51	2.05	14	1
3:B:360:PX4:O3	3:B:360:PX4:H9	0.51	2.06	1	2
3:B:347:PX4:O1	3:B:347:PX4:H3	0.51	2.06	13	2
3:C:312:PX4:H3	3:C:312:PX4:C6	0.51	2.36	4	1
3:B:363:PX4:H5	3:C:302:PX4:O2	0.51	2.05	14	1
3:B:369:PX4:H11	3:B:370:PX4:O6	0.51	2.05	14	1
3:A:613:PX4:O1	3:A:628:PX4:H4	0.51	2.05	1	1
3:B:390:PX4:H7	3:B:390:PX4:O3	0.51	2.05	3	4
3:B:370:PX4:O2	3:B:378:PX4:H5	0.51	2.06	15	1
3:C:327:PX4:H9	3:C:327:PX4:O2	0.51	2.05	8	2
3:A:606:PX4:H6	3:B:383:PX4:O3	0.51	2.06	9	1
3:A:618:PX4:H13	3:A:620:PX4:O3	0.51	2.05	2	1
3:C:351:PX4:O3	3:C:351:PX4:H13	0.51	2.06	6	4
3:B:367:PX4:H10	3:B:367:PX4:O3	0.51	2.06	6	3
3:A:644:PX4:H4	3:A:644:PX4:O2	0.51	2.05	11	2
3:A:614:PX4:H5	3:C:350:PX4:O2	0.51	2.05	14	1
3:A:621:PX4:O4	3:A:621:PX4:H6	0.51	2.05	2	1
3:C:302:PX4:H9	3:C:302:PX4:O1	0.51	2.05	2	1
3:A:627:PX4:O1	3:A:643:PX4:H13	0.51	2.04	4	1
3:B:341:PX4:O1	3:B:341:PX4:H3	0.51	2.05	7	1
3:C:342:PX4:O1	3:C:342:PX4:H3	0.51	2.06	13	1
3:A:610:PX4:O1	3:A:610:PX4:H3	0.51	2.05	15	2
2:C:173:ARG:HH11	2:C:177:HIS:CE1	0.51	2.24	14	1
3:A:611:PX4:C22	3:B:394:PX4:H44	0.51	2.36	10	1
3:A:623:PX4:H3	3:B:398:PX4:O8	0.51	2.05	11	1
3:B:312:PX4:H9	3:B:356:PX4:O1	0.51	2.05	2	1
3:C:358:PX4:O6	3:C:358:PX4:H8	0.51	2.06	2	2
3:B:355:PX4:O4	3:B:355:PX4:H4	0.51	2.06	8	1
3:A:618:PX4:O2	3:A:618:PX4:H4	0.51	2.05	10	1
3:B:369:PX4:O3	3:B:369:PX4:H13	0.51	2.06	14	1
3:C:353:PX4:O3	3:C:353:PX4:H12	0.51	2.06	6	1
3:B:354:PX4:O6	3:B:354:PX4:H12	0.51	2.06	7	1
2:B:72:TRP:NE1	3:B:341:PX4:H4	0.51	2.21	10	1
3:C:359:PX4:H3	3:C:359:PX4:O6	0.51	2.06	8	1
3:B:356:PX4:H43	3:C:333:PX4:H66	0.51	1.83	9	1
3:C:352:PX4:O3	3:C:352:PX4:H12	0.51	2.06	11	1
3:C:301:PX4:O3	3:C:301:PX4:H13	0.50	2.06	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:307:PX4:H4	3:B:318:PX4:O2	0.50	2.06	8	2
3:A:626:PX4:H6	3:C:362:PX4:O2	0.50	2.06	12	1
3:B:373:PX4:H3	3:B:380:PX4:O3	0.50	2.05	14	1
3:C:305:PX4:O1	3:C:324:PX4:H7	0.50	2.07	3	1
3:A:604:PX4:H3	3:B:392:PX4:O2	0.50	2.06	5	1
3:A:643:PX4:O3	3:A:643:PX4:H10	0.50	2.06	15	2
3:C:315:PX4:O3	3:C:348:PX4:H5	0.50	2.06	6	1
3:B:322:PX4:H4	3:B:322:PX4:O2	0.50	2.05	12	1
3:B:351:PX4:H7	3:B:354:PX4:H1	0.50	1.83	14	1
3:B:388:PX4:H9	3:B:388:PX4:O3	0.50	2.06	15	1
1:A:360:PHE:O	3:A:644:PX4:H10	0.50	2.06	4	2
3:B:310:PX4:H9	3:B:310:PX4:O3	0.50	2.06	8	2
1:A:405:GLU:OE2	3:A:641:PX4:H4	0.50	2.06	8	2
3:C:338:PX4:O2	3:C:345:PX4:H7	0.50	2.06	15	2
3:B:400:PX4:H11	3:C:363:PX4:H14	0.50	1.83	13	1
3:A:645:PX4:H4	3:A:645:PX4:O2	0.50	2.06	10	3
3:B:308:PX4:O3	3:B:308:PX4:H13	0.50	2.07	15	2
1:A:358:GLY:O	3:A:650:PX4:H4	0.50	2.06	15	1
3:A:623:PX4:H7	3:B:398:PX4:O1	0.50	2.06	15	1
3:A:650:PX4:O8	3:A:654:PX4:H11	0.50	2.07	2	1
3:B:322:PX4:O2	3:B:350:PX4:H11	0.50	2.07	4	2
3:A:602:PX4:O1	3:B:375:PX4:H3	0.50	2.07	13	1
3:B:338:PX4:H12	3:B:338:PX4:O3	0.50	2.07	4	3
3:B:354:PX4:H6	3:B:354:PX4:O6	0.50	2.07	2	1
3:A:651:PX4:O3	3:A:651:PX4:H7	0.50	2.07	3	3
2:B:177:HIS:CE1	2:C:133:GLU:OE1	0.50	2.65	6	1
3:B:359:PX4:O2	3:B:373:PX4:H11	0.50	2.06	8	1
3:B:309:PX4:H9	3:B:336:PX4:O1	0.50	2.06	9	1
3:C:304:PX4:H9	3:C:304:PX4:O3	0.50	2.07	9	2
3:A:654:PX4:O3	3:A:654:PX4:H6	0.50	2.06	11	1
3:B:351:PX4:H4	3:B:354:PX4:O2	0.50	2.07	11	1
3:C:331:PX4:H7	3:C:331:PX4:O3	0.50	2.07	3	1
3:A:615:PX4:H5	3:C:360:PX4:O8	0.50	2.07	4	1
3:A:654:PX4:O2	3:A:654:PX4:H3	0.50	2.07	7	2
3:C:344:PX4:H3	3:C:364:PX4:O8	0.50	2.06	7	1
3:B:359:PX4:O2	3:B:359:PX4:H4	0.50	2.06	9	1
3:C:320:PX4:H4	3:C:341:PX4:O4	0.50	2.06	10	1
3:B:337:PX4:O2	3:B:337:PX4:H13	0.50	2.06	13	2
3:A:616:PX4:O1	3:A:634:PX4:H5	0.50	2.07	14	2
3:B:334:PX4:H4	3:B:352:PX4:O2	0.50	2.07	13	1
3:B:306:PX4:H4	3:B:348:PX4:O1	0.50	2.06	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:354:PX4:O3	3:C:354:PX4:H10	0.50	2.07	4	1
3:C:320:PX4:H3	3:C:341:PX4:O1	0.50	2.07	6	1
1:A:484:TRP:CE2	1:A:498:PRO:HB3	0.50	2.41	7	2
2:B:205:GLU:OE1	3:B:321:PX4:H4	0.50	2.06	7	2
3:A:646:PX4:O2	3:A:646:PX4:H3	0.50	2.06	8	1
3:A:646:PX4:O1	3:A:646:PX4:H3	0.50	2.07	15	2
2:B:72:TRP:CG	3:B:341:PX4:H13	0.50	2.42	12	1
3:B:315:PX4:H9	3:B:336:PX4:O6	0.50	2.07	2	1
3:C:349:PX4:O2	3:C:349:PX4:H4	0.50	2.06	7	2
1:A:398:GLY:O	3:A:652:PX4:H6	0.50	2.07	13	2
2:B:263:ASN:OD1	3:B:331:PX4:H10	0.50	2.07	7	1
3:B:302:PX4:H72	3:C:306:PX4:H70	0.50	1.83	9	1
3:B:321:PX4:H3	3:B:321:PX4:O2	0.50	2.05	9	1
3:C:305:PX4:O4	3:C:311:PX4:H10	0.50	2.06	9	1
3:C:335:PX4:H6	3:C:335:PX4:O3	0.50	2.07	9	1
3:B:334:PX4:O2	3:B:348:PX4:H12	0.50	2.07	15	2
3:B:338:PX4:O1	3:B:338:PX4:H12	0.50	2.07	14	1
3:A:626:PX4:H13	3:C:362:PX4:C1	0.49	2.36	2	1
3:B:313:PX4:O3	3:B:313:PX4:H9	0.49	2.07	5	2
3:B:397:PX4:O3	3:B:397:PX4:H9	0.49	2.07	6	1
3:C:330:PX4:O3	3:C:330:PX4:H9	0.49	2.07	7	3
3:B:384:PX4:O2	3:B:384:PX4:H4	0.49	2.07	13	3
3:A:619:PX4:O3	3:A:619:PX4:H12	0.49	2.06	11	1
3:A:634:PX4:H6	3:A:634:PX4:O3	0.49	2.07	12	2
2:B:72:TRP:CE2	3:B:341:PX4:H13	0.49	2.42	14	1
3:B:320:PX4:H17	3:B:320:PX4:H3	0.49	1.84	14	1
3:C:313:PX4:H8	3:C:337:PX4:C6	0.49	2.37	15	1
3:B:382:PX4:O2	3:B:382:PX4:H3	0.49	2.06	9	1
3:A:620:PX4:H6	3:A:620:PX4:O1	0.49	2.07	13	1
3:B:351:PX4:O1	3:B:351:PX4:H3	0.49	2.08	12	4
2:B:76:GLU:CD	3:B:305:PX4:H10	0.49	2.32	3	1
3:C:336:PX4:O1	3:C:336:PX4:H3	0.49	2.07	3	1
3:C:326:PX4:H10	3:C:326:PX4:O3	0.49	2.07	4	2
3:A:640:PX4:H7	3:A:640:PX4:O4	0.49	2.07	7	1
3:A:616:PX4:O8	3:A:634:PX4:H11	0.49	2.07	11	1
3:B:327:PX4:H4	3:B:327:PX4:O2	0.49	2.06	11	6
3:C:361:PX4:O2	3:C:361:PX4:H4	0.49	2.08	2	2
3:A:620:PX4:H7	3:C:348:PX4:H17	0.49	1.84	5	1
3:B:339:PX4:H9	3:B:339:PX4:O3	0.49	2.06	6	1
3:B:361:PX4:O1	3:B:368:PX4:H12	0.49	2.07	6	2
3:C:364:PX4:O2	3:C:364:PX4:H4	0.49	2.06	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:225:LEU:HD23	2:C:82:LEU:HD21	0.49	1.84	10	1
2:B:245:GLU:O	2:B:249:VAL:HG23	0.49	2.08	13	1
3:B:378:PX4:H3	3:B:378:PX4:O4	0.49	2.07	15	2
3:B:334:PX4:H10	3:B:334:PX4:O3	0.49	2.07	2	1
3:C:312:PX4:H3	3:C:312:PX4:O4	0.49	2.07	15	3
3:C:322:PX4:O4	3:C:351:PX4:H4	0.49	2.08	6	1
3:B:301:PX4:O1	3:B:303:PX4:H13	0.49	2.07	13	1
3:C:331:PX4:H10	3:C:331:PX4:O1	0.49	2.08	15	1
3:A:605:PX4:O3	3:A:605:PX4:H12	0.49	2.07	3	2
3:A:610:PX4:H13	3:B:389:PX4:O2	0.49	2.07	6	1
3:B:362:PX4:H8	3:B:366:PX4:O2	0.49	2.07	1	1
3:B:376:PX4:O3	3:B:376:PX4:H6	0.49	2.07	1	2
3:B:326:PX4:O1	3:B:355:PX4:H3	0.49	2.07	2	1
3:A:642:PX4:O3	3:A:642:PX4:H7	0.49	2.08	3	1
3:B:400:PX4:O8	3:B:400:PX4:H12	0.49	2.08	12	1
3:B:365:PX4:H12	3:B:365:PX4:O2	0.49	2.08	13	2
2:C:80:GLU:OE1	3:C:304:PX4:H4	0.49	2.06	14	1
3:B:353:PX4:O2	3:B:369:PX4:H3	0.49	2.07	1	1
3:C:362:PX4:O2	3:C:362:PX4:H9	0.49	2.08	1	1
3:B:325:PX4:H6	3:B:357:PX4:O8	0.49	2.08	2	1
3:A:610:PX4:O2	3:B:379:PX4:H3	0.49	2.08	3	1
3:A:645:PX4:O1	3:A:648:PX4:H8	0.49	2.07	10	1
3:B:332:PX4:O3	3:B:332:PX4:H9	0.49	2.07	13	2
3:A:638:PX4:H10	3:A:648:PX4:O3	0.49	2.07	1	1
3:A:614:PX4:O2	3:A:625:PX4:H4	0.49	2.08	5	2
3:A:649:PX4:O4	3:A:652:PX4:H5	0.49	2.07	3	1
3:B:306:PX4:H4	3:B:348:PX4:O4	0.49	2.07	6	1
3:C:346:PX4:O1	3:C:346:PX4:H3	0.49	2.07	7	1
3:A:605:PX4:H3	3:B:379:PX4:O3	0.49	2.08	9	2
3:B:356:PX4:H7	3:B:356:PX4:O2	0.49	2.07	8	1
3:B:387:PX4:H6	3:B:387:PX4:O1	0.49	2.08	10	2
3:C:344:PX4:O1	3:C:344:PX4:H6	0.49	2.08	14	1
3:C:354:PX4:O3	3:C:354:PX4:H12	0.49	2.08	15	1
3:A:611:PX4:H8	3:B:394:PX4:O1	0.49	2.08	11	2
3:A:635:PX4:O6	3:A:637:PX4:H5	0.49	2.08	4	1
3:B:400:PX4:O4	3:B:400:PX4:H3	0.49	2.08	13	3
3:A:640:PX4:O3	3:A:640:PX4:H9	0.49	2.08	6	2
3:B:386:PX4:H10	3:B:386:PX4:O3	0.49	2.07	8	1
3:A:631:PX4:O4	3:A:642:PX4:H10	0.49	2.07	10	1
3:C:349:PX4:O4	3:C:349:PX4:H4	0.49	2.08	13	1
3:A:615:PX4:H8	3:C:345:PX4:O1	0.48	2.09	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:650:PX4:O3	3:A:650:PX4:H7	0.48	2.08	8	1
3:B:362:PX4:O3	3:B:366:PX4:H3	0.48	2.08	10	1
3:B:396:PX4:H37	3:C:361:PX4:H43	0.48	1.85	10	1
3:B:359:PX4:H18	3:B:373:PX4:H5	0.48	1.83	13	1
3:A:620:PX4:O8	3:A:636:PX4:H10	0.48	2.08	15	1
3:A:621:PX4:O1	3:A:621:PX4:H3	0.48	2.07	7	2
3:B:356:PX4:H5	3:B:373:PX4:O2	0.48	2.08	6	1
3:B:336:PX4:O3	3:B:336:PX4:H9	0.48	2.07	7	1
3:C:329:PX4:O2	3:C:329:PX4:H4	0.48	2.08	9	1
3:A:610:PX4:H3	3:B:389:PX4:O4	0.48	2.08	10	1
3:A:623:PX4:O1	3:A:640:PX4:C2	0.48	2.61	15	1
3:B:374:PX4:O1	3:B:384:PX4:H13	0.48	2.08	1	1
3:A:631:PX4:O8	3:A:642:PX4:H10	0.48	2.07	3	1
3:C:307:PX4:H9	3:C:343:PX4:O2	0.48	2.07	3	1
3:A:641:PX4:O1	3:A:651:PX4:H3	0.48	2.08	4	1
3:B:315:PX4:H4	3:B:315:PX4:O4	0.48	2.07	4	1
3:B:329:PX4:O4	3:B:355:PX4:H8	0.48	2.07	5	1
3:A:608:PX4:H3	3:A:611:PX4:O1	0.48	2.08	7	1
3:B:355:PX4:O2	3:B:377:PX4:H12	0.48	2.08	8	1
3:C:351:PX4:O5	3:C:351:PX4:H12	0.48	2.08	9	1
3:A:647:PX4:H4	3:A:652:PX4:O1	0.48	2.08	15	1
3:B:320:PX4:O2	3:B:340:PX4:H8	0.48	2.07	1	1
3:B:326:PX4:O1	3:B:355:PX4:H9	0.48	2.08	3	3
3:C:317:PX4:H12	3:C:317:PX4:O3	0.48	2.09	9	3
3:A:603:PX4:H3	3:A:603:PX4:O1	0.48	2.08	8	1
3:C:351:PX4:O1	3:C:359:PX4:H6	0.48	2.09	11	1
3:B:350:PX4:O1	3:B:374:PX4:H13	0.48	2.09	13	1
3:B:383:PX4:H10	3:B:383:PX4:H14	0.48	1.83	1	1
3:C:344:PX4:O2	3:C:344:PX4:H4	0.48	2.09	1	2
3:A:621:PX4:O2	3:A:621:PX4:H6	0.48	2.09	3	1
3:B:315:PX4:H3	3:B:336:PX4:O1	0.48	2.09	10	2
3:A:652:PX4:O3	3:A:652:PX4:H13	0.48	2.09	10	2
3:B:327:PX4:O8	3:B:354:PX4:H13	0.48	2.08	10	1
2:C:76:GLU:OE1	3:C:304:PX4:H12	0.48	2.08	12	1
1:A:365:PRO:HG2	1:A:388:TRP:CZ2	0.48	2.43	1	1
1:A:393:ALA:O	3:A:644:PX4:H9	0.48	2.08	4	2
3:B:338:PX4:H48	3:B:343:PX4:H11	0.48	1.86	2	1
3:A:644:PX4:O1	3:A:644:PX4:H6	0.48	2.08	3	1
3:B:325:PX4:H13	3:B:325:PX4:O3	0.48	2.07	10	1
2:B:72:TRP:CZ2	3:B:341:PX4:H6	0.48	2.43	14	2
3:B:359:PX4:O2	3:B:380:PX4:H4	0.48	2.09	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:332:PX4:H7	3:B:332:PX4:O3	0.48	2.09	3	1
3:B:391:PX4:H12	3:B:391:PX4:O3	0.48	2.09	15	3
3:B:321:PX4:O3	3:B:321:PX4:H9	0.48	2.08	6	1
3:C:355:PX4:H10	3:C:355:PX4:O3	0.48	2.09	6	4
3:A:631:PX4:O2	3:A:631:PX4:H7	0.48	2.09	8	1
3:B:322:PX4:O4	3:B:350:PX4:H5	0.48	2.09	4	1
3:B:399:PX4:O2	3:B:399:PX4:H4	0.48	2.08	7	1
2:B:262:LEU:O	3:B:331:PX4:H5	0.48	2.07	11	1
3:C:345:PX4:H12	3:C:345:PX4:O3	0.48	2.07	14	2
3:C:358:PX4:H9	3:C:361:PX4:O1	0.48	2.09	12	1
2:B:221:HIS:CD2	2:C:86:MET:HG2	0.48	2.43	14	1
3:A:634:PX4:H3	3:A:634:PX4:O7	0.48	2.08	15	1
3:B:341:PX4:O2	3:B:346:PX4:H3	0.48	2.09	1	1
3:A:644:PX4:O3	3:A:650:PX4:H4	0.48	2.09	2	1
3:B:322:PX4:O2	3:B:322:PX4:H3	0.48	2.08	3	1
3:C:324:PX4:O2	3:C:345:PX4:H7	0.48	2.09	4	1
3:C:354:PX4:O8	3:C:354:PX4:H12	0.48	2.09	6	1
3:C:331:PX4:O2	3:C:331:PX4:H4	0.48	2.08	7	1
3:A:614:PX4:H10	3:A:628:PX4:O2	0.48	2.09	10	1
3:B:376:PX4:O1	3:B:390:PX4:H12	0.48	2.09	10	1
3:B:359:PX4:H4	3:B:359:PX4:O4	0.48	2.08	11	1
3:B:303:PX4:H22	3:C:334:PX4:H70	0.48	1.84	12	1
3:A:645:PX4:H6	3:A:646:PX4:O2	0.47	2.08	11	5
3:B:325:PX4:H3	3:B:357:PX4:O8	0.47	2.09	3	1
3:C:320:PX4:H3	3:C:341:PX4:O4	0.47	2.08	4	1
3:B:320:PX4:O2	3:B:320:PX4:H9	0.47	2.09	8	1
3:B:315:PX4:O3	3:B:315:PX4:H7	0.47	2.09	10	1
3:C:303:PX4:O3	3:C:303:PX4:H12	0.47	2.09	13	2
3:B:373:PX4:H13	3:B:380:PX4:O4	0.47	2.09	13	1
3:B:334:PX4:O3	3:B:334:PX4:H12	0.47	2.09	14	1
3:B:359:PX4:O4	3:B:373:PX4:H13	0.47	2.09	15	1
3:A:626:PX4:H13	3:C:362:PX4:H2	0.47	1.86	2	1
3:B:350:PX4:O1	3:B:374:PX4:H11	0.47	2.09	8	2
2:C:80:GLU:CD	3:C:304:PX4:H4	0.47	2.34	14	1
3:A:637:PX4:O3	3:A:637:PX4:H7	0.47	2.08	3	3
3:C:341:PX4:O3	3:C:341:PX4:H6	0.47	2.09	6	2
3:B:373:PX4:H10	3:B:373:PX4:O3	0.47	2.08	8	3
3:C:315:PX4:O3	3:C:348:PX4:H6	0.47	2.09	5	1
2:B:130:TRP:HE1	2:C:177:HIS:CE1	0.47	2.27	8	1
3:C:306:PX4:H12	3:C:306:PX4:O3	0.47	2.08	12	2
3:B:378:PX4:H5	3:B:386:PX4:H46	0.47	1.85	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:389:PX4:O2	3:B:389:PX4:H4	0.47	2.08	14	1
3:A:639:PX4:O1	3:A:639:PX4:H3	0.47	2.09	3	1
3:C:305:PX4:O2	3:C:305:PX4:H4	0.47	2.10	14	2
3:C:328:PX4:H10	3:C:328:PX4:O3	0.47	2.10	4	1
3:B:316:PX4:H3	3:B:316:PX4:O2	0.47	2.10	5	1
3:B:330:PX4:O4	3:B:330:PX4:H3	0.47	2.09	12	1
3:B:366:PX4:O3	3:B:366:PX4:H13	0.47	2.09	14	2
3:B:346:PX4:H10	3:B:346:PX4:O3	0.47	2.10	15	1
3:C:358:PX4:O3	3:C:358:PX4:H12	0.47	2.09	2	4
3:C:339:PX4:H10	3:C:339:PX4:O3	0.47	2.09	5	1
3:A:610:PX4:O3	3:A:610:PX4:H9	0.47	2.10	10	3
3:B:376:PX4:O2	3:B:392:PX4:H9	0.47	2.09	7	1
3:A:638:PX4:H7	3:A:648:PX4:O2	0.47	2.09	8	1
3:A:638:PX4:H6	3:A:638:PX4:O3	0.47	2.09	14	1
3:A:629:PX4:O4	3:A:631:PX4:H13	0.47	2.10	4	4
2:B:55:SER:N	2:B:58:SER:HG	0.47	2.08	2	2
2:B:120:GLU:OE1	3:B:311:PX4:H7	0.47	2.10	8	1
3:A:604:PX4:O3	3:B:392:PX4:H4	0.47	2.09	12	1
3:B:399:PX4:H6	3:C:357:PX4:O3	0.47	2.10	14	1
3:B:320:PX4:O3	3:B:320:PX4:H9	0.47	2.10	12	3
3:B:333:PX4:O3	3:B:333:PX4:H6	0.47	2.09	1	2
3:B:320:PX4:O4	3:B:340:PX4:H7	0.47	2.10	2	1
3:B:367:PX4:C4	3:B:367:PX4:O3	0.47	2.62	5	1
3:A:631:PX4:O6	3:A:642:PX4:H10	0.47	2.09	6	1
3:B:365:PX4:H6	3:B:365:PX4:O3	0.47	2.10	6	1
3:A:628:PX4:H6	3:A:628:PX4:O3	0.47	2.09	7	1
3:A:642:PX4:O2	3:A:651:PX4:H5	0.47	2.09	11	2
3:A:632:PX4:H10	3:A:632:PX4:O4	0.47	2.09	9	1
3:B:323:PX4:O6	3:B:346:PX4:H13	0.47	2.09	10	2
3:B:335:PX4:O2	3:B:335:PX4:H4	0.47	2.10	12	1
3:C:331:PX4:H10	3:C:331:PX4:O3	0.47	2.08	14	1
3:A:613:PX4:H11	3:C:345:PX4:O4	0.47	2.09	15	1
3:B:399:PX4:H3	3:C:357:PX4:O4	0.47	2.10	15	1
1:A:323:PHE:CE2	1:A:506:MET:HE3	0.47	2.45	12	2
3:B:372:PX4:O2	3:B:372:PX4:H4	0.47	2.10	2	2
3:A:632:PX4:H9	3:A:647:PX4:O2	0.47	2.10	6	1
3:B:352:PX4:H10	3:B:368:PX4:O6	0.47	2.10	12	1
3:C:311:PX4:H7	3:C:311:PX4:O3	0.47	2.10	15	1
3:A:626:PX4:H5	3:A:638:PX4:O1	0.47	2.10	1	1
3:A:633:PX4:H15	3:A:633:PX4:H10	0.47	1.87	1	1
3:C:306:PX4:H11	3:C:350:PX4:O1	0.47	2.09	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:350:PX4:H10	3:C:350:PX4:O3	0.47	2.10	2	1
3:C:320:PX4:H11	3:C:330:PX4:H9	0.47	1.86	4	1
3:B:338:PX4:C25	3:B:343:PX4:H8	0.47	2.40	8	1
3:C:316:PX4:H9	3:C:342:PX4:O2	0.47	2.10	9	1
3:B:336:PX4:H8	3:B:343:PX4:O1	0.47	2.10	10	2
3:A:602:PX4:H10	3:A:602:PX4:O3	0.47	2.10	11	1
3:B:351:PX4:H7	3:B:354:PX4:C1	0.47	2.40	14	1
1:A:392:GLU:O	3:A:644:PX4:H9	0.47	2.10	1	1
3:B:344:PX4:O3	3:B:344:PX4:H7	0.47	2.10	1	2
3:B:343:PX4:C20	3:C:336:PX4:H70	0.47	2.40	2	1
3:A:639:PX4:H6	3:A:639:PX4:O3	0.47	2.10	13	5
3:B:338:PX4:P1	3:B:358:PX4:H6	0.47	2.50	6	1
3:C:307:PX4:H12	3:C:307:PX4:O3	0.47	2.10	6	1
2:B:105:GLN:OE1	3:B:303:PX4:H13	0.47	2.10	9	1
3:B:364:PX4:H11	3:C:301:PX4:O1	0.47	2.08	10	1
3:C:320:PX4:H5	3:C:330:PX4:O3	0.47	2.10	10	1
2:C:83:ARG:HA	3:C:312:PX4:H59	0.47	1.87	12	1
3:C:339:PX4:O3	3:C:339:PX4:H7	0.47	2.10	14	1
3:A:641:PX4:O4	3:A:641:PX4:H3	0.47	2.10	15	1
3:C:363:PX4:O3	3:C:363:PX4:H10	0.46	2.10	1	1
3:A:627:PX4:O2	3:A:643:PX4:H13	0.46	2.11	3	1
3:B:338:PX4:O4	3:B:338:PX4:H3	0.46	2.09	3	1
3:A:631:PX4:H11	3:A:646:PX4:O1	0.46	2.09	14	2
3:A:604:PX4:C6	3:A:604:PX4:H4	0.46	2.40	12	1
3:C:323:PX4:O2	3:C:342:PX4:H4	0.46	2.10	12	1
3:C:327:PX4:H5	3:C:334:PX4:O2	0.46	2.09	13	1
3:A:618:PX4:P1	3:A:633:PX4:H3	0.46	2.50	14	1
1:A:368:ILE:H	1:A:368:ILE:HD13	0.46	1.69	2	1
3:C:312:PX4:H7	3:C:312:PX4:C6	0.46	2.39	5	1
3:B:342:PX4:O3	3:B:350:PX4:H13	0.46	2.10	7	2
3:A:626:PX4:H13	3:C:362:PX4:O3	0.46	2.09	2	1
3:B:395:PX4:H12	3:C:358:PX4:O3	0.46	2.11	3	1
3:C:303:PX4:O1	3:C:303:PX4:H4	0.46	2.10	3	1
3:C:311:PX4:H4	3:C:311:PX4:O2	0.46	2.10	4	1
3:A:632:PX4:H10	3:A:632:PX4:O3	0.46	2.09	14	2
2:B:80:GLU:OE1	3:B:305:PX4:H10	0.46	2.09	6	1
3:A:614:PX4:H10	3:A:614:PX4:O4	0.46	2.10	11	1
3:A:624:PX4:O4	3:A:639:PX4:H9	0.46	2.11	7	1
2:B:72:TRP:CE2	3:B:341:PX4:H4	0.46	2.46	10	1
3:B:353:PX4:O2	3:B:369:PX4:H4	0.46	2.11	11	1
3:B:312:PX4:H12	3:B:312:PX4:O3	0.46	2.10	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:615:PX4:H12	3:A:615:PX4:O3	0.46	2.10	14	1
3:C:307:PX4:H9	3:C:343:PX4:O1	0.46	2.11	1	1
3:C:357:PX4:O3	3:C:357:PX4:H6	0.46	2.11	1	2
3:C:305:PX4:O2	3:C:311:PX4:H9	0.46	2.10	3	1
3:C:308:PX4:O1	3:C:308:PX4:H12	0.46	2.10	3	1
3:B:392:PX4:H3	3:B:392:PX4:H14	0.46	1.86	4	1
3:B:391:PX4:H4	3:C:303:PX4:O2	0.46	2.11	1	1
3:B:388:PX4:O3	3:B:388:PX4:H7	0.46	2.09	9	3
3:B:327:PX4:O2	3:B:327:PX4:H4	0.46	2.10	5	1
3:B:392:PX4:H3	3:B:392:PX4:H15	0.46	1.88	5	1
3:C:333:PX4:H29	3:C:333:PX4:H38	0.46	1.86	7	1
3:B:400:PX4:H9	3:B:400:PX4:O3	0.46	2.11	9	1
3:C:329:PX4:O1	3:C:354:PX4:H8	0.46	2.10	9	1
3:A:607:PX4:O2	3:A:612:PX4:H12	0.46	2.10	10	1
3:A:601:PX4:O2	3:B:372:PX4:H9	0.46	2.11	13	1
3:B:340:PX4:O4	3:B:340:PX4:H4	0.46	2.10	13	2
2:C:173:ARG:HE	2:C:177:HIS:CD2	0.46	2.28	13	1
3:A:640:PX4:O1	3:A:640:PX4:H4	0.46	2.10	2	1
3:A:605:PX4:H11	3:B:379:PX4:O3	0.46	2.10	3	1
3:C:323:PX4:O2	3:C:342:PX4:H8	0.46	2.09	3	1
1:A:371:ALA:HB2	1:A:381:PHE:CD2	0.46	2.45	4	1
3:A:605:PX4:H13	3:B:379:PX4:C6	0.46	2.40	9	3
3:B:397:PX4:O1	3:B:397:PX4:H3	0.46	2.11	8	1
3:C:315:PX4:O4	3:C:315:PX4:H4	0.46	2.11	10	1
3:B:309:PX4:O3	3:B:309:PX4:H6	0.46	2.11	14	1
3:C:357:PX4:O3	3:C:357:PX4:C3	0.46	2.64	1	1
3:B:400:PX4:H9	3:B:400:PX4:O8	0.46	2.11	3	1
3:A:631:PX4:H8	3:A:646:PX4:O4	0.46	2.10	4	2
2:B:262:LEU:O	3:B:331:PX4:H9	0.46	2.11	5	1
3:A:624:PX4:O1	3:A:639:PX4:H9	0.46	2.10	8	1
3:A:616:PX4:O2	3:A:616:PX4:H7	0.46	2.11	11	1
1:A:387:HIS:CE1	1:A:406:LEU:HB2	0.46	2.46	12	1
3:C:343:PX4:O3	3:C:343:PX4:H12	0.46	2.11	12	1
3:A:632:PX4:H9	3:A:647:PX4:C6	0.46	2.41	13	1
3:C:305:PX4:O6	3:C:311:PX4:H3	0.46	2.11	14	1
3:B:373:PX4:H13	3:B:380:PX4:O3	0.46	2.10	6	2
3:B:364:PX4:O3	3:B:364:PX4:H7	0.46	2.11	6	2
3:B:310:PX4:H9	3:B:310:PX4:P1	0.46	2.51	10	2
3:A:630:PX4:O2	3:A:633:PX4:H13	0.46	2.11	10	1
3:B:361:PX4:H4	3:B:368:PX4:C1	0.46	2.41	10	1
3:B:383:PX4:O3	3:B:383:PX4:C4	0.46	2.64	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:362:PX4:O3	3:C:362:PX4:H7	0.46	2.10	14	1
3:A:605:PX4:O3	3:B:379:PX4:H3	0.46	2.11	1	1
3:A:630:PX4:O3	3:A:630:PX4:H6	0.46	2.11	3	1
3:A:642:PX4:O3	3:A:642:PX4:C3	0.46	2.64	3	1
3:C:320:PX4:H8	3:C:330:PX4:O3	0.46	2.11	6	1
3:B:387:PX4:H7	3:B:390:PX4:O3	0.46	2.11	10	1
3:C:315:PX4:O2	3:C:315:PX4:H4	0.46	2.11	15	1
3:B:306:PX4:H3	3:B:339:PX4:O8	0.45	2.11	8	2
3:A:649:PX4:H18	3:A:649:PX4:H13	0.45	1.87	9	1
3:C:307:PX4:H4	3:C:343:PX4:O2	0.45	2.11	10	1
3:C:323:PX4:O2	3:C:342:PX4:H3	0.45	2.11	11	1
3:B:326:PX4:O4	3:B:326:PX4:H3	0.45	2.11	1	1
3:B:337:PX4:O1	3:B:337:PX4:H3	0.45	2.11	1	1
2:C:180:ALA:O	2:C:184:HIS:CD2	0.45	2.70	2	1
3:C:320:PX4:H11	3:C:330:PX4:O4	0.45	2.11	3	1
3:A:620:PX4:H12	3:C:348:PX4:O1	0.45	2.11	4	1
3:C:352:PX4:O2	3:C:352:PX4:H3	0.45	2.11	8	1
3:B:320:PX4:O2	3:B:340:PX4:H7	0.45	2.10	11	1
2:B:142:GLU:OE1	3:B:328:PX4:H10	0.45	2.11	13	1
3:C:309:PX4:H10	3:C:309:PX4:O3	0.45	2.11	8	3
3:A:636:PX4:H9	3:A:636:PX4:O3	0.45	2.11	4	1
3:B:392:PX4:O3	3:B:392:PX4:C5	0.45	2.64	4	1
3:C:324:PX4:H3	3:C:324:PX4:O1	0.45	2.11	4	2
3:A:633:PX4:H44	3:A:633:PX4:H68	0.45	1.89	6	1
3:B:388:PX4:O1	3:B:388:PX4:H9	0.45	2.12	11	1
3:B:335:PX4:H10	3:B:353:PX4:O2	0.45	2.11	12	1
3:B:380:PX4:O1	3:B:387:PX4:H8	0.45	2.10	12	1
3:B:331:PX4:O1	3:B:331:PX4:H3	0.45	2.11	2	1
3:B:380:PX4:O1	3:B:387:PX4:H10	0.45	2.11	3	2
2:C:207:GLY:HA2	2:C:210:ARG:NH2	0.45	2.26	3	1
3:C:305:PX4:H6	3:C:324:PX4:H6	0.45	1.88	3	1
3:B:326:PX4:C1	3:B:355:PX4:H7	0.45	2.41	5	1
3:B:370:PX4:H6	3:B:386:PX4:O1	0.45	2.12	5	1
3:B:334:PX4:H10	3:B:334:PX4:P1	0.45	2.51	6	1
3:C:342:PX4:H9	3:C:342:PX4:O3	0.45	2.11	7	1
3:A:618:PX4:H3	3:A:620:PX4:O8	0.45	2.12	8	1
3:A:648:PX4:H72	3:A:653:PX4:H34	0.45	1.88	10	1
3:A:615:PX4:O1	3:A:615:PX4:H3	0.45	2.11	11	1
3:B:400:PX4:H3	3:B:400:PX4:O8	0.45	2.12	13	1
3:B:362:PX4:O3	3:B:362:PX4:H13	0.45	2.12	4	2
3:A:645:PX4:H6	3:A:646:PX4:O3	0.45	2.12	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:622:PX4:O4	3:A:622:PX4:H3	0.45	2.12	5	1
3:B:336:PX4:H72	3:C:305:PX4:H37	0.45	1.87	5	1
3:A:635:PX4:O6	3:A:637:PX4:H11	0.45	2.12	6	1
3:A:644:PX4:O2	3:A:650:PX4:H4	0.45	2.12	6	1
3:C:330:PX4:O2	3:C:330:PX4:H9	0.45	2.12	11	1
1:A:347:ASN:HA	1:A:505:TRP:O	0.45	2.12	12	1
3:B:345:PX4:O3	3:B:345:PX4:H7	0.45	2.12	14	1
3:C:347:PX4:O3	3:C:347:PX4:C5	0.45	2.64	14	1
3:A:633:PX4:C1	3:A:638:PX4:H6	0.45	2.42	5	1
3:A:632:PX4:H3	3:A:643:PX4:O1	0.45	2.12	9	2
3:B:351:PX4:H12	3:B:351:PX4:O3	0.45	2.12	9	1
3:B:302:PX4:O2	3:B:302:PX4:H7	0.45	2.11	11	1
3:A:635:PX4:O1	3:A:637:PX4:H5	0.45	2.12	15	1
3:B:322:PX4:H12	3:B:322:PX4:O3	0.45	2.11	1	1
3:C:343:PX4:H3	3:C:343:PX4:O1	0.45	2.12	5	2
3:A:610:PX4:H45	3:A:649:PX4:H44	0.45	1.89	6	1
3:B:342:PX4:O4	3:B:350:PX4:H13	0.45	2.12	10	2
3:B:364:PX4:H15	3:C:303:PX4:H10	0.45	1.89	6	1
3:C:316:PX4:O8	3:C:316:PX4:H4	0.45	2.12	9	1
2:C:131:GLN:OE1	2:C:131:GLN:HA	0.45	2.12	12	1
3:A:611:PX4:H13	3:A:611:PX4:O3	0.45	2.12	13	1
3:A:618:PX4:O1	3:A:633:PX4:H3	0.45	2.12	14	1
3:A:637:PX4:O2	3:A:637:PX4:H3	0.45	2.10	14	1
3:A:650:PX4:H9	3:A:650:PX4:O3	0.45	2.12	14	1
3:B:373:PX4:H3	3:B:380:PX4:C1	0.45	2.40	14	1
3:B:400:PX4:O3	3:B:400:PX4:H6	0.45	2.12	2	2
3:B:353:PX4:H8	3:B:382:PX4:O2	0.45	2.11	3	2
3:B:360:PX4:O2	3:B:362:PX4:H10	0.45	2.12	5	1
3:B:397:PX4:H7	3:C:347:PX4:H10	0.45	1.89	6	1
3:A:627:PX4:H45	3:A:647:PX4:H69	0.45	1.89	7	1
3:A:634:PX4:H47	3:A:634:PX4:H7	0.45	1.87	12	1
3:C:304:PX4:O2	3:C:347:PX4:H6	0.45	2.12	12	1
3:B:395:PX4:O3	3:B:395:PX4:H13	0.45	2.12	1	1
3:B:363:PX4:H7	3:C:302:PX4:O1	0.45	2.11	7	1
3:B:349:PX4:O3	3:B:349:PX4:H13	0.45	2.11	11	1
3:C:309:PX4:O4	3:C:327:PX4:H12	0.44	2.11	4	2
3:B:342:PX4:O6	3:B:367:PX4:H6	0.44	2.11	5	1
3:B:367:PX4:O3	3:B:367:PX4:H10	0.44	2.12	5	1
2:C:234:GLU:CD	2:C:237:ARG:HH11	0.44	2.20	5	1
3:A:608:PX4:H10	3:A:611:PX4:O2	0.44	2.12	8	1
3:B:370:PX4:H9	3:B:378:PX4:H10	0.44	1.89	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:133:GLU:CD	2:C:173:ARG:HH22	0.44	2.20	14	1
3:C:301:PX4:H4	3:C:301:PX4:O2	0.44	2.12	15	1
3:B:360:PX4:O1	3:B:362:PX4:H10	0.44	2.13	4	1
3:C:316:PX4:H7	3:C:342:PX4:P1	0.44	2.52	7	1
3:C:350:PX4:O2	3:C:355:PX4:H7	0.44	2.13	9	1
3:B:378:PX4:H13	3:B:386:PX4:O1	0.44	2.13	15	1
3:B:364:PX4:H3	3:B:364:PX4:O1	0.44	2.13	1	1
3:A:653:PX4:H7	3:A:653:PX4:O2	0.44	2.13	2	2
3:B:331:PX4:O3	3:B:331:PX4:H12	0.44	2.12	4	2
2:B:106:LYS:NZ	2:B:110:GLU:OE1	0.44	2.50	8	2
3:B:326:PX4:H13	3:B:355:PX4:O3	0.44	2.13	6	1
3:C:334:PX4:O2	3:C:334:PX4:H4	0.44	2.13	8	1
3:A:645:PX4:O3	3:A:648:PX4:H5	0.44	2.12	9	1
3:B:338:PX4:O6	3:B:358:PX4:H4	0.44	2.12	11	1
3:A:636:PX4:H3	3:A:636:PX4:C6	0.44	2.42	12	1
3:A:605:PX4:H8	3:B:344:PX4:C5	0.44	2.43	13	1
3:B:360:PX4:H12	3:B:360:PX4:O6	0.44	2.12	13	1
3:A:610:PX4:O1	3:B:379:PX4:H8	0.44	2.11	7	1
3:A:627:PX4:O6	3:C:361:PX4:H8	0.44	2.12	7	1
3:C:323:PX4:O3	3:C:323:PX4:H7	0.44	2.12	10	1
3:B:380:PX4:O6	3:B:387:PX4:H10	0.44	2.13	1	1
3:B:371:PX4:H6	3:B:371:PX4:O1	0.44	2.12	7	1
3:A:611:PX4:O3	3:A:611:PX4:H13	0.44	2.12	8	1
3:A:619:PX4:H4	3:A:632:PX4:O2	0.44	2.12	11	1
3:A:642:PX4:H69	3:A:648:PX4:H59	0.44	1.90	13	1
3:C:317:PX4:O6	3:C:344:PX4:H9	0.44	2.13	2	1
3:A:629:PX4:O6	3:A:631:PX4:H13	0.44	2.13	5	1
2:B:175:ARG:HG2	3:B:318:PX4:H13	0.44	1.89	7	1
3:C:340:PX4:H7	3:C:340:PX4:O3	0.44	2.13	9	2
2:B:200:LEU:C	2:B:200:LEU:HD23	0.44	2.38	15	1
2:B:212:ALA:HB2	3:B:322:PX4:H12	0.44	1.88	15	1
3:C:320:PX4:H11	3:C:330:PX4:O3	0.44	2.13	9	2
3:A:605:PX4:O1	3:A:609:PX4:H10	0.44	2.13	4	1
3:A:609:PX4:H6	3:A:609:PX4:O3	0.44	2.12	4	1
3:B:303:PX4:H4	3:B:303:PX4:O2	0.44	2.13	5	1
3:C:315:PX4:O3	3:C:315:PX4:H7	0.44	2.12	6	1
3:B:320:PX4:H6	3:B:340:PX4:C6	0.44	2.43	7	1
3:B:377:PX4:O3	3:B:377:PX4:H6	0.44	2.13	7	1
3:B:375:PX4:O2	3:B:392:PX4:H4	0.44	2.12	15	1
3:B:307:PX4:O3	3:B:307:PX4:H12	0.44	2.13	3	1
3:B:337:PX4:O2	3:B:337:PX4:H3	0.44	2.11	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:627:PX4:O1	3:A:643:PX4:H3	0.44	2.13	5	1
3:C:322:PX4:C1	3:C:322:PX4:H15	0.44	2.43	7	1
3:C:351:PX4:O1	3:C:359:PX4:H4	0.44	2.12	12	2
3:C:358:PX4:O8	3:C:361:PX4:H7	0.44	2.13	7	1
3:A:626:PX4:H10	3:C:346:PX4:H47	0.44	1.89	9	1
3:B:304:PX4:H14	3:B:345:PX4:H6	0.44	1.90	14	1
3:B:400:PX4:O8	3:B:400:PX4:H3	0.44	2.12	3	1
3:B:398:PX4:H10	3:B:398:PX4:O3	0.44	2.12	4	1
3:C:334:PX4:O3	3:C:334:PX4:H13	0.44	2.12	15	4
3:B:400:PX4:H11	3:C:347:PX4:C6	0.44	2.43	9	1
3:B:374:PX4:H10	3:B:374:PX4:O3	0.44	2.13	11	1
1:A:382:PHE:CD1	1:A:387:HIS:HB3	0.44	2.48	12	1
3:A:631:PX4:H45	3:B:381:PX4:H43	0.43	1.89	3	1
3:C:351:PX4:O1	3:C:351:PX4:H13	0.43	2.13	4	1
3:B:312:PX4:O2	3:B:317:PX4:H4	0.43	2.13	6	1
3:B:376:PX4:O1	3:B:390:PX4:H6	0.43	2.12	8	1
3:B:379:PX4:O1	3:B:379:PX4:H9	0.43	2.13	12	1
3:B:378:PX4:H4	3:B:386:PX4:O4	0.43	2.13	14	1
3:B:311:PX4:O1	3:B:345:PX4:H12	0.43	2.13	3	1
3:A:633:PX4:O3	3:A:638:PX4:H6	0.43	2.13	5	1
3:A:641:PX4:O3	3:A:641:PX4:C4	0.43	2.66	7	2
3:B:340:PX4:O2	3:B:340:PX4:H4	0.43	2.13	15	2
3:B:400:PX4:H11	3:C:347:PX4:O7	0.43	2.14	7	1
3:A:608:PX4:H5	3:A:611:PX4:H2	0.43	1.89	12	1
3:C:345:PX4:O1	3:C:345:PX4:H3	0.43	2.13	13	2
2:B:262:LEU:O	3:B:331:PX4:H13	0.43	2.13	14	1
3:B:367:PX4:H13	3:B:377:PX4:O2	0.43	2.13	15	1
3:B:357:PX4:O4	3:B:357:PX4:H4	0.43	2.13	2	1
3:A:605:PX4:H8	3:B:379:PX4:O2	0.43	2.14	3	1
3:A:615:PX4:O2	3:A:615:PX4:H3	0.43	2.13	5	1
3:C:323:PX4:H16	3:C:323:PX4:H4	0.43	1.90	5	1
1:A:402:HIS:HE1	3:A:649:PX4:H12	0.43	1.62	7	1
3:C:301:PX4:C6	3:C:301:PX4:H2	0.43	2.43	8	1
3:C:362:PX4:O2	3:C:362:PX4:H4	0.43	2.13	10	1
3:A:630:PX4:H40	3:B:391:PX4:H72	0.43	1.90	14	1
3:A:633:PX4:O3	3:A:633:PX4:H10	0.43	2.13	3	2
3:B:327:PX4:O8	3:B:354:PX4:H5	0.43	2.13	5	1
3:C:315:PX4:C1	3:C:348:PX4:H6	0.43	2.44	5	1
3:C:310:PX4:H65	3:C:343:PX4:H71	0.43	1.89	10	1
3:B:321:PX4:H7	3:B:321:PX4:O3	0.43	2.13	12	1
3:A:606:PX4:O2	3:C:302:PX4:H10	0.43	2.13	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:323:PX4:H4	3:C:323:PX4:H16	0.43	1.90	4	1
3:B:313:PX4:O3	3:B:313:PX4:C4	0.43	2.66	5	1
3:B:397:PX4:O8	3:C:312:PX4:H17	0.43	2.13	5	1
3:B:390:PX4:O2	3:B:392:PX4:H6	0.43	2.14	7	1
3:B:379:PX4:O3	3:B:379:PX4:H9	0.43	2.14	9	1
3:B:398:PX4:C9	3:B:398:PX4:H26	0.43	2.43	9	1
3:B:357:PX4:O1	3:B:357:PX4:H4	0.43	2.13	1	1
3:A:620:PX4:H4	3:C:348:PX4:O1	0.43	2.14	3	1
3:A:636:PX4:O8	3:A:636:PX4:H15	0.43	2.13	4	1
3:B:374:PX4:O3	3:B:374:PX4:H7	0.43	2.14	4	1
3:B:397:PX4:H5	3:C:304:PX4:O1	0.43	2.14	4	1
3:A:617:PX4:O1	3:A:617:PX4:H3	0.43	2.13	9	1
3:B:399:PX4:O1	3:C:326:PX4:H3	0.43	2.14	9	1
3:B:387:PX4:O1	3:B:390:PX4:H9	0.43	2.13	10	1
3:A:631:PX4:O1	3:A:642:PX4:H10	0.43	2.13	15	1
3:C:316:PX4:H13	3:C:323:PX4:O1	0.43	2.14	15	1
3:A:646:PX4:H9	3:A:646:PX4:O3	0.43	2.14	14	2
3:B:324:PX4:H3	3:B:324:PX4:O1	0.43	2.13	5	1
3:B:316:PX4:H8	3:B:321:PX4:O1	0.43	2.13	6	1
3:C:310:PX4:O3	3:C:310:PX4:H13	0.43	2.13	11	2
3:C:318:PX4:O3	3:C:318:PX4:H6	0.43	2.14	10	2
1:A:399:TYR:CD1	1:A:401:LYS:HG3	0.43	2.48	12	1
3:A:632:PX4:O3	3:A:632:PX4:C4	0.43	2.67	12	1
3:B:326:PX4:O1	3:B:326:PX4:H3	0.43	2.13	12	1
3:B:335:PX4:O3	3:B:335:PX4:H7	0.43	2.13	12	1
3:B:394:PX4:O3	3:B:394:PX4:H7	0.43	2.14	12	1
3:C:349:PX4:H10	3:C:349:PX4:O8	0.43	2.14	13	1
3:A:644:PX4:H9	3:A:650:PX4:O1	0.43	2.14	14	1
1:A:362:ARG:NH2	3:A:650:PX4:H9	0.43	2.29	15	1
3:A:635:PX4:H15	3:A:637:PX4:H8	0.43	1.91	15	1
3:B:342:PX4:O3	3:B:342:PX4:H13	0.43	2.14	4	2
3:A:614:PX4:H13	3:A:628:PX4:O1	0.43	2.14	9	1
3:B:365:PX4:O3	3:B:365:PX4:H12	0.43	2.12	10	1
3:C:335:PX4:O1	3:C:335:PX4:H3	0.43	2.14	10	1
3:B:308:PX4:H63	3:B:323:PX4:H38	0.43	1.91	14	1
3:B:335:PX4:O3	3:B:335:PX4:H13	0.43	2.14	3	1
3:B:375:PX4:O1	3:B:376:PX4:H8	0.43	2.14	3	1
3:B:328:PX4:O3	3:B:328:PX4:H13	0.43	2.14	5	1
3:C:359:PX4:H9	3:C:359:PX4:O3	0.43	2.14	12	1
3:B:312:PX4:H3	3:B:312:PX4:C6	0.43	2.44	14	1
3:A:641:PX4:C6	3:A:641:PX4:H3	0.43	2.44	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:395:PX4:H4	3:B:395:PX4:O2	0.43	2.13	7	2
3:B:353:PX4:O4	3:B:369:PX4:H10	0.43	2.14	3	1
2:C:113:GLU:OE1	3:C:330:PX4:H13	0.43	2.14	6	1
3:B:311:PX4:O4	3:B:311:PX4:H3	0.43	2.13	8	2
3:B:359:PX4:H5	3:B:371:PX4:H9	0.42	1.91	2	1
3:B:325:PX4:O3	3:B:325:PX4:H7	0.42	2.13	3	1
3:C:352:PX4:O3	3:C:352:PX4:C3	0.42	2.67	4	1
3:A:608:PX4:H13	3:A:608:PX4:O3	0.42	2.14	5	1
3:C:344:PX4:O1	3:C:364:PX4:H4	0.42	2.13	5	1
3:A:605:PX4:O4	3:A:605:PX4:H12	0.42	2.14	7	1
3:A:643:PX4:O2	3:A:643:PX4:H4	0.42	2.12	8	1
3:B:378:PX4:H9	3:B:378:PX4:O3	0.42	2.14	8	1
3:C:355:PX4:H10	3:C:355:PX4:O1	0.42	2.14	11	1
3:A:632:PX4:O3	3:A:632:PX4:H10	0.42	2.14	12	1
3:B:355:PX4:H39	3:B:399:PX4:H43	0.42	1.91	4	1
3:C:302:PX4:O2	3:C:302:PX4:H4	0.42	2.14	7	1
3:C:340:PX4:H8	3:C:360:PX4:C6	0.42	2.44	10	1
3:B:375:PX4:O2	3:B:376:PX4:H5	0.42	2.15	12	1
3:A:632:PX4:O1	3:A:632:PX4:H4	0.42	2.14	2	1
3:B:312:PX4:H15	3:B:312:PX4:H10	0.42	1.90	2	1
3:B:313:PX4:O1	3:B:313:PX4:H4	0.42	2.14	2	1
3:A:616:PX4:H3	3:C:356:PX4:O4	0.42	2.13	4	1
3:B:307:PX4:H4	3:B:318:PX4:O1	0.42	2.15	4	1
3:B:373:PX4:H13	3:B:380:PX4:C1	0.42	2.44	6	1
3:C:342:PX4:H3	3:C:342:PX4:O4	0.42	2.13	6	2
1:A:382:PHE:CD1	1:A:415:ILE:HD12	0.42	2.50	8	1
3:B:350:PX4:O3	3:B:350:PX4:H9	0.42	2.14	15	2
3:A:629:PX4:O2	3:A:631:PX4:H6	0.42	2.14	11	1
3:C:338:PX4:H9	3:C:338:PX4:O3	0.42	2.15	13	1
3:A:619:PX4:H7	3:B:397:PX4:O2	0.42	2.14	14	1
3:B:377:PX4:O2	3:B:377:PX4:H6	0.42	2.14	15	1
3:B:382:PX4:O2	3:B:382:PX4:H4	0.42	2.14	15	1
2:B:80:GLU:OE2	3:B:305:PX4:H6	0.42	2.15	1	1
3:B:320:PX4:H11	3:B:340:PX4:H14	0.42	1.92	8	1
3:A:636:PX4:H3	3:A:636:PX4:O4	0.42	2.13	11	1
3:B:306:PX4:H8	3:B:339:PX4:O8	0.42	2.15	1	1
1:A:360:PHE:O	3:A:644:PX4:H12	0.42	2.14	3	1
1:A:386:LYS:HE3	1:A:402:HIS:CE1	0.42	2.49	5	1
3:B:357:PX4:H4	3:B:357:PX4:O2	0.42	2.15	6	1
3:C:306:PX4:H17	3:C:306:PX4:O8	0.42	2.15	10	1
3:B:350:PX4:O1	3:B:374:PX4:H8	0.42	2.15	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:400:PX4:H3	3:B:400:PX4:H16	0.42	1.89	12	1
3:C:351:PX4:O6	3:C:351:PX4:H12	0.42	2.14	13	1
3:B:353:PX4:O3	3:B:369:PX4:H4	0.42	2.13	3	1
3:A:653:PX4:O3	3:A:653:PX4:H9	0.42	2.14	5	1
3:B:316:PX4:O3	3:B:316:PX4:C5	0.42	2.67	6	1
3:B:389:PX4:O3	3:B:389:PX4:C4	0.42	2.66	8	1
3:A:626:PX4:H48	3:A:634:PX4:H9	0.42	1.90	9	1
3:B:311:PX4:O8	3:B:345:PX4:H3	0.42	2.15	14	1
3:B:316:PX4:H53	3:B:344:PX4:C27	0.42	2.44	1	1
3:B:369:PX4:O2	3:B:386:PX4:H8	0.42	2.14	1	1
3:B:302:PX4:H4	3:B:302:PX4:O2	0.42	2.13	7	2
3:B:334:PX4:O2	3:B:348:PX4:H13	0.42	2.15	4	1
3:B:337:PX4:O3	3:B:337:PX4:H6	0.42	2.13	4	2
3:B:363:PX4:H11	3:B:381:PX4:P1	0.42	2.54	5	1
2:B:205:GLU:CD	3:B:321:PX4:H4	0.42	2.40	7	1
3:B:386:PX4:C1	3:B:388:PX4:H10	0.42	2.44	7	1
3:C:340:PX4:H4	3:C:340:PX4:O2	0.42	2.14	7	1
3:B:378:PX4:O1	3:C:302:PX4:H10	0.42	2.14	8	1
3:B:333:PX4:O1	3:B:333:PX4:H13	0.42	2.14	10	1
3:A:644:PX4:H29	3:A:654:PX4:H8	0.42	1.92	11	1
3:A:609:PX4:H5	3:B:384:PX4:O4	0.42	2.14	13	1
3:B:303:PX4:H43	3:C:327:PX4:H72	0.42	1.92	13	1
3:B:346:PX4:O1	3:B:371:PX4:H3	0.42	2.14	13	1
3:C:322:PX4:O1	3:C:351:PX4:H10	0.42	2.15	2	1
3:C:325:PX4:H24	3:C:359:PX4:H22	0.42	1.92	2	1
3:A:635:PX4:O4	3:A:637:PX4:H12	0.42	2.14	6	1
3:B:363:PX4:H5	3:B:381:PX4:O1	0.42	2.15	6	1
3:A:641:PX4:O2	3:A:651:PX4:H10	0.42	2.14	8	1
3:B:307:PX4:H2	3:B:307:PX4:C6	0.42	2.44	10	1
3:B:371:PX4:H10	3:B:371:PX4:O1	0.42	2.15	11	1
3:C:341:PX4:O1	3:C:349:PX4:H5	0.42	2.15	12	1
3:A:610:PX4:H6	3:A:612:PX4:O2	0.42	2.14	13	1
3:B:304:PX4:H39	3:B:340:PX4:H72	0.42	1.90	13	1
3:A:602:PX4:O2	3:A:602:PX4:H4	0.42	2.14	14	1
3:B:361:PX4:H12	3:B:361:PX4:O3	0.42	2.14	1	1
3:B:387:PX4:C1	3:B:387:PX4:C6	0.42	2.98	1	1
3:C:309:PX4:H34	3:C:315:PX4:H33	0.42	1.91	4	1
3:B:360:PX4:O2	3:B:362:PX4:H12	0.42	2.15	10	1
3:B:363:PX4:O8	3:B:363:PX4:H13	0.42	2.15	15	1
3:A:626:PX4:H13	3:C:362:PX4:H17	0.42	1.91	1	1
3:A:617:PX4:H11	3:A:625:PX4:O1	0.42	2.15	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:325:PX4:H38	3:B:331:PX4:H64	0.42	1.91	3	1
3:A:609:PX4:O1	3:A:609:PX4:H6	0.42	2.15	5	2
3:B:320:PX4:O4	3:B:320:PX4:H7	0.42	2.15	8	1
3:B:400:PX4:H5	3:C:347:PX4:H2	0.42	1.89	9	1
3:A:647:PX4:H9	3:A:647:PX4:O3	0.42	2.14	13	1
2:C:58:SER:OG	3:C:332:PX4:H4	0.42	2.15	14	1
3:C:325:PX4:H4	3:C:334:PX4:O8	0.41	2.14	1	1
3:C:316:PX4:H7	3:C:316:PX4:O3	0.41	2.14	2	1
3:C:362:PX4:O6	3:C:362:PX4:H3	0.41	2.15	3	1
3:B:385:PX4:H6	3:B:385:PX4:O3	0.41	2.15	5	1
3:A:623:PX4:O3	3:A:623:PX4:H13	0.41	2.15	6	1
2:B:158:GLU:OE1	2:C:155:LYS:NZ	0.41	2.48	8	1
3:B:341:PX4:H45	3:C:344:PX4:H65	0.41	1.92	8	1
3:B:390:PX4:O3	3:B:390:PX4:H7	0.41	2.15	10	1
3:A:620:PX4:O3	3:A:620:PX4:H13	0.41	2.14	11	1
3:B:359:PX4:O3	3:B:359:PX4:H12	0.41	2.15	11	1
3:B:338:PX4:H11	3:B:365:PX4:C1	0.41	2.45	12	1
3:A:616:PX4:H7	3:A:616:PX4:O4	0.41	2.15	5	1
3:B:334:PX4:H9	3:B:352:PX4:O1	0.41	2.15	7	1
3:A:601:PX4:O1	3:B:377:PX4:C2	0.41	2.68	9	1
3:C:340:PX4:H10	3:C:360:PX4:O8	0.41	2.15	9	1
3:B:311:PX4:O3	3:B:311:PX4:H12	0.41	2.15	10	1
3:B:354:PX4:O3	3:B:354:PX4:H7	0.41	2.16	11	1
3:C:341:PX4:O2	3:C:349:PX4:H8	0.41	2.15	12	1
1:A:364:LEU:HD11	1:A:368:ILE:CG2	0.41	2.45	13	1
3:B:374:PX4:H7	3:B:374:PX4:O1	0.41	2.14	2	1
3:A:634:PX4:O2	3:A:634:PX4:H3	0.41	2.14	4	1
3:A:603:PX4:H5	3:A:609:PX4:O1	0.41	2.15	5	1
3:A:633:PX4:O2	3:A:633:PX4:H4	0.41	2.14	6	1
3:B:356:PX4:O3	3:B:356:PX4:H9	0.41	2.15	6	1
1:A:402:HIS:HE1	3:A:649:PX4:H4	0.41	1.74	8	1
3:A:627:PX4:H10	3:A:627:PX4:O3	0.41	2.16	9	1
3:B:323:PX4:O5	3:B:323:PX4:C23	0.41	2.68	12	1
3:C:332:PX4:H9	3:C:332:PX4:O3	0.41	2.15	13	1
3:A:621:PX4:O4	3:A:621:PX4:H13	0.41	2.15	3	1
3:B:361:PX4:H4	3:B:368:PX4:O1	0.41	2.15	4	1
3:C:305:PX4:H7	3:C:305:PX4:O3	0.41	2.15	7	1
2:B:130:TRP:NE1	2:C:177:HIS:CE1	0.41	2.89	8	1
3:C:332:PX4:H13	3:C:335:PX4:O2	0.41	2.15	9	1
3:A:622:PX4:O3	3:A:622:PX4:H12	0.41	2.14	11	1
3:B:357:PX4:H13	3:B:357:PX4:O3	0.41	2.16	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:C:113:GLU:OE1	3:C:330:PX4:H11	0.41	2.16	11	1
3:B:378:PX4:H12	3:B:386:PX4:O4	0.41	2.16	12	1
3:B:380:PX4:O2	3:B:387:PX4:H11	0.41	2.15	14	1
3:B:322:PX4:H10	3:B:350:PX4:C4	0.41	2.45	1	1
3:C:345:PX4:O4	3:C:345:PX4:H3	0.41	2.15	3	1
3:A:618:PX4:H10	3:A:618:PX4:O3	0.41	2.16	6	1
3:B:337:PX4:H45	3:B:368:PX4:H70	0.41	1.91	6	1
3:B:338:PX4:O1	3:B:358:PX4:H4	0.41	2.15	7	1
3:C:344:PX4:H3	3:C:364:PX4:O3	0.41	2.16	8	1
3:A:616:PX4:H22	3:C:337:PX4:H24	0.41	1.92	9	1
3:A:626:PX4:H5	3:C:362:PX4:O2	0.41	2.16	9	1
3:C:309:PX4:H7	3:C:315:PX4:O1	0.41	2.15	9	1
3:C:337:PX4:H10	3:C:337:PX4:O3	0.41	2.16	13	2
3:C:320:PX4:H10	3:C:341:PX4:O4	0.41	2.15	11	1
2:B:72:TRP:CD1	3:B:341:PX4:H4	0.41	2.50	12	1
3:A:614:PX4:H12	3:A:614:PX4:O2	0.41	2.16	13	1
3:B:323:PX4:O4	3:B:323:PX4:H4	0.41	2.15	14	1
3:B:387:PX4:O6	3:B:390:PX4:H12	0.41	2.15	15	1
3:C:307:PX4:H2	3:C:343:PX4:H14	0.41	1.93	1	1
3:A:604:PX4:H7	3:B:392:PX4:C1	0.41	2.45	2	1
3:A:652:PX4:H13	3:A:652:PX4:O3	0.41	2.15	2	1
3:B:390:PX4:O3	3:B:392:PX4:H8	0.41	2.15	2	1
3:C:319:PX4:H10	3:C:319:PX4:O1	0.41	2.16	3	1
2:B:201:GLU:CD	3:B:313:PX4:H4	0.41	2.41	6	1
3:A:634:PX4:H54	3:A:640:PX4:H44	0.41	1.91	8	1
3:C:340:PX4:H9	3:C:340:PX4:O1	0.41	2.15	8	1
3:B:314:PX4:O3	3:B:314:PX4:H12	0.41	2.15	9	1
3:A:605:PX4:O6	3:A:609:PX4:H3	0.41	2.16	13	2
3:B:382:PX4:H4	3:B:393:PX4:O1	0.41	2.16	10	1
3:B:304:PX4:H9	3:B:304:PX4:O3	0.41	2.16	11	1
3:C:346:PX4:H9	3:C:346:PX4:O3	0.41	2.15	11	1
3:A:616:PX4:H46	3:A:634:PX4:H8	0.41	1.92	12	1
3:C:349:PX4:H4	3:C:349:PX4:O8	0.41	2.15	13	1
3:B:312:PX4:H65	3:C:328:PX4:H39	0.41	1.91	15	1
3:A:614:PX4:H13	3:A:628:PX4:O2	0.41	2.15	1	1
3:B:338:PX4:H3	3:B:338:PX4:C6	0.41	2.45	2	1
3:C:357:PX4:H3	3:C:357:PX4:O4	0.41	2.14	2	1
3:B:310:PX4:H7	3:B:310:PX4:O2	0.41	2.15	4	1
1:A:361:TRP:HE1	1:A:364:LEU:HD22	0.41	1.76	5	1
3:B:368:PX4:O3	3:B:368:PX4:C4	0.41	2.67	7	1
3:B:382:PX4:H4	3:B:393:PX4:O2	0.41	2.16	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:612:PX4:C1	3:A:612:PX4:C6	0.41	2.99	9	1
3:C:329:PX4:H7	3:C:329:PX4:O3	0.41	2.16	13	1
3:B:329:PX4:H3	3:B:329:PX4:O1	0.41	2.16	1	1
3:C:357:PX4:H3	3:C:357:PX4:C6	0.41	2.45	3	1
3:A:602:PX4:H57	3:B:357:PX4:H30	0.41	1.92	4	1
3:A:641:PX4:O3	3:A:641:PX4:H9	0.41	2.16	4	1
3:C:318:PX4:H6	3:C:318:PX4:O3	0.41	2.16	4	1
3:C:306:PX4:O2	3:C:336:PX4:H5	0.41	2.16	6	1
3:A:635:PX4:O1	3:A:635:PX4:H3	0.41	2.16	10	1
3:B:362:PX4:H7	3:B:366:PX4:H2	0.41	1.91	12	1
3:B:316:PX4:O3	3:B:316:PX4:H12	0.41	2.16	13	1
2:C:153:ARG:O	2:C:157:HIS:CD2	0.41	2.74	14	1
3:A:602:PX4:H8	3:A:603:PX4:O2	0.41	2.15	1	1
3:B:335:PX4:H4	3:B:335:PX4:O2	0.41	2.16	1	1
3:B:359:PX4:H10	3:B:359:PX4:O3	0.41	2.16	1	1
3:B:365:PX4:O3	3:B:365:PX4:C4	0.41	2.69	2	1
3:B:312:PX4:H8	3:B:356:PX4:O4	0.41	2.16	4	1
3:B:329:PX4:O4	3:B:355:PX4:H5	0.41	2.16	4	1
3:B:339:PX4:H4	3:B:360:PX4:O2	0.41	2.15	4	1
3:B:391:PX4:H13	3:C:303:PX4:H15	0.41	1.92	4	1
3:C:323:PX4:H4	3:C:323:PX4:C7	0.41	2.46	4	1
3:B:343:PX4:H4	3:B:343:PX4:O4	0.41	2.16	5	1
3:B:378:PX4:O1	3:B:378:PX4:H3	0.41	2.16	5	1
3:A:645:PX4:H13	3:A:646:PX4:O2	0.41	2.16	6	1
3:B:387:PX4:H13	3:B:387:PX4:O3	0.41	2.16	6	1
3:C:344:PX4:C1	3:C:364:PX4:H6	0.41	2.46	6	1
3:B:342:PX4:O6	3:B:367:PX4:H7	0.41	2.16	7	1
3:B:400:PX4:C6	3:B:400:PX4:H3	0.41	2.46	7	1
3:B:317:PX4:O2	3:B:317:PX4:H9	0.41	2.15	8	1
3:C:332:PX4:H6	3:C:335:PX4:O4	0.41	2.16	9	1
3:C:323:PX4:O3	3:C:323:PX4:C3	0.41	2.69	10	1
3:B:312:PX4:O3	3:B:312:PX4:C5	0.41	2.69	13	1
3:A:617:PX4:O2	3:A:617:PX4:H4	0.41	2.15	15	1
3:B:306:PX4:C2	3:B:339:PX4:O8	0.41	2.69	15	1
3:B:330:PX4:H3	3:B:330:PX4:H16	0.41	1.93	15	1
3:C:357:PX4:H6	3:C:357:PX4:O3	0.41	2.15	15	1
1:A:399:TYR:HA	1:A:400:PRO:C	0.41	2.41	2	1
3:A:625:PX4:H12	3:A:625:PX4:O3	0.41	2.16	2	1
3:C:323:PX4:H19	3:C:342:PX4:H27	0.41	1.93	4	1
3:A:622:PX4:H3	3:A:622:PX4:C6	0.41	2.46	5	1
3:B:322:PX4:O6	3:B:350:PX4:H5	0.41	2.15	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:B:359:PX4:O3	3:B:359:PX4:H10	0.41	2.16	8	1
1:A:362:ARG:HE	3:A:650:PX4:C6	0.41	2.28	11	1
3:A:605:PX4:H3	3:B:379:PX4:C6	0.41	2.46	12	1
3:B:314:PX4:O1	3:B:314:PX4:H3	0.41	2.15	13	1
3:B:375:PX4:H9	3:B:375:PX4:O3	0.40	2.16	1	1
3:B:392:PX4:H15	3:B:392:PX4:H13	0.40	1.93	3	1
3:C:316:PX4:H13	3:C:342:PX4:O1	0.40	2.16	3	1
3:B:387:PX4:O1	3:B:387:PX4:H13	0.40	2.15	4	1
3:A:614:PX4:H12	3:A:614:PX4:O3	0.40	2.16	10	1
3:B:331:PX4:H4	3:B:331:PX4:H15	0.40	1.92	13	1
3:A:626:PX4:H4	3:C:346:PX4:O1	0.40	2.16	14	1
3:A:605:PX4:H12	3:A:605:PX4:O3	0.40	2.16	4	1
3:C:333:PX4:O3	3:C:333:PX4:H12	0.40	2.16	4	1
3:A:601:PX4:H11	3:A:601:PX4:O6	0.40	2.16	6	1
3:C:352:PX4:O4	3:C:352:PX4:H13	0.40	2.17	8	1
3:B:315:PX4:H10	3:B:336:PX4:O1	0.40	2.16	9	1
3:B:358:PX4:O3	3:B:358:PX4:H9	0.40	2.16	9	1
2:B:115:TYR:CE2	2:B:119:VAL:CG2	0.40	3.04	10	1
3:B:353:PX4:H9	3:B:369:PX4:O2	0.40	2.15	12	1
3:C:313:PX4:H8	3:C:337:PX4:H14	0.40	1.92	15	1
3:B:386:PX4:O3	3:B:386:PX4:H9	0.40	2.16	1	1
3:C:342:PX4:O3	3:C:342:PX4:H9	0.40	2.17	1	1
3:B:363:PX4:O2	3:B:368:PX4:H5	0.40	2.17	2	1
3:A:617:PX4:H26	3:C:355:PX4:H69	0.40	1.93	3	1
3:A:628:PX4:O3	3:A:628:PX4:H16	0.40	2.16	3	1
3:C:320:PX4:O3	3:C:320:PX4:H13	0.40	2.16	3	1
3:C:314:PX4:H13	3:C:314:PX4:O2	0.40	2.17	4	1
3:A:649:PX4:H58	3:A:649:PX4:C13	0.40	2.46	5	1
3:B:325:PX4:H11	3:B:357:PX4:O2	0.40	2.16	6	1
3:C:310:PX4:H13	3:C:310:PX4:O3	0.40	2.17	8	1
3:B:398:PX4:H6	3:C:357:PX4:O3	0.40	2.17	10	1
2:C:91:GLU:OE1	3:C:314:PX4:H6	0.40	2.17	10	1
3:C:340:PX4:H8	3:C:360:PX4:H14	0.40	1.92	10	1
3:C:322:PX4:O3	3:C:322:PX4:H13	0.40	2.16	11	1
3:B:350:PX4:O1	3:B:350:PX4:H3	0.40	2.17	13	1
1:A:443:ARG:HD2	3:A:651:PX4:H7	0.40	1.93	14	1
3:B:395:PX4:O1	3:C:312:PX4:H8	0.40	2.16	15	1
3:B:360:PX4:O3	3:B:360:PX4:C4	0.40	2.70	3	1
1:A:359:GLN:OE1	3:A:650:PX4:H8	0.40	2.16	4	1
3:C:315:PX4:H3	3:C:353:PX4:O2	0.40	2.17	4	1
3:A:649:PX4:H58	3:A:649:PX4:H26	0.40	1.93	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:317:PX4:H4	3:C:333:PX4:C8	0.40	2.46	5	1
3:B:375:PX4:C6	3:B:376:PX4:H5	0.40	2.47	6	1
3:B:387:PX4:H13	3:B:387:PX4:O1	0.40	2.16	6	1
3:C:344:PX4:O3	3:C:364:PX4:H6	0.40	2.17	6	1
3:B:363:PX4:H8	3:B:381:PX4:H1	0.40	1.93	7	1
2:C:226:SER:OG	3:C:317:PX4:H10	0.40	2.16	11	1
3:B:341:PX4:H7	3:B:341:PX4:O4	0.40	2.16	12	1
3:B:341:PX4:H54	3:B:373:PX4:C11	0.40	2.46	14	1
3:A:619:PX4:H58	3:A:632:PX4:H8	0.40	1.93	15	1
3:B:316:PX4:H8	3:B:322:PX4:O1	0.40	2.16	1	1
2:C:164:SER:OG	3:C:305:PX4:H8	0.40	2.15	2	1
3:A:607:PX4:O2	3:A:607:PX4:H4	0.40	2.16	3	1
3:B:368:PX4:O3	3:B:368:PX4:H9	0.40	2.17	3	1
3:C:332:PX4:O3	3:C:332:PX4:H9	0.40	2.16	9	1
3:B:396:PX4:H3	3:B:396:PX4:O1	0.40	2.16	10	1
3:B:356:PX4:H9	3:B:356:PX4:O1	0.40	2.16	11	1
3:B:399:PX4:O2	3:C:326:PX4:H3	0.40	2.17	12	1
1:A:364:LEU:HD11	1:A:368:ILE:HG21	0.40	1.93	13	1
3:B:363:PX4:H3	3:B:363:PX4:O4	0.40	2.17	13	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±1%)	15±3 (8±1%)	3±1 (2±1%)	10	55
2	B	209/211 (99%)	205±2 (98±1%)	4±2 (2±1%)	0±0 (0±0%)	44	80
2	C	207/211 (98%)	202±2 (98±1%)	4±2 (2±1%)	1±1 (0±0%)	37	78
All	All	9150/9270 (99%)	8751 (96%)	338 (4%)	61 (1%)	20	70

All 34 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	448	GLU	5

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Mol	Chain	Res	Type	Models (Total)
1	A	367	SER	4
1	A	411	PRO	4
1	A	510	SER	3
2	C	65	GLY	3
1	A	491	LEU	3
1	A	322	ASN	3
1	A	472	GLU	2
1	A	446	ASP	2
1	A	466	SER	2
1	A	479	LYS	2
1	A	338	GLU	2
1	A	354	PRO	2
2	B	65	GLY	2
2	C	100	TYR	2
1	A	454	LYS	2
1	A	443	ARG	1
1	A	463	PRO	1
1	A	347	ASN	1
1	A	395	LEU	1
1	A	394	SER	1
1	A	375	LYS	1
2	C	121	PRO	1
1	A	404	LYS	1
1	A	366	ALA	1
1	A	370	THR	1
1	A	393	ALA	1
2	B	187	PRO	1
1	A	368	ILE	1
2	B	66	PRO	1
2	C	99	PRO	1
1	A	450	PRO	1
2	B	98	GLN	1
2	C	142	GLU	1

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	169/169 (100%)	164±2 (97±1%)	5±2 (3±1%)	35 84
2	B	187/187 (100%)	182±1 (98±1%)	5±1 (2±1%)	42 88
2	C	184/187 (98%)	180±1 (98±1%)	4±1 (2±1%)	46 90
All	All	8100/8145 (99%)	7892 (97%)	208 (3%)	41 88

All 101 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	15
1	A	492	LYS	14
2	B	145	ARG	12
1	A	325	THR	8
1	A	368	ILE	8
1	A	370	THR	8
2	C	106	LYS	6
1	A	412	THR	5
2	B	156	LEU	4
1	A	342	TRP	4
2	B	243	VAL	4
1	A	365	PRO	3
1	A	388	TRP	3
2	B	261	LYS	3
2	C	119	VAL	3
1	A	445	VAL	2
2	B	68	THR	2
2	C	56	THR	2
1	A	349	VAL	2
2	C	99	PRO	2
2	C	114	LEU	2
2	C	141	VAL	2
1	A	372	TYR	2
1	A	411	PRO	2
2	B	183	THR	2
2	C	127	GLN	2
2	C	154	GLN	2
2	B	194	GLN	2
2	C	183	THR	2
1	A	433	ASN	2
1	A	361	TRP	2
1	A	509	PRO	2
2	B	106	LYS	2

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Mol	Chain	Res	Type	Models (Total)
2	C	192	LEU	2
2	C	213	GLU	2
1	A	344	VAL	2
2	B	165	PRO	2
1	A	394	SER	1
1	A	415	ILE	1
2	B	56	THR	1
2	B	178	VAL	1
2	C	71	PHE	1
2	C	105	GLN	1
2	C	140	LYS	1
2	C	231	PRO	1
2	C	259	THR	1
1	A	390	PHE	1
2	C	67	VAL	1
1	A	423	PRO	1
1	A	486	PHE	1
2	B	90	LEU	1
2	C	121	PRO	1
2	C	123	LEU	1
2	C	139	GLN	1
1	A	397	PRO	1
2	B	87	SER	1
2	B	114	LEU	1
2	B	116	ARG	1
2	B	160	GLN	1
2	C	86	MET	1
2	C	120	GLU	1
2	B	69	GLN	1
2	B	93	VAL	1
2	B	215	HIS	1
2	C	78	GLU	1
2	C	91	GLU	1
2	C	129	LYS	1
2	C	179	ASP	1
2	B	191	GLU	1
2	C	133	GLU	1
1	A	422	MET	1
2	B	245	GLU	1
2	C	243	VAL	1
1	A	453	ILE	1
2	C	69	GLN	1

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Mol	Chain	Res	Type	Models (Total)
1	A	362	ARG	1
2	B	118	LYS	1
2	C	100	TYR	1
2	C	250	SER	1
2	B	166	LEU	1
2	B	231	PRO	1
2	C	211	LEU	1
2	C	245	GLU	1
2	C	251	PHE	1
2	B	63	GLN	1
2	C	66	PRO	1
2	C	68	THR	1
2	C	144	LEU	1
2	C	224	THR	1
2	C	234	GLU	1
1	A	341	PHE	1
2	B	141	VAL	1
2	C	221	HIS	1
1	A	402	HIS	1
2	B	154	GLN	1
2	B	242	PRO	1
2	C	227	GLU	1
2	B	84	GLN	1
2	B	108	TRP	1
2	C	103	ASP	1
1	A	340	TRP	1

6.3.3 RNA

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates

There are no 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	A	608	-	45,45,45	1.04±0.08	3±2 (6±3%)
3	PX4	A	631	-	45,45,45	1.11±0.12	3±2 (7±3%)
3	PX4	C	318	-	45,45,45	1.07±0.14	3±1 (5±2%)
3	PX4	B	351	-	45,45,45	1.07±0.14	3±2 (5±3%)
3	PX4	B	325	-	45,45,45	1.05±0.08	2±2 (5±3%)
3	PX4	C	362	-	45,45,45	1.09±0.13	3±2 (6±3%)
3	PX4	C	331	-	45,45,45	1.03±0.11	2±1 (5±2%)
3	PX4	C	350	-	45,45,45	1.09±0.11	3±1 (6±2%)
3	PX4	A	640	-	45,45,45	1.07±0.09	3±1 (6±2%)
3	PX4	C	357	-	45,45,45	1.04±0.13	2±1 (5±2%)
3	PX4	A	620	-	45,45,45	1.04±0.10	3±1 (5±2%)
3	PX4	B	395	-	45,45,45	1.04±0.11	2±1 (4±2%)
3	PX4	C	335	-	45,45,45	1.14±0.12	3±1 (6±3%)
3	PX4	C	308	-	45,45,45	1.11±0.11	4±2 (8±3%)
3	PX4	C	338	-	45,45,45	1.03±0.11	3±2 (6±4%)
3	PX4	C	351	-	45,45,45	1.06±0.09	3±1 (6±2%)
3	PX4	A	606	-	45,45,45	1.10±0.10	4±2 (8±3%)
3	PX4	B	369	-	45,45,45	1.06±0.14	3±2 (6±4%)
3	PX4	A	637	-	45,45,45	1.06±0.10	3±2 (6±3%)
3	PX4	B	310	-	45,45,45	1.10±0.16	3±1 (6±3%)
3	PX4	B	363	-	45,45,45	1.04±0.11	2±1 (5±2%)
3	PX4	C	319	-	45,45,45	1.04±0.10	3±1 (5±2%)
3	PX4	B	330	-	45,45,45	1.09±0.09	3±1 (6±2%)
3	PX4	B	390	-	45,45,45	1.07±0.10	3±1 (7±3%)
3	PX4	B	394	-	45,45,45	1.09±0.12	3±2 (7±3%)
3	PX4	B	399	-	45,45,45	1.04±0.11	3±2 (6±3%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
3	PX4	A	621	-	45,45,45	1.04±0.10	3±1 (5±3%)
3	PX4	B	396	-	45,45,45	1.10±0.14	4±2 (8±3%)
3	PX4	C	312	-	45,45,45	1.08±0.11	3±2 (7±3%)
3	PX4	C	325	-	45,45,45	1.06±0.11	3±1 (6±2%)
3	PX4	C	309	-	45,45,45	1.10±0.17	3±2 (6±4%)
3	PX4	A	607	-	45,45,45	1.11±0.13	3±1 (6±2%)
3	PX4	B	385	-	45,45,45	1.10±0.12	3±1 (7±3%)
3	PX4	C	333	-	45,45,45	1.08±0.14	3±2 (6±3%)
3	PX4	C	311	-	45,45,45	1.06±0.09	3±1 (6±2%)
3	PX4	B	386	-	45,45,45	1.06±0.12	3±1 (6±3%)
3	PX4	B	368	-	45,45,45	1.10±0.09	3±1 (7±2%)
3	PX4	B	357	-	45,45,45	1.07±0.12	3±1 (6±3%)
3	PX4	B	344	-	45,45,45	1.07±0.12	4±2 (7±3%)
3	PX4	B	400	-	45,45,45	1.07±0.12	3±1 (6±3%)
3	PX4	B	375	-	45,45,45	1.02±0.08	3±1 (5±1%)
3	PX4	A	605	-	45,45,45	1.11±0.09	3±1 (7±2%)
3	PX4	A	653	-	45,45,45	1.11±0.13	4±2 (8±3%)
3	PX4	B	379	-	45,45,45	1.06±0.10	3±1 (7±2%)
3	PX4	C	306	-	45,45,45	1.10±0.12	3±1 (7±2%)
3	PX4	A	641	-	45,45,45	1.04±0.11	3±1 (5±2%)
3	PX4	C	347	-	45,45,45	1.08±0.14	3±1 (6±3%)
3	PX4	B	336	-	45,45,45	1.03±0.12	3±2 (5±4%)
3	PX4	C	313	-	45,45,45	1.04±0.12	2±2 (5±3%)
3	PX4	B	382	-	45,45,45	1.09±0.10	3±1 (7±2%)
3	PX4	B	309	-	45,45,45	1.07±0.10	3±1 (6±3%)
3	PX4	C	344	-	45,45,45	1.02±0.14	3±1 (5±3%)
3	PX4	C	343	-	45,45,45	1.09±0.10	3±1 (6±1%)
3	PX4	B	301	-	45,45,45	1.11±0.11	4±2 (7±3%)
3	PX4	C	358	-	45,45,45	1.03±0.10	3±1 (5±2%)
3	PX4	A	618	-	45,45,45	1.05±0.10	2±1 (5±2%)
3	PX4	C	345	-	45,45,45	1.09±0.13	3±2 (6±3%)
3	PX4	A	654	-	45,45,45	1.05±0.11	3±2 (6±3%)
3	PX4	A	646	-	45,45,45	1.03±0.07	2±1 (4±2%)
3	PX4	C	346	-	45,45,45	1.09±0.09	3±2 (5±3%)
3	PX4	B	350	-	45,45,45	1.09±0.08	3±1 (7±3%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
3	PX4	B	302	-	45,45,45	1.09±0.13	3±2 (7±4%)
3	PX4	A	614	-	45,45,45	1.10±0.09	3±1 (6±2%)
3	PX4	B	316	-	45,45,45	1.07±0.11	3±1 (7±3%)
3	PX4	A	602	-	45,45,45	1.08±0.11	3±2 (6±3%)
3	PX4	B	341	-	45,45,45	1.07±0.07	3±1 (5±3%)
3	PX4	A	644	-	45,45,45	1.03±0.13	3±2 (6±3%)
3	PX4	C	301	-	45,45,45	1.08±0.08	3±1 (7±2%)
3	PX4	A	611	-	45,45,45	1.08±0.09	3±1 (6±2%)
3	PX4	B	362	-	45,45,45	1.06±0.11	3±1 (6±3%)
3	PX4	B	393	-	45,45,45	1.11±0.14	3±2 (7±4%)
3	PX4	B	338	-	45,45,45	1.08±0.11	3±1 (6±1%)
3	PX4	C	339	-	45,45,45	1.06±0.10	3±1 (6±2%)
3	PX4	B	333	-	45,45,45	1.09±0.11	3±1 (6±3%)
3	PX4	A	648	-	45,45,45	1.10±0.09	3±1 (7±2%)
3	PX4	A	652	-	45,45,45	1.05±0.07	3±1 (6±2%)
3	PX4	A	636	-	45,45,45	1.06±0.07	2±1 (5±2%)
3	PX4	A	639	-	45,45,45	1.13±0.14	4±2 (9±4%)
3	PX4	A	613	-	45,45,45	1.11±0.12	3±1 (7±2%)
3	PX4	C	302	-	45,45,45	1.05±0.07	3±1 (7±1%)
3	PX4	B	327	-	45,45,45	1.10±0.13	3±2 (7±3%)
3	PX4	A	643	-	45,45,45	1.04±0.13	3±2 (6±4%)
3	PX4	B	313	-	45,45,45	1.06±0.14	3±2 (6±3%)
3	PX4	A	601	-	45,45,45	1.10±0.08	3±1 (7±2%)
3	PX4	B	373	-	45,45,45	1.08±0.13	3±1 (5±2%)
3	PX4	B	381	-	45,45,45	1.06±0.10	3±1 (6±2%)
3	PX4	A	626	-	45,45,45	1.05±0.14	2±1 (5±3%)
3	PX4	C	353	-	45,45,45	1.08±0.10	3±1 (7±2%)
3	PX4	B	397	-	45,45,45	1.07±0.11	3±1 (7±2%)
3	PX4	A	603	-	45,45,45	1.09±0.13	3±2 (6±3%)
3	PX4	B	355	-	45,45,45	1.11±0.12	4±2 (8±4%)
3	PX4	B	322	-	45,45,45	1.10±0.12	3±1 (7±2%)
3	PX4	B	354	-	45,45,45	1.08±0.08	3±1 (6±2%)
3	PX4	A	617	-	45,45,45	1.08±0.10	3±2 (7±4%)
3	PX4	A	627	-	45,45,45	1.11±0.12	4±1 (7±3%)
3	PX4	C	317	-	45,45,45	1.08±0.14	3±2 (6±4%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
3	PX4	A	642	-	45,45,45	1.08±0.09	3±1 (7±2%)
3	PX4	B	326	-	45,45,45	1.08±0.14	3±2 (6±4%)
3	PX4	B	392	-	45,45,45	1.05±0.11	3±1 (6±2%)
3	PX4	B	398	-	45,45,45	1.06±0.11	3±1 (6±2%)
3	PX4	B	365	-	45,45,45	1.06±0.14	3±2 (6±3%)
3	PX4	B	307	-	45,45,45	1.08±0.08	4±1 (8±3%)
3	PX4	C	354	-	45,45,45	1.11±0.09	3±1 (7±3%)
3	PX4	C	360	-	45,45,45	1.09±0.10	3±1 (7±2%)
3	PX4	B	345	-	45,45,45	1.09±0.14	3±2 (7±3%)
3	PX4	C	321	-	45,45,45	1.10±0.13	4±2 (8±4%)
3	PX4	B	339	-	45,45,45	1.05±0.09	3±1 (6±3%)
3	PX4	C	330	-	45,45,45	1.08±0.12	3±2 (7±4%)
3	PX4	B	323	-	45,45,45	1.08±0.13	3±2 (6±3%)
3	PX4	A	612	-	45,45,45	1.02±0.11	2±1 (5±2%)
3	PX4	C	356	-	45,45,45	1.05±0.16	3±2 (6±3%)
3	PX4	B	352	-	45,45,45	1.09±0.16	3±1 (6±3%)
3	PX4	B	359	-	45,45,45	1.08±0.09	3±1 (6±3%)
3	PX4	B	324	-	45,45,45	1.06±0.09	2±1 (5±2%)
3	PX4	B	311	-	45,45,45	1.15±0.12	4±1 (9±2%)
3	PX4	A	651	-	45,45,45	1.06±0.07	3±1 (7±2%)
3	PX4	C	349	-	45,45,45	1.05±0.12	3±2 (6±4%)
3	PX4	B	384	-	45,45,45	1.11±0.11	3±1 (7±3%)
3	PX4	A	630	-	45,45,45	1.05±0.09	3±2 (6±3%)
3	PX4	C	336	-	45,45,45	1.06±0.08	3±1 (6±2%)
3	PX4	C	332	-	45,45,45	1.06±0.11	3±1 (7±3%)
3	PX4	B	317	-	45,45,45	1.05±0.11	3±1 (6±2%)
3	PX4	B	366	-	45,45,45	1.02±0.11	3±1 (6±2%)
3	PX4	B	321	-	45,45,45	1.11±0.10	3±2 (7±3%)
3	PX4	C	337	-	45,45,45	1.07±0.09	3±2 (6±3%)
3	PX4	C	359	-	45,45,45	1.12±0.12	3±1 (6±3%)
3	PX4	B	349	-	45,45,45	1.09±0.06	3±1 (7±2%)
3	PX4	B	360	-	45,45,45	1.09±0.11	3±2 (7±3%)
3	PX4	B	329	-	45,45,45	1.12±0.11	4±1 (8±2%)
3	PX4	B	334	-	45,45,45	1.07±0.09	3±1 (6±2%)
3	PX4	B	377	-	45,45,45	1.08±0.11	3±1 (7±3%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
3	PX4	C	305	-	45,45,45	1.09±0.13	3±2 (7±4%)
3	PX4	B	358	-	45,45,45	1.07±0.09	3±1 (6±2%)
3	PX4	C	320	-	45,45,45	1.08±0.12	3±1 (5±2%)
3	PX4	C	327	-	45,45,45	1.06±0.08	3±1 (6±2%)
3	PX4	A	604	-	45,45,45	1.06±0.10	3±1 (6±2%)
3	PX4	B	378	-	45,45,45	1.06±0.12	3±1 (6±2%)
3	PX4	B	391	-	45,45,45	1.04±0.07	2±1 (5±2%)
3	PX4	C	348	-	45,45,45	1.06±0.10	3±1 (6±2%)
3	PX4	B	389	-	45,45,45	1.08±0.13	3±1 (6±2%)
3	PX4	A	632	-	45,45,45	1.07±0.16	3±1 (7±3%)
3	PX4	B	308	-	45,45,45	1.10±0.13	4±1 (8±2%)
3	PX4	B	374	-	45,45,45	1.08±0.14	3±2 (6±3%)
3	PX4	C	328	-	45,45,45	1.10±0.11	3±1 (7±2%)
3	PX4	B	305	-	45,45,45	1.09±0.08	3±1 (6±2%)
3	PX4	B	315	-	45,45,45	1.04±0.12	3±1 (6±2%)
3	PX4	A	628	-	45,45,45	1.05±0.11	3±2 (6±3%)
3	PX4	C	361	-	45,45,45	1.07±0.15	3±2 (5±3%)
3	PX4	B	383	-	45,45,45	1.10±0.13	4±2 (8±3%)
3	PX4	A	638	-	45,45,45	1.04±0.12	2±1 (5±3%)
3	PX4	A	623	-	45,45,45	1.03±0.13	2±2 (5±3%)
3	PX4	B	331	-	45,45,45	1.08±0.12	3±2 (6±3%)
3	PX4	A	619	-	45,45,45	1.07±0.12	3±1 (6±2%)
3	PX4	C	316	-	45,45,45	1.05±0.11	3±1 (6±2%)
3	PX4	C	355	-	45,45,45	1.11±0.11	4±2 (8±4%)
3	PX4	A	624	-	45,45,45	1.05±0.10	2±2 (5±3%)
3	PX4	B	361	-	45,45,45	1.09±0.11	3±2 (7±4%)
3	PX4	B	314	-	45,45,45	1.11±0.11	3±1 (6±2%)
3	PX4	C	342	-	45,45,45	1.04±0.13	3±1 (6±3%)
3	PX4	B	347	-	45,45,45	1.07±0.06	3±1 (7±2%)
3	PX4	C	322	-	45,45,45	1.05±0.13	3±1 (6±2%)
3	PX4	A	609	-	45,45,45	1.09±0.11	4±1 (7±3%)
3	PX4	C	303	-	45,45,45	1.08±0.17	3±2 (6±3%)
3	PX4	A	633	-	45,45,45	1.07±0.13	3±1 (5±3%)
3	PX4	A	616	-	45,45,45	1.08±0.11	3±1 (6±2%)
3	PX4	A	615	-	45,45,45	1.05±0.13	2±1 (5±3%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
3	PX4	C	329	-	45,45,45	1.16±0.12	4±2 (8±4%)
3	PX4	C	352	-	45,45,45	1.14±0.11	3±1 (7±2%)
3	PX4	A	625	-	45,45,45	1.08±0.11	3±2 (6±3%)
3	PX4	A	622	-	45,45,45	1.07±0.09	3±1 (6±2%)
3	PX4	C	334	-	45,45,45	1.05±0.14	3±2 (6±3%)
3	PX4	C	340	-	45,45,45	1.06±0.09	3±1 (6±3%)
3	PX4	C	315	-	45,45,45	1.07±0.10	2±1 (5±2%)
3	PX4	A	649	-	45,45,45	1.08±0.12	3±1 (6±3%)
3	PX4	B	348	-	45,45,45	1.07±0.11	3±1 (6±2%)
3	PX4	A	634	-	45,45,45	1.04±0.10	3±1 (6±3%)
3	PX4	B	304	-	45,45,45	1.03±0.13	2±2 (5±3%)
3	PX4	C	363	-	45,45,45	1.09±0.12	3±2 (7±3%)
3	PX4	B	342	-	45,45,45	1.11±0.10	3±2 (6±3%)
3	PX4	C	314	-	45,45,45	1.06±0.11	2±1 (5±3%)
3	PX4	B	343	-	45,45,45	1.05±0.12	3±1 (5±3%)
3	PX4	B	303	-	45,45,45	1.02±0.14	3±2 (5±3%)
3	PX4	B	380	-	45,45,45	1.07±0.10	3±1 (6±2%)
3	PX4	B	353	-	45,45,45	1.10±0.13	3±1 (6±3%)
3	PX4	C	326	-	45,45,45	1.11±0.12	3±1 (7±3%)
3	PX4	A	645	-	45,45,45	1.11±0.09	3±1 (6±1%)
3	PX4	B	370	-	45,45,45	1.06±0.10	3±1 (5±2%)
3	PX4	B	346	-	45,45,45	1.09±0.12	3±1 (6±2%)
3	PX4	C	323	-	45,45,45	1.06±0.17	3±2 (6±4%)
3	PX4	A	650	-	45,45,45	1.07±0.08	3±1 (6±2%)
3	PX4	B	367	-	45,45,45	1.09±0.11	3±1 (5±3%)
3	PX4	B	318	-	45,45,45	1.04±0.11	3±2 (5±3%)
3	PX4	C	341	-	45,45,45	1.10±0.11	3±1 (7±2%)
3	PX4	B	371	-	45,45,45	1.05±0.12	3±2 (5±3%)
3	PX4	B	376	-	45,45,45	1.10±0.09	3±2 (7±3%)
3	PX4	B	319	-	45,45,45	1.08±0.10	3±1 (5±3%)
3	PX4	B	337	-	45,45,45	1.06±0.13	3±2 (7±3%)
3	PX4	A	610	-	45,45,45	1.07±0.12	3±2 (6±3%)
3	PX4	B	328	-	45,45,45	1.10±0.08	3±1 (7±2%)
3	PX4	C	324	-	45,45,45	1.04±0.09	2±2 (5±3%)
3	PX4	B	332	-	45,45,45	1.11±0.11	3±1 (7±3%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
3	PX4	B	364	-	45,45,45	1.07±0.14	3±2 (7±4%)
3	PX4	B	306	-	45,45,45	1.06±0.13	3±2 (6±3%)
3	PX4	C	364	-	45,45,45	1.10±0.11	3±2 (7±3%)
3	PX4	B	335	-	45,45,45	1.04±0.10	3±1 (5±2%)
3	PX4	B	387	-	45,45,45	1.06±0.11	3±2 (5±3%)
3	PX4	A	635	-	45,45,45	1.07±0.13	3±2 (7±4%)
3	PX4	C	307	-	45,45,45	1.10±0.16	3±2 (7±4%)
3	PX4	B	388	-	45,45,45	1.07±0.11	3±2 (6±3%)
3	PX4	A	629	-	45,45,45	1.07±0.10	3±1 (5±2%)
3	PX4	B	312	-	45,45,45	1.10±0.14	4±2 (8±4%)
3	PX4	B	320	-	45,45,45	1.08±0.11	3±1 (6±2%)
3	PX4	A	647	-	45,45,45	1.08±0.08	3±2 (7±3%)
3	PX4	C	310	-	45,45,45	1.06±0.11	3±1 (5±2%)
3	PX4	B	356	-	45,45,45	1.04±0.14	3±2 (5±3%)
3	PX4	B	340	-	45,45,45	1.10±0.13	3±2 (6±3%)
3	PX4	B	372	-	45,45,45	1.04±0.12	3±2 (6±3%)
3	PX4	C	304	-	45,45,45	1.12±0.10	3±2 (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	A	608	-	51,53,53	0.96±0.19	3±2 (4±3%)
3	PX4	A	631	-	51,53,53	0.95±0.10	2±1 (4±2%)
3	PX4	C	318	-	51,53,53	0.95±0.12	2±1 (4±2%)
3	PX4	B	351	-	51,53,53	0.93±0.11	2±1 (4±2%)
3	PX4	B	325	-	51,53,53	0.95±0.12	2±2 (3±3%)
3	PX4	C	362	-	51,53,53	0.93±0.11	2±2 (4±3%)
3	PX4	C	331	-	51,53,53	0.92±0.11	2±1 (4±2%)
3	PX4	C	350	-	51,53,53	1.07±0.13	3±2 (6±3%)
3	PX4	A	640	-	51,53,53	0.98±0.09	2±1 (4±2%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
3	PX4	C	357	-	51,53,53	0.96±0.08	2±1 (4±2%)
3	PX4	A	620	-	51,53,53	0.93±0.12	2±1 (4±2%)
3	PX4	B	395	-	51,53,53	0.93±0.12	2±1 (4±2%)
3	PX4	C	335	-	51,53,53	0.99±0.11	3±2 (6±3%)
3	PX4	C	308	-	51,53,53	0.92±0.13	2±1 (3±2%)
3	PX4	C	338	-	51,53,53	0.96±0.12	2±1 (4±2%)
3	PX4	C	351	-	51,53,53	0.97±0.10	2±2 (4±3%)
3	PX4	A	606	-	51,53,53	0.92±0.10	2±2 (4±3%)
3	PX4	B	369	-	51,53,53	0.98±0.13	3±2 (5±3%)
3	PX4	A	637	-	51,53,53	0.95±0.08	2±1 (4±1%)
3	PX4	B	310	-	51,53,53	0.92±0.10	2±1 (3±1%)
3	PX4	B	363	-	51,53,53	0.97±0.10	2±1 (4±2%)
3	PX4	C	319	-	51,53,53	0.90±0.09	2±1 (3±1%)
3	PX4	B	330	-	51,53,53	0.93±0.10	2±1 (3±2%)
3	PX4	B	390	-	51,53,53	0.91±0.10	2±1 (3±2%)
3	PX4	B	394	-	51,53,53	0.99±0.11	2±1 (4±2%)
3	PX4	B	399	-	51,53,53	0.96±0.11	2±1 (4±2%)
3	PX4	A	621	-	51,53,53	0.97±0.11	3±1 (5±2%)
3	PX4	B	396	-	51,53,53	0.99±0.10	2±1 (4±2%)
3	PX4	C	312	-	51,53,53	0.92±0.11	2±2 (4±4%)
3	PX4	C	325	-	51,53,53	0.98±0.07	3±1 (5±2%)
3	PX4	C	309	-	51,53,53	0.93±0.11	2±1 (4±2%)
3	PX4	A	607	-	51,53,53	0.97±0.11	2±2 (4±3%)
3	PX4	B	385	-	51,53,53	1.01±0.16	3±1 (5±2%)
3	PX4	C	333	-	51,53,53	0.95±0.13	2±2 (4±3%)
3	PX4	C	311	-	51,53,53	1.00±0.10	2±1 (4±2%)
3	PX4	B	386	-	51,53,53	0.95±0.10	2±1 (3±2%)
3	PX4	B	368	-	51,53,53	0.97±0.14	2±1 (4±2%)
3	PX4	B	357	-	51,53,53	0.98±0.14	3±2 (5±4%)
3	PX4	B	344	-	51,53,53	1.00±0.10	2±1 (4±1%)
3	PX4	B	400	-	51,53,53	0.93±0.11	2±1 (4±2%)
3	PX4	B	375	-	51,53,53	0.89±0.13	2±1 (3±2%)
3	PX4	A	605	-	51,53,53	0.97±0.12	3±1 (5±2%)
3	PX4	A	653	-	51,53,53	1.00±0.12	2±1 (4±2%)
3	PX4	B	379	-	51,53,53	0.96±0.11	2±2 (4±3%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
3	PX4	C	306	-	51,53,53	1.00±0.09	3±1 (5±2%)
3	PX4	A	641	-	51,53,53	0.91±0.12	2±1 (3±2%)
3	PX4	C	347	-	51,53,53	0.95±0.09	2±1 (4±2%)
3	PX4	B	336	-	51,53,53	0.95±0.10	2±2 (3±2%)
3	PX4	C	313	-	51,53,53	0.98±0.09	2±2 (4±3%)
3	PX4	B	382	-	51,53,53	0.96±0.08	2±1 (4±2%)
3	PX4	B	309	-	51,53,53	0.99±0.13	3±1 (5±2%)
3	PX4	C	344	-	51,53,53	0.99±0.12	2±1 (4±2%)
3	PX4	C	343	-	51,53,53	0.93±0.09	2±2 (4±3%)
3	PX4	B	301	-	51,53,53	0.95±0.11	2±1 (3±2%)
3	PX4	C	358	-	51,53,53	0.99±0.10	2±1 (4±2%)
3	PX4	A	618	-	51,53,53	0.99±0.13	3±2 (6±3%)
3	PX4	C	345	-	51,53,53	0.95±0.13	2±1 (4±2%)
3	PX4	A	654	-	51,53,53	0.91±0.11	2±1 (3±2%)
3	PX4	A	646	-	51,53,53	0.91±0.14	2±1 (4±2%)
3	PX4	C	346	-	51,53,53	0.97±0.09	2±1 (4±2%)
3	PX4	B	350	-	51,53,53	0.97±0.14	3±2 (5±4%)
3	PX4	B	302	-	51,53,53	0.90±0.11	2±1 (3±2%)
3	PX4	A	614	-	51,53,53	0.93±0.13	2±2 (4±3%)
3	PX4	B	316	-	51,53,53	0.91±0.14	2±1 (4±2%)
3	PX4	A	602	-	51,53,53	0.92±0.11	2±2 (4±3%)
3	PX4	B	341	-	51,53,53	1.05±0.12	3±1 (6±2%)
3	PX4	A	644	-	51,53,53	0.94±0.09	2±1 (4±1%)
3	PX4	C	301	-	51,53,53	0.95±0.09	2±2 (4±3%)
3	PX4	A	611	-	51,53,53	0.93±0.13	2±1 (3±1%)
3	PX4	B	362	-	51,53,53	0.95±0.10	2±2 (4±2%)
3	PX4	B	393	-	51,53,53	0.96±0.08	2±1 (4±1%)
3	PX4	B	338	-	51,53,53	0.91±0.12	2±1 (4±2%)
3	PX4	C	339	-	51,53,53	0.94±0.13	2±1 (3±2%)
3	PX4	B	333	-	51,53,53	0.95±0.10	2±2 (4±3%)
3	PX4	A	648	-	51,53,53	0.97±0.10	2±1 (4±2%)
3	PX4	A	652	-	51,53,53	0.99±0.10	3±1 (5±2%)
3	PX4	A	636	-	51,53,53	0.98±0.11	2±1 (4±2%)
3	PX4	A	639	-	51,53,53	0.93±0.08	2±1 (4±2%)
3	PX4	A	613	-	51,53,53	0.88±0.08	2±1 (3±1%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
3	PX4	C	302	-	51,53,53	0.98±0.13	3±2 (5±3%)
3	PX4	B	327	-	51,53,53	0.95±0.15	2±2 (4±3%)
3	PX4	A	643	-	51,53,53	0.97±0.08	2±2 (4±3%)
3	PX4	B	313	-	51,53,53	0.98±0.10	2±1 (4±2%)
3	PX4	A	601	-	51,53,53	0.97±0.14	3±1 (5±2%)
3	PX4	B	373	-	51,53,53	0.95±0.09	2±1 (4±2%)
3	PX4	B	381	-	51,53,53	0.93±0.09	2±1 (3±2%)
3	PX4	A	626	-	51,53,53	0.96±0.15	2±2 (4±2%)
3	PX4	C	353	-	51,53,53	0.97±0.09	2±1 (4±2%)
3	PX4	B	397	-	51,53,53	0.94±0.12	2±1 (4±2%)
3	PX4	A	603	-	51,53,53	0.97±0.12	3±1 (5±2%)
3	PX4	B	355	-	51,53,53	0.94±0.13	2±1 (4±2%)
3	PX4	B	322	-	51,53,53	0.92±0.12	2±1 (3±2%)
3	PX4	B	354	-	51,53,53	0.97±0.12	2±2 (4±3%)
3	PX4	A	617	-	51,53,53	0.98±0.12	2±1 (4±2%)
3	PX4	A	627	-	51,53,53	0.93±0.11	2±1 (4±2%)
3	PX4	C	317	-	51,53,53	1.05±0.11	4±2 (7±3%)
3	PX4	A	642	-	51,53,53	0.98±0.11	3±2 (5±2%)
3	PX4	B	326	-	51,53,53	0.96±0.12	2±2 (4±3%)
3	PX4	B	392	-	51,53,53	0.96±0.09	3±1 (4±2%)
3	PX4	B	398	-	51,53,53	0.90±0.09	2±1 (3±2%)
3	PX4	B	365	-	51,53,53	0.94±0.13	2±1 (3±2%)
3	PX4	B	307	-	51,53,53	0.95±0.07	2±1 (4±2%)
3	PX4	C	354	-	51,53,53	0.98±0.11	3±1 (5±2%)
3	PX4	C	360	-	51,53,53	0.95±0.16	2±1 (3±2%)
3	PX4	B	345	-	51,53,53	0.93±0.10	2±1 (3±1%)
3	PX4	C	321	-	51,53,53	0.97±0.08	2±1 (4±2%)
3	PX4	B	339	-	51,53,53	0.91±0.12	2±1 (4±2%)
3	PX4	C	330	-	51,53,53	0.96±0.11	2±1 (4±1%)
3	PX4	B	323	-	51,53,53	0.90±0.08	2±1 (3±2%)
3	PX4	A	612	-	51,53,53	1.00±0.15	2±1 (4±2%)
3	PX4	C	356	-	51,53,53	0.94±0.12	2±2 (4±2%)
3	PX4	B	352	-	51,53,53	0.94±0.10	2±1 (3±2%)
3	PX4	B	359	-	51,53,53	0.95±0.10	2±2 (3±3%)
3	PX4	B	324	-	51,53,53	0.91±0.10	2±1 (4±2%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
3	PX4	B	311	-	51,53,53	0.96±0.08	2±1 (3±2%)
3	PX4	A	651	-	51,53,53	1.03±0.13	3±1 (6±2%)
3	PX4	C	349	-	51,53,53	1.00±0.14	3±2 (5±3%)
3	PX4	B	384	-	51,53,53	1.03±0.10	3±1 (5±2%)
3	PX4	A	630	-	51,53,53	0.92±0.11	2±1 (4±2%)
3	PX4	C	336	-	51,53,53	0.93±0.10	2±1 (4±2%)
3	PX4	C	332	-	51,53,53	0.97±0.14	2±2 (4±3%)
3	PX4	B	317	-	51,53,53	0.91±0.10	2±1 (3±2%)
3	PX4	B	366	-	51,53,53	0.93±0.09	2±1 (3±2%)
3	PX4	B	321	-	51,53,53	0.95±0.13	3±2 (5±3%)
3	PX4	C	337	-	51,53,53	0.93±0.11	2±1 (3±2%)
3	PX4	C	359	-	51,53,53	0.85±0.11	1±1 (2±2%)
3	PX4	B	349	-	51,53,53	0.95±0.10	2±1 (3±2%)
3	PX4	B	360	-	51,53,53	0.96±0.11	2±2 (3±3%)
3	PX4	B	329	-	51,53,53	0.95±0.13	2±1 (4±2%)
3	PX4	B	334	-	51,53,53	0.89±0.11	1±1 (2±2%)
3	PX4	B	377	-	51,53,53	0.94±0.11	2±1 (3±2%)
3	PX4	C	305	-	51,53,53	0.94±0.09	2±1 (4±2%)
3	PX4	B	358	-	51,53,53	0.96±0.13	2±2 (4±3%)
3	PX4	C	320	-	51,53,53	1.00±0.10	3±1 (5±2%)
3	PX4	C	327	-	51,53,53	0.97±0.13	3±2 (5±3%)
3	PX4	A	604	-	51,53,53	0.96±0.09	3±1 (5±2%)
3	PX4	B	378	-	51,53,53	0.96±0.12	2±1 (4±2%)
3	PX4	B	391	-	51,53,53	0.91±0.13	2±2 (3±3%)
3	PX4	C	348	-	51,53,53	0.93±0.09	2±2 (4±3%)
3	PX4	B	389	-	51,53,53	0.96±0.09	2±1 (4±1%)
3	PX4	A	632	-	51,53,53	0.94±0.12	2±2 (4±3%)
3	PX4	B	308	-	51,53,53	0.93±0.16	2±2 (4±4%)
3	PX4	B	374	-	51,53,53	0.92±0.10	2±1 (4±2%)
3	PX4	C	328	-	51,53,53	0.95±0.11	2±1 (4±2%)
3	PX4	B	305	-	51,53,53	0.95±0.08	3±1 (5±2%)
3	PX4	B	315	-	51,53,53	0.99±0.12	2±1 (4±2%)
3	PX4	A	628	-	51,53,53	0.93±0.06	2±1 (4±2%)
3	PX4	C	361	-	51,53,53	0.95±0.09	2±1 (4±2%)
3	PX4	B	383	-	51,53,53	1.02±0.08	3±1 (5±2%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
3	PX4	A	638	-	51,53,53	0.94±0.09	2±1 (4±2%)
3	PX4	A	623	-	51,53,53	0.95±0.09	2±1 (4±2%)
3	PX4	B	331	-	51,53,53	0.89±0.13	2±2 (3±3%)
3	PX4	A	619	-	51,53,53	0.93±0.09	2±1 (3±2%)
3	PX4	C	316	-	51,53,53	0.90±0.08	2±1 (3±2%)
3	PX4	C	355	-	51,53,53	0.99±0.12	3±1 (5±2%)
3	PX4	A	624	-	51,53,53	0.93±0.14	2±2 (4±3%)
3	PX4	B	361	-	51,53,53	0.94±0.11	2±2 (4±3%)
3	PX4	B	314	-	51,53,53	0.88±0.11	2±1 (3±1%)
3	PX4	C	342	-	51,53,53	0.92±0.11	2±1 (3±2%)
3	PX4	B	347	-	51,53,53	0.99±0.12	3±1 (4±1%)
3	PX4	C	322	-	51,53,53	0.96±0.10	2±1 (4±2%)
3	PX4	A	609	-	51,53,53	0.97±0.12	2±2 (4±3%)
3	PX4	C	303	-	51,53,53	0.93±0.10	2±1 (3±2%)
3	PX4	A	633	-	51,53,53	0.94±0.10	2±1 (3±1%)
3	PX4	A	616	-	51,53,53	0.95±0.11	3±1 (5±2%)
3	PX4	A	615	-	51,53,53	0.93±0.11	2±1 (3±2%)
3	PX4	C	329	-	51,53,53	0.99±0.14	3±2 (5±3%)
3	PX4	C	352	-	51,53,53	0.95±0.08	2±1 (4±2%)
3	PX4	A	625	-	51,53,53	0.98±0.09	2±1 (3±2%)
3	PX4	A	622	-	51,53,53	0.97±0.14	3±1 (4±2%)
3	PX4	C	334	-	51,53,53	0.93±0.10	2±1 (3±2%)
3	PX4	C	340	-	51,53,53	0.96±0.13	2±2 (4±3%)
3	PX4	C	315	-	51,53,53	0.97±0.10	3±1 (4±2%)
3	PX4	A	649	-	51,53,53	1.01±0.11	3±2 (5±3%)
3	PX4	B	348	-	51,53,53	0.99±0.10	3±1 (5±2%)
3	PX4	A	634	-	51,53,53	0.95±0.12	2±2 (4±3%)
3	PX4	B	304	-	51,53,53	0.94±0.10	2±1 (3±2%)
3	PX4	C	363	-	51,53,53	1.01±0.13	3±2 (5±3%)
3	PX4	B	342	-	51,53,53	0.99±0.13	3±2 (5±3%)
3	PX4	C	314	-	51,53,53	0.94±0.08	2±1 (3±2%)
3	PX4	B	343	-	51,53,53	0.95±0.09	2±2 (3±3%)
3	PX4	B	303	-	51,53,53	0.92±0.12	2±1 (4±2%)
3	PX4	B	380	-	51,53,53	0.98±0.12	3±2 (5±3%)
3	PX4	B	353	-	51,53,53	0.96±0.12	2±1 (4±2%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
3	PX4	C	326	-	51,53,53	0.97±0.09	2±1 (4±2%)
3	PX4	A	645	-	51,53,53	0.90±0.14	2±2 (4±3%)
3	PX4	B	370	-	51,53,53	0.96±0.09	2±1 (4±2%)
3	PX4	B	346	-	51,53,53	0.88±0.07	1±1 (2±1%)
3	PX4	C	323	-	51,53,53	0.96±0.10	2±1 (4±2%)
3	PX4	A	650	-	51,53,53	0.94±0.12	2±1 (4±2%)
3	PX4	B	367	-	51,53,53	0.97±0.11	2±1 (4±1%)
3	PX4	B	318	-	51,53,53	0.94±0.12	2±1 (3±2%)
3	PX4	C	341	-	51,53,53	0.97±0.09	3±1 (4±2%)
3	PX4	B	371	-	51,53,53	0.96±0.12	2±1 (4±2%)
3	PX4	B	376	-	51,53,53	0.92±0.10	2±1 (4±2%)
3	PX4	B	319	-	51,53,53	1.00±0.10	3±2 (5±3%)
3	PX4	B	337	-	51,53,53	0.93±0.09	2±1 (4±2%)
3	PX4	A	610	-	51,53,53	0.92±0.12	2±1 (3±2%)
3	PX4	B	328	-	51,53,53	0.95±0.07	2±1 (3±1%)
3	PX4	C	324	-	51,53,53	0.97±0.12	3±1 (4±2%)
3	PX4	B	332	-	51,53,53	0.96±0.15	3±2 (5±2%)
3	PX4	B	364	-	51,53,53	0.94±0.13	2±1 (3±2%)
3	PX4	B	306	-	51,53,53	1.00±0.12	3±1 (6±2%)
3	PX4	C	364	-	51,53,53	0.94±0.09	2±1 (4±2%)
3	PX4	B	335	-	51,53,53	0.94±0.12	2±1 (4±2%)
3	PX4	B	387	-	51,53,53	0.89±0.10	2±1 (3±2%)
3	PX4	A	635	-	51,53,53	0.90±0.07	2±1 (3±1%)
3	PX4	C	307	-	51,53,53	0.94±0.09	2±1 (3±1%)
3	PX4	B	388	-	51,53,53	0.98±0.13	3±2 (4±3%)
3	PX4	A	629	-	51,53,53	0.88±0.13	2±1 (3±2%)
3	PX4	B	312	-	51,53,53	0.99±0.08	2±2 (4±2%)
3	PX4	B	320	-	51,53,53	0.99±0.13	3±2 (4±3%)
3	PX4	A	647	-	51,53,53	0.96±0.10	2±1 (4±2%)
3	PX4	C	310	-	51,53,53	1.03±0.14	3±1 (6±2%)
3	PX4	B	356	-	51,53,53	0.98±0.13	3±2 (5±3%)
3	PX4	B	340	-	51,53,53	0.92±0.09	2±1 (4±2%)
3	PX4	B	372	-	51,53,53	1.02±0.10	3±1 (6±2%)
3	PX4	C	304	-	51,53,53	0.96±0.15	3±2 (5±3%)

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	308	-	-	0±0,49,49,49	-
3	PX4	C	335	-	-	0±0,49,49,49	-
3	PX4	B	330	-	-	0±0,49,49,49	-
3	PX4	B	396	-	-	0±0,49,49,49	-
3	PX4	C	309	-	-	0±0,49,49,49	-
3	PX4	C	347	-	-	0±0,49,49,49	-
3	PX4	A	654	-	-	0±0,49,49,49	-
3	PX4	B	386	-	-	0±0,49,49,49	-
3	PX4	B	381	-	-	0±0,49,49,49	-
3	PX4	C	330	-	-	0±0,49,49,49	-
3	PX4	B	339	-	-	0±0,49,49,49	-
3	PX4	C	337	-	-	0±0,49,49,49	-
3	PX4	C	332	-	-	0±0,49,49,49	-
3	PX4	B	359	-	-	0±0,49,49,49	-
3	PX4	C	338	-	-	0±0,49,49,49	-
3	PX4	C	316	-	-	0±0,49,49,49	-
3	PX4	C	321	-	-	0±0,49,49,49	-
3	PX4	B	393	-	-	0±0,49,49,49	-
3	PX4	A	609	-	-	0±0,49,49,49	-
3	PX4	A	649	-	-	0±0,49,49,49	-
3	PX4	B	347	-	-	0±0,49,49,49	-
3	PX4	A	601	-	-	0±0,49,49,49	-
3	PX4	B	342	-	-	0±0,49,49,49	-
3	PX4	B	303	-	-	0±0,49,49,49	-
3	PX4	B	360	-	-	0±0,49,49,49	-
3	PX4	B	304	-	-	0±0,49,49,49	-
3	PX4	C	360	-	-	0±0,49,49,49	-
3	PX4	B	355	-	-	0±0,49,49,49	-
3	PX4	B	334	-	-	0±0,49,49,49	-
3	PX4	A	622	-	-	0±0,49,49,49	-
3	PX4	C	313	-	-	0±0,49,49,49	-
3	PX4	B	328	-	-	0±0,49,49,49	-
3	PX4	C	352	-	-	0±0,49,49,49	-
3	PX4	C	306	-	-	0±0,49,49,49	-
3	PX4	B	361	-	-	0±0,49,49,49	-
3	PX4	A	639	-	-	0±0,49,49,49	-
3	PX4	C	345	-	-	0±0,49,49,49	-
3	PX4	B	311	-	-	0±0,49,49,49	-
3	PX4	A	615	-	-	0±0,49,49,49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PX4	B	335	-	-	0±0,49,49,49	-
3	PX4	A	632	-	-	0±0,49,49,49	-
3	PX4	C	350	-	-	0±0,49,49,49	-
3	PX4	B	373	-	-	0±0,49,49,49	-
3	PX4	B	320	-	-	0±0,49,49,49	-
3	PX4	B	343	-	-	0±0,49,49,49	-
3	PX4	A	610	-	-	0±0,49,49,49	-
3	PX4	A	614	-	-	0±0,49,49,49	-
3	PX4	B	326	-	-	0±0,49,49,49	-
3	PX4	A	618	-	-	0±0,49,49,49	-
3	PX4	A	638	-	-	0±0,49,49,49	-
3	PX4	A	603	-	-	0±0,49,49,49	-
3	PX4	A	628	-	-	0±0,49,49,49	-
3	PX4	B	384	-	-	0±0,49,49,49	-
3	PX4	C	305	-	-	0±0,49,49,49	-
3	PX4	C	357	-	-	0±0,49,49,49	-
3	PX4	C	339	-	-	0±0,49,49,49	-
3	PX4	B	395	-	-	0±0,49,49,49	-
3	PX4	C	307	-	-	0±0,49,49,49	-
3	PX4	A	619	-	-	0±0,49,49,49	-
3	PX4	A	627	-	-	0±0,49,49,49	-
3	PX4	B	305	-	-	0±0,49,49,49	-
3	PX4	C	329	-	-	0±0,49,49,49	-
3	PX4	A	617	-	-	0±0,49,49,49	-
3	PX4	B	317	-	-	0±0,49,49,49	-
3	PX4	B	385	-	-	0±0,49,49,49	-
3	PX4	C	310	-	-	0±0,49,49,49	-
3	PX4	B	399	-	-	0±0,49,49,49	-
3	PX4	B	352	-	-	0±0,49,49,49	-
3	PX4	C	359	-	-	0±0,49,49,49	-
3	PX4	B	371	-	-	0±0,49,49,49	-
3	PX4	B	309	-	-	0±0,49,49,49	-
3	PX4	C	328	-	-	0±0,49,49,49	-
3	PX4	A	637	-	-	0±0,49,49,49	-
3	PX4	C	361	-	-	0±0,49,49,49	-
3	PX4	C	301	-	-	0±0,49,49,49	-
3	PX4	A	651	-	-	0±0,49,49,49	-
3	PX4	A	645	-	-	0±0,49,49,49	-
3	PX4	A	616	-	-	0±0,49,49,49	-
3	PX4	B	331	-	-	0±0,49,49,49	-
3	PX4	B	306	-	-	0±0,49,49,49	-
3	PX4	B	376	-	-	0±0,49,49,49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PX4	A	613	-	-	0±0,49,49,49	-
3	PX4	C	311	-	-	0±0,49,49,49	-
3	PX4	B	349	-	-	0±0,49,49,49	-
3	PX4	A	652	-	-	0±0,49,49,49	-
3	PX4	C	363	-	-	0±0,49,49,49	-
3	PX4	B	312	-	-	0±0,49,49,49	-
3	PX4	A	643	-	-	0±0,49,49,49	-
3	PX4	B	391	-	-	0±0,49,49,49	-
3	PX4	B	356	-	-	0±0,49,49,49	-
3	PX4	C	356	-	-	0±0,49,49,49	-
3	PX4	C	318	-	-	0±0,49,49,49	-
3	PX4	A	604	-	-	0±0,49,49,49	-
3	PX4	C	349	-	-	0±0,49,49,49	-
3	PX4	A	635	-	-	0±0,49,49,49	-
3	PX4	A	612	-	-	0±0,49,49,49	-
3	PX4	B	392	-	-	0±0,49,49,49	-
3	PX4	C	320	-	-	0±0,49,49,49	-
3	PX4	B	337	-	-	0±0,49,49,49	-
3	PX4	C	312	-	-	0±0,49,49,49	-
3	PX4	B	332	-	-	0±0,49,49,49	-
3	PX4	C	353	-	-	0±0,49,49,49	-
3	PX4	B	367	-	-	0±0,49,49,49	-
3	PX4	A	629	-	-	0±0,49,49,49	-
3	PX4	B	333	-	-	0±0,49,49,49	-
3	PX4	A	608	-	-	0±0,49,49,49	-
3	PX4	B	350	-	-	0±0,49,49,49	-
3	PX4	C	362	-	-	0±0,49,49,49	-
3	PX4	C	336	-	-	0±0,49,49,49	-
3	PX4	A	605	-	-	0±0,49,49,49	-
3	PX4	B	368	-	-	0±0,49,49,49	-
3	PX4	A	644	-	-	0±0,49,49,49	-
3	PX4	A	621	-	-	0±0,49,49,49	-
3	PX4	B	325	-	-	0±0,49,49,49	-
3	PX4	C	325	-	-	0±0,49,49,49	-
3	PX4	B	323	-	-	0±0,49,49,49	-
3	PX4	C	303	-	-	0±0,49,49,49	-
3	PX4	A	631	-	-	0±0,49,49,49	-
3	PX4	C	333	-	-	0±0,49,49,49	-
3	PX4	B	351	-	-	0±0,49,49,49	-
3	PX4	B	329	-	-	0±0,49,49,49	-
3	PX4	A	602	-	-	0±0,49,49,49	-
3	PX4	A	620	-	-	0±0,49,49,49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PX4	B	364	-	-	0±0,49,49,49	-
3	PX4	B	363	-	-	0±0,49,49,49	-
3	PX4	C	344	-	-	0±0,49,49,49	-
3	PX4	B	379	-	-	0±0,49,49,49	-
3	PX4	A	647	-	-	0±0,49,49,49	-
3	PX4	C	348	-	-	0±0,49,49,49	-
3	PX4	C	322	-	-	0±0,49,49,49	-
3	PX4	C	334	-	-	0±0,49,49,49	-
3	PX4	B	370	-	-	0±0,49,49,49	-
3	PX4	B	314	-	-	0±0,49,49,49	-
3	PX4	B	315	-	-	0±0,49,49,49	-
3	PX4	C	327	-	-	0±0,49,49,49	-
3	PX4	B	383	-	-	0±0,49,49,49	-
3	PX4	B	307	-	-	0±0,49,49,49	-
3	PX4	C	319	-	-	0±0,49,49,49	-
3	PX4	B	338	-	-	0±0,49,49,49	-
3	PX4	C	341	-	-	0±0,49,49,49	-
3	PX4	B	346	-	-	0±0,49,49,49	-
3	PX4	B	324	-	-	0±0,49,49,49	-
3	PX4	B	336	-	-	0±0,49,49,49	-
3	PX4	A	626	-	-	0±0,49,49,49	-
3	PX4	B	389	-	-	0±0,49,49,49	-
3	PX4	B	380	-	-	0±0,49,49,49	-
3	PX4	B	366	-	-	0±0,49,49,49	-
3	PX4	B	322	-	-	0±0,49,49,49	-
3	PX4	B	398	-	-	0±0,49,49,49	-
3	PX4	C	326	-	-	0±0,49,49,49	-
3	PX4	C	346	-	-	0±0,49,49,49	-
3	PX4	B	397	-	-	0±0,49,49,49	-
3	PX4	A	648	-	-	0±0,49,49,49	-
3	PX4	B	362	-	-	0±0,49,49,49	-
3	PX4	B	313	-	-	0±0,49,49,49	-
3	PX4	C	343	-	-	0±0,49,49,49	-
3	PX4	A	623	-	-	0±0,49,49,49	-
3	PX4	B	319	-	-	0±0,49,49,49	-
3	PX4	B	354	-	-	0±0,49,49,49	-
3	PX4	A	634	-	-	0±0,49,49,49	-
3	PX4	B	358	-	-	0±0,49,49,49	-
3	PX4	B	382	-	-	0±0,49,49,49	-
3	PX4	A	624	-	-	0±0,49,49,49	-
3	PX4	B	394	-	-	0±0,49,49,49	-
3	PX4	B	327	-	-	0±0,49,49,49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PX4	C	340	-	-	0±0,49,49,49	-
3	PX4	C	302	-	-	0±0,49,49,49	-
3	PX4	B	390	-	-	0±0,49,49,49	-
3	PX4	B	341	-	-	0±0,49,49,49	-
3	PX4	B	310	-	-	0±0,49,49,49	-
3	PX4	B	387	-	-	0±0,49,49,49	-
3	PX4	C	324	-	-	0±0,49,49,49	-
3	PX4	C	317	-	-	0±0,49,49,49	-
3	PX4	B	369	-	-	0±0,49,49,49	-
3	PX4	B	344	-	-	0±0,49,49,49	-
3	PX4	A	650	-	-	0±0,49,49,49	-
3	PX4	B	302	-	-	0±0,49,49,49	-
3	PX4	B	357	-	-	0±0,49,49,49	-
3	PX4	B	340	-	-	0±0,49,49,49	-
3	PX4	B	400	-	-	0±0,49,49,49	-
3	PX4	C	314	-	-	0±0,49,49,49	-
3	PX4	A	646	-	-	0±0,49,49,49	-
3	PX4	C	304	-	-	0±0,49,49,49	-
3	PX4	B	365	-	-	0±0,49,49,49	-
3	PX4	B	316	-	-	0±0,49,49,49	-
3	PX4	B	378	-	-	0±0,49,49,49	-
3	PX4	B	321	-	-	0±0,49,49,49	-
3	PX4	B	353	-	-	0±0,49,49,49	-
3	PX4	B	388	-	-	0±0,49,49,49	-
3	PX4	B	348	-	-	0±0,49,49,49	-
3	PX4	A	606	-	-	0±0,49,49,49	-
3	PX4	A	633	-	-	0±0,49,49,49	-
3	PX4	A	641	-	-	0±0,49,49,49	-
3	PX4	A	630	-	-	0±0,49,49,49	-
3	PX4	A	607	-	-	0±0,49,49,49	-
3	PX4	C	331	-	-	0±0,49,49,49	-
3	PX4	A	642	-	-	0±0,49,49,49	-
3	PX4	A	640	-	-	0±0,49,49,49	-
3	PX4	A	611	-	-	0±0,49,49,49	-
3	PX4	C	355	-	-	0±0,49,49,49	-
3	PX4	A	625	-	-	0±0,49,49,49	-
3	PX4	B	301	-	-	0±0,49,49,49	-
3	PX4	A	653	-	-	0±0,49,49,49	-
3	PX4	B	375	-	-	0±0,49,49,49	-
3	PX4	B	374	-	-	0±0,49,49,49	-
3	PX4	C	354	-	-	0±0,49,49,49	-
3	PX4	C	358	-	-	0±0,49,49,49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PX4	C	323	-	-	0±0,49,49,49	-
3	PX4	B	372	-	-	0±0,49,49,49	-
3	PX4	B	308	-	-	0±0,49,49,49	-
3	PX4	C	364	-	-	0±0,49,49,49	-
3	PX4	B	345	-	-	0±0,49,49,49	-
3	PX4	A	636	-	-	0±0,49,49,49	-
3	PX4	B	377	-	-	0±0,49,49,49	-
3	PX4	C	342	-	-	0±0,49,49,49	-
3	PX4	C	351	-	-	0±0,49,49,49	-
3	PX4	C	315	-	-	0±0,49,49,49	-
3	PX4	B	318	-	-	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	C	322	PX4	C2-C1	5.97	1.69	1.51	1	5
3	B	352	PX4	C2-C1	5.78	1.68	1.51	2	6
3	B	313	PX4	C6-C7	5.46	1.67	1.50	7	6
3	B	357	PX4	C8-C7	5.44	1.67	1.50	10	5
3	A	611	PX4	C10-C9	5.39	1.66	1.50	3	5
3	B	372	PX4	C8-C7	5.28	1.67	1.50	5	8
3	C	356	PX4	C8-C7	5.19	1.67	1.50	1	11
3	A	638	PX4	C8-C7	5.18	1.67	1.50	8	6
3	B	338	PX4	C6-C7	5.16	1.67	1.50	9	8
3	B	365	PX4	C6-C7	5.13	1.66	1.50	7	6
3	B	353	PX4	O7-C7	5.12	1.34	1.46	11	4
3	B	356	PX4	O7-C7	5.12	1.34	1.46	2	2
3	C	303	PX4	C8-C7	5.11	1.66	1.50	3	7
3	B	370	PX4	C6-C7	5.10	1.66	1.50	5	7
3	C	352	PX4	C8-C7	5.07	1.66	1.50	8	3
3	B	346	PX4	C8-C7	5.06	1.66	1.50	7	5
3	C	346	PX4	C24-C23	5.06	1.65	1.50	14	3
3	C	306	PX4	C24-C23	5.03	1.65	1.50	4	3
3	B	386	PX4	C24-C23	5.02	1.65	1.50	6	5
3	A	618	PX4	C24-C23	5.00	1.65	1.50	10	3
3	B	388	PX4	C6-C7	5.00	1.66	1.50	10	7
3	C	347	PX4	C8-C7	4.99	1.66	1.50	5	7
3	C	309	PX4	C6-C7	4.93	1.66	1.50	12	6
3	B	303	PX4	C6-C7	4.92	1.66	1.50	5	9
3	A	631	PX4	O7-C23	4.91	1.20	1.34	14	6
3	A	613	PX4	C2-C1	4.90	1.66	1.51	8	7

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	A	603	PX4	C2-C1	4.89	1.66	1.51	1	5
3	B	393	PX4	O7-C7	4.87	1.35	1.46	11	3
3	A	645	PX4	C6-C7	4.82	1.65	1.50	2	6
3	C	353	PX4	O7-C7	4.79	1.35	1.46	1	3
3	A	612	PX4	C2-C1	4.78	1.65	1.51	5	4
3	C	359	PX4	O7-C23	4.78	1.20	1.34	11	3
3	C	352	PX4	C10-C9	4.77	1.64	1.50	2	4
3	A	607	PX4	C6-C7	4.73	1.65	1.50	15	5
3	C	333	PX4	C8-C7	4.70	1.65	1.50	1	5
3	B	350	PX4	C6-C7	4.69	1.65	1.50	13	9
3	C	305	PX4	C8-C7	4.68	1.65	1.50	2	9
3	B	393	PX4	C8-C7	4.67	1.65	1.50	6	6
3	B	301	PX4	C24-C23	4.66	1.64	1.50	9	4
3	B	373	PX4	C8-C7	4.65	1.65	1.50	14	6
3	B	343	PX4	C8-C7	4.64	1.65	1.50	7	7
3	B	306	PX4	O5-C8	4.63	1.55	1.45	4	1
3	C	313	PX4	C8-C7	4.61	1.65	1.50	2	8
3	B	340	PX4	C8-C7	4.61	1.65	1.50	15	7
3	B	318	PX4	C8-C7	4.60	1.65	1.50	10	7
3	B	314	PX4	C8-C7	4.58	1.65	1.50	9	8
3	B	324	PX4	C6-C7	4.58	1.65	1.50	9	4
3	B	351	PX4	C2-N1	4.58	1.65	1.51	1	4
3	B	308	PX4	C2-C1	4.57	1.65	1.51	4	6
3	B	373	PX4	C10-C9	4.56	1.63	1.50	9	4
3	B	381	PX4	C6-C7	4.55	1.65	1.50	13	6
3	B	330	PX4	C6-C7	4.55	1.65	1.50	2	7
3	C	351	PX4	C6-C7	4.55	1.65	1.50	6	8
3	B	396	PX4	O7-C23	4.55	1.21	1.34	3	5
3	B	385	PX4	C2-C1	4.54	1.65	1.51	3	5
3	B	326	PX4	C6-C7	4.53	1.65	1.50	10	8
3	A	619	PX4	C8-C7	4.52	1.64	1.50	13	9
3	B	314	PX4	C2-C1	4.52	1.65	1.51	3	6
3	B	342	PX4	O7-C7	4.52	1.36	1.46	7	3
3	A	627	PX4	C8-C7	4.49	1.64	1.50	6	9
3	B	331	PX4	C8-C7	4.49	1.64	1.50	13	7
3	B	380	PX4	C6-C7	4.49	1.64	1.50	3	6
3	B	338	PX4	C8-C7	4.48	1.64	1.50	7	5
3	C	304	PX4	C8-C7	4.48	1.64	1.50	2	6
3	B	322	PX4	C2-C1	4.47	1.64	1.51	1	8
3	B	368	PX4	C8-C7	4.45	1.64	1.50	2	7
3	C	343	PX4	C6-C7	4.44	1.64	1.50	10	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	A	619	PX4	C6-C7	4.44	1.64	1.50	5	6
3	B	319	PX4	C8-C7	4.43	1.64	1.50	11	8
3	B	374	PX4	C6-C7	4.44	1.64	1.50	15	7
3	B	315	PX4	C8-C7	4.43	1.64	1.50	10	5
3	B	349	PX4	C10-C9	4.43	1.63	1.50	2	2
3	B	333	PX4	C2-C1	4.42	1.64	1.51	14	1
3	B	330	PX4	C2-C1	4.41	1.64	1.51	1	7
3	B	351	PX4	C2-C1	4.41	1.64	1.51	13	5
3	B	395	PX4	C2-C1	4.40	1.64	1.51	11	2
3	C	323	PX4	C8-C7	4.40	1.64	1.50	5	7
3	A	639	PX4	C2-C1	4.40	1.64	1.51	9	9
3	A	632	PX4	C6-C7	4.40	1.64	1.50	4	6
3	B	376	PX4	C6-C7	4.38	1.64	1.50	12	6
3	B	332	PX4	C8-C7	4.38	1.64	1.50	3	9
3	A	648	PX4	C8-C7	4.38	1.64	1.50	4	6
3	A	650	PX4	C8-C7	4.38	1.64	1.50	13	9
3	C	350	PX4	C6-C7	4.38	1.64	1.50	1	10
3	B	380	PX4	C8-C7	4.38	1.64	1.50	7	5
3	C	335	PX4	C2-C1	4.37	1.64	1.51	5	9
3	C	320	PX4	C2-C1	4.37	1.64	1.51	14	1
3	B	385	PX4	C8-C7	4.37	1.64	1.50	14	6
3	B	308	PX4	C8-C7	4.36	1.64	1.50	10	8
3	B	364	PX4	C24-C23	4.36	1.63	1.50	4	4
3	C	314	PX4	C6-C7	4.36	1.64	1.50	5	4
3	C	347	PX4	C6-C7	4.36	1.64	1.50	3	6
3	A	641	PX4	C8-C7	4.35	1.64	1.50	12	6
3	B	378	PX4	C2-C1	4.34	1.64	1.51	9	4
3	B	347	PX4	C8-C7	4.33	1.64	1.50	8	9
3	B	389	PX4	O5-C9	4.33	1.46	1.33	10	2
3	B	304	PX4	O7-C23	4.33	1.22	1.34	7	2
3	B	323	PX4	O7-C7	4.33	1.56	1.46	1	5
3	B	327	PX4	C8-C7	4.32	1.64	1.50	5	7
3	A	645	PX4	C24-C23	4.32	1.63	1.50	10	5
3	A	635	PX4	O7-C23	4.32	1.22	1.34	10	3
3	B	396	PX4	C8-C7	4.32	1.64	1.50	13	5
3	B	380	PX4	C2-C1	4.31	1.64	1.51	1	4
3	C	335	PX4	C24-C23	4.31	1.63	1.50	14	3
3	B	305	PX4	C5-N1	4.31	1.37	1.50	14	1
3	C	326	PX4	C10-C9	4.31	1.63	1.50	2	5
3	B	333	PX4	C8-C7	4.31	1.64	1.50	8	6
3	C	307	PX4	C2-C1	4.31	1.64	1.51	8	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	C	361	PX4	C10-C9	4.30	1.63	1.50	7	5
3	B	369	PX4	C6-C7	4.30	1.64	1.50	15	7
3	B	327	PX4	C6-C7	4.30	1.64	1.50	2	6
3	B	382	PX4	C8-C7	4.30	1.64	1.50	9	6
3	B	398	PX4	C8-C7	4.29	1.64	1.50	2	7
3	C	350	PX4	C8-C7	4.29	1.64	1.50	8	8
3	B	312	PX4	C10-C9	4.27	1.63	1.50	13	7
3	A	612	PX4	O7-C7	4.26	1.36	1.46	5	2
3	A	648	PX4	C10-C9	4.26	1.63	1.50	10	3
3	C	306	PX4	C8-C7	4.26	1.64	1.50	11	9
3	B	390	PX4	C2-C1	4.26	1.64	1.51	12	6
3	C	345	PX4	C2-C1	4.26	1.64	1.51	7	8
3	B	346	PX4	C2-C1	4.24	1.64	1.51	1	5
3	B	353	PX4	C2-C1	4.24	1.64	1.51	12	6
3	C	336	PX4	O7-C7	4.24	1.36	1.46	14	4
3	A	611	PX4	C6-C7	4.24	1.64	1.50	11	7
3	B	362	PX4	O7-C7	4.23	1.36	1.46	3	3
3	C	301	PX4	C2-C1	4.23	1.64	1.51	5	8
3	C	317	PX4	O5-C8	4.23	1.35	1.45	5	3
3	B	354	PX4	C10-C9	4.23	1.63	1.50	15	4
3	B	305	PX4	C6-C7	4.22	1.64	1.50	4	7
3	B	321	PX4	C6-C7	4.22	1.64	1.50	1	8
3	B	367	PX4	C8-C7	4.22	1.64	1.50	5	6
3	C	348	PX4	C6-C7	4.22	1.64	1.50	15	7
3	C	357	PX4	C6-C7	4.21	1.64	1.50	9	4
3	A	624	PX4	C6-C7	4.21	1.64	1.50	2	7
3	A	629	PX4	C24-C23	4.20	1.62	1.50	4	3
3	A	649	PX4	C6-C7	4.20	1.63	1.50	9	7
3	A	639	PX4	C8-C7	4.19	1.63	1.50	14	6
3	B	343	PX4	O7-C7	4.18	1.36	1.46	15	3
3	B	333	PX4	C6-C7	4.18	1.63	1.50	15	5
3	A	628	PX4	O7-C7	4.18	1.36	1.46	2	2
3	C	313	PX4	C6-C7	4.18	1.63	1.50	5	4
3	C	334	PX4	O7-C23	4.18	1.22	1.34	8	3
3	B	360	PX4	C10-C9	4.17	1.62	1.50	4	3
3	B	389	PX4	C24-C23	4.17	1.62	1.50	13	2
3	C	360	PX4	C6-C7	4.17	1.63	1.50	14	4
3	C	359	PX4	C6-C7	4.17	1.63	1.50	9	8
3	C	357	PX4	C2-C1	4.16	1.63	1.51	8	6
3	B	383	PX4	C24-C23	4.16	1.62	1.50	8	5
3	B	384	PX4	C2-C1	4.15	1.63	1.51	11	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	355	PX4	O7-C23	4.15	1.22	1.34	12	4
3	B	324	PX4	C8-C7	4.15	1.63	1.50	2	5
3	B	345	PX4	C24-C23	4.14	1.62	1.50	1	4
3	A	637	PX4	C10-C9	4.14	1.62	1.50	7	4
3	B	373	PX4	O5-C8	4.14	1.54	1.45	4	3
3	C	343	PX4	O7-C7	4.14	1.36	1.46	3	2
3	C	335	PX4	C10-C9	4.13	1.62	1.50	13	7
3	B	349	PX4	C6-C7	4.13	1.63	1.50	12	7
3	B	351	PX4	C6-C7	4.13	1.63	1.50	3	6
3	B	316	PX4	C8-C7	4.12	1.63	1.50	12	6
3	B	306	PX4	O7-C7	4.12	1.36	1.46	8	4
3	B	309	PX4	C2-C1	4.12	1.63	1.51	14	8
3	B	363	PX4	O7-C7	4.12	1.36	1.46	13	4
3	C	308	PX4	O5-C8	4.12	1.54	1.45	6	4
3	A	642	PX4	C2-C1	4.11	1.63	1.51	15	2
3	B	387	PX4	C6-C7	4.10	1.63	1.50	7	5
3	C	364	PX4	C6-C7	4.10	1.63	1.50	9	7
3	A	605	PX4	C8-C7	4.10	1.63	1.50	10	6
3	A	646	PX4	C2-C1	4.10	1.63	1.51	12	7
3	B	382	PX4	C2-C1	4.09	1.63	1.51	2	7
3	C	341	PX4	C6-C7	4.09	1.63	1.50	5	7
3	C	362	PX4	C6-C7	4.09	1.63	1.50	3	6
3	C	360	PX4	C2-C1	4.09	1.63	1.51	1	3
3	B	394	PX4	C6-C7	4.09	1.63	1.50	8	6
3	A	649	PX4	C8-C7	4.09	1.63	1.50	15	5
3	B	383	PX4	C10-C9	4.09	1.62	1.50	9	5
3	C	329	PX4	C6-C7	4.09	1.63	1.50	3	9
3	C	336	PX4	C2-C1	4.08	1.63	1.51	15	3
3	B	322	PX4	C6-C7	4.08	1.63	1.50	1	7
3	C	320	PX4	C10-C9	4.08	1.62	1.50	4	5
3	C	358	PX4	O5-C9	4.08	1.21	1.33	10	2
3	B	324	PX4	C24-C23	4.07	1.62	1.50	10	3
3	A	603	PX4	C6-C7	4.06	1.63	1.50	15	8
3	B	383	PX4	C6-C7	4.06	1.63	1.50	2	6
3	B	370	PX4	C24-C23	4.06	1.62	1.50	15	3
3	A	641	PX4	O5-C9	4.06	1.21	1.33	7	1
3	C	345	PX4	C24-C23	4.06	1.62	1.50	14	1
3	B	310	PX4	O5-C8	4.06	1.36	1.45	6	4
3	B	342	PX4	C8-C7	4.06	1.63	1.50	6	9
3	C	325	PX4	C10-C9	4.06	1.62	1.50	8	3
3	A	644	PX4	O5-C8	4.05	1.36	1.45	5	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	A	613	PX4	C6-C7	4.05	1.63	1.50	2	5
3	B	395	PX4	C8-C7	4.05	1.63	1.50	10	5
3	C	318	PX4	C8-C7	4.05	1.63	1.50	8	3
3	A	654	PX4	C2-C1	4.04	1.63	1.51	2	3
3	B	301	PX4	C8-C7	4.04	1.63	1.50	15	3
3	C	343	PX4	C8-C7	4.04	1.63	1.50	15	6
3	A	604	PX4	C8-C7	4.04	1.63	1.50	10	3
3	B	377	PX4	C2-C1	4.03	1.63	1.51	8	6
3	C	339	PX4	C2-C1	4.03	1.63	1.51	2	9
3	C	344	PX4	C8-C7	4.03	1.63	1.50	8	6
3	A	647	PX4	C2-C1	4.03	1.63	1.51	9	5
3	B	311	PX4	C6-C7	4.03	1.63	1.50	3	7
3	A	611	PX4	O5-C9	4.03	1.45	1.33	10	2
3	C	301	PX4	C8-C7	4.03	1.63	1.50	14	7
3	A	645	PX4	C2-C1	4.02	1.63	1.51	15	6
3	B	326	PX4	C24-C23	4.02	1.62	1.50	10	3
3	C	323	PX4	O5-C8	4.02	1.36	1.45	5	2
3	B	395	PX4	C6-C7	4.01	1.63	1.50	2	5
3	B	314	PX4	O7-C7	4.01	1.37	1.46	4	5
3	B	316	PX4	C4-N1	4.01	1.38	1.50	6	1
3	B	320	PX4	C6-C7	4.00	1.63	1.50	7	6
3	B	381	PX4	C11-C10	4.00	1.66	1.52	13	1
3	B	336	PX4	C8-C7	4.00	1.63	1.50	14	5
3	B	344	PX4	O7-C7	4.00	1.37	1.46	3	4
3	C	339	PX4	C6-C7	4.00	1.63	1.50	12	4
3	C	311	PX4	C8-C7	3.99	1.63	1.50	15	8
3	B	372	PX4	C6-C7	3.99	1.63	1.50	3	5
3	C	336	PX4	C6-C7	3.99	1.63	1.50	3	2
3	B	354	PX4	O7-C7	3.99	1.37	1.46	11	4
3	B	397	PX4	C2-C1	3.98	1.63	1.51	1	4
3	B	363	PX4	C6-C7	3.98	1.63	1.50	1	5
3	C	315	PX4	C2-N1	3.98	1.63	1.51	5	2
3	C	342	PX4	C8-C7	3.98	1.63	1.50	2	8
3	C	355	PX4	C8-C7	3.98	1.63	1.50	4	4
3	B	376	PX4	C2-C1	3.98	1.63	1.51	8	8
3	C	313	PX4	C24-C23	3.98	1.62	1.50	5	2
3	C	333	PX4	C3-N1	3.98	1.38	1.50	9	2
3	B	316	PX4	C6-C7	3.98	1.63	1.50	15	9
3	B	327	PX4	O7-C7	3.98	1.37	1.46	6	5
3	C	329	PX4	O5-C8	3.98	1.36	1.45	1	5
3	C	306	PX4	O7-C7	3.97	1.37	1.46	7	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	C	309	PX4	C8-C7	3.97	1.63	1.50	2	8
3	B	311	PX4	C8-C7	3.97	1.63	1.50	14	10
3	C	364	PX4	O7-C7	3.96	1.37	1.46	13	3
3	A	637	PX4	O7-C7	3.96	1.37	1.46	10	3
3	A	606	PX4	O7-C23	3.96	1.23	1.34	8	5
3	A	640	PX4	C10-C9	3.96	1.62	1.50	3	3
3	C	359	PX4	C2-C1	3.96	1.63	1.51	6	4
3	C	328	PX4	C2-C1	3.95	1.63	1.51	4	4
3	C	346	PX4	C6-C7	3.95	1.63	1.50	11	5
3	C	332	PX4	C24-C23	3.95	1.62	1.50	8	5
3	C	305	PX4	C6-C7	3.95	1.63	1.50	3	7
3	C	335	PX4	C6-C7	3.95	1.63	1.50	14	6
3	A	606	PX4	C8-C7	3.94	1.63	1.50	8	6
3	B	310	PX4	C6-C7	3.94	1.63	1.50	6	6
3	B	362	PX4	C8-C7	3.94	1.63	1.50	1	5
3	A	639	PX4	O7-C7	3.93	1.37	1.46	7	6
3	B	323	PX4	C8-C7	3.93	1.63	1.50	13	7
3	C	303	PX4	C6-C7	3.93	1.63	1.50	11	8
3	C	323	PX4	C6-C7	3.93	1.63	1.50	6	6
3	C	328	PX4	C8-C7	3.93	1.63	1.50	4	7
3	B	345	PX4	C11-C10	3.93	1.66	1.52	9	3
3	B	337	PX4	O5-C8	3.92	1.36	1.45	9	5
3	A	632	PX4	C8-C7	3.92	1.63	1.50	6	11
3	B	360	PX4	C6-C7	3.92	1.63	1.50	14	6
3	A	620	PX4	C2-C1	3.92	1.63	1.51	9	5
3	B	327	PX4	C2-C1	3.92	1.63	1.51	3	4
3	B	367	PX4	O7-C23	3.92	1.23	1.34	6	2
3	C	304	PX4	C11-C10	3.91	1.66	1.52	6	2
3	B	326	PX4	O7-C23	3.91	1.23	1.34	3	2
3	A	648	PX4	C2-C1	3.91	1.63	1.51	5	6
3	B	378	PX4	C6-C7	3.91	1.63	1.50	14	6
3	A	636	PX4	C8-C7	3.91	1.63	1.50	12	3
3	B	356	PX4	C6-C7	3.91	1.63	1.50	12	7
3	B	305	PX4	O5-C8	3.91	1.36	1.45	13	2
3	B	374	PX4	C8-C7	3.90	1.63	1.50	2	6
3	B	337	PX4	C2-C1	3.90	1.63	1.51	14	4
3	A	637	PX4	C8-C7	3.90	1.63	1.50	1	3
3	B	376	PX4	O7-C7	3.90	1.37	1.46	2	5
3	C	322	PX4	C6-C7	3.90	1.63	1.50	5	7
3	C	363	PX4	O5-C8	3.90	1.36	1.45	4	2
3	B	386	PX4	C2-C1	3.89	1.63	1.51	8	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	383	PX4	C8-C7	3.89	1.63	1.50	9	9
3	A	605	PX4	C6-C7	3.89	1.63	1.50	6	6
3	B	310	PX4	C8-C7	3.88	1.62	1.50	5	8
3	B	384	PX4	C6-C7	3.88	1.62	1.50	8	8
3	B	375	PX4	C24-C23	3.88	1.62	1.50	7	2
3	C	359	PX4	C8-C7	3.88	1.62	1.50	5	5
3	A	637	PX4	O7-C23	3.87	1.23	1.34	3	1
3	C	307	PX4	C24-C23	3.87	1.61	1.50	2	5
3	B	377	PX4	C8-C7	3.87	1.62	1.50	8	8
3	A	633	PX4	C6-C7	3.87	1.62	1.50	7	4
3	C	327	PX4	C2-C1	3.87	1.63	1.51	4	6
3	A	651	PX4	C8-C7	3.86	1.62	1.50	14	9
3	B	374	PX4	C4-N1	3.86	1.38	1.50	5	1
3	B	364	PX4	C2-C1	3.86	1.63	1.51	11	7
3	B	367	PX4	C24-C23	3.86	1.61	1.50	5	3
3	A	649	PX4	O5-C8	3.85	1.53	1.45	10	2
3	B	323	PX4	C2-C1	3.85	1.63	1.51	10	3
3	B	390	PX4	C10-C9	3.85	1.61	1.50	11	2
3	C	329	PX4	C2-C1	3.85	1.63	1.51	3	6
3	B	332	PX4	C10-C9	3.85	1.61	1.50	15	3
3	C	361	PX4	C6-C7	3.85	1.62	1.50	3	4
3	A	622	PX4	O7-C7	3.85	1.37	1.46	7	4
3	C	310	PX4	C10-C9	3.85	1.61	1.50	10	2
3	B	302	PX4	C3-N1	3.84	1.61	1.50	2	3
3	C	311	PX4	O7-C7	3.84	1.37	1.46	4	3
3	B	323	PX4	C24-C23	3.84	1.61	1.50	10	5
3	C	306	PX4	C6-C7	3.84	1.62	1.50	14	8
3	A	604	PX4	C2-C1	3.84	1.62	1.51	11	3
3	C	357	PX4	C8-C7	3.83	1.62	1.50	5	7
3	B	350	PX4	O7-C7	3.83	1.37	1.46	14	5
3	C	310	PX4	C2-C1	3.83	1.62	1.51	1	8
3	A	611	PX4	O7-C7	3.82	1.37	1.46	7	3
3	A	639	PX4	C5-N1	3.82	1.61	1.50	5	5
3	B	347	PX4	C2-C1	3.82	1.62	1.51	9	6
3	B	359	PX4	C11-C10	3.82	1.66	1.52	14	1
3	B	320	PX4	C2-N1	3.82	1.63	1.51	14	2
3	B	392	PX4	O7-C7	3.82	1.37	1.46	5	4
3	B	393	PX4	C24-C23	3.81	1.61	1.50	10	5
3	B	398	PX4	C2-C1	3.81	1.62	1.51	5	5
3	B	338	PX4	C24-C23	3.81	1.61	1.50	2	3
3	B	311	PX4	C10-C9	3.81	1.61	1.50	3	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	312	PX4	C25-C24	3.81	1.66	1.52	15	2
3	B	371	PX4	C6-C7	3.81	1.62	1.50	14	7
3	B	399	PX4	C2-N1	3.81	1.63	1.51	2	1
3	C	307	PX4	O7-C7	3.81	1.37	1.46	6	2
3	A	631	PX4	C8-C7	3.80	1.62	1.50	10	10
3	C	308	PX4	C3-N1	3.80	1.61	1.50	13	4
3	A	618	PX4	C8-C7	3.80	1.62	1.50	5	7
3	A	631	PX4	C10-C9	3.80	1.61	1.50	10	1
3	A	635	PX4	C6-C7	3.80	1.62	1.50	15	5
3	B	385	PX4	C6-C7	3.80	1.62	1.50	7	6
3	B	392	PX4	C10-C9	3.80	1.61	1.50	7	6
3	A	653	PX4	C6-C7	3.79	1.62	1.50	7	8
3	A	612	PX4	O7-C23	3.79	1.23	1.34	4	2
3	C	308	PX4	C24-C23	3.79	1.39	1.50	4	5
3	B	348	PX4	O7-C7	3.79	1.37	1.46	11	4
3	A	610	PX4	C6-C7	3.79	1.62	1.50	9	7
3	B	321	PX4	C8-C7	3.79	1.62	1.50	15	9
3	B	346	PX4	C10-C9	3.79	1.61	1.50	10	5
3	C	354	PX4	C6-C7	3.79	1.62	1.50	3	8
3	B	317	PX4	C2-C1	3.79	1.62	1.51	6	6
3	B	371	PX4	O7-C7	3.78	1.37	1.46	15	4
3	C	330	PX4	C6-C7	3.78	1.62	1.50	3	9
3	C	310	PX4	C8-C7	3.78	1.62	1.50	12	4
3	A	633	PX4	C24-C23	3.77	1.61	1.50	6	5
3	B	399	PX4	C6-C7	3.77	1.62	1.50	12	5
3	C	302	PX4	C6-C7	3.77	1.62	1.50	3	4
3	C	307	PX4	C8-C7	3.76	1.62	1.50	8	7
3	C	311	PX4	C2-N1	3.77	1.62	1.51	3	3
3	C	335	PX4	O5-C8	3.77	1.53	1.45	9	2
3	B	312	PX4	C8-C7	3.76	1.62	1.50	6	7
3	C	326	PX4	C6-C7	3.76	1.62	1.50	6	3
3	B	369	PX4	C8-C7	3.75	1.62	1.50	10	4
3	A	650	PX4	C6-C7	3.75	1.62	1.50	8	5
3	B	309	PX4	O7-C7	3.75	1.37	1.46	3	4
3	B	331	PX4	C6-C7	3.75	1.62	1.50	7	4
3	C	337	PX4	C10-C9	3.75	1.61	1.50	1	4
3	B	348	PX4	C2-C1	3.75	1.62	1.51	7	6
3	C	362	PX4	C8-C7	3.75	1.62	1.50	14	6
3	B	380	PX4	C24-C23	3.74	1.61	1.50	12	3
3	B	393	PX4	C2-C1	3.74	1.62	1.51	13	6
3	A	615	PX4	C8-C7	3.74	1.62	1.50	7	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	351	PX4	O7-C7	3.74	1.37	1.46	13	4
3	B	334	PX4	O5-C8	3.73	1.36	1.45	1	5
3	B	305	PX4	O5-C9	3.73	1.22	1.33	10	4
3	B	392	PX4	O7-C23	3.73	1.23	1.34	7	4
3	C	358	PX4	O7-C23	3.73	1.23	1.34	2	2
3	A	608	PX4	C6-C7	3.73	1.62	1.50	15	8
3	B	345	PX4	C2-C1	3.72	1.62	1.51	2	4
3	C	333	PX4	C24-C23	3.72	1.61	1.50	1	5
3	A	602	PX4	O7-C7	3.72	1.37	1.46	2	4
3	A	616	PX4	C24-C23	3.72	1.61	1.50	5	2
3	A	623	PX4	C2-C1	3.72	1.62	1.51	4	3
3	B	312	PX4	C2-C1	3.72	1.62	1.51	9	5
3	C	312	PX4	C6-C7	3.72	1.62	1.50	1	6
3	C	326	PX4	C24-C23	3.72	1.61	1.50	15	4
3	B	387	PX4	C2-C1	3.72	1.62	1.51	15	4
3	B	351	PX4	C10-C9	3.71	1.61	1.50	7	2
3	B	356	PX4	O7-C23	3.71	1.23	1.34	5	2
3	C	356	PX4	C6-C7	3.72	1.62	1.50	8	5
3	B	377	PX4	C6-C7	3.71	1.62	1.50	5	8
3	B	328	PX4	C24-C23	3.71	1.61	1.50	10	3
3	C	333	PX4	C10-C9	3.71	1.61	1.50	11	3
3	A	607	PX4	C8-C7	3.71	1.62	1.50	3	9
3	B	315	PX4	C6-C7	3.71	1.62	1.50	13	6
3	C	349	PX4	O7-C23	3.71	1.23	1.34	2	5
3	A	625	PX4	C8-C7	3.71	1.62	1.50	8	6
3	B	319	PX4	C11-C10	3.71	1.65	1.52	2	2
3	C	361	PX4	O5-C9	3.71	1.44	1.33	1	2
3	C	363	PX4	C2-C1	3.71	1.62	1.51	7	6
3	B	369	PX4	C11-C10	3.70	1.65	1.52	13	2
3	B	317	PX4	C6-C7	3.70	1.62	1.50	4	6
3	A	607	PX4	C5-N1	3.70	1.60	1.50	11	2
3	A	626	PX4	C2-C1	3.69	1.62	1.51	12	8
3	A	649	PX4	O7-C7	3.69	1.37	1.46	12	4
3	B	346	PX4	C6-C7	3.69	1.62	1.50	6	8
3	A	620	PX4	O5-C8	3.69	1.36	1.45	6	2
3	B	345	PX4	O5-C8	3.68	1.53	1.45	13	2
3	B	368	PX4	O7-C7	3.68	1.37	1.46	12	3
3	C	303	PX4	C2-C1	3.68	1.62	1.51	1	2
3	A	652	PX4	C10-C9	3.68	1.61	1.50	13	5
3	B	308	PX4	C6-C7	3.68	1.62	1.50	2	5
3	A	625	PX4	C2-C1	3.68	1.62	1.51	7	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	C	328	PX4	C6-C7	3.68	1.62	1.50	9	5
3	B	367	PX4	C6-C7	3.68	1.62	1.50	14	3
3	B	322	PX4	C8-C7	3.67	1.62	1.50	6	5
3	B	347	PX4	C10-C9	3.67	1.61	1.50	7	4
3	C	348	PX4	C8-C7	3.68	1.62	1.50	12	7
3	B	329	PX4	C6-C7	3.67	1.62	1.50	5	6
3	A	627	PX4	C6-C7	3.67	1.62	1.50	4	8
3	A	640	PX4	C8-C7	3.67	1.62	1.50	6	8
3	B	359	PX4	C10-C9	3.67	1.61	1.50	4	4
3	A	638	PX4	O5-C8	3.67	1.37	1.45	15	3
3	B	326	PX4	C8-C7	3.67	1.62	1.50	3	7
3	B	359	PX4	C6-C7	3.67	1.62	1.50	9	6
3	B	343	PX4	C2-C1	3.67	1.62	1.51	13	4
3	C	317	PX4	C8-C7	3.67	1.62	1.50	6	9
3	B	306	PX4	C24-C23	3.66	1.61	1.50	1	3
3	A	617	PX4	C8-C7	3.66	1.62	1.50	11	10
3	C	325	PX4	O7-C23	3.66	1.23	1.34	3	5
3	C	355	PX4	C10-C9	3.66	1.61	1.50	9	4
3	B	302	PX4	C2-C1	3.66	1.62	1.51	8	6
3	A	610	PX4	C2-C1	3.65	1.62	1.51	1	2
3	A	649	PX4	C2-C1	3.65	1.62	1.51	11	5
3	A	654	PX4	C24-C23	3.65	1.61	1.50	14	3
3	A	613	PX4	O5-C8	3.65	1.53	1.45	12	5
3	A	654	PX4	C10-C9	3.65	1.61	1.50	6	4
3	B	313	PX4	C8-C7	3.65	1.62	1.50	13	6
3	B	368	PX4	C2-C1	3.65	1.62	1.51	3	6
3	C	352	PX4	C24-C23	3.65	1.40	1.50	3	3
3	A	646	PX4	C24-C23	3.65	1.61	1.50	9	2
3	B	372	PX4	C24-C23	3.65	1.61	1.50	10	3
3	A	648	PX4	C6-C7	3.64	1.62	1.50	11	7
3	C	305	PX4	C25-C24	3.64	1.65	1.52	7	1
3	C	314	PX4	C3-N1	3.64	1.39	1.50	3	2
3	C	329	PX4	C8-C7	3.64	1.62	1.50	15	7
3	A	606	PX4	C6-C7	3.64	1.62	1.50	3	6
3	A	609	PX4	C8-C7	3.64	1.62	1.50	4	8
3	A	630	PX4	C2-C1	3.64	1.62	1.51	9	3
3	C	343	PX4	C2-C1	3.64	1.62	1.51	3	3
3	A	621	PX4	C2-C1	3.63	1.62	1.51	1	3
3	B	343	PX4	O7-C23	3.63	1.24	1.34	12	3
3	B	301	PX4	O7-C7	3.63	1.38	1.46	9	5
3	B	329	PX4	O7-C7	3.63	1.38	1.46	3	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	C	310	PX4	C6-C7	3.63	1.62	1.50	1	5
3	C	339	PX4	C8-C7	3.63	1.62	1.50	1	4
3	A	646	PX4	C8-C7	3.62	1.62	1.50	9	6
3	B	379	PX4	C8-C7	3.62	1.62	1.50	13	10
3	C	314	PX4	O5-C8	3.62	1.53	1.45	13	2
3	C	315	PX4	C8-C7	3.62	1.62	1.50	2	5
3	B	384	PX4	C10-C9	3.62	1.61	1.50	5	4
3	B	321	PX4	C2-C1	3.62	1.62	1.51	10	3
3	B	325	PX4	C2-C1	3.62	1.62	1.51	15	7
3	B	348	PX4	C8-C7	3.62	1.62	1.50	13	7
3	B	364	PX4	O5-C8	3.62	1.37	1.45	8	5
3	A	622	PX4	C6-C7	3.61	1.62	1.50	6	6
3	A	603	PX4	C8-C7	3.61	1.62	1.50	14	6
3	B	328	PX4	C2-C1	3.61	1.62	1.51	7	4
3	B	335	PX4	C2-C1	3.61	1.62	1.51	3	5
3	C	352	PX4	C6-C7	3.60	1.62	1.50	1	10
3	B	376	PX4	C8-C7	3.60	1.62	1.50	6	7
3	C	318	PX4	C24-C23	3.60	1.61	1.50	8	1
3	C	347	PX4	C2-N1	3.60	1.62	1.51	5	1
3	C	319	PX4	C8-C7	3.60	1.62	1.50	7	10
3	C	344	PX4	O7-C7	3.60	1.38	1.46	13	5
3	C	353	PX4	C2-C1	3.60	1.62	1.51	15	10
3	A	614	PX4	C6-C7	3.60	1.62	1.50	2	6
3	B	399	PX4	O7-C7	3.59	1.38	1.46	11	3
3	C	362	PX4	O7-C7	3.59	1.38	1.46	1	2
3	B	329	PX4	C10-C9	3.59	1.61	1.50	14	4
3	B	359	PX4	C2-C1	3.59	1.62	1.51	13	4
3	C	302	PX4	C2-C1	3.59	1.62	1.51	4	6
3	C	364	PX4	C8-C7	3.59	1.62	1.50	12	7
3	C	326	PX4	C2-C1	3.59	1.62	1.51	2	3
3	C	347	PX4	C2-C1	3.59	1.62	1.51	15	2
3	C	340	PX4	O5-C8	3.58	1.53	1.45	2	3
3	C	359	PX4	C10-C9	3.58	1.61	1.50	4	5
3	A	624	PX4	C2-C1	3.58	1.62	1.51	3	5
3	C	355	PX4	O5-C9	3.58	1.22	1.33	2	2
3	C	317	PX4	C24-C23	3.58	1.61	1.50	13	5
3	B	389	PX4	C8-C7	3.58	1.62	1.50	2	6
3	A	621	PX4	C24-C23	3.57	1.61	1.50	13	2
3	C	317	PX4	C2-C1	3.58	1.62	1.51	5	5
3	C	320	PX4	C24-C23	3.57	1.61	1.50	7	4
3	A	618	PX4	C6-C7	3.57	1.62	1.50	13	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	C	316	PX4	O7-C7	3.57	1.38	1.46	10	2
3	A	619	PX4	O7-C7	3.57	1.38	1.46	1	3
3	B	340	PX4	C2-C1	3.57	1.62	1.51	3	4
3	B	307	PX4	O7-C7	3.57	1.38	1.46	15	1
3	C	318	PX4	C6-C7	3.57	1.62	1.50	14	7
3	C	341	PX4	C8-C7	3.57	1.62	1.50	2	8
3	A	616	PX4	O5-C9	3.57	1.23	1.33	14	1
3	B	361	PX4	C6-C7	3.57	1.62	1.50	8	10
3	B	360	PX4	O7-C7	3.56	1.38	1.46	7	4
3	C	358	PX4	C24-C23	3.56	1.61	1.50	9	6
3	A	610	PX4	C8-C7	3.56	1.61	1.50	13	5
3	A	626	PX4	C2-N1	3.56	1.62	1.51	14	2
3	B	307	PX4	C2-C1	3.56	1.62	1.51	4	5
3	C	360	PX4	C25-C24	3.56	1.65	1.52	12	2
3	A	615	PX4	C6-C7	3.55	1.61	1.50	6	4
3	C	321	PX4	O7-C7	3.55	1.38	1.46	2	3
3	A	602	PX4	C2-C1	3.55	1.62	1.51	1	8
3	B	342	PX4	C24-C23	3.55	1.61	1.50	10	3
3	C	363	PX4	C6-C7	3.55	1.61	1.50	14	3
3	C	320	PX4	C8-C7	3.55	1.61	1.50	4	8
3	A	640	PX4	C6-C7	3.54	1.61	1.50	4	5
3	B	318	PX4	C2-N1	3.54	1.62	1.51	15	1
3	B	365	PX4	C8-C7	3.54	1.61	1.50	4	5
3	B	377	PX4	C25-C24	3.54	1.65	1.52	5	2
3	C	328	PX4	C2-N1	3.54	1.62	1.51	3	2
3	A	620	PX4	C8-C7	3.54	1.61	1.50	4	5
3	C	312	PX4	O7-C7	3.54	1.38	1.46	12	2
3	B	328	PX4	C3-N1	3.54	1.60	1.50	1	3
3	B	355	PX4	C2-C1	3.54	1.62	1.51	10	5
3	C	308	PX4	C2-C1	3.54	1.62	1.51	13	6
3	C	334	PX4	C24-C23	3.53	1.61	1.50	2	4
3	A	601	PX4	C10-C9	3.53	1.60	1.50	5	5
3	A	625	PX4	C10-C9	3.53	1.61	1.50	1	6
3	B	396	PX4	C6-C7	3.53	1.61	1.50	7	7
3	C	311	PX4	C24-C23	3.53	1.61	1.50	1	3
3	B	361	PX4	C8-C7	3.53	1.61	1.50	10	5
3	C	354	PX4	C2-C1	3.53	1.62	1.51	4	7
3	A	612	PX4	C6-C7	3.52	1.61	1.50	1	5
3	A	628	PX4	C8-C7	3.52	1.61	1.50	5	5
3	B	400	PX4	C2-N1	3.52	1.62	1.51	7	4
3	B	307	PX4	C25-C24	3.52	1.65	1.52	11	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	333	PX4	O5-C8	3.52	1.37	1.45	10	4
3	C	361	PX4	C8-C7	3.52	1.61	1.50	3	5
3	C	355	PX4	C4-N1	3.52	1.39	1.50	14	1
3	B	306	PX4	C2-C1	3.52	1.62	1.51	12	4
3	C	327	PX4	C6-C7	3.52	1.61	1.50	6	7
3	C	352	PX4	C2-C1	3.52	1.62	1.51	9	5
3	B	302	PX4	C6-C7	3.51	1.61	1.50	11	5
3	B	374	PX4	C24-C23	3.51	1.60	1.50	14	4
3	C	337	PX4	C8-C7	3.51	1.61	1.50	2	5
3	B	335	PX4	C6-C7	3.51	1.61	1.50	3	7
3	A	637	PX4	C6-C7	3.51	1.61	1.50	11	5
3	C	335	PX4	O7-C7	3.51	1.38	1.46	14	2
3	A	642	PX4	C24-C23	3.51	1.60	1.50	14	3
3	C	328	PX4	C24-C23	3.51	1.60	1.50	12	2
3	C	351	PX4	C24-C23	3.51	1.60	1.50	9	5
3	A	653	PX4	C10-C9	3.51	1.60	1.50	7	1
3	B	378	PX4	O5-C9	3.50	1.23	1.33	1	2
3	B	336	PX4	C2-C1	3.50	1.61	1.51	2	3
3	B	341	PX4	C2-C1	3.50	1.61	1.51	10	4
3	C	302	PX4	O7-C7	3.50	1.38	1.46	7	3
3	C	323	PX4	O5-C9	3.50	1.43	1.33	3	2
3	B	340	PX4	C4-N1	3.50	1.39	1.50	11	1
3	B	394	PX4	O7-C23	3.49	1.24	1.34	13	3
3	B	366	PX4	C2-N1	3.49	1.62	1.51	7	2
3	B	382	PX4	C4-N1	3.49	1.39	1.50	10	3
3	C	326	PX4	O7-C7	3.49	1.38	1.46	6	4
3	B	334	PX4	C2-C1	3.49	1.61	1.51	7	6
3	B	341	PX4	C6-C7	3.49	1.61	1.50	12	8
3	B	397	PX4	C10-C9	3.49	1.60	1.50	8	5
3	A	605	PX4	C24-C23	3.48	1.60	1.50	11	4
3	A	636	PX4	C6-C7	3.48	1.61	1.50	7	7
3	C	334	PX4	C10-C9	3.48	1.60	1.50	2	6
3	A	650	PX4	C2-N1	3.48	1.62	1.51	6	3
3	B	363	PX4	C2-C1	3.48	1.61	1.51	1	5
3	B	352	PX4	O7-C23	3.48	1.44	1.34	4	3
3	B	396	PX4	C2-C1	3.48	1.61	1.51	2	7
3	C	354	PX4	C8-C7	3.48	1.61	1.50	10	10
3	A	653	PX4	O7-C7	3.48	1.38	1.46	6	6
3	A	635	PX4	C2-N1	3.47	1.62	1.51	3	1
3	C	356	PX4	C2-C1	3.48	1.61	1.51	9	4
3	B	332	PX4	C6-C7	3.47	1.61	1.50	4	7

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	C	331	PX4	C8-C7	3.47	1.61	1.50	13	6
3	C	336	PX4	C10-C9	3.47	1.60	1.50	8	6
3	B	334	PX4	C8-C7	3.47	1.61	1.50	8	8
3	C	321	PX4	O5-C9	3.47	1.43	1.33	12	3
3	B	309	PX4	C24-C23	3.47	1.60	1.50	10	4
3	A	619	PX4	C10-C9	3.47	1.60	1.50	1	5
3	B	311	PX4	C2-C1	3.47	1.61	1.51	3	6
3	B	316	PX4	O7-C7	3.47	1.38	1.46	9	4
3	A	610	PX4	C24-C23	3.46	1.60	1.50	4	4
3	A	630	PX4	O5-C8	3.46	1.52	1.45	14	3
3	C	315	PX4	O3-C1	3.46	1.30	1.44	1	1
3	C	345	PX4	C6-C7	3.46	1.61	1.50	14	7
3	A	623	PX4	C6-C7	3.46	1.61	1.50	4	4
3	C	338	PX4	C6-C7	3.46	1.61	1.50	5	3
3	A	616	PX4	C2-C1	3.46	1.61	1.51	13	5
3	B	363	PX4	C8-C7	3.46	1.61	1.50	15	8
3	C	343	PX4	C10-C9	3.46	1.60	1.50	14	2
3	B	352	PX4	O7-C7	3.46	1.38	1.46	2	4
3	C	363	PX4	C4-N1	3.46	1.40	1.50	12	1
3	A	636	PX4	C24-C23	3.45	1.60	1.50	5	6
3	C	308	PX4	C6-C7	3.45	1.61	1.50	5	5
3	C	350	PX4	O7-C23	3.45	1.24	1.34	15	4
3	B	340	PX4	O5-C9	3.45	1.23	1.33	6	2
3	A	643	PX4	O5-C9	3.45	1.23	1.33	3	2
3	B	322	PX4	C24-C23	3.45	1.60	1.50	5	3
3	A	629	PX4	C8-C7	3.45	1.61	1.50	13	6
3	B	314	PX4	C24-C23	3.45	1.60	1.50	14	1
3	B	366	PX4	C6-C7	3.45	1.61	1.50	15	3
3	B	400	PX4	C8-C7	3.45	1.61	1.50	5	9
3	C	355	PX4	C6-C7	3.45	1.61	1.50	1	9
3	A	631	PX4	C2-C1	3.44	1.61	1.51	11	6
3	C	329	PX4	C3-N1	3.44	1.60	1.50	9	2
3	B	336	PX4	C6-C7	3.44	1.61	1.50	5	8
3	B	328	PX4	O7-C7	3.44	1.38	1.46	12	4
3	B	378	PX4	C8-C7	3.44	1.61	1.50	1	9
3	A	650	PX4	C25-C24	3.44	1.64	1.52	12	1
3	C	316	PX4	C24-C23	3.44	1.60	1.50	7	5
3	A	633	PX4	O7-C23	3.43	1.24	1.34	2	2
3	A	630	PX4	C8-C7	3.43	1.61	1.50	5	5
3	A	643	PX4	C8-C7	3.43	1.61	1.50	1	6
3	B	344	PX4	C24-C23	3.43	1.60	1.50	1	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	360	PX4	C8-C7	3.43	1.61	1.50	14	6
3	B	386	PX4	C8-C7	3.43	1.61	1.50	5	7
3	B	310	PX4	C2-C1	3.43	1.61	1.51	15	7
3	B	388	PX4	C8-C7	3.43	1.61	1.50	6	6
3	B	389	PX4	C10-C9	3.43	1.60	1.50	5	4
3	A	646	PX4	O7-C23	3.42	1.24	1.34	8	2
3	B	305	PX4	C8-C7	3.42	1.61	1.50	8	8
3	B	357	PX4	C6-C7	3.42	1.61	1.50	3	4
3	B	354	PX4	O5-C9	3.42	1.43	1.33	10	1
3	B	327	PX4	C10-C9	3.42	1.60	1.50	14	3
3	B	359	PX4	C24-C23	3.42	1.60	1.50	6	4
3	B	373	PX4	C2-C1	3.42	1.61	1.51	6	6
3	A	632	PX4	O7-C23	3.42	1.24	1.34	11	4
3	B	331	PX4	C2-C1	3.42	1.61	1.51	12	4
3	C	331	PX4	C10-C9	3.42	1.60	1.50	6	5
3	C	316	PX4	C8-C7	3.42	1.61	1.50	7	8
3	B	400	PX4	C2-C1	3.41	1.61	1.51	2	4
3	B	382	PX4	C6-C7	3.41	1.61	1.50	5	9
3	B	397	PX4	O5-C8	3.41	1.52	1.45	5	2
3	A	635	PX4	C24-C23	3.41	1.60	1.50	1	4
3	A	621	PX4	C6-C7	3.41	1.61	1.50	14	7
3	B	344	PX4	C2-C1	3.41	1.61	1.51	2	9
3	B	394	PX4	O7-C7	3.41	1.38	1.46	1	3
3	C	305	PX4	C2-C1	3.41	1.61	1.51	5	2
3	B	338	PX4	C10-C9	3.40	1.60	1.50	10	2
3	B	387	PX4	C8-C7	3.40	1.61	1.50	13	7
3	C	350	PX4	O7-C7	3.40	1.38	1.46	8	3
3	C	353	PX4	C24-C23	3.40	1.60	1.50	13	3
3	A	629	PX4	C11-C10	3.40	1.64	1.52	1	2
3	A	636	PX4	C2-C1	3.40	1.61	1.51	14	5
3	B	379	PX4	C2-C1	3.40	1.61	1.51	12	4
3	C	321	PX4	C10-C9	3.40	1.60	1.50	3	4
3	C	342	PX4	C6-C7	3.40	1.61	1.50	15	6
3	C	302	PX4	C8-C7	3.40	1.61	1.50	1	7
3	B	347	PX4	C6-C7	3.40	1.61	1.50	13	6
3	C	336	PX4	C8-C7	3.40	1.61	1.50	10	7
3	A	640	PX4	O7-C23	3.39	1.43	1.34	11	1
3	B	396	PX4	C10-C9	3.39	1.60	1.50	10	5
3	A	636	PX4	O7-C7	3.39	1.38	1.46	8	4
3	B	335	PX4	C8-C7	3.39	1.61	1.50	4	5
3	C	335	PX4	C4-N1	3.39	1.59	1.50	9	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	C	359	PX4	O7-C7	3.39	1.38	1.46	4	3
3	C	303	PX4	O7-C7	3.39	1.38	1.46	5	3
3	B	340	PX4	C6-C7	3.39	1.61	1.50	11	4
3	B	328	PX4	C6-C7	3.39	1.61	1.50	12	8
3	B	381	PX4	C8-C7	3.39	1.61	1.50	11	7
3	A	601	PX4	O5-C8	3.38	1.37	1.45	14	1
3	C	318	PX4	C2-C1	3.39	1.61	1.51	10	3
3	A	635	PX4	C8-C7	3.38	1.61	1.50	11	7
3	C	307	PX4	C6-C7	3.38	1.61	1.50	1	5
3	C	316	PX4	O7-C23	3.38	1.24	1.34	1	3
3	B	326	PX4	C2-C1	3.38	1.61	1.51	6	3
3	B	358	PX4	C5-N1	3.38	1.59	1.50	6	1
3	B	355	PX4	C24-C23	3.38	1.60	1.50	4	5
3	C	325	PX4	C8-C7	3.38	1.61	1.50	7	4
3	B	397	PX4	C5-N1	3.38	1.59	1.50	10	1
3	A	609	PX4	C6-C7	3.37	1.61	1.50	4	9
3	B	339	PX4	C2-C1	3.37	1.61	1.51	1	5
3	B	355	PX4	C6-C7	3.37	1.61	1.50	1	7
3	C	302	PX4	C25-C24	3.37	1.64	1.52	9	3
3	C	304	PX4	C6-C7	3.37	1.61	1.50	13	7
3	C	314	PX4	C8-C7	3.37	1.61	1.50	8	9
3	C	341	PX4	O7-C7	3.37	1.38	1.46	4	5
3	A	601	PX4	C6-C7	3.36	1.61	1.50	6	9
3	B	353	PX4	C6-C7	3.37	1.61	1.50	11	8
3	B	388	PX4	C2-C1	3.37	1.61	1.51	2	7
3	C	326	PX4	P1-O1	3.37	1.39	1.55	1	4
3	C	308	PX4	C10-C9	3.36	1.60	1.50	14	4
3	B	342	PX4	C19-C18	3.36	1.68	1.51	9	1
3	C	331	PX4	C6-C7	3.36	1.61	1.50	4	6
3	C	332	PX4	C2-C1	3.36	1.61	1.51	6	4
3	C	354	PX4	C10-C9	3.36	1.60	1.50	3	3
3	B	319	PX4	C24-C23	3.36	1.60	1.50	6	3
3	C	349	PX4	C10-C9	3.36	1.60	1.50	10	3
3	A	635	PX4	C2-C1	3.36	1.61	1.51	10	6
3	B	303	PX4	C2-C1	3.36	1.61	1.51	5	7
3	A	607	PX4	O5-C9	3.36	1.43	1.33	11	4
3	A	627	PX4	C2-C1	3.36	1.61	1.51	8	4
3	B	370	PX4	C10-C9	3.36	1.60	1.50	14	3
3	C	301	PX4	C6-C7	3.35	1.61	1.50	13	5
3	C	306	PX4	C5-N1	3.36	1.59	1.50	9	2
3	B	356	PX4	C24-C23	3.35	1.60	1.50	5	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	369	PX4	O7-C23	3.35	1.24	1.34	8	2
3	A	616	PX4	O7-C23	3.35	1.24	1.34	10	3
3	B	320	PX4	O7-C7	3.35	1.38	1.46	1	3
3	C	347	PX4	O5-C8	3.35	1.37	1.45	10	1
3	A	651	PX4	C10-C9	3.35	1.60	1.50	8	4
3	B	327	PX4	O5-C8	3.35	1.52	1.45	11	1
3	A	601	PX4	C2-N1	3.35	1.61	1.51	10	2
3	C	335	PX4	O7-C23	3.35	1.24	1.34	8	1
3	A	652	PX4	C8-C7	3.34	1.61	1.50	13	10
3	A	608	PX4	C8-C7	3.34	1.61	1.50	3	8
3	C	354	PX4	C24-C23	3.34	1.60	1.50	1	4
3	C	310	PX4	O7-C23	3.34	1.43	1.34	15	1
3	A	628	PX4	C2-N1	3.34	1.61	1.51	14	2
3	A	639	PX4	O7-C23	3.34	1.43	1.34	11	3
3	C	331	PX4	O7-C7	3.34	1.38	1.46	5	4
3	C	312	PX4	C8-C7	3.34	1.61	1.50	14	7
3	C	333	PX4	O7-C7	3.34	1.38	1.46	8	3
3	A	633	PX4	C2-N1	3.33	1.61	1.51	12	3
3	A	653	PX4	C8-C7	3.33	1.61	1.50	7	7
3	A	616	PX4	C8-C7	3.33	1.61	1.50	14	10
3	C	334	PX4	C8-C7	3.33	1.61	1.50	5	6
3	A	634	PX4	C8-C7	3.33	1.61	1.50	9	10
3	B	314	PX4	C3-N1	3.33	1.59	1.50	7	2
3	B	376	PX4	C24-C23	3.33	1.60	1.50	5	4
3	B	328	PX4	C2-N1	3.33	1.61	1.51	8	2
3	C	360	PX4	C8-C7	3.33	1.61	1.50	5	9
3	C	353	PX4	O5-C8	3.32	1.37	1.45	8	4
3	A	601	PX4	C8-C7	3.32	1.61	1.50	14	6
3	A	638	PX4	C4-N1	3.32	1.59	1.50	13	2
3	B	372	PX4	O7-C23	3.32	1.24	1.34	10	2
3	C	346	PX4	C10-C9	3.32	1.60	1.50	7	3
3	C	363	PX4	C8-C7	3.32	1.61	1.50	11	8
3	B	358	PX4	C2-C1	3.32	1.61	1.51	9	7
3	B	364	PX4	C8-C7	3.32	1.61	1.50	10	5
3	A	609	PX4	O7-C23	3.32	1.24	1.34	4	2
3	B	319	PX4	C6-C7	3.32	1.61	1.50	10	4
3	B	331	PX4	O7-C7	3.32	1.38	1.46	12	3
3	B	389	PX4	O7-C7	3.32	1.38	1.46	5	2
3	A	647	PX4	C8-C7	3.31	1.61	1.50	15	8
3	B	307	PX4	C24-C23	3.31	1.60	1.50	15	5
3	B	360	PX4	C2-C1	3.31	1.61	1.51	11	7

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	A	602	PX4	C25-C24	3.31	1.64	1.52	12	2
3	C	321	PX4	C5-N1	3.31	1.59	1.50	3	3
3	C	333	PX4	O5-C8	3.31	1.52	1.45	1	3
3	C	345	PX4	C8-C7	3.31	1.61	1.50	6	7
3	B	304	PX4	O5-C9	3.31	1.43	1.33	10	2
3	B	325	PX4	C10-C9	3.31	1.60	1.50	2	3
3	B	371	PX4	C2-C1	3.31	1.61	1.51	15	2
3	C	338	PX4	C8-C7	3.31	1.61	1.50	8	6
3	A	645	PX4	C5-N1	3.31	1.59	1.50	7	3
3	B	333	PX4	C24-C23	3.31	1.60	1.50	12	5
3	B	380	PX4	O5-C9	3.31	1.43	1.33	1	5
3	A	627	PX4	C11-C10	3.31	1.64	1.52	13	2
3	A	653	PX4	C24-C23	3.31	1.60	1.50	12	2
3	C	333	PX4	C6-C7	3.31	1.61	1.50	6	6
3	C	335	PX4	C8-C7	3.31	1.61	1.50	1	7
3	B	301	PX4	O5-C8	3.30	1.52	1.45	6	2
3	B	351	PX4	C8-C7	3.30	1.61	1.50	4	2
3	B	358	PX4	C10-C9	3.30	1.60	1.50	14	2
3	B	389	PX4	O7-C23	3.30	1.24	1.34	12	1
3	A	642	PX4	C8-C7	3.30	1.61	1.50	15	6
3	C	357	PX4	O7-C23	3.30	1.43	1.34	14	2
3	B	311	PX4	O7-C7	3.30	1.38	1.46	9	3
3	B	374	PX4	C2-C1	3.30	1.61	1.51	2	6
3	C	358	PX4	O7-C7	3.30	1.38	1.46	6	2
3	C	307	PX4	O5-C8	3.30	1.37	1.45	9	4
3	A	617	PX4	C11-C10	3.30	1.64	1.52	11	2
3	A	653	PX4	C11-C10	3.30	1.64	1.52	12	1
3	B	362	PX4	C2-C1	3.30	1.61	1.51	6	5
3	B	316	PX4	O5-C8	3.29	1.52	1.45	6	7
3	B	383	PX4	C2-C1	3.30	1.61	1.51	5	4
3	C	319	PX4	C6-C7	3.29	1.61	1.50	14	3
3	A	622	PX4	C10-C9	3.29	1.60	1.50	5	3
3	C	322	PX4	O7-C7	3.29	1.38	1.46	4	2
3	B	325	PX4	C8-C7	3.29	1.61	1.50	3	7
3	B	330	PX4	C24-C23	3.29	1.60	1.50	15	3
3	B	335	PX4	C24-C23	3.29	1.60	1.50	2	2
3	C	310	PX4	C2-N1	3.29	1.61	1.51	3	1
3	C	337	PX4	C6-C7	3.29	1.61	1.50	14	5
3	A	604	PX4	C6-C7	3.29	1.61	1.50	6	4
3	A	609	PX4	C2-C1	3.29	1.61	1.51	13	7
3	A	602	PX4	C6-C7	3.29	1.61	1.50	7	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	336	PX4	C5-N1	3.29	1.59	1.50	7	1
3	B	375	PX4	C10-C9	3.29	1.60	1.50	2	5
3	A	607	PX4	O7-C7	3.28	1.38	1.46	9	3
3	A	625	PX4	O5-C8	3.28	1.52	1.45	13	2
3	C	302	PX4	C4-N1	3.29	1.59	1.50	10	2
3	B	339	PX4	C6-C7	3.28	1.61	1.50	13	10
3	C	342	PX4	O5-C8	3.29	1.52	1.45	2	2
3	A	652	PX4	C11-C10	3.28	1.64	1.52	3	3
3	B	333	PX4	O5-C9	3.28	1.42	1.33	3	2
3	B	340	PX4	C24-C23	3.28	1.60	1.50	13	5
3	A	616	PX4	C6-C7	3.28	1.61	1.50	15	5
3	B	320	PX4	C8-C7	3.28	1.61	1.50	13	4
3	B	342	PX4	C6-C7	3.28	1.61	1.50	6	5
3	B	389	PX4	C6-C7	3.28	1.61	1.50	15	4
3	C	351	PX4	C4-N1	3.28	1.40	1.50	1	1
3	B	369	PX4	C2-C1	3.27	1.61	1.51	5	4
3	B	398	PX4	C24-C23	3.27	1.60	1.50	13	2
3	B	310	PX4	C10-C9	3.27	1.60	1.50	10	5
3	C	328	PX4	C10-C9	3.27	1.60	1.50	1	5
3	B	355	PX4	C10-C9	3.27	1.60	1.50	2	5
3	C	318	PX4	O5-C8	3.27	1.52	1.45	15	1
3	A	601	PX4	O7-C7	3.26	1.38	1.46	12	4
3	A	629	PX4	C6-C7	3.26	1.61	1.50	8	2
3	C	321	PX4	O7-C23	3.26	1.25	1.34	8	3
3	C	309	PX4	C2-N1	3.26	1.61	1.51	14	2
3	C	315	PX4	C6-C7	3.26	1.61	1.50	9	7
3	A	605	PX4	O5-C8	3.25	1.52	1.45	5	5
3	A	653	PX4	O5-C8	3.26	1.37	1.45	15	2
3	B	304	PX4	C2-C1	3.26	1.61	1.51	1	7
3	B	312	PX4	O7-C7	3.26	1.38	1.46	9	6
3	C	336	PX4	O7-C23	3.26	1.25	1.34	13	2
3	A	617	PX4	C6-C7	3.25	1.61	1.50	8	6
3	A	643	PX4	O5-C8	3.25	1.37	1.45	7	3
3	C	320	PX4	O5-C9	3.25	1.23	1.33	13	2
3	A	617	PX4	C2-C1	3.25	1.61	1.51	1	4
3	A	613	PX4	C8-C7	3.25	1.61	1.50	12	7
3	A	652	PX4	C6-C7	3.25	1.61	1.50	15	6
3	B	339	PX4	C8-C7	3.25	1.61	1.50	4	9
3	B	333	PX4	O7-C7	3.25	1.39	1.46	13	4
3	B	364	PX4	C6-C7	3.25	1.61	1.50	8	6
3	B	391	PX4	C2-C1	3.25	1.61	1.51	11	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	C	350	PX4	C2-N1	3.25	1.61	1.51	14	1
3	B	342	PX4	C10-C9	3.25	1.60	1.50	9	4
3	B	356	PX4	C10-C9	3.25	1.60	1.50	6	4
3	B	368	PX4	C6-C7	3.25	1.61	1.50	11	5
3	B	317	PX4	O5-C9	3.25	1.42	1.33	14	2
3	C	317	PX4	O7-C23	3.25	1.25	1.34	6	2
3	C	344	PX4	C24-C23	3.25	1.60	1.50	9	4
3	B	307	PX4	C11-C10	3.24	1.64	1.52	9	5
3	B	345	PX4	C4-N1	3.24	1.40	1.50	1	1
3	A	615	PX4	C2-C1	3.24	1.61	1.51	7	2
3	B	378	PX4	C4-N1	3.24	1.40	1.50	9	2
3	C	314	PX4	C10-C9	3.24	1.60	1.50	8	2
3	C	329	PX4	O5-C9	3.24	1.23	1.33	3	3
3	A	604	PX4	C10-C9	3.23	1.60	1.50	5	6
3	A	614	PX4	C2-C1	3.23	1.61	1.51	8	5
3	A	642	PX4	O7-C7	3.23	1.39	1.46	7	3
3	A	645	PX4	C8-C7	3.23	1.60	1.50	1	5
3	B	340	PX4	C10-C9	3.23	1.60	1.50	12	5
3	C	338	PX4	C10-C9	3.23	1.60	1.50	14	3
3	A	610	PX4	O5-C8	3.23	1.52	1.45	1	2
3	A	629	PX4	O7-C23	3.23	1.25	1.34	13	2
3	B	319	PX4	C2-C1	3.23	1.61	1.51	3	3
3	B	302	PX4	C8-C7	3.23	1.60	1.50	6	5
3	B	345	PX4	C10-C9	3.23	1.60	1.50	11	4
3	C	323	PX4	C2-C1	3.23	1.61	1.51	1	2
3	A	633	PX4	C8-C7	3.23	1.60	1.50	2	6
3	C	326	PX4	O5-C8	3.23	1.38	1.45	13	3
3	C	317	PX4	C10-C9	3.23	1.60	1.50	5	3
3	B	301	PX4	C6-C7	3.22	1.60	1.50	2	6
3	B	342	PX4	C2-C1	3.22	1.61	1.51	1	3
3	B	386	PX4	O7-C7	3.22	1.39	1.46	6	5
3	C	322	PX4	C10-C9	3.22	1.60	1.50	2	6
3	B	389	PX4	C4-N1	3.22	1.59	1.50	5	2
3	C	340	PX4	C2-C1	3.22	1.61	1.51	10	6
3	C	341	PX4	C10-C9	3.22	1.60	1.50	12	5
3	C	347	PX4	O7-C23	3.22	1.25	1.34	15	3
3	B	361	PX4	C10-C9	3.22	1.60	1.50	2	4
3	B	336	PX4	C2-N1	3.22	1.61	1.51	15	2
3	A	637	PX4	C2-C1	3.22	1.61	1.51	3	6
3	A	610	PX4	O7-C7	3.21	1.39	1.46	6	2
3	A	624	PX4	O7-C23	3.22	1.43	1.34	6	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	329	PX4	C24-C23	3.21	1.60	1.50	8	2
3	B	357	PX4	C10-C9	3.21	1.60	1.50	10	3
3	B	361	PX4	C11-C10	3.21	1.64	1.52	10	2
3	A	641	PX4	C2-N1	3.21	1.61	1.51	5	2
3	A	643	PX4	C2-C1	3.21	1.61	1.51	7	5
3	C	361	PX4	C2-C1	3.21	1.61	1.51	12	4
3	A	604	PX4	O5-C8	3.21	1.38	1.45	7	3
3	C	329	PX4	C2-N1	3.21	1.61	1.51	10	2
3	B	333	PX4	C4-N1	3.21	1.59	1.50	15	2
3	B	349	PX4	O7-C23	3.21	1.43	1.34	9	3
3	B	307	PX4	O5-C8	3.20	1.38	1.45	14	5
3	B	400	PX4	C6-C7	3.20	1.60	1.50	5	4
3	C	341	PX4	O4-C6	3.20	1.32	1.44	8	1
3	C	363	PX4	C5-N1	3.20	1.59	1.50	9	2
3	A	642	PX4	C10-C9	3.20	1.60	1.50	1	3
3	B	308	PX4	O5-C9	3.20	1.24	1.33	3	2
3	B	358	PX4	C8-C7	3.20	1.60	1.50	2	6
3	B	386	PX4	C6-C7	3.20	1.60	1.50	2	7
3	C	323	PX4	C24-C23	3.20	1.60	1.50	5	4
3	B	307	PX4	C8-C7	3.20	1.60	1.50	11	5
3	B	351	PX4	C25-C24	3.20	1.63	1.52	12	2
3	C	332	PX4	O5-C8	3.20	1.52	1.45	6	3
3	C	340	PX4	C8-C7	3.20	1.60	1.50	13	6
3	A	605	PX4	O7-C7	3.20	1.39	1.46	11	2
3	A	602	PX4	C24-C23	3.20	1.60	1.50	15	5
3	B	362	PX4	C10-C9	3.20	1.60	1.50	8	2
3	B	369	PX4	O5-C8	3.19	1.52	1.45	14	4
3	B	380	PX4	O7-C23	3.19	1.25	1.34	9	1
3	C	330	PX4	C8-C7	3.19	1.60	1.50	11	4
3	B	355	PX4	C3-N1	3.19	1.59	1.50	8	4
3	A	632	PX4	O5-C8	3.19	1.38	1.45	4	3
3	A	639	PX4	C10-C9	3.19	1.60	1.50	2	6
3	B	309	PX4	C8-C7	3.19	1.60	1.50	15	2
3	B	329	PX4	C8-C7	3.19	1.60	1.50	2	8
3	B	392	PX4	C6-C7	3.19	1.60	1.50	7	3
3	B	393	PX4	O7-C23	3.19	1.25	1.34	5	3
3	A	623	PX4	C8-C7	3.19	1.60	1.50	2	4
3	B	343	PX4	C3-N1	3.19	1.40	1.50	1	1
3	B	397	PX4	C8-C7	3.19	1.60	1.50	14	5
3	B	399	PX4	C8-C7	3.19	1.60	1.50	6	8
3	C	358	PX4	C6-C7	3.19	1.60	1.50	6	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	A	602	PX4	O5-C8	3.19	1.52	1.45	14	3
3	B	315	PX4	C24-C23	3.19	1.59	1.50	2	4
3	C	337	PX4	C24-C23	3.19	1.59	1.50	9	5
3	A	652	PX4	O7-C23	3.18	1.43	1.34	4	1
3	B	370	PX4	C2-C1	3.18	1.61	1.51	11	3
3	B	371	PX4	C24-C23	3.18	1.59	1.50	3	3
3	C	340	PX4	O7-C7	3.18	1.39	1.46	6	6
3	B	352	PX4	C6-C7	3.18	1.60	1.50	13	10
3	A	616	PX4	O5-C8	3.18	1.52	1.45	8	3
3	B	355	PX4	C8-C7	3.18	1.60	1.50	1	6
3	B	317	PX4	O7-C7	3.18	1.39	1.46	14	5
3	B	360	PX4	O5-C9	3.18	1.42	1.33	5	1
3	A	606	PX4	C2-C1	3.17	1.60	1.51	7	6
3	A	629	PX4	O7-C7	3.17	1.39	1.46	1	3
3	B	346	PX4	C4-N1	3.17	1.40	1.50	2	1
3	B	343	PX4	C6-C7	3.17	1.60	1.50	5	5
3	B	391	PX4	C6-C7	3.17	1.60	1.50	10	9
3	C	330	PX4	C10-C9	3.17	1.41	1.50	9	4
3	A	607	PX4	C4-N1	3.17	1.59	1.50	2	3
3	C	354	PX4	O5-C9	3.17	1.24	1.33	15	3
3	C	342	PX4	C10-C9	3.17	1.59	1.50	15	5
3	C	342	PX4	C24-C23	3.17	1.59	1.50	10	3
3	A	612	PX4	C2-N1	3.16	1.61	1.51	11	2
3	B	337	PX4	C6-C7	3.16	1.60	1.50	15	5
3	A	621	PX4	O7-C7	3.16	1.39	1.46	14	1
3	B	346	PX4	O5-C8	3.16	1.52	1.45	13	4
3	B	350	PX4	C2-C1	3.16	1.60	1.51	5	5
3	B	353	PX4	C8-C7	3.16	1.60	1.50	7	6
3	B	391	PX4	C10-C9	3.16	1.59	1.50	4	1
3	C	311	PX4	C3-N1	3.16	1.40	1.50	8	1
3	A	604	PX4	C25-C24	3.16	1.63	1.52	13	1
3	A	618	PX4	C4-N1	3.16	1.40	1.50	14	2
3	B	355	PX4	C4-N1	3.16	1.59	1.50	12	3
3	C	348	PX4	C2-N1	3.16	1.61	1.51	7	1
3	B	370	PX4	C8-C7	3.15	1.60	1.50	6	7
3	B	392	PX4	C8-C7	3.15	1.60	1.50	5	7
3	A	623	PX4	O5-C8	3.15	1.38	1.45	7	1
3	A	633	PX4	C2-C1	3.15	1.60	1.51	7	4
3	B	397	PX4	O7-C7	3.15	1.39	1.46	6	5
3	C	316	PX4	C2-C1	3.15	1.60	1.51	4	4
3	A	615	PX4	C25-C24	3.15	1.63	1.52	2	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	350	PX4	C11-C10	3.15	1.63	1.52	15	3
3	B	385	PX4	O7-C7	3.15	1.39	1.46	5	6
3	C	352	PX4	O7-C23	3.15	1.25	1.34	15	3
3	A	653	PX4	C3-N1	3.15	1.59	1.50	12	1
3	B	390	PX4	C6-C7	3.15	1.60	1.50	4	7
3	B	383	PX4	O5-C8	3.14	1.52	1.45	14	7
3	B	400	PX4	C10-C9	3.14	1.59	1.50	1	3
3	B	362	PX4	C6-C7	3.14	1.60	1.50	8	3
3	C	334	PX4	O7-C7	3.14	1.39	1.46	2	5
3	B	344	PX4	C11-C10	3.14	1.63	1.52	12	3
3	B	366	PX4	O7-C23	3.14	1.25	1.34	14	2
3	A	602	PX4	C8-C7	3.14	1.60	1.50	1	4
3	B	341	PX4	C8-C7	3.14	1.60	1.50	5	5
3	C	324	PX4	C6-C7	3.14	1.60	1.50	7	3
3	A	617	PX4	C24-C23	3.14	1.59	1.50	7	2
3	B	306	PX4	C10-C9	3.13	1.59	1.50	3	4
3	B	332	PX4	C2-C1	3.13	1.60	1.51	3	6
3	B	347	PX4	O5-C8	3.13	1.38	1.45	9	2
3	B	350	PX4	C8-C7	3.13	1.60	1.50	3	7
3	B	397	PX4	C6-C7	3.13	1.60	1.50	12	4
3	C	323	PX4	O7-C7	3.13	1.39	1.46	2	4
3	B	302	PX4	O5-C9	3.13	1.24	1.33	6	4
3	B	333	PX4	C10-C9	3.13	1.59	1.50	11	2
3	B	366	PX4	C8-C7	3.13	1.60	1.50	8	8
3	B	387	PX4	O7-C7	3.13	1.39	1.46	3	3
3	A	626	PX4	C8-C7	3.13	1.60	1.50	11	5
3	B	340	PX4	C11-C10	3.13	1.63	1.52	7	2
3	C	351	PX4	C11-C10	3.13	1.63	1.52	2	2
3	B	310	PX4	C25-C24	3.13	1.63	1.52	13	2
3	C	309	PX4	O7-C7	3.12	1.39	1.46	15	3
3	C	360	PX4	C24-C23	3.12	1.59	1.50	10	5
3	A	611	PX4	C25-C24	3.12	1.63	1.52	5	3
3	A	628	PX4	C25-C24	3.12	1.63	1.52	13	1
3	C	337	PX4	O7-C23	3.12	1.25	1.34	2	4
3	C	357	PX4	C11-C10	3.12	1.63	1.52	2	1
3	A	620	PX4	C2-N1	3.12	1.61	1.51	12	4
3	B	391	PX4	C25-C24	3.12	1.63	1.52	15	1
3	C	353	PX4	C10-C9	3.12	1.59	1.50	10	6
3	A	630	PX4	C6-C7	3.11	1.60	1.50	3	6
3	A	642	PX4	C6-C7	3.11	1.60	1.50	11	7
3	B	365	PX4	C2-C1	3.11	1.60	1.51	13	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	C	329	PX4	C11-C10	3.11	1.63	1.52	11	2
3	A	614	PX4	O7-C7	3.11	1.39	1.46	1	5
3	A	635	PX4	C5-N1	3.11	1.59	1.50	7	2
3	A	643	PX4	C2-N1	3.11	1.61	1.51	4	2
3	B	381	PX4	P1-O1	3.11	1.40	1.55	2	2
3	A	644	PX4	C2-C1	3.11	1.60	1.51	4	7
3	B	379	PX4	C11-C10	3.11	1.63	1.52	9	4
3	B	389	PX4	C2-N1	3.11	1.60	1.51	1	2
3	B	390	PX4	O7-C23	3.11	1.25	1.34	10	4
3	C	324	PX4	O5-C9	3.11	1.24	1.33	1	2
3	B	359	PX4	O7-C7	3.11	1.39	1.46	10	3
3	A	625	PX4	C6-C7	3.10	1.60	1.50	3	6
3	A	614	PX4	C24-C23	3.10	1.59	1.50	1	3
3	A	647	PX4	C10-C9	3.10	1.59	1.50	3	3
3	B	367	PX4	C2-C1	3.10	1.60	1.51	1	3
3	B	379	PX4	C3-N1	3.10	1.41	1.50	1	2
3	C	304	PX4	O5-C8	3.10	1.38	1.45	8	3
3	C	315	PX4	C24-C23	3.10	1.59	1.50	9	1
3	C	348	PX4	O7-C7	3.10	1.39	1.46	6	1
3	A	614	PX4	O5-C9	3.10	1.42	1.33	5	1
3	B	349	PX4	C25-C24	3.09	1.63	1.52	6	7
3	C	325	PX4	C2-C1	3.09	1.60	1.51	1	3
3	C	301	PX4	C11-C10	3.09	1.63	1.52	8	2
3	C	349	PX4	O5-C8	3.09	1.38	1.45	4	2
3	A	605	PX4	C10-C9	3.09	1.59	1.50	5	4
3	A	618	PX4	C10-C9	3.09	1.59	1.50	2	4
3	B	368	PX4	C10-C9	3.09	1.59	1.50	15	2
3	B	384	PX4	C3-N1	3.09	1.59	1.50	12	2
3	C	355	PX4	C11-C10	3.09	1.63	1.52	8	3
3	B	384	PX4	C24-C23	3.09	1.59	1.50	5	4
3	C	318	PX4	O5-C9	3.09	1.42	1.33	9	2
3	B	382	PX4	O5-C8	3.08	1.38	1.45	3	2
3	C	350	PX4	C24-C23	3.09	1.59	1.50	14	1
3	A	613	PX4	O7-C23	3.08	1.25	1.34	10	6
3	B	334	PX4	C10-C9	3.08	1.59	1.50	6	3
3	B	381	PX4	C10-C9	3.08	1.59	1.50	15	2
3	C	349	PX4	C8-C7	3.08	1.60	1.50	14	3
3	A	609	PX4	O5-C9	3.08	1.24	1.33	7	3
3	B	306	PX4	C6-C7	3.08	1.60	1.50	13	3
3	B	354	PX4	C6-C7	3.08	1.60	1.50	3	6
3	B	364	PX4	C10-C9	3.08	1.59	1.50	11	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	C	341	PX4	C2-C1	3.08	1.60	1.51	7	4
3	C	362	PX4	O5-C9	3.08	1.42	1.33	14	3
3	B	308	PX4	O7-C23	3.08	1.25	1.34	3	3
3	B	317	PX4	O7-C23	3.08	1.25	1.34	9	2
3	B	383	PX4	C4-N1	3.08	1.58	1.50	4	3
3	B	398	PX4	C6-C7	3.08	1.60	1.50	10	4
3	C	303	PX4	O5-C8	3.08	1.38	1.45	15	2
3	C	309	PX4	C2-C1	3.08	1.60	1.51	15	4
3	B	305	PX4	C4-N1	3.08	1.58	1.50	14	1
3	C	354	PX4	O7-C7	3.08	1.39	1.46	10	2
3	A	651	PX4	C11-C10	3.07	1.63	1.52	1	1
3	B	345	PX4	C6-C7	3.07	1.60	1.50	13	4
3	C	334	PX4	C6-C7	3.07	1.60	1.50	5	3
3	A	615	PX4	C10-C9	3.07	1.59	1.50	2	3
3	C	319	PX4	C2-C1	3.07	1.60	1.51	14	6
3	C	328	PX4	O5-C9	3.07	1.42	1.33	15	3
3	B	345	PX4	O7-C23	3.07	1.25	1.34	11	1
3	A	616	PX4	C25-C24	3.07	1.63	1.52	10	3
3	B	329	PX4	C2-C1	3.07	1.60	1.51	2	7
3	C	314	PX4	C24-C23	3.07	1.59	1.50	8	2
3	B	312	PX4	O5-C8	3.07	1.52	1.45	3	3
3	B	325	PX4	C24-C23	3.07	1.59	1.50	10	3
3	C	320	PX4	C6-C7	3.07	1.60	1.50	2	6
3	C	351	PX4	C8-C7	3.07	1.60	1.50	8	4
3	C	362	PX4	O7-C23	3.07	1.25	1.34	10	2
3	B	379	PX4	C6-C7	3.07	1.60	1.50	8	6
3	A	612	PX4	C8-C7	3.06	1.60	1.50	2	4
3	C	304	PX4	O7-C23	3.06	1.25	1.34	13	4
3	B	321	PX4	C11-C10	3.06	1.63	1.52	6	4
3	B	361	PX4	O5-C8	3.06	1.38	1.45	5	1
3	B	367	PX4	O7-C7	3.06	1.39	1.46	6	2
3	B	371	PX4	C5-N1	3.06	1.58	1.50	11	1
3	C	341	PX4	O5-C8	3.06	1.38	1.45	7	6
3	A	616	PX4	C10-C9	3.06	1.59	1.50	2	1
3	A	603	PX4	O7-C23	3.06	1.25	1.34	15	2
3	B	369	PX4	O7-C7	3.06	1.39	1.46	13	1
3	B	349	PX4	O7-C7	3.06	1.39	1.46	10	2
3	B	370	PX4	O5-C8	3.06	1.38	1.45	15	3
3	B	384	PX4	C8-C7	3.06	1.60	1.50	4	7
3	B	386	PX4	O7-C23	3.06	1.25	1.34	5	1
3	B	386	PX4	O5-C8	3.06	1.52	1.45	14	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	C	326	PX4	O7-C23	3.06	1.42	1.34	15	3
3	C	359	PX4	C24-C23	3.06	1.59	1.50	7	3
3	A	653	PX4	C25-C24	3.05	1.63	1.52	9	3
3	C	305	PX4	O5-C9	3.05	1.42	1.33	5	1
3	B	313	PX4	O5-C8	3.05	1.38	1.45	13	1
3	C	317	PX4	C2-N1	3.05	1.60	1.51	3	1
3	C	337	PX4	C2-C1	3.05	1.60	1.51	5	4
3	B	329	PX4	C25-C24	3.05	1.63	1.52	10	1
3	B	339	PX4	C10-C9	3.05	1.59	1.50	15	2
3	C	341	PX4	C24-C23	3.05	1.59	1.50	1	2
3	C	336	PX4	C24-C23	3.05	1.59	1.50	15	6
3	C	358	PX4	C4-N1	3.05	1.58	1.50	12	2
3	A	614	PX4	C8-C7	3.04	1.60	1.50	6	5
3	A	611	PX4	C8-C7	3.04	1.60	1.50	12	6
3	A	619	PX4	C2-N1	3.04	1.60	1.51	12	2
3	B	321	PX4	O7-C23	3.04	1.25	1.34	2	3
3	A	644	PX4	C10-C9	3.04	1.59	1.50	6	3
3	B	313	PX4	O5-C9	3.04	1.42	1.33	13	1
3	B	352	PX4	C10-C9	3.04	1.59	1.50	9	2
3	B	374	PX4	C11-C10	3.04	1.63	1.52	14	2
3	B	385	PX4	O7-C23	3.04	1.25	1.34	4	2
3	A	607	PX4	C2-C1	3.04	1.60	1.51	15	1
3	C	343	PX4	C24-C23	3.04	1.59	1.50	7	4
3	B	318	PX4	C10-C9	3.04	1.59	1.50	2	3
3	B	337	PX4	C10-C9	3.03	1.41	1.50	4	3
3	B	378	PX4	O5-C8	3.03	1.51	1.45	1	2
3	C	342	PX4	O7-C7	3.03	1.39	1.46	8	2
3	B	366	PX4	C2-C1	3.03	1.60	1.51	13	6
3	B	344	PX4	C2-N1	3.03	1.60	1.51	2	1
3	C	301	PX4	C10-C9	3.03	1.59	1.50	4	7
3	B	309	PX4	O7-C23	3.03	1.25	1.34	6	2
3	B	357	PX4	O7-C23	3.03	1.25	1.34	3	2
3	B	390	PX4	C8-C7	3.03	1.60	1.50	5	8
3	A	634	PX4	C2-C1	3.03	1.60	1.51	6	6
3	C	316	PX4	C6-C7	3.02	1.60	1.50	14	7
3	A	617	PX4	P1-O1	3.02	1.41	1.55	14	3
3	A	647	PX4	C24-C23	3.02	1.59	1.50	10	5
3	B	341	PX4	C24-C23	3.02	1.59	1.50	15	3
3	B	353	PX4	P1-O1	3.02	1.41	1.55	15	2
3	B	390	PX4	C25-C24	3.02	1.63	1.52	11	2
3	A	605	PX4	C2-C1	3.02	1.60	1.51	2	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	A	626	PX4	O5-C8	3.02	1.38	1.45	2	2
3	B	316	PX4	C5-N1	3.02	1.58	1.50	7	2
3	B	348	PX4	C10-C9	3.02	1.59	1.50	1	2
3	C	323	PX4	C25-C24	3.02	1.63	1.52	4	2
3	A	623	PX4	O5-C9	3.01	1.42	1.33	10	2
3	A	643	PX4	C5-N1	3.01	1.58	1.50	9	2
3	B	339	PX4	C11-C10	3.01	1.63	1.52	3	1
3	C	313	PX4	C5-N1	3.01	1.58	1.50	4	2
3	C	338	PX4	C2-C1	3.01	1.60	1.51	8	3
3	C	342	PX4	C2-C1	3.01	1.60	1.51	6	5
3	A	628	PX4	C2-C1	3.01	1.60	1.51	4	3
3	B	313	PX4	C11-C10	3.01	1.63	1.52	9	3
3	C	340	PX4	C6-C7	3.01	1.60	1.50	15	5
3	A	633	PX4	O7-C7	3.01	1.39	1.46	7	3
3	A	639	PX4	C24-C23	3.01	1.59	1.50	9	3
3	B	304	PX4	C6-C7	3.01	1.60	1.50	7	4
3	B	354	PX4	C8-C7	3.01	1.60	1.50	13	4
3	B	359	PX4	C2-N1	3.01	1.60	1.51	11	1
3	B	381	PX4	C2-N1	3.01	1.42	1.51	6	1
3	B	358	PX4	C6-C7	3.01	1.60	1.50	6	9
3	A	648	PX4	O5-C8	3.01	1.51	1.45	13	4
3	B	368	PX4	C11-C10	3.01	1.63	1.52	8	2
3	B	303	PX4	C24-C23	3.01	1.59	1.50	14	2
3	B	318	PX4	C5-N1	3.01	1.41	1.50	6	2
3	A	622	PX4	C24-C23	3.00	1.59	1.50	12	2
3	B	354	PX4	C24-C23	3.00	1.59	1.50	6	2
3	A	644	PX4	O7-C23	3.00	1.25	1.34	7	3
3	B	308	PX4	C10-C9	3.00	1.59	1.50	6	2
3	B	394	PX4	O5-C9	3.00	1.24	1.33	12	2
3	B	398	PX4	C10-C9	3.00	1.59	1.50	5	3
3	B	306	PX4	C5-N1	3.00	1.41	1.50	5	1
3	B	333	PX4	P1-O1	3.00	1.41	1.55	1	1
3	C	331	PX4	C2-C1	3.00	1.60	1.51	6	3
3	C	356	PX4	O7-C23	3.00	1.25	1.34	4	3
3	B	346	PX4	O5-C9	3.00	1.42	1.33	6	4
3	B	366	PX4	C24-C23	3.00	1.59	1.50	8	3
3	C	303	PX4	C2-N1	2.99	1.60	1.51	5	4
3	A	630	PX4	C3-N1	2.99	1.58	1.50	3	1
3	A	639	PX4	C6-C7	2.99	1.60	1.50	3	5
3	A	618	PX4	C5-N1	2.99	1.41	1.50	1	1
3	A	640	PX4	O5-C8	2.99	1.38	1.45	6	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	324	PX4	O7-C7	2.99	1.39	1.46	8	2
3	B	324	PX4	C28-C27	2.99	1.66	1.51	12	3
3	B	325	PX4	O7-C7	2.99	1.39	1.46	12	2
3	B	382	PX4	C2-N1	2.99	1.60	1.51	12	2
3	C	338	PX4	O5-C8	2.99	1.38	1.45	12	1
3	A	648	PX4	O7-C7	2.99	1.39	1.46	9	4
3	B	313	PX4	C25-C24	2.99	1.63	1.52	9	5
3	B	360	PX4	C17-C16	2.99	1.66	1.51	14	1
3	B	393	PX4	C4-N1	2.99	1.41	1.50	10	1
3	B	330	PX4	C8-C7	2.98	1.60	1.50	9	4
3	B	379	PX4	O7-C7	2.99	1.39	1.46	9	5
3	C	353	PX4	C6-C7	2.99	1.60	1.50	4	7
3	C	306	PX4	O5-C8	2.98	1.38	1.45	15	1
3	C	348	PX4	P1-O1	2.98	1.41	1.55	13	3
3	C	363	PX4	C3-N1	2.98	1.58	1.50	8	2
3	A	635	PX4	O7-C7	2.98	1.39	1.46	8	2
3	A	638	PX4	C6-C7	2.98	1.60	1.50	3	6
3	A	640	PX4	C2-N1	2.98	1.60	1.51	8	2
3	B	328	PX4	C8-C7	2.98	1.60	1.50	11	8
3	B	394	PX4	C24-C23	2.98	1.59	1.50	4	2
3	B	331	PX4	O5-C8	2.98	1.38	1.45	10	5
3	B	394	PX4	C2-N1	2.98	1.60	1.51	3	2
3	C	301	PX4	O7-C23	2.98	1.25	1.34	2	1
3	B	368	PX4	C4-N1	2.98	1.41	1.50	4	2
3	C	345	PX4	C10-C9	2.98	1.59	1.50	13	3
3	C	345	PX4	C25-C24	2.98	1.63	1.52	7	2
3	C	353	PX4	O5-C9	2.98	1.24	1.33	1	3
3	B	360	PX4	C24-C23	2.97	1.59	1.50	10	2
3	C	318	PX4	C3-N1	2.98	1.58	1.50	12	3
3	B	304	PX4	C8-C7	2.97	1.60	1.50	14	5
3	B	318	PX4	P1-O1	2.97	1.41	1.55	9	2
3	B	399	PX4	C11-C10	2.97	1.63	1.52	6	2
3	B	332	PX4	O5-C9	2.97	1.42	1.33	8	4
3	B	388	PX4	P1-O1	2.97	1.41	1.55	7	4
3	B	390	PX4	C2-N1	2.97	1.42	1.51	8	1
3	B	353	PX4	O5-C9	2.97	1.42	1.33	6	1
3	B	309	PX4	C4-N1	2.97	1.58	1.50	11	6
3	B	344	PX4	C8-C7	2.97	1.60	1.50	7	8
3	B	345	PX4	C8-C7	2.97	1.60	1.50	8	7
3	B	354	PX4	P1-O3	2.97	1.47	1.59	2	1
3	B	391	PX4	O5-C9	2.97	1.42	1.33	12	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	324	PX4	C25-C24	2.97	1.63	1.52	15	2
3	B	330	PX4	O5-C8	2.97	1.51	1.45	6	2
3	C	312	PX4	C2-C1	2.97	1.60	1.51	13	6
3	A	617	PX4	C10-C9	2.96	1.59	1.50	13	5
3	A	627	PX4	C24-C23	2.96	1.59	1.50	6	6
3	C	340	PX4	C24-C23	2.96	1.59	1.50	6	2
3	B	318	PX4	C2-C1	2.96	1.60	1.51	12	6
3	A	613	PX4	O7-C7	2.96	1.39	1.46	5	3
3	B	349	PX4	C18-C17	2.96	1.66	1.51	1	1
3	A	630	PX4	C11-C10	2.96	1.63	1.52	5	2
3	A	634	PX4	O5-C9	2.96	1.42	1.33	2	3
3	C	315	PX4	O7-C7	2.96	1.39	1.46	5	4
3	C	323	PX4	C2-N1	2.96	1.60	1.51	6	2
3	A	640	PX4	C2-C1	2.96	1.60	1.51	2	4
3	A	643	PX4	C6-C7	2.96	1.60	1.50	4	4
3	A	646	PX4	O5-C8	2.96	1.38	1.45	13	1
3	A	647	PX4	C5-N1	2.96	1.41	1.50	5	1
3	B	347	PX4	C24-C23	2.96	1.59	1.50	6	1
3	B	383	PX4	O7-C23	2.95	1.25	1.34	12	2
3	B	389	PX4	C25-C24	2.95	1.63	1.52	15	2
3	C	343	PX4	O7-C23	2.96	1.25	1.34	5	4
3	B	323	PX4	C6-C7	2.95	1.60	1.50	8	2
3	A	606	PX4	C11-C10	2.95	1.63	1.52	14	5
3	A	607	PX4	C10-C9	2.95	1.59	1.50	7	2
3	B	317	PX4	C25-C24	2.95	1.63	1.52	9	1
3	B	319	PX4	O7-C7	2.95	1.39	1.46	2	1
3	B	329	PX4	C11-C10	2.95	1.63	1.52	15	4
3	B	304	PX4	O5-C8	2.95	1.38	1.45	5	1
3	A	644	PX4	C6-C7	2.95	1.60	1.50	5	3
3	B	311	PX4	C5-N1	2.95	1.58	1.50	7	5
3	B	388	PX4	C11-C10	2.95	1.63	1.52	10	3
3	A	651	PX4	O5-C8	2.95	1.51	1.45	1	5
3	B	331	PX4	C24-C23	2.95	1.59	1.50	14	2
3	A	651	PX4	O5-C9	2.94	1.41	1.33	6	2
3	B	367	PX4	C11-C10	2.94	1.63	1.52	15	2
3	C	306	PX4	C10-C9	2.94	1.59	1.50	1	3
3	C	352	PX4	O7-C7	2.94	1.39	1.46	3	1
3	B	323	PX4	O4-C6	2.94	1.33	1.44	7	1
3	A	604	PX4	C5-N1	2.94	1.58	1.50	9	3
3	B	307	PX4	C10-C9	2.94	1.59	1.50	13	5
3	B	337	PX4	C3-N1	2.94	1.41	1.50	9	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	A	603	PX4	O7-C7	2.94	1.39	1.46	5	2
3	C	361	PX4	C11-C10	2.94	1.63	1.52	3	1
3	A	608	PX4	C24-C23	2.94	1.59	1.50	6	2
3	A	627	PX4	C5-N1	2.94	1.58	1.50	13	2
3	B	303	PX4	O5-C8	2.93	1.38	1.45	14	1
3	B	327	PX4	C2-N1	2.93	1.60	1.51	4	1
3	B	359	PX4	O5-C8	2.93	1.51	1.45	10	2
3	B	389	PX4	C11-C10	2.93	1.62	1.52	10	2
3	C	363	PX4	C24-C23	2.93	1.59	1.50	6	1
3	B	315	PX4	O5-C9	2.93	1.41	1.33	12	2
3	B	360	PX4	O5-C8	2.93	1.38	1.45	9	3
3	B	304	PX4	C11-C10	2.93	1.62	1.52	5	1
3	B	339	PX4	O5-C8	2.93	1.38	1.45	3	2
3	B	386	PX4	C10-C9	2.93	1.59	1.50	11	3
3	C	307	PX4	C10-C9	2.93	1.59	1.50	2	3
3	C	360	PX4	O7-C7	2.93	1.39	1.46	6	2
3	C	338	PX4	O7-C7	2.93	1.39	1.46	7	1
3	C	349	PX4	C6-C7	2.93	1.60	1.50	10	7
3	A	605	PX4	C11-C10	2.92	1.62	1.52	15	2
3	C	309	PX4	P1-O1	2.92	1.41	1.55	7	4
3	C	325	PX4	C25-C24	2.92	1.62	1.52	12	3
3	C	337	PX4	C25-C24	2.92	1.62	1.52	12	1
3	C	344	PX4	C6-C7	2.92	1.59	1.50	7	6
3	A	652	PX4	C24-C23	2.92	1.59	1.50	5	4
3	B	306	PX4	C8-C7	2.92	1.59	1.50	5	5
3	B	322	PX4	O7-C23	2.92	1.26	1.34	4	3
3	B	356	PX4	C4-N1	2.92	1.58	1.50	2	2
3	A	645	PX4	C25-C24	2.92	1.62	1.52	3	2
3	A	649	PX4	C24-C23	2.92	1.59	1.50	2	2
3	B	311	PX4	C24-C23	2.92	1.59	1.50	11	6
3	B	338	PX4	O7-C7	2.92	1.39	1.46	2	1
3	B	368	PX4	C5-N1	2.92	1.58	1.50	6	1
3	A	634	PX4	C11-C10	2.92	1.62	1.52	14	4
3	B	332	PX4	C24-C23	2.92	1.59	1.50	11	1
3	B	394	PX4	O5-C8	2.92	1.51	1.45	9	3
3	C	311	PX4	C2-C1	2.91	1.60	1.51	6	5
3	C	346	PX4	O7-C7	2.91	1.39	1.46	7	4
3	C	356	PX4	C24-C23	2.91	1.59	1.50	8	2
3	A	621	PX4	C8-C7	2.91	1.59	1.50	3	4
3	B	303	PX4	C2-N1	2.91	1.60	1.51	13	1
3	B	388	PX4	O7-C23	2.91	1.26	1.34	13	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	C	346	PX4	C2-C1	2.91	1.60	1.51	2	2
3	C	364	PX4	C2-C1	2.91	1.60	1.51	1	3
3	B	387	PX4	C25-C24	2.91	1.62	1.52	11	1
3	A	628	PX4	C6-C7	2.91	1.59	1.50	7	5
3	A	646	PX4	O7-C7	2.91	1.39	1.46	13	2
3	C	309	PX4	C3-N1	2.91	1.58	1.50	7	1
3	C	344	PX4	C11-C10	2.91	1.62	1.52	8	2
3	A	601	PX4	C24-C23	2.91	1.59	1.50	3	3
3	A	648	PX4	O7-C23	2.91	1.26	1.34	13	5
3	B	335	PX4	C10-C9	2.91	1.59	1.50	9	3
3	B	378	PX4	O7-C7	2.91	1.39	1.46	8	3
3	A	620	PX4	O5-C9	2.90	1.24	1.33	13	1
3	A	638	PX4	C11-C10	2.90	1.62	1.52	13	1
3	B	345	PX4	C25-C24	2.90	1.62	1.52	2	3
3	A	653	PX4	C2-C1	2.90	1.60	1.51	8	6
3	C	312	PX4	C10-C9	2.90	1.59	1.50	7	4
3	C	349	PX4	C2-C1	2.90	1.60	1.51	1	3
3	B	381	PX4	C3-N1	2.90	1.58	1.50	15	2
3	B	363	PX4	C24-C23	2.90	1.59	1.50	4	2
3	B	366	PX4	C5-N1	2.90	1.58	1.50	6	2
3	B	375	PX4	O7-C7	2.90	1.39	1.46	11	3
3	C	334	PX4	P1-O1	2.90	1.41	1.55	14	3
3	B	354	PX4	O7-C23	2.90	1.26	1.34	3	3
3	C	317	PX4	C6-C7	2.90	1.59	1.50	7	5
3	B	357	PX4	O7-C7	2.90	1.39	1.46	1	3
3	C	352	PX4	O5-C8	2.90	1.51	1.45	8	4
3	B	305	PX4	C2-C1	2.89	1.60	1.51	2	3
3	B	323	PX4	C2-N1	2.89	1.60	1.51	12	1
3	B	371	PX4	C11-C10	2.89	1.62	1.52	13	4
3	B	356	PX4	C2-C1	2.89	1.60	1.51	3	6
3	A	622	PX4	C8-C7	2.89	1.59	1.50	4	7
3	B	376	PX4	C10-C9	2.89	1.59	1.50	4	3
3	B	301	PX4	C2-N1	2.89	1.60	1.51	9	1
3	B	319	PX4	O5-C8	2.89	1.51	1.45	14	3
3	B	337	PX4	O7-C7	2.89	1.53	1.46	10	3
3	A	623	PX4	O7-C7	2.88	1.39	1.46	4	2
3	A	601	PX4	O5-C9	2.88	1.25	1.33	2	1
3	B	321	PX4	C24-C23	2.88	1.59	1.50	14	4
3	C	333	PX4	C2-C1	2.88	1.60	1.51	2	3
3	A	626	PX4	O7-C23	2.88	1.26	1.34	13	3
3	C	301	PX4	C25-C24	2.88	1.62	1.52	9	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	A	614	PX4	O5-C8	2.88	1.51	1.45	14	2
3	A	639	PX4	C25-C24	2.88	1.62	1.52	14	2
3	C	302	PX4	C2-N1	2.88	1.60	1.51	15	3
3	B	366	PX4	C11-C10	2.88	1.62	1.52	11	2
3	C	324	PX4	O7-C7	2.88	1.39	1.46	11	2
3	C	331	PX4	O5-C8	2.88	1.38	1.45	4	3
3	B	395	PX4	O5-C9	2.88	1.41	1.33	12	2
3	C	336	PX4	C3-N1	2.88	1.58	1.50	11	1
3	C	349	PX4	O7-C7	2.88	1.39	1.46	5	2
3	B	342	PX4	O5-C8	2.88	1.38	1.45	6	1
3	B	307	PX4	C6-C7	2.88	1.59	1.50	1	4
3	C	364	PX4	O5-C8	2.88	1.38	1.45	2	2
3	A	638	PX4	C24-C23	2.87	1.59	1.50	12	1
3	B	351	PX4	O5-C9	2.87	1.41	1.33	2	2
3	B	363	PX4	C10-C9	2.87	1.59	1.50	13	3
3	B	385	PX4	O5-C8	2.87	1.51	1.45	2	2
3	C	361	PX4	O5-C8	2.87	1.38	1.45	4	1
3	C	363	PX4	O7-C7	2.87	1.39	1.46	9	4
3	B	302	PX4	O7-C7	2.87	1.39	1.46	1	4
3	B	366	PX4	O7-C7	2.87	1.39	1.46	8	2
3	B	368	PX4	P1-O1	2.87	1.42	1.55	12	4
3	B	350	PX4	C10-C9	2.87	1.59	1.50	1	5
3	C	305	PX4	C11-C10	2.87	1.62	1.52	8	6
3	A	605	PX4	O7-C23	2.87	1.26	1.34	9	6
3	B	396	PX4	O7-C7	2.87	1.39	1.46	15	2
3	B	358	PX4	O7-C7	2.87	1.39	1.46	3	3
3	C	303	PX4	C11-C10	2.87	1.62	1.52	15	2
3	B	394	PX4	C8-C7	2.87	1.59	1.50	12	4
3	B	398	PX4	C2-N1	2.87	1.60	1.51	6	1
3	C	330	PX4	O7-C23	2.87	1.26	1.34	5	4
3	A	607	PX4	C24-C23	2.86	1.59	1.50	14	3
3	C	337	PX4	O5-C9	2.86	1.25	1.33	3	5
3	A	628	PX4	C11-C10	2.86	1.62	1.52	15	3
3	C	305	PX4	O5-C8	2.86	1.51	1.45	8	2
3	A	623	PX4	C25-C24	2.86	1.62	1.52	13	1
3	B	318	PX4	O5-C8	2.86	1.51	1.45	10	3
3	B	317	PX4	C10-C9	2.86	1.59	1.50	1	2
3	C	340	PX4	C10-C9	2.86	1.59	1.50	5	3
3	A	610	PX4	C10-C9	2.86	1.59	1.50	4	2
3	B	306	PX4	O7-C23	2.86	1.26	1.34	7	2
3	B	317	PX4	C24-C23	2.86	1.59	1.50	14	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	338	PX4	C5-N1	2.85	1.41	1.50	15	2
3	B	373	PX4	C6-C7	2.85	1.59	1.50	11	4
3	B	337	PX4	C8-C7	2.85	1.59	1.50	13	10
3	B	352	PX4	C8-C7	2.85	1.59	1.50	7	6
3	C	348	PX4	O7-C23	2.85	1.42	1.34	2	2
3	B	364	PX4	O5-C9	2.85	1.41	1.33	8	2
3	C	328	PX4	O7-C7	2.85	1.39	1.46	8	4
3	B	335	PX4	O7-C7	2.85	1.39	1.46	5	1
3	C	321	PX4	C26-C25	2.85	1.65	1.51	9	1
3	A	610	PX4	O5-C9	2.84	1.41	1.33	2	4
3	A	602	PX4	P1-O1	2.84	1.42	1.55	12	3
3	A	638	PX4	O5-C9	2.84	1.41	1.33	7	1
3	A	642	PX4	O5-C8	2.84	1.38	1.45	14	4
3	B	312	PX4	C6-C7	2.84	1.59	1.50	9	4
3	B	327	PX4	C11-C10	2.84	1.62	1.52	1	2
3	C	339	PX4	C3-N1	2.84	1.41	1.50	5	2
3	B	328	PX4	P1-O1	2.84	1.42	1.55	11	3
3	C	308	PX4	C8-C7	2.84	1.59	1.50	1	9
3	A	627	PX4	O5-C8	2.84	1.38	1.45	3	3
3	A	633	PX4	O5-C9	2.84	1.41	1.33	14	2
3	C	303	PX4	C10-C9	2.84	1.58	1.50	10	2
3	C	309	PX4	O5-C9	2.84	1.41	1.33	15	1
3	C	325	PX4	O7-C7	2.84	1.39	1.46	4	1
3	B	388	PX4	C10-C9	2.84	1.58	1.50	6	5
3	B	393	PX4	C15-C14	2.84	1.65	1.51	10	1
3	C	357	PX4	O7-C7	2.84	1.39	1.46	10	4
3	A	625	PX4	C25-C24	2.83	1.62	1.52	7	1
3	B	333	PX4	O7-C23	2.83	1.26	1.34	4	3
3	C	312	PX4	C24-C23	2.83	1.58	1.50	14	4
3	A	618	PX4	O7-C23	2.83	1.42	1.34	4	2
3	C	310	PX4	P1-O1	2.83	1.42	1.55	13	3
3	A	627	PX4	C25-C24	2.83	1.62	1.52	7	1
3	C	312	PX4	P1-O2	2.83	1.41	1.50	14	2
3	C	315	PX4	C10-C9	2.83	1.58	1.50	2	2
3	C	342	PX4	C11-C10	2.83	1.62	1.52	7	2
3	A	641	PX4	C5-N1	2.83	1.58	1.50	4	2
3	B	341	PX4	C10-C9	2.83	1.58	1.50	2	4
3	A	621	PX4	C3-N1	2.82	1.58	1.50	1	3
3	A	629	PX4	C2-C1	2.82	1.59	1.51	9	6
3	A	645	PX4	C10-C9	2.82	1.58	1.50	15	4
3	B	302	PX4	C10-C9	2.82	1.58	1.50	15	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	354	PX4	C25-C24	2.82	1.62	1.52	1	1
3	B	357	PX4	C24-C23	2.82	1.58	1.50	12	1
3	C	304	PX4	C2-C1	2.82	1.59	1.51	6	5
3	C	319	PX4	C10-C9	2.82	1.58	1.50	5	2
3	A	634	PX4	C6-C7	2.82	1.59	1.50	1	5
3	A	648	PX4	P1-O4	2.82	1.48	1.59	12	1
3	B	334	PX4	P1-O2	2.82	1.41	1.50	5	2
3	C	315	PX4	O7-C23	2.82	1.26	1.34	4	3
3	A	610	PX4	C15-C14	2.82	1.65	1.51	6	1
3	B	326	PX4	C25-C24	2.82	1.62	1.52	6	3
3	B	332	PX4	C4-N1	2.82	1.41	1.50	9	1
3	B	371	PX4	C8-C7	2.82	1.59	1.50	2	5
3	B	379	PX4	C5-N1	2.82	1.58	1.50	10	1
3	C	313	PX4	O7-C7	2.82	1.40	1.46	3	1
3	C	354	PX4	C3-N1	2.82	1.41	1.50	4	2
3	C	356	PX4	C10-C9	2.82	1.58	1.50	8	1
3	B	311	PX4	O5-C9	2.81	1.25	1.33	15	2
3	B	356	PX4	O5-C8	2.81	1.51	1.45	12	2
3	B	360	PX4	C2-N1	2.81	1.60	1.51	15	2
3	B	394	PX4	C2-C1	2.81	1.59	1.51	2	6
3	C	305	PX4	O7-C7	2.81	1.40	1.46	8	3
3	C	321	PX4	C6-C7	2.81	1.59	1.50	10	3
3	B	301	PX4	C10-C9	2.81	1.58	1.50	12	5
3	B	359	PX4	P1-O1	2.81	1.42	1.55	8	3
3	C	327	PX4	C24-C23	2.81	1.58	1.50	1	3
3	A	634	PX4	C24-C23	2.81	1.58	1.50	10	1
3	C	346	PX4	C8-C7	2.81	1.59	1.50	11	3
3	B	328	PX4	C10-C9	2.81	1.58	1.50	4	5
3	A	618	PX4	C2-C1	2.81	1.59	1.51	6	2
3	C	344	PX4	C2-C1	2.81	1.59	1.51	10	2
3	C	358	PX4	C10-C9	2.81	1.58	1.50	12	2
3	A	647	PX4	O5-C9	2.81	1.41	1.33	14	2
3	B	321	PX4	C4-N1	2.81	1.41	1.50	1	2
3	B	379	PX4	C24-C23	2.81	1.58	1.50	8	4
3	B	381	PX4	O7-C23	2.81	1.26	1.34	10	3
3	B	382	PX4	O5-C9	2.81	1.41	1.33	13	4
3	B	389	PX4	C2-C1	2.81	1.59	1.51	4	5
3	C	348	PX4	C24-C23	2.81	1.58	1.50	10	1
3	C	363	PX4	C25-C24	2.81	1.62	1.52	11	4
3	B	383	PX4	C5-N1	2.81	1.41	1.50	2	1
3	B	375	PX4	C8-C7	2.81	1.59	1.50	9	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	C	359	PX4	O5-C9	2.80	1.25	1.33	15	3
3	A	608	PX4	C25-C24	2.80	1.62	1.52	2	3
3	B	301	PX4	C4-N1	2.80	1.58	1.50	5	3
3	B	301	PX4	O5-C9	2.80	1.25	1.33	14	1
3	B	359	PX4	C4-N1	2.80	1.41	1.50	14	3
3	B	364	PX4	O7-C23	2.80	1.26	1.34	9	1
3	C	337	PX4	P1-O2	2.80	1.41	1.50	1	2
3	A	654	PX4	C8-C7	2.80	1.59	1.50	13	10
3	A	635	PX4	C25-C24	2.80	1.62	1.52	1	1
3	A	654	PX4	C6-C7	2.80	1.59	1.50	10	8
3	B	391	PX4	C24-C23	2.80	1.58	1.50	1	2
3	C	338	PX4	C4-N1	2.80	1.58	1.50	13	1
3	A	627	PX4	O7-C23	2.80	1.26	1.34	4	2
3	B	305	PX4	P1-O1	2.80	1.42	1.55	4	5
3	B	322	PX4	O5-C8	2.80	1.51	1.45	8	4
3	B	364	PX4	C11-C10	2.80	1.62	1.52	1	3
3	A	616	PX4	O7-C7	2.80	1.53	1.46	11	2
3	B	345	PX4	C2-N1	2.80	1.60	1.51	15	1
3	C	330	PX4	C24-C23	2.79	1.58	1.50	14	3
3	C	355	PX4	C24-C23	2.80	1.58	1.50	9	4
3	A	605	PX4	O5-C9	2.79	1.25	1.33	5	3
3	A	614	PX4	C3-N1	2.79	1.58	1.50	10	2
3	A	645	PX4	P1-O4	2.79	1.70	1.59	6	1
3	A	604	PX4	C34-C33	2.79	1.65	1.51	8	1
3	B	337	PX4	O7-C23	2.79	1.26	1.34	13	2
3	B	372	PX4	C10-C9	2.79	1.58	1.50	13	2
3	C	324	PX4	C8-C7	2.79	1.59	1.50	15	5
3	B	371	PX4	O7-C23	2.79	1.26	1.34	2	2
3	C	339	PX4	C24-C23	2.79	1.58	1.50	12	3
3	A	620	PX4	C6-C7	2.79	1.59	1.50	1	5
3	A	627	PX4	C3-N1	2.79	1.58	1.50	9	2
3	B	393	PX4	C5-N1	2.79	1.41	1.50	2	3
3	C	346	PX4	C4-N1	2.79	1.58	1.50	8	2
3	B	371	PX4	C10-C9	2.79	1.58	1.50	10	2
3	C	320	PX4	O7-C7	2.79	1.53	1.46	10	3
3	A	606	PX4	C15-C14	2.79	1.65	1.51	2	1
3	B	373	PX4	C5-N1	2.79	1.58	1.50	9	2
3	B	387	PX4	C11-C10	2.79	1.62	1.52	10	2
3	B	385	PX4	C10-C9	2.79	1.58	1.50	3	4
3	B	400	PX4	C11-C10	2.79	1.62	1.52	11	2
3	C	361	PX4	P1-O1	2.79	1.42	1.55	2	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	C	308	PX4	C25-C24	2.79	1.62	1.52	3	2
3	C	313	PX4	C20-C19	2.79	1.65	1.51	7	1
3	C	364	PX4	C10-C9	2.79	1.58	1.50	3	1
3	A	641	PX4	C6-C7	2.79	1.59	1.50	10	4
3	A	646	PX4	C6-C7	2.79	1.59	1.50	8	3
3	A	652	PX4	C25-C24	2.78	1.62	1.52	3	2
3	B	302	PX4	C24-C23	2.78	1.58	1.50	10	2
3	B	324	PX4	O5-C8	2.78	1.38	1.45	3	2
3	C	312	PX4	O7-C23	2.79	1.26	1.34	13	2
3	B	343	PX4	C26-C25	2.78	1.65	1.51	10	1
3	B	386	PX4	C3-N1	2.78	1.58	1.50	5	1
3	C	311	PX4	C10-C9	2.78	1.58	1.50	12	1
3	C	322	PX4	P1-O1	2.78	1.42	1.55	5	4
3	B	334	PX4	C6-C7	2.78	1.59	1.50	6	5
3	B	360	PX4	O7-C23	2.78	1.26	1.34	12	2
3	A	606	PX4	C4-N1	2.78	1.41	1.50	11	2
3	A	608	PX4	C4-N1	2.78	1.58	1.50	6	2
3	B	352	PX4	C2-N1	2.78	1.59	1.51	5	1
3	B	379	PX4	C10-C9	2.78	1.58	1.50	14	1
3	C	330	PX4	O5-C9	2.78	1.25	1.33	2	2
3	A	632	PX4	C24-C23	2.78	1.58	1.50	6	5
3	A	628	PX4	C10-C9	2.77	1.58	1.50	6	3
3	A	637	PX4	C25-C24	2.77	1.62	1.52	11	3
3	A	638	PX4	P1-O1	2.77	1.42	1.55	10	3
3	B	397	PX4	C3-N1	2.77	1.58	1.50	8	3
3	B	398	PX4	P1-O4	2.77	1.48	1.59	13	1
3	A	622	PX4	C2-C1	2.77	1.59	1.51	15	5
3	A	634	PX4	O3-C1	2.77	1.33	1.44	9	1
3	A	630	PX4	C34-C33	2.77	1.65	1.51	6	1
3	C	333	PX4	O5-C9	2.77	1.25	1.33	15	1
3	C	330	PX4	C4-N1	2.77	1.58	1.50	11	1
3	A	602	PX4	C3-N1	2.77	1.58	1.50	3	1
3	B	341	PX4	C2-N1	2.77	1.59	1.51	11	3
3	C	327	PX4	C10-C9	2.77	1.58	1.50	13	3
3	A	641	PX4	C10-C9	2.77	1.58	1.50	7	4
3	C	332	PX4	C6-C7	2.77	1.59	1.50	2	8
3	B	306	PX4	C11-C10	2.77	1.62	1.52	14	1
3	B	350	PX4	C24-C23	2.77	1.58	1.50	7	3
3	C	355	PX4	C25-C24	2.77	1.62	1.52	8	3
3	A	641	PX4	C2-C1	2.76	1.59	1.51	6	4
3	B	338	PX4	C2-C1	2.76	1.59	1.51	12	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	C	348	PX4	C34-C33	2.77	1.65	1.51	11	1
3	C	357	PX4	C24-C23	2.77	1.58	1.50	15	3
3	B	340	PX4	C25-C24	2.76	1.62	1.52	11	5
3	B	348	PX4	C28-C27	2.76	1.65	1.51	14	1
3	C	318	PX4	C16-C15	2.76	1.65	1.51	14	1
3	A	614	PX4	C25-C24	2.76	1.62	1.52	11	1
3	B	305	PX4	C2-N1	2.76	1.59	1.51	2	4
3	C	342	PX4	P1-O1	2.76	1.42	1.55	8	2
3	A	627	PX4	O3-C1	2.76	1.33	1.44	5	1
3	A	628	PX4	O5-C8	2.76	1.39	1.45	12	3
3	A	642	PX4	O5-C9	2.76	1.25	1.33	6	6
3	A	652	PX4	O5-C8	2.76	1.51	1.45	12	4
3	C	306	PX4	C2-C1	2.76	1.59	1.51	3	4
3	B	330	PX4	O7-C7	2.76	1.40	1.46	15	3
3	B	359	PX4	P1-O3	2.76	1.70	1.59	5	2
3	B	355	PX4	O7-C7	2.76	1.40	1.46	7	3
3	B	395	PX4	O7-C7	2.76	1.40	1.46	9	2
3	C	349	PX4	O5-C9	2.76	1.25	1.33	2	3
3	C	316	PX4	C27-C26	2.76	1.65	1.51	11	1
3	A	630	PX4	C24-C23	2.75	1.58	1.50	1	3
3	B	352	PX4	P1-O4	2.76	1.48	1.59	8	1
3	C	322	PX4	C24-C23	2.76	1.58	1.50	7	5
3	C	339	PX4	C2-N1	2.76	1.59	1.51	3	3
3	B	369	PX4	P1-O4	2.75	1.48	1.59	1	1
3	B	308	PX4	O5-C8	2.75	1.51	1.45	11	2
3	B	367	PX4	C4-N1	2.75	1.58	1.50	12	3
3	B	370	PX4	C2-N1	2.75	1.59	1.51	5	3
3	C	301	PX4	C4-N1	2.75	1.58	1.50	9	2
3	A	613	PX4	C2-N1	2.75	1.59	1.51	11	4
3	A	616	PX4	C3-N1	2.75	1.58	1.50	13	1
3	A	638	PX4	C25-C24	2.75	1.62	1.52	12	2
3	B	338	PX4	O7-C23	2.75	1.26	1.34	3	1
3	B	364	PX4	C2-N1	2.75	1.59	1.51	9	1
3	C	304	PX4	C4-N1	2.75	1.42	1.50	3	4
3	B	393	PX4	O5-C8	2.75	1.39	1.45	14	3
3	A	654	PX4	O7-C7	2.75	1.40	1.46	8	4
3	B	306	PX4	O5-C9	2.75	1.41	1.33	7	3
3	C	332	PX4	C25-C24	2.75	1.62	1.52	7	3
3	C	363	PX4	P1-O1	2.75	1.42	1.55	15	2
3	A	628	PX4	P1-O1	2.75	1.42	1.55	14	4
3	A	643	PX4	C25-C24	2.75	1.62	1.52	7	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	316	PX4	O5-C9	2.75	1.25	1.33	14	2
3	B	320	PX4	C10-C9	2.75	1.42	1.50	7	1
3	C	361	PX4	C3-N1	2.75	1.42	1.50	1	2
3	C	348	PX4	O5-C8	2.74	1.51	1.45	15	2
3	C	355	PX4	C2-C1	2.74	1.59	1.51	1	5
3	C	362	PX4	C24-C23	2.74	1.58	1.50	5	4
3	A	608	PX4	O7-C7	2.74	1.40	1.46	6	3
3	A	643	PX4	O7-C23	2.74	1.26	1.34	8	1
3	B	344	PX4	O5-C9	2.74	1.25	1.33	5	1
3	B	305	PX4	O7-C7	2.74	1.40	1.46	15	3
3	B	346	PX4	C3-N1	2.74	1.42	1.50	1	2
3	A	609	PX4	C24-C23	2.74	1.58	1.50	15	6
3	B	323	PX4	O5-C8	2.74	1.39	1.45	8	2
3	C	312	PX4	P1-O1	2.74	1.42	1.55	5	4
3	C	342	PX4	O7-C23	2.74	1.26	1.34	11	2
3	C	347	PX4	O7-C7	2.74	1.40	1.46	12	3
3	B	310	PX4	O5-C9	2.73	1.41	1.33	14	1
3	B	334	PX4	P1-O1	2.73	1.42	1.55	5	4
3	B	367	PX4	P1-O2	2.73	1.41	1.50	1	1
3	C	306	PX4	O7-C23	2.73	1.26	1.34	4	2
3	C	329	PX4	C24-C23	2.74	1.58	1.50	2	2
3	C	353	PX4	C11-C10	2.73	1.62	1.52	11	4
3	A	619	PX4	O5-C8	2.73	1.51	1.45	15	3
3	B	319	PX4	O5-C9	2.73	1.25	1.33	15	2
3	B	328	PX4	C11-C10	2.73	1.62	1.52	8	2
3	A	624	PX4	C5-N1	2.73	1.57	1.50	2	1
3	B	318	PX4	C25-C24	2.73	1.62	1.52	1	2
3	B	365	PX4	O7-C7	2.73	1.40	1.46	15	2
3	A	642	PX4	C11-C10	2.73	1.62	1.52	1	1
3	B	318	PX4	C4-N1	2.73	1.42	1.50	9	1
3	B	381	PX4	C2-C1	2.73	1.59	1.51	11	7
3	C	361	PX4	C25-C24	2.73	1.62	1.52	13	2
3	C	348	PX4	C2-C1	2.73	1.59	1.51	14	8
3	C	362	PX4	C2-C1	2.73	1.59	1.51	7	2
3	A	613	PX4	C25-C24	2.73	1.62	1.52	8	2
3	B	329	PX4	O7-C23	2.73	1.26	1.34	9	2
3	B	362	PX4	C24-C23	2.73	1.58	1.50	3	3
3	B	364	PX4	C3-N1	2.73	1.57	1.50	6	1
3	C	323	PX4	P1-O1	2.73	1.42	1.55	4	5
3	A	626	PX4	C24-C23	2.73	1.58	1.50	15	1
3	B	381	PX4	C24-C23	2.73	1.58	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	C11-C10	2.73	1.62	1.52	8	2
3	B	340	PX4	C34-C33	2.72	1.65	1.51	10	1
3	C	306	PX4	C3-N1	2.72	1.57	1.50	10	3
3	C	363	PX4	C15-C14	2.72	1.65	1.51	7	1
3	B	356	PX4	C11-C10	2.72	1.62	1.52	5	1
3	A	633	PX4	C10-C9	2.72	1.58	1.50	9	2
3	A	635	PX4	C11-C10	2.72	1.62	1.52	9	3
3	A	644	PX4	C2-N1	2.72	1.59	1.51	15	2
3	B	350	PX4	O5-C8	2.72	1.39	1.45	9	2
3	A	606	PX4	O5-C9	2.72	1.41	1.33	15	3
3	B	377	PX4	C34-C33	2.72	1.65	1.51	12	1
3	A	654	PX4	O5-C8	2.72	1.51	1.45	8	1
3	C	325	PX4	C6-C7	2.72	1.59	1.50	8	6
3	C	351	PX4	C10-C9	2.72	1.58	1.50	10	5
3	B	349	PX4	C8-C7	2.72	1.59	1.50	14	7
3	B	389	PX4	C33-C32	2.72	1.65	1.51	3	1
3	A	608	PX4	O5-C8	2.72	1.51	1.45	6	3
3	B	344	PX4	C10-C9	2.72	1.58	1.50	10	3
3	B	367	PX4	O5-C8	2.71	1.51	1.45	11	4
3	B	310	PX4	C3-N1	2.71	1.57	1.50	1	2
3	B	349	PX4	C2-C1	2.71	1.59	1.51	12	4
3	B	397	PX4	C4-N1	2.71	1.57	1.50	3	1
3	C	310	PX4	C4-N1	2.71	1.42	1.50	3	1
3	A	632	PX4	O5-C9	2.71	1.25	1.33	3	2
3	B	308	PX4	O7-C7	2.71	1.40	1.46	6	7
3	B	349	PX4	P1-O1	2.71	1.42	1.55	7	3
3	C	362	PX4	P1-O1	2.71	1.42	1.55	6	3
3	A	612	PX4	C24-C23	2.71	1.42	1.50	3	1
3	B	307	PX4	P1-O1	2.71	1.42	1.55	2	7
3	B	382	PX4	O7-C7	2.71	1.40	1.46	2	3
3	A	645	PX4	C3-N1	2.71	1.42	1.50	9	1
3	A	623	PX4	P1-O3	2.71	1.48	1.59	7	1
3	A	650	PX4	C10-C9	2.71	1.58	1.50	4	1
3	B	323	PX4	O7-C23	2.71	1.41	1.34	8	1
3	B	359	PX4	O7-C23	2.71	1.26	1.34	7	2
3	B	383	PX4	P1-O1	2.71	1.42	1.55	1	2
3	B	392	PX4	P1-O4	2.71	1.70	1.59	9	1
3	B	357	PX4	C25-C24	2.71	1.62	1.52	13	2
3	C	305	PX4	C2-N1	2.71	1.43	1.51	11	1
3	C	321	PX4	C8-C7	2.71	1.59	1.50	12	5
3	C	322	PX4	C8-C7	2.71	1.59	1.50	12	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	C	352	PX4	P1-O1	2.71	1.42	1.55	15	4
3	B	336	PX4	O7-C23	2.71	1.26	1.34	13	3
3	B	354	PX4	C2-C1	2.71	1.59	1.51	1	3
3	B	399	PX4	C10-C9	2.71	1.42	1.50	14	4
3	B	363	PX4	C4-N1	2.70	1.42	1.50	7	1
3	B	365	PX4	C10-C9	2.70	1.58	1.50	15	4
3	B	399	PX4	C2-C1	2.70	1.59	1.51	7	4
3	C	322	PX4	C4-N1	2.70	1.57	1.50	10	1
3	A	617	PX4	C25-C24	2.70	1.62	1.52	4	1
3	B	315	PX4	C2-C1	2.70	1.59	1.51	3	3
3	C	324	PX4	C24-C23	2.70	1.58	1.50	12	4
3	B	332	PX4	O5-C8	2.70	1.51	1.45	11	2
3	B	349	PX4	P1-O3	2.70	1.48	1.59	13	1
3	B	377	PX4	C2-N1	2.70	1.59	1.51	2	2
3	B	379	PX4	C28-C27	2.70	1.65	1.51	12	2
3	C	325	PX4	C11-C10	2.70	1.62	1.52	7	4
3	A	604	PX4	C3-N1	2.70	1.42	1.50	6	1
3	A	644	PX4	C24-C23	2.70	1.58	1.50	2	3
3	B	341	PX4	C3-N1	2.70	1.42	1.50	15	1
3	C	324	PX4	C2-C1	2.70	1.59	1.51	10	3
3	C	325	PX4	O5-C9	2.70	1.41	1.33	14	2
3	A	631	PX4	C4-N1	2.70	1.57	1.50	2	4
3	A	631	PX4	C6-C7	2.70	1.59	1.50	7	3
3	B	317	PX4	C8-C7	2.70	1.59	1.50	2	7
3	B	322	PX4	C10-C9	2.70	1.58	1.50	11	1
3	B	372	PX4	O7-C7	2.70	1.40	1.46	7	3
3	C	323	PX4	C3-N1	2.70	1.42	1.50	6	2
3	C	346	PX4	P1-O3	2.70	1.48	1.59	5	2
3	A	624	PX4	O5-C9	2.70	1.25	1.33	8	2
3	C	349	PX4	C2-N1	2.69	1.59	1.51	13	3
3	C	362	PX4	C25-C24	2.70	1.62	1.52	15	3
3	B	339	PX4	O7-C7	2.69	1.40	1.46	14	3
3	B	348	PX4	C24-C23	2.69	1.58	1.50	13	2
3	A	609	PX4	C18-C17	2.69	1.65	1.51	12	2
3	A	649	PX4	C5-N1	2.69	1.57	1.50	6	1
3	B	322	PX4	C25-C24	2.69	1.62	1.52	7	3
3	C	347	PX4	C3-N1	2.69	1.57	1.50	15	2
3	A	645	PX4	O5-C8	2.69	1.39	1.45	8	1
3	A	651	PX4	O7-C23	2.69	1.41	1.34	7	2
3	B	324	PX4	P1-O3	2.69	1.48	1.59	5	1
3	B	384	PX4	C4-N1	2.69	1.57	1.50	13	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	C	327	PX4	C8-C7	2.69	1.59	1.50	1	4
3	A	622	PX4	C3-N1	2.69	1.57	1.50	14	2
3	B	369	PX4	C24-C23	2.69	1.58	1.50	8	1
3	B	342	PX4	C3-N1	2.69	1.57	1.50	10	2
3	B	349	PX4	C3-N1	2.69	1.42	1.50	7	1
3	C	313	PX4	O5-C8	2.69	1.39	1.45	5	3
3	A	610	PX4	C4-N1	2.68	1.57	1.50	5	1
3	B	372	PX4	C2-C1	2.68	1.59	1.51	10	6
3	B	360	PX4	C5-N1	2.68	1.57	1.50	1	1
3	B	366	PX4	C25-C24	2.68	1.62	1.52	13	2
3	C	359	PX4	C3-N1	2.68	1.57	1.50	8	3
3	A	654	PX4	P1-O1	2.68	1.42	1.55	13	3
3	C	325	PX4	O5-C8	2.68	1.51	1.45	12	1
3	B	349	PX4	C34-C33	2.68	1.65	1.51	6	2
3	C	321	PX4	P1-O1	2.68	1.42	1.55	7	4
3	C	355	PX4	C31-C30	2.68	1.65	1.51	10	1
3	A	604	PX4	C11-C10	2.68	1.62	1.52	13	3
3	A	638	PX4	O7-C7	2.68	1.40	1.46	14	2
3	B	322	PX4	O5-C9	2.68	1.25	1.33	7	3
3	A	619	PX4	C2-C1	2.68	1.59	1.51	9	2
3	A	651	PX4	O7-C7	2.68	1.40	1.46	5	3
3	B	368	PX4	O7-C23	2.68	1.26	1.34	8	3
3	C	314	PX4	C4-N1	2.68	1.42	1.50	3	1
3	B	361	PX4	C25-C24	2.68	1.62	1.52	4	1
3	C	315	PX4	C25-C24	2.68	1.62	1.52	12	3
3	B	339	PX4	C3-N1	2.67	1.57	1.50	6	1
3	C	343	PX4	C2-N1	2.67	1.59	1.51	1	2
3	C	354	PX4	C11-C10	2.67	1.62	1.52	1	1
3	B	372	PX4	P1-O1	2.67	1.43	1.55	12	1
3	C	307	PX4	P1-O1	2.67	1.43	1.55	1	1
3	C	335	PX4	C3-N1	2.67	1.57	1.50	4	2
3	C	345	PX4	O7-C23	2.67	1.26	1.34	14	3
3	A	601	PX4	P1-O2	2.67	1.41	1.50	15	2
3	A	606	PX4	C24-C23	2.67	1.58	1.50	13	1
3	A	647	PX4	O7-C7	2.67	1.40	1.46	11	3
3	A	650	PX4	O5-C8	2.67	1.39	1.45	12	2
3	B	303	PX4	C8-C7	2.67	1.59	1.50	8	4
3	A	625	PX4	P1-O2	2.67	1.41	1.50	7	2
3	B	334	PX4	C24-C23	2.67	1.58	1.50	11	1
3	B	339	PX4	C25-C24	2.67	1.62	1.52	3	1
3	B	378	PX4	C11-C10	2.67	1.62	1.52	5	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	C	317	PX4	O7-C7	2.67	1.40	1.46	15	2
3	A	603	PX4	P1-O2	2.67	1.41	1.50	11	2
3	B	302	PX4	P1-O4	2.67	1.48	1.59	3	2
3	B	312	PX4	C24-C23	2.67	1.58	1.50	8	4
3	C	311	PX4	C6-C7	2.67	1.59	1.50	11	4
3	C	330	PX4	C2-N1	2.67	1.43	1.51	5	3
3	C	360	PX4	C3-N1	2.67	1.42	1.50	8	1
3	A	618	PX4	C11-C10	2.66	1.62	1.52	8	1
3	B	320	PX4	C4-N1	2.66	1.57	1.50	8	2
3	B	320	PX4	C11-C10	2.66	1.61	1.52	5	1
3	B	339	PX4	O5-C9	2.66	1.25	1.33	9	1
3	B	392	PX4	C25-C24	2.67	1.62	1.52	9	1
3	B	355	PX4	C11-C10	2.66	1.61	1.52	6	2
3	B	367	PX4	C2-N1	2.66	1.59	1.51	3	2
3	C	310	PX4	C3-N1	2.66	1.57	1.50	5	2
3	C	339	PX4	O7-C7	2.66	1.40	1.46	8	5
3	A	633	PX4	O5-C8	2.66	1.39	1.45	10	1
3	A	609	PX4	C11-C10	2.66	1.61	1.52	13	3
3	A	644	PX4	C8-C7	2.66	1.59	1.50	3	2
3	A	647	PX4	C2-N1	2.66	1.59	1.51	10	3
3	A	647	PX4	C6-C7	2.66	1.59	1.50	12	4
3	B	317	PX4	O5-C8	2.66	1.39	1.45	7	2
3	B	377	PX4	C15-C14	2.66	1.65	1.51	12	1
3	C	318	PX4	P1-O1	2.66	1.43	1.55	1	3
3	B	344	PX4	P1-O1	2.66	1.43	1.55	5	5
3	A	633	PX4	C11-C10	2.66	1.61	1.52	3	3
3	C	331	PX4	C5-N1	2.66	1.57	1.50	12	1
3	C	358	PX4	O5-C8	2.66	1.51	1.45	8	1
3	C	359	PX4	P1-O4	2.66	1.49	1.59	7	1
3	B	367	PX4	C3-N1	2.66	1.42	1.50	12	2
3	C	307	PX4	C25-C24	2.66	1.61	1.52	11	1
3	A	604	PX4	C24-C23	2.66	1.58	1.50	8	3
3	B	390	PX4	O7-C7	2.66	1.40	1.46	4	2
3	B	392	PX4	O5-C9	2.66	1.25	1.33	5	1
3	C	321	PX4	C4-N1	2.66	1.57	1.50	6	2
3	A	639	PX4	P1-O1	2.66	1.43	1.55	6	7
3	B	309	PX4	C11-C10	2.66	1.61	1.52	14	2
3	B	337	PX4	O5-C9	2.66	1.41	1.33	8	2
3	C	301	PX4	C24-C23	2.66	1.58	1.50	12	3
3	C	332	PX4	O4-C6	2.66	1.34	1.44	7	1
3	C	354	PX4	C20-C19	2.65	1.65	1.51	8	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	C	361	PX4	C4-N1	2.65	1.42	1.50	13	2
3	A	630	PX4	O7-C23	2.65	1.26	1.34	4	3
3	B	379	PX4	C25-C24	2.65	1.61	1.52	7	2
3	C	304	PX4	C10-C9	2.65	1.58	1.50	6	4
3	C	359	PX4	C4-N1	2.65	1.57	1.50	14	1
3	B	353	PX4	C31-C30	2.65	1.65	1.51	12	1
3	C	332	PX4	C8-C7	2.65	1.59	1.50	15	5
3	B	336	PX4	O5-C9	2.65	1.41	1.33	13	1
3	B	348	PX4	C6-C7	2.65	1.59	1.50	11	6
3	C	342	PX4	C25-C24	2.65	1.61	1.52	7	3
3	A	640	PX4	C25-C24	2.65	1.61	1.52	5	3
3	B	334	PX4	O7-C7	2.65	1.52	1.46	1	1
3	B	388	PX4	C3-N1	2.65	1.42	1.50	1	2
3	A	632	PX4	O7-C7	2.65	1.40	1.46	4	4
3	B	347	PX4	C25-C24	2.65	1.61	1.52	1	2
3	B	317	PX4	P1-O1	2.65	1.43	1.55	15	5
3	C	351	PX4	O7-C23	2.65	1.26	1.34	10	1
3	C	353	PX4	C8-C7	2.65	1.59	1.50	11	4
3	A	613	PX4	C24-C23	2.65	1.58	1.50	1	4
3	B	329	PX4	C5-N1	2.65	1.42	1.50	7	1
3	B	321	PX4	C25-C24	2.64	1.61	1.52	1	2
3	B	400	PX4	C25-C24	2.64	1.61	1.52	15	2
3	C	338	PX4	C11-C10	2.64	1.61	1.52	2	3
3	A	615	PX4	O7-C7	2.64	1.40	1.46	15	2
3	C	309	PX4	O5-C8	2.64	1.51	1.45	3	2
3	C	339	PX4	O5-C8	2.64	1.51	1.45	15	3
3	C	360	PX4	O5-C8	2.64	1.51	1.45	14	2
3	A	632	PX4	C4-N1	2.64	1.57	1.50	7	2
3	B	308	PX4	C24-C23	2.64	1.43	1.50	7	6
3	B	397	PX4	O5-C9	2.64	1.41	1.33	14	3
3	C	302	PX4	O3-C1	2.64	1.34	1.44	4	1
3	C	334	PX4	C4-N1	2.64	1.42	1.50	9	2
3	A	635	PX4	C33-C32	2.64	1.64	1.51	11	1
3	B	310	PX4	C2-N1	2.64	1.59	1.51	10	2
3	B	338	PX4	C25-C24	2.64	1.61	1.52	1	1
3	B	390	PX4	O5-C8	2.64	1.51	1.45	15	1
3	C	347	PX4	C24-C23	2.64	1.58	1.50	9	2
3	A	624	PX4	C8-C7	2.63	1.59	1.50	12	5
3	B	329	PX4	O5-C8	2.63	1.51	1.45	2	1
3	B	371	PX4	C3-N1	2.63	1.57	1.50	5	1
3	B	400	PX4	P1-O1	2.63	1.43	1.55	3	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	400	PX4	C4-N1	2.63	1.42	1.50	12	1
3	C	324	PX4	O7-C23	2.63	1.41	1.34	4	1
3	C	360	PX4	P1-O1	2.63	1.43	1.55	4	2
3	B	311	PX4	O5-C8	2.63	1.51	1.45	5	4
3	B	315	PX4	C4-N1	2.63	1.57	1.50	12	2
3	B	332	PX4	C11-C10	2.63	1.61	1.52	1	4
3	B	336	PX4	C10-C9	2.63	1.58	1.50	2	1
3	B	388	PX4	O7-C7	2.63	1.40	1.46	15	2
3	A	653	PX4	P1-O1	2.63	1.43	1.55	6	2
3	B	301	PX4	P1-O1	2.63	1.43	1.55	12	4
3	B	384	PX4	P1-O3	2.63	1.49	1.59	12	2
3	B	334	PX4	C25-C24	2.63	1.61	1.52	7	2
3	B	363	PX4	C5-N1	2.63	1.42	1.50	4	1
3	B	391	PX4	O7-C7	2.63	1.40	1.46	1	2
3	C	351	PX4	C2-C1	2.63	1.59	1.51	2	6
3	C	359	PX4	C28-C27	2.63	1.64	1.51	5	1
3	C	361	PX4	C24-C23	2.63	1.58	1.50	6	3
3	B	389	PX4	P1-O1	2.63	1.43	1.55	2	4
3	A	620	PX4	C4-N1	2.63	1.57	1.50	3	1
3	B	314	PX4	C25-C24	2.63	1.61	1.52	9	2
3	C	355	PX4	O5-C8	2.62	1.39	1.45	14	4
3	A	617	PX4	C4-N1	2.62	1.57	1.50	7	3
3	A	617	PX4	C15-C14	2.62	1.64	1.51	9	1
3	A	626	PX4	C10-C9	2.62	1.58	1.50	14	2
3	B	360	PX4	C25-C24	2.62	1.61	1.52	13	2
3	B	375	PX4	C25-C24	2.62	1.61	1.52	3	4
3	C	308	PX4	C5-N1	2.62	1.57	1.50	14	2
3	B	349	PX4	C4-N1	2.62	1.42	1.50	9	3
3	A	604	PX4	O7-C7	2.62	1.40	1.46	3	3
3	B	322	PX4	O7-C7	2.62	1.40	1.46	8	3
3	B	326	PX4	C10-C9	2.62	1.58	1.50	2	2
3	B	358	PX4	O7-C23	2.62	1.26	1.34	3	1
3	C	356	PX4	O5-C8	2.62	1.51	1.45	11	2
3	A	641	PX4	P1-O2	2.62	1.41	1.50	1	1
3	A	652	PX4	O5-C9	2.62	1.25	1.33	10	1
3	A	638	PX4	C2-C1	2.62	1.59	1.51	12	3
3	B	327	PX4	C24-C23	2.61	1.58	1.50	8	1
3	B	353	PX4	C24-C23	2.61	1.58	1.50	11	3
3	A	620	PX4	C10-C9	2.61	1.58	1.50	7	2
3	B	368	PX4	P1-O4	2.61	1.49	1.59	10	1
3	B	391	PX4	C8-C7	2.61	1.59	1.50	15	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	A	651	PX4	C6-C7	2.61	1.59	1.50	2	5
3	B	377	PX4	C11-C10	2.61	1.61	1.52	13	2
3	C	318	PX4	C20-C19	2.61	1.64	1.51	15	1
3	A	612	PX4	O5-C8	2.61	1.51	1.45	15	3
3	A	639	PX4	C28-C27	2.61	1.64	1.51	3	1
3	C	303	PX4	P1-O1	2.61	1.43	1.55	15	4
3	C	313	PX4	P1-O1	2.61	1.43	1.55	11	3
3	B	354	PX4	C4-N1	2.61	1.57	1.50	5	2
3	B	398	PX4	O5-C8	2.61	1.51	1.45	9	4
3	C	360	PX4	C10-C9	2.61	1.58	1.50	13	5
3	A	606	PX4	C2-N1	2.61	1.59	1.51	6	2
3	B	354	PX4	C5-N1	2.61	1.42	1.50	10	2
3	A	608	PX4	C2-C1	2.60	1.59	1.51	12	4
3	B	339	PX4	C15-C14	2.60	1.64	1.51	14	1
3	B	344	PX4	C6-C7	2.60	1.59	1.50	5	6
3	B	367	PX4	C10-C9	2.60	1.58	1.50	2	2
3	A	640	PX4	C24-C23	2.60	1.58	1.50	4	1
3	B	373	PX4	P1-O1	2.60	1.43	1.55	2	4
3	B	303	PX4	C10-C9	2.60	1.58	1.50	15	3
3	B	350	PX4	C4-N1	2.60	1.42	1.50	6	1
3	B	376	PX4	C5-N1	2.60	1.42	1.50	1	1
3	C	308	PX4	C28-C27	2.60	1.64	1.51	11	1
3	C	314	PX4	C5-N1	2.60	1.57	1.50	4	2
3	C	325	PX4	C4-N1	2.60	1.42	1.50	6	1
3	C	355	PX4	C5-N1	2.60	1.57	1.50	7	1
3	C	321	PX4	C24-C23	2.60	1.58	1.50	15	5
3	C	338	PX4	O7-C23	2.60	1.41	1.34	9	2
3	C	348	PX4	C3-N1	2.60	1.42	1.50	13	1
3	C	364	PX4	O7-C23	2.60	1.26	1.34	1	1
3	A	638	PX4	C3-N1	2.60	1.57	1.50	4	1
3	B	303	PX4	O7-C7	2.60	1.40	1.46	15	3
3	B	367	PX4	C5-N1	2.60	1.57	1.50	6	1
3	A	638	PX4	C2-N1	2.60	1.59	1.51	5	1
3	B	313	PX4	C5-N1	2.60	1.57	1.50	11	2
3	B	342	PX4	O7-C23	2.59	1.26	1.34	10	2
3	B	345	PX4	O5-C9	2.60	1.25	1.33	12	3
3	B	313	PX4	C24-C23	2.59	1.58	1.50	5	1
3	B	347	PX4	P1-O1	2.59	1.43	1.55	5	2
3	B	353	PX4	C19-C18	2.59	1.64	1.51	9	1
3	C	302	PX4	C3-N1	2.59	1.42	1.50	8	2
3	A	603	PX4	O5-C8	2.59	1.39	1.45	1	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	331	PX4	C3-N1	2.59	1.57	1.50	8	1
3	B	378	PX4	C24-C23	2.59	1.58	1.50	15	4
3	C	355	PX4	O7-C23	2.59	1.26	1.34	14	1
3	C	357	PX4	C10-C9	2.59	1.58	1.50	10	2
3	B	305	PX4	P1-O2	2.59	1.41	1.50	12	1
3	A	631	PX4	C2-N1	2.59	1.59	1.51	9	2
3	B	311	PX4	C11-C10	2.59	1.61	1.52	6	2
3	C	337	PX4	O7-C7	2.59	1.40	1.46	11	3
3	C	354	PX4	C2-N1	2.59	1.59	1.51	9	1
3	C	356	PX4	O7-C7	2.59	1.40	1.46	2	2
3	B	314	PX4	O5-C8	2.59	1.39	1.45	11	5
3	B	315	PX4	C5-N1	2.59	1.42	1.50	7	1
3	B	326	PX4	C32-C31	2.59	1.64	1.51	3	1
3	A	606	PX4	P1-O1	2.59	1.43	1.55	9	2
3	B	392	PX4	C2-C1	2.59	1.59	1.51	13	5
3	C	348	PX4	C10-C9	2.59	1.58	1.50	4	2
3	A	624	PX4	C10-C9	2.59	1.58	1.50	9	1
3	B	398	PX4	C11-C10	2.59	1.61	1.52	13	2
3	C	346	PX4	C20-C19	2.59	1.64	1.51	8	1
3	A	632	PX4	C30-C29	2.58	1.64	1.51	12	1
3	A	603	PX4	C3-N1	2.58	1.57	1.50	7	1
3	A	610	PX4	P1-O1	2.58	1.43	1.55	8	2
3	A	619	PX4	C5-N1	2.58	1.42	1.50	8	1
3	B	304	PX4	C14-C13	2.58	1.64	1.51	4	1
3	B	322	PX4	C11-C10	2.58	1.61	1.52	1	1
3	B	330	PX4	P1-O1	2.58	1.43	1.55	6	2
3	B	395	PX4	C24-C23	2.58	1.58	1.50	6	4
3	C	313	PX4	C2-C1	2.58	1.59	1.51	8	5
3	C	346	PX4	P1-O1	2.58	1.43	1.55	3	4
3	C	346	PX4	C3-N1	2.58	1.42	1.50	6	1
3	A	626	PX4	C25-C24	2.58	1.61	1.52	10	2
3	B	316	PX4	C2-C1	2.58	1.59	1.51	2	5
3	C	339	PX4	C10-C9	2.58	1.58	1.50	10	2
3	A	612	PX4	P1-O1	2.58	1.43	1.55	2	4
3	A	634	PX4	C20-C19	2.58	1.64	1.51	3	1
3	B	301	PX4	O7-C23	2.58	1.27	1.34	5	3
3	B	324	PX4	C11-C10	2.58	1.61	1.52	13	1
3	C	364	PX4	C3-N1	2.58	1.42	1.50	3	2
3	A	642	PX4	C4-N1	2.58	1.57	1.50	4	2
3	A	637	PX4	P1-O3	2.57	1.49	1.59	3	1
3	A	650	PX4	C15-C14	2.57	1.64	1.51	3	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	327	PX4	C3-N1	2.57	1.57	1.50	9	3
3	B	330	PX4	C4-N1	2.57	1.57	1.50	12	2
3	A	640	PX4	C11-C10	2.57	1.61	1.52	6	1
3	B	356	PX4	C25-C24	2.57	1.61	1.52	9	1
3	C	346	PX4	C2-N1	2.57	1.59	1.51	12	1
3	B	382	PX4	C10-C9	2.57	1.58	1.50	5	2
3	C	317	PX4	P1-O1	2.57	1.43	1.55	3	2
3	A	627	PX4	P1-O1	2.57	1.43	1.55	8	5
3	C	321	PX4	C11-C10	2.57	1.61	1.52	9	3
3	C	327	PX4	O5-C9	2.57	1.40	1.33	4	2
3	C	352	PX4	C3-N1	2.57	1.57	1.50	11	1
3	C	359	PX4	O5-C8	2.57	1.39	1.45	4	1
3	B	372	PX4	P1-O3	2.57	1.49	1.59	5	1
3	B	340	PX4	O7-C23	2.57	1.27	1.34	2	1
3	C	303	PX4	C5-N1	2.57	1.57	1.50	1	1
3	B	346	PX4	C11-C10	2.57	1.61	1.52	15	1
3	B	371	PX4	C4-N1	2.56	1.42	1.50	14	1
3	C	305	PX4	C13-C12	2.57	1.64	1.51	2	2
3	A	623	PX4	C10-C9	2.56	1.58	1.50	14	2
3	A	650	PX4	C4-N1	2.56	1.42	1.50	2	2
3	B	386	PX4	P1-O1	2.56	1.43	1.55	15	1
3	B	396	PX4	O5-C8	2.56	1.39	1.45	6	3
3	C	357	PX4	C34-C33	2.56	1.64	1.51	5	1
3	A	645	PX4	C2-N1	2.56	1.59	1.51	4	1
3	B	308	PX4	C11-C10	2.56	1.61	1.52	3	5
3	C	319	PX4	O7-C7	2.56	1.40	1.46	10	1
3	A	611	PX4	C5-N1	2.56	1.57	1.50	7	2
3	C	310	PX4	C28-C27	2.56	1.64	1.51	3	1
3	C	337	PX4	C4-N1	2.56	1.57	1.50	15	1
3	A	635	PX4	C10-C9	2.56	1.58	1.50	4	4
3	A	647	PX4	O3-C1	2.56	1.34	1.44	1	1
3	A	644	PX4	C25-C24	2.56	1.61	1.52	14	1
3	C	316	PX4	C25-C24	2.56	1.61	1.52	6	3
3	A	642	PX4	O3-C1	2.56	1.34	1.44	4	1
3	B	301	PX4	C2-C1	2.56	1.59	1.51	8	4
3	B	317	PX4	C29-C28	2.56	1.64	1.51	8	1
3	B	348	PX4	P1-O1	2.56	1.43	1.55	4	3
3	B	373	PX4	C24-C23	2.56	1.58	1.50	12	1
3	B	374	PX4	O5-C9	2.56	1.25	1.33	13	2
3	B	387	PX4	C3-N1	2.56	1.42	1.50	13	1
3	B	344	PX4	O5-C8	2.55	1.50	1.45	6	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	381	PX4	O7-C7	2.55	1.40	1.46	14	3
3	C	318	PX4	O7-C23	2.56	1.27	1.34	11	2
3	C	330	PX4	O7-C7	2.56	1.40	1.46	15	4
3	B	321	PX4	O7-C7	2.55	1.40	1.46	4	1
3	B	344	PX4	P1-O4	2.55	1.49	1.59	12	1
3	B	385	PX4	C4-N1	2.55	1.57	1.50	4	1
3	C	364	PX4	C5-N1	2.55	1.57	1.50	13	2
3	A	628	PX4	C5-N1	2.55	1.57	1.50	15	3
3	B	375	PX4	O5-C9	2.55	1.40	1.33	6	2
3	B	377	PX4	C10-C9	2.55	1.58	1.50	10	2
3	B	380	PX4	C11-C10	2.55	1.61	1.52	2	3
3	C	315	PX4	C2-C1	2.55	1.59	1.51	3	2
3	A	624	PX4	O5-C8	2.55	1.50	1.45	9	1
3	B	305	PX4	C10-C9	2.55	1.58	1.50	1	1
3	C	326	PX4	P1-O4	2.55	1.49	1.59	7	1
3	C	350	PX4	O3-C1	2.55	1.34	1.44	14	1
3	B	325	PX4	C2-N1	2.55	1.59	1.51	10	1
3	B	384	PX4	O7-C7	2.55	1.40	1.46	10	2
3	B	400	PX4	O7-C7	2.55	1.40	1.46	4	4
3	C	321	PX4	C2-C1	2.55	1.59	1.51	2	5
3	A	650	PX4	P1-O1	2.55	1.43	1.55	10	2
3	B	400	PX4	C5-N1	2.55	1.57	1.50	9	2
3	B	311	PX4	O7-C23	2.55	1.27	1.34	3	3
3	C	323	PX4	C10-C9	2.55	1.58	1.50	8	2
3	B	314	PX4	C10-C9	2.55	1.58	1.50	10	5
3	B	325	PX4	O7-C23	2.54	1.27	1.34	9	3
3	B	369	PX4	C10-C9	2.55	1.58	1.50	10	2
3	A	637	PX4	C3-N1	2.54	1.57	1.50	11	2
3	B	373	PX4	P1-O4	2.54	1.49	1.59	6	1
3	B	323	PX4	C10-C9	2.54	1.58	1.50	7	1
3	B	396	PX4	C33-C32	2.54	1.64	1.51	2	1
3	B	396	PX4	C24-C23	2.54	1.58	1.50	6	2
3	B	359	PX4	C5-N1	2.54	1.57	1.50	15	1
3	C	310	PX4	O4-C6	2.54	1.35	1.44	4	1
3	C	320	PX4	C3-N1	2.54	1.42	1.50	11	3
3	C	332	PX4	O7-C23	2.54	1.41	1.34	6	1
3	A	641	PX4	O7-C23	2.54	1.27	1.34	5	2
3	B	365	PX4	C4-N1	2.54	1.57	1.50	8	2
3	C	310	PX4	P1-O2	2.54	1.42	1.50	6	2
3	C	345	PX4	C29-C28	2.54	1.64	1.51	13	1
3	A	608	PX4	O7-C23	2.54	1.27	1.34	11	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	313	PX4	P1-O4	2.54	1.49	1.59	7	1
3	A	631	PX4	P1-O1	2.54	1.43	1.55	1	3
3	A	651	PX4	C25-C24	2.54	1.61	1.52	13	2
3	B	399	PX4	C13-C12	2.54	1.64	1.51	13	1
3	C	346	PX4	C32-C31	2.54	1.64	1.51	15	1
3	B	362	PX4	C2-N1	2.54	1.43	1.51	7	4
3	C	326	PX4	C3-N1	2.53	1.42	1.50	13	2
3	A	613	PX4	P1-O1	2.53	1.43	1.55	10	3
3	A	626	PX4	C6-C7	2.53	1.58	1.50	11	2
3	B	361	PX4	C2-C1	2.53	1.59	1.51	5	6
3	B	384	PX4	P1-O1	2.53	1.43	1.55	14	3
3	B	393	PX4	C6-C7	2.53	1.58	1.50	2	4
3	C	304	PX4	C24-C23	2.53	1.58	1.50	5	3
3	C	327	PX4	C5-N1	2.53	1.57	1.50	2	3
3	B	397	PX4	O7-C23	2.53	1.41	1.34	15	2
3	C	332	PX4	C11-C10	2.53	1.61	1.52	9	1
3	C	339	PX4	P1-O4	2.53	1.49	1.59	11	1
3	C	355	PX4	C2-N1	2.53	1.59	1.51	15	2
3	C	356	PX4	P1-O4	2.53	1.49	1.59	2	1
3	C	358	PX4	P1-O3	2.53	1.49	1.59	4	1
3	B	352	PX4	C25-C24	2.53	1.61	1.52	14	2
3	A	649	PX4	O3-C1	2.53	1.34	1.44	7	1
3	B	384	PX4	O3-C1	2.53	1.34	1.44	1	1
3	B	395	PX4	C25-C24	2.53	1.61	1.52	5	2
3	C	301	PX4	C5-N1	2.53	1.57	1.50	15	4
3	C	337	PX4	P1-O3	2.53	1.49	1.59	12	1
3	A	625	PX4	C11-C10	2.53	1.61	1.52	15	4
3	A	641	PX4	O7-C7	2.53	1.40	1.46	6	2
3	C	326	PX4	C8-C7	2.53	1.58	1.50	11	6
3	C	343	PX4	C4-N1	2.53	1.57	1.50	4	2
3	A	631	PX4	C25-C24	2.53	1.61	1.52	12	3
3	A	618	PX4	C3-N1	2.52	1.57	1.50	6	2
3	A	639	PX4	C2-N1	2.53	1.59	1.51	2	1
3	B	337	PX4	P1-O1	2.53	1.43	1.55	2	3
3	B	388	PX4	C12-C11	2.52	1.64	1.51	5	1
3	C	336	PX4	C11-C10	2.53	1.61	1.52	12	2
3	C	352	PX4	C11-C10	2.53	1.61	1.52	3	3
3	A	601	PX4	C3-N1	2.52	1.42	1.50	5	1
3	B	329	PX4	P1-O3	2.52	1.49	1.59	9	1
3	A	650	PX4	C24-C23	2.52	1.58	1.50	7	3
3	B	314	PX4	C6-C7	2.52	1.58	1.50	2	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	316	PX4	C11-C10	2.52	1.61	1.52	10	3
3	B	337	PX4	C25-C24	2.52	1.61	1.52	6	2
3	C	302	PX4	P1-O1	2.52	1.43	1.55	10	4
3	C	327	PX4	C2-N1	2.52	1.43	1.51	1	1
3	A	647	PX4	O7-C23	2.52	1.27	1.34	11	1
3	A	605	PX4	P1-O1	2.52	1.43	1.55	15	4
3	B	359	PX4	C8-C7	2.52	1.58	1.50	7	6
3	C	320	PX4	C25-C24	2.52	1.61	1.52	4	1
3	B	309	PX4	C2-N1	2.52	1.59	1.51	4	1
3	B	338	PX4	P1-O1	2.52	1.43	1.55	4	4
3	B	365	PX4	P1-O3	2.52	1.49	1.59	9	1
3	B	378	PX4	C10-C9	2.52	1.58	1.50	10	1
3	B	381	PX4	C19-C18	2.52	1.64	1.51	15	1
3	C	310	PX4	C11-C10	2.52	1.61	1.52	11	2
3	B	352	PX4	O3-C1	2.52	1.34	1.44	9	1
3	A	639	PX4	C17-C16	2.51	1.64	1.51	6	1
3	B	301	PX4	C27-C26	2.51	1.64	1.51	14	1
3	B	389	PX4	C3-N1	2.52	1.57	1.50	15	3
3	C	319	PX4	P1-O1	2.51	1.43	1.55	11	4
3	C	361	PX4	P1-O4	2.52	1.49	1.59	12	1
3	A	605	PX4	C4-N1	2.51	1.42	1.50	3	1
3	B	318	PX4	C11-C10	2.51	1.61	1.52	9	3
3	B	347	PX4	C5-N1	2.51	1.42	1.50	6	3
3	B	354	PX4	P1-O1	2.51	1.43	1.55	1	4
3	C	320	PX4	C2-N1	2.51	1.59	1.51	3	3
3	C	350	PX4	O4-C6	2.51	1.35	1.44	10	2
3	C	364	PX4	P1-O1	2.51	1.43	1.55	11	4
3	A	603	PX4	C10-C9	2.51	1.58	1.50	6	4
3	C	308	PX4	C2-N1	2.51	1.59	1.51	7	1
3	C	313	PX4	C10-C9	2.51	1.58	1.50	15	1
3	C	309	PX4	C10-C9	2.51	1.58	1.50	7	3
3	C	310	PX4	C29-C28	2.51	1.64	1.51	8	1
3	C	360	PX4	P1-O4	2.51	1.69	1.59	2	1
3	B	368	PX4	O5-C8	2.51	1.39	1.45	7	1
3	B	377	PX4	O5-C9	2.51	1.40	1.33	4	1
3	B	383	PX4	O5-C9	2.51	1.40	1.33	14	1
3	C	319	PX4	C25-C24	2.51	1.61	1.52	4	2
3	A	625	PX4	P1-O1	2.51	1.43	1.55	12	4
3	B	391	PX4	C16-C15	2.51	1.64	1.51	3	1
3	C	328	PX4	O7-C23	2.51	1.27	1.34	9	1
3	C	335	PX4	O4-C6	2.51	1.35	1.44	8	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	332	PX4	O7-C7	2.51	1.40	1.46	2	4
3	B	358	PX4	C15-C14	2.51	1.64	1.51	11	1
3	B	375	PX4	C6-C7	2.51	1.58	1.50	8	3
3	B	391	PX4	P1-O3	2.51	1.49	1.59	15	2
3	A	651	PX4	C2-C1	2.51	1.58	1.51	13	2
3	A	647	PX4	C18-C17	2.50	1.64	1.51	12	1
3	A	653	PX4	O5-C9	2.50	1.26	1.33	9	2
3	A	601	PX4	C11-C10	2.50	1.61	1.52	4	2
3	A	637	PX4	O3-C1	2.50	1.34	1.44	14	1
3	A	608	PX4	P1-O4	2.50	1.49	1.59	4	2
3	A	639	PX4	C4-N1	2.50	1.57	1.50	13	2
3	A	653	PX4	C17-C16	2.50	1.64	1.51	14	1
3	B	301	PX4	C3-N1	2.50	1.42	1.50	1	1
3	B	353	PX4	C25-C24	2.50	1.61	1.52	12	2
3	C	318	PX4	C34-C33	2.50	1.64	1.51	14	1
3	C	344	PX4	C10-C9	2.50	1.58	1.50	8	2
3	C	350	PX4	C11-C10	2.50	1.61	1.52	13	3
3	B	302	PX4	C25-C24	2.50	1.61	1.52	12	1
3	B	361	PX4	O7-C7	2.50	1.40	1.46	11	6
3	B	377	PX4	O7-C7	2.50	1.40	1.46	14	4
3	B	377	PX4	C17-C16	2.50	1.64	1.51	7	1
3	C	302	PX4	P1-O2	2.50	1.42	1.50	14	1
3	A	615	PX4	C24-C23	2.50	1.58	1.50	8	1
3	B	354	PX4	C11-C10	2.50	1.61	1.52	4	2
3	A	604	PX4	C4-N1	2.50	1.57	1.50	3	2
3	B	346	PX4	C24-C23	2.50	1.58	1.50	8	3
3	C	333	PX4	C4-N1	2.50	1.42	1.50	15	2
3	C	343	PX4	P1-O1	2.50	1.43	1.55	7	6
3	A	611	PX4	C28-C27	2.50	1.64	1.51	15	1
3	B	343	PX4	C2-N1	2.50	1.59	1.51	5	2
3	B	348	PX4	C5-N1	2.50	1.57	1.50	4	1
3	B	366	PX4	C34-C33	2.50	1.64	1.51	13	1
3	B	350	PX4	C2-N1	2.50	1.59	1.51	7	1
3	B	385	PX4	O5-C9	2.50	1.26	1.33	9	2
3	C	305	PX4	O7-C23	2.50	1.41	1.34	12	2
3	C	338	PX4	C25-C24	2.50	1.61	1.52	5	3
3	C	339	PX4	O5-C9	2.50	1.40	1.33	7	2
3	B	328	PX4	P1-O4	2.49	1.49	1.59	15	1
3	B	354	PX4	O5-C8	2.49	1.39	1.45	14	1
3	A	641	PX4	C4-N1	2.49	1.57	1.50	7	1
3	B	394	PX4	C25-C24	2.49	1.61	1.52	12	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	357	PX4	C2-C1	2.49	1.58	1.51	10	5
3	B	397	PX4	P1-O2	2.49	1.42	1.50	11	2
3	A	614	PX4	C10-C9	2.49	1.43	1.50	1	3
3	A	619	PX4	C3-N1	2.49	1.57	1.50	10	3
3	A	632	PX4	C11-C10	2.49	1.61	1.52	5	3
3	B	318	PX4	C6-C7	2.49	1.58	1.50	1	3
3	C	355	PX4	P1-O1	2.49	1.43	1.55	6	3
3	B	333	PX4	C25-C24	2.49	1.61	1.52	14	1
3	A	635	PX4	P1-O1	2.49	1.43	1.55	12	2
3	B	334	PX4	C2-N1	2.49	1.59	1.51	12	2
3	B	355	PX4	C25-C24	2.49	1.61	1.52	8	1
3	B	384	PX4	O5-C9	2.49	1.40	1.33	13	2
3	C	318	PX4	P1-O2	2.49	1.42	1.50	1	2
3	A	641	PX4	C17-C16	2.49	1.64	1.51	3	1
3	A	646	PX4	C10-C9	2.49	1.57	1.50	15	1
3	A	645	PX4	C28-C27	2.49	1.64	1.51	8	1
3	B	321	PX4	C28-C27	2.49	1.64	1.51	13	1
3	B	331	PX4	C5-N1	2.49	1.57	1.50	3	2
3	B	302	PX4	C30-C29	2.49	1.64	1.51	7	1
3	B	343	PX4	C4-N1	2.49	1.57	1.50	15	2
3	C	330	PX4	C2-C1	2.49	1.58	1.51	9	3
3	B	346	PX4	P1-O1	2.49	1.43	1.55	7	3
3	C	338	PX4	P1-O1	2.49	1.43	1.55	4	2
3	C	329	PX4	O7-C7	2.48	1.40	1.46	11	5
3	B	321	PX4	P1-O2	2.48	1.42	1.50	10	1
3	B	346	PX4	C31-C30	2.48	1.64	1.51	2	1
3	C	333	PX4	P1-O1	2.48	1.43	1.55	9	3
3	B	388	PX4	O5-C9	2.48	1.26	1.33	11	1
3	C	304	PX4	C25-C24	2.48	1.61	1.52	9	2
3	C	311	PX4	P1-O2	2.48	1.42	1.50	14	3
3	C	344	PX4	C3-N1	2.48	1.42	1.50	9	1
3	B	326	PX4	C4-N1	2.48	1.57	1.50	13	3
3	C	308	PX4	O7-C7	2.48	1.40	1.46	1	2
3	C	360	PX4	C11-C10	2.48	1.61	1.52	7	1
3	A	615	PX4	O5-C8	2.48	1.39	1.45	14	2
3	A	632	PX4	C3-N1	2.48	1.42	1.50	2	1
3	B	323	PX4	C3-N1	2.48	1.42	1.50	13	2
3	B	312	PX4	C4-N1	2.48	1.57	1.50	2	1
3	B	348	PX4	P1-O4	2.48	1.49	1.59	9	1
3	B	366	PX4	C3-N1	2.48	1.42	1.50	15	1
3	B	377	PX4	O7-C23	2.48	1.27	1.34	8	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	C	332	PX4	C2-N1	2.48	1.59	1.51	8	2
3	C	338	PX4	C34-C33	2.48	1.64	1.51	5	1
3	C	339	PX4	C5-N1	2.48	1.42	1.50	13	1
3	C	344	PX4	O5-C9	2.48	1.40	1.33	13	1
3	C	354	PX4	P1-O1	2.48	1.43	1.55	4	1
3	A	631	PX4	O7-C7	2.48	1.40	1.46	4	2
3	A	643	PX4	C10-C9	2.48	1.57	1.50	8	3
3	B	315	PX4	C15-C14	2.48	1.64	1.51	7	1
3	C	320	PX4	P1-O3	2.48	1.49	1.59	4	1
3	B	384	PX4	O4-C6	2.47	1.54	1.44	14	1
3	C	356	PX4	C4-N1	2.48	1.42	1.50	13	1
3	A	625	PX4	C4-N1	2.47	1.42	1.50	5	1
3	A	634	PX4	C25-C24	2.47	1.61	1.52	5	3
3	A	625	PX4	C24-C23	2.47	1.43	1.50	5	1
3	A	646	PX4	P1-O1	2.47	1.43	1.55	14	1
3	B	362	PX4	C4-N1	2.47	1.57	1.50	6	2
3	B	365	PX4	P1-O1	2.47	1.43	1.55	10	3
3	B	381	PX4	C20-C19	2.47	1.64	1.51	2	1
3	C	329	PX4	C4-N1	2.47	1.42	1.50	8	3
3	C	334	PX4	C2-C1	2.47	1.58	1.51	2	4
3	C	352	PX4	C25-C24	2.47	1.61	1.52	3	2
3	B	313	PX4	O7-C7	2.47	1.40	1.46	15	2
3	C	358	PX4	C3-N1	2.47	1.57	1.50	6	2
3	A	603	PX4	C24-C23	2.47	1.57	1.50	4	3
3	A	614	PX4	C33-C32	2.47	1.64	1.51	3	1
3	A	621	PX4	C31-C30	2.47	1.64	1.51	2	2
3	B	310	PX4	C5-N1	2.47	1.42	1.50	6	1
3	C	341	PX4	C5-N1	2.47	1.57	1.50	3	1
3	A	645	PX4	P1-O1	2.47	1.43	1.55	12	1
3	C	311	PX4	O7-C23	2.47	1.41	1.34	4	2
3	A	628	PX4	C24-C23	2.47	1.57	1.50	4	2
3	A	615	PX4	P1-O1	2.47	1.43	1.55	11	3
3	A	644	PX4	C31-C30	2.47	1.64	1.51	2	1
3	B	304	PX4	C3-N1	2.47	1.57	1.50	14	1
3	B	364	PX4	P1-O2	2.47	1.42	1.50	5	1
3	B	394	PX4	C5-N1	2.47	1.57	1.50	13	1
3	B	365	PX4	O7-C23	2.47	1.27	1.34	15	2
3	B	375	PX4	C27-C26	2.47	1.64	1.51	4	1
3	B	387	PX4	O5-C9	2.47	1.40	1.33	2	1
3	B	308	PX4	C4-N1	2.46	1.57	1.50	2	2
3	B	345	PX4	P1-O1	2.46	1.43	1.55	5	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	382	PX4	C21-C20	2.46	1.66	1.51	15	1
3	A	611	PX4	C2-C1	2.46	1.58	1.51	13	3
3	A	614	PX4	C28-C27	2.46	1.64	1.51	5	1
3	B	358	PX4	C25-C24	2.46	1.61	1.52	15	2
3	B	364	PX4	O7-C7	2.46	1.52	1.46	13	2
3	B	399	PX4	C24-C23	2.46	1.57	1.50	12	2
3	B	314	PX4	C2-N1	2.46	1.59	1.51	15	1
3	C	330	PX4	C3-N1	2.46	1.42	1.50	15	3
3	A	615	PX4	C27-C26	2.46	1.64	1.51	14	1
3	A	620	PX4	C24-C23	2.46	1.57	1.50	15	4
3	A	640	PX4	C5-N1	2.46	1.57	1.50	15	2
3	A	649	PX4	P1-O1	2.46	1.43	1.55	8	1
3	B	331	PX4	O7-C23	2.46	1.41	1.34	9	3
3	B	353	PX4	C10-C9	2.46	1.57	1.50	4	2
3	B	361	PX4	C4-N1	2.46	1.57	1.50	5	1
3	B	387	PX4	O5-C8	2.46	1.39	1.45	13	2
3	A	637	PX4	C31-C30	2.46	1.64	1.51	12	3
3	A	648	PX4	O5-C9	2.46	1.26	1.33	1	1
3	A	653	PX4	C2-N1	2.46	1.59	1.51	8	1
3	B	324	PX4	O7-C23	2.46	1.27	1.34	4	3
3	C	310	PX4	O5-C8	2.46	1.39	1.45	6	3
3	B	304	PX4	C12-C11	2.46	1.64	1.51	3	1
3	A	622	PX4	O5-C8	2.45	1.39	1.45	10	3
3	B	308	PX4	C25-C24	2.45	1.61	1.52	8	3
3	B	326	PX4	O5-C8	2.46	1.50	1.45	14	4
3	B	374	PX4	O5-C8	2.46	1.39	1.45	14	4
3	C	360	PX4	C4-N1	2.46	1.57	1.50	5	3
3	B	374	PX4	C10-C9	2.45	1.57	1.50	14	1
3	B	378	PX4	C20-C19	2.45	1.64	1.51	9	1
3	C	302	PX4	C24-C23	2.45	1.57	1.50	12	1
3	C	320	PX4	C16-C15	2.45	1.64	1.51	1	1
3	A	636	PX4	C19-C18	2.45	1.64	1.51	2	1
3	B	326	PX4	P1-O1	2.45	1.44	1.55	2	2
3	B	327	PX4	C5-N1	2.45	1.42	1.50	15	3
3	C	327	PX4	O7-C7	2.45	1.40	1.46	5	4
3	C	359	PX4	C13-C12	2.45	1.64	1.51	10	1
3	A	622	PX4	C25-C24	2.45	1.61	1.52	4	3
3	B	336	PX4	O7-C7	2.45	1.40	1.46	12	1
3	C	306	PX4	P1-O1	2.45	1.44	1.55	5	3
3	C	357	PX4	C5-N1	2.45	1.57	1.50	6	1
3	B	302	PX4	C4-N1	2.45	1.57	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	C11-C10	2.45	1.61	1.52	13	1
3	A	613	PX4	C3-N1	2.45	1.42	1.50	6	1
3	B	309	PX4	O5-C8	2.45	1.50	1.45	5	1
3	B	321	PX4	C3-N1	2.45	1.57	1.50	4	2
3	A	602	PX4	C10-C9	2.44	1.57	1.50	10	4
3	A	624	PX4	C17-C16	2.44	1.63	1.51	2	1
3	B	312	PX4	P1-O4	2.44	1.49	1.59	12	2
3	B	371	PX4	C13-C12	2.44	1.63	1.51	11	1
3	B	375	PX4	C2-N1	2.45	1.58	1.51	11	4
3	C	308	PX4	P1-O1	2.44	1.44	1.55	2	4
3	B	316	PX4	C24-C23	2.44	1.57	1.50	5	4
3	B	338	PX4	C2-N1	2.44	1.58	1.51	3	2
3	C	328	PX4	P1-O1	2.44	1.44	1.55	3	3
3	A	639	PX4	C20-C19	2.44	1.63	1.51	6	1
3	A	644	PX4	C5-N1	2.44	1.42	1.50	11	2
3	B	301	PX4	C5-N1	2.44	1.42	1.50	4	2
3	B	328	PX4	C25-C24	2.44	1.61	1.52	13	1
3	B	337	PX4	C24-C23	2.44	1.57	1.50	2	1
3	B	349	PX4	O5-C8	2.44	1.50	1.45	5	1
3	B	368	PX4	C24-C23	2.44	1.57	1.50	12	2
3	B	380	PX4	C4-N1	2.44	1.57	1.50	8	1
3	A	645	PX4	O7-C7	2.44	1.40	1.46	11	3
3	B	382	PX4	O7-C23	2.44	1.41	1.34	5	3
3	A	611	PX4	C3-N1	2.44	1.57	1.50	13	2
3	B	349	PX4	C24-C23	2.44	1.57	1.50	10	2
3	A	615	PX4	C32-C31	2.43	1.63	1.51	8	2
3	B	352	PX4	C11-C10	2.43	1.61	1.52	3	1
3	B	372	PX4	O5-C9	2.44	1.40	1.33	1	2
3	B	340	PX4	O7-C7	2.43	1.40	1.46	3	2
3	B	376	PX4	C3-N1	2.43	1.57	1.50	1	1
3	B	393	PX4	O5-C9	2.43	1.26	1.33	2	3
3	A	653	PX4	O7-C23	2.43	1.27	1.34	3	4
3	B	306	PX4	C34-C33	2.43	1.63	1.51	8	1
3	B	324	PX4	C2-C1	2.43	1.58	1.51	8	2
3	B	328	PX4	P1-O3	2.43	1.49	1.59	13	1
3	B	358	PX4	C12-C11	2.43	1.63	1.51	12	1
3	B	387	PX4	P1-O1	2.43	1.44	1.55	3	2
3	B	398	PX4	P1-O1	2.43	1.44	1.55	10	1
3	C	324	PX4	C5-N1	2.43	1.42	1.50	8	2
3	C	358	PX4	C8-C7	2.43	1.58	1.50	3	1
3	B	336	PX4	P1-O1	2.43	1.44	1.55	1	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	343	PX4	C5-N1	2.43	1.42	1.50	7	2
3	B	357	PX4	C14-C13	2.43	1.63	1.51	1	1
3	C	327	PX4	C25-C24	2.43	1.61	1.52	11	2
3	A	619	PX4	P1-O2	2.43	1.42	1.50	7	3
3	A	639	PX4	C11-C10	2.43	1.61	1.52	13	1
3	A	639	PX4	P1-O3	2.43	1.49	1.59	14	1
3	C	350	PX4	C2-C1	2.43	1.58	1.51	9	7
3	B	304	PX4	C2-N1	2.43	1.44	1.51	7	4
3	B	341	PX4	C4-N1	2.43	1.57	1.50	5	1
3	B	391	PX4	P1-O1	2.43	1.44	1.55	9	1
3	C	303	PX4	C18-C17	2.43	1.63	1.51	3	1
3	C	326	PX4	C25-C24	2.43	1.61	1.52	3	2
3	A	651	PX4	C19-C18	2.43	1.63	1.51	15	1
3	A	631	PX4	O5-C9	2.43	1.40	1.33	9	1
3	B	356	PX4	P1-O1	2.43	1.44	1.55	8	4
3	B	400	PX4	C24-C23	2.43	1.57	1.50	7	3
3	C	302	PX4	O5-C8	2.43	1.50	1.45	2	3
3	C	303	PX4	C24-C23	2.42	1.43	1.50	4	2
3	C	326	PX4	P1-O3	2.42	1.49	1.59	12	1
3	C	344	PX4	C2-N1	2.42	1.44	1.51	10	3
3	C	345	PX4	C31-C30	2.43	1.63	1.51	4	1
3	A	640	PX4	C4-N1	2.42	1.43	1.50	11	2
3	C	303	PX4	O7-C23	2.42	1.41	1.34	10	3
3	A	644	PX4	C33-C32	2.42	1.63	1.51	14	1
3	C	307	PX4	C3-N1	2.42	1.57	1.50	9	3
3	C	321	PX4	C25-C24	2.42	1.61	1.52	5	3
3	C	313	PX4	O7-C23	2.42	1.27	1.34	14	3
3	C	325	PX4	P1-O1	2.42	1.44	1.55	6	2
3	C	341	PX4	C25-C24	2.42	1.61	1.52	11	3
3	C	356	PX4	O5-C9	2.42	1.26	1.33	4	1
3	B	302	PX4	C15-C14	2.42	1.63	1.51	4	2
3	B	373	PX4	O5-C9	2.42	1.40	1.33	10	1
3	B	387	PX4	C30-C29	2.42	1.63	1.51	11	2
3	C	304	PX4	C13-C12	2.42	1.63	1.51	12	1
3	C	314	PX4	C27-C26	2.42	1.63	1.51	12	1
3	A	649	PX4	C14-C13	2.42	1.63	1.51	11	1
3	C	325	PX4	C24-C23	2.42	1.57	1.50	14	2
3	A	602	PX4	C4-N1	2.42	1.57	1.50	12	1
3	A	624	PX4	P1-O1	2.42	1.44	1.55	9	3
3	A	634	PX4	C10-C9	2.42	1.57	1.50	8	3
3	B	319	PX4	C2-N1	2.42	1.44	1.51	2	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	366	PX4	P1-O1	2.42	1.44	1.55	3	2
3	B	399	PX4	C25-C24	2.42	1.61	1.52	5	1
3	C	301	PX4	C15-C14	2.42	1.63	1.51	12	1
3	B	321	PX4	C10-C9	2.42	1.57	1.50	3	2
3	A	606	PX4	P1-O2	2.41	1.42	1.50	14	1
3	A	609	PX4	C3-N1	2.42	1.43	1.50	13	2
3	B	333	PX4	C29-C28	2.42	1.63	1.51	2	1
3	B	361	PX4	C29-C28	2.42	1.63	1.51	8	1
3	B	391	PX4	C5-N1	2.42	1.57	1.50	13	2
3	B	395	PX4	C10-C9	2.42	1.57	1.50	1	4
3	C	360	PX4	O7-C23	2.42	1.27	1.34	9	2
3	A	622	PX4	O4-C6	2.41	1.53	1.44	7	1
3	B	384	PX4	C20-C19	2.41	1.63	1.51	8	1
3	C	312	PX4	C11-C10	2.42	1.61	1.52	10	3
3	A	601	PX4	P1-O1	2.41	1.44	1.55	4	5
3	A	627	PX4	O5-C9	2.41	1.40	1.33	10	2
3	A	615	PX4	C19-C18	2.41	1.63	1.51	11	1
3	B	309	PX4	C3-N1	2.41	1.57	1.50	2	1
3	B	347	PX4	O7-C7	2.41	1.52	1.46	8	4
3	B	357	PX4	C2-N1	2.41	1.58	1.51	4	3
3	C	324	PX4	C2-N1	2.41	1.44	1.51	13	1
3	A	621	PX4	C5-N1	2.41	1.57	1.50	9	1
3	A	638	PX4	C5-N1	2.41	1.43	1.50	3	2
3	C	314	PX4	C2-C1	2.41	1.58	1.51	10	2
3	C	345	PX4	O7-C7	2.41	1.40	1.46	4	1
3	C	349	PX4	C4-N1	2.41	1.57	1.50	7	1
3	B	342	PX4	C11-C10	2.41	1.61	1.52	9	2
3	B	375	PX4	C4-N1	2.41	1.57	1.50	9	2
3	B	320	PX4	P1-O4	2.41	1.50	1.59	13	2
3	C	314	PX4	O7-C23	2.41	1.27	1.34	1	1
3	C	326	PX4	C2-N1	2.41	1.58	1.51	9	1
3	A	609	PX4	C5-N1	2.41	1.57	1.50	5	3
3	B	399	PX4	C4-N1	2.41	1.43	1.50	2	2
3	C	304	PX4	O3-C1	2.41	1.35	1.44	4	1
3	C	327	PX4	C4-N1	2.41	1.57	1.50	15	3
3	A	605	PX4	C5-N1	2.40	1.57	1.50	9	1
3	A	626	PX4	C4-N1	2.41	1.57	1.50	2	1
3	B	322	PX4	C5-N1	2.41	1.43	1.50	4	1
3	B	334	PX4	C4-N1	2.41	1.43	1.50	7	1
3	B	351	PX4	O5-C8	2.41	1.39	1.45	12	1
3	B	397	PX4	C24-C23	2.40	1.57	1.50	11	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	365	PX4	O3-C1	2.40	1.35	1.44	5	1
3	B	370	PX4	C11-C10	2.40	1.61	1.52	4	1
3	C	340	PX4	P1-O1	2.40	1.44	1.55	8	4
3	B	331	PX4	C10-C9	2.40	1.57	1.50	9	3
3	B	383	PX4	C25-C24	2.40	1.61	1.52	2	2
3	B	395	PX4	P1-O2	2.40	1.42	1.50	2	1
3	C	307	PX4	O7-C23	2.40	1.41	1.34	10	2
3	C	350	PX4	P1-O1	2.40	1.44	1.55	9	2
3	A	626	PX4	O3-C1	2.40	1.35	1.44	13	1
3	A	644	PX4	P1-O1	2.40	1.44	1.55	6	4
3	B	316	PX4	C10-C9	2.40	1.57	1.50	3	1
3	A	612	PX4	C10-C9	2.40	1.57	1.50	9	1
3	B	390	PX4	C30-C29	2.40	1.63	1.51	13	1
3	B	363	PX4	O7-C23	2.40	1.27	1.34	2	2
3	C	358	PX4	C2-C1	2.40	1.58	1.51	3	6
3	B	322	PX4	P1-O1	2.40	1.44	1.55	3	2
3	B	344	PX4	C20-C19	2.40	1.63	1.51	5	1
3	C	332	PX4	C31-C30	2.40	1.63	1.51	10	1
3	C	334	PX4	C2-N1	2.40	1.58	1.51	6	2
3	C	335	PX4	O5-C9	2.40	1.40	1.33	11	1
3	C	354	PX4	C16-C15	2.40	1.63	1.51	14	1
3	A	629	PX4	O5-C8	2.39	1.50	1.45	3	2
3	B	309	PX4	C5-N1	2.39	1.57	1.50	5	1
3	B	330	PX4	C25-C24	2.39	1.61	1.52	5	1
3	A	653	PX4	O4-C6	2.39	1.35	1.44	3	1
3	B	329	PX4	O3-C1	2.39	1.35	1.44	12	1
3	B	357	PX4	P1-O1	2.39	1.44	1.55	12	3
3	C	324	PX4	C26-C25	2.39	1.63	1.51	6	1
3	C	340	PX4	C31-C30	2.39	1.63	1.51	11	1
3	C	356	PX4	C11-C10	2.39	1.61	1.52	8	1
3	B	324	PX4	C4-N1	2.39	1.43	1.50	1	2
3	B	330	PX4	C3-N1	2.39	1.56	1.50	7	1
3	B	381	PX4	O5-C8	2.39	1.39	1.45	12	1
3	C	314	PX4	P1-O4	2.39	1.50	1.59	9	1
3	A	606	PX4	O5-C8	2.39	1.50	1.45	9	2
3	B	348	PX4	C25-C24	2.39	1.61	1.52	8	3
3	C	312	PX4	C32-C31	2.39	1.63	1.51	5	1
3	C	338	PX4	P1-O2	2.39	1.42	1.50	7	2
3	C	352	PX4	P1-O4	2.39	1.68	1.59	8	1
3	B	353	PX4	O5-C8	2.39	1.50	1.45	12	1
3	A	603	PX4	C11-C10	2.39	1.60	1.52	7	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	307	PX4	C3-N1	2.39	1.56	1.50	7	2
3	B	353	PX4	C3-N1	2.39	1.56	1.50	7	2
3	B	400	PX4	C18-C17	2.39	1.63	1.51	12	1
3	C	348	PX4	P1-O2	2.39	1.42	1.50	11	2
3	C	356	PX4	C25-C24	2.39	1.60	1.52	10	1
3	B	344	PX4	C3-N1	2.39	1.56	1.50	14	2
3	C	363	PX4	O7-C23	2.39	1.41	1.34	9	2
3	C	304	PX4	O8-C23	2.39	1.15	1.22	2	1
3	C	311	PX4	C25-C24	2.39	1.60	1.52	1	1
3	A	602	PX4	C11-C10	2.39	1.60	1.52	2	2
3	C	312	PX4	C4-N1	2.39	1.43	1.50	9	1
3	C	345	PX4	P1-O1	2.39	1.44	1.55	8	3
3	A	604	PX4	O7-C23	2.38	1.27	1.34	8	1
3	A	643	PX4	C24-C23	2.39	1.57	1.50	11	2
3	C	305	PX4	P1-O4	2.39	1.50	1.59	1	2
3	C	362	PX4	C27-C26	2.39	1.63	1.51	11	1
3	A	646	PX4	C5-N1	2.38	1.56	1.50	1	3
3	B	315	PX4	O5-C8	2.38	1.39	1.45	11	3
3	A	607	PX4	O7-C23	2.38	1.41	1.34	9	3
3	A	648	PX4	O4-C6	2.38	1.35	1.44	2	1
3	B	301	PX4	C11-C10	2.38	1.60	1.52	1	4
3	B	363	PX4	C11-C10	2.38	1.60	1.52	14	1
3	C	334	PX4	C11-C10	2.38	1.60	1.52	9	1
3	C	350	PX4	C10-C9	2.38	1.57	1.50	11	2
3	B	327	PX4	O7-C23	2.38	1.27	1.34	13	1
3	B	338	PX4	C18-C17	2.38	1.63	1.51	10	1
3	B	358	PX4	O5-C9	2.38	1.26	1.33	4	1
3	B	371	PX4	C25-C24	2.38	1.60	1.52	14	1
3	B	356	PX4	C33-C32	2.38	1.63	1.51	10	1
3	C	328	PX4	O5-C8	2.38	1.39	1.45	12	2
3	B	369	PX4	C25-C24	2.38	1.60	1.52	8	2
3	B	376	PX4	O5-C8	2.38	1.39	1.45	7	1
3	B	324	PX4	C16-C15	2.38	1.63	1.51	3	1
3	B	326	PX4	O5-C9	2.38	1.26	1.33	9	1
3	B	382	PX4	P1-O1	2.38	1.44	1.55	2	2
3	B	390	PX4	P1-O3	2.38	1.50	1.59	2	1
3	B	390	PX4	C4-N1	2.38	1.43	1.50	6	3
3	B	396	PX4	C18-C17	2.38	1.63	1.51	5	1
3	C	349	PX4	P1-O4	2.38	1.68	1.59	15	1
3	A	602	PX4	C19-C18	2.38	1.63	1.51	15	1
3	B	333	PX4	C5-N1	2.38	1.43	1.50	13	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	A	610	PX4	C25-C24	2.37	1.60	1.52	12	2
3	A	652	PX4	C2-C1	2.38	1.58	1.51	7	2
3	B	320	PX4	C24-C23	2.38	1.57	1.50	3	1
3	B	326	PX4	C34-C33	2.38	1.63	1.51	13	1
3	B	380	PX4	C10-C9	2.38	1.57	1.50	10	2
3	A	640	PX4	P1-O4	2.37	1.68	1.59	6	1
3	A	647	PX4	C3-N1	2.37	1.43	1.50	6	1
3	A	648	PX4	C24-C23	2.37	1.57	1.50	14	3
3	B	325	PX4	C27-C26	2.37	1.63	1.51	10	1
3	B	328	PX4	C16-C15	2.37	1.63	1.51	9	1
3	B	362	PX4	P1-O1	2.37	1.44	1.55	12	3
3	A	629	PX4	C10-C9	2.37	1.57	1.50	13	2
3	B	309	PX4	C6-C7	2.37	1.58	1.50	11	3
3	B	323	PX4	C27-C26	2.37	1.63	1.51	7	1
3	B	399	PX4	O7-C23	2.37	1.27	1.34	2	1
3	C	341	PX4	O5-C9	2.37	1.40	1.33	10	1
3	A	603	PX4	C25-C24	2.37	1.60	1.52	8	2
3	A	636	PX4	C25-C24	2.37	1.60	1.52	7	2
3	B	344	PX4	C18-C17	2.37	1.63	1.51	7	1
3	B	376	PX4	P1-O1	2.37	1.44	1.55	1	4
3	B	386	PX4	C11-C10	2.37	1.60	1.52	9	1
3	C	311	PX4	C11-C10	2.37	1.60	1.52	14	1
3	C	330	PX4	O5-C8	2.37	1.50	1.45	6	2
3	B	387	PX4	C24-C23	2.37	1.57	1.50	2	1
3	C	355	PX4	C3-N1	2.37	1.43	1.50	15	2
3	B	312	PX4	C20-C19	2.37	1.63	1.51	12	1
3	B	371	PX4	C30-C29	2.37	1.63	1.51	2	1
3	B	392	PX4	C5-N1	2.37	1.56	1.50	6	1
3	A	639	PX4	O5-C8	2.37	1.50	1.45	13	1
3	B	308	PX4	C32-C31	2.37	1.63	1.51	7	1
3	C	313	PX4	C31-C30	2.37	1.63	1.51	11	1
3	C	331	PX4	C12-C11	2.37	1.63	1.51	8	1
3	B	400	PX4	C31-C30	2.36	1.63	1.51	15	1
3	C	328	PX4	C26-C25	2.36	1.63	1.51	1	1
3	C	329	PX4	P1-O1	2.36	1.44	1.55	1	4
3	C	335	PX4	C2-N1	2.36	1.44	1.51	11	2
3	C	349	PX4	C24-C23	2.36	1.57	1.50	15	4
3	A	626	PX4	P1-O4	2.36	1.50	1.59	10	1
3	A	632	PX4	C33-C32	2.36	1.63	1.51	13	1
3	B	380	PX4	P1-O1	2.36	1.44	1.55	8	2
3	C	353	PX4	C4-N1	2.36	1.43	1.50	14	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	A	617	PX4	O3-C1	2.36	1.35	1.44	5	1
3	A	617	PX4	C3-N1	2.36	1.56	1.50	6	3
3	A	630	PX4	C5-N1	2.36	1.56	1.50	11	2
3	B	340	PX4	P1-O3	2.36	1.50	1.59	9	1
3	B	376	PX4	C11-C10	2.36	1.60	1.52	1	1
3	C	307	PX4	C11-C10	2.36	1.60	1.52	1	2
3	C	305	PX4	C10-C9	2.36	1.57	1.50	12	3
3	C	331	PX4	C24-C23	2.36	1.57	1.50	15	1
3	B	321	PX4	C5-N1	2.36	1.43	1.50	8	1
3	B	347	PX4	O7-C23	2.36	1.27	1.34	1	2
3	C	332	PX4	P1-O3	2.36	1.50	1.59	8	1
3	C	334	PX4	C26-C25	2.36	1.63	1.51	1	2
3	A	623	PX4	C11-C10	2.36	1.60	1.52	13	1
3	A	614	PX4	O7-C23	2.36	1.27	1.34	12	2
3	A	629	PX4	C3-N1	2.36	1.56	1.50	13	2
3	B	305	PX4	O7-C23	2.36	1.27	1.34	12	1
3	B	309	PX4	P1-O1	2.36	1.44	1.55	1	2
3	B	364	PX4	C28-C27	2.36	1.63	1.51	5	1
3	A	605	PX4	P1-O4	2.35	1.68	1.59	9	1
3	A	644	PX4	C28-C27	2.36	1.63	1.51	12	1
3	A	654	PX4	C5-N1	2.36	1.43	1.50	7	1
3	B	348	PX4	O5-C9	2.35	1.40	1.33	3	1
3	A	635	PX4	O3-C1	2.35	1.35	1.44	12	1
3	A	645	PX4	C32-C31	2.35	1.63	1.51	14	1
3	B	323	PX4	P1-O1	2.35	1.44	1.55	1	2
3	B	377	PX4	C3-N1	2.35	1.43	1.50	12	1
3	B	399	PX4	O5-C9	2.35	1.26	1.33	4	2
3	A	601	PX4	C4-N1	2.35	1.43	1.50	5	2
3	A	626	PX4	C14-C13	2.35	1.63	1.51	15	1
3	A	643	PX4	P1-O4	2.35	1.50	1.59	14	1
3	B	342	PX4	C4-N1	2.35	1.43	1.50	5	1
3	A	611	PX4	P1-O1	2.35	1.44	1.55	3	2
3	A	622	PX4	P1-O1	2.35	1.44	1.55	8	3
3	A	631	PX4	C11-C10	2.35	1.60	1.52	9	1
3	A	649	PX4	O5-C9	2.35	1.26	1.33	10	2
3	A	651	PX4	C20-C19	2.35	1.63	1.51	4	1
3	B	330	PX4	C10-C9	2.35	1.57	1.50	4	3
3	B	358	PX4	O5-C8	2.35	1.39	1.45	15	1
3	B	360	PX4	C11-C10	2.35	1.60	1.52	4	2
3	B	365	PX4	O5-C9	2.35	1.40	1.33	9	1
3	B	378	PX4	P1-O1	2.35	1.44	1.55	13	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	397	PX4	C2-N1	2.35	1.58	1.51	5	2
3	A	623	PX4	C24-C23	2.35	1.57	1.50	2	2
3	B	302	PX4	C26-C25	2.35	1.63	1.51	15	1
3	B	388	PX4	C24-C23	2.35	1.43	1.50	3	1
3	B	394	PX4	P1-O1	2.35	1.44	1.55	9	3
3	A	614	PX4	C4-N1	2.34	1.43	1.50	4	1
3	A	653	PX4	P1-O4	2.35	1.50	1.59	2	1
3	B	320	PX4	C2-C1	2.35	1.58	1.51	10	4
3	C	354	PX4	O7-C23	2.35	1.27	1.34	13	1
3	B	331	PX4	C11-C10	2.35	1.43	1.52	7	2
3	B	308	PX4	P1-O1	2.34	1.44	1.55	8	1
3	B	352	PX4	C26-C25	2.34	1.63	1.51	8	1
3	B	383	PX4	C3-N1	2.34	1.56	1.50	9	2
3	B	385	PX4	C24-C23	2.35	1.57	1.50	9	2
3	B	394	PX4	C10-C9	2.35	1.57	1.50	9	2
3	B	391	PX4	C11-C10	2.34	1.60	1.52	7	1
3	C	313	PX4	C11-C10	2.34	1.60	1.52	15	1
3	C	326	PX4	C33-C32	2.34	1.63	1.51	14	1
3	C	342	PX4	C4-N1	2.34	1.43	1.50	7	1
3	A	611	PX4	O5-C8	2.34	1.39	1.45	12	2
3	B	306	PX4	C25-C24	2.34	1.60	1.52	7	1
3	B	338	PX4	O5-C8	2.34	1.39	1.45	9	1
3	C	331	PX4	C25-C24	2.34	1.60	1.52	9	2
3	C	339	PX4	P1-O2	2.34	1.42	1.50	12	1
3	B	341	PX4	O5-C8	2.34	1.50	1.45	8	3
3	B	360	PX4	C28-C27	2.34	1.63	1.51	4	1
3	B	365	PX4	C25-C24	2.34	1.60	1.52	15	1
3	C	348	PX4	C25-C24	2.34	1.60	1.52	9	2
3	B	309	PX4	C14-C13	2.34	1.63	1.51	5	1
3	B	311	PX4	P1-O1	2.34	1.44	1.55	8	5
3	B	337	PX4	P1-O4	2.34	1.50	1.59	15	1
3	A	641	PX4	C24-C23	2.34	1.57	1.50	11	2
3	B	327	PX4	P1-O4	2.34	1.50	1.59	14	2
3	B	385	PX4	C25-C24	2.34	1.60	1.52	11	3
3	B	386	PX4	O6-C9	2.34	1.29	1.22	14	1
3	B	390	PX4	C24-C23	2.34	1.57	1.50	14	1
3	A	602	PX4	C32-C31	2.34	1.63	1.51	14	2
3	A	611	PX4	C24-C23	2.34	1.57	1.50	4	2
3	A	607	PX4	P1-O1	2.34	1.44	1.55	12	3
3	A	607	PX4	O5-C8	2.34	1.50	1.45	9	1
3	A	617	PX4	C27-C26	2.34	1.63	1.51	10	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	A	620	PX4	C30-C29	2.34	1.63	1.51	7	1
3	B	342	PX4	C2-N1	2.34	1.58	1.51	1	1
3	B	392	PX4	O5-C8	2.34	1.50	1.45	9	1
3	B	394	PX4	P1-O3	2.34	1.50	1.59	8	1
3	B	400	PX4	O5-C9	2.34	1.40	1.33	3	1
3	A	624	PX4	O7-C7	2.34	1.41	1.46	1	1
3	B	368	PX4	C2-N1	2.34	1.58	1.51	5	2
3	B	373	PX4	O7-C7	2.34	1.41	1.46	10	1
3	B	398	PX4	O7-C23	2.34	1.27	1.34	5	3
3	C	336	PX4	O5-C9	2.34	1.40	1.33	10	3
3	B	313	PX4	C2-C1	2.34	1.58	1.51	2	4
3	C	303	PX4	C4-N1	2.34	1.56	1.50	7	2
3	A	608	PX4	C30-C29	2.33	1.63	1.51	14	1
3	A	620	PX4	C17-C16	2.33	1.63	1.51	5	1
3	A	623	PX4	P1-O4	2.33	1.68	1.59	13	2
3	B	308	PX4	P1-O2	2.33	1.42	1.50	13	1
3	B	318	PX4	C24-C23	2.33	1.57	1.50	3	1
3	B	359	PX4	O5-C9	2.33	1.26	1.33	7	1
3	B	373	PX4	C13-C12	2.33	1.63	1.51	5	1
3	C	343	PX4	C25-C24	2.33	1.60	1.52	14	1
3	C	358	PX4	C25-C24	2.33	1.60	1.52	7	2
3	C	339	PX4	O7-C23	2.33	1.27	1.34	1	2
3	A	606	PX4	O7-C7	2.33	1.41	1.46	11	1
3	B	306	PX4	P1-O4	2.33	1.50	1.59	9	1
3	B	339	PX4	C4-N1	2.33	1.43	1.50	15	1
3	B	355	PX4	C2-N1	2.33	1.58	1.51	1	1
3	A	621	PX4	O4-C6	2.33	1.35	1.44	6	1
3	A	643	PX4	O7-C7	2.33	1.41	1.46	7	1
3	A	653	PX4	C4-N1	2.33	1.56	1.50	5	2
3	B	303	PX4	P1-O1	2.33	1.44	1.55	9	4
3	B	362	PX4	O7-C23	2.33	1.27	1.34	6	3
3	C	305	PX4	C24-C23	2.33	1.57	1.50	13	2
3	C	343	PX4	C11-C10	2.33	1.60	1.52	13	2
3	B	332	PX4	P1-O1	2.33	1.44	1.55	12	3
3	B	368	PX4	C17-C16	2.33	1.63	1.51	9	1
3	C	309	PX4	O7-C23	2.33	1.27	1.34	7	2
3	B	307	PX4	C27-C26	2.33	1.63	1.51	11	3
3	B	376	PX4	O7-C23	2.33	1.27	1.34	4	2
3	B	358	PX4	C4-N1	2.33	1.56	1.50	11	2
3	B	377	PX4	C24-C23	2.33	1.57	1.50	1	2
3	C	337	PX4	C32-C31	2.33	1.63	1.51	14	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	C	346	PX4	O5-C8	2.33	1.40	1.45	8	3
3	A	616	PX4	P1-O1	2.32	1.44	1.55	8	2
3	A	621	PX4	C19-C18	2.32	1.63	1.51	5	1
3	A	650	PX4	O5-C9	2.32	1.40	1.33	13	2
3	B	310	PX4	C13-C12	2.32	1.63	1.51	3	1
3	B	335	PX4	C27-C26	2.32	1.63	1.51	11	1
3	C	357	PX4	C29-C28	2.33	1.63	1.51	10	1
3	A	636	PX4	O7-C23	2.32	1.27	1.34	13	1
3	B	377	PX4	C19-C18	2.32	1.63	1.51	10	1
3	B	390	PX4	P1-O1	2.32	1.44	1.55	12	1
3	C	304	PX4	O7-C7	2.32	1.41	1.46	2	3
3	C	350	PX4	P1-O4	2.32	1.68	1.59	11	1
3	C	360	PX4	C16-C15	2.32	1.63	1.51	6	2
3	B	313	PX4	C10-C9	2.32	1.57	1.50	5	2
3	B	368	PX4	C32-C31	2.32	1.63	1.51	15	1
3	B	382	PX4	C17-C16	2.32	1.63	1.51	9	1
3	C	314	PX4	C25-C24	2.32	1.60	1.52	9	1
3	A	635	PX4	C14-C13	2.32	1.63	1.51	11	1
3	B	301	PX4	C31-C30	2.32	1.63	1.51	1	1
3	C	364	PX4	C4-N1	2.32	1.43	1.50	12	5
3	A	636	PX4	C28-C27	2.32	1.63	1.51	3	1
3	B	303	PX4	C25-C24	2.32	1.60	1.52	15	1
3	A	602	PX4	P1-O2	2.32	1.42	1.50	9	1
3	A	624	PX4	C2-N1	2.32	1.58	1.51	15	1
3	A	648	PX4	P1-O1	2.32	1.44	1.55	9	4
3	B	327	PX4	C25-C24	2.32	1.60	1.52	14	3
3	B	357	PX4	O5-C8	2.32	1.50	1.45	12	3
3	C	307	PX4	C2-N1	2.32	1.44	1.51	3	2
3	B	391	PX4	O7-C23	2.32	1.27	1.34	9	1
3	C	347	PX4	P1-O2	2.32	1.42	1.50	8	1
3	A	607	PX4	C25-C24	2.32	1.60	1.52	13	4
3	A	603	PX4	P1-O1	2.32	1.44	1.55	12	2
3	A	610	PX4	C3-N1	2.32	1.56	1.50	12	2
3	A	625	PX4	O5-C9	2.32	1.26	1.33	8	3
3	B	328	PX4	O4-C6	2.32	1.35	1.44	9	1
3	B	321	PX4	C2-N1	2.32	1.58	1.51	10	2
3	C	328	PX4	C25-C24	2.32	1.60	1.52	2	2
3	A	652	PX4	C29-C28	2.31	1.63	1.51	14	1
3	B	342	PX4	C13-C12	2.31	1.63	1.51	7	2
3	B	350	PX4	P1-O1	2.31	1.44	1.55	11	4
3	C	311	PX4	P1-O1	2.31	1.44	1.55	7	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	C	316	PX4	C26-C25	2.31	1.63	1.51	10	1
3	C	338	PX4	C2-N1	2.31	1.58	1.51	7	1
3	C	351	PX4	O3-C1	2.31	1.35	1.44	3	2
3	C	363	PX4	P1-O4	2.31	1.50	1.59	1	1
3	B	378	PX4	C15-C14	2.31	1.63	1.51	2	1
3	B	384	PX4	O7-C23	2.31	1.40	1.34	2	1
3	C	304	PX4	P1-O1	2.31	1.44	1.55	2	2
3	C	324	PX4	C29-C28	2.31	1.63	1.51	15	1
3	B	312	PX4	C15-C14	2.31	1.63	1.51	10	1
3	B	331	PX4	C33-C32	2.31	1.63	1.51	14	1
3	C	340	PX4	C3-N1	2.31	1.43	1.50	9	1
3	B	309	PX4	C13-C12	2.31	1.63	1.51	14	1
3	B	344	PX4	C4-N1	2.31	1.43	1.50	14	1
3	B	322	PX4	C3-N1	2.31	1.56	1.50	5	2
3	B	330	PX4	O7-C23	2.31	1.27	1.34	9	2
3	B	355	PX4	P1-O1	2.31	1.44	1.55	11	4
3	B	367	PX4	C13-C12	2.31	1.63	1.51	13	1
3	C	347	PX4	C13-C12	2.31	1.63	1.51	13	1
3	B	356	PX4	C32-C31	2.30	1.63	1.51	9	1
3	A	631	PX4	O3-C1	2.30	1.35	1.44	8	1
3	A	649	PX4	C18-C17	2.30	1.63	1.51	2	2
3	A	604	PX4	C2-N1	2.30	1.58	1.51	6	1
3	A	630	PX4	C25-C24	2.30	1.60	1.52	4	2
3	A	651	PX4	C2-N1	2.30	1.58	1.51	1	1
3	B	322	PX4	C4-N1	2.30	1.56	1.50	4	1
3	C	322	PX4	C3-N1	2.30	1.56	1.50	14	3
3	A	651	PX4	C5-N1	2.30	1.43	1.50	3	1
3	A	612	PX4	C25-C24	2.30	1.60	1.52	7	3
3	A	615	PX4	C3-N1	2.30	1.43	1.50	7	3
3	A	628	PX4	O4-C6	2.30	1.35	1.44	14	1
3	A	638	PX4	C27-C26	2.30	1.63	1.51	11	1
3	B	325	PX4	C25-C24	2.30	1.60	1.52	3	2
3	B	302	PX4	C28-C27	2.30	1.63	1.51	13	1
3	B	336	PX4	C24-C23	2.30	1.57	1.50	13	1
3	C	322	PX4	C5-N1	2.30	1.56	1.50	7	1
3	A	650	PX4	C19-C18	2.30	1.63	1.51	1	1
3	C	332	PX4	O7-C7	2.30	1.52	1.46	9	2
3	C	353	PX4	P1-O1	2.30	1.44	1.55	8	2
3	A	621	PX4	P1-O3	2.30	1.50	1.59	1	1
3	A	622	PX4	C14-C13	2.30	1.63	1.51	15	1
3	A	625	PX4	P1-O4	2.30	1.50	1.59	10	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	A	625	PX4	C26-C25	2.30	1.63	1.51	3	1
3	B	398	PX4	O7-C7	2.30	1.41	1.46	12	4
3	C	310	PX4	C24-C23	2.30	1.57	1.50	13	1
3	C	323	PX4	C12-C11	2.30	1.63	1.51	6	1
3	B	336	PX4	C26-C25	2.30	1.63	1.51	11	1
3	C	332	PX4	C3-N1	2.30	1.43	1.50	9	1
3	C	338	PX4	C33-C32	2.30	1.63	1.51	2	1
3	A	621	PX4	O5-C8	2.29	1.50	1.45	10	3
3	A	625	PX4	O7-C23	2.29	1.27	1.34	9	1
3	B	307	PX4	C26-C25	2.29	1.63	1.51	14	1
3	C	311	PX4	C5-N1	2.30	1.56	1.50	12	1
3	C	361	PX4	C19-C18	2.30	1.63	1.51	1	1
3	B	343	PX4	O4-C6	2.29	1.35	1.44	4	1
3	B	398	PX4	C4-N1	2.29	1.43	1.50	13	1
3	C	322	PX4	O5-C8	2.29	1.40	1.45	4	1
3	A	651	PX4	C24-C23	2.29	1.57	1.50	1	3
3	A	651	PX4	C16-C15	2.29	1.63	1.51	3	1
3	B	306	PX4	C2-N1	2.29	1.44	1.51	6	3
3	B	329	PX4	P1-O2	2.29	1.42	1.50	14	2
3	C	316	PX4	C4-N1	2.29	1.43	1.50	10	1
3	C	336	PX4	P1-O1	2.29	1.44	1.55	1	3
3	C	345	PX4	O5-C9	2.29	1.40	1.33	6	2
3	A	606	PX4	O4-C6	2.29	1.35	1.44	5	1
3	A	630	PX4	C10-C9	2.29	1.57	1.50	7	3
3	B	305	PX4	C11-C10	2.29	1.60	1.52	12	1
3	B	307	PX4	C5-N1	2.29	1.56	1.50	15	3
3	B	357	PX4	O5-C9	2.29	1.40	1.33	6	1
3	B	361	PX4	O5-C9	2.29	1.40	1.33	5	2
3	B	367	PX4	C29-C28	2.29	1.63	1.51	8	1
3	B	395	PX4	C31-C30	2.29	1.63	1.51	2	1
3	C	318	PX4	C25-C24	2.29	1.60	1.52	14	3
3	C	319	PX4	O7-C23	2.29	1.27	1.34	14	4
3	A	624	PX4	C24-C23	2.29	1.57	1.50	6	2
3	B	337	PX4	C2-N1	2.29	1.58	1.51	8	3
3	B	340	PX4	P1-O1	2.29	1.44	1.55	12	1
3	B	380	PX4	C2-N1	2.29	1.58	1.51	6	1
3	B	394	PX4	C3-N1	2.29	1.56	1.50	5	2
3	C	302	PX4	O5-C9	2.29	1.26	1.33	5	1
3	B	365	PX4	P1-O2	2.29	1.42	1.50	9	2
3	B	368	PX4	O5-C9	2.29	1.40	1.33	4	2
3	C	303	PX4	C15-C14	2.29	1.63	1.51	3	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	C	321	PX4	C34-C33	2.29	1.63	1.51	2	1
3	C	345	PX4	C2-N1	2.29	1.58	1.51	15	1
3	C	349	PX4	P1-O2	2.29	1.42	1.50	14	1
3	A	631	PX4	O5-C8	2.29	1.40	1.45	2	2
3	A	645	PX4	O5-C9	2.29	1.40	1.33	15	2
3	B	317	PX4	C11-C10	2.29	1.60	1.52	2	1
3	B	338	PX4	C33-C32	2.29	1.63	1.51	6	1
3	B	351	PX4	P1-O1	2.29	1.44	1.55	12	1
3	C	364	PX4	C25-C24	2.29	1.60	1.52	5	2
3	B	311	PX4	C13-C12	2.28	1.63	1.51	9	1
3	B	324	PX4	C34-C33	2.28	1.63	1.51	11	1
3	B	327	PX4	P1-O1	2.29	1.44	1.55	7	3
3	A	642	PX4	O7-C23	2.28	1.27	1.34	3	2
3	B	338	PX4	C3-N1	2.28	1.56	1.50	4	2
3	B	338	PX4	O4-C6	2.28	1.36	1.44	13	1
3	B	361	PX4	C20-C19	2.28	1.63	1.51	13	1
3	A	611	PX4	C2-N1	2.28	1.44	1.51	2	2
3	B	303	PX4	O7-C23	2.28	1.27	1.34	6	1
3	B	315	PX4	O7-C23	2.28	1.27	1.34	6	3
3	B	339	PX4	C24-C23	2.28	1.57	1.50	11	2
3	B	379	PX4	P1-O1	2.28	1.44	1.55	7	1
3	B	392	PX4	C17-C16	2.28	1.63	1.51	6	1
3	A	618	PX4	C25-C24	2.28	1.60	1.52	1	1
3	A	637	PX4	C2-N1	2.28	1.58	1.51	2	1
3	B	315	PX4	C30-C29	2.28	1.63	1.51	7	1
3	C	324	PX4	C10-C9	2.28	1.57	1.50	1	2
3	C	336	PX4	C5-N1	2.28	1.56	1.50	8	1
3	B	326	PX4	C11-C10	2.28	1.60	1.52	5	1
3	A	610	PX4	O7-C23	2.28	1.27	1.34	12	2
3	A	619	PX4	P1-O1	2.28	1.44	1.55	9	1
3	A	642	PX4	C2-N1	2.28	1.44	1.51	14	1
3	A	654	PX4	O5-C9	2.28	1.26	1.33	3	1
3	B	348	PX4	C11-C10	2.28	1.60	1.52	8	2
3	B	369	PX4	O5-C9	2.28	1.40	1.33	6	3
3	C	337	PX4	C3-N1	2.28	1.56	1.50	11	1
3	A	619	PX4	O5-C9	2.28	1.40	1.33	14	1
3	B	323	PX4	C11-C10	2.28	1.60	1.52	4	2
3	B	323	PX4	C13-C12	2.28	1.63	1.51	4	1
3	B	354	PX4	C2-N1	2.28	1.58	1.51	8	2
3	B	370	PX4	C33-C32	2.28	1.63	1.51	10	1
3	C	314	PX4	C11-C10	2.28	1.60	1.52	14	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	C	317	PX4	P1-O4	2.28	1.50	1.59	5	2
3	C	324	PX4	O5-C8	2.28	1.40	1.45	7	2
3	C	364	PX4	C11-C10	2.28	1.60	1.52	14	2
3	A	614	PX4	C31-C30	2.28	1.63	1.51	9	1
3	B	335	PX4	O7-C23	2.28	1.27	1.34	11	2
3	B	361	PX4	C2-N1	2.28	1.58	1.51	8	1
3	B	378	PX4	C2-N1	2.28	1.58	1.51	2	1
3	B	394	PX4	C11-C10	2.28	1.60	1.52	4	3
3	C	346	PX4	C30-C29	2.28	1.63	1.51	3	1
3	A	623	PX4	O7-C23	2.28	1.27	1.34	7	2
3	B	349	PX4	C16-C15	2.28	1.63	1.51	8	1
3	C	312	PX4	C3-N1	2.28	1.56	1.50	7	1
3	C	362	PX4	C3-N1	2.28	1.43	1.50	9	2
3	B	388	PX4	O5-C8	2.27	1.40	1.45	7	1
3	C	305	PX4	C3-N1	2.28	1.43	1.50	7	1
3	B	366	PX4	C28-C27	2.27	1.63	1.51	1	1
3	B	372	PX4	C2-N1	2.27	1.58	1.51	1	2
3	C	335	PX4	C25-C24	2.27	1.60	1.52	6	1
3	A	610	PX4	P1-O3	2.27	1.50	1.59	4	1
3	A	622	PX4	C4-N1	2.27	1.43	1.50	11	2
3	B	314	PX4	C5-N1	2.27	1.43	1.50	15	1
3	C	322	PX4	O5-C9	2.27	1.26	1.33	15	3
3	C	338	PX4	C26-C25	2.27	1.63	1.51	12	1
3	C	356	PX4	C2-N1	2.27	1.58	1.51	13	2
3	A	614	PX4	C5-N1	2.27	1.43	1.50	4	2
3	A	621	PX4	C25-C24	2.27	1.60	1.52	9	1
3	A	637	PX4	C24-C23	2.27	1.57	1.50	5	1
3	B	343	PX4	O5-C8	2.27	1.40	1.45	7	1
3	B	356	PX4	C16-C15	2.27	1.63	1.51	12	1
3	B	396	PX4	O6-C9	2.27	1.15	1.22	8	2
3	C	347	PX4	P1-O1	2.27	1.44	1.55	6	4
3	A	648	PX4	C11-C10	2.27	1.60	1.52	9	2
3	B	329	PX4	C26-C25	2.27	1.63	1.51	11	2
3	B	392	PX4	C24-C23	2.27	1.57	1.50	12	1
3	C	301	PX4	C2-N1	2.27	1.58	1.51	6	2
3	A	615	PX4	C29-C28	2.27	1.63	1.51	9	1
3	A	629	PX4	C5-N1	2.27	1.56	1.50	8	1
3	B	304	PX4	C30-C29	2.27	1.63	1.51	10	1
3	B	311	PX4	O4-C6	2.27	1.36	1.44	12	1
3	B	315	PX4	C19-C18	2.27	1.63	1.51	3	1
3	B	342	PX4	P1-O1	2.27	1.44	1.55	14	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	A	625	PX4	O7-C7	2.27	1.51	1.46	10	1
3	A	641	PX4	C11-C10	2.27	1.60	1.52	15	2
3	A	654	PX4	C3-N1	2.27	1.56	1.50	8	1
3	B	319	PX4	P1-O1	2.27	1.44	1.55	2	4
3	B	327	PX4	C20-C19	2.27	1.63	1.51	1	2
3	B	339	PX4	O3-C1	2.27	1.35	1.44	4	1
3	A	610	PX4	C11-C10	2.26	1.60	1.52	12	2
3	B	329	PX4	O5-C9	2.26	1.40	1.33	9	3
3	B	353	PX4	P1-O3	2.27	1.68	1.59	7	1
3	B	384	PX4	O5-C8	2.27	1.50	1.45	4	2
3	C	347	PX4	C10-C9	2.27	1.57	1.50	7	2
3	A	618	PX4	O7-C7	2.26	1.41	1.46	15	2
3	B	315	PX4	C12-C11	2.26	1.63	1.51	12	1
3	B	329	PX4	P1-O1	2.26	1.44	1.55	2	2
3	B	372	PX4	C3-N1	2.26	1.56	1.50	5	1
3	C	359	PX4	C25-C24	2.26	1.60	1.52	4	1
3	A	653	PX4	C5-N1	2.26	1.56	1.50	6	1
3	B	379	PX4	C2-N1	2.26	1.44	1.51	4	2
3	B	384	PX4	C18-C17	2.26	1.63	1.51	3	1
3	B	387	PX4	C31-C30	2.26	1.63	1.51	15	1
3	C	332	PX4	C16-C15	2.26	1.63	1.51	3	1
3	A	617	PX4	O7-C7	2.26	1.41	1.46	12	2
3	B	326	PX4	O7-C7	2.26	1.41	1.46	3	1
3	B	357	PX4	C12-C11	2.26	1.63	1.51	5	1
3	B	367	PX4	C27-C26	2.26	1.63	1.51	6	1
3	B	382	PX4	C29-C28	2.26	1.63	1.51	4	1
3	A	611	PX4	C32-C31	2.26	1.63	1.51	15	1
3	B	398	PX4	O5-C9	2.26	1.26	1.33	9	1
3	A	621	PX4	O3-C1	2.26	1.35	1.44	15	1
3	B	327	PX4	O5-C9	2.26	1.26	1.33	12	1
3	C	314	PX4	P1-O2	2.26	1.43	1.50	13	1
3	B	375	PX4	C11-C10	2.26	1.60	1.52	15	1
3	C	362	PX4	C12-C11	2.26	1.63	1.51	1	1
3	A	606	PX4	P1-O3	2.26	1.50	1.59	11	2
3	B	396	PX4	P1-O4	2.26	1.50	1.59	3	1
3	C	329	PX4	O7-C23	2.26	1.27	1.34	12	2
3	C	361	PX4	C5-N1	2.26	1.56	1.50	1	1
3	A	637	PX4	C20-C19	2.25	1.63	1.51	15	2
3	A	650	PX4	O7-C7	2.25	1.41	1.46	1	2
3	B	323	PX4	C5-N1	2.25	1.43	1.50	1	2
3	A	614	PX4	C2-N1	2.25	1.58	1.51	5	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	A	624	PX4	C11-C10	2.25	1.60	1.52	2	1
3	A	649	PX4	C11-C10	2.25	1.60	1.52	13	3
3	B	339	PX4	C26-C25	2.25	1.63	1.51	14	1
3	B	388	PX4	C19-C18	2.25	1.63	1.51	6	1
3	C	312	PX4	C25-C24	2.25	1.60	1.52	5	1
3	C	332	PX4	C10-C9	2.25	1.57	1.50	12	2
3	B	309	PX4	C31-C30	2.25	1.63	1.51	6	1
3	B	320	PX4	O3-C1	2.25	1.35	1.44	4	1
3	B	336	PX4	C4-N1	2.25	1.43	1.50	2	3
3	B	350	PX4	C17-C16	2.25	1.63	1.51	2	1
3	A	623	PX4	P1-O1	2.25	1.44	1.55	11	2
3	B	369	PX4	O3-C1	2.25	1.35	1.44	6	1
3	B	396	PX4	C34-C33	2.25	1.63	1.51	13	1
3	C	302	PX4	C18-C17	2.25	1.63	1.51	7	1
3	C	306	PX4	C14-C13	2.25	1.63	1.51	14	1
3	B	371	PX4	P1-O1	2.25	1.44	1.55	1	2
3	C	322	PX4	O7-C23	2.25	1.27	1.34	7	2
3	C	356	PX4	P1-O1	2.25	1.44	1.55	15	3
3	C	357	PX4	P1-O2	2.25	1.43	1.50	15	2
3	A	618	PX4	P1-O3	2.25	1.50	1.59	15	1
3	A	620	PX4	C3-N1	2.25	1.56	1.50	9	1
3	B	304	PX4	O7-C7	2.25	1.51	1.46	13	2
3	B	359	PX4	C3-N1	2.25	1.56	1.50	15	1
3	C	302	PX4	O7-C23	2.25	1.40	1.34	14	4
3	C	343	PX4	C20-C19	2.25	1.63	1.51	6	1
3	A	642	PX4	O4-C6	2.25	1.36	1.44	6	1
3	A	642	PX4	P1-O1	2.25	1.44	1.55	14	1
3	A	654	PX4	C11-C10	2.25	1.60	1.52	8	1
3	B	318	PX4	O7-C7	2.25	1.41	1.46	2	2
3	B	318	PX4	O5-C9	2.25	1.39	1.33	2	1
3	B	361	PX4	C3-N1	2.25	1.43	1.50	5	1
3	B	385	PX4	P1-O1	2.25	1.44	1.55	5	3
3	C	340	PX4	C20-C19	2.25	1.63	1.51	5	1
3	C	359	PX4	C11-C10	2.25	1.60	1.52	15	1
3	B	349	PX4	P1-O2	2.25	1.43	1.50	1	1
3	C	336	PX4	C2-N1	2.25	1.58	1.51	1	2
3	A	627	PX4	C2-N1	2.24	1.58	1.51	8	2
3	B	312	PX4	C11-C10	2.24	1.60	1.52	10	2
3	B	320	PX4	O7-C23	2.25	1.27	1.34	2	2
3	B	330	PX4	O6-C9	2.24	1.15	1.22	15	1
3	B	344	PX4	C5-N1	2.24	1.56	1.50	7	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	362	PX4	C12-C11	2.24	1.62	1.51	3	1
3	B	376	PX4	C31-C30	2.24	1.62	1.51	2	1
3	C	320	PX4	P1-O1	2.25	1.44	1.55	4	1
3	A	607	PX4	C32-C31	2.24	1.62	1.51	3	1
3	A	624	PX4	C4-N1	2.24	1.56	1.50	10	1
3	A	604	PX4	O3-C1	2.24	1.35	1.44	9	1
3	A	606	PX4	C10-C9	2.24	1.57	1.50	2	2
3	A	610	PX4	C33-C32	2.24	1.62	1.51	5	1
3	B	326	PX4	C33-C32	2.24	1.62	1.51	7	1
3	B	373	PX4	C31-C30	2.24	1.62	1.51	4	1
3	B	385	PX4	P1-O2	2.24	1.43	1.50	2	1
3	B	396	PX4	C2-N1	2.24	1.44	1.51	5	2
3	C	306	PX4	P1-O2	2.24	1.43	1.50	11	1
3	C	328	PX4	O4-C6	2.24	1.36	1.44	5	1
3	A	622	PX4	P1-O2	2.24	1.43	1.50	14	1
3	B	304	PX4	P1-O1	2.24	1.45	1.55	4	2
3	B	374	PX4	C12-C11	2.24	1.62	1.51	2	1
3	A	621	PX4	P1-O2	2.24	1.43	1.50	7	1
3	B	393	PX4	C27-C26	2.24	1.62	1.51	1	1
3	B	374	PX4	O7-C7	2.24	1.41	1.46	6	2
3	B	381	PX4	C25-C24	2.24	1.60	1.52	4	2
3	B	396	PX4	C3-N1	2.24	1.56	1.50	10	1
3	C	318	PX4	O7-C7	2.24	1.41	1.46	7	1
3	C	343	PX4	O3-C1	2.24	1.53	1.44	11	1
3	C	344	PX4	P1-O1	2.24	1.45	1.55	3	3
3	B	307	PX4	O5-C9	2.24	1.26	1.33	3	2
3	B	324	PX4	C14-C13	2.24	1.62	1.51	1	1
3	B	327	PX4	P1-O3	2.24	1.50	1.59	2	1
3	B	345	PX4	C3-N1	2.24	1.56	1.50	12	3
3	B	389	PX4	C29-C28	2.24	1.62	1.51	14	2
3	C	307	PX4	O5-C9	2.24	1.39	1.33	8	2
3	C	309	PX4	C24-C23	2.24	1.57	1.50	15	2
3	C	314	PX4	C20-C19	2.24	1.62	1.51	8	1
3	A	635	PX4	O5-C8	2.24	1.40	1.45	5	1
3	A	601	PX4	C2-C1	2.23	1.58	1.51	2	4
3	A	614	PX4	P1-O1	2.23	1.45	1.55	15	1
3	B	302	PX4	O5-C8	2.23	1.40	1.45	13	1
3	B	395	PX4	O4-C6	2.24	1.36	1.44	1	1
3	C	338	PX4	C12-C11	2.24	1.62	1.51	14	1
3	B	310	PX4	C20-C19	2.23	1.62	1.51	9	1
3	B	323	PX4	C25-C24	2.23	1.60	1.52	3	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	351	PX4	C4-N1	2.23	1.56	1.50	2	2
3	B	354	PX4	C12-C11	2.23	1.62	1.51	8	1
3	B	373	PX4	C11-C10	2.23	1.60	1.52	2	1
3	C	321	PX4	C30-C29	2.23	1.62	1.51	5	1
3	C	364	PX4	C24-C23	2.23	1.57	1.50	6	1
3	C	301	PX4	O7-C7	2.23	1.41	1.46	3	2
3	B	397	PX4	C33-C32	2.23	1.62	1.51	14	1
3	C	338	PX4	C30-C29	2.23	1.62	1.51	3	1
3	C	352	PX4	O5-C9	2.23	1.39	1.33	8	1
3	B	303	PX4	C32-C31	2.23	1.62	1.51	5	1
3	B	308	PX4	P1-O3	2.23	1.50	1.59	10	1
3	B	312	PX4	P1-O1	2.23	1.45	1.55	2	4
3	C	361	PX4	O7-C7	2.23	1.41	1.46	1	1
3	C	363	PX4	O5-C9	2.23	1.39	1.33	15	1
3	A	640	PX4	C28-C27	2.23	1.62	1.51	7	1
3	C	321	PX4	C31-C30	2.23	1.62	1.51	15	1
3	A	652	PX4	O7-C7	2.23	1.41	1.46	7	2
3	B	324	PX4	C12-C11	2.23	1.62	1.51	6	1
3	B	364	PX4	C17-C16	2.23	1.62	1.51	15	1
3	B	378	PX4	O7-C23	2.23	1.28	1.34	11	1
3	C	351	PX4	C18-C17	2.23	1.62	1.51	7	1
3	B	369	PX4	C17-C16	2.23	1.62	1.51	11	1
3	C	361	PX4	C2-N1	2.23	1.58	1.51	6	1
3	B	390	PX4	C5-N1	2.23	1.56	1.50	13	2
3	C	305	PX4	C28-C27	2.23	1.62	1.51	2	1
3	A	636	PX4	C11-C10	2.23	1.60	1.52	10	1
3	B	313	PX4	C17-C16	2.23	1.62	1.51	12	1
3	B	328	PX4	C28-C27	2.23	1.62	1.51	13	1
3	B	399	PX4	P1-O1	2.23	1.45	1.55	1	2
3	C	358	PX4	P1-O1	2.23	1.45	1.55	4	2
3	A	652	PX4	P1-O1	2.22	1.45	1.55	2	2
3	A	649	PX4	C20-C19	2.22	1.62	1.51	2	1
3	B	308	PX4	O3-C1	2.22	1.35	1.44	8	1
3	C	306	PX4	O4-C6	2.22	1.36	1.44	7	1
3	C	309	PX4	C26-C25	2.22	1.62	1.51	3	1
3	C	351	PX4	O5-C9	2.22	1.26	1.33	5	1
3	B	310	PX4	C11-C10	2.22	1.60	1.52	9	1
3	B	339	PX4	O7-C23	2.22	1.28	1.34	7	1
3	B	369	PX4	P1-O1	2.22	1.45	1.55	7	4
3	B	397	PX4	P1-O1	2.22	1.45	1.55	13	2
3	C	315	PX4	O5-C9	2.22	1.39	1.33	15	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	A	643	PX4	P1-O2	2.22	1.43	1.50	14	2
3	C	317	PX4	O5-C9	2.22	1.39	1.33	13	1
3	A	609	PX4	P1-O1	2.22	1.45	1.55	2	2
3	A	623	PX4	C34-C33	2.22	1.62	1.51	8	1
3	B	302	PX4	P1-O1	2.22	1.45	1.55	15	1
3	B	305	PX4	C24-C23	2.22	1.57	1.50	1	1
3	B	343	PX4	C11-C10	2.22	1.60	1.52	8	1
3	B	347	PX4	O5-C9	2.22	1.39	1.33	12	2
3	B	360	PX4	C33-C32	2.22	1.62	1.51	1	1
3	C	324	PX4	C17-C16	2.22	1.62	1.51	8	1
3	C	327	PX4	C16-C15	2.22	1.62	1.51	7	2
3	A	629	PX4	P1-O1	2.22	1.45	1.55	5	3
3	A	643	PX4	C17-C16	2.22	1.62	1.51	4	1
3	B	319	PX4	C10-C9	2.22	1.57	1.50	13	5
3	A	646	PX4	C15-C14	2.22	1.62	1.51	14	1
3	A	652	PX4	O8-C23	2.22	1.29	1.22	9	1
3	B	351	PX4	C11-C10	2.22	1.60	1.52	9	2
3	B	383	PX4	C31-C30	2.22	1.62	1.51	7	1
3	C	307	PX4	C15-C14	2.22	1.62	1.51	6	1
3	B	320	PX4	C15-C14	2.22	1.62	1.51	6	2
3	A	613	PX4	O5-C9	2.21	1.26	1.33	9	1
3	B	331	PX4	C12-C11	2.22	1.62	1.51	8	1
3	B	361	PX4	C19-C18	2.22	1.62	1.51	11	1
3	B	355	PX4	C34-C33	2.21	1.62	1.51	13	1
3	B	305	PX4	C20-C19	2.21	1.62	1.51	8	1
3	B	315	PX4	P1-O1	2.21	1.45	1.55	2	2
3	A	608	PX4	C10-C9	2.21	1.57	1.50	8	2
3	A	609	PX4	O7-C7	2.21	1.41	1.46	15	2
3	B	356	PX4	C19-C18	2.21	1.62	1.51	15	1
3	B	380	PX4	O7-C7	2.21	1.41	1.46	2	1
3	B	382	PX4	C5-N1	2.21	1.56	1.50	7	1
3	B	396	PX4	C29-C28	2.21	1.62	1.51	13	1
3	C	307	PX4	C12-C11	2.21	1.62	1.51	11	1
3	C	363	PX4	C10-C9	2.21	1.57	1.50	10	3
3	A	642	PX4	C16-C15	2.21	1.62	1.51	15	1
3	B	304	PX4	C10-C9	2.21	1.57	1.50	2	2
3	B	361	PX4	C24-C23	2.21	1.57	1.50	11	2
3	B	362	PX4	P1-O2	2.21	1.43	1.50	2	3
3	C	308	PX4	O7-C23	2.21	1.28	1.34	7	1
3	A	610	PX4	C2-N1	2.21	1.58	1.51	10	1
3	A	621	PX4	C2-N1	2.21	1.58	1.51	7	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	305	PX4	C25-C24	2.21	1.60	1.52	12	1
3	B	320	PX4	C21-C20	2.21	1.65	1.51	12	1
3	B	333	PX4	C3-N1	2.21	1.43	1.50	8	1
3	B	352	PX4	O5-C8	2.21	1.50	1.45	15	2
3	C	317	PX4	C25-C24	2.21	1.60	1.52	9	3
3	B	393	PX4	C13-C12	2.21	1.62	1.51	15	1
3	C	316	PX4	O5-C8	2.21	1.50	1.45	5	1
3	C	321	PX4	O5-C8	2.21	1.40	1.45	12	2
3	A	635	PX4	O5-C9	2.21	1.39	1.33	15	3
3	A	638	PX4	C10-C9	2.21	1.57	1.50	3	1
3	B	301	PX4	P1-O2	2.21	1.43	1.50	12	1
3	B	322	PX4	P1-O2	2.21	1.43	1.50	9	1
3	C	346	PX4	C11-C10	2.21	1.60	1.52	14	2
3	A	603	PX4	C5-N1	2.21	1.56	1.50	1	1
3	A	636	PX4	C4-N1	2.21	1.56	1.50	7	2
3	B	322	PX4	C2-N1	2.21	1.44	1.51	14	2
3	B	334	PX4	C18-C17	2.21	1.62	1.51	11	2
3	B	351	PX4	C27-C26	2.21	1.62	1.51	6	2
3	B	358	PX4	C2-N1	2.21	1.58	1.51	1	1
3	C	328	PX4	P1-O2	2.21	1.43	1.50	2	1
3	C	356	PX4	C27-C26	2.21	1.62	1.51	8	1
3	A	636	PX4	P1-O1	2.21	1.45	1.55	7	2
3	A	640	PX4	C19-C18	2.21	1.62	1.51	3	1
3	B	330	PX4	C28-C27	2.21	1.62	1.51	14	1
3	B	365	PX4	C5-N1	2.21	1.56	1.50	9	5
3	B	376	PX4	C33-C32	2.20	1.62	1.51	9	1
3	B	393	PX4	C11-C10	2.21	1.60	1.52	14	3
3	B	390	PX4	C3-N1	2.20	1.56	1.50	1	2
3	B	398	PX4	C34-C33	2.20	1.62	1.51	9	1
3	C	304	PX4	C3-N1	2.21	1.56	1.50	8	1
3	A	619	PX4	C11-C10	2.20	1.60	1.52	5	1
3	A	647	PX4	C25-C24	2.20	1.60	1.52	15	1
3	B	320	PX4	C3-N1	2.20	1.43	1.50	9	3
3	A	633	PX4	C31-C30	2.20	1.62	1.51	2	1
3	A	643	PX4	C12-C11	2.20	1.62	1.51	1	1
3	B	323	PX4	P1-O4	2.20	1.50	1.59	4	1
3	B	374	PX4	C25-C24	2.20	1.60	1.52	3	1
3	B	395	PX4	O3-C1	2.20	1.35	1.44	9	1
3	C	324	PX4	C25-C24	2.20	1.60	1.52	5	1
3	B	316	PX4	C17-C16	2.20	1.62	1.51	14	1
3	B	323	PX4	O5-C9	2.20	1.39	1.33	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	346	PX4	C29-C28	2.20	1.62	1.51	13	2
3	B	378	PX4	C3-N1	2.20	1.56	1.50	1	1
3	B	379	PX4	O5-C8	2.20	1.40	1.45	5	1
3	C	326	PX4	C11-C10	2.20	1.60	1.52	1	1
3	B	350	PX4	C25-C24	2.20	1.60	1.52	12	1
3	B	352	PX4	C3-N1	2.20	1.56	1.50	15	1
3	B	353	PX4	C11-C10	2.20	1.60	1.52	6	1
3	B	377	PX4	P1-O1	2.20	1.45	1.55	10	1
3	B	381	PX4	C14-C13	2.20	1.62	1.51	14	1
3	B	389	PX4	C5-N1	2.20	1.56	1.50	11	1
3	C	343	PX4	O5-C8	2.20	1.40	1.45	15	3
3	C	345	PX4	P1-O4	2.20	1.50	1.59	12	2
3	C	363	PX4	C11-C10	2.20	1.60	1.52	10	1
3	A	611	PX4	C13-C12	2.20	1.62	1.51	11	1
3	B	340	PX4	C3-N1	2.20	1.56	1.50	13	1
3	B	358	PX4	C28-C27	2.20	1.62	1.51	4	1
3	B	400	PX4	O5-C8	2.20	1.40	1.45	14	3
3	C	319	PX4	C13-C12	2.20	1.62	1.51	9	1
3	C	321	PX4	C33-C32	2.20	1.62	1.51	1	1
3	A	629	PX4	O5-C9	2.20	1.39	1.33	12	1
3	C	328	PX4	C29-C28	2.20	1.62	1.51	8	1
3	B	394	PX4	C4-N1	2.19	1.56	1.50	4	2
3	B	395	PX4	P1-O3	2.19	1.50	1.59	13	1
3	C	305	PX4	P1-O1	2.20	1.45	1.55	12	3
3	C	339	PX4	P1-O1	2.20	1.45	1.55	8	1
3	C	355	PX4	C20-C19	2.20	1.62	1.51	11	1
3	C	360	PX4	C27-C26	2.20	1.62	1.51	14	1
3	C	362	PX4	C4-N1	2.20	1.56	1.50	4	1
3	C	362	PX4	P1-O2	2.20	1.43	1.50	8	1
3	A	612	PX4	C11-C10	2.19	1.60	1.52	7	1
3	A	619	PX4	C19-C18	2.19	1.62	1.51	15	1
3	B	309	PX4	C10-C9	2.19	1.57	1.50	5	2
3	B	325	PX4	C6-C7	2.19	1.57	1.50	4	2
3	B	334	PX4	C28-C27	2.19	1.62	1.51	13	1
3	B	354	PX4	O3-C1	2.19	1.36	1.44	3	1
3	C	309	PX4	P1-O4	2.19	1.50	1.59	6	1
3	C	331	PX4	P1-O1	2.19	1.45	1.55	3	2
3	A	613	PX4	C10-C9	2.19	1.57	1.50	12	2
3	B	361	PX4	P1-O1	2.19	1.45	1.55	5	1
3	C	328	PX4	C17-C16	2.19	1.62	1.51	5	1
3	C	351	PX4	O5-C8	2.19	1.40	1.45	3	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	310	PX4	C24-C23	2.19	1.57	1.50	4	1
3	B	312	PX4	O7-C23	2.19	1.28	1.34	2	2
3	C	307	PX4	C32-C31	2.19	1.62	1.51	7	1
3	C	331	PX4	P1-O4	2.19	1.50	1.59	14	1
3	A	606	PX4	C25-C24	2.19	1.60	1.52	12	2
3	A	627	PX4	C10-C9	2.19	1.57	1.50	10	2
3	B	318	PX4	P1-O2	2.19	1.43	1.50	9	1
3	B	350	PX4	C5-N1	2.19	1.56	1.50	2	1
3	B	374	PX4	O7-C23	2.19	1.28	1.34	12	2
3	C	348	PX4	C11-C10	2.19	1.60	1.52	9	4
3	A	604	PX4	P1-O1	2.19	1.45	1.55	9	2
3	A	629	PX4	P1-O2	2.19	1.43	1.50	5	1
3	C	326	PX4	C13-C12	2.19	1.62	1.51	4	1
3	C	326	PX4	C4-N1	2.19	1.56	1.50	14	1
3	C	362	PX4	C20-C19	2.19	1.62	1.51	12	1
3	B	364	PX4	P1-O1	2.19	1.45	1.55	2	2
3	C	337	PX4	P1-O1	2.19	1.45	1.55	2	3
3	A	651	PX4	P1-O1	2.18	1.45	1.55	12	1
3	A	654	PX4	C25-C24	2.18	1.60	1.52	8	2
3	C	323	PX4	C13-C12	2.18	1.62	1.51	11	1
3	C	325	PX4	C13-C12	2.18	1.62	1.51	1	1
3	B	362	PX4	C5-N1	2.18	1.56	1.50	10	1
3	C	341	PX4	C13-C12	2.18	1.62	1.51	1	1
3	A	647	PX4	C4-N1	2.18	1.56	1.50	5	3
3	A	651	PX4	C12-C11	2.18	1.62	1.51	11	1
3	B	384	PX4	C30-C29	2.18	1.62	1.51	8	1
3	B	362	PX4	C25-C24	2.18	1.60	1.52	9	1
3	B	387	PX4	C4-N1	2.18	1.56	1.50	7	2
3	C	364	PX4	C19-C18	2.18	1.62	1.51	5	1
3	A	617	PX4	C34-C33	2.18	1.62	1.51	9	1
3	A	621	PX4	C14-C13	2.18	1.62	1.51	1	1
3	A	650	PX4	C5-N1	2.18	1.56	1.50	3	1
3	C	319	PX4	C11-C10	2.18	1.60	1.52	10	1
3	C	324	PX4	C16-C15	2.18	1.62	1.51	3	1
3	C	347	PX4	C4-N1	2.18	1.56	1.50	2	1
3	A	633	PX4	C5-N1	2.18	1.56	1.50	11	1
3	C	301	PX4	C3-N1	2.18	1.56	1.50	10	1
3	B	312	PX4	C13-C12	2.18	1.62	1.51	11	1
3	B	361	PX4	C5-N1	2.18	1.56	1.50	6	1
3	B	372	PX4	C13-C12	2.18	1.62	1.51	1	1
3	B	373	PX4	C25-C24	2.18	1.60	1.52	7	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	C	315	PX4	P1-O1	2.18	1.45	1.55	15	3
3	C	321	PX4	O4-C6	2.18	1.36	1.44	3	1
3	C	324	PX4	C3-N1	2.18	1.56	1.50	7	1
3	C	355	PX4	C29-C28	2.18	1.62	1.51	12	1
3	B	374	PX4	C17-C16	2.18	1.62	1.51	14	1
3	B	397	PX4	C11-C10	2.18	1.60	1.52	8	1
3	B	380	PX4	C3-N1	2.18	1.56	1.50	1	1
3	B	393	PX4	P1-O1	2.18	1.45	1.55	4	2
3	C	349	PX4	C11-C10	2.18	1.60	1.52	12	3
3	A	650	PX4	C2-C1	2.18	1.57	1.51	6	2
3	A	652	PX4	C26-C25	2.17	1.62	1.51	12	1
3	C	312	PX4	C28-C27	2.18	1.62	1.51	4	1
3	A	649	PX4	C4-N1	2.17	1.43	1.50	12	1
3	B	352	PX4	C24-C23	2.17	1.57	1.50	14	1
3	B	365	PX4	C24-C23	2.17	1.57	1.50	11	1
3	B	380	PX4	C25-C24	2.17	1.60	1.52	4	1
3	B	366	PX4	C10-C9	2.17	1.57	1.50	2	1
3	B	382	PX4	C12-C11	2.17	1.62	1.51	10	1
3	C	321	PX4	C32-C31	2.17	1.62	1.51	7	1
3	C	347	PX4	C16-C15	2.17	1.62	1.51	9	1
3	B	309	PX4	C25-C24	2.17	1.60	1.52	11	2
3	B	313	PX4	O7-C23	2.17	1.28	1.34	6	2
3	B	328	PX4	O7-C23	2.17	1.28	1.34	6	2
3	B	336	PX4	C16-C15	2.17	1.62	1.51	1	1
3	A	615	PX4	O5-C9	2.17	1.27	1.33	12	1
3	B	338	PX4	C30-C29	2.17	1.62	1.51	8	2
3	B	359	PX4	C25-C24	2.17	1.60	1.52	9	1
3	B	375	PX4	O7-C23	2.17	1.28	1.34	3	1
3	B	385	PX4	C5-N1	2.17	1.43	1.50	13	2
3	C	317	PX4	C3-N1	2.17	1.56	1.50	3	1
3	A	644	PX4	C4-N1	2.17	1.56	1.50	6	1
3	C	340	PX4	C25-C24	2.17	1.60	1.52	5	1
3	B	380	PX4	C15-C14	2.17	1.62	1.51	4	1
3	B	345	PX4	C19-C18	2.17	1.62	1.51	9	1
3	C	326	PX4	O6-C9	2.17	1.29	1.22	3	1
3	A	623	PX4	C4-N1	2.17	1.56	1.50	13	1
3	A	630	PX4	O4-C6	2.17	1.36	1.44	14	1
3	A	649	PX4	C10-C9	2.17	1.57	1.50	10	1
3	C	328	PX4	C34-C33	2.17	1.62	1.51	15	1
3	C	330	PX4	C18-C17	2.17	1.62	1.51	5	1
3	A	634	PX4	O7-C23	2.17	1.28	1.34	5	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	A	643	PX4	P1-O3	2.17	1.50	1.59	3	1
3	B	334	PX4	P1-O3	2.17	1.50	1.59	3	2
3	B	335	PX4	C16-C15	2.17	1.62	1.51	10	1
3	B	335	PX4	C11-C10	2.17	1.60	1.52	14	1
3	B	343	PX4	P1-O2	2.17	1.43	1.50	10	1
3	B	359	PX4	O4-C6	2.17	1.36	1.44	7	1
3	C	333	PX4	O7-C23	2.17	1.28	1.34	1	3
3	A	637	PX4	C27-C26	2.17	1.62	1.51	14	1
3	A	639	PX4	C18-C17	2.16	1.62	1.51	4	1
3	A	644	PX4	O7-C7	2.16	1.41	1.46	2	2
3	B	312	PX4	C2-N1	2.16	1.44	1.51	5	1
3	C	341	PX4	P1-O3	2.16	1.50	1.59	5	1
3	C	354	PX4	C4-N1	2.17	1.43	1.50	6	1
3	B	385	PX4	C15-C14	2.16	1.62	1.51	11	1
3	B	329	PX4	C15-C14	2.16	1.62	1.51	1	1
3	A	626	PX4	P1-O1	2.16	1.45	1.55	1	3
3	A	649	PX4	P1-O4	2.16	1.67	1.59	7	1
3	A	654	PX4	C2-N1	2.16	1.58	1.51	10	1
3	B	330	PX4	C2-N1	2.16	1.58	1.51	15	3
3	C	347	PX4	C18-C17	2.16	1.62	1.51	9	2
3	B	348	PX4	O7-C23	2.16	1.28	1.34	4	1
3	B	356	PX4	C2-N1	2.16	1.44	1.51	9	1
3	A	612	PX4	C34-C33	2.16	1.62	1.51	12	1
3	A	620	PX4	O7-C7	2.16	1.41	1.46	13	2
3	A	635	PX4	C3-N1	2.16	1.43	1.50	4	1
3	B	369	PX4	P1-O2	2.16	1.43	1.50	8	2
3	C	329	PX4	C28-C27	2.16	1.62	1.51	10	1
3	C	354	PX4	C17-C16	2.16	1.62	1.51	14	1
3	C	355	PX4	C15-C14	2.16	1.62	1.51	12	1
3	C	364	PX4	C17-C16	2.16	1.62	1.51	5	1
3	A	610	PX4	C5-N1	2.16	1.56	1.50	4	2
3	B	346	PX4	C25-C24	2.16	1.60	1.52	11	1
3	C	301	PX4	P1-O1	2.16	1.45	1.55	9	1
3	A	654	PX4	C4-N1	2.16	1.43	1.50	14	1
3	C	318	PX4	C2-N1	2.16	1.44	1.51	15	2
3	C	347	PX4	C19-C18	2.16	1.62	1.51	9	1
3	B	371	PX4	C2-N1	2.16	1.44	1.51	1	1
3	B	393	PX4	C18-C17	2.16	1.62	1.51	9	1
3	B	399	PX4	C19-C18	2.16	1.62	1.51	9	1
3	C	326	PX4	C29-C28	2.16	1.62	1.51	12	1
3	A	632	PX4	C10-C9	2.16	1.57	1.50	15	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	C	359	PX4	P1-O1	2.16	1.45	1.55	7	1
3	B	314	PX4	P1-O1	2.15	1.45	1.55	11	1
3	B	361	PX4	C26-C25	2.15	1.62	1.51	10	1
3	B	370	PX4	O7-C23	2.15	1.28	1.34	3	1
3	A	616	PX4	C4-N1	2.15	1.56	1.50	6	2
3	A	633	PX4	P1-O1	2.15	1.45	1.55	13	2
3	B	319	PX4	C5-N1	2.15	1.56	1.50	12	1
3	B	397	PX4	C31-C30	2.15	1.62	1.51	14	1
3	B	362	PX4	C16-C15	2.15	1.62	1.51	1	1
3	B	366	PX4	P1-O4	2.15	1.51	1.59	7	1
3	C	333	PX4	C20-C19	2.15	1.62	1.51	1	1
3	C	353	PX4	C3-N1	2.15	1.43	1.50	5	1
3	A	621	PX4	P1-O1	2.15	1.45	1.55	12	2
3	A	638	PX4	O7-C23	2.15	1.28	1.34	3	1
3	B	375	PX4	P1-O4	2.15	1.51	1.59	15	1
3	A	608	PX4	O4-C6	2.15	1.36	1.44	13	2
3	B	320	PX4	C19-C18	2.15	1.62	1.51	13	1
3	B	321	PX4	O5-C8	2.15	1.50	1.45	4	1
3	B	357	PX4	P1-O4	2.15	1.51	1.59	15	1
3	B	358	PX4	C24-C23	2.15	1.56	1.50	10	2
3	C	311	PX4	C33-C32	2.15	1.62	1.51	5	2
3	A	624	PX4	C28-C27	2.15	1.62	1.51	15	1
3	A	630	PX4	C19-C18	2.15	1.62	1.51	15	2
3	B	363	PX4	C25-C24	2.15	1.60	1.52	11	1
3	B	396	PX4	C27-C26	2.15	1.62	1.51	11	1
3	B	399	PX4	O5-C8	2.15	1.40	1.45	2	1
3	C	338	PX4	O5-C9	2.15	1.27	1.33	7	1
3	A	642	PX4	C25-C24	2.15	1.60	1.52	5	1
3	A	646	PX4	C25-C24	2.14	1.60	1.52	6	1
3	B	326	PX4	P1-O2	2.14	1.43	1.50	2	1
3	B	345	PX4	O3-C1	2.14	1.36	1.44	15	1
3	B	393	PX4	C3-N1	2.14	1.43	1.50	5	1
3	C	312	PX4	P1-O3	2.14	1.51	1.59	1	1
3	C	319	PX4	O5-C8	2.14	1.40	1.45	3	2
3	C	354	PX4	O8-C23	2.14	1.16	1.22	7	1
3	C	364	PX4	C28-C27	2.14	1.62	1.51	15	1
3	A	639	PX4	P1-O2	2.14	1.43	1.50	3	1
3	A	612	PX4	C4-N1	2.14	1.56	1.50	4	1
3	A	621	PX4	C4-N1	2.14	1.43	1.50	15	1
3	A	640	PX4	O5-C9	2.14	1.39	1.33	14	3
3	A	645	PX4	C31-C30	2.14	1.62	1.51	12	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	327	PX4	C16-C15	2.14	1.62	1.51	2	1
3	B	330	PX4	P1-O4	2.14	1.51	1.59	3	1
3	B	306	PX4	C32-C31	2.14	1.62	1.51	5	1
3	B	314	PX4	P1-O4	2.14	1.51	1.59	13	1
3	B	375	PX4	C5-N1	2.14	1.56	1.50	14	1
3	C	319	PX4	C15-C14	2.14	1.62	1.51	3	1
3	B	313	PX4	C2-N1	2.14	1.58	1.51	7	2
3	B	380	PX4	C18-C17	2.14	1.62	1.51	5	1
3	B	396	PX4	O5-C9	2.14	1.39	1.33	4	2
3	C	332	PX4	C4-N1	2.14	1.43	1.50	2	2
3	C	345	PX4	O5-C8	2.14	1.49	1.45	3	2
3	C	347	PX4	C12-C11	2.14	1.62	1.51	8	1
3	B	347	PX4	P1-O3	2.14	1.67	1.59	15	2
3	B	336	PX4	P1-O3	2.14	1.51	1.59	13	1
3	B	350	PX4	C26-C25	2.14	1.62	1.51	12	1
3	B	365	PX4	C2-N1	2.14	1.58	1.51	3	1
3	C	314	PX4	C34-C33	2.14	1.62	1.51	12	1
3	C	341	PX4	O7-C23	2.14	1.28	1.34	2	1
3	B	364	PX4	C31-C30	2.14	1.62	1.51	1	1
3	C	312	PX4	P1-O4	2.14	1.51	1.59	1	1
3	C	333	PX4	C34-C33	2.14	1.62	1.51	15	1
3	A	645	PX4	C11-C10	2.13	1.60	1.52	1	1
3	B	306	PX4	O8-C23	2.14	1.16	1.22	12	1
3	B	314	PX4	C34-C33	2.14	1.62	1.51	10	1
3	C	338	PX4	C13-C12	2.14	1.62	1.51	8	1
3	A	651	PX4	C17-C16	2.13	1.62	1.51	8	1
3	B	342	PX4	C28-C27	2.13	1.62	1.51	10	1
3	B	355	PX4	O5-C8	2.13	1.49	1.45	6	2
3	B	387	PX4	C20-C19	2.13	1.62	1.51	3	1
3	C	324	PX4	P1-O3	2.14	1.67	1.59	12	2
3	C	334	PX4	C3-N1	2.13	1.56	1.50	10	1
3	C	330	PX4	C11-C10	2.13	1.60	1.52	8	1
3	C	332	PX4	O5-C9	2.13	1.39	1.33	1	1
3	C	341	PX4	C27-C26	2.13	1.62	1.51	5	2
3	C	344	PX4	O7-C23	2.13	1.28	1.34	5	1
3	A	633	PX4	P1-O2	2.13	1.43	1.50	3	1
3	C	335	PX4	C13-C12	2.13	1.62	1.51	14	2
3	C	338	PX4	C5-N1	2.13	1.56	1.50	5	1
3	A	648	PX4	P1-O2	2.13	1.43	1.50	5	1
3	A	651	PX4	C4-N1	2.13	1.56	1.50	2	1
3	B	329	PX4	C33-C32	2.13	1.62	1.51	15	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	360	PX4	P1-O1	2.13	1.45	1.55	14	3
3	B	392	PX4	C11-C10	2.13	1.60	1.52	12	1
3	C	302	PX4	C31-C30	2.13	1.62	1.51	10	1
3	C	319	PX4	C24-C23	2.13	1.56	1.50	15	1
3	B	351	PX4	C24-C23	2.13	1.56	1.50	4	1
3	B	311	PX4	P1-O4	2.13	1.51	1.59	5	1
3	B	314	PX4	C11-C10	2.13	1.60	1.52	14	2
3	B	317	PX4	C17-C16	2.13	1.62	1.51	9	1
3	B	337	PX4	C4-N1	2.13	1.56	1.50	8	1
3	B	341	PX4	C27-C26	2.13	1.62	1.51	3	1
3	B	343	PX4	C10-C9	2.13	1.56	1.50	10	2
3	C	320	PX4	C4-N1	2.13	1.56	1.50	11	1
3	C	329	PX4	C10-C9	2.13	1.56	1.50	13	1
3	C	304	PX4	P1-O4	2.13	1.51	1.59	12	1
3	C	360	PX4	C17-C16	2.13	1.62	1.51	3	1
3	A	622	PX4	C15-C14	2.13	1.62	1.51	2	1
3	A	634	PX4	P1-O1	2.13	1.45	1.55	9	1
3	A	641	PX4	P1-O1	2.13	1.45	1.55	1	2
3	A	653	PX4	C33-C32	2.13	1.62	1.51	3	1
3	B	311	PX4	P1-O2	2.13	1.43	1.50	1	1
3	B	335	PX4	C28-C27	2.13	1.62	1.51	8	1
3	B	348	PX4	C18-C17	2.13	1.62	1.51	12	1
3	B	349	PX4	C28-C27	2.13	1.62	1.51	4	1
3	C	308	PX4	C14-C13	2.13	1.62	1.51	12	1
3	B	347	PX4	C28-C27	2.13	1.62	1.51	5	1
3	B	396	PX4	C14-C13	2.13	1.62	1.51	13	1
3	C	345	PX4	C5-N1	2.13	1.43	1.50	2	1
3	C	364	PX4	O5-C9	2.13	1.27	1.33	4	1
3	A	617	PX4	P1-O3	2.13	1.51	1.59	10	1
3	B	301	PX4	C25-C24	2.13	1.60	1.52	8	1
3	B	372	PX4	C30-C29	2.13	1.62	1.51	14	1
3	C	325	PX4	C14-C13	2.13	1.62	1.51	13	1
3	A	608	PX4	C5-N1	2.12	1.43	1.50	8	1
3	A	604	PX4	P1-O4	2.12	1.51	1.59	10	1
3	B	317	PX4	C27-C26	2.12	1.62	1.51	2	1
3	B	351	PX4	C3-N1	2.12	1.56	1.50	9	1
3	B	376	PX4	C4-N1	2.12	1.56	1.50	1	1
3	B	383	PX4	C11-C10	2.12	1.60	1.52	8	1
3	B	315	PX4	O4-C6	2.12	1.36	1.44	3	1
3	B	315	PX4	C10-C9	2.12	1.56	1.50	8	2
3	C	344	PX4	C12-C11	2.12	1.62	1.51	15	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	C	354	PX4	C5-N1	2.12	1.43	1.50	8	1
3	C	358	PX4	C13-C12	2.12	1.62	1.51	10	1
3	B	320	PX4	P1-O1	2.12	1.45	1.55	11	2
3	B	353	PX4	C15-C14	2.12	1.62	1.51	2	1
3	C	348	PX4	C17-C16	2.12	1.62	1.51	10	1
3	A	621	PX4	C17-C16	2.12	1.62	1.51	14	1
3	B	374	PX4	C16-C15	2.12	1.62	1.51	1	1
3	B	380	PX4	O3-C1	2.12	1.53	1.44	5	1
3	C	340	PX4	P1-O2	2.12	1.43	1.50	2	1
3	C	340	PX4	C30-C29	2.12	1.62	1.51	6	1
3	A	613	PX4	C28-C27	2.12	1.62	1.51	3	1
3	B	373	PX4	O7-C23	2.12	1.28	1.34	7	1
3	B	375	PX4	C2-C1	2.12	1.57	1.51	4	2
3	B	396	PX4	P1-O2	2.12	1.43	1.50	11	1
3	A	619	PX4	C17-C16	2.12	1.62	1.51	1	1
3	A	632	PX4	P1-O1	2.12	1.45	1.55	6	2
3	C	303	PX4	O5-C9	2.12	1.27	1.33	7	1
3	A	637	PX4	C5-N1	2.12	1.56	1.50	5	1
3	B	316	PX4	C3-N1	2.12	1.43	1.50	13	1
3	B	373	PX4	C4-N1	2.12	1.43	1.50	12	1
3	C	344	PX4	C4-N1	2.12	1.56	1.50	2	1
3	B	327	PX4	O3-C1	2.12	1.36	1.44	7	1
3	B	388	PX4	C16-C15	2.12	1.62	1.51	7	1
3	B	306	PX4	C14-C13	2.11	1.62	1.51	13	1
3	A	622	PX4	C5-N1	2.11	1.43	1.50	3	1
3	A	624	PX4	C25-C24	2.11	1.59	1.52	2	1
3	B	336	PX4	C19-C18	2.11	1.62	1.51	12	1
3	B	362	PX4	C15-C14	2.11	1.62	1.51	14	1
3	B	377	PX4	C12-C11	2.11	1.62	1.51	14	1
3	B	394	PX4	C12-C11	2.11	1.62	1.51	13	1
3	C	317	PX4	C11-C10	2.11	1.44	1.52	11	1
3	C	338	PX4	C24-C23	2.11	1.56	1.50	14	2
3	C	344	PX4	C30-C29	2.11	1.62	1.51	14	1
3	C	351	PX4	C17-C16	2.11	1.62	1.51	8	1
3	A	653	PX4	C28-C27	2.11	1.62	1.51	10	1
3	B	302	PX4	C2-N1	2.11	1.45	1.51	7	1
3	B	315	PX4	O7-C7	2.11	1.41	1.46	3	3
3	B	332	PX4	C3-N1	2.11	1.43	1.50	11	1
3	B	335	PX4	C3-N1	2.11	1.56	1.50	2	1
3	C	351	PX4	P1-O2	2.11	1.43	1.50	14	2
3	C	306	PX4	C15-C14	2.11	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	331	PX4	C31-C30	2.11	1.62	1.51	2	1
3	B	302	PX4	C19-C18	2.11	1.62	1.51	12	1
3	B	345	PX4	O7-C7	2.11	1.41	1.46	6	1
3	B	330	PX4	C11-C10	2.11	1.59	1.52	2	1
3	B	335	PX4	P1-O1	2.11	1.45	1.55	13	5
3	B	355	PX4	C15-C14	2.11	1.62	1.51	14	1
3	B	342	PX4	C25-C24	2.11	1.59	1.52	15	1
3	B	358	PX4	P1-O1	2.11	1.45	1.55	13	1
3	B	370	PX4	O7-C7	2.11	1.51	1.46	13	2
3	B	387	PX4	O3-C1	2.11	1.36	1.44	7	1
3	C	314	PX4	P1-O1	2.11	1.45	1.55	4	1
3	C	338	PX4	P1-O4	2.11	1.51	1.59	7	1
3	B	394	PX4	C21-C20	2.11	1.64	1.51	3	1
3	C	312	PX4	C2-N1	2.11	1.57	1.51	15	1
3	C	319	PX4	O5-C9	2.11	1.27	1.33	13	1
3	C	352	PX4	C5-N1	2.11	1.56	1.50	11	1
3	C	364	PX4	P1-O4	2.11	1.51	1.59	12	1
3	A	603	PX4	C14-C13	2.11	1.62	1.51	4	1
3	A	620	PX4	O7-C23	2.11	1.28	1.34	12	1
3	B	310	PX4	C4-N1	2.11	1.43	1.50	6	1
3	C	309	PX4	C18-C17	2.11	1.62	1.51	13	1
3	C	324	PX4	P1-O1	2.11	1.45	1.55	15	1
3	A	627	PX4	C16-C15	2.11	1.62	1.51	14	1
3	C	301	PX4	C30-C29	2.11	1.62	1.51	11	1
3	C	326	PX4	C12-C11	2.11	1.62	1.51	2	1
3	A	623	PX4	C3-N1	2.10	1.43	1.50	7	3
3	A	637	PX4	C32-C31	2.10	1.62	1.51	14	1
3	B	373	PX4	C26-C25	2.10	1.62	1.51	2	1
3	B	398	PX4	C30-C29	2.10	1.62	1.51	1	1
3	C	328	PX4	C4-N1	2.11	1.56	1.50	6	1
3	C	364	PX4	C20-C19	2.11	1.62	1.51	9	1
3	A	636	PX4	C5-N1	2.10	1.43	1.50	10	2
3	A	604	PX4	C15-C14	2.10	1.62	1.51	1	1
3	A	608	PX4	C28-C27	2.10	1.62	1.51	11	1
3	A	611	PX4	C12-C11	2.10	1.62	1.51	12	1
3	A	649	PX4	O4-C6	2.10	1.36	1.44	8	1
3	A	653	PX4	C18-C17	2.10	1.62	1.51	15	1
3	B	305	PX4	C30-C29	2.10	1.62	1.51	13	1
3	B	320	PX4	C17-C16	2.10	1.62	1.51	11	1
3	B	326	PX4	C35-C34	2.10	1.64	1.51	15	1
3	B	372	PX4	C16-C15	2.10	1.62	1.51	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	364	PX4	C18-C17	2.10	1.62	1.51	9	1
3	B	372	PX4	C11-C10	2.10	1.59	1.52	11	1
3	B	375	PX4	C16-C15	2.10	1.62	1.51	8	1
3	B	376	PX4	C25-C24	2.10	1.59	1.52	11	1
3	B	390	PX4	C26-C25	2.10	1.62	1.51	15	2
3	B	397	PX4	C26-C25	2.10	1.62	1.51	4	1
3	C	327	PX4	C3-N1	2.10	1.56	1.50	15	1
3	C	310	PX4	O7-C7	2.10	1.41	1.46	8	1
3	C	337	PX4	O5-C8	2.10	1.49	1.45	1	2
3	B	315	PX4	C13-C12	2.10	1.62	1.51	1	1
3	B	338	PX4	C4-N1	2.10	1.43	1.50	11	1
3	C	316	PX4	O6-C9	2.10	1.28	1.22	4	1
3	C	323	PX4	C11-C10	2.10	1.59	1.52	6	2
3	C	341	PX4	P1-O1	2.10	1.45	1.55	8	1
3	B	349	PX4	C17-C16	2.10	1.62	1.51	6	1
3	C	345	PX4	C28-C27	2.10	1.62	1.51	15	1
3	A	650	PX4	P1-O3	2.10	1.51	1.59	14	1
3	B	371	PX4	C26-C25	2.10	1.62	1.51	4	1
3	C	322	PX4	P1-O4	2.10	1.51	1.59	7	1
3	A	631	PX4	C26-C25	2.10	1.62	1.51	2	1
3	B	311	PX4	C26-C25	2.10	1.62	1.51	2	1
3	B	343	PX4	C28-C27	2.10	1.62	1.51	2	1
3	C	318	PX4	C11-C10	2.10	1.59	1.52	6	1
3	C	323	PX4	C5-N1	2.10	1.56	1.50	14	1
3	C	330	PX4	C32-C31	2.10	1.62	1.51	9	1
3	A	620	PX4	C25-C24	2.10	1.59	1.52	8	1
3	A	644	PX4	C11-C10	2.10	1.59	1.52	11	1
3	B	341	PX4	O7-C23	2.10	1.28	1.34	8	1
3	C	349	PX4	P1-O1	2.10	1.45	1.55	10	2
3	B	365	PX4	C17-C16	2.10	1.62	1.51	3	1
3	B	370	PX4	C5-N1	2.09	1.43	1.50	15	1
3	B	394	PX4	P1-O2	2.09	1.43	1.50	14	1
3	C	307	PX4	C20-C19	2.10	1.62	1.51	1	1
3	C	332	PX4	P1-O2	2.10	1.43	1.50	10	1
3	A	608	PX4	C11-C10	2.09	1.59	1.52	5	1
3	A	637	PX4	P1-O1	2.09	1.45	1.55	10	2
3	A	642	PX4	C31-C30	2.09	1.62	1.51	7	1
3	A	607	PX4	C2-N1	2.09	1.57	1.51	10	1
3	A	619	PX4	C29-C28	2.09	1.62	1.51	12	1
3	B	368	PX4	C3-N1	2.09	1.56	1.50	14	1
3	C	303	PX4	C25-C24	2.09	1.59	1.52	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	C	304	PX4	C2-N1	2.09	1.57	1.51	6	1
3	A	641	PX4	C20-C19	2.09	1.62	1.51	15	1
3	A	608	PX4	P1-O1	2.09	1.45	1.55	13	1
3	A	618	PX4	C28-C27	2.09	1.62	1.51	9	1
3	A	624	PX4	C19-C18	2.09	1.62	1.51	8	1
3	A	647	PX4	P1-O3	2.09	1.51	1.59	15	1
3	B	339	PX4	P1-O2	2.09	1.43	1.50	13	1
3	A	650	PX4	C11-C10	2.09	1.59	1.52	5	1
3	B	312	PX4	C26-C25	2.09	1.62	1.51	6	1
3	B	320	PX4	O5-C9	2.09	1.27	1.33	14	1
3	B	369	PX4	C3-N1	2.09	1.56	1.50	14	2
3	B	369	PX4	C2-N1	2.09	1.57	1.51	8	1
3	B	385	PX4	C14-C13	2.09	1.62	1.51	1	1
3	B	387	PX4	P1-O3	2.09	1.51	1.59	14	1
3	B	399	PX4	C31-C30	2.09	1.62	1.51	9	1
3	C	349	PX4	C20-C19	2.09	1.62	1.51	3	1
3	C	358	PX4	C20-C19	2.09	1.62	1.51	2	1
3	A	604	PX4	C32-C31	2.09	1.62	1.51	15	2
3	A	630	PX4	C33-C32	2.09	1.62	1.51	3	1
3	A	631	PX4	C29-C28	2.09	1.62	1.51	14	1
3	B	301	PX4	P1-O3	2.09	1.51	1.59	12	1
3	B	320	PX4	C28-C27	2.09	1.62	1.51	7	1
3	B	345	PX4	C5-N1	2.09	1.56	1.50	1	1
3	B	364	PX4	O3-C1	2.09	1.36	1.44	15	1
3	B	390	PX4	C11-C10	2.09	1.59	1.52	15	3
3	B	396	PX4	P1-O3	2.09	1.67	1.59	4	1
3	C	329	PX4	C36-C35	2.09	1.65	1.50	1	1
3	A	629	PX4	C4-N1	2.09	1.56	1.50	3	1
3	B	379	PX4	C19-C18	2.09	1.62	1.51	6	1
3	C	309	PX4	O4-C6	2.09	1.36	1.44	15	1
3	A	609	PX4	C10-C9	2.09	1.56	1.50	6	3
3	A	634	PX4	C3-N1	2.09	1.56	1.50	5	1
3	A	652	PX4	C17-C16	2.09	1.62	1.51	7	1
3	B	331	PX4	O5-C9	2.09	1.27	1.33	11	1
3	B	320	PX4	C5-N1	2.09	1.56	1.50	6	1
3	B	326	PX4	C17-C16	2.09	1.62	1.51	5	1
3	C	306	PX4	C12-C11	2.09	1.62	1.51	10	1
3	C	346	PX4	C21-C20	2.09	1.64	1.51	9	1
3	B	316	PX4	C21-C20	2.08	1.64	1.51	14	1
3	B	332	PX4	C25-C24	2.09	1.59	1.52	10	2
3	B	319	PX4	P1-O2	2.08	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	335	PX4	C25-C24	2.08	1.59	1.52	14	1
3	B	336	PX4	C28-C27	2.09	1.62	1.51	5	1
3	A	628	PX4	C28-C27	2.08	1.62	1.51	15	1
3	A	639	PX4	C30-C29	2.08	1.62	1.51	13	1
3	C	342	PX4	O5-C9	2.09	1.27	1.33	4	1
3	A	631	PX4	C27-C26	2.08	1.62	1.51	15	1
3	B	350	PX4	O4-C6	2.08	1.36	1.44	8	1
3	B	356	PX4	C12-C11	2.08	1.62	1.51	13	1
3	C	302	PX4	C17-C16	2.08	1.62	1.51	1	1
3	C	354	PX4	O5-C8	2.08	1.40	1.45	5	1
3	C	355	PX4	O7-C7	2.08	1.41	1.46	2	1
3	A	604	PX4	C19-C18	2.08	1.62	1.51	13	1
3	B	369	PX4	C34-C33	2.08	1.62	1.51	2	1
3	B	384	PX4	P1-O2	2.08	1.43	1.50	2	1
3	B	399	PX4	C16-C15	2.08	1.62	1.51	15	1
3	A	625	PX4	O3-C1	2.08	1.36	1.44	8	2
3	A	632	PX4	C2-C1	2.08	1.57	1.51	5	1
3	B	318	PX4	O3-C1	2.08	1.36	1.44	3	1
3	B	348	PX4	P1-O3	2.08	1.51	1.59	7	1
3	A	647	PX4	C11-C10	2.08	1.59	1.52	2	2
3	B	351	PX4	C5-N1	2.08	1.56	1.50	3	2
3	B	368	PX4	C25-C24	2.08	1.59	1.52	7	1
3	B	400	PX4	O4-C6	2.08	1.36	1.44	4	1
3	B	391	PX4	C15-C14	2.08	1.62	1.51	5	1
3	C	343	PX4	C5-N1	2.08	1.56	1.50	5	1
3	C	347	PX4	O6-C9	2.08	1.28	1.22	1	1
3	B	304	PX4	C25-C24	2.08	1.59	1.52	4	1
3	B	323	PX4	C28-C27	2.08	1.62	1.51	6	1
3	A	617	PX4	O7-C23	2.08	1.40	1.34	12	1
3	A	618	PX4	O5-C8	2.08	1.40	1.45	5	1
3	B	370	PX4	O4-C6	2.08	1.36	1.44	14	1
3	C	334	PX4	C25-C24	2.08	1.59	1.52	6	1
3	C	354	PX4	P1-O3	2.08	1.67	1.59	10	1
3	C	359	PX4	C32-C31	2.08	1.62	1.51	14	1
3	A	614	PX4	O4-C6	2.08	1.52	1.44	15	2
3	A	647	PX4	O8-C23	2.08	1.16	1.22	5	1
3	B	337	PX4	C33-C32	2.08	1.62	1.51	8	2
3	B	387	PX4	C10-C9	2.08	1.56	1.50	8	1
3	B	392	PX4	C26-C25	2.08	1.62	1.51	14	1
3	A	617	PX4	C5-N1	2.07	1.44	1.50	10	1
3	A	626	PX4	C11-C10	2.07	1.59	1.52	13	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	336	PX4	C25-C24	2.07	1.59	1.52	8	2
3	B	360	PX4	O4-C6	2.07	1.36	1.44	5	1
3	B	362	PX4	C11-C10	2.07	1.59	1.52	13	2
3	B	366	PX4	C4-N1	2.07	1.44	1.50	13	2
3	C	334	PX4	C15-C14	2.07	1.62	1.51	15	1
3	B	331	PX4	O4-C6	2.07	1.36	1.44	7	1
3	B	308	PX4	C20-C19	2.07	1.62	1.51	12	1
3	B	324	PX4	P1-O1	2.07	1.45	1.55	12	1
3	B	340	PX4	C30-C29	2.07	1.62	1.51	11	2
3	B	352	PX4	C5-N1	2.07	1.56	1.50	12	1
3	B	353	PX4	C4-N1	2.07	1.56	1.50	7	1
3	C	339	PX4	P1-O3	2.07	1.51	1.59	12	1
3	C	339	PX4	C17-C16	2.07	1.62	1.51	13	1
3	C	343	PX4	C27-C26	2.07	1.62	1.51	13	1
3	C	360	PX4	O5-C9	2.07	1.27	1.33	12	1
3	C	362	PX4	C19-C18	2.07	1.62	1.51	1	1
3	B	323	PX4	C15-C14	2.07	1.62	1.51	12	1
3	B	341	PX4	C25-C24	2.07	1.59	1.52	13	1
3	B	381	PX4	P1-O2	2.07	1.43	1.50	1	1
3	C	306	PX4	C18-C17	2.07	1.62	1.51	15	1
3	C	356	PX4	O3-C1	2.07	1.36	1.44	6	1
3	C	343	PX4	C3-N1	2.07	1.44	1.50	3	2
3	A	628	PX4	P1-O3	2.07	1.51	1.59	4	1
3	B	317	PX4	O6-C9	2.07	1.16	1.22	6	1
3	B	320	PX4	O5-C8	2.07	1.49	1.45	6	1
3	B	347	PX4	O3-C1	2.07	1.36	1.44	5	1
3	C	318	PX4	C4-N1	2.07	1.44	1.50	15	1
3	A	639	PX4	C15-C14	2.07	1.62	1.51	10	1
3	C	308	PX4	O5-C9	2.07	1.39	1.33	7	2
3	C	316	PX4	P1-O1	2.07	1.45	1.55	13	2
3	C	363	PX4	C18-C17	2.07	1.62	1.51	2	1
3	A	620	PX4	P1-O1	2.07	1.45	1.55	11	2
3	A	652	PX4	C2-N1	2.07	1.45	1.51	5	1
3	A	654	PX4	O4-C6	2.07	1.36	1.44	4	1
3	B	314	PX4	C32-C31	2.07	1.62	1.51	11	1
3	B	368	PX4	C27-C26	2.07	1.62	1.51	12	1
3	B	375	PX4	C13-C12	2.07	1.62	1.51	3	1
3	C	351	PX4	C15-C14	2.07	1.41	1.51	1	1
3	A	606	PX4	C29-C28	2.06	1.62	1.51	9	1
3	B	337	PX4	C32-C31	2.06	1.62	1.51	11	1
3	B	360	PX4	O3-C1	2.06	1.36	1.44	7	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	A	605	PX4	C21-C20	2.06	1.64	1.51	4	1
3	B	364	PX4	C34-C33	2.06	1.62	1.51	11	1
3	A	616	PX4	C28-C27	2.06	1.62	1.51	7	2
3	A	637	PX4	O5-C8	2.06	1.40	1.45	5	1
3	B	318	PX4	O7-C23	2.06	1.28	1.34	11	1
3	B	328	PX4	O5-C9	2.06	1.39	1.33	14	1
3	B	336	PX4	C12-C11	2.06	1.62	1.51	9	1
3	B	377	PX4	P1-O2	2.06	1.43	1.50	1	1
3	B	358	PX4	C11-C10	2.06	1.59	1.52	9	1
3	B	368	PX4	C13-C12	2.06	1.62	1.51	13	1
3	B	379	PX4	C4-N1	2.06	1.56	1.50	9	1
3	C	327	PX4	O8-C23	2.06	1.16	1.22	5	1
3	A	609	PX4	C25-C24	2.06	1.59	1.52	4	1
3	A	630	PX4	P1-O1	2.06	1.45	1.55	14	2
3	A	641	PX4	C18-C17	2.06	1.62	1.51	4	1
3	B	307	PX4	C31-C30	2.06	1.62	1.51	11	1
3	B	386	PX4	C2-N1	2.06	1.57	1.51	7	1
3	B	310	PX4	P1-O1	2.06	1.45	1.55	7	2
3	B	390	PX4	O5-C9	2.06	1.27	1.33	8	1
3	C	341	PX4	C11-C10	2.06	1.59	1.52	10	1
3	A	651	PX4	C18-C17	2.06	1.62	1.51	7	1
3	B	321	PX4	O5-C9	2.06	1.39	1.33	1	1
3	B	359	PX4	P1-O2	2.06	1.43	1.50	10	1
3	B	375	PX4	C30-C29	2.06	1.62	1.51	9	1
3	C	363	PX4	C27-C26	2.06	1.62	1.51	4	1
3	A	619	PX4	C25-C24	2.06	1.44	1.52	10	1
3	A	647	PX4	O5-C8	2.06	1.40	1.45	3	2
3	B	303	PX4	C34-C33	2.06	1.62	1.51	1	1
3	B	316	PX4	P1-O2	2.06	1.43	1.50	7	1
3	B	325	PX4	C19-C18	2.06	1.62	1.51	12	1
3	C	302	PX4	C34-C33	2.06	1.62	1.51	2	1
3	C	323	PX4	P1-O2	2.06	1.43	1.50	6	1
3	B	352	PX4	P1-O3	2.06	1.67	1.59	12	1
3	A	632	PX4	C25-C24	2.06	1.59	1.52	2	1
3	A	648	PX4	C2-N1	2.06	1.45	1.51	2	1
3	B	344	PX4	C19-C18	2.06	1.62	1.51	7	1
3	C	309	PX4	O3-C1	2.06	1.36	1.44	2	1
3	B	331	PX4	P1-O1	2.06	1.45	1.55	13	2
3	B	340	PX4	C20-C19	2.06	1.62	1.51	10	2
3	B	380	PX4	C30-C29	2.06	1.62	1.51	8	1
3	C	330	PX4	P1-O1	2.06	1.45	1.55	4	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	A	606	PX4	C27-C26	2.05	1.62	1.51	15	1
3	A	618	PX4	O5-C9	2.06	1.39	1.33	11	1
3	C	304	PX4	C28-C27	2.06	1.62	1.51	10	1
3	A	626	PX4	C34-C33	2.05	1.62	1.51	1	1
3	B	341	PX4	P1-O4	2.05	1.51	1.59	15	1
3	B	345	PX4	C14-C13	2.05	1.62	1.51	2	1
3	B	369	PX4	C15-C14	2.05	1.62	1.51	13	1
3	C	363	PX4	C17-C16	2.05	1.62	1.51	10	1
3	A	612	PX4	C14-C13	2.05	1.62	1.51	7	1
3	B	302	PX4	C17-C16	2.05	1.62	1.51	6	1
3	B	372	PX4	C25-C24	2.05	1.59	1.52	8	1
3	C	348	PX4	P1-O3	2.05	1.51	1.59	7	1
3	B	355	PX4	C31-C30	2.05	1.62	1.51	14	1
3	B	392	PX4	C33-C32	2.05	1.62	1.51	6	1
3	A	626	PX4	O7-C7	2.05	1.41	1.46	7	1
3	A	644	PX4	C32-C31	2.05	1.62	1.51	11	1
3	B	312	PX4	C27-C26	2.05	1.62	1.51	7	1
3	B	332	PX4	C13-C12	2.05	1.62	1.51	11	2
3	B	302	PX4	O7-C23	2.05	1.28	1.34	12	1
3	B	358	PX4	C34-C33	2.05	1.62	1.51	14	1
3	B	377	PX4	O4-C6	2.05	1.36	1.44	11	1
3	C	311	PX4	O5-C9	2.05	1.27	1.33	3	2
3	B	306	PX4	C28-C27	2.05	1.62	1.51	14	1
3	B	323	PX4	C4-N1	2.05	1.55	1.50	15	1
3	B	330	PX4	P1-O2	2.05	1.43	1.50	15	1
3	C	351	PX4	C34-C33	2.05	1.62	1.51	15	1
3	A	637	PX4	C4-N1	2.04	1.55	1.50	1	1
3	B	335	PX4	C2-N1	2.04	1.57	1.51	10	2
3	B	368	PX4	C26-C25	2.04	1.62	1.51	5	1
3	B	380	PX4	C33-C32	2.04	1.61	1.51	13	1
3	C	301	PX4	O5-C8	2.04	1.49	1.45	4	1
3	C	343	PX4	C12-C11	2.04	1.61	1.51	12	1
3	A	605	PX4	C12-C11	2.04	1.61	1.51	11	1
3	A	637	PX4	C30-C29	2.04	1.61	1.51	14	1
3	A	644	PX4	P1-O2	2.04	1.43	1.50	6	1
3	A	645	PX4	C33-C32	2.04	1.61	1.51	9	1
3	B	319	PX4	C27-C26	2.04	1.61	1.51	6	1
3	B	329	PX4	C17-C16	2.04	1.61	1.51	7	1
3	B	342	PX4	P1-O3	2.04	1.67	1.59	5	1
3	B	355	PX4	P1-O3	2.04	1.51	1.59	7	1
3	C	321	PX4	P1-O2	2.04	1.43	1.50	11	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	A	619	PX4	C13-C12	2.04	1.61	1.51	13	1
3	A	630	PX4	O5-C9	2.04	1.27	1.33	3	1
3	B	308	PX4	C3-N1	2.04	1.44	1.50	4	1
3	B	325	PX4	C17-C16	2.04	1.61	1.51	11	1
3	B	383	PX4	P1-O4	2.04	1.51	1.59	11	1
3	C	312	PX4	O5-C9	2.04	1.27	1.33	14	1
3	C	330	PX4	C14-C13	2.04	1.61	1.51	9	1
3	C	313	PX4	C25-C24	2.04	1.59	1.52	11	1
3	C	314	PX4	O5-C9	2.04	1.39	1.33	1	1
3	C	316	PX4	C10-C9	2.04	1.56	1.50	15	1
3	C	355	PX4	C33-C32	2.04	1.61	1.51	13	1
3	C	364	PX4	O3-C1	2.04	1.36	1.44	1	1
3	B	368	PX4	C30-C29	2.04	1.61	1.51	14	1
3	B	382	PX4	C24-C23	2.04	1.56	1.50	4	1
3	C	352	PX4	C31-C30	2.04	1.61	1.51	9	1
3	A	650	PX4	O4-C6	2.04	1.36	1.44	4	1
3	B	316	PX4	O7-C23	2.04	1.28	1.34	6	1
3	B	357	PX4	C34-C33	2.04	1.61	1.51	11	1
3	C	303	PX4	C30-C29	2.04	1.41	1.51	5	1
3	C	358	PX4	C19-C18	2.04	1.61	1.51	3	1
3	C	360	PX4	C12-C11	2.04	1.61	1.51	4	1
3	A	603	PX4	C2-N1	2.04	1.45	1.51	8	1
3	A	612	PX4	C5-N1	2.04	1.55	1.50	11	1
3	A	650	PX4	C16-C15	2.04	1.61	1.51	14	1
3	B	343	PX4	C13-C12	2.04	1.61	1.51	5	1
3	B	355	PX4	C13-C12	2.04	1.61	1.51	9	1
3	B	370	PX4	C14-C13	2.03	1.61	1.51	11	2
3	B	376	PX4	C20-C19	2.03	1.61	1.51	15	2
3	B	380	PX4	C19-C18	2.04	1.61	1.51	3	1
3	B	386	PX4	C5-N1	2.04	1.55	1.50	3	2
3	B	331	PX4	P1-O3	2.03	1.51	1.59	1	1
3	B	341	PX4	C28-C27	2.03	1.61	1.51	8	1
3	B	377	PX4	C20-C19	2.03	1.61	1.51	5	1
3	B	398	PX4	P1-O3	2.03	1.51	1.59	9	1
3	C	306	PX4	C33-C32	2.03	1.61	1.51	4	1
3	C	362	PX4	P1-O4	2.03	1.51	1.59	9	1
3	C	363	PX4	C28-C27	2.03	1.61	1.51	12	1
3	A	601	PX4	C16-C15	2.03	1.61	1.51	13	1
3	A	613	PX4	C4-N1	2.03	1.55	1.50	10	1
3	C	307	PX4	C27-C26	2.03	1.61	1.51	8	1
3	C	309	PX4	P1-O3	2.03	1.51	1.59	3	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	A	620	PX4	O3-C1	2.03	1.36	1.44	10	1
3	B	353	PX4	C18-C17	2.03	1.61	1.51	11	1
3	A	622	PX4	O7-C23	2.03	1.40	1.34	13	1
3	C	362	PX4	O3-C1	2.03	1.52	1.44	5	1
3	C	364	PX4	C27-C26	2.03	1.61	1.51	5	1
3	A	629	PX4	C32-C31	2.03	1.61	1.51	8	1
3	B	332	PX4	C19-C18	2.03	1.61	1.51	9	1
3	B	341	PX4	P1-O1	2.03	1.45	1.55	8	1
3	B	392	PX4	P1-O1	2.03	1.45	1.55	11	2
3	C	302	PX4	C10-C9	2.03	1.56	1.50	13	1
3	C	325	PX4	O4-C6	2.03	1.36	1.44	2	1
3	C	325	PX4	O3-C1	2.03	1.36	1.44	5	1
3	A	618	PX4	P1-O1	2.03	1.45	1.55	3	1
3	A	606	PX4	C19-C18	2.03	1.61	1.51	1	1
3	A	642	PX4	P1-O2	2.03	1.43	1.50	9	1
3	B	310	PX4	P1-O4	2.03	1.51	1.59	13	1
3	B	310	PX4	C29-C28	2.03	1.61	1.51	5	1
3	B	331	PX4	C25-C24	2.03	1.59	1.52	11	1
3	B	343	PX4	C33-C32	2.03	1.61	1.51	11	1
3	C	305	PX4	C26-C25	2.03	1.61	1.51	2	1
3	C	344	PX4	C29-C28	2.03	1.61	1.51	9	1
3	A	607	PX4	P1-O3	2.02	1.51	1.59	10	1
3	A	639	PX4	C3-N1	2.02	1.44	1.50	8	1
3	A	645	PX4	C4-N1	2.03	1.55	1.50	12	1
3	B	350	PX4	C3-N1	2.02	1.44	1.50	7	1
3	B	321	PX4	P1-O1	2.02	1.46	1.55	14	1
3	B	338	PX4	C20-C19	2.02	1.61	1.51	1	1
3	B	351	PX4	O7-C23	2.02	1.40	1.34	3	1
3	B	354	PX4	C18-C17	2.02	1.61	1.51	4	1
3	B	354	PX4	C3-N1	2.03	1.44	1.50	8	1
3	B	383	PX4	C33-C32	2.03	1.61	1.51	3	1
3	C	315	PX4	C12-C11	2.02	1.61	1.51	12	1
3	C	341	PX4	C20-C19	2.03	1.61	1.51	7	1
3	B	383	PX4	O7-C7	2.02	1.41	1.46	12	1
3	C	319	PX4	P1-O3	2.02	1.67	1.59	11	1
3	C	338	PX4	C19-C18	2.02	1.61	1.51	4	1
3	C	348	PX4	O3-C1	2.02	1.36	1.44	3	1
3	A	648	PX4	C34-C33	2.02	1.61	1.51	6	1
3	A	618	PX4	O4-C6	2.02	1.52	1.44	10	1
3	A	619	PX4	P1-O3	2.02	1.51	1.59	8	1
3	B	302	PX4	C29-C28	2.02	1.61	1.51	11	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	B	313	PX4	C27-C26	2.02	1.61	1.51	1	1
3	A	644	PX4	C13-C12	2.02	1.61	1.51	13	1
3	B	313	PX4	P1-O1	2.02	1.46	1.55	15	1
3	B	357	PX4	C28-C27	2.02	1.61	1.51	9	1
3	C	330	PX4	C33-C32	2.02	1.61	1.51	3	1
3	C	332	PX4	P1-O1	2.02	1.46	1.55	10	2
3	C	340	PX4	O6-C9	2.02	1.28	1.22	15	1
3	C	351	PX4	C3-N1	2.02	1.55	1.50	4	1
3	A	642	PX4	C28-C27	2.02	1.61	1.51	9	1
3	B	303	PX4	C29-C28	2.02	1.61	1.51	5	1
3	B	317	PX4	C5-N1	2.02	1.55	1.50	11	1
3	B	335	PX4	C17-C16	2.02	1.61	1.51	6	1
3	B	338	PX4	O5-C9	2.02	1.39	1.33	11	1
3	C	336	PX4	C17-C16	2.02	1.61	1.51	15	1
3	C	340	PX4	C5-N1	2.02	1.44	1.50	5	1
3	B	391	PX4	C2-N1	2.02	1.57	1.51	7	2
3	B	396	PX4	C13-C12	2.02	1.61	1.51	6	1
3	C	318	PX4	C29-C28	2.02	1.61	1.51	6	1
3	C	327	PX4	P1-O2	2.02	1.43	1.50	4	1
3	C	351	PX4	P1-O1	2.02	1.46	1.55	3	1
3	C	349	PX4	C25-C24	2.02	1.59	1.52	10	1
3	C	352	PX4	C27-C26	2.02	1.61	1.51	2	1
3	A	621	PX4	C30-C29	2.02	1.61	1.51	13	1
3	A	632	PX4	C13-C12	2.02	1.61	1.51	11	1
3	A	628	PX4	C32-C31	2.02	1.61	1.51	6	1
3	A	637	PX4	C17-C16	2.02	1.61	1.51	14	1
3	B	315	PX4	C11-C10	2.02	1.59	1.52	2	1
3	B	324	PX4	C2-N1	2.02	1.45	1.51	4	1
3	B	323	PX4	C14-C13	2.02	1.61	1.51	7	1
3	B	353	PX4	C5-N1	2.02	1.44	1.50	12	1
3	C	345	PX4	O3-C1	2.02	1.36	1.44	15	1
3	A	602	PX4	C12-C11	2.01	1.61	1.51	11	1
3	B	332	PX4	C16-C15	2.01	1.61	1.51	14	1
3	B	374	PX4	C3-N1	2.02	1.55	1.50	4	2
3	C	307	PX4	P1-O3	2.02	1.51	1.59	4	1
3	C	362	PX4	C10-C9	2.01	1.56	1.50	13	1
3	A	622	PX4	C19-C18	2.01	1.61	1.51	15	1
3	A	646	PX4	C26-C25	2.01	1.61	1.51	10	1
3	B	330	PX4	C5-N1	2.01	1.55	1.50	1	1
3	B	337	PX4	C5-N1	2.01	1.44	1.50	13	1
3	C	316	PX4	P1-O3	2.01	1.51	1.59	8	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	C	340	PX4	C15-C14	2.01	1.61	1.51	5	1
3	A	606	PX4	C3-N1	2.01	1.44	1.50	12	1
3	A	615	PX4	P1-O3	2.01	1.51	1.59	9	1
3	B	341	PX4	O4-C6	2.01	1.37	1.44	9	1
3	B	367	PX4	O8-C23	2.01	1.28	1.22	4	1
3	C	309	PX4	C11-C10	2.01	1.59	1.52	2	1
3	C	340	PX4	C19-C18	2.01	1.61	1.51	9	1
3	B	370	PX4	C30-C29	2.01	1.61	1.51	7	1
3	B	379	PX4	O7-C23	2.01	1.40	1.34	4	1
3	B	387	PX4	O7-C23	2.01	1.28	1.34	11	1
3	C	321	PX4	P1-O4	2.01	1.51	1.59	10	1
3	C	356	PX4	C19-C18	2.01	1.61	1.51	4	1
3	A	625	PX4	C3-N1	2.01	1.55	1.50	15	1
3	A	644	PX4	C17-C16	2.01	1.61	1.51	15	1
3	B	325	PX4	O4-C6	2.01	1.52	1.44	9	1
3	B	346	PX4	O7-C23	2.01	1.28	1.34	2	1
3	B	347	PX4	C11-C10	2.01	1.59	1.52	13	1
3	C	325	PX4	C20-C19	2.01	1.61	1.51	9	1
3	C	333	PX4	C2-N1	2.01	1.57	1.51	12	1
3	C	352	PX4	C34-C33	2.01	1.61	1.51	6	1
3	C	352	PX4	C12-C11	2.01	1.61	1.51	10	1
3	A	614	PX4	C18-C17	2.01	1.61	1.51	12	1
3	A	646	PX4	C31-C30	2.01	1.61	1.51	9	1
3	A	620	PX4	P1-O2	2.01	1.43	1.50	11	1
3	A	628	PX4	C4-N1	2.01	1.55	1.50	6	1
3	B	363	PX4	P1-O1	2.01	1.46	1.55	11	2
3	C	308	PX4	C11-C10	2.01	1.59	1.52	13	1
3	B	370	PX4	C13-C12	2.01	1.61	1.51	7	1
3	C	311	PX4	C12-C11	2.01	1.61	1.51	1	1
3	A	632	PX4	C12-C11	2.01	1.61	1.51	15	1
3	A	634	PX4	O4-C6	2.01	1.37	1.44	7	1
3	B	357	PX4	C11-C10	2.01	1.59	1.52	10	1
3	B	393	PX4	C17-C16	2.01	1.61	1.51	5	1
3	B	358	PX4	C19-C18	2.01	1.61	1.51	11	1
3	B	399	PX4	C5-N1	2.01	1.55	1.50	3	1
3	B	399	PX4	C29-C28	2.01	1.61	1.51	5	1
3	C	309	PX4	C5-N1	2.01	1.44	1.50	6	1
3	C	352	PX4	O8-C23	2.01	1.16	1.22	6	1
3	C	364	PX4	C30-C29	2.01	1.61	1.51	15	1
3	A	643	PX4	C3-N1	2.00	1.55	1.50	3	1
3	B	374	PX4	C13-C12	2.00	1.61	1.51	9	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
3	C	329	PX4	P1-O3	2.00	1.51	1.59	2	1
3	A	627	PX4	C28-C27	2.00	1.61	1.51	12	1
3	B	308	PX4	C13-C12	2.00	1.61	1.51	12	1
3	B	321	PX4	O8-C23	2.00	1.28	1.22	1	1
3	B	341	PX4	O7-C7	2.00	1.41	1.46	13	1
3	B	374	PX4	C2-N1	2.00	1.57	1.51	13	1
3	B	362	PX4	C3-N1	2.00	1.55	1.50	15	1
3	B	387	PX4	C2-N1	2.00	1.57	1.51	13	1
3	B	399	PX4	O3-C1	2.00	1.36	1.44	10	1
3	C	328	PX4	C15-C14	2.00	1.61	1.51	5	1
3	C	350	PX4	C3-N1	2.00	1.44	1.50	2	1
3	A	602	PX4	O4-C6	2.00	1.37	1.44	1	1
3	B	384	PX4	C15-C14	2.00	1.61	1.51	4	1
3	B	396	PX4	C15-C14	2.00	1.61	1.51	7	1
3	C	332	PX4	C5-N1	2.00	1.44	1.50	5	1
3	B	313	PX4	C4-N1	2.00	1.55	1.50	12	1
3	C	317	PX4	C5-N1	2.00	1.44	1.50	5	1
3	C	327	PX4	P1-O1	2.00	1.46	1.55	3	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	C	349	PX4	C7-O7-C23	5.89	103.71	117.80	4	6
3	A	653	PX4	O7-C23-C24	5.81	98.91	111.48	12	5
3	B	343	PX4	C7-O7-C23	5.60	104.38	117.80	4	5
3	C	318	PX4	C7-O7-C23	5.56	104.48	117.80	15	4
3	B	341	PX4	C7-O7-C23	5.54	104.54	117.80	11	9
3	B	342	PX4	O7-C23-C24	5.50	99.59	111.48	1	5
3	B	385	PX4	O7-C23-C24	5.35	99.91	111.48	3	6
3	A	636	PX4	C7-O7-C23	5.34	105.02	117.80	2	3
3	A	612	PX4	C7-O7-C23	5.30	105.11	117.80	12	8
3	B	329	PX4	C8-C7-C6	5.24	99.56	111.78	6	3
3	C	310	PX4	O7-C23-C24	5.18	100.27	111.48	1	8
3	B	341	PX4	O5-C8-C7	5.18	123.32	108.40	6	6
3	A	622	PX4	O7-C23-C24	5.11	100.42	111.48	6	5
3	C	311	PX4	C7-O7-C23	5.05	105.72	117.80	1	7
3	B	379	PX4	O7-C23-C24	5.01	100.63	111.48	3	8
3	C	320	PX4	O5-C8-C7	5.02	122.85	108.40	1	6
3	B	372	PX4	O7-C23-C24	5.00	100.66	111.48	15	6
3	C	361	PX4	O5-C8-C7	4.98	122.77	108.40	12	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	330	PX4	C7-O7-C23	4.97	105.89	117.80	4	8
3	B	348	PX4	C7-O7-C23	4.95	129.64	117.80	9	3
3	A	651	PX4	O7-C23-C24	4.91	100.87	111.48	12	5
3	C	325	PX4	C8-C7-C6	4.90	100.35	111.78	11	1
3	C	360	PX4	O7-C23-C24	4.85	100.98	111.48	2	3
3	B	340	PX4	O7-C23-C24	4.84	101.02	111.48	9	2
3	A	608	PX4	C7-O7-C23	4.83	106.25	117.80	7	4
3	C	327	PX4	C7-O7-C23	4.82	106.26	117.80	4	4
3	B	313	PX4	C7-O7-C23	4.81	106.29	117.80	7	2
3	C	324	PX4	C7-O7-C23	4.80	106.30	117.80	12	6
3	B	331	PX4	C7-O7-C23	4.79	106.34	117.80	14	3
3	B	378	PX4	O7-C23-C24	4.76	101.19	111.48	3	3
3	A	614	PX4	O7-C23-C24	4.75	101.20	111.48	3	3
3	B	384	PX4	O5-C8-C7	4.72	122.01	108.40	9	6
3	B	399	PX4	C8-C7-C6	4.69	122.71	111.78	15	3
3	B	328	PX4	C7-O7-C23	4.66	106.65	117.80	6	5
3	A	616	PX4	C7-O7-C23	4.65	106.66	117.80	6	7
3	B	320	PX4	O7-C23-C24	4.65	101.41	111.48	6	4
3	B	319	PX4	C7-O7-C23	4.65	106.67	117.80	1	11
3	C	344	PX4	O7-C23-C24	4.64	101.44	111.48	7	5
3	C	353	PX4	O7-C23-C24	4.64	101.45	111.48	14	3
3	B	349	PX4	O7-C23-C24	4.64	101.45	111.48	10	2
3	B	325	PX4	O7-C23-C24	4.63	101.46	111.48	12	2
3	C	302	PX4	O5-C8-C7	4.60	121.66	108.40	6	9
3	C	344	PX4	C7-O7-C23	4.59	106.81	117.80	15	3
3	A	653	PX4	O5-C8-C7	4.58	121.59	108.40	14	9
3	A	612	PX4	C5-N1-C4	4.55	120.93	108.98	11	3
3	A	626	PX4	O7-C23-C24	4.54	101.66	111.48	4	7
3	C	329	PX4	C7-O7-C23	4.54	106.94	117.80	5	4
3	A	620	PX4	O7-C23-C24	4.52	101.70	111.48	13	4
3	C	360	PX4	C5-N1-C3	4.52	97.10	108.98	13	2
3	A	601	PX4	C8-C7-C6	4.52	101.25	111.78	11	5
3	B	344	PX4	C8-C7-C6	4.52	101.25	111.78	13	3
3	B	328	PX4	O7-C23-O8	4.51	134.25	123.70	10	1
3	C	346	PX4	C7-O7-C23	4.50	107.03	117.80	5	4
3	A	605	PX4	O7-C23-O8	4.49	134.19	123.70	10	8
3	C	339	PX4	O7-C23-C24	4.47	101.81	111.48	3	4
3	B	354	PX4	O5-C8-C7	4.46	121.24	108.40	13	4
3	C	363	PX4	O7-C23-C24	4.45	101.84	111.48	9	7
3	A	637	PX4	O5-C8-C7	4.44	121.20	108.40	10	5
3	C	363	PX4	O7-C23-O8	4.44	134.09	123.70	9	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	A	651	PX4	C8-C7-C6	4.43	101.47	111.78	3	5
3	B	308	PX4	C5-N1-C4	4.42	97.36	108.98	13	3
3	B	356	PX4	C7-O7-C23	4.42	107.21	117.80	12	4
3	C	309	PX4	C8-C7-C6	4.42	101.48	111.78	11	1
3	B	399	PX4	C7-O7-C23	4.41	107.23	117.80	8	5
3	C	333	PX4	O7-C23-O8	4.40	133.99	123.70	1	1
3	B	369	PX4	C4-N1-C3	4.40	97.42	108.98	12	2
3	C	329	PX4	O5-C8-C7	4.38	121.03	108.40	1	6
3	B	318	PX4	C7-O7-C23	4.37	107.33	117.80	5	4
3	B	315	PX4	O7-C23-C24	4.36	102.04	111.48	4	1
3	C	348	PX4	O5-C8-C7	4.36	120.98	108.40	11	6
3	C	355	PX4	C7-O7-C23	4.36	107.37	117.80	8	4
3	A	605	PX4	O7-C23-C24	4.35	102.07	111.48	10	5
3	C	338	PX4	O5-C8-C7	4.34	120.92	108.40	14	4
3	B	316	PX4	C7-O7-C23	4.33	107.44	117.80	11	4
3	A	612	PX4	O5-C8-C7	4.32	120.85	108.40	3	6
3	A	611	PX4	O5-C8-C7	4.32	120.84	108.40	10	5
3	A	640	PX4	C7-O7-C23	4.32	107.46	117.80	14	5
3	C	363	PX4	C7-O7-C23	4.32	107.46	117.80	11	3
3	C	336	PX4	O7-C23-C24	4.31	102.15	111.48	13	4
3	A	650	PX4	O5-C8-C7	4.31	120.82	108.40	5	3
3	B	396	PX4	C8-C7-C6	4.31	101.74	111.78	12	4
3	C	329	PX4	O7-C23-C24	4.31	102.16	111.48	1	7
3	A	625	PX4	C8-C7-C6	4.30	101.75	111.78	6	1
3	C	339	PX4	C7-O7-C23	4.30	107.50	117.80	13	3
3	B	365	PX4	O7-C23-C24	4.30	102.18	111.48	2	3
3	B	381	PX4	O5-C8-C7	4.29	120.77	108.40	5	4
3	A	610	PX4	O7-C23-C24	4.27	102.24	111.48	4	3
3	B	323	PX4	C7-O7-C23	4.27	107.58	117.80	8	3
3	B	359	PX4	C5-N1-C4	4.27	97.77	108.98	3	2
3	B	338	PX4	O7-C23-C24	4.26	102.26	111.48	11	4
3	A	649	PX4	C7-O7-C23	4.26	107.60	117.80	7	3
3	C	331	PX4	C7-O7-C23	4.26	107.61	117.80	13	2
3	B	380	PX4	C7-O7-C23	4.25	107.62	117.80	11	6
3	C	351	PX4	O7-C23-C24	4.25	102.30	111.48	4	5
3	B	316	PX4	C8-C7-C6	4.24	101.89	111.78	11	1
3	C	331	PX4	C1-C2-N1	4.24	129.44	115.82	12	1
3	A	633	PX4	C7-O7-C23	4.24	107.66	117.80	15	3
3	A	625	PX4	C7-O7-C23	4.23	107.66	117.80	5	4
3	A	621	PX4	O7-C23-C24	4.23	102.33	111.48	5	6
3	B	369	PX4	C7-O7-C23	4.23	107.68	117.80	12	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	C	304	PX4	O7-C23-C24	4.22	102.34	111.48	12	4
3	B	354	PX4	C8-C7-C6	4.22	121.61	111.78	4	3
3	B	337	PX4	C8-C7-C6	4.21	101.96	111.78	15	5
3	C	338	PX4	C7-O7-C23	4.21	107.71	117.80	3	3
3	B	360	PX4	C7-O7-C23	4.20	107.73	117.80	13	4
3	C	338	PX4	O7-C23-C24	4.20	102.40	111.48	10	4
3	C	310	PX4	C7-O7-C23	4.20	107.75	117.80	1	5
3	C	350	PX4	C7-O7-C23	4.20	127.84	117.80	1	8
3	C	360	PX4	C7-O7-C23	4.20	107.75	117.80	2	4
3	B	326	PX4	O7-C23-C24	4.19	102.41	111.48	14	5
3	C	350	PX4	O7-C23-C24	4.19	102.42	111.48	11	5
3	B	353	PX4	O5-C8-C7	4.18	120.45	108.40	13	3
3	C	346	PX4	O5-C8-C7	4.18	120.44	108.40	11	4
3	B	360	PX4	O5-C8-C7	4.16	120.39	108.40	7	2
3	C	303	PX4	C7-O7-C23	4.16	107.84	117.80	11	7
3	C	351	PX4	C7-O7-C23	4.16	107.83	117.80	12	4
3	B	315	PX4	O5-C8-C7	4.16	120.39	108.40	13	3
3	A	611	PX4	C7-O7-C23	4.15	107.86	117.80	14	4
3	A	615	PX4	C7-O7-C23	4.15	107.86	117.80	15	3
3	C	326	PX4	C7-O7-C23	4.15	107.86	117.80	6	5
3	C	344	PX4	C5-N1-C3	4.15	119.88	108.98	1	3
3	B	396	PX4	O5-C8-C7	4.14	120.34	108.40	2	5
3	C	335	PX4	C7-O7-C23	4.14	107.88	117.80	3	4
3	A	624	PX4	C1-C2-N1	4.14	129.10	115.82	3	5
3	B	394	PX4	C5-N1-C3	4.14	119.85	108.98	3	5
3	C	342	PX4	C7-O7-C23	4.14	107.89	117.80	7	3
3	A	649	PX4	O7-C23-C24	4.14	102.53	111.48	2	3
3	B	364	PX4	C8-C7-C6	4.13	102.15	111.78	15	3
3	C	342	PX4	C5-N1-C4	4.13	119.83	108.98	15	2
3	A	631	PX4	O7-C23-C24	4.13	102.54	111.48	1	6
3	C	319	PX4	C7-O7-C23	4.13	107.91	117.80	13	5
3	B	309	PX4	C7-O7-C23	4.13	127.67	117.80	10	7
3	C	313	PX4	O5-C8-C7	4.12	120.28	108.40	5	6
3	A	608	PX4	O5-C9-C10	4.12	99.27	111.83	2	5
3	B	306	PX4	O7-C23-C24	4.12	102.57	111.48	5	1
3	A	642	PX4	C5-N1-C3	4.12	98.16	108.98	14	3
3	A	635	PX4	O5-C8-C7	4.11	120.25	108.40	11	1
3	C	336	PX4	C7-O7-C23	4.11	107.96	117.80	12	3
3	B	308	PX4	C7-O7-C23	4.11	107.97	117.80	11	2
3	C	337	PX4	C7-O7-C23	4.11	107.97	117.80	9	4
3	B	318	PX4	O7-C23-C24	4.10	102.61	111.48	3	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	C	314	PX4	O7-C23-C24	4.10	102.61	111.48	12	1
3	C	355	PX4	O7-C23-C24	4.09	102.62	111.48	12	5
3	B	315	PX4	C7-O7-C23	4.09	108.00	117.80	12	9
3	B	360	PX4	O5-C9-O6	4.09	133.86	123.63	12	3
3	A	606	PX4	O7-C23-C24	4.09	102.64	111.48	4	4
3	B	341	PX4	O7-C23-C24	4.09	102.64	111.48	15	4
3	B	333	PX4	C5-N1-C4	4.08	119.70	108.98	6	3
3	C	309	PX4	O7-C23-C24	4.07	102.67	111.48	10	2
3	B	368	PX4	O7-C23-C24	4.07	102.68	111.48	3	7
3	C	335	PX4	O7-C23-C24	4.07	102.68	111.48	10	3
3	C	345	PX4	C5-N1-C3	4.07	119.66	108.98	10	3
3	C	328	PX4	O7-C23-C24	4.06	102.69	111.48	10	6
3	A	639	PX4	C7-O7-C23	4.06	108.08	117.80	13	3
3	B	328	PX4	O7-C23-C24	4.05	102.71	111.48	5	6
3	C	313	PX4	C7-O7-C23	4.05	108.10	117.80	2	4
3	C	353	PX4	O5-C8-C7	4.04	120.06	108.40	12	4
3	A	617	PX4	O7-C23-C24	4.04	102.75	111.48	5	6
3	A	636	PX4	C8-C7-C6	4.04	121.19	111.78	14	5
3	C	361	PX4	C8-C7-C6	4.04	102.38	111.78	8	5
3	B	389	PX4	O7-C23-C24	4.02	102.78	111.48	12	3
3	C	308	PX4	O5-C9-C10	4.02	99.58	111.83	9	2
3	B	347	PX4	C7-O7-C23	4.02	108.18	117.80	15	7
3	B	307	PX4	C7-O7-C23	4.01	108.19	117.80	1	2
3	A	652	PX4	C7-O7-C23	4.01	108.20	117.80	12	6
3	A	651	PX4	O7-C23-O8	4.01	133.07	123.70	12	4
3	B	304	PX4	C8-C7-C6	4.01	121.12	111.78	12	4
3	B	350	PX4	O7-C23-C24	4.01	102.81	111.48	2	1
3	C	315	PX4	O7-C23-C24	4.01	102.81	111.48	14	5
3	C	343	PX4	O5-C8-C7	4.00	119.93	108.40	11	6
3	A	633	PX4	O5-C8-C7	4.00	119.93	108.40	4	1
3	A	622	PX4	C7-O7-C23	4.00	108.23	117.80	13	3
3	B	388	PX4	C8-C7-C6	4.00	121.10	111.78	13	5
3	C	307	PX4	O5-C8-C7	3.99	119.90	108.40	8	10
3	A	652	PX4	O5-C8-C7	3.99	119.89	108.40	9	5
3	B	311	PX4	O7-C23-C24	3.99	102.85	111.48	3	4
3	C	321	PX4	O5-C8-C7	3.99	119.88	108.40	12	4
3	C	350	PX4	C5-N1-C3	3.97	98.55	108.98	7	1
3	C	332	PX4	C7-O7-C23	3.97	108.30	117.80	15	3
3	B	312	PX4	C5-N1-C3	3.96	98.57	108.98	13	2
3	B	348	PX4	O7-C23-C24	3.96	102.91	111.48	12	3
3	C	354	PX4	C8-C7-C6	3.96	121.02	111.78	6	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	306	PX4	O5-C8-C7	3.96	119.80	108.40	5	9
3	B	348	PX4	C8-C7-C6	3.96	121.01	111.78	2	4
3	C	306	PX4	O7-C23-C24	3.96	102.92	111.48	9	3
3	C	317	PX4	C7-O7-C23	3.96	127.26	117.80	4	4
3	B	388	PX4	O7-C23-C24	3.95	102.93	111.48	1	5
3	A	618	PX4	O5-C8-C7	3.95	119.79	108.40	1	9
3	C	358	PX4	O7-C23-C24	3.95	102.93	111.48	8	4
3	B	393	PX4	O7-C23-C24	3.95	102.94	111.48	10	4
3	C	350	PX4	C5-N1-C4	3.95	98.61	108.98	13	1
3	A	607	PX4	O5-C9-C10	3.94	99.81	111.83	6	3
3	B	386	PX4	O7-C23-C24	3.94	102.95	111.48	14	6
3	B	336	PX4	C1-C2-N1	3.93	128.45	115.82	8	2
3	A	622	PX4	C8-C7-C6	3.93	120.95	111.78	13	6
3	A	651	PX4	C7-O7-C23	3.93	108.39	117.80	14	2
3	B	384	PX4	C7-O7-C23	3.92	108.41	117.80	13	6
3	B	327	PX4	C7-O7-C23	3.92	108.41	117.80	10	3
3	C	358	PX4	C8-C7-C6	3.92	120.92	111.78	1	2
3	A	627	PX4	C7-O7-C23	3.92	108.42	117.80	6	4
3	B	346	PX4	C7-O7-C23	3.92	108.42	117.80	7	1
3	B	327	PX4	C5-N1-C4	3.91	98.69	108.98	3	3
3	B	382	PX4	O7-C23-C24	3.91	103.01	111.48	3	4
3	B	345	PX4	C4-N1-C3	3.90	119.23	108.98	3	1
3	C	313	PX4	O5-C9-O6	3.90	133.39	123.63	14	2
3	B	367	PX4	C7-O7-C23	3.90	108.47	117.80	1	7
3	C	352	PX4	C7-O7-C23	3.89	108.49	117.80	4	5
3	A	630	PX4	C8-C7-C6	3.88	102.73	111.78	3	5
3	B	372	PX4	O7-C23-O8	3.89	132.79	123.70	15	5
3	B	362	PX4	O5-C8-C7	3.88	119.59	108.40	7	6
3	C	304	PX4	O5-C8-C7	3.88	119.59	108.40	12	2
3	C	364	PX4	O5-C8-C7	3.88	119.57	108.40	6	4
3	B	349	PX4	O5-C8-C7	3.88	119.57	108.40	14	3
3	B	393	PX4	C7-O7-C23	3.87	108.53	117.80	12	1
3	C	310	PX4	C5-N1-C4	3.87	98.80	108.98	4	1
3	B	344	PX4	O5-C8-C7	3.87	119.56	108.40	5	4
3	A	609	PX4	C7-O7-C23	3.87	108.53	117.80	6	3
3	B	336	PX4	O7-C23-O8	3.87	132.75	123.70	14	2
3	B	392	PX4	C7-O7-C23	3.87	108.54	117.80	10	7
3	B	334	PX4	C7-O7-C23	3.87	108.54	117.80	14	3
3	B	306	PX4	C7-O7-C23	3.86	108.55	117.80	14	5
3	B	322	PX4	O7-C23-O8	3.86	132.74	123.70	12	2
3	B	399	PX4	O7-C23-C24	3.86	103.13	111.48	15	7

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	389	PX4	C7-O7-C23	3.86	108.56	117.80	9	8
3	B	308	PX4	O7-C23-C24	3.86	103.14	111.48	9	5
3	B	385	PX4	O5-C8-C7	3.86	119.51	108.40	7	1
3	A	604	PX4	O7-C23-C24	3.85	103.15	111.48	3	4
3	B	310	PX4	C5-N1-C4	3.85	98.86	108.98	4	3
3	B	326	PX4	C4-N1-C3	3.85	119.09	108.98	4	2
3	C	354	PX4	O7-C23-C24	3.85	103.15	111.48	13	7
3	C	320	PX4	C8-C7-C6	3.84	120.75	111.78	15	2
3	C	357	PX4	O7-C23-C24	3.84	103.17	111.48	10	5
3	A	626	PX4	O7-C23-O8	3.83	132.66	123.70	13	2
3	B	307	PX4	O5-C8-C7	3.83	119.44	108.40	14	5
3	B	352	PX4	O5-C8-C7	3.83	119.44	108.40	15	5
3	B	361	PX4	O7-C23-C24	3.83	103.20	111.48	12	5
3	B	351	PX4	O5-C8-C7	3.82	119.42	108.40	2	6
3	B	301	PX4	C7-O7-C23	3.82	108.65	117.80	3	2
3	B	353	PX4	O7-C23-O8	3.82	132.64	123.70	14	3
3	B	398	PX4	C7-O7-C23	3.82	108.66	117.80	5	6
3	A	636	PX4	O7-C23-O8	3.82	132.63	123.70	10	1
3	B	332	PX4	C7-O7-C23	3.81	108.67	117.80	1	5
3	C	307	PX4	O7-C23-C24	3.82	103.23	111.48	8	4
3	B	365	PX4	O7-C23-O8	3.81	132.62	123.70	15	3
3	B	385	PX4	C5-N1-C4	3.80	118.97	108.98	8	1
3	B	304	PX4	C7-O7-C23	3.80	108.71	117.80	11	7
3	A	610	PX4	C7-O7-C23	3.79	108.71	117.80	1	4
3	A	626	PX4	O5-C8-C7	3.79	119.33	108.40	2	3
3	C	322	PX4	C8-C7-C6	3.79	102.94	111.78	7	2
3	A	633	PX4	O7-C23-C24	3.79	103.28	111.48	5	6
3	B	344	PX4	O5-C9-C10	3.79	100.28	111.83	3	3
3	B	306	PX4	C8-C7-C6	3.79	102.95	111.78	9	4
3	B	360	PX4	O7-C23-C24	3.78	103.29	111.48	1	3
3	A	654	PX4	C7-O7-C23	3.78	108.74	117.80	6	7
3	A	603	PX4	O5-C8-C7	3.78	119.30	108.40	14	4
3	A	619	PX4	C1-C2-N1	3.78	127.95	115.82	9	3
3	B	364	PX4	O7-C23-C24	3.78	103.31	111.48	13	5
3	A	603	PX4	O7-C23-O8	3.77	132.53	123.70	12	7
3	A	641	PX4	O7-C23-C24	3.77	103.32	111.48	4	3
3	B	339	PX4	C7-O7-C23	3.77	108.77	117.80	1	6
3	B	381	PX4	C4-N1-C3	3.77	99.07	108.98	14	2
3	A	602	PX4	C7-O7-C23	3.76	108.79	117.80	11	5
3	B	334	PX4	C8-C7-C6	3.76	103.01	111.78	7	2
3	B	398	PX4	O5-C8-C7	3.76	119.24	108.40	4	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	A	604	PX4	C7-O7-C23	3.75	108.82	117.80	6	8
3	B	388	PX4	O5-C8-C7	3.75	119.21	108.40	15	3
3	B	356	PX4	O7-C23-O8	3.75	132.47	123.70	4	2
3	A	646	PX4	C5-N1-C3	3.75	99.13	108.98	12	5
3	A	646	PX4	C5-N1-C4	3.74	99.14	108.98	6	2
3	C	305	PX4	O5-C9-C10	3.74	100.42	111.83	14	2
3	C	324	PX4	O5-C8-C7	3.74	119.18	108.40	10	4
3	A	621	PX4	C7-O7-C23	3.74	108.84	117.80	5	6
3	A	644	PX4	C4-N1-C3	3.74	99.16	108.98	11	1
3	B	312	PX4	O7-C23-C24	3.73	103.40	111.48	12	1
3	B	376	PX4	C7-O7-C23	3.73	108.86	117.80	6	3
3	C	364	PX4	O7-C23-O8	3.73	132.44	123.70	2	3
3	B	358	PX4	C7-O7-C23	3.73	108.86	117.80	4	4
3	B	379	PX4	C7-O7-C23	3.73	126.72	117.80	4	4
3	B	380	PX4	C5-N1-C3	3.73	99.19	108.98	2	3
3	C	301	PX4	O5-C8-C7	3.72	119.13	108.40	15	4
3	C	305	PX4	O7-C23-O8	3.73	132.41	123.70	13	1
3	C	350	PX4	O5-C8-C7	3.72	119.13	108.40	10	8
3	C	353	PX4	C1-C2-N1	3.72	127.77	115.82	3	4
3	C	321	PX4	O7-C23-C24	3.71	103.45	111.48	6	5
3	B	313	PX4	O7-C23-C24	3.71	103.45	111.48	10	2
3	B	308	PX4	O7-C23-O8	3.71	132.37	123.70	3	3
3	B	320	PX4	C7-O7-C23	3.70	108.94	117.80	5	6
3	A	647	PX4	C8-C7-C6	3.70	103.17	111.78	10	2
3	B	367	PX4	C8-O5-C9	3.69	103.63	117.12	15	1
3	C	317	PX4	C8-C7-C6	3.69	120.39	111.78	4	9
3	C	310	PX4	O5-C8-C7	3.69	119.03	108.40	5	6
3	A	634	PX4	O5-C9-O6	3.69	132.85	123.63	4	2
3	B	371	PX4	C7-O7-C23	3.69	108.97	117.80	7	3
3	B	335	PX4	C5-N1-C3	3.68	118.65	108.98	8	3
3	B	313	PX4	O7-C23-O8	3.68	132.31	123.70	14	4
3	C	330	PX4	C8-C7-C6	3.68	103.20	111.78	12	4
3	C	333	PX4	C4-N1-C3	3.68	99.32	108.98	14	2
3	C	332	PX4	O5-C9-C10	3.67	100.66	111.83	2	4
3	A	645	PX4	O7-C23-C24	3.66	103.55	111.48	8	3
3	C	358	PX4	C26-C25-C24	3.66	99.67	113.13	11	1
3	A	603	PX4	O7-C23-C24	3.66	103.56	111.48	15	3
3	A	638	PX4	C4-N1-C3	3.66	99.36	108.98	2	2
3	A	631	PX4	C7-O7-C23	3.66	109.04	117.80	7	3
3	B	394	PX4	C1-C2-N1	3.65	127.55	115.82	4	1
3	A	608	PX4	O5-C9-O6	3.65	132.77	123.63	2	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	375	PX4	C7-O7-C23	3.65	109.06	117.80	7	6
3	A	607	PX4	O7-C23-C24	3.65	103.58	111.48	14	4
3	A	632	PX4	C8-C7-C6	3.65	103.28	111.78	11	2
3	B	364	PX4	C7-O7-C23	3.65	109.07	117.80	7	5
3	B	400	PX4	O7-C23-C24	3.64	103.60	111.48	5	5
3	B	311	PX4	O7-C23-O8	3.64	132.21	123.70	3	2
3	B	397	PX4	O7-C23-C24	3.64	103.61	111.48	2	5
3	B	341	PX4	O5-C9-O6	3.64	132.73	123.63	6	4
3	C	328	PX4	O5-C8-C7	3.64	118.89	108.40	9	6
3	B	353	PX4	C4-N1-C3	3.64	99.42	108.98	4	3
3	C	312	PX4	C7-O7-C23	3.64	109.09	117.80	12	2
3	B	309	PX4	C8-C7-C6	3.63	103.31	111.78	10	3
3	B	392	PX4	O5-C8-C7	3.63	118.87	108.40	8	6
3	A	643	PX4	C7-O7-C23	3.63	109.11	117.80	4	4
3	B	356	PX4	C8-C7-C6	3.63	103.32	111.78	12	4
3	C	358	PX4	C7-O7-C23	3.63	109.11	117.80	9	4
3	B	376	PX4	O7-C23-O8	3.62	132.18	123.70	15	3
3	B	354	PX4	C7-O7-C23	3.62	109.13	117.80	8	3
3	B	329	PX4	C5-N1-C4	3.61	99.49	108.98	13	3
3	B	372	PX4	C4-N1-C3	3.61	99.49	108.98	12	3
3	C	324	PX4	C5-N1-C3	3.61	99.49	108.98	7	1
3	A	654	PX4	O5-C9-O6	3.61	132.66	123.63	6	2
3	B	353	PX4	C5-N1-C3	3.61	118.45	108.98	11	5
3	B	319	PX4	O7-C23-C24	3.61	103.68	111.48	4	5
3	A	642	PX4	O7-C23-C24	3.60	103.70	111.48	15	1
3	C	340	PX4	C7-O7-C23	3.60	109.18	117.80	1	2
3	B	355	PX4	O7-C23-C24	3.60	103.70	111.48	12	6
3	A	640	PX4	C4-N1-C3	3.59	99.54	108.98	12	1
3	A	635	PX4	C5-N1-C3	3.59	118.41	108.98	1	2
3	B	308	PX4	O5-C9-O6	3.59	132.60	123.63	3	3
3	B	317	PX4	C4-N1-C3	3.59	99.56	108.98	3	2
3	B	319	PX4	O7-C23-O8	3.59	132.09	123.70	10	3
3	A	624	PX4	C7-O7-C23	3.58	109.22	117.80	2	3
3	C	307	PX4	C7-O7-C23	3.59	109.22	117.80	4	2
3	B	359	PX4	C4-N1-C3	3.58	118.39	108.98	3	3
3	A	617	PX4	O5-C9-C10	3.58	100.92	111.83	8	1
3	A	623	PX4	C8-C7-C6	3.58	120.13	111.78	7	4
3	B	338	PX4	O5-C8-C7	3.58	118.72	108.40	7	5
3	C	303	PX4	O5-C8-C7	3.58	118.71	108.40	12	4
3	B	390	PX4	C7-O7-C23	3.58	109.24	117.80	8	2
3	C	331	PX4	C5-N1-C3	3.57	99.59	108.98	15	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	A	608	PX4	O5-C8-C7	3.57	118.69	108.40	2	4
3	B	332	PX4	O5-C8-C7	3.57	118.69	108.40	13	4
3	B	377	PX4	O5-C8-C7	3.57	118.69	108.40	11	4
3	C	347	PX4	O7-C23-O8	3.57	132.05	123.70	15	3
3	B	395	PX4	O7-C23-C24	3.57	103.76	111.48	11	6
3	C	362	PX4	O7-C23-C24	3.56	103.77	111.48	6	5
3	B	335	PX4	C7-O7-C23	3.56	109.27	117.80	3	3
3	C	320	PX4	C7-O7-C23	3.56	109.27	117.80	10	6
3	C	326	PX4	O5-C8-C7	3.56	118.66	108.40	11	4
3	A	612	PX4	O7-C23-O8	3.55	132.00	123.70	14	1
3	A	629	PX4	O5-C8-C7	3.55	118.62	108.40	9	3
3	C	325	PX4	O7-C23-O8	3.54	131.99	123.70	9	6
3	B	336	PX4	C4-N1-C3	3.54	118.28	108.98	2	2
3	C	332	PX4	C5-N1-C4	3.54	118.28	108.98	8	2
3	B	342	PX4	C11-C10-C9	3.54	126.66	113.69	7	2
3	B	387	PX4	O7-C23-O8	3.54	131.98	123.70	12	2
3	A	640	PX4	O5-C8-C7	3.54	118.59	108.40	9	4
3	A	645	PX4	C8-O5-C9	3.53	130.04	117.12	1	3
3	A	652	PX4	O7-C23-C24	3.53	103.84	111.48	6	4
3	B	347	PX4	C4-N1-C3	3.53	99.70	108.98	4	4
3	C	311	PX4	O5-C8-C7	3.53	118.58	108.40	14	4
3	C	355	PX4	O5-C9-C10	3.53	101.07	111.83	9	4
3	C	322	PX4	O7-C23-C24	3.53	103.84	111.48	4	4
3	C	323	PX4	O5-C9-C10	3.53	101.08	111.83	3	3
3	C	306	PX4	O5-C8-C7	3.53	118.56	108.40	12	2
3	C	308	PX4	O7-C23-C24	3.52	103.86	111.48	9	2
3	C	347	PX4	C7-O7-C23	3.52	109.36	117.80	8	3
3	B	366	PX4	C8-C7-C6	3.52	103.58	111.78	15	1
3	B	395	PX4	O7-C7-C8	3.52	120.97	108.34	3	3
3	C	364	PX4	C8-C7-C6	3.52	103.58	111.78	10	3
3	A	633	PX4	C5-N1-C4	3.52	99.74	108.98	15	1
3	A	621	PX4	O7-C23-O8	3.51	131.92	123.70	1	6
3	C	333	PX4	C7-O7-C23	3.51	109.39	117.80	13	3
3	B	324	PX4	O5-C8-C7	3.51	118.51	108.40	11	3
3	C	349	PX4	O5-C9-O6	3.51	132.40	123.63	15	3
3	B	312	PX4	C4-N1-C3	3.50	99.77	108.98	3	4
3	B	353	PX4	O7-C23-C24	3.50	103.90	111.48	9	1
3	B	383	PX4	C8-C7-C6	3.50	103.62	111.78	8	3
3	B	379	PX4	O5-C8-C7	3.50	118.48	108.40	12	2
3	C	328	PX4	C4-N1-C3	3.50	118.17	108.98	6	4
3	A	615	PX4	O7-C23-C24	3.50	103.92	111.48	7	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	A	622	PX4	C4-N1-C3	3.50	99.79	108.98	13	2
3	C	354	PX4	C7-O7-C23	3.50	109.43	117.80	15	4
3	C	333	PX4	C8-C7-C6	3.49	103.64	111.78	2	4
3	C	355	PX4	O5-C9-O6	3.49	132.36	123.63	9	2
3	B	310	PX4	C7-O7-C23	3.49	109.44	117.80	12	3
3	C	321	PX4	C8-C7-C6	3.49	103.65	111.78	10	4
3	C	334	PX4	C5-N1-C3	3.49	99.81	108.98	13	3
3	A	607	PX4	C7-O7-C23	3.49	109.45	117.80	6	6
3	B	313	PX4	O5-C8-C7	3.49	118.45	108.40	12	3
3	B	332	PX4	O7-C23-C24	3.48	103.94	111.48	7	5
3	B	380	PX4	O5-C8-C7	3.48	118.44	108.40	10	8
3	C	342	PX4	O7-C23-C24	3.48	103.94	111.48	3	3
3	B	381	PX4	C1-C2-N1	3.48	126.99	115.82	6	3
3	B	301	PX4	C4-N1-C3	3.47	99.85	108.98	14	2
3	B	367	PX4	O7-C23-C24	3.47	103.97	111.48	11	3
3	C	305	PX4	O5-C8-C7	3.47	118.41	108.40	15	4
3	B	366	PX4	C5-N1-C3	3.47	99.86	108.98	9	3
3	C	340	PX4	C8-C7-C6	3.47	103.69	111.78	12	5
3	B	301	PX4	O5-C9-O6	3.47	132.31	123.63	15	1
3	A	615	PX4	O5-C8-C7	3.47	118.39	108.40	1	2
3	B	373	PX4	O7-C23-C24	3.47	103.98	111.48	3	5
3	A	651	PX4	O5-C8-C7	3.47	118.39	108.40	5	10
3	C	318	PX4	O5-C8-C7	3.47	118.39	108.40	14	4
3	A	629	PX4	C7-O7-C23	3.47	109.50	117.80	6	4
3	A	624	PX4	C4-N1-C3	3.46	99.88	108.98	10	4
3	C	337	PX4	O7-C23-C24	3.46	103.99	111.48	12	5
3	A	618	PX4	O7-C23-O8	3.46	131.79	123.70	12	3
3	B	350	PX4	O5-C9-O6	3.46	132.28	123.63	4	5
3	B	357	PX4	C4-N1-C3	3.46	99.89	108.98	13	4
3	A	644	PX4	O5-C8-C7	3.46	118.36	108.40	5	5
3	B	325	PX4	O5-C8-C7	3.45	118.36	108.40	4	4
3	B	352	PX4	C8-C7-C6	3.46	103.73	111.78	5	3
3	B	375	PX4	O7-C23-C24	3.46	104.01	111.48	7	1
3	C	302	PX4	O5-C9-O6	3.46	132.27	123.63	5	2
3	C	326	PX4	O7-C23-O8	3.45	131.78	123.70	9	2
3	B	321	PX4	O5-C9-O6	3.45	132.27	123.63	8	3
3	A	643	PX4	C8-C7-C6	3.45	103.74	111.78	5	3
3	A	636	PX4	C1-C2-N1	3.45	126.89	115.82	1	1
3	B	329	PX4	C4-N1-C3	3.45	99.92	108.98	1	2
3	B	363	PX4	C11-C10-C9	3.45	101.06	113.69	7	2
3	B	378	PX4	O5-C9-C10	3.45	101.32	111.83	15	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	378	PX4	C5-N1-C3	3.45	99.92	108.98	13	3
3	A	625	PX4	O5-C8-C7	3.44	118.32	108.40	6	5
3	B	394	PX4	O5-C9-O6	3.44	132.24	123.63	1	3
3	B	309	PX4	O7-C23-C24	3.44	104.04	111.48	10	5
3	C	317	PX4	O7-C7-C6	3.44	120.69	108.34	1	6
3	B	355	PX4	C5-N1-C3	3.44	99.94	108.98	8	2
3	A	601	PX4	O5-C9-O6	3.44	132.23	123.63	6	2
3	C	306	PX4	C8-C7-C6	3.44	119.80	111.78	11	4
3	C	330	PX4	C7-O7-C23	3.44	126.03	117.80	14	6
3	B	370	PX4	C1-C2-N1	3.43	126.85	115.82	1	3
3	A	608	PX4	O7-C23-C24	3.43	104.05	111.48	13	2
3	A	638	PX4	C7-O7-C23	3.43	109.58	117.80	7	2
3	B	377	PX4	C8-C7-C6	3.43	119.79	111.78	2	4
3	A	601	PX4	O7-C23-C24	3.43	104.06	111.48	4	3
3	A	602	PX4	O5-C9-O6	3.43	132.21	123.63	9	2
3	A	649	PX4	C5-N1-C3	3.43	99.97	108.98	13	6
3	B	344	PX4	O7-C23-C24	3.43	104.06	111.48	4	5
3	B	396	PX4	O7-C23-C24	3.43	104.06	111.48	13	3
3	C	333	PX4	O5-C9-O6	3.43	132.21	123.63	4	1
3	B	334	PX4	O5-C8-C7	3.43	118.28	108.40	6	3
3	C	331	PX4	O5-C8-C7	3.43	118.28	108.40	15	8
3	A	644	PX4	C8-C7-C6	3.42	103.80	111.78	5	4
3	A	648	PX4	C7-O7-C23	3.42	109.60	117.80	1	5
3	C	340	PX4	O5-C8-C7	3.43	118.27	108.40	1	3
3	A	644	PX4	C7-O7-C23	3.42	109.60	117.80	15	2
3	C	308	PX4	C7-O7-C23	3.42	109.60	117.80	12	6
3	A	620	PX4	O5-C8-C7	3.42	118.26	108.40	12	5
3	B	346	PX4	C5-N1-C4	3.41	100.01	108.98	5	3
3	C	358	PX4	O5-C9-C10	3.41	101.43	111.83	4	2
3	A	621	PX4	C5-N1-C3	3.41	100.01	108.98	6	2
3	B	312	PX4	C5-N1-C4	3.41	117.94	108.98	4	3
3	A	634	PX4	C4-N1-C3	3.41	117.93	108.98	8	3
3	C	358	PX4	O7-C23-O8	3.41	131.68	123.70	2	3
3	A	615	PX4	O7-C23-O8	3.41	131.67	123.70	10	3
3	B	344	PX4	O7-C23-O8	3.41	131.67	123.70	11	3
3	B	399	PX4	O5-C8-C7	3.41	118.22	108.40	14	2
3	B	336	PX4	O7-C23-C24	3.40	104.12	111.48	1	5
3	A	611	PX4	C8-C7-C6	3.40	103.85	111.78	14	2
3	B	323	PX4	O5-C8-C7	3.40	118.20	108.40	6	3
3	A	616	PX4	O5-C9-O6	3.40	132.13	123.63	1	4
3	B	310	PX4	C8-C7-C6	3.40	103.86	111.78	8	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	C	318	PX4	O7-C23-C24	3.40	104.13	111.48	12	3
3	B	342	PX4	C4-N1-C3	3.40	100.06	108.98	5	3
3	B	393	PX4	C25-C24-C23	3.40	101.25	113.69	15	1
3	C	324	PX4	O7-C23-C24	3.40	104.13	111.48	4	7
3	C	306	PX4	C4-N1-C3	3.39	100.06	108.98	12	2
3	C	318	PX4	C8-C7-C6	3.39	103.87	111.78	12	2
3	C	330	PX4	O7-C23-C24	3.39	104.14	111.48	11	6
3	B	354	PX4	O7-C23-C24	3.39	104.14	111.48	14	3
3	C	315	PX4	C7-O7-C23	3.39	109.68	117.80	11	6
3	A	607	PX4	O5-C8-C7	3.39	118.17	108.40	3	5
3	A	624	PX4	C5-N1-C3	3.39	100.07	108.98	11	2
3	A	654	PX4	C8-C7-C6	3.39	103.88	111.78	15	4
3	B	374	PX4	C7-O7-C23	3.39	109.68	117.80	2	5
3	C	333	PX4	O7-C23-C24	3.39	104.15	111.48	10	4
3	A	652	PX4	O5-C9-O6	3.39	132.10	123.63	10	3
3	B	397	PX4	O5-C8-C7	3.39	118.16	108.40	8	4
3	C	361	PX4	O5-C9-O6	3.39	132.10	123.63	9	1
3	C	316	PX4	O5-C8-C7	3.39	118.16	108.40	12	1
3	C	332	PX4	O7-C23-C24	3.39	104.16	111.48	2	1
3	C	306	PX4	C5-N1-C3	3.38	117.86	108.98	1	4
3	C	327	PX4	O5-C8-C7	3.38	118.15	108.40	8	4
3	A	640	PX4	O7-C7-C8	3.38	120.47	108.34	13	2
3	B	321	PX4	C4-N1-C3	3.38	117.85	108.98	12	3
3	B	362	PX4	C4-N1-C3	3.38	117.85	108.98	3	2
3	B	396	PX4	O5-C9-O6	3.38	132.08	123.63	8	4
3	C	342	PX4	C25-C24-C23	3.38	101.31	113.69	2	1
3	B	339	PX4	C8-C7-C6	3.38	103.91	111.78	7	5
3	C	301	PX4	C8-C7-C6	3.38	103.91	111.78	8	2
3	B	337	PX4	C7-O7-C23	3.38	109.71	117.80	5	6
3	C	354	PX4	O5-C9-C10	3.38	101.54	111.83	13	2
3	B	376	PX4	O7-C23-C24	3.38	104.18	111.48	8	6
3	A	637	PX4	C7-O7-C23	3.37	109.72	117.80	9	5
3	B	393	PX4	C8-C7-C6	3.38	119.66	111.78	15	2
3	C	301	PX4	O7-C23-C24	3.37	104.18	111.48	13	5
3	B	347	PX4	O5-C8-C7	3.37	118.11	108.40	3	3
3	A	628	PX4	C7-O7-C23	3.37	109.73	117.80	4	3
3	B	395	PX4	C8-O5-C9	3.37	104.80	117.12	14	1
3	B	317	PX4	C7-O7-C23	3.37	109.74	117.80	15	6
3	C	329	PX4	O7-C23-O8	3.37	131.58	123.70	14	3
3	B	301	PX4	C5-N1-C3	3.36	100.14	108.98	13	2
3	B	310	PX4	C5-N1-C3	3.36	117.81	108.98	5	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	373	PX4	O5-C9-C10	3.37	101.57	111.83	4	4
3	B	361	PX4	C7-O7-C23	3.36	109.74	117.80	6	6
3	C	354	PX4	C5-N1-C3	3.36	117.81	108.98	3	3
3	C	356	PX4	O5-C9-C10	3.36	101.58	111.83	14	2
3	B	335	PX4	O7-C23-O8	3.36	131.56	123.70	5	3
3	C	306	PX4	C7-O7-C23	3.36	109.76	117.80	6	4
3	C	358	PX4	O5-C9-O6	3.36	132.03	123.63	10	1
3	B	347	PX4	O7-C23-C24	3.36	104.22	111.48	6	4
3	A	648	PX4	O5-C9-C10	3.36	101.60	111.83	4	1
3	B	366	PX4	C26-C25-C24	3.36	100.79	113.13	8	2
3	B	372	PX4	C7-O7-C23	3.36	125.83	117.80	7	4
3	B	386	PX4	C5-N1-C3	3.36	100.16	108.98	15	2
3	C	311	PX4	O5-C9-C10	3.36	101.60	111.83	6	4
3	B	373	PX4	C7-O7-C23	3.35	109.77	117.80	11	6
3	A	608	PX4	C8-C7-C6	3.35	103.97	111.78	2	3
3	B	301	PX4	C8-C7-C6	3.35	103.97	111.78	11	2
3	A	618	PX4	C7-O7-C23	3.35	109.78	117.80	10	5
3	C	345	PX4	O5-C9-O6	3.35	132.01	123.63	9	3
3	A	607	PX4	C8-C7-C6	3.35	119.59	111.78	5	2
3	B	355	PX4	C4-N1-C3	3.35	100.18	108.98	6	4
3	A	636	PX4	O7-C23-C24	3.34	104.25	111.48	15	5
3	A	647	PX4	C7-O7-C23	3.34	109.79	117.80	4	7
3	B	356	PX4	O5-C8-C7	3.34	118.03	108.40	15	3
3	C	323	PX4	O5-C8-C7	3.34	118.03	108.40	13	6
3	A	601	PX4	O7-C7-C6	3.34	120.33	108.34	7	3
3	C	338	PX4	O7-C23-O8	3.34	131.52	123.70	15	1
3	A	628	PX4	O7-C23-O8	3.34	131.51	123.70	10	3
3	B	396	PX4	C7-O7-C23	3.34	109.81	117.80	8	4
3	C	307	PX4	C1-C2-N1	3.33	126.52	115.82	10	2
3	C	309	PX4	O5-C8-C7	3.33	118.00	108.40	8	3
3	C	323	PX4	C8-C7-C6	3.33	119.56	111.78	8	2
3	C	334	PX4	O7-C23-O8	3.33	131.50	123.70	2	1
3	C	348	PX4	C7-O7-C23	3.33	109.82	117.80	8	6
3	B	358	PX4	O7-C23-C24	3.33	104.28	111.48	9	4
3	B	393	PX4	O7-C23-O8	3.33	131.49	123.70	5	2
3	C	349	PX4	C4-N1-C2	3.33	123.14	109.91	15	2
3	A	610	PX4	O5-C9-O6	3.33	131.95	123.63	7	1
3	B	331	PX4	C4-N1-C3	3.33	100.24	108.98	8	1
3	A	613	PX4	O7-C23-O8	3.32	131.47	123.70	1	2
3	B	311	PX4	O5-C8-C7	3.32	117.98	108.40	6	5
3	B	339	PX4	O7-C23-O8	3.32	131.48	123.70	9	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	347	PX4	C5-N1-C3	3.32	100.25	108.98	15	3
3	C	305	PX4	C7-O7-C23	3.32	109.85	117.80	11	5
3	C	353	PX4	C8-O5-C9	3.32	104.98	117.12	2	4
3	C	339	PX4	O7-C23-O8	3.32	131.46	123.70	10	4
3	B	357	PX4	O7-C23-C24	3.32	104.30	111.48	11	4
3	C	364	PX4	C5-N1-C3	3.32	100.26	108.98	9	3
3	B	341	PX4	C4-N1-C3	3.32	100.27	108.98	13	4
3	A	640	PX4	O7-C23-C24	3.31	104.32	111.48	12	6
3	C	315	PX4	O5-C9-O6	3.31	131.91	123.63	3	1
3	A	635	PX4	O5-C9-O6	3.31	131.91	123.63	10	3
3	B	333	PX4	C7-O7-C23	3.31	109.88	117.80	10	3
3	C	316	PX4	O7-C23-C24	3.31	104.32	111.48	10	4
3	C	342	PX4	O5-C8-C7	3.31	117.94	108.40	5	2
3	B	374	PX4	C8-C7-C6	3.31	104.07	111.78	1	6
3	B	397	PX4	C5-N1-C4	3.31	100.29	108.98	10	2
3	C	363	PX4	O5-C8-C7	3.31	117.94	108.40	7	6
3	B	400	PX4	C5-N1-C4	3.31	117.66	108.98	7	3
3	C	311	PX4	O5-C9-O6	3.31	131.90	123.63	1	2
3	A	601	PX4	C5-N1-C4	3.30	100.30	108.98	12	2
3	A	652	PX4	C8-C7-C6	3.30	119.49	111.78	6	3
3	B	391	PX4	O5-C9-C10	3.30	101.76	111.83	7	1
3	A	648	PX4	O5-C9-O6	3.30	131.88	123.63	2	4
3	B	318	PX4	C5-N1-C3	3.30	117.65	108.98	14	2
3	B	378	PX4	C5-N1-C4	3.30	100.31	108.98	5	3
3	C	357	PX4	O7-C23-O8	3.30	131.42	123.70	1	3
3	B	345	PX4	C7-O7-C23	3.29	109.91	117.80	7	4
3	A	647	PX4	O5-C8-C7	3.29	117.89	108.40	5	5
3	B	311	PX4	C8-C7-C6	3.29	104.11	111.78	4	2
3	B	316	PX4	C5-N1-C3	3.29	100.33	108.98	8	2
3	B	398	PX4	C8-O5-C9	3.29	105.08	117.12	3	3
3	C	314	PX4	O5-C8-C7	3.29	117.89	108.40	10	6
3	C	342	PX4	O7-C7-C8	3.29	120.15	108.34	4	3
3	B	309	PX4	O7-C23-O8	3.29	131.40	123.70	3	4
3	A	636	PX4	O5-C9-C10	3.29	101.81	111.83	1	3
3	A	648	PX4	C8-C7-C6	3.29	104.12	111.78	14	1
3	A	653	PX4	C7-O7-C23	3.29	109.93	117.80	13	3
3	B	307	PX4	O7-C23-C24	3.29	104.37	111.48	10	3
3	B	359	PX4	C8-C7-C6	3.29	119.45	111.78	2	3
3	B	385	PX4	C7-O7-C23	3.29	109.93	117.80	9	1
3	A	618	PX4	O5-C9-C10	3.28	101.83	111.83	10	3
3	B	314	PX4	O7-C23-C24	3.28	104.38	111.48	10	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	325	PX4	O7-C23-O8	3.28	131.38	123.70	9	4
3	B	319	PX4	O5-C9-C10	3.27	101.86	111.83	15	1
3	B	372	PX4	C5-N1-C4	3.27	117.58	108.98	12	3
3	B	329	PX4	C7-O7-C23	3.27	109.96	117.80	11	4
3	C	317	PX4	C5-N1-C3	3.27	100.38	108.98	15	4
3	B	343	PX4	C16-C15-C14	3.27	130.90	114.37	12	1
3	B	335	PX4	O5-C8-C7	3.27	117.81	108.40	6	6
3	A	618	PX4	O7-C23-C24	3.27	104.42	111.48	8	5
3	A	642	PX4	C7-O7-C23	3.26	109.99	117.80	6	6
3	B	343	PX4	O7-C7-C8	3.26	120.04	108.34	5	2
3	B	365	PX4	O5-C9-C10	3.26	101.89	111.83	15	2
3	A	640	PX4	C8-C7-C6	3.26	104.19	111.78	10	4
3	C	307	PX4	C11-C10-C9	3.26	101.76	113.69	9	1
3	C	302	PX4	O5-C9-C10	3.26	101.91	111.83	5	3
3	A	630	PX4	O7-C23-C24	3.25	104.44	111.48	13	3
3	B	351	PX4	C7-O7-C23	3.25	110.01	117.80	7	6
3	C	349	PX4	C4-N1-C3	3.25	100.43	108.98	3	2
3	B	361	PX4	C1-C2-N1	3.25	126.26	115.82	14	2
3	A	637	PX4	O7-C23-C24	3.25	104.45	111.48	7	2
3	B	345	PX4	O5-C8-C7	3.25	117.77	108.40	14	6
3	A	641	PX4	O5-C9-C10	3.25	101.93	111.83	15	2
3	B	320	PX4	O5-C9-O6	3.25	131.76	123.63	9	2
3	B	306	PX4	O7-C23-O8	3.25	131.30	123.70	7	6
3	A	603	PX4	O7-C7-C8	3.25	119.99	108.34	15	1
3	A	634	PX4	O5-C8-C7	3.24	117.75	108.40	11	7
3	B	309	PX4	O4-P1-O2	3.24	121.79	108.94	1	1
3	C	319	PX4	C5-N1-C3	3.24	100.45	108.98	4	1
3	B	312	PX4	O5-C9-C10	3.24	101.95	111.83	15	4
3	B	313	PX4	O5-C9-O6	3.24	131.73	123.63	10	1
3	B	377	PX4	O5-C9-C10	3.24	101.95	111.83	7	4
3	C	316	PX4	C7-O7-C23	3.24	110.04	117.80	5	1
3	B	329	PX4	O7-C23-O8	3.24	131.28	123.70	9	1
3	C	339	PX4	C8-C7-C6	3.24	104.23	111.78	1	2
3	A	616	PX4	O7-C23-O8	3.24	131.27	123.70	10	4
3	B	394	PX4	C8-C7-C6	3.24	104.24	111.78	12	5
3	C	362	PX4	C5-N1-C4	3.24	100.47	108.98	15	3
3	A	643	PX4	O5-C8-C7	3.23	117.72	108.40	3	6
3	C	344	PX4	C8-C7-C6	3.24	119.33	111.78	12	2
3	C	349	PX4	C5-N1-C3	3.23	100.48	108.98	1	1
3	B	383	PX4	O5-C9-O6	3.23	131.71	123.63	10	3
3	B	393	PX4	O7-C7-C8	3.23	119.94	108.34	11	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	329	PX4	C8-O5-C9	3.23	105.31	117.12	1	2
3	B	384	PX4	O7-C23-C24	3.23	104.49	111.48	10	6
3	B	358	PX4	O7-C23-O8	3.23	131.26	123.70	3	3
3	B	391	PX4	O7-C23-C24	3.23	104.50	111.48	12	5
3	C	346	PX4	O7-C7-C6	3.23	119.92	108.34	10	2
3	A	650	PX4	C7-O7-C23	3.23	110.08	117.80	4	2
3	B	366	PX4	C5-N1-C4	3.23	100.50	108.98	5	2
3	B	384	PX4	C8-C7-C6	3.23	104.26	111.78	15	2
3	C	351	PX4	O5-C9-O6	3.23	131.69	123.63	2	2
3	C	352	PX4	O5-C9-C10	3.22	102.00	111.83	13	2
3	B	384	PX4	O7-C23-O8	3.22	131.24	123.70	10	3
3	C	341	PX4	C5-N1-C3	3.22	100.51	108.98	3	2
3	B	321	PX4	O5-C8-C7	3.22	117.68	108.40	8	3
3	B	312	PX4	C8-C7-C6	3.22	119.28	111.78	9	3
3	B	329	PX4	C5-N1-C3	3.22	117.42	108.98	12	1
3	B	317	PX4	C8-C7-C6	3.21	104.29	111.78	15	3
3	B	364	PX4	O5-C8-C7	3.21	117.66	108.40	4	1
3	C	328	PX4	C7-O7-C23	3.21	110.11	117.80	3	3
3	B	371	PX4	O5-C8-C7	3.21	117.66	108.40	1	4
3	C	335	PX4	O5-C8-C7	3.21	117.66	108.40	9	8
3	A	640	PX4	C12-C11-C10	3.21	101.34	113.13	5	1
3	A	622	PX4	O5-C8-C7	3.20	117.64	108.40	1	6
3	A	627	PX4	O7-C23-C24	3.20	104.55	111.48	8	7
3	B	357	PX4	O5-C8-C7	3.21	117.64	108.40	4	5
3	C	322	PX4	C7-O7-C23	3.20	110.13	117.80	9	5
3	C	324	PX4	C8-C7-C6	3.20	119.26	111.78	8	4
3	C	340	PX4	O7-C7-C8	3.20	119.84	108.34	1	3
3	C	362	PX4	C8-C7-C6	3.21	104.31	111.78	11	2
3	B	301	PX4	O7-C23-O8	3.20	131.19	123.70	4	2
3	B	328	PX4	C5-N1-C4	3.20	117.39	108.98	4	1
3	A	616	PX4	O7-C7-C8	3.20	119.83	108.34	14	4
3	C	355	PX4	O5-C8-C7	3.20	117.62	108.40	4	7
3	B	334	PX4	O7-C23-C24	3.20	104.56	111.48	15	3
3	B	343	PX4	C1-C2-N1	3.20	126.09	115.82	15	2
3	C	341	PX4	C7-O7-C23	3.20	110.14	117.80	7	3
3	C	350	PX4	O7-C23-O8	3.20	131.18	123.70	11	4
3	C	358	PX4	C25-C24-C23	3.20	101.97	113.69	1	1
3	B	384	PX4	C4-N1-C3	3.20	100.58	108.98	2	3
3	C	317	PX4	C11-C10-C9	3.20	125.40	113.69	4	3
3	C	360	PX4	O5-C8-C7	3.20	117.61	108.40	15	2
3	B	388	PX4	C5-N1-C4	3.19	100.59	108.98	2	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	C	323	PX4	C7-O7-C23	3.19	110.16	117.80	13	4
3	A	619	PX4	C7-O7-C23	3.19	110.16	117.80	5	3
3	B	321	PX4	C7-O7-C23	3.19	125.43	117.80	10	5
3	A	621	PX4	O5-C8-C7	3.19	117.58	108.40	4	2
3	B	391	PX4	C26-C25-C24	3.19	124.84	113.13	7	1
3	C	306	PX4	O7-C23-O8	3.18	131.15	123.70	4	4
3	A	614	PX4	C5-N1-C4	3.18	117.32	108.98	2	3
3	B	382	PX4	O7-C7-C6	3.18	96.94	108.34	1	2
3	B	383	PX4	O5-C9-C10	3.18	102.15	111.83	14	5
3	C	340	PX4	O5-C9-C10	3.18	102.15	111.83	12	1
3	A	624	PX4	O7-C23-O8	3.18	131.13	123.70	2	2
3	B	302	PX4	C7-O7-C23	3.17	110.20	117.80	2	3
3	C	343	PX4	C8-C7-C6	3.17	104.39	111.78	4	2
3	C	349	PX4	C5-N1-C4	3.17	117.31	108.98	9	7
3	C	317	PX4	O5-C8-C7	3.17	117.54	108.40	7	7
3	B	335	PX4	O5-C9-C10	3.17	102.17	111.83	2	2
3	B	342	PX4	C7-O7-C23	3.17	110.21	117.80	12	6
3	B	400	PX4	O5-C9-C10	3.17	102.17	111.83	12	2
3	B	362	PX4	O7-C23-O8	3.17	131.11	123.70	7	5
3	B	395	PX4	O5-C8-C7	3.17	117.52	108.40	8	3
3	C	323	PX4	C5-N1-C3	3.17	117.29	108.98	9	2
3	C	323	PX4	O7-C23-C24	3.17	104.63	111.48	13	3
3	C	363	PX4	C4-N1-C3	3.17	100.66	108.98	1	2
3	A	639	PX4	O7-C7-C6	3.16	119.70	108.34	7	3
3	B	331	PX4	C5-N1-C4	3.16	100.67	108.98	6	3
3	C	341	PX4	O7-C23-O8	3.16	131.10	123.70	6	3
3	C	314	PX4	C7-O7-C23	3.16	110.23	117.80	1	5
3	B	383	PX4	O7-C23-O8	3.16	131.09	123.70	2	1
3	C	345	PX4	O5-C8-C7	3.16	117.51	108.40	2	4
3	A	601	PX4	C7-O7-C23	3.16	110.24	117.80	15	5
3	A	602	PX4	C5-N1-C4	3.16	100.68	108.98	15	1
3	A	630	PX4	O5-C9-O6	3.16	131.53	123.63	11	4
3	C	357	PX4	C7-O7-C23	3.16	110.24	117.80	14	5
3	A	615	PX4	C5-N1-C4	3.16	100.69	108.98	2	3
3	B	315	PX4	C5-N1-C4	3.16	117.27	108.98	2	2
3	A	623	PX4	O5-C8-C7	3.15	117.48	108.40	2	2
3	C	329	PX4	C5-N1-C3	3.15	100.70	108.98	15	4
3	C	362	PX4	O7-C23-O8	3.15	131.07	123.70	10	3
3	A	614	PX4	O8-C23-C24	3.15	136.10	123.78	3	1
3	A	619	PX4	O5-C9-C10	3.15	102.24	111.83	11	3
3	B	382	PX4	C5-N1-C4	3.15	117.24	108.98	5	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	399	PX4	O5-C9-C10	3.15	102.24	111.83	5	2
3	C	330	PX4	O5-C8-C7	3.15	117.47	108.40	15	3
3	A	642	PX4	C4-N1-C3	3.14	100.72	108.98	3	3
3	A	646	PX4	C7-O7-C23	3.14	110.27	117.80	5	4
3	A	653	PX4	C4-N1-C3	3.14	117.23	108.98	13	1
3	B	320	PX4	O5-C8-C7	3.14	117.46	108.40	14	3
3	B	347	PX4	O7-C23-O8	3.14	131.06	123.70	1	3
3	B	385	PX4	O5-C9-C10	3.14	102.25	111.83	5	3
3	C	355	PX4	C25-C24-C23	3.14	125.21	113.69	14	1
3	B	348	PX4	C4-N1-C3	3.14	100.73	108.98	1	2
3	B	375	PX4	O7-C7-C8	3.14	119.61	108.34	6	2
3	B	393	PX4	C12-C11-C10	3.14	101.59	113.13	6	2
3	A	606	PX4	C8-C7-C6	3.14	104.47	111.78	1	4
3	A	634	PX4	O5-C9-C10	3.14	102.27	111.83	4	3
3	B	316	PX4	O5-C8-C7	3.14	117.44	108.40	3	2
3	C	326	PX4	C5-N1-C4	3.14	100.74	108.98	15	3
3	C	356	PX4	C8-C7-C6	3.13	119.09	111.78	5	4
3	B	352	PX4	O7-C23-C24	3.13	104.71	111.48	4	2
3	A	632	PX4	O5-C8-C7	3.13	117.42	108.40	2	5
3	B	378	PX4	C8-C7-C6	3.13	104.49	111.78	11	3
3	B	397	PX4	O7-C23-O8	3.13	131.02	123.70	11	1
3	C	350	PX4	O7-C7-C8	3.13	119.57	108.34	12	3
3	C	322	PX4	C11-C10-C9	3.13	125.15	113.69	8	2
3	C	353	PX4	O7-C7-C8	3.13	119.56	108.34	7	2
3	A	642	PX4	O5-C8-C7	3.12	117.40	108.40	15	6
3	B	320	PX4	O7-C23-O8	3.12	131.01	123.70	10	2
3	B	392	PX4	C4-N1-C3	3.12	117.18	108.98	6	3
3	C	362	PX4	O5-C9-C10	3.12	102.31	111.83	13	2
3	C	341	PX4	O5-C8-C7	3.12	117.40	108.40	3	6
3	B	301	PX4	C3-N1-C2	3.12	122.31	109.91	11	1
3	B	350	PX4	C7-O7-C23	3.12	110.34	117.80	2	7
3	B	392	PX4	C8-C7-C6	3.12	104.52	111.78	10	2
3	B	302	PX4	O7-C23-C24	3.12	104.74	111.48	13	4
3	B	341	PX4	C12-C11-C10	3.12	101.68	113.13	7	2
3	B	391	PX4	C5-N1-C4	3.11	100.80	108.98	7	4
3	B	326	PX4	C7-O7-C23	3.11	110.35	117.80	5	4
3	A	653	PX4	O7-C23-O8	3.11	130.98	123.70	12	4
3	C	346	PX4	O7-C23-C24	3.11	104.75	111.48	14	3
3	B	382	PX4	O5-C9-C10	3.11	102.36	111.83	8	4
3	B	362	PX4	C1-C2-N1	3.11	125.80	115.82	14	1
3	C	310	PX4	C8-C7-C6	3.11	104.54	111.78	4	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	341	PX4	O5-C9-C10	3.11	102.36	111.83	14	2
3	B	382	PX4	O5-C8-C7	3.11	117.35	108.40	2	5
3	A	632	PX4	O5-C9-C10	3.10	102.37	111.83	6	1
3	A	608	PX4	O7-C7-C8	3.10	119.47	108.34	7	2
3	A	637	PX4	P1-O3-C1	3.10	136.03	121.26	12	2
3	B	318	PX4	O5-C8-C7	3.10	117.34	108.40	9	4
3	B	324	PX4	C7-O7-C23	3.10	110.38	117.80	2	3
3	B	383	PX4	O7-C23-C24	3.10	104.78	111.48	11	5
3	C	340	PX4	C1-C2-N1	3.10	125.77	115.82	12	1
3	A	624	PX4	O7-C23-C24	3.10	104.78	111.48	2	5
3	B	368	PX4	C8-O5-C9	3.10	105.79	117.12	4	1
3	A	650	PX4	O7-C23-O8	3.10	130.94	123.70	14	3
3	B	321	PX4	C8-C7-C6	3.10	119.00	111.78	9	6
3	B	334	PX4	O7-C23-O8	3.10	130.94	123.70	11	2
3	B	370	PX4	O7-C23-C24	3.10	104.78	111.48	3	5
3	C	335	PX4	O5-C9-O6	3.10	131.37	123.63	14	2
3	B	365	PX4	C1-C2-N1	3.09	125.75	115.82	13	1
3	B	387	PX4	O7-C23-C24	3.09	104.79	111.48	2	3
3	B	383	PX4	C4-N1-C3	3.09	100.85	108.98	5	2
3	A	634	PX4	O3-C1-C2	3.09	124.53	109.65	2	2
3	B	358	PX4	C1-C2-N1	3.09	125.74	115.82	1	1
3	B	369	PX4	O7-C23-O8	3.09	130.93	123.70	2	4
3	C	327	PX4	O7-C23-C24	3.09	104.80	111.48	7	6
3	C	313	PX4	O7-C23-C24	3.08	104.81	111.48	2	3
3	B	309	PX4	C12-C11-C10	3.08	124.45	113.13	5	1
3	B	304	PX4	O7-C23-O8	3.08	130.91	123.70	8	2
3	B	358	PX4	O5-C9-C10	3.08	102.44	111.83	7	2
3	C	364	PX4	C7-O7-C23	3.08	110.42	117.80	8	7
3	B	356	PX4	C5-N1-C3	3.08	100.89	108.98	14	4
3	B	391	PX4	C7-O7-C23	3.08	110.43	117.80	8	1
3	A	617	PX4	C5-N1-C3	3.08	100.89	108.98	7	2
3	B	363	PX4	C8-C7-C6	3.08	118.96	111.78	9	3
3	B	373	PX4	C8-C7-C6	3.08	104.61	111.78	8	2
3	B	372	PX4	O5-C9-C10	3.08	102.45	111.83	11	4
3	B	385	PX4	C4-N1-C3	3.08	100.89	108.98	6	3
3	B	388	PX4	C11-C10-C9	3.08	102.42	113.69	9	3
3	A	622	PX4	C5-N1-C4	3.08	117.06	108.98	10	2
3	C	319	PX4	O5-C8-C7	3.08	117.26	108.40	5	4
3	B	359	PX4	O5-C8-C7	3.07	117.26	108.40	9	3
3	C	334	PX4	O5-C8-C7	3.07	117.26	108.40	6	3
3	C	357	PX4	C5-N1-C4	3.08	117.06	108.98	13	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	A	614	PX4	O7-C23-O8	3.07	130.89	123.70	10	3
3	A	644	PX4	O7-C23-C24	3.07	104.83	111.48	3	3
3	C	334	PX4	O7-C7-C6	3.07	119.37	108.34	12	1
3	A	617	PX4	O5-C8-C7	3.07	117.25	108.40	1	5
3	B	351	PX4	C5-N1-C3	3.07	100.91	108.98	10	2
3	B	357	PX4	C8-O5-C9	3.07	105.89	117.12	10	2
3	C	316	PX4	C1-C2-N1	3.07	125.68	115.82	12	1
3	C	335	PX4	C25-C24-C23	3.07	102.43	113.69	4	1
3	C	341	PX4	O7-C23-C24	3.07	104.84	111.48	7	4
3	B	332	PX4	O5-C9-O6	3.07	131.30	123.63	2	2
3	B	371	PX4	O5-C9-C10	3.07	102.48	111.83	14	2
3	A	609	PX4	O5-C9-O6	3.06	131.29	123.63	7	2
3	A	647	PX4	O5-C9-C10	3.06	102.49	111.83	3	1
3	A	652	PX4	O5-C9-C10	3.06	102.49	111.83	3	3
3	B	348	PX4	O7-C7-C6	3.06	119.33	108.34	13	3
3	B	368	PX4	O3-P1-O2	3.06	96.80	108.94	1	1
3	C	336	PX4	O5-C8-C7	3.06	117.22	108.40	2	7
3	A	633	PX4	C8-C7-C6	3.06	118.92	111.78	4	1
3	C	315	PX4	O7-C7-C6	3.06	119.32	108.34	1	1
3	B	350	PX4	O5-C9-C10	3.06	102.51	111.83	4	3
3	A	645	PX4	C7-O7-C23	3.06	110.48	117.80	11	3
3	B	340	PX4	C26-C25-C24	3.06	101.90	113.13	3	1
3	B	350	PX4	C8-C7-C6	3.06	104.66	111.78	6	3
3	B	354	PX4	P1-O3-C1	3.06	135.81	121.26	3	1
3	B	391	PX4	C8-C7-C6	3.06	104.65	111.78	4	3
3	B	385	PX4	C11-C10-C9	3.06	102.49	113.69	9	1
3	C	305	PX4	C4-N1-C3	3.06	117.01	108.98	7	2
3	C	352	PX4	O7-C23-O8	3.06	130.85	123.70	4	3
3	B	303	PX4	O7-C23-C24	3.06	104.87	111.48	11	6
3	B	308	PX4	O5-C9-C10	3.05	102.52	111.83	6	3
3	B	356	PX4	O7-C23-C24	3.05	104.88	111.48	4	5
3	B	371	PX4	O7-C23-C24	3.05	104.87	111.48	7	3
3	B	372	PX4	O5-C8-C7	3.05	117.19	108.40	5	2
3	C	336	PX4	C5-N1-C3	3.05	100.96	108.98	12	3
3	C	353	PX4	O7-C23-O8	3.05	130.84	123.70	14	1
3	B	349	PX4	C7-O7-C23	3.05	110.50	117.80	11	5
3	A	606	PX4	C7-O7-C23	3.05	110.50	117.80	11	3
3	A	649	PX4	C4-N1-C3	3.05	116.98	108.98	4	3
3	C	347	PX4	O5-C9-C10	3.05	102.54	111.83	8	1
3	A	639	PX4	C8-C7-C6	3.05	104.68	111.78	14	2
3	B	355	PX4	O5-C8-C7	3.05	117.18	108.40	2	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	C	316	PX4	C8-O5-C9	3.05	105.98	117.12	12	1
3	C	356	PX4	C7-O7-C23	3.05	110.50	117.80	9	3
3	C	320	PX4	O5-C9-O6	3.05	131.25	123.63	2	3
3	C	358	PX4	C1-C2-N1	3.05	125.60	115.82	2	1
3	C	326	PX4	O7-C23-C24	3.04	104.90	111.48	9	6
3	C	340	PX4	O7-C23-O8	3.04	130.82	123.70	11	1
3	A	608	PX4	C5-N1-C3	3.04	100.99	108.98	2	2
3	C	346	PX4	C5-N1-C3	3.04	100.98	108.98	12	1
3	B	367	PX4	O5-C9-O6	3.04	131.24	123.63	4	3
3	A	625	PX4	C26-C25-C24	3.04	101.96	113.13	11	1
3	B	303	PX4	C1-C2-N1	3.04	125.57	115.82	9	3
3	B	303	PX4	O5-C9-O6	3.04	131.23	123.63	5	1
3	B	370	PX4	O5-C8-C7	3.04	117.16	108.40	2	5
3	C	347	PX4	O7-C23-C24	3.04	104.91	111.48	11	5
3	A	623	PX4	C7-O7-C23	3.04	110.53	117.80	1	3
3	A	641	PX4	C5-N1-C4	3.04	116.95	108.98	8	1
3	C	364	PX4	O5-C9-C10	3.04	102.58	111.83	14	2
3	B	369	PX4	O7-C23-C24	3.03	104.92	111.48	15	5
3	C	359	PX4	C8-C7-C6	3.04	118.86	111.78	12	2
3	A	604	PX4	C4-N1-C3	3.03	101.01	108.98	12	2
3	B	358	PX4	C4-N1-C3	3.03	116.94	108.98	1	2
3	B	307	PX4	C8-C7-C6	3.03	118.85	111.78	13	1
3	B	368	PX4	C8-C7-C6	3.03	104.72	111.78	3	3
3	C	318	PX4	C8-O5-C9	3.03	106.04	117.12	10	1
3	C	357	PX4	C12-C11-C10	3.03	124.26	113.13	9	2
3	A	627	PX4	O5-C8-C7	3.03	117.12	108.40	14	4
3	B	394	PX4	O7-C23-C24	3.03	104.93	111.48	2	1
3	C	309	PX4	C5-N1-C3	3.02	101.03	108.98	14	3
3	C	335	PX4	C8-C7-C6	3.02	104.74	111.78	4	1
3	B	348	PX4	O5-C8-C7	3.02	117.10	108.40	15	7
3	C	348	PX4	O5-C9-C10	3.02	102.62	111.83	9	2
3	C	345	PX4	C5-N1-C2	3.02	97.91	109.91	10	1
3	B	306	PX4	C5-N1-C3	3.02	101.05	108.98	15	2
3	B	305	PX4	O7-C23-C24	3.01	104.96	111.48	9	5
3	C	344	PX4	O5-C8-C7	3.01	117.08	108.40	3	2
3	B	301	PX4	O5-C8-C7	3.01	117.08	108.40	8	4
3	B	339	PX4	O5-C8-C7	3.01	117.08	108.40	3	3
3	B	345	PX4	C8-C7-C6	3.01	104.77	111.78	6	4
3	B	374	PX4	O5-C9-O6	3.01	131.16	123.63	1	1
3	C	317	PX4	O7-C23-O8	3.01	130.74	123.70	4	4
3	C	332	PX4	O5-C9-O6	3.01	131.16	123.63	10	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	C	309	PX4	C7-O7-C23	3.01	110.60	117.80	8	4
3	A	623	PX4	C5-N1-C3	3.01	116.87	108.98	4	4
3	C	310	PX4	C5-N1-C3	3.00	101.08	108.98	5	4
3	C	350	PX4	C1-C2-N1	3.00	125.46	115.82	13	2
3	A	603	PX4	C1-C2-N1	3.00	125.46	115.82	5	2
3	A	619	PX4	O5-C8-C7	3.00	117.05	108.40	8	3
3	A	651	PX4	C5-N1-C3	3.00	116.86	108.98	1	4
3	B	375	PX4	C4-N1-C3	3.00	116.86	108.98	13	1
3	B	343	PX4	O5-C8-C7	3.00	117.05	108.40	3	3
3	C	344	PX4	C5-N1-C4	3.00	101.09	108.98	1	2
3	C	352	PX4	O7-C23-C24	3.00	104.99	111.48	14	5
3	A	603	PX4	O5-C9-O6	3.00	131.13	123.63	5	6
3	A	635	PX4	C4-N1-C3	3.00	101.10	108.98	10	4
3	B	386	PX4	O5-C8-C7	3.00	117.04	108.40	7	1
3	B	305	PX4	C4-N1-C3	3.00	101.10	108.98	4	6
3	B	311	PX4	O7-C7-C8	3.00	119.10	108.34	7	1
3	B	327	PX4	C4-N1-C3	3.00	116.85	108.98	1	4
3	A	609	PX4	O5-C8-C7	3.00	117.04	108.40	5	5
3	C	354	PX4	O5-C8-C7	3.00	117.04	108.40	14	4
3	C	355	PX4	O8-C23-C24	3.00	135.50	123.78	12	1
3	B	303	PX4	C7-O7-C23	2.99	110.63	117.80	1	3
3	B	326	PX4	C8-C7-C6	2.99	104.81	111.78	10	1
3	B	396	PX4	O5-C9-C10	2.99	102.71	111.83	8	2
3	C	309	PX4	O7-C7-C8	2.99	119.08	108.34	14	4
3	C	355	PX4	C4-N1-C2	2.99	98.01	109.91	12	1
3	B	320	PX4	C5-N1-C4	2.99	116.83	108.98	9	3
3	B	390	PX4	O5-C9-O6	2.99	131.11	123.63	8	1
3	B	400	PX4	O5-C8-C7	2.99	117.02	108.40	8	5
3	B	314	PX4	C8-C7-C6	2.99	104.82	111.78	14	4
3	C	350	PX4	C8-C7-C6	2.99	118.75	111.78	11	2
3	B	358	PX4	C5-N1-C3	2.98	116.81	108.98	1	4
3	B	341	PX4	O7-C23-O8	2.98	130.68	123.70	15	2
3	B	324	PX4	O7-C23-O8	2.98	130.67	123.70	10	1
3	B	368	PX4	O7-C23-O8	2.98	130.68	123.70	8	4
3	B	372	PX4	O5-C9-O6	2.98	131.08	123.63	2	5
3	A	617	PX4	C7-O7-C23	2.98	124.92	117.80	4	5
3	B	329	PX4	C11-C10-C9	2.98	102.78	113.69	14	2
3	B	379	PX4	O5-C9-C10	2.98	102.75	111.83	9	2
3	A	613	PX4	O5-C8-C7	2.98	116.98	108.40	5	3
3	B	345	PX4	C1-C2-N1	2.98	125.38	115.82	6	2
3	C	337	PX4	O5-C8-C7	2.98	116.98	108.40	4	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	344	PX4	C5-N1-C4	2.98	101.16	108.98	10	1
3	B	349	PX4	O5-C9-O6	2.97	131.07	123.63	4	1
3	B	381	PX4	O7-C23-O8	2.97	130.66	123.70	4	1
3	C	304	PX4	C1-C2-N1	2.97	125.37	115.82	4	3
3	A	642	PX4	O5-C9-C10	2.97	102.77	111.83	13	6
3	B	311	PX4	C11-C10-C9	2.97	124.58	113.69	9	1
3	B	353	PX4	C5-N1-C4	2.97	101.17	108.98	2	2
3	B	385	PX4	C8-C7-C6	2.97	104.85	111.78	6	2
3	C	303	PX4	O5-C9-C10	2.97	102.77	111.83	10	3
3	B	370	PX4	C7-O7-C23	2.97	110.69	117.80	8	3
3	A	636	PX4	C5-N1-C4	2.97	116.77	108.98	14	2
3	B	353	PX4	C7-O7-C23	2.97	110.69	117.80	8	7
3	A	650	PX4	O5-C9-O6	2.97	131.05	123.63	2	2
3	B	314	PX4	O7-C23-O8	2.97	130.64	123.70	14	2
3	B	378	PX4	C7-O7-C23	2.97	110.69	117.80	13	7
3	C	316	PX4	C5-N1-C3	2.97	101.18	108.98	13	1
3	A	616	PX4	O5-C9-C10	2.97	102.79	111.83	9	1
3	B	305	PX4	C7-O7-C23	2.96	110.70	117.80	1	7
3	B	313	PX4	C4-N1-C3	2.96	101.19	108.98	9	3
3	B	330	PX4	O5-C8-C7	2.97	116.94	108.40	8	3
3	B	391	PX4	C5-N1-C3	2.97	101.19	108.98	5	1
3	C	326	PX4	C8-C7-C6	2.97	104.87	111.78	15	2
3	C	341	PX4	O5-C9-C10	2.97	102.79	111.83	1	2
3	C	320	PX4	O7-C23-C24	2.96	105.07	111.48	14	3
3	C	335	PX4	P1-O4-C6	2.96	138.33	121.35	13	1
3	B	350	PX4	C5-N1-C3	2.96	116.75	108.98	4	1
3	C	327	PX4	O7-C7-C6	2.96	118.97	108.34	14	2
3	B	379	PX4	O7-C7-C8	2.96	118.96	108.34	4	2
3	C	325	PX4	O7-C23-C24	2.96	105.08	111.48	10	5
3	C	356	PX4	O7-C23-C24	2.96	105.08	111.48	7	3
3	B	345	PX4	O7-C23-C24	2.96	105.08	111.48	5	3
3	B	363	PX4	O7-C23-O8	2.96	130.62	123.70	6	3
3	B	365	PX4	C7-O7-C23	2.96	110.72	117.80	2	5
3	C	318	PX4	C4-N1-C3	2.96	101.20	108.98	5	3
3	A	625	PX4	C4-N1-C3	2.96	101.21	108.98	1	2
3	B	304	PX4	C4-N1-C3	2.96	101.21	108.98	10	2
3	C	304	PX4	C11-C10-C9	2.96	102.86	113.69	11	3
3	C	359	PX4	O5-C8-C7	2.96	116.92	108.40	7	2
3	B	362	PX4	O5-C9-C10	2.96	102.82	111.83	14	2
3	C	356	PX4	C1-C2-N1	2.96	125.31	115.82	5	2
3	B	354	PX4	C8-O5-C9	2.95	127.92	117.12	1	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	A	604	PX4	C8-C7-C6	2.95	104.90	111.78	13	3
3	B	323	PX4	C5-N1-C4	2.95	101.22	108.98	15	2
3	A	612	PX4	C8-C7-C6	2.95	118.66	111.78	13	3
3	A	615	PX4	C5-N1-C3	2.95	116.73	108.98	10	3
3	C	309	PX4	C5-N1-C4	2.95	101.23	108.98	5	3
3	B	379	PX4	C25-C24-C23	2.95	124.49	113.69	13	1
3	B	394	PX4	O5-C8-C7	2.94	116.89	108.40	5	3
3	A	601	PX4	O5-C8-C7	2.94	116.88	108.40	9	6
3	B	373	PX4	O7-C23-O8	2.94	130.58	123.70	10	2
3	C	329	PX4	C1-C2-N1	2.94	125.27	115.82	7	2
3	A	621	PX4	C5-N1-C2	2.94	121.60	109.91	1	1
3	B	351	PX4	C12-C11-C10	2.94	102.32	113.13	14	1
3	C	325	PX4	O5-C9-O6	2.94	130.99	123.63	12	4
3	B	390	PX4	O5-C8-C7	2.94	116.87	108.40	7	6
3	A	645	PX4	C4-N1-C3	2.94	101.26	108.98	11	3
3	B	361	PX4	C8-C7-C6	2.94	104.94	111.78	4	2
3	C	335	PX4	C5-N1-C3	2.94	116.69	108.98	7	3
3	B	368	PX4	O5-C8-C7	2.94	116.86	108.40	14	6
3	B	376	PX4	C5-N1-C4	2.94	101.26	108.98	8	3
3	B	305	PX4	C1-C2-N1	2.94	125.24	115.82	10	2
3	B	387	PX4	O7-C7-C8	2.94	118.88	108.34	8	2
3	B	322	PX4	C7-O7-C23	2.93	110.77	117.80	12	6
3	B	330	PX4	O7-C23-O8	2.93	130.56	123.70	9	3
3	C	360	PX4	O5-C9-O6	2.93	130.97	123.63	5	1
3	A	610	PX4	O5-C9-C10	2.93	102.89	111.83	10	2
3	C	317	PX4	C8-O5-C9	2.93	127.83	117.12	5	2
3	C	349	PX4	C8-C7-C6	2.93	118.62	111.78	9	3
3	A	605	PX4	C8-C7-C6	2.93	118.61	111.78	7	2
3	B	362	PX4	C7-O7-C23	2.93	110.78	117.80	2	4
3	C	334	PX4	C5-N1-C4	2.93	101.28	108.98	6	4
3	C	353	PX4	O5-C9-O6	2.93	130.96	123.63	4	2
3	B	345	PX4	C5-N1-C3	2.93	101.28	108.98	9	1
3	B	355	PX4	C7-O7-C23	2.93	110.79	117.80	6	1
3	B	370	PX4	C8-C7-C6	2.93	104.96	111.78	10	2
3	B	374	PX4	O7-C7-C8	2.93	118.85	108.34	13	2
3	C	301	PX4	C1-C2-N1	2.93	125.22	115.82	8	3
3	C	352	PX4	O5-C8-C7	2.93	116.84	108.40	10	4
3	A	637	PX4	O7-C7-C6	2.93	118.84	108.34	3	1
3	B	342	PX4	O7-C23-O8	2.93	130.54	123.70	1	6
3	B	388	PX4	O7-C23-O8	2.93	130.54	123.70	12	3
3	B	394	PX4	C7-O7-C23	2.93	110.79	117.80	2	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	A	607	PX4	O5-C9-O6	2.92	130.94	123.63	6	1
3	A	603	PX4	O5-C9-C10	2.92	102.92	111.83	4	4
3	A	625	PX4	O7-C23-C24	2.92	105.16	111.48	12	2
3	B	306	PX4	C5-N1-C4	2.92	101.30	108.98	10	2
3	B	363	PX4	O7-C23-C24	2.92	105.16	111.48	7	5
3	B	370	PX4	O5-C9-O6	2.92	130.94	123.63	3	4
3	B	377	PX4	C5-N1-C2	2.92	121.53	109.91	11	1
3	B	311	PX4	O5-C9-O6	2.92	130.94	123.63	5	2
3	B	341	PX4	C8-C7-C6	2.92	104.97	111.78	3	2
3	C	345	PX4	O7-C23-C24	2.92	105.16	111.48	15	3
3	A	643	PX4	O7-C23-O8	2.92	130.53	123.70	1	3
3	B	307	PX4	O5-C9-O6	2.92	130.93	123.63	2	2
3	B	340	PX4	C5-N1-C3	2.92	101.31	108.98	13	1
3	B	363	PX4	O5-C9-C10	2.92	102.93	111.83	14	3
3	A	620	PX4	C5-N1-C3	2.92	116.64	108.98	4	3
3	B	369	PX4	O5-C9-O6	2.92	130.93	123.63	11	3
3	A	654	PX4	O7-C23-C24	2.92	105.17	111.48	12	3
3	B	306	PX4	C11-C10-C9	2.91	103.01	113.69	8	1
3	B	311	PX4	C7-O7-C23	2.92	110.82	117.80	12	4
3	C	322	PX4	O7-C23-O8	2.91	130.52	123.70	7	4
3	B	361	PX4	O5-C8-C7	2.91	116.79	108.40	13	3
3	A	630	PX4	C8-O5-C9	2.91	106.48	117.12	11	2
3	B	302	PX4	O5-C8-C7	2.91	116.79	108.40	1	4
3	B	374	PX4	O3-C1-C2	2.91	123.66	109.65	3	1
3	B	368	PX4	O5-C9-O6	2.91	130.91	123.63	1	1
3	C	324	PX4	C12-C11-C10	2.91	123.81	113.13	5	3
3	C	325	PX4	O5-C8-C7	2.91	116.78	108.40	5	4
3	A	608	PX4	C8-O5-C9	2.91	106.49	117.12	2	3
3	A	628	PX4	O7-C23-C24	2.91	105.19	111.48	14	2
3	B	330	PX4	C5-N1-C3	2.90	101.35	108.98	7	2
3	B	347	PX4	O7-C7-C8	2.90	118.76	108.34	6	4
3	C	332	PX4	C8-C7-C6	2.90	105.01	111.78	15	2
3	C	330	PX4	O5-C9-O6	2.90	130.89	123.63	11	3
3	C	335	PX4	O7-C23-O8	2.90	130.49	123.70	3	3
3	B	311	PX4	C4-N1-C3	2.90	116.59	108.98	8	1
3	B	368	PX4	C26-C25-C24	2.90	123.78	113.13	15	1
3	B	391	PX4	C11-C10-C9	2.90	103.06	113.69	2	1
3	B	397	PX4	C7-O7-C23	2.90	110.85	117.80	5	4
3	A	629	PX4	C5-N1-C4	2.90	101.36	108.98	9	1
3	A	639	PX4	C5-N1-C4	2.90	101.36	108.98	5	3
3	C	320	PX4	C5-N1-C3	2.90	116.59	108.98	13	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	A	647	PX4	C31-C30-C29	2.90	99.72	114.37	13	1
3	A	648	PX4	C5-N1-C3	2.90	101.36	108.98	12	3
3	B	374	PX4	O5-C8-C7	2.90	116.75	108.40	15	4
3	B	378	PX4	C1-C2-N1	2.90	125.12	115.82	10	1
3	A	626	PX4	O5-C9-C10	2.90	103.00	111.83	3	3
3	B	325	PX4	O5-C9-C10	2.90	103.00	111.83	8	1
3	B	341	PX4	C25-C24-C23	2.90	124.31	113.69	2	1
3	B	367	PX4	C8-C7-C6	2.89	105.04	111.78	6	7
3	C	353	PX4	C7-O7-C23	2.89	110.87	117.80	7	5
3	B	371	PX4	C8-C7-C6	2.89	105.04	111.78	13	3
3	A	631	PX4	O5-C8-C7	2.89	116.73	108.40	10	5
3	A	653	PX4	O5-C9-O6	2.89	130.86	123.63	10	1
3	A	606	PX4	O7-C23-O8	2.89	130.46	123.70	10	4
3	A	623	PX4	O7-C23-O8	2.89	130.46	123.70	13	4
3	B	370	PX4	O7-C7-C8	2.89	118.70	108.34	5	1
3	C	312	PX4	O5-C8-C7	2.89	116.72	108.40	2	3
3	A	609	PX4	C5-N1-C4	2.89	101.40	108.98	10	4
3	C	362	PX4	C7-O7-C23	2.89	110.89	117.80	6	5
3	A	625	PX4	C5-N1-C3	2.89	101.40	108.98	10	3
3	A	626	PX4	C4-N1-C2	2.88	121.37	109.91	13	1
3	B	324	PX4	O7-C7-C8	2.88	118.69	108.34	9	2
3	C	362	PX4	O5-C8-C7	2.88	116.70	108.40	3	3
3	A	608	PX4	O1-P1-O2	2.88	125.85	112.44	2	1
3	B	301	PX4	O5-C9-C10	2.88	103.05	111.83	15	1
3	C	307	PX4	O7-C7-C8	2.88	118.68	108.34	14	1
3	A	602	PX4	O5-C8-C7	2.88	116.69	108.40	7	5
3	B	350	PX4	C5-N1-C4	2.88	101.42	108.98	4	3
3	B	359	PX4	O7-C23-C24	2.88	117.70	111.48	5	4
3	B	386	PX4	O5-C9-O6	2.88	130.82	123.63	6	2
3	B	387	PX4	C7-O7-C23	2.88	110.92	117.80	11	5
3	C	315	PX4	O5-C9-C10	2.87	103.07	111.83	3	4
3	B	326	PX4	O7-C23-O8	2.87	130.42	123.70	12	3
3	B	344	PX4	C8-O5-C9	2.87	127.62	117.12	12	2
3	C	350	PX4	O7-C7-C6	2.87	118.65	108.34	8	4
3	C	334	PX4	C4-N1-C3	2.87	101.43	108.98	12	3
3	A	627	PX4	C8-C7-C6	2.87	118.48	111.78	1	2
3	C	312	PX4	C8-C7-C6	2.87	105.09	111.78	13	3
3	B	366	PX4	O5-C8-C7	2.87	116.67	108.40	10	3
3	C	314	PX4	C5-N1-C3	2.87	101.44	108.98	8	1
3	C	306	PX4	O7-C7-C6	2.87	118.63	108.34	13	5
3	C	349	PX4	O5-C8-C7	2.87	116.67	108.40	6	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	C	341	PX4	O7-C7-C6	2.87	118.63	108.34	11	2
3	B	397	PX4	C8-C7-C6	2.87	105.10	111.78	12	1
3	C	362	PX4	O7-C7-C6	2.87	118.63	108.34	13	2
3	A	641	PX4	C7-O7-C23	2.87	110.94	117.80	11	3
3	B	380	PX4	C8-C7-C6	2.86	105.11	111.78	9	3
3	C	319	PX4	C8-C7-C6	2.86	118.46	111.78	14	4
3	C	319	PX4	O5-C9-C10	2.86	103.10	111.83	13	2
3	C	340	PX4	O7-C23-C24	2.87	105.28	111.48	9	5
3	C	326	PX4	C4-N1-C3	2.86	101.45	108.98	2	2
3	C	344	PX4	O5-C9-O6	2.86	130.79	123.63	7	2
3	B	321	PX4	O7-C23-C24	2.86	105.29	111.48	4	2
3	C	324	PX4	P1-O3-C1	2.86	134.88	121.26	5	1
3	C	333	PX4	C1-C2-N1	2.86	125.01	115.82	3	2
3	A	620	PX4	O7-C23-O8	2.86	130.39	123.70	4	4
3	A	634	PX4	C5-N1-C4	2.86	116.49	108.98	3	2
3	B	382	PX4	C7-O7-C23	2.86	110.95	117.80	1	1
3	B	395	PX4	C5-N1-C2	2.86	121.27	109.91	11	1
3	C	346	PX4	C8-C7-C6	2.86	118.45	111.78	4	4
3	A	625	PX4	C5-N1-C4	2.85	101.48	108.98	2	2
3	A	631	PX4	C1-C2-N1	2.85	124.98	115.82	9	2
3	A	640	PX4	C5-N1-C3	2.86	116.48	108.98	7	2
3	B	327	PX4	O7-C23-C24	2.85	105.31	111.48	12	5
3	B	348	PX4	O5-C9-O6	2.86	130.77	123.63	8	4
3	B	356	PX4	C4-N1-C3	2.86	116.48	108.98	5	2
3	B	389	PX4	O5-C8-C7	2.85	116.62	108.40	13	3
3	B	320	PX4	C5-N1-C3	2.85	116.47	108.98	14	2
3	B	357	PX4	C5-N1-C4	2.85	101.48	108.98	10	2
3	A	621	PX4	P1-O3-C1	2.85	134.82	121.26	12	2
3	B	344	PX4	C5-N1-C3	2.85	101.49	108.98	5	3
3	B	372	PX4	C5-N1-C3	2.85	101.49	108.98	14	2
3	C	308	PX4	C8-C7-C6	2.85	118.43	111.78	8	2
3	B	354	PX4	O7-C7-C6	2.85	118.56	108.34	8	1
3	C	306	PX4	O7-C7-C8	2.85	118.56	108.34	3	6
3	A	601	PX4	O7-C23-O8	2.85	130.36	123.70	4	2
3	A	649	PX4	O7-C23-O8	2.85	130.36	123.70	7	3
3	B	317	PX4	O5-C9-C10	2.85	103.15	111.83	3	1
3	B	382	PX4	C25-C24-C23	2.85	103.26	113.69	2	1
3	C	355	PX4	C8-C7-C6	2.85	105.14	111.78	6	3
3	B	326	PX4	C5-N1-C3	2.85	116.45	108.98	14	3
3	A	605	PX4	C4-N1-C3	2.84	101.51	108.98	14	2
3	B	319	PX4	C8-C7-C6	2.84	118.42	111.78	3	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	381	PX4	O7-C23-C24	2.84	105.33	111.48	2	1
3	C	345	PX4	C7-O7-C23	2.84	110.99	117.80	10	5
3	A	613	PX4	O5-C9-C10	2.84	103.17	111.83	9	1
3	A	638	PX4	O5-C8-C7	2.84	116.59	108.40	4	6
3	B	352	PX4	C5-N1-C3	2.84	101.51	108.98	10	2
3	B	373	PX4	C12-C11-C10	2.84	123.56	113.13	6	1
3	C	305	PX4	O5-C9-O6	2.84	130.73	123.63	14	2
3	B	391	PX4	C4-N1-C3	2.84	116.44	108.98	6	5
3	C	318	PX4	C5-N1-C3	2.84	116.44	108.98	11	2
3	A	636	PX4	O5-C8-C7	2.84	116.58	108.40	10	3
3	B	352	PX4	O5-C9-C10	2.84	103.18	111.83	4	3
3	A	632	PX4	C1-C2-N1	2.84	124.93	115.82	4	1
3	A	645	PX4	C5-N1-C3	2.84	116.43	108.98	11	1
3	B	388	PX4	C7-O7-C23	2.84	111.01	117.80	6	3
3	B	319	PX4	O5-C9-O6	2.84	130.72	123.63	15	3
3	B	318	PX4	C26-C25-C24	2.83	123.54	113.13	8	1
3	B	355	PX4	C3-N1-C2	2.83	121.18	109.91	14	2
3	C	308	PX4	C26-C25-C24	2.84	123.55	113.13	7	2
3	C	342	PX4	C3-N1-C2	2.84	121.18	109.91	11	1
3	B	368	PX4	O7-C7-C8	2.83	118.51	108.34	14	2
3	B	375	PX4	C5-N1-C3	2.83	101.53	108.98	11	2
3	B	383	PX4	C7-O7-C23	2.83	111.01	117.80	2	4
3	B	386	PX4	O7-C7-C8	2.83	118.51	108.34	10	2
3	B	309	PX4	O7-C7-C6	2.83	118.50	108.34	15	2
3	B	362	PX4	C5-N1-C4	2.83	101.55	108.98	2	2
3	B	374	PX4	C1-C2-N1	2.83	124.90	115.82	11	1
3	C	301	PX4	O5-C9-O6	2.83	130.70	123.63	5	2
3	A	616	PX4	O7-C23-C24	2.83	105.37	111.48	13	2
3	A	630	PX4	C4-N1-C3	2.83	101.55	108.98	1	2
3	B	390	PX4	C1-C2-N1	2.83	124.89	115.82	1	1
3	B	385	PX4	O1-P1-O2	2.82	125.59	112.44	15	1
3	C	329	PX4	C4-N1-C3	2.83	116.40	108.98	15	2
3	B	304	PX4	C25-C24-C23	2.82	124.04	113.69	5	1
3	B	305	PX4	O7-C23-O8	2.82	130.31	123.70	9	1
3	B	311	PX4	C5-N1-C3	2.82	116.39	108.98	9	3
3	B	379	PX4	C5-N1-C3	2.82	101.57	108.98	4	1
3	B	333	PX4	O8-C23-C24	2.82	134.81	123.78	5	1
3	B	326	PX4	C1-C2-N1	2.82	124.87	115.82	14	2
3	B	385	PX4	O7-C23-O8	2.82	130.29	123.70	12	3
3	C	304	PX4	O5-C9-O6	2.82	130.68	123.63	8	4
3	C	317	PX4	C15-C14-C13	2.82	100.13	114.37	15	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	A	605	PX4	C7-O7-C23	2.81	111.06	117.80	1	6
3	A	605	PX4	O5-C8-C7	2.81	116.51	108.40	6	3
3	B	369	PX4	O5-C8-C7	2.81	116.51	108.40	9	2
3	B	399	PX4	O7-C23-O8	2.81	130.28	123.70	14	2
3	A	612	PX4	O7-C23-C24	2.81	105.40	111.48	4	4
3	A	616	PX4	C5-N1-C4	2.81	101.59	108.98	1	3
3	A	639	PX4	O5-C8-C7	2.81	116.50	108.40	9	4
3	B	303	PX4	C4-N1-C3	2.81	101.59	108.98	12	1
3	A	644	PX4	C11-C10-C9	2.81	123.99	113.69	12	1
3	B	332	PX4	C5-N1-C4	2.81	116.36	108.98	1	2
3	B	357	PX4	O5-C9-O6	2.81	130.66	123.63	4	2
3	B	303	PX4	C8-C7-C6	2.81	118.33	111.78	14	3
3	A	601	PX4	C5-N1-C3	2.81	101.60	108.98	2	1
3	A	609	PX4	O7-C23-O8	2.81	130.27	123.70	13	3
3	A	614	PX4	C3-N1-C2	2.81	121.07	109.91	8	1
3	B	387	PX4	O5-C9-C10	2.81	103.28	111.83	7	3
3	B	317	PX4	C1-C2-N1	2.80	124.82	115.82	9	1
3	B	399	PX4	O5-C9-O6	2.80	130.64	123.63	5	3
3	C	316	PX4	C8-C7-C6	2.80	118.32	111.78	2	2
3	C	357	PX4	O5-C8-C7	2.80	116.48	108.40	12	4
3	B	319	PX4	O7-C7-C8	2.80	118.40	108.34	2	2
3	B	333	PX4	O7-C23-C24	2.80	105.42	111.48	7	3
3	B	314	PX4	C7-O7-C23	2.80	111.09	117.80	4	3
3	C	332	PX4	C1-C2-N1	2.80	124.82	115.82	8	2
3	C	349	PX4	O7-C23-C24	2.80	105.42	111.48	8	3
3	C	359	PX4	C29-C28-C27	2.80	100.20	114.37	9	1
3	B	344	PX4	O7-C7-C8	2.80	118.39	108.34	2	1
3	C	317	PX4	O7-C7-C8	2.80	118.39	108.34	9	3
3	A	603	PX4	C7-O7-C23	2.80	111.10	117.80	10	3
3	A	649	PX4	O5-C9-C10	2.80	103.30	111.83	8	3
3	B	303	PX4	O5-C9-C10	2.80	103.30	111.83	13	2
3	B	383	PX4	C1-C2-N1	2.80	124.80	115.82	3	2
3	C	312	PX4	O7-C23-O8	2.80	130.25	123.70	8	1
3	A	601	PX4	C34-C33-C32	2.80	100.23	114.37	12	1
3	A	606	PX4	O7-C7-C8	2.80	118.38	108.34	1	4
3	B	387	PX4	O5-C9-O6	2.80	130.62	123.63	4	2
3	B	378	PX4	O5-C8-C7	2.80	116.46	108.40	2	4
3	A	632	PX4	O7-C23-O8	2.79	130.24	123.70	11	4
3	B	327	PX4	C26-C25-C24	2.79	102.86	113.13	7	1
3	B	336	PX4	O5-C9-O6	2.79	130.62	123.63	4	2
3	B	355	PX4	O7-C7-C8	2.79	118.37	108.34	8	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	313	PX4	C5-N1-C4	2.79	116.31	108.98	1	1
3	B	379	PX4	O7-C23-O8	2.79	130.23	123.70	3	1
3	A	603	PX4	C5-N1-C4	2.79	101.65	108.98	7	1
3	A	652	PX4	C12-C11-C10	2.79	102.88	113.13	4	1
3	B	363	PX4	O5-C9-O6	2.79	130.60	123.63	15	3
3	A	613	PX4	C8-C7-C6	2.79	105.29	111.78	3	2
3	A	613	PX4	O7-C23-C24	2.79	105.45	111.48	1	2
3	A	640	PX4	O7-C23-O8	2.79	130.22	123.70	5	1
3	B	339	PX4	C1-C2-N1	2.79	124.77	115.82	4	2
3	B	370	PX4	C5-N1-C3	2.79	101.65	108.98	3	3
3	B	385	PX4	O5-C9-O6	2.79	130.60	123.63	8	1
3	A	630	PX4	C7-O7-C23	2.78	111.13	117.80	1	4
3	B	335	PX4	C1-C2-N1	2.78	124.76	115.82	2	1
3	B	306	PX4	C8-O5-C9	2.78	106.95	117.12	5	2
3	C	315	PX4	O7-C23-O8	2.78	130.21	123.70	12	5
3	C	359	PX4	C5-N1-C4	2.78	101.67	108.98	2	2
3	A	614	PX4	C7-O7-C23	2.78	111.14	117.80	2	5
3	B	330	PX4	C4-N1-C3	2.78	101.67	108.98	14	1
3	C	317	PX4	O5-C9-O6	2.78	130.59	123.63	5	3
3	C	335	PX4	P1-O3-C1	2.78	134.50	121.26	2	2
3	A	619	PX4	O7-C23-O8	2.78	130.20	123.70	7	2
3	B	316	PX4	O7-C23-C24	2.78	105.47	111.48	13	5
3	B	339	PX4	O7-C23-C24	2.78	105.47	111.48	9	4
3	B	367	PX4	O7-C7-C6	2.78	118.32	108.34	4	2
3	B	394	PX4	O5-C9-C10	2.78	103.36	111.83	9	1
3	B	339	PX4	C5-N1-C3	2.78	116.27	108.98	4	2
3	C	320	PX4	O5-C9-C10	2.78	103.36	111.83	4	3
3	A	646	PX4	O7-C23-O8	2.78	130.19	123.70	11	2
3	B	335	PX4	O7-C7-C8	2.78	118.30	108.34	4	1
3	B	362	PX4	O7-C23-C24	2.78	105.48	111.48	10	2
3	C	312	PX4	O7-C7-C6	2.78	118.30	108.34	13	2
3	A	613	PX4	C1-C2-N1	2.77	124.72	115.82	2	1
3	B	383	PX4	C5-N1-C4	2.77	101.69	108.98	6	3
3	C	329	PX4	C25-C24-C23	2.77	103.53	113.69	6	3
3	A	635	PX4	O5-C9-C10	2.77	103.38	111.83	8	2
3	B	346	PX4	O5-C9-C10	2.77	103.39	111.83	12	2
3	B	369	PX4	C5-N1-C3	2.77	101.70	108.98	5	3
3	B	381	PX4	O5-C9-C10	2.77	103.38	111.83	6	4
3	C	303	PX4	C5-N1-C4	2.77	101.69	108.98	9	1
3	A	649	PX4	C26-C25-C24	2.77	102.95	113.13	7	2
3	B	397	PX4	O7-C7-C8	2.77	118.28	108.34	2	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	C	304	PX4	C3-N1-C2	2.77	120.92	109.91	1	1
3	C	310	PX4	C1-C2-N1	2.77	124.71	115.82	12	2
3	B	320	PX4	O5-C9-C10	2.77	103.40	111.83	7	3
3	B	347	PX4	O5-C9-C10	2.77	103.40	111.83	14	1
3	B	396	PX4	C5-N1-C3	2.77	101.71	108.98	12	2
3	C	315	PX4	C25-C24-C23	2.77	103.56	113.69	7	1
3	B	322	PX4	O7-C23-C24	2.76	105.50	111.48	7	3
3	C	304	PX4	C5-N1-C4	2.76	101.72	108.98	1	2
3	B	392	PX4	O5-C9-C10	2.76	103.41	111.83	15	3
3	C	302	PX4	O7-C23-O8	2.76	117.25	123.70	1	1
3	C	327	PX4	C5-N1-C3	2.76	116.23	108.98	12	2
3	B	317	PX4	O5-C9-O6	2.76	130.53	123.63	3	2
3	B	318	PX4	O5-C9-C10	2.76	103.42	111.83	9	3
3	B	396	PX4	O7-C23-O8	2.76	130.16	123.70	13	3
3	C	310	PX4	O5-C9-C10	2.76	103.42	111.83	1	3
3	B	389	PX4	C1-C2-N1	2.76	124.67	115.82	6	2
3	C	321	PX4	C7-O7-C23	2.76	111.20	117.80	1	4
3	C	327	PX4	C5-N1-C4	2.76	101.73	108.98	14	4
3	C	331	PX4	O7-C23-C24	2.76	105.51	111.48	14	3
3	A	606	PX4	O5-C9-C10	2.76	103.43	111.83	5	3
3	A	601	PX4	C1-C2-N1	2.76	124.67	115.82	5	2
3	B	321	PX4	C8-O5-C9	2.76	107.04	117.12	6	4
3	B	380	PX4	O7-C23-C24	2.76	105.52	111.48	12	5
3	C	302	PX4	C11-C10-C9	2.76	123.79	113.69	4	1
3	C	320	PX4	P1-O4-C6	2.76	137.14	121.35	5	1
3	C	348	PX4	O7-C23-C24	2.76	105.52	111.48	5	2
3	A	642	PX4	C5-N1-C4	2.75	101.74	108.98	11	3
3	B	346	PX4	O5-C8-C7	2.75	116.33	108.40	15	3
3	C	361	PX4	C8-O5-C9	2.75	127.17	117.12	5	1
3	A	611	PX4	C5-N1-C3	2.75	116.20	108.98	5	2
3	A	622	PX4	O7-C23-O8	2.75	130.13	123.70	6	1
3	A	641	PX4	O5-C8-C7	2.75	116.32	108.40	8	3
3	C	304	PX4	O5-C9-C10	2.75	103.45	111.83	2	2
3	C	351	PX4	O7-C23-O8	2.75	130.13	123.70	11	4
3	A	626	PX4	C7-O7-C23	2.75	111.22	117.80	12	2
3	B	333	PX4	O5-C9-C10	2.75	103.46	111.83	4	3
3	B	349	PX4	C5-N1-C3	2.75	116.19	108.98	14	2
3	C	305	PX4	O7-C7-C6	2.75	98.49	108.34	10	1
3	C	308	PX4	O7-C7-C8	2.75	118.20	108.34	6	2
3	B	365	PX4	C5-N1-C4	2.75	116.19	108.98	9	2
3	B	377	PX4	C7-O7-C23	2.75	111.22	117.80	9	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	C	364	PX4	C4-N1-C3	2.75	101.76	108.98	9	2
3	C	305	PX4	C8-C7-C6	2.74	105.39	111.78	8	3
3	C	334	PX4	C8-C7-C6	2.75	105.38	111.78	12	2
3	C	338	PX4	C25-C24-C23	2.74	103.64	113.69	7	1
3	A	612	PX4	C5-N1-C2	2.74	99.01	109.91	15	1
3	C	305	PX4	O7-C23-C24	2.74	105.55	111.48	6	3
3	C	329	PX4	O5-C9-O6	2.74	130.49	123.63	13	4
3	A	642	PX4	O1-P1-O3	2.74	119.99	107.57	13	1
3	B	364	PX4	C1-C2-N1	2.74	124.62	115.82	9	2
3	C	356	PX4	O5-C9-O6	2.74	130.48	123.63	12	3
3	C	301	PX4	O5-C9-C10	2.73	103.50	111.83	5	3
3	C	348	PX4	C5-N1-C3	2.74	116.16	108.98	4	2
3	A	643	PX4	O7-C7-C8	2.73	118.15	108.34	14	3
3	A	645	PX4	O5-C8-C7	2.73	116.28	108.40	11	4
3	B	318	PX4	C8-C7-C6	2.73	105.41	111.78	1	2
3	B	348	PX4	C5-N1-C3	2.73	116.16	108.98	15	4
3	B	357	PX4	C5-N1-C3	2.73	101.80	108.98	13	1
3	A	604	PX4	C11-C10-C9	2.73	103.69	113.69	3	1
3	B	303	PX4	C5-N1-C4	2.73	101.81	108.98	4	2
3	C	361	PX4	O7-C23-C24	2.73	105.58	111.48	12	4
3	B	400	PX4	O7-C23-O8	2.73	130.08	123.70	13	1
3	B	332	PX4	C8-C7-C6	2.72	118.14	111.78	2	4
3	B	305	PX4	O5-C8-C7	2.72	116.25	108.40	7	2
3	B	310	PX4	O5-C9-C10	2.72	103.53	111.83	9	2
3	C	347	PX4	O1-P1-O2	2.72	125.11	112.44	6	2
3	A	652	PX4	C11-C10-C9	2.72	103.72	113.69	3	3
3	B	326	PX4	O5-C9-O6	2.72	130.44	123.63	8	4
3	B	344	PX4	C7-O7-C23	2.72	111.28	117.80	14	3
3	A	618	PX4	C11-C10-C9	2.72	123.66	113.69	6	2
3	B	390	PX4	C5-N1-C3	2.72	101.83	108.98	14	1
3	B	312	PX4	O7-C7-C8	2.72	118.10	108.34	6	1
3	C	309	PX4	C12-C11-C10	2.72	123.12	113.13	11	1
3	C	331	PX4	C8-C7-C6	2.72	105.44	111.78	2	3
3	B	322	PX4	C1-C2-N1	2.72	124.55	115.82	9	1
3	B	321	PX4	O7-C23-O8	2.72	130.06	123.70	8	5
3	B	350	PX4	C1-C2-N1	2.72	124.55	115.82	11	1
3	B	389	PX4	C11-C10-C9	2.71	123.64	113.69	1	1
3	C	331	PX4	C5-N1-C4	2.71	101.85	108.98	9	2
3	C	347	PX4	C4-N1-C3	2.71	101.85	108.98	11	4
3	A	623	PX4	O7-C23-C24	2.71	105.61	111.48	8	3
3	A	636	PX4	O6-C9-C10	2.71	134.39	123.78	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	A	641	PX4	C1-C2-N1	2.71	124.53	115.82	12	1
3	B	323	PX4	C1-C2-N1	2.71	124.53	115.82	13	2
3	B	381	PX4	O4-P1-O2	2.71	119.68	108.94	9	1
3	A	614	PX4	O7-C7-C6	2.71	118.07	108.34	11	1
3	C	360	PX4	O7-C23-O8	2.71	130.04	123.70	2	1
3	B	397	PX4	C28-C27-C26	2.71	100.67	114.37	1	1
3	A	620	PX4	O5-C9-C10	2.71	103.58	111.83	14	1
3	B	394	PX4	C5-N1-C4	2.71	101.86	108.98	7	3
3	C	323	PX4	C11-C10-C9	2.71	103.77	113.69	3	2
3	A	621	PX4	C4-N1-C3	2.71	101.86	108.98	1	1
3	B	302	PX4	C4-N1-C3	2.71	116.09	108.98	11	4
3	B	330	PX4	C8-C7-C6	2.71	105.47	111.78	13	4
3	B	400	PX4	O5-C9-O6	2.71	130.40	123.63	6	3
3	A	634	PX4	C8-C7-C6	2.70	118.09	111.78	3	2
3	B	388	PX4	C8-O5-C9	2.71	107.23	117.12	15	1
3	C	313	PX4	C11-C10-C9	2.71	123.61	113.69	7	1
3	C	336	PX4	O7-C23-O8	2.70	130.03	123.70	5	2
3	A	645	PX4	C8-C7-C6	2.70	118.09	111.78	13	3
3	B	336	PX4	O5-C9-C10	2.70	103.59	111.83	7	2
3	A	648	PX4	C12-C11-C10	2.70	103.20	113.13	2	4
3	A	613	PX4	C12-C11-C10	2.70	103.21	113.13	15	1
3	B	309	PX4	C26-C25-C24	2.70	103.21	113.13	9	2
3	A	606	PX4	O5-C8-C7	2.70	116.17	108.40	3	1
3	A	621	PX4	C8-O5-C9	2.70	107.26	117.12	11	1
3	A	632	PX4	C33-C32-C31	2.70	128.00	114.37	6	1
3	B	359	PX4	C4-N1-C2	2.70	99.19	109.91	8	1
3	B	367	PX4	O7-C23-O8	2.70	130.01	123.70	10	3
3	B	393	PX4	C31-C30-C29	2.70	100.74	114.37	3	1
3	B	398	PX4	C8-C7-C6	2.70	105.50	111.78	10	2
3	C	346	PX4	P1-O3-C1	2.70	134.10	121.26	10	2
3	B	304	PX4	C1-C2-N1	2.69	124.47	115.82	8	1
3	B	340	PX4	C25-C24-C23	2.70	123.57	113.69	2	3
3	B	301	PX4	C5-N1-C4	2.69	101.90	108.98	8	2
3	B	323	PX4	C5-N1-C3	2.69	116.05	108.98	4	2
3	C	348	PX4	C4-N1-C3	2.69	101.90	108.98	8	2
3	B	337	PX4	O7-C23-C24	2.69	105.66	111.48	2	4
3	B	365	PX4	O5-C8-C7	2.69	116.16	108.40	13	6
3	B	396	PX4	C25-C24-C23	2.69	103.83	113.69	11	3
3	B	377	PX4	C5-N1-C4	2.69	101.91	108.98	3	1
3	C	305	PX4	C1-C2-N1	2.69	124.46	115.82	6	2
3	C	313	PX4	C5-N1-C3	2.69	101.91	108.98	10	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	A	653	PX4	O7-C7-C8	2.69	118.00	108.34	10	2
3	B	354	PX4	C4-N1-C3	2.69	101.91	108.98	4	5
3	A	615	PX4	C8-C7-C6	2.69	105.52	111.78	15	1
3	A	630	PX4	O7-C23-O8	2.69	129.99	123.70	4	3
3	A	604	PX4	O7-C7-C6	2.69	117.98	108.34	7	6
3	B	315	PX4	C8-O5-C9	2.69	107.29	117.12	15	1
3	B	352	PX4	C8-O5-C9	2.69	107.29	117.12	2	1
3	A	651	PX4	C8-O5-C9	2.69	107.30	117.12	14	1
3	C	327	PX4	O7-C23-O8	2.69	129.99	123.70	3	2
3	A	614	PX4	C8-C7-C6	2.69	105.52	111.78	7	2
3	A	620	PX4	C4-N1-C3	2.69	101.92	108.98	14	1
3	A	632	PX4	C12-C11-C10	2.69	122.99	113.13	14	1
3	B	375	PX4	C8-O5-C9	2.69	107.30	117.12	14	2
3	C	334	PX4	O5-C9-C10	2.68	103.65	111.83	7	1
3	C	337	PX4	O7-C7-C8	2.68	117.97	108.34	5	2
3	A	612	PX4	C8-O5-C9	2.68	107.31	117.12	2	2
3	B	358	PX4	C11-C10-C9	2.68	123.52	113.69	11	1
3	B	363	PX4	C25-C24-C23	2.68	103.86	113.69	4	2
3	B	384	PX4	C8-O5-C9	2.68	107.31	117.12	11	1
3	B	333	PX4	O5-C9-O6	2.68	130.33	123.63	9	1
3	C	312	PX4	O5-C9-C10	2.68	103.66	111.83	7	4
3	C	335	PX4	C1-C2-N1	2.68	124.43	115.82	7	3
3	A	608	PX4	C5-N1-C4	2.68	101.94	108.98	13	2
3	A	651	PX4	O5-C9-C10	2.68	103.67	111.83	8	1
3	B	307	PX4	C12-C11-C10	2.68	103.28	113.13	12	3
3	B	337	PX4	O7-C23-O8	2.68	129.97	123.70	5	2
3	C	304	PX4	C7-O7-C23	2.68	111.38	117.80	4	4
3	C	310	PX4	O7-C23-O8	2.68	129.97	123.70	1	4
3	B	349	PX4	C8-O5-C9	2.68	107.33	117.12	2	1
3	B	383	PX4	O5-C8-C7	2.68	116.12	108.40	6	7
3	C	314	PX4	C12-C11-C10	2.68	122.97	113.13	3	1
3	C	314	PX4	O7-C7-C6	2.68	98.73	108.34	7	1
3	C	352	PX4	C8-O5-C9	2.68	126.91	117.12	5	3
3	A	619	PX4	O7-C23-C24	2.68	105.69	111.48	7	4
3	B	331	PX4	C12-C11-C10	2.68	103.29	113.13	1	2
3	B	355	PX4	C5-N1-C4	2.68	116.01	108.98	7	1
3	C	347	PX4	C12-C11-C10	2.68	103.29	113.13	2	1
3	B	354	PX4	C26-C25-C24	2.67	103.30	113.13	11	1
3	C	326	PX4	C12-C11-C10	2.67	103.30	113.13	5	1
3	C	347	PX4	C3-N1-C2	2.67	120.54	109.91	1	1
3	A	613	PX4	C7-O7-C23	2.67	111.40	117.80	11	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	315	PX4	O7-C23-O8	2.67	129.95	123.70	11	1
3	C	324	PX4	O5-C9-C10	2.67	103.69	111.83	3	2
3	C	356	PX4	C5-N1-C4	2.67	101.96	108.98	9	3
3	B	336	PX4	C7-O7-C23	2.67	111.41	117.80	14	4
3	B	359	PX4	O5-C9-C10	2.67	103.70	111.83	1	1
3	C	343	PX4	C5-N1-C4	2.67	115.99	108.98	13	2
3	C	349	PX4	O5-C9-C10	2.67	103.69	111.83	15	2
3	A	631	PX4	C5-N1-C4	2.67	101.97	108.98	14	3
3	B	385	PX4	C12-C11-C10	2.67	122.93	113.13	5	1
3	A	607	PX4	C5-N1-C4	2.67	115.98	108.98	13	2
3	B	327	PX4	O5-C9-O6	2.67	130.30	123.63	10	2
3	B	364	PX4	C5-N1-C3	2.67	101.97	108.98	3	2
3	C	301	PX4	O7-C23-O8	2.67	129.94	123.70	7	4
3	C	303	PX4	O7-C7-C8	2.67	117.91	108.34	15	1
3	C	343	PX4	C7-O7-C23	2.67	111.41	117.80	9	5
3	C	320	PX4	C5-N1-C4	2.67	115.98	108.98	10	3
3	C	360	PX4	C8-C7-C6	2.67	105.57	111.78	12	4
3	C	360	PX4	C8-O5-C9	2.67	107.37	117.12	5	2
3	B	337	PX4	C8-O5-C9	2.67	107.37	117.12	4	1
3	B	393	PX4	C8-O5-C9	2.66	126.86	117.12	7	1
3	C	313	PX4	C26-C25-C24	2.67	103.33	113.13	9	1
3	B	313	PX4	C5-N1-C3	2.66	101.98	108.98	11	1
3	A	616	PX4	C25-C24-C23	2.66	103.94	113.69	15	1
3	A	637	PX4	C8-O5-C9	2.66	107.38	117.12	12	3
3	C	345	PX4	O7-C7-C6	2.66	117.90	108.34	6	1
3	B	305	PX4	O5-C9-O6	2.66	130.29	123.63	10	2
3	B	313	PX4	C26-C25-C24	2.66	122.90	113.13	5	1
3	B	333	PX4	P1-O3-C1	2.66	108.59	121.26	4	1
3	B	373	PX4	C5-N1-C3	2.66	101.99	108.98	9	1
3	B	384	PX4	C27-C26-C25	2.66	127.82	114.37	7	1
3	C	320	PX4	C25-C24-C23	2.66	103.94	113.69	10	1
3	A	616	PX4	O5-C8-C7	2.66	116.06	108.40	4	1
3	A	614	PX4	O5-C9-O6	2.66	130.27	123.63	1	2
3	A	644	PX4	O5-C9-O6	2.66	130.27	123.63	9	2
3	B	338	PX4	C8-C7-C6	2.66	117.98	111.78	13	5
3	B	354	PX4	O5-C9-O6	2.66	130.28	123.63	1	3
3	B	380	PX4	C4-N1-C3	2.66	115.96	108.98	13	1
3	B	335	PX4	C8-C7-C6	2.66	105.59	111.78	5	2
3	B	352	PX4	C7-O7-C23	2.66	111.44	117.80	12	2
3	A	625	PX4	C3-N1-C2	2.65	120.46	109.91	13	1
3	B	357	PX4	O7-C7-C8	2.65	117.87	108.34	7	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	C	342	PX4	O5-C9-C10	2.65	103.74	111.83	12	2
3	C	361	PX4	C1-C2-N1	2.66	124.34	115.82	15	1
3	B	338	PX4	O5-C9-O6	2.65	130.26	123.63	4	1
3	C	343	PX4	C4-N1-C3	2.65	115.94	108.98	15	4
3	C	361	PX4	C5-N1-C3	2.65	102.01	108.98	8	2
3	A	638	PX4	C11-C10-C9	2.65	103.98	113.69	14	1
3	B	337	PX4	O5-C8-C7	2.65	116.03	108.40	13	4
3	C	358	PX4	C5-N1-C3	2.65	115.94	108.98	14	2
3	A	603	PX4	O7-C7-C6	2.65	117.84	108.34	7	1
3	A	637	PX4	C8-C7-C6	2.65	105.61	111.78	10	1
3	B	370	PX4	O5-C9-C10	2.65	103.76	111.83	2	2
3	A	648	PX4	C4-N1-C3	2.65	102.02	108.98	6	2
3	B	382	PX4	O5-C9-O6	2.65	130.25	123.63	7	2
3	B	384	PX4	O5-C9-C10	2.65	103.77	111.83	6	2
3	C	363	PX4	C8-C7-C6	2.65	105.61	111.78	5	5
3	A	618	PX4	C8-C7-C6	2.65	105.62	111.78	3	1
3	A	649	PX4	O5-C8-C7	2.65	116.02	108.40	15	5
3	B	312	PX4	C7-O7-C23	2.64	111.47	117.80	10	2
3	B	333	PX4	C1-C2-N1	2.65	124.31	115.82	12	1
3	B	335	PX4	O5-C9-O6	2.65	130.25	123.63	4	3
3	C	304	PX4	C8-C7-C6	2.65	117.95	111.78	4	2
3	C	333	PX4	O7-C7-C8	2.65	117.84	108.34	3	1
3	B	345	PX4	C5-N1-C4	2.64	102.03	108.98	12	1
3	C	353	PX4	C5-N1-C4	2.64	102.03	108.98	15	3
3	A	633	PX4	C4-N1-C3	2.64	115.91	108.98	11	3
3	B	360	PX4	C8-C7-C6	2.64	105.63	111.78	1	1
3	C	328	PX4	C11-C10-C9	2.64	104.02	113.69	12	1
3	B	366	PX4	C1-C2-N1	2.64	124.29	115.82	5	2
3	C	361	PX4	C11-C10-C9	2.64	104.03	113.69	12	1
3	C	363	PX4	C5-N1-C3	2.64	102.05	108.98	15	2
3	B	327	PX4	O5-C8-C7	2.64	116.00	108.40	14	1
3	B	395	PX4	O1-P1-O2	2.64	124.71	112.44	10	1
3	B	306	PX4	O5-C9-C10	2.64	103.80	111.83	1	1
3	B	327	PX4	C8-O5-C9	2.63	107.49	117.12	8	1
3	C	313	PX4	O7-C23-O8	2.64	129.87	123.70	6	1
3	A	638	PX4	O5-C9-O6	2.63	130.22	123.63	3	4
3	B	306	PX4	C4-N1-C3	2.63	115.89	108.98	4	2
3	C	302	PX4	C8-C7-C6	2.63	105.64	111.78	4	2
3	A	634	PX4	C7-O7-C23	2.63	111.50	117.80	2	1
3	A	637	PX4	O5-C9-O6	2.63	130.21	123.63	5	3
3	C	327	PX4	C8-C7-C6	2.63	105.65	111.78	12	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	A	618	PX4	C4-N1-C3	2.63	102.07	108.98	15	2
3	A	638	PX4	C5-N1-C3	2.63	102.07	108.98	4	1
3	B	308	PX4	C4-N1-C3	2.63	102.07	108.98	15	1
3	B	339	PX4	O5-C9-O6	2.63	130.20	123.63	8	1
3	B	357	PX4	C25-C24-C23	2.63	104.06	113.69	6	2
3	C	330	PX4	C5-N1-C4	2.63	102.07	108.98	15	2
3	B	374	PX4	C3-N1-C2	2.63	99.47	109.91	4	1
3	B	328	PX4	O5-C9-C10	2.63	103.83	111.83	11	2
3	C	323	PX4	O7-C23-O8	2.63	129.85	123.70	6	5
3	C	363	PX4	O5-C9-C10	2.63	103.83	111.83	15	2
3	C	307	PX4	C20-C19-C18	2.62	101.10	114.37	6	1
3	C	325	PX4	C26-C25-C24	2.62	103.48	113.13	3	2
3	A	633	PX4	C5-N1-C3	2.62	102.09	108.98	10	3
3	C	324	PX4	C4-N1-C3	2.62	102.09	108.98	9	1
3	C	352	PX4	C5-N1-C4	2.62	102.08	108.98	11	1
3	A	636	PX4	C4-N1-C3	2.62	102.09	108.98	7	1
3	A	652	PX4	C8-O5-C9	2.62	107.54	117.12	15	2
3	B	398	PX4	O7-C23-O8	2.62	129.84	123.70	5	3
3	C	317	PX4	C34-C33-C32	2.62	101.12	114.37	1	1
3	C	341	PX4	C1-C2-N1	2.62	124.24	115.82	12	1
3	B	322	PX4	C5-N1-C3	2.62	102.10	108.98	10	1
3	B	338	PX4	O6-C9-C10	2.62	113.54	123.78	1	1
3	A	641	PX4	O7-C23-O8	2.62	129.82	123.70	9	5
3	B	330	PX4	C5-N1-C4	2.62	102.10	108.98	12	1
3	B	331	PX4	O7-C7-C6	2.62	117.73	108.34	13	2
3	B	332	PX4	C1-C2-N1	2.62	124.22	115.82	1	2
3	C	351	PX4	O5-C8-C7	2.62	115.94	108.40	14	4
3	B	327	PX4	C11-C10-C9	2.61	123.27	113.69	10	1
3	A	621	PX4	O7-C7-C8	2.61	117.72	108.34	2	4
3	A	648	PX4	O5-C8-C7	2.61	115.93	108.40	14	4
3	B	342	PX4	C8-C7-C6	2.61	105.69	111.78	15	2
3	B	365	PX4	C25-C24-C23	2.61	104.12	113.69	15	2
3	C	329	PX4	C8-C7-C6	2.61	117.88	111.78	3	3
3	B	350	PX4	C4-N1-C3	2.61	102.11	108.98	4	2
3	B	360	PX4	O7-C23-O8	2.61	129.81	123.70	1	5
3	B	380	PX4	O7-C23-O8	2.61	129.81	123.70	5	4
3	C	325	PX4	C4-N1-C3	2.61	102.12	108.98	12	2
3	A	616	PX4	C4-N1-C3	2.61	102.12	108.98	3	3
3	A	609	PX4	O1-P1-O2	2.61	124.58	112.44	12	1
3	A	624	PX4	O5-C9-O6	2.61	130.15	123.63	2	1
3	A	647	PX4	C5-N1-C4	2.61	102.12	108.98	4	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	A	649	PX4	O7-C7-C6	2.61	117.70	108.34	2	1
3	A	632	PX4	O7-C7-C8	2.61	117.69	108.34	3	3
3	B	323	PX4	O7-C23-C24	2.61	105.84	111.48	5	3
3	B	325	PX4	C26-C25-C24	2.61	103.55	113.13	5	1
3	A	604	PX4	O5-C8-C7	2.60	115.90	108.40	3	2
3	A	627	PX4	O4-P1-O2	2.60	98.62	108.94	8	1
3	B	375	PX4	C1-C2-N1	2.60	124.18	115.82	12	4
3	B	306	PX4	O7-C7-C6	2.60	117.68	108.34	8	1
3	B	364	PX4	O7-C23-O8	2.60	129.79	123.70	9	4
3	C	323	PX4	C3-N1-C2	2.60	120.25	109.91	2	1
3	A	602	PX4	O7-C7-C6	2.60	117.67	108.34	1	2
3	B	368	PX4	C1-C2-N1	2.60	124.17	115.82	5	2
3	C	363	PX4	C1-C2-N1	2.60	124.17	115.82	15	1
3	A	611	PX4	P1-O3-C1	2.60	133.63	121.26	10	2
3	B	316	PX4	O7-C7-C8	2.60	117.67	108.34	1	2
3	C	364	PX4	O7-C23-C24	2.60	105.86	111.48	2	3
3	B	324	PX4	O5-C9-O6	2.60	130.12	123.63	15	2
3	C	331	PX4	O5-C9-O6	2.60	130.12	123.63	3	1
3	A	611	PX4	O7-C23-C24	2.59	105.87	111.48	8	2
3	A	632	PX4	C7-O7-C23	2.59	111.59	117.80	9	2
3	B	349	PX4	O7-C23-O8	2.59	129.77	123.70	13	3
3	C	339	PX4	C5-N1-C4	2.59	102.16	108.98	11	3
3	C	345	PX4	O7-C7-C8	2.59	117.65	108.34	1	2
3	C	354	PX4	C5-N1-C4	2.59	102.16	108.98	8	1
3	A	647	PX4	C1-C2-N1	2.59	124.14	115.82	3	4
3	B	305	PX4	O7-C7-C8	2.59	117.64	108.34	3	1
3	C	314	PX4	O7-C7-C8	2.59	117.65	108.34	5	2
3	B	350	PX4	O7-C7-C6	2.59	117.64	108.34	7	2
3	B	384	PX4	C5-N1-C3	2.59	102.17	108.98	3	2
3	B	329	PX4	O5-C8-C7	2.59	115.86	108.40	9	2
3	B	337	PX4	C1-C2-N1	2.59	124.14	115.82	3	2
3	A	621	PX4	O1-P1-O2	2.59	124.49	112.44	6	1
3	A	634	PX4	O7-C7-C6	2.59	117.63	108.34	8	2
3	B	313	PX4	C8-C7-C6	2.59	117.82	111.78	7	3
3	C	309	PX4	O4-P1-O2	2.59	98.67	108.94	5	1
3	C	315	PX4	C11-C10-C9	2.59	104.21	113.69	9	2
3	C	357	PX4	P1-O3-C1	2.59	133.59	121.26	12	1
3	A	618	PX4	C5-N1-C3	2.59	102.18	108.98	10	1
3	A	609	PX4	C1-C2-N1	2.59	124.12	115.82	3	3
3	A	634	PX4	C1-C2-N1	2.59	124.12	115.82	5	3
3	B	304	PX4	C12-C11-C10	2.59	103.62	113.13	4	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	C	317	PX4	O7-C23-C24	2.59	105.88	111.48	2	3
3	B	322	PX4	C4-N1-C3	2.59	102.18	108.98	11	2
3	A	602	PX4	O5-C9-C10	2.59	103.95	111.83	8	1
3	A	644	PX4	C5-N1-C4	2.59	102.19	108.98	3	1
3	A	646	PX4	O7-C23-C24	2.58	105.89	111.48	5	5
3	B	307	PX4	C25-C24-C23	2.59	123.17	113.69	3	1
3	A	647	PX4	O7-C23-C24	2.58	105.89	111.48	11	3
3	B	322	PX4	C5-N1-C4	2.58	115.76	108.98	5	2
3	B	324	PX4	O7-C23-C24	2.58	105.89	111.48	6	3
3	B	353	PX4	O1-P1-O2	2.59	124.47	112.44	3	2
3	B	392	PX4	C1-C2-N1	2.58	124.11	115.82	2	2
3	B	351	PX4	O7-C23-C24	2.58	105.89	111.48	7	4
3	A	644	PX4	O1-P1-O4	2.58	119.27	107.57	4	1
3	B	306	PX4	C31-C30-C29	2.58	101.33	114.37	12	1
3	B	327	PX4	P1-O3-C1	2.58	108.98	121.26	3	1
3	B	327	PX4	O7-C7-C8	2.58	117.60	108.34	8	4
3	B	377	PX4	O7-C23-O8	2.58	129.74	123.70	13	1
3	B	389	PX4	C25-C24-C23	2.58	104.24	113.69	6	2
3	A	605	PX4	O5-C9-C10	2.58	103.98	111.83	1	2
3	A	632	PX4	C5-N1-C4	2.58	115.75	108.98	10	1
3	B	360	PX4	C1-C2-N1	2.58	124.10	115.82	5	2
3	A	640	PX4	O5-C9-C10	2.58	103.97	111.83	8	3
3	C	301	PX4	C12-C11-C10	2.58	122.60	113.13	10	2
3	C	313	PX4	C1-C2-N1	2.58	124.10	115.82	6	1
3	C	351	PX4	O5-C9-C10	2.58	119.70	111.83	14	2
3	B	373	PX4	C1-C2-N1	2.58	124.09	115.82	7	1
3	B	376	PX4	O7-C7-C8	2.58	117.59	108.34	14	1
3	C	334	PX4	O5-C9-O6	2.58	130.07	123.63	7	1
3	B	352	PX4	C11-C10-C9	2.58	123.13	113.69	6	1
3	B	310	PX4	O7-C23-C24	2.57	105.91	111.48	14	5
3	C	335	PX4	C11-C10-C9	2.57	104.26	113.69	8	1
3	B	311	PX4	C5-N1-C2	2.57	120.14	109.91	12	1
3	B	389	PX4	C5-N1-C4	2.57	102.22	108.98	10	4
3	C	311	PX4	O7-C23-C24	2.57	105.92	111.48	1	3
3	C	349	PX4	O7-C23-O8	2.57	129.72	123.70	8	1
3	A	633	PX4	O5-C9-O6	2.57	130.06	123.63	9	2
3	B	348	PX4	O5-C9-C10	2.57	103.99	111.83	15	3
3	C	363	PX4	C5-N1-C2	2.57	120.14	109.91	7	2
3	B	376	PX4	C25-C24-C23	2.57	104.27	113.69	10	1
3	B	392	PX4	O7-C23-C24	2.57	105.92	111.48	10	4
3	A	617	PX4	C8-C7-C6	2.57	105.79	111.78	9	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	346	PX4	C8-C7-C6	2.57	117.78	111.78	9	1
3	C	325	PX4	C7-O7-C23	2.57	111.64	117.80	1	5
3	C	348	PX4	C1-C2-N1	2.57	124.07	115.82	3	1
3	C	359	PX4	O5-C9-C10	2.57	104.00	111.83	2	1
3	B	359	PX4	O5-C9-O6	2.57	130.06	123.63	1	1
3	B	393	PX4	C1-C2-N1	2.57	124.07	115.82	9	2
3	B	340	PX4	O7-C7-C8	2.57	117.56	108.34	1	1
3	B	383	PX4	C8-O5-C9	2.57	107.73	117.12	7	1
3	A	614	PX4	O5-C8-C7	2.57	115.79	108.40	10	5
3	A	634	PX4	C3-N1-C2	2.57	120.11	109.91	4	1
3	C	355	PX4	O7-C7-C8	2.57	117.55	108.34	1	1
3	B	357	PX4	C7-O7-C23	2.57	111.65	117.80	1	2
3	B	324	PX4	C1-C2-N1	2.57	124.06	115.82	5	4
3	B	385	PX4	O7-C7-C6	2.56	117.54	108.34	9	1
3	C	306	PX4	P1-O3-C1	2.56	133.47	121.26	3	1
3	C	364	PX4	O5-C9-O6	2.57	130.04	123.63	5	2
3	A	631	PX4	O7-C23-O8	2.56	129.70	123.70	1	3
3	A	648	PX4	O7-C7-C6	2.56	117.54	108.34	7	1
3	A	650	PX4	C25-C24-C23	2.56	104.31	113.69	12	1
3	C	312	PX4	O7-C23-C24	2.56	117.03	111.48	2	2
3	B	304	PX4	O7-C23-C24	2.56	105.94	111.48	9	1
3	B	322	PX4	P1-O3-C1	2.56	109.07	121.26	12	1
3	C	302	PX4	C7-O7-C23	2.56	111.66	117.80	8	3
3	B	389	PX4	O7-C7-C8	2.56	117.53	108.34	14	2
3	C	321	PX4	C4-N1-C3	2.56	102.25	108.98	4	1
3	B	316	PX4	C8-O5-C9	2.56	107.76	117.12	11	1
3	B	388	PX4	O7-C7-C8	2.56	99.16	108.34	7	2
3	B	400	PX4	C5-N1-C3	2.56	102.25	108.98	9	2
3	C	312	PX4	C25-C24-C23	2.56	123.07	113.69	7	1
3	C	322	PX4	C1-C2-N1	2.56	124.04	115.82	10	3
3	A	634	PX4	C34-C33-C32	2.56	101.44	114.37	10	1
3	A	645	PX4	O7-C7-C8	2.56	117.52	108.34	13	2
3	B	362	PX4	C8-O5-C9	2.56	107.77	117.12	6	1
3	B	390	PX4	O7-C7-C8	2.56	117.52	108.34	9	2
3	B	399	PX4	C8-O5-C9	2.56	107.77	117.12	4	1
3	C	322	PX4	C5-N1-C3	2.56	115.69	108.98	8	3
3	A	653	PX4	O5-C9-C10	2.56	104.04	111.83	7	1
3	B	340	PX4	C7-O7-C23	2.56	111.68	117.80	9	4
3	B	384	PX4	C25-C24-C23	2.56	104.33	113.69	11	1
3	A	637	PX4	C5-N1-C3	2.55	102.27	108.98	3	4
3	B	328	PX4	C5-N1-C3	2.55	115.69	108.98	1	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	333	PX4	O7-C23-O8	2.55	117.73	123.70	5	2
3	B	346	PX4	O7-C23-C24	2.55	105.96	111.48	8	2
3	C	342	PX4	O5-C9-O6	2.55	130.02	123.63	6	2
3	C	301	PX4	O7-C7-C6	2.55	117.50	108.34	4	1
3	C	351	PX4	C3-N1-C2	2.55	120.06	109.91	7	1
3	B	343	PX4	C5-N1-C3	2.55	115.68	108.98	7	2
3	B	349	PX4	C4-N1-C3	2.55	102.27	108.98	5	2
3	C	338	PX4	O7-C7-C8	2.55	117.50	108.34	13	5
3	A	639	PX4	C1-C2-N1	2.55	124.00	115.82	2	2
3	A	650	PX4	C11-C10-C9	2.55	104.35	113.69	6	2
3	A	652	PX4	C4-N1-C3	2.55	102.28	108.98	1	2
3	B	395	PX4	O1-P1-O3	2.55	119.13	107.57	5	1
3	A	609	PX4	C25-C24-C23	2.55	104.36	113.69	10	2
3	A	654	PX4	O7-C23-O8	2.55	129.66	123.70	12	2
3	B	304	PX4	C8-O5-C9	2.55	107.80	117.12	13	1
3	B	317	PX4	O1-P1-O2	2.55	124.30	112.44	7	1
3	C	328	PX4	C14-C13-C12	2.55	101.48	114.37	14	1
3	C	361	PX4	O5-C9-C10	2.55	104.06	111.83	7	1
3	B	319	PX4	O3-C1-C2	2.55	121.91	109.65	7	1
3	B	319	PX4	P1-O3-C1	2.55	133.38	121.26	11	1
3	B	342	PX4	O5-C8-C7	2.55	115.74	108.40	14	6
3	B	371	PX4	C26-C25-C24	2.55	122.49	113.13	5	1
3	B	395	PX4	O5-C9-C10	2.55	104.07	111.83	10	2
3	B	400	PX4	O7-C7-C6	2.55	99.21	108.34	11	1
3	B	367	PX4	C5-N1-C3	2.54	115.66	108.98	9	1
3	B	377	PX4	O6-C9-C10	2.55	133.74	123.78	4	2
3	B	388	PX4	C26-C25-C24	2.55	103.77	113.13	8	1
3	C	315	PX4	C8-O5-C9	2.55	107.81	117.12	12	2
3	A	610	PX4	C5-N1-C4	2.54	102.29	108.98	1	1
3	A	615	PX4	C12-C11-C10	2.55	103.77	113.13	5	1
3	B	321	PX4	C5-N1-C4	2.55	102.29	108.98	4	1
3	C	339	PX4	O7-C7-C6	2.55	117.48	108.34	1	2
3	A	641	PX4	C11-C10-C9	2.54	104.37	113.69	12	1
3	A	645	PX4	O7-C23-O8	2.54	129.66	123.70	10	2
3	C	303	PX4	O7-C23-O8	2.54	129.66	123.70	5	1
3	C	346	PX4	C8-O5-C9	2.55	107.81	117.12	6	1
3	A	647	PX4	O7-C23-O8	2.54	129.65	123.70	15	1
3	B	332	PX4	C5-N1-C3	2.54	102.29	108.98	7	1
3	B	304	PX4	C5-N1-C3	2.54	102.30	108.98	4	1
3	B	315	PX4	O7-C7-C6	2.54	117.47	108.34	6	3
3	A	623	PX4	C1-C2-N1	2.54	123.98	115.82	5	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	A	630	PX4	O5-C9-C10	2.54	104.09	111.83	9	1
3	B	331	PX4	C5-N1-C3	2.54	115.65	108.98	1	1
3	B	343	PX4	C5-N1-C4	2.54	115.66	108.98	2	1
3	B	348	PX4	O7-C7-C8	2.54	117.47	108.34	8	3
3	B	389	PX4	O5-C9-O6	2.54	129.99	123.63	2	1
3	B	363	PX4	C8-O5-C9	2.54	107.83	117.12	15	1
3	B	393	PX4	O5-C8-C7	2.54	115.73	108.40	1	3
3	B	394	PX4	O7-C7-C8	2.54	99.22	108.34	2	2
3	C	345	PX4	C11-C10-C9	2.54	104.38	113.69	11	1
3	A	654	PX4	O7-C7-C8	2.54	117.45	108.34	11	3
3	B	310	PX4	O5-C9-O6	2.54	129.98	123.63	11	1
3	B	328	PX4	O5-C9-O6	2.54	129.98	123.63	5	1
3	C	347	PX4	C5-N1-C3	2.54	102.30	108.98	1	1
3	B	311	PX4	C26-C25-C24	2.54	103.80	113.13	13	2
3	A	630	PX4	C3-N1-C2	2.54	120.00	109.91	1	1
3	A	645	PX4	P1-O3-C1	2.54	133.34	121.26	8	1
3	A	650	PX4	O7-C7-C8	2.54	117.44	108.34	5	3
3	B	336	PX4	C33-C32-C31	2.54	101.54	114.37	3	1
3	B	322	PX4	O5-C8-C7	2.54	115.71	108.40	15	2
3	B	371	PX4	P1-O3-C1	2.54	133.33	121.26	11	1
3	C	345	PX4	C1-C2-N1	2.54	123.96	115.82	11	4
3	B	309	PX4	C1-C2-N1	2.53	123.96	115.82	9	3
3	C	327	PX4	O8-C23-C24	2.54	133.70	123.78	11	2
3	C	313	PX4	C4-N1-C3	2.53	102.32	108.98	14	1
3	C	351	PX4	C1-C2-N1	2.53	123.96	115.82	4	1
3	A	617	PX4	O4-P1-O2	2.53	98.90	108.94	15	2
3	A	638	PX4	O7-C7-C8	2.53	117.43	108.34	15	2
3	A	643	PX4	O1-P1-O4	2.53	119.05	107.57	5	2
3	B	326	PX4	O5-C8-C7	2.53	115.70	108.40	11	2
3	B	341	PX4	C1-C2-N1	2.53	123.95	115.82	13	2
3	B	359	PX4	C1-C2-N1	2.53	123.95	115.82	3	1
3	C	337	PX4	C25-C24-C23	2.53	104.41	113.69	2	2
3	C	337	PX4	O5-C9-C10	2.53	104.11	111.83	3	1
3	A	609	PX4	C5-N1-C3	2.53	115.62	108.98	3	3
3	B	305	PX4	C8-O5-C9	2.53	126.37	117.12	4	2
3	C	362	PX4	C1-C2-N1	2.53	123.95	115.82	10	3
3	A	632	PX4	C11-C10-C9	2.53	104.42	113.69	5	1
3	A	642	PX4	O6-C9-C10	2.53	133.68	123.78	13	1
3	A	607	PX4	C8-O5-C9	2.53	126.36	117.12	10	1
3	B	387	PX4	C1-C2-N1	2.53	123.94	115.82	2	1
3	C	311	PX4	O7-C7-C8	2.53	117.41	108.34	9	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	A	604	PX4	O5-C9-C10	2.53	104.14	111.83	5	1
3	A	623	PX4	C11-C10-C9	2.53	122.95	113.69	4	1
3	A	648	PX4	C8-O5-C9	2.53	126.35	117.12	6	2
3	B	392	PX4	C30-C29-C28	2.53	101.59	114.37	15	1
3	A	634	PX4	C8-O5-C9	2.53	107.89	117.12	6	1
3	B	337	PX4	C5-N1-C3	2.52	115.61	108.98	13	1
3	B	371	PX4	O7-C23-O8	2.53	129.61	123.70	7	2
3	C	332	PX4	O7-C23-O8	2.52	129.60	123.70	14	2
3	C	345	PX4	C5-N1-C4	2.52	115.60	108.98	2	1
3	C	353	PX4	C12-C11-C10	2.52	122.40	113.13	15	2
3	B	329	PX4	O5-C9-O6	2.52	129.94	123.63	8	1
3	B	337	PX4	C11-C10-C9	2.52	122.93	113.69	10	1
3	B	352	PX4	C5-N1-C4	2.52	115.60	108.98	12	1
3	A	610	PX4	C1-C2-N1	2.52	123.91	115.82	12	1
3	A	646	PX4	O5-C9-C10	2.52	104.15	111.83	6	1
3	B	351	PX4	C5-N1-C4	2.52	102.36	108.98	8	3
3	B	302	PX4	O3-P1-O2	2.52	98.95	108.94	10	1
3	B	331	PX4	O5-C8-C7	2.52	115.66	108.40	13	3
3	B	342	PX4	O5-C9-C10	2.52	104.15	111.83	13	1
3	B	359	PX4	O7-C23-O8	2.52	129.60	123.70	4	2
3	B	369	PX4	C5-N1-C2	2.52	119.92	109.91	6	1
3	B	395	PX4	C7-O7-C23	2.52	111.77	117.80	7	4
3	A	601	PX4	C8-O5-C9	2.52	107.92	117.12	14	2
3	A	604	PX4	C1-C2-N1	2.52	123.90	115.82	15	1
3	B	331	PX4	O7-C23-C24	2.52	106.04	111.48	7	1
3	B	357	PX4	C1-C2-N1	2.52	123.90	115.82	1	3
3	B	358	PX4	O5-C9-O6	2.52	129.93	123.63	7	3
3	B	389	PX4	C8-O5-C9	2.52	107.91	117.12	10	1
3	C	309	PX4	O5-C9-C10	2.52	104.15	111.83	2	1
3	C	356	PX4	C5-N1-C3	2.52	102.36	108.98	14	1
3	A	607	PX4	C26-C25-C24	2.52	122.37	113.13	11	2
3	A	618	PX4	C3-N1-C2	2.52	119.91	109.91	5	1
3	B	362	PX4	C5-N1-C2	2.52	119.91	109.91	2	1
3	B	399	PX4	O8-C23-C24	2.51	133.62	123.78	5	1
3	C	304	PX4	C26-C25-C24	2.52	103.89	113.13	9	1
3	C	315	PX4	C1-C2-N1	2.52	123.90	115.82	2	1
3	C	322	PX4	O5-C9-O6	2.52	129.92	123.63	15	1
3	C	333	PX4	P1-O3-C1	2.52	133.23	121.26	4	1
3	C	335	PX4	O7-C7-C6	2.52	117.37	108.34	9	1
3	A	611	PX4	C25-C24-C23	2.51	104.48	113.69	6	1
3	A	612	PX4	O5-C9-O6	2.51	129.92	123.63	13	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	A	654	PX4	O3-C1-C2	2.51	121.75	109.65	4	1
3	B	305	PX4	O5-C9-C10	2.51	104.17	111.83	8	4
3	B	350	PX4	O5-C8-C7	2.51	115.64	108.40	8	1
3	B	390	PX4	C4-N1-C3	2.51	115.58	108.98	3	2
3	C	303	PX4	O7-C23-C24	2.51	106.05	111.48	4	3
3	B	314	PX4	O5-C8-C7	2.51	115.64	108.40	9	3
3	A	635	PX4	C7-O7-C23	2.51	111.79	117.80	1	3
3	B	339	PX4	C12-C11-C10	2.51	103.90	113.13	8	1
3	B	353	PX4	C8-C7-C6	2.51	105.93	111.78	5	2
3	C	303	PX4	O5-C9-O6	2.51	129.91	123.63	7	2
3	C	322	PX4	O5-C8-C7	2.51	115.64	108.40	10	2
3	C	326	PX4	O5-C9-C10	2.51	104.18	111.83	11	1
3	C	348	PX4	O7-C23-O8	2.51	129.57	123.70	4	1
3	A	607	PX4	O1-P1-O2	2.51	124.12	112.44	5	2
3	A	640	PX4	C5-N1-C4	2.51	102.39	108.98	7	2
3	B	316	PX4	C1-C2-N1	2.51	123.87	115.82	2	2
3	B	321	PX4	C5-N1-C3	2.51	115.56	108.98	9	1
3	B	361	PX4	C8-O5-C9	2.51	107.95	117.12	4	3
3	C	332	PX4	O5-C8-C7	2.51	115.62	108.40	10	1
3	C	312	PX4	C8-O5-C9	2.50	107.96	117.12	4	2
3	A	623	PX4	C4-N1-C3	2.50	102.41	108.98	6	2
3	A	631	PX4	C5-N1-C3	2.50	102.41	108.98	3	1
3	C	307	PX4	P1-O3-C1	2.50	133.16	121.26	11	1
3	B	361	PX4	O5-C9-C10	2.50	104.21	111.83	15	1
3	B	373	PX4	C25-C24-C23	2.50	104.53	113.69	5	3
3	C	318	PX4	O5-C9-C10	2.50	104.21	111.83	8	1
3	C	330	PX4	C5-N1-C3	2.50	102.41	108.98	11	3
3	C	341	PX4	C8-C7-C6	2.50	105.95	111.78	10	6
3	C	345	PX4	C8-C7-C6	2.50	105.95	111.78	5	1
3	A	628	PX4	O5-C8-C7	2.50	115.60	108.40	4	3
3	B	327	PX4	C1-C2-N1	2.50	123.85	115.82	6	3
3	C	363	PX4	C8-O5-C9	2.50	107.98	117.12	15	2
3	A	607	PX4	C25-C24-C23	2.50	104.54	113.69	7	1
3	A	610	PX4	C11-C10-C9	2.50	104.54	113.69	12	1
3	A	602	PX4	C4-N1-C3	2.50	115.54	108.98	15	2
3	A	628	PX4	P1-O3-C1	2.50	109.37	121.26	11	1
3	B	306	PX4	O5-C9-O6	2.50	129.88	123.63	5	1
3	B	336	PX4	C3-N1-C2	2.50	119.84	109.91	14	1
3	B	340	PX4	O1-P1-O2	2.50	124.07	112.44	13	1
3	B	386	PX4	O1-P1-O2	2.50	124.07	112.44	13	3
3	C	318	PX4	O5-C9-O6	2.50	129.88	123.63	8	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	A	643	PX4	C8-O5-C9	2.50	126.24	117.12	14	2
3	C	318	PX4	C1-C2-N1	2.50	123.84	115.82	6	2
3	A	620	PX4	C5-N1-C4	2.49	102.42	108.98	2	3
3	B	317	PX4	O7-C7-C8	2.49	117.29	108.34	3	3
3	B	367	PX4	C4-N1-C3	2.49	102.42	108.98	6	1
3	B	328	PX4	O5-C8-C7	2.49	115.58	108.40	12	3
3	B	333	PX4	O5-C8-C7	2.49	115.58	108.40	14	4
3	B	355	PX4	C8-C7-C6	2.49	105.97	111.78	8	1
3	A	602	PX4	C12-C11-C10	2.49	103.98	113.13	9	1
3	B	301	PX4	O7-C23-C24	2.49	106.09	111.48	4	3
3	B	389	PX4	C4-N1-C2	2.49	119.81	109.91	13	1
3	A	602	PX4	C5-N1-C3	2.49	115.51	108.98	3	2
3	A	652	PX4	C26-C25-C24	2.49	122.27	113.13	7	1
3	B	303	PX4	C8-O5-C9	2.49	126.22	117.12	12	1
3	B	362	PX4	O3-C1-C2	2.49	121.62	109.65	9	1
3	C	324	PX4	C5-N1-C4	2.49	115.52	108.98	7	1
3	B	316	PX4	O7-C23-O8	2.49	129.52	123.70	15	6
3	C	309	PX4	C8-O5-C9	2.49	108.03	117.12	3	3
3	C	310	PX4	C29-C28-C27	2.49	101.80	114.37	12	1
3	C	361	PX4	O7-C23-O8	2.49	129.52	123.70	9	3
3	A	620	PX4	O5-C9-O6	2.49	129.84	123.63	13	2
3	B	301	PX4	C26-C25-C24	2.49	122.26	113.13	1	1
3	A	653	PX4	C8-C7-C6	2.48	117.58	111.78	14	2
3	A	611	PX4	C26-C25-C24	2.48	104.00	113.13	7	1
3	A	651	PX4	C4-N1-C3	2.48	102.45	108.98	2	3
3	B	315	PX4	C8-C7-C6	2.48	105.99	111.78	6	2
3	B	323	PX4	O7-C23-O8	2.48	129.51	123.70	9	2
3	C	324	PX4	O7-C23-O8	2.49	129.52	123.70	3	2
3	C	315	PX4	C5-N1-C4	2.48	102.45	108.98	4	1
3	C	329	PX4	C11-C10-C9	2.48	104.59	113.69	1	2
3	B	328	PX4	C8-O5-C9	2.48	108.04	117.12	3	1
3	C	304	PX4	O7-C23-O8	2.48	129.51	123.70	9	1
3	C	361	PX4	O7-C7-C8	2.48	117.25	108.34	1	2
3	C	363	PX4	C25-C24-C23	2.48	122.80	113.69	9	1
3	A	611	PX4	C4-N1-C3	2.48	102.46	108.98	13	2
3	A	650	PX4	O7-C23-C24	2.48	106.11	111.48	1	2
3	A	616	PX4	O1-P1-O2	2.48	123.98	112.44	6	2
3	A	648	PX4	O7-C23-O8	2.48	129.50	123.70	9	1
3	A	651	PX4	O5-C9-O6	2.48	129.83	123.63	5	3
3	B	337	PX4	O5-C9-O6	2.48	129.83	123.63	4	2
3	B	373	PX4	O5-C8-C7	2.48	115.55	108.40	10	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	384	PX4	C12-C11-C10	2.48	122.24	113.13	5	1
3	B	313	PX4	O7-C7-C6	2.48	117.23	108.34	1	2
3	B	321	PX4	O5-C9-C10	2.48	104.28	111.83	4	3
3	B	345	PX4	O7-C7-C6	2.48	117.23	108.34	11	1
3	C	307	PX4	C8-O5-C9	2.48	108.06	117.12	14	1
3	C	309	PX4	O7-C23-O8	2.48	129.50	123.70	5	3
3	B	395	PX4	O7-C23-O8	2.48	129.50	123.70	4	2
3	C	308	PX4	O5-C9-O6	2.48	129.82	123.63	9	3
3	C	320	PX4	O3-P1-O2	2.48	118.75	108.94	3	1
3	A	642	PX4	O7-C23-O8	2.48	129.49	123.70	15	2
3	C	350	PX4	C12-C11-C10	2.48	104.03	113.13	14	3
3	B	356	PX4	O5-C9-C10	2.48	104.29	111.83	5	3
3	A	619	PX4	C5-N1-C4	2.47	102.48	108.98	5	1
3	B	358	PX4	C25-C24-C23	2.48	104.62	113.69	5	1
3	B	394	PX4	C13-C12-C11	2.48	126.88	114.37	4	1
3	B	398	PX4	C5-N1-C3	2.48	102.47	108.98	11	2
3	B	335	PX4	P1-O3-C1	2.47	109.48	121.26	5	2
3	B	380	PX4	C1-C2-N1	2.47	123.76	115.82	9	2
3	C	345	PX4	C15-C14-C13	2.47	101.86	114.37	5	2
3	C	303	PX4	C4-N1-C3	2.47	115.47	108.98	13	1
3	C	324	PX4	C8-O5-C9	2.47	108.08	117.12	14	1
3	C	337	PX4	O7-C7-C6	2.47	99.47	108.34	8	1
3	A	630	PX4	C11-C10-C9	2.47	104.64	113.69	14	1
3	B	328	PX4	C11-C10-C9	2.47	122.75	113.69	8	2
3	B	340	PX4	O5-C9-C10	2.47	104.30	111.83	15	2
3	B	345	PX4	C26-C25-C24	2.47	104.04	113.13	11	2
3	B	363	PX4	O5-C8-C7	2.47	115.52	108.40	14	3
3	C	302	PX4	C5-N1-C3	2.47	115.47	108.98	13	3
3	C	313	PX4	O7-C7-C8	2.47	117.21	108.34	12	2
3	C	321	PX4	O7-C7-C8	2.47	117.21	108.34	12	4
3	C	325	PX4	P1-O3-C1	2.47	133.02	121.26	4	1
3	C	354	PX4	C12-C11-C10	2.47	104.05	113.13	15	1
3	B	309	PX4	O5-C9-C10	2.47	104.31	111.83	4	1
3	B	331	PX4	C11-C10-C9	2.47	122.74	113.69	14	2
3	C	341	PX4	C8-O5-C9	2.47	108.09	117.12	4	2
3	B	324	PX4	C17-C16-C15	2.47	101.89	114.37	13	1
3	B	345	PX4	C8-O5-C9	2.47	108.10	117.12	13	1
3	B	374	PX4	O5-C9-C10	2.47	104.31	111.83	7	1
3	A	618	PX4	C5-N1-C4	2.47	115.45	108.98	15	2
3	A	638	PX4	C5-N1-C4	2.47	102.50	108.98	3	2
3	A	650	PX4	O5-C9-C10	2.47	104.31	111.83	10	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	305	PX4	C5-N1-C4	2.47	102.50	108.98	1	1
3	B	310	PX4	O7-C7-C8	2.47	117.19	108.34	13	1
3	C	301	PX4	C7-O7-C23	2.47	111.89	117.80	8	2
3	B	325	PX4	C25-C24-C23	2.47	122.73	113.69	8	3
3	B	343	PX4	O7-C23-C24	2.47	106.15	111.48	3	2
3	A	648	PX4	P1-O3-C1	2.46	132.99	121.26	15	1
3	B	309	PX4	O7-C7-C8	2.46	117.19	108.34	14	1
3	B	326	PX4	O3-P1-O2	2.46	99.17	108.94	1	1
3	B	333	PX4	C8-C7-C6	2.46	117.53	111.78	7	1
3	B	307	PX4	C1-C2-N1	2.46	123.73	115.82	10	1
3	B	359	PX4	C5-N1-C3	2.46	102.51	108.98	1	1
3	B	375	PX4	O5-C9-C10	2.46	104.33	111.83	7	2
3	B	400	PX4	C8-C7-C6	2.46	117.53	111.78	9	3
3	C	322	PX4	C25-C24-C23	2.46	122.72	113.69	6	1
3	A	617	PX4	C12-C11-C10	2.46	104.08	113.13	1	1
3	A	628	PX4	O5-C9-C10	2.46	104.33	111.83	15	2
3	A	629	PX4	O1-P1-O2	2.46	123.90	112.44	8	1
3	C	354	PX4	C26-C25-C24	2.46	122.18	113.13	15	1
3	B	309	PX4	C5-N1-C3	2.46	102.51	108.98	5	2
3	A	634	PX4	O7-C23-C24	2.46	106.16	111.48	2	1
3	B	379	PX4	P1-O4-C6	2.46	135.45	121.35	9	1
3	B	385	PX4	O3-C1-C2	2.46	121.49	109.65	3	1
3	B	348	PX4	C5-N1-C4	2.46	102.52	108.98	12	2
3	B	362	PX4	C8-C7-C6	2.46	106.05	111.78	6	1
3	B	385	PX4	C16-C15-C14	2.46	101.94	114.37	3	1
3	B	400	PX4	C7-O7-C23	2.46	111.91	117.80	14	2
3	C	322	PX4	C5-N1-C4	2.46	102.52	108.98	1	1
3	A	629	PX4	C8-C7-C6	2.46	106.06	111.78	15	2
3	B	347	PX4	C34-C33-C32	2.46	126.79	114.37	13	1
3	C	323	PX4	C1-C2-N1	2.46	123.71	115.82	7	1
3	C	336	PX4	C25-C24-C23	2.46	104.69	113.69	9	2
3	A	603	PX4	C4-N1-C3	2.46	102.53	108.98	11	2
3	A	602	PX4	C8-C7-C6	2.45	117.51	111.78	9	2
3	A	603	PX4	C12-C11-C10	2.45	104.11	113.13	9	1
3	A	613	PX4	C26-C25-C24	2.45	122.15	113.13	1	1
3	B	390	PX4	C8-C7-C6	2.45	117.51	111.78	5	2
3	B	329	PX4	O7-C23-C24	2.45	106.17	111.48	15	4
3	B	337	PX4	C25-C24-C23	2.45	104.70	113.69	6	2
3	A	604	PX4	O7-C23-O8	2.45	129.44	123.70	1	3
3	A	605	PX4	O7-C7-C6	2.45	117.14	108.34	8	5
3	A	619	PX4	C25-C24-C23	2.45	122.69	113.69	6	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	361	PX4	O7-C23-O8	2.45	129.44	123.70	12	2
3	B	394	PX4	C12-C11-C10	2.45	122.14	113.13	1	2
3	C	330	PX4	C26-C25-C24	2.45	122.14	113.13	14	1
3	C	357	PX4	C26-C25-C24	2.45	104.11	113.13	6	1
3	A	616	PX4	C12-C11-C10	2.45	104.12	113.13	15	1
3	A	621	PX4	C8-C7-C6	2.45	117.50	111.78	6	2
3	A	627	PX4	O7-C23-O8	2.45	129.44	123.70	1	2
3	A	644	PX4	O7-C23-O8	2.45	129.44	123.70	3	4
3	A	641	PX4	C26-C25-C24	2.45	122.13	113.13	12	2
3	B	320	PX4	C1-C2-N1	2.45	123.69	115.82	3	2
3	C	332	PX4	O7-C7-C6	2.45	117.14	108.34	6	2
3	B	329	PX4	C32-C31-C30	2.45	101.98	114.37	5	1
3	B	332	PX4	O6-C9-C10	2.45	133.37	123.78	11	1
3	C	336	PX4	C4-N1-C3	2.45	115.42	108.98	12	2
3	C	344	PX4	O7-C7-C6	2.45	117.14	108.34	5	2
3	C	357	PX4	O7-C7-C6	2.45	117.14	108.34	15	2
3	B	336	PX4	C26-C25-C24	2.45	122.13	113.13	5	2
3	B	371	PX4	O1-P1-O2	2.45	123.85	112.44	6	1
3	C	316	PX4	O5-C9-C10	2.45	104.36	111.83	1	4
3	C	325	PX4	C1-C2-N1	2.45	123.69	115.82	12	1
3	B	354	PX4	O7-C23-O8	2.45	129.43	123.70	9	4
3	A	644	PX4	P1-O3-C1	2.45	132.91	121.26	1	1
3	B	312	PX4	C12-C11-C10	2.45	104.13	113.13	14	1
3	B	340	PX4	O5-C9-O6	2.45	129.75	123.63	15	4
3	B	376	PX4	O5-C9-C10	2.45	104.37	111.83	9	2
3	B	386	PX4	C7-O7-C23	2.45	123.65	117.80	7	2
3	A	610	PX4	O5-C8-C7	2.44	115.44	108.40	9	2
3	C	303	PX4	C8-C7-C6	2.45	106.08	111.78	9	1
3	C	340	PX4	C8-O5-C9	2.44	126.06	117.12	14	1
3	A	610	PX4	C4-N1-C3	2.44	102.56	108.98	11	2
3	A	621	PX4	O5-C9-O6	2.44	129.74	123.63	12	1
3	A	622	PX4	C5-N1-C3	2.44	102.56	108.98	15	2
3	A	643	PX4	C12-C11-C10	2.44	104.15	113.13	14	1
3	A	649	PX4	O5-C9-O6	2.44	129.74	123.63	15	5
3	B	314	PX4	C8-O5-C9	2.44	108.19	117.12	3	1
3	B	348	PX4	C13-C12-C11	2.44	102.02	114.37	7	1
3	C	344	PX4	O7-C23-O8	2.44	129.42	123.70	3	3
3	B	388	PX4	C1-C2-N1	2.44	123.66	115.82	1	2
3	B	392	PX4	O7-C23-O8	2.44	129.41	123.70	12	5
3	B	361	PX4	C3-N1-C2	2.44	100.21	109.91	7	1
3	C	314	PX4	C4-N1-C3	2.44	102.56	108.98	11	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	C	335	PX4	O3-C1-C2	2.44	121.39	109.65	13	1
3	A	608	PX4	O7-C23-O8	2.44	129.41	123.70	11	3
3	A	639	PX4	C3-N1-C2	2.44	100.21	109.91	2	3
3	B	369	PX4	C1-C2-N1	2.44	123.65	115.82	7	1
3	C	346	PX4	O5-C9-O6	2.44	129.73	123.63	7	1
3	B	323	PX4	O5-C9-O6	2.44	129.73	123.63	12	2
3	A	609	PX4	C8-C7-C6	2.44	106.10	111.78	7	1
3	A	626	PX4	O5-C9-O6	2.44	129.72	123.63	2	2
3	B	400	PX4	C4-N1-C3	2.44	115.38	108.98	9	2
3	A	627	PX4	O5-C9-C10	2.44	104.41	111.83	2	1
3	B	315	PX4	C16-C15-C14	2.44	102.06	114.37	6	1
3	B	330	PX4	O7-C23-C24	2.44	106.21	111.48	3	1
3	B	353	PX4	O7-C7-C8	2.44	117.08	108.34	1	1
3	B	353	PX4	C11-C10-C9	2.44	104.77	113.69	14	2
3	C	308	PX4	C8-O5-C9	2.44	108.21	117.12	5	2
3	B	366	PX4	O5-C9-O6	2.43	129.72	123.63	11	1
3	B	372	PX4	C11-C10-C9	2.44	122.62	113.69	11	2
3	B	394	PX4	O7-C23-O8	2.44	129.40	123.70	2	2
3	B	398	PX4	O5-C9-O6	2.44	129.72	123.63	11	2
3	B	346	PX4	C12-C11-C10	2.43	122.07	113.13	5	1
3	C	302	PX4	O7-C23-C24	2.43	106.21	111.48	7	3
3	A	638	PX4	O7-C23-C24	2.43	116.74	111.48	4	2
3	C	323	PX4	C4-N1-C3	2.43	102.58	108.98	14	1
3	B	378	PX4	C8-O5-C9	2.43	108.23	117.12	9	1
3	C	306	PX4	C5-N1-C4	2.43	115.36	108.98	10	1
3	C	328	PX4	C8-C7-C6	2.43	117.46	111.78	5	2
3	A	646	PX4	C12-C11-C10	2.43	104.19	113.13	8	2
3	C	340	PX4	O7-C7-C6	2.43	117.07	108.34	2	1
3	A	615	PX4	O5-C9-O6	2.43	129.71	123.63	3	2
3	B	304	PX4	O5-C8-C7	2.43	115.40	108.40	2	1
3	B	340	PX4	C8-C7-C6	2.43	106.12	111.78	5	4
3	C	346	PX4	C1-C2-N1	2.43	123.63	115.82	7	2
3	B	356	PX4	O7-C7-C8	2.43	117.06	108.34	4	2
3	A	642	PX4	C13-C12-C11	2.43	126.64	114.37	2	1
3	B	350	PX4	C8-O5-C9	2.43	108.24	117.12	8	2
3	B	388	PX4	O5-C9-O6	2.43	129.70	123.63	2	4
3	C	315	PX4	C5-N1-C3	2.43	115.35	108.98	15	2
3	C	338	PX4	C15-C14-C13	2.43	102.09	114.37	10	1
3	A	631	PX4	C25-C24-C23	2.43	104.80	113.69	12	1
3	B	356	PX4	C3-N1-C2	2.43	119.56	109.91	14	1
3	C	343	PX4	O7-C7-C8	2.43	117.05	108.34	4	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	A	620	PX4	C11-C10-C9	2.42	122.58	113.69	7	3
3	C	323	PX4	O5-C9-O6	2.42	129.69	123.63	13	1
3	C	340	PX4	O5-C9-O6	2.42	129.69	123.63	8	1
3	B	312	PX4	O5-C8-C7	2.42	115.38	108.40	15	2
3	B	316	PX4	O5-C9-O6	2.42	129.69	123.63	13	1
3	B	333	PX4	C11-C10-C9	2.42	122.57	113.69	11	2
3	B	333	PX4	C4-N1-C3	2.42	102.61	108.98	6	4
3	C	335	PX4	C4-N1-C3	2.42	102.61	108.98	11	4
3	C	343	PX4	C1-C2-N1	2.42	123.60	115.82	1	1
3	C	358	PX4	O5-C8-C7	2.42	101.41	108.40	12	5
3	B	368	PX4	C7-O7-C23	2.42	112.00	117.80	5	2
3	C	303	PX4	C25-C24-C23	2.42	104.82	113.69	3	1
3	C	344	PX4	C11-C10-C9	2.42	104.83	113.69	12	1
3	A	616	PX4	C11-C10-C9	2.42	104.83	113.69	13	2
3	B	331	PX4	C26-C25-C24	2.42	122.01	113.13	14	1
3	B	332	PX4	O7-C23-O8	2.42	129.36	123.70	4	3
3	B	339	PX4	O7-C7-C6	2.42	117.02	108.34	4	2
3	B	342	PX4	C26-C25-C24	2.42	104.24	113.13	13	1
3	B	395	PX4	C8-C7-C6	2.42	106.14	111.78	11	2
3	A	636	PX4	C12-C11-C10	2.42	122.01	113.13	11	1
3	A	646	PX4	O5-C9-O6	2.42	129.67	123.63	8	1
3	A	618	PX4	C8-O5-C9	2.42	108.29	117.12	6	1
3	B	310	PX4	O5-C8-C7	2.42	115.36	108.40	2	1
3	B	312	PX4	O5-C9-O6	2.42	129.67	123.63	15	1
3	B	356	PX4	O8-C23-C24	2.42	133.23	123.78	7	1
3	B	366	PX4	C7-O7-C23	2.41	112.02	117.80	9	5
3	B	398	PX4	C5-N1-C4	2.42	115.32	108.98	15	1
3	C	302	PX4	C4-N1-C3	2.42	102.63	108.98	2	3
3	C	362	PX4	C11-C10-C9	2.42	122.55	113.69	6	1
3	A	628	PX4	O5-C9-O6	2.41	129.67	123.63	15	1
3	A	646	PX4	C4-N1-C3	2.41	102.63	108.98	10	1
3	B	324	PX4	C4-N1-C3	2.41	102.63	108.98	12	2
3	B	398	PX4	O1-P1-O2	2.41	123.67	112.44	5	1
3	B	309	PX4	P1-O4-C6	2.41	107.53	121.35	14	1
3	B	315	PX4	O4-P1-O2	2.41	99.38	108.94	1	1
3	B	335	PX4	C26-C25-C24	2.41	121.99	113.13	1	2
3	C	341	PX4	C25-C24-C23	2.41	104.86	113.69	13	2
3	B	361	PX4	O5-C9-O6	2.41	129.66	123.63	15	1
3	B	390	PX4	O7-C23-C24	2.41	106.27	111.48	10	1
3	C	304	PX4	C13-C12-C11	2.41	102.19	114.37	5	1
3	C	306	PX4	O5-C9-C10	2.41	104.48	111.83	4	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	C	319	PX4	C8-O5-C9	2.41	108.31	117.12	14	1
3	C	351	PX4	C8-C7-C6	2.41	106.16	111.78	11	1
3	B	311	PX4	O3-P1-O2	2.41	99.38	108.94	5	1
3	B	342	PX4	O7-C7-C6	2.41	116.99	108.34	12	2
3	B	391	PX4	O5-C8-C7	2.41	115.34	108.40	12	3
3	C	320	PX4	C1-C2-N1	2.41	123.56	115.82	6	1
3	A	606	PX4	C5-N1-C4	2.41	115.30	108.98	5	1
3	A	624	PX4	C27-C26-C25	2.41	102.20	114.37	11	1
3	B	315	PX4	C26-C25-C24	2.41	104.28	113.13	10	1
3	B	338	PX4	O7-C23-O8	2.41	129.33	123.70	7	5
3	B	357	PX4	C8-C7-C6	2.41	106.17	111.78	8	2
3	B	373	PX4	C8-O5-C9	2.41	108.32	117.12	2	1
3	C	314	PX4	C1-C2-N1	2.41	123.55	115.82	13	2
3	B	382	PX4	C8-C7-C6	2.41	117.40	111.78	6	2
3	B	395	PX4	C5-N1-C3	2.41	102.65	108.98	7	1
3	C	356	PX4	P1-O3-C1	2.41	132.72	121.26	4	2
3	B	360	PX4	C26-C25-C24	2.41	104.29	113.13	7	1
3	C	336	PX4	O5-C9-O6	2.41	129.64	123.63	4	2
3	C	351	PX4	C12-C11-C10	2.41	104.29	113.13	13	2
3	B	313	PX4	C1-C2-N1	2.40	123.54	115.82	11	3
3	B	374	PX4	C26-C25-C24	2.40	104.30	113.13	2	1
3	B	385	PX4	C1-C2-N1	2.40	123.54	115.82	15	3
3	C	354	PX4	O7-C7-C8	2.40	116.97	108.34	4	1
3	A	622	PX4	O5-C9-C10	2.40	104.51	111.83	6	1
3	A	636	PX4	C26-C25-C24	2.40	121.96	113.13	11	1
3	B	303	PX4	O7-C23-O8	2.40	129.32	123.70	7	2
3	B	347	PX4	O1-P1-O2	2.40	123.62	112.44	14	3
3	B	349	PX4	O7-C7-C8	2.40	116.96	108.34	7	1
3	A	608	PX4	P1-O4-C6	2.40	107.59	121.35	14	1
3	A	619	PX4	O1-P1-O2	2.40	123.61	112.44	11	1
3	A	654	PX4	O5-C9-C10	2.40	104.51	111.83	6	3
3	A	654	PX4	C20-C19-C18	2.40	102.23	114.37	3	1
3	B	390	PX4	C12-C11-C10	2.40	121.95	113.13	4	1
3	C	308	PX4	C5-N1-C2	2.40	119.46	109.91	10	1
3	B	306	PX4	C1-C2-N1	2.40	123.53	115.82	6	1
3	B	322	PX4	O5-C9-C10	2.40	104.51	111.83	1	1
3	B	358	PX4	C5-N1-C4	2.40	115.28	108.98	14	1
3	A	639	PX4	O7-C7-C8	2.40	116.95	108.34	5	4
3	B	314	PX4	C4-N1-C3	2.40	102.67	108.98	15	2
3	B	378	PX4	C26-C25-C24	2.40	104.31	113.13	3	1
3	B	333	PX4	C25-C24-C23	2.40	104.91	113.69	7	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	C	345	PX4	O7-C23-O8	2.40	129.31	123.70	12	1
3	B	377	PX4	C25-C24-C23	2.40	104.91	113.69	10	1
3	A	638	PX4	C5-N1-C2	2.40	119.43	109.91	12	1
3	C	332	PX4	C11-C10-C9	2.40	104.91	113.69	2	1
3	A	630	PX4	C1-C2-N1	2.39	123.51	115.82	10	1
3	B	324	PX4	C27-C26-C25	2.39	102.27	114.37	12	1
3	B	313	PX4	C19-C18-C17	2.39	102.28	114.37	12	1
3	B	325	PX4	C8-C7-C6	2.39	106.20	111.78	12	2
3	C	308	PX4	C12-C11-C10	2.39	121.92	113.13	7	2
3	C	351	PX4	C16-C15-C14	2.39	102.27	114.37	11	1
3	A	609	PX4	O7-C23-C24	2.39	106.31	111.48	12	1
3	A	627	PX4	O7-C7-C8	2.39	116.92	108.34	10	2
3	A	645	PX4	C34-C33-C32	2.39	102.29	114.37	15	1
3	B	315	PX4	O7-C7-C8	2.39	116.92	108.34	3	2
3	B	321	PX4	O7-C7-C6	2.39	116.92	108.34	1	1
3	B	385	PX4	C8-O5-C9	2.39	108.38	117.12	8	1
3	C	311	PX4	C5-N1-C3	2.39	102.70	108.98	5	2
3	C	318	PX4	O7-C7-C8	2.39	116.92	108.34	15	1
3	C	337	PX4	O7-C23-O8	2.39	129.29	123.70	10	2
3	A	611	PX4	O7-C23-O8	2.39	129.29	123.70	2	1
3	A	654	PX4	C25-C24-C23	2.39	104.94	113.69	8	1
3	B	352	PX4	O7-C7-C6	2.39	99.78	108.34	6	1
3	B	367	PX4	O5-C9-C10	2.39	104.56	111.83	14	2
3	B	382	PX4	C11-C10-C9	2.39	122.44	113.69	6	1
3	C	321	PX4	C15-C14-C13	2.39	102.30	114.37	14	1
3	A	618	PX4	O8-C23-C24	2.39	133.11	123.78	4	2
3	A	638	PX4	O3-C1-C2	2.39	121.13	109.65	13	2
3	B	326	PX4	C8-O5-C9	2.39	108.40	117.12	3	3
3	C	328	PX4	O7-C23-O8	2.39	129.28	123.70	1	2
3	A	645	PX4	O7-C7-C6	2.38	116.90	108.34	8	1
3	B	350	PX4	O7-C23-O8	2.39	129.28	123.70	2	2
3	B	378	PX4	O5-C9-O6	2.39	129.59	123.63	1	2
3	C	333	PX4	O1-P1-O2	2.38	123.54	112.44	1	1
3	C	338	PX4	C8-C7-C6	2.39	106.22	111.78	9	2
3	B	342	PX4	C5-N1-C4	2.38	102.71	108.98	10	3
3	C	347	PX4	O7-C7-C8	2.38	116.90	108.34	1	1
3	C	356	PX4	C25-C24-C23	2.38	104.95	113.69	8	1
3	B	349	PX4	C1-C2-N1	2.38	123.47	115.82	8	2
3	B	351	PX4	O7-C7-C8	2.38	116.89	108.34	10	1
3	B	370	PX4	O1-P1-O2	2.38	123.53	112.44	11	1
3	A	617	PX4	O5-C9-O6	2.38	129.59	123.63	1	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	383	PX4	O3-C1-C2	2.38	121.11	109.65	1	1
3	B	385	PX4	O8-C23-C24	2.38	133.10	123.78	5	1
3	C	316	PX4	O7-C7-C6	2.38	116.89	108.34	8	1
3	C	349	PX4	C25-C24-C23	2.38	104.97	113.69	13	1
3	A	627	PX4	C11-C10-C9	2.38	122.42	113.69	6	1
3	A	649	PX4	C20-C19-C18	2.38	102.33	114.37	8	1
3	A	650	PX4	C4-N1-C3	2.38	115.23	108.98	1	4
3	B	313	PX4	C14-C13-C12	2.38	102.34	114.37	14	1
3	B	325	PX4	C8-O5-C9	2.38	108.42	117.12	8	1
3	B	397	PX4	O5-C9-O6	2.38	129.58	123.63	5	2
3	C	361	PX4	C4-N1-C2	2.38	119.37	109.91	4	1
3	A	617	PX4	C4-N1-C3	2.38	102.73	108.98	2	3
3	B	326	PX4	O1-P1-O2	2.38	123.50	112.44	2	1
3	B	332	PX4	C25-C24-C23	2.38	104.98	113.69	15	1
3	C	362	PX4	C26-C25-C24	2.38	121.87	113.13	11	2
3	A	602	PX4	O7-C23-O8	2.38	129.26	123.70	9	2
3	B	349	PX4	O5-C9-C10	2.38	104.59	111.83	4	3
3	B	370	PX4	C4-N1-C3	2.38	115.22	108.98	13	1
3	B	386	PX4	O7-C23-O8	2.38	129.26	123.70	7	1
3	B	397	PX4	O5-C9-C10	2.38	104.59	111.83	14	1
3	C	333	PX4	C5-N1-C3	2.38	102.73	108.98	9	1
3	B	352	PX4	O1-P1-O2	2.37	123.49	112.44	1	2
3	A	624	PX4	C5-N1-C4	2.37	102.74	108.98	1	1
3	A	641	PX4	O7-C7-C8	2.37	116.86	108.34	6	3
3	A	644	PX4	O5-C9-C10	2.37	104.60	111.83	13	1
3	C	331	PX4	C34-C33-C32	2.37	102.36	114.37	15	2
3	A	650	PX4	C5-N1-C4	2.37	102.74	108.98	1	2
3	B	307	PX4	O5-C9-C10	2.37	104.60	111.83	11	3
3	B	384	PX4	C32-C31-C30	2.37	102.37	114.37	9	1
3	C	327	PX4	O5-C9-C10	2.37	104.60	111.83	14	2
3	C	363	PX4	O6-C9-C10	2.37	133.06	123.78	15	1
3	A	603	PX4	C15-C14-C13	2.37	102.38	114.37	2	1
3	B	303	PX4	O5-C8-C7	2.37	115.23	108.40	9	3
3	B	312	PX4	O7-C23-O8	2.37	129.25	123.70	10	3
3	B	325	PX4	C4-N1-C3	2.37	115.21	108.98	12	1
3	C	353	PX4	C8-C7-C6	2.37	106.26	111.78	12	2
3	C	315	PX4	C5-N1-C2	2.37	100.49	109.91	1	1
3	C	339	PX4	C25-C24-C23	2.37	122.38	113.69	9	1
3	C	364	PX4	C1-C2-N1	2.37	123.43	115.82	15	1
3	A	628	PX4	O7-C7-C8	2.37	116.83	108.34	11	1
3	B	385	PX4	C28-C27-C26	2.37	102.40	114.37	11	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	314	PX4	O5-C9-O6	2.37	129.55	123.63	8	1
3	B	320	PX4	C4-N1-C3	2.37	115.19	108.98	4	2
3	B	332	PX4	C8-O5-C9	2.37	108.47	117.12	11	1
3	B	399	PX4	C4-N1-C3	2.37	102.76	108.98	11	1
3	C	317	PX4	O5-C9-C10	2.37	119.05	111.83	4	3
3	C	329	PX4	C5-N1-C2	2.37	119.32	109.91	5	1
3	B	364	PX4	O3-P1-O2	2.36	118.31	108.94	4	1
3	C	341	PX4	C26-C25-C24	2.37	104.44	113.13	15	1
3	C	355	PX4	O6-C9-C10	2.37	133.03	123.78	11	1
3	B	392	PX4	O7-C7-C8	2.36	116.83	108.34	7	1
3	B	365	PX4	O5-C9-O6	2.36	129.54	123.63	4	1
3	B	394	PX4	C3-N1-C2	2.36	119.31	109.91	12	2
3	A	628	PX4	C8-C7-C6	2.36	117.29	111.78	10	3
3	B	308	PX4	C1-C2-N1	2.36	123.40	115.82	11	2
3	C	346	PX4	O7-C7-C8	2.36	116.82	108.34	7	3
3	B	320	PX4	O6-C9-C10	2.36	133.02	123.78	1	1
3	C	332	PX4	C4-N1-C3	2.36	115.18	108.98	9	2
3	B	308	PX4	C5-N1-C3	2.36	102.78	108.98	3	1
3	C	309	PX4	C26-C25-C24	2.36	104.46	113.13	15	1
3	C	315	PX4	O7-C7-C8	2.36	116.80	108.34	13	2
3	A	621	PX4	O5-C9-C10	2.35	104.66	111.83	14	1
3	A	623	PX4	O5-C9-C10	2.35	104.66	111.83	6	3
3	A	645	PX4	O1-P1-O2	2.35	123.40	112.44	10	1
3	C	319	PX4	C1-C2-N1	2.36	123.38	115.82	1	2
3	B	331	PX4	O7-C23-O8	2.35	129.21	123.70	5	2
3	B	379	PX4	C4-N1-C3	2.35	115.16	108.98	5	2
3	C	321	PX4	O5-C9-O6	2.35	129.52	123.63	8	2
3	C	359	PX4	O7-C23-O8	2.35	129.21	123.70	15	2
3	C	359	PX4	C11-C10-C9	2.35	122.32	113.69	9	2
3	B	347	PX4	C5-N1-C4	2.35	102.80	108.98	9	1
3	B	381	PX4	C5-N1-C4	2.35	115.15	108.98	7	1
3	A	639	PX4	C26-C25-C24	2.35	121.76	113.13	5	2
3	B	361	PX4	C5-N1-C3	2.35	102.80	108.98	4	3
3	B	379	PX4	C12-C11-C10	2.35	104.49	113.13	8	1
3	B	360	PX4	C4-N1-C3	2.35	115.15	108.98	6	3
3	B	371	PX4	O5-C9-O6	2.35	129.51	123.63	14	2
3	B	371	PX4	C25-C24-C23	2.35	122.30	113.69	9	1
3	C	311	PX4	C31-C30-C29	2.35	102.49	114.37	5	2
3	A	614	PX4	O5-C9-C10	2.35	104.68	111.83	4	3
3	A	617	PX4	O7-C23-O8	2.35	129.19	123.70	14	2
3	A	625	PX4	O5-C9-O6	2.35	129.50	123.63	4	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	327	PX4	C4-N1-C2	2.35	119.24	109.91	14	1
3	B	351	PX4	C1-C2-N1	2.35	123.36	115.82	7	2
3	B	397	PX4	C19-C18-C17	2.35	102.50	114.37	6	1
3	C	314	PX4	O7-C23-O8	2.35	129.20	123.70	12	2
3	C	326	PX4	O7-C7-C8	2.35	116.77	108.34	5	2
3	B	391	PX4	O3-P1-O2	2.35	99.64	108.94	5	1
3	C	310	PX4	C8-O5-C9	2.35	108.54	117.12	10	1
3	C	347	PX4	O5-C9-O6	2.35	129.50	123.63	13	3
3	A	628	PX4	C5-N1-C4	2.35	102.81	108.98	14	2
3	C	332	PX4	C32-C31-C30	2.35	102.51	114.37	8	1
3	A	651	PX4	C5-N1-C4	2.34	102.82	108.98	14	4
3	B	343	PX4	C8-C7-C6	2.34	106.32	111.78	11	1
3	C	349	PX4	C1-C2-N1	2.34	123.35	115.82	15	1
3	C	355	PX4	O7-C23-O8	2.34	129.19	123.70	4	1
3	B	304	PX4	C11-C10-C9	2.34	122.28	113.69	9	2
3	B	318	PX4	C5-N1-C4	2.34	115.13	108.98	15	3
3	B	320	PX4	O8-C23-C24	2.34	132.94	123.78	6	1
3	B	376	PX4	C8-C7-C6	2.34	117.25	111.78	13	1
3	B	377	PX4	O7-C7-C8	2.34	116.74	108.34	8	1
3	C	310	PX4	C4-N1-C3	2.34	115.13	108.98	15	3
3	C	328	PX4	O5-C9-C10	2.34	104.69	111.83	11	3
3	C	330	PX4	C25-C24-C23	2.34	122.28	113.69	3	1
3	C	331	PX4	C4-N1-C2	2.34	119.22	109.91	3	1
3	B	324	PX4	C8-C7-C6	2.34	117.25	111.78	15	3
3	C	338	PX4	O5-C9-O6	2.34	129.49	123.63	4	3
3	B	318	PX4	C11-C10-C9	2.34	122.27	113.69	4	1
3	C	338	PX4	O3-C1-C2	2.34	120.91	109.65	14	2
3	A	620	PX4	C8-C7-C6	2.34	106.33	111.78	13	1
3	B	368	PX4	O7-C7-C6	2.34	99.96	108.34	14	1
3	B	399	PX4	O7-C7-C6	2.34	99.96	108.34	6	2
3	C	326	PX4	C19-C18-C17	2.34	126.19	114.37	12	1
3	A	601	PX4	C4-N1-C3	2.34	115.11	108.98	2	1
3	A	604	PX4	C4-N1-C2	2.34	119.20	109.91	15	1
3	B	316	PX4	C5-N1-C4	2.34	115.11	108.98	6	2
3	B	346	PX4	O5-C9-O6	2.34	129.47	123.63	12	2
3	C	301	PX4	C5-N1-C3	2.34	102.84	108.98	13	1
3	C	313	PX4	C12-C11-C10	2.34	121.72	113.13	8	2
3	C	352	PX4	C18-C17-C16	2.34	102.55	114.37	13	1
3	C	353	PX4	C5-N1-C2	2.34	119.20	109.91	9	1
3	A	622	PX4	O7-C7-C6	2.33	116.72	108.34	6	1
3	A	627	PX4	P1-O3-C1	2.34	110.14	121.26	13	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	A	629	PX4	O5-C9-C10	2.34	104.71	111.83	2	1
3	A	638	PX4	C8-C7-C6	2.33	117.23	111.78	13	2
3	B	348	PX4	O7-C23-O8	2.34	129.16	123.70	12	3
3	B	360	PX4	C25-C24-C23	2.34	105.14	113.69	14	1
3	C	318	PX4	O1-P1-O2	2.34	123.31	112.44	4	2
3	B	395	PX4	C11-C10-C9	2.34	105.14	113.69	11	1
3	C	319	PX4	P1-O3-C1	2.33	132.38	121.26	9	1
3	A	639	PX4	C4-N1-C3	2.33	102.85	108.98	1	1
3	B	302	PX4	C8-C7-C6	2.33	106.34	111.78	10	3
3	B	321	PX4	O7-C7-C8	2.33	116.71	108.34	3	3
3	B	371	PX4	C5-N1-C4	2.33	102.85	108.98	11	2
3	C	312	PX4	P1-O3-C1	2.33	132.37	121.26	12	1
3	C	321	PX4	C5-N1-C3	2.33	115.11	108.98	11	2
3	C	349	PX4	O4-P1-O2	2.33	99.68	108.94	7	1
3	A	629	PX4	C4-N1-C2	2.33	119.18	109.91	12	1
3	A	647	PX4	O7-C7-C8	2.33	116.71	108.34	7	2
3	B	355	PX4	O5-C9-C10	2.33	104.72	111.83	5	1
3	B	356	PX4	C25-C24-C23	2.33	122.24	113.69	5	2
3	B	358	PX4	C8-C7-C6	2.33	106.35	111.78	11	3
3	C	343	PX4	O7-C23-C24	2.33	106.44	111.48	10	2
3	A	631	PX4	C8-O5-C9	2.33	108.60	117.12	3	1
3	A	635	PX4	O7-C7-C6	2.33	99.98	108.34	3	2
3	B	319	PX4	C12-C11-C10	2.33	121.69	113.13	4	1
3	B	337	PX4	C26-C25-C24	2.33	104.56	113.13	8	1
3	C	346	PX4	C4-N1-C3	2.33	115.10	108.98	12	2
3	C	309	PX4	O1-P1-O2	2.33	123.28	112.44	12	1
3	C	348	PX4	C8-C7-C6	2.33	106.35	111.78	15	2
3	A	621	PX4	O3-C1-C2	2.33	120.85	109.65	14	1
3	B	307	PX4	C5-N1-C3	2.33	115.09	108.98	5	1
3	A	627	PX4	C28-C27-C26	2.33	102.61	114.37	3	1
3	A	643	PX4	O5-C9-C10	2.33	104.74	111.83	1	2
3	B	371	PX4	O1-P1-O4	2.33	118.11	107.57	9	1
3	C	324	PX4	C26-C25-C24	2.33	104.58	113.13	15	1
3	C	328	PX4	C29-C28-C27	2.33	102.60	114.37	7	1
3	B	302	PX4	O1-P1-O2	2.33	123.26	112.44	13	1
3	B	381	PX4	C26-C25-C24	2.33	104.58	113.13	8	1
3	B	391	PX4	O6-C9-C10	2.33	132.88	123.78	7	1
3	A	628	PX4	C12-C11-C10	2.32	121.66	113.13	1	1
3	B	315	PX4	C1-C2-N1	2.32	123.28	115.82	1	2
3	C	358	PX4	C4-N1-C3	2.32	115.08	108.98	8	1
3	B	355	PX4	O7-C23-O8	2.32	129.14	123.70	4	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	A	644	PX4	O7-C7-C6	2.32	116.67	108.34	5	1
3	A	646	PX4	C13-C12-C11	2.32	102.63	114.37	8	1
3	B	376	PX4	O7-C7-C6	2.32	116.68	108.34	2	2
3	B	390	PX4	C5-N1-C4	2.32	102.87	108.98	11	2
3	C	317	PX4	C4-N1-C3	2.32	102.87	108.98	14	1
3	A	653	PX4	C5-N1-C3	2.32	102.88	108.98	6	1
3	B	315	PX4	O5-C9-O6	2.32	129.44	123.63	10	1
3	C	320	PX4	C12-C11-C10	2.32	104.60	113.13	5	1
3	C	322	PX4	O1-P1-O3	2.32	118.09	107.57	10	1
3	A	602	PX4	O7-C7-C8	2.32	116.67	108.34	8	1
3	C	356	PX4	P1-O4-C6	2.32	134.65	121.35	2	2
3	A	620	PX4	O7-C7-C6	2.32	116.66	108.34	9	2
3	A	628	PX4	C5-N1-C3	2.32	115.07	108.98	6	2
3	B	357	PX4	O5-C9-C10	2.32	104.76	111.83	11	2
3	A	623	PX4	O5-C9-O6	2.32	129.43	123.63	14	1
3	B	319	PX4	O4-P1-O2	2.32	118.12	108.94	10	2
3	B	317	PX4	C5-N1-C3	2.32	115.06	108.98	13	1
3	C	316	PX4	O5-C9-O6	2.32	129.43	123.63	3	2
3	C	329	PX4	C5-N1-C4	2.32	102.89	108.98	14	1
3	C	353	PX4	O5-C9-C10	2.32	104.77	111.83	4	1
3	A	632	PX4	O7-C23-C24	2.32	106.47	111.48	5	2
3	B	363	PX4	C26-C25-C24	2.32	121.64	113.13	7	2
3	B	395	PX4	C12-C11-C10	2.31	104.62	113.13	15	1
3	C	324	PX4	C11-C10-C9	2.32	105.21	113.69	7	1
3	C	337	PX4	C1-C2-N1	2.32	123.25	115.82	7	2
3	B	302	PX4	C5-N1-C4	2.31	102.90	108.98	7	1
3	B	360	PX4	C4-N1-C2	2.31	119.11	109.91	7	1
3	B	376	PX4	O5-C9-O6	2.31	129.41	123.63	15	2
3	B	380	PX4	C5-N1-C4	2.31	102.90	108.98	13	1
3	B	396	PX4	C11-C10-C9	2.31	105.22	113.69	7	1
3	A	620	PX4	C7-O7-C23	2.31	112.26	117.80	7	3
3	B	301	PX4	C12-C11-C10	2.31	104.63	113.13	4	1
3	B	326	PX4	O8-C23-C24	2.31	132.82	123.78	14	1
3	B	347	PX4	C8-C7-C6	2.31	106.39	111.78	4	1
3	C	331	PX4	O7-C7-C6	2.31	116.64	108.34	5	2
3	B	337	PX4	C4-N1-C3	2.31	115.04	108.98	4	1
3	B	351	PX4	C31-C30-C29	2.31	126.05	114.37	11	1
3	B	396	PX4	O4-P1-O2	2.31	118.09	108.94	5	1
3	C	317	PX4	C12-C11-C10	2.31	104.64	113.13	3	1
3	C	320	PX4	O8-C23-C24	2.31	132.82	123.78	14	1
3	C	336	PX4	C12-C11-C10	2.31	104.64	113.13	4	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	A	630	PX4	C13-C12-C11	2.31	102.70	114.37	12	1
3	B	361	PX4	C4-N1-C3	2.31	102.91	108.98	5	1
3	B	367	PX4	C11-C10-C9	2.31	122.15	113.69	10	2
3	B	376	PX4	C1-C2-N1	2.31	123.23	115.82	4	2
3	B	384	PX4	O3-C1-C2	2.31	120.76	109.65	4	1
3	C	343	PX4	O7-C23-O8	2.31	129.10	123.70	3	3
3	A	625	PX4	O7-C7-C8	2.31	116.62	108.34	6	2
3	A	639	PX4	O5-C9-C10	2.31	104.80	111.83	12	1
3	C	325	PX4	O7-C7-C6	2.31	116.62	108.34	14	1
3	C	336	PX4	C8-O5-C9	2.31	108.68	117.12	9	1
3	A	609	PX4	C12-C11-C10	2.31	104.65	113.13	3	1
3	B	320	PX4	C12-C11-C10	2.31	121.60	113.13	9	1
3	B	333	PX4	C3-N1-C2	2.31	119.08	109.91	4	1
3	B	379	PX4	O5-C9-O6	2.31	129.40	123.63	8	1
3	C	338	PX4	C1-C2-N1	2.31	123.23	115.82	9	1
3	C	321	PX4	O7-C23-O8	2.31	129.09	123.70	5	2
3	C	333	PX4	O8-C23-C24	2.31	132.80	123.78	14	1
3	C	345	PX4	C12-C11-C10	2.31	104.66	113.13	2	1
3	C	349	PX4	C12-C11-C10	2.30	121.59	113.13	11	1
3	B	381	PX4	C8-C7-C6	2.30	106.41	111.78	14	1
3	B	369	PX4	O1-P1-O4	2.30	97.13	107.57	9	2
3	C	342	PX4	C11-C10-C9	2.30	105.25	113.69	15	1
3	B	324	PX4	O3-C1-C2	2.30	120.73	109.65	8	1
3	A	631	PX4	C4-N1-C3	2.30	115.02	108.98	3	1
3	A	646	PX4	C8-C7-C6	2.30	117.15	111.78	8	2
3	A	648	PX4	O7-C23-C24	2.30	106.50	111.48	6	2
3	B	400	PX4	C1-C2-N1	2.30	123.21	115.82	3	1
3	C	326	PX4	C33-C32-C31	2.30	126.00	114.37	3	1
3	C	361	PX4	O7-C7-C6	2.30	116.60	108.34	2	1
3	A	653	PX4	C1-C2-N1	2.30	123.20	115.82	4	2
3	B	331	PX4	P1-O4-C6	2.30	134.53	121.35	11	1
3	C	304	PX4	O1-P1-O3	2.30	118.00	107.57	13	2
3	B	326	PX4	C34-C33-C32	2.30	125.99	114.37	11	1
3	C	315	PX4	O1-P1-O3	2.30	117.99	107.57	1	1
3	C	342	PX4	C8-O5-C9	2.30	108.71	117.12	9	1
3	B	380	PX4	C20-C19-C18	2.30	102.75	114.37	8	1
3	B	303	PX4	C12-C11-C10	2.30	121.57	113.13	12	1
3	B	400	PX4	C25-C24-C23	2.30	105.27	113.69	13	1
3	B	343	PX4	C4-N1-C3	2.30	115.01	108.98	12	2
3	B	352	PX4	C26-C25-C24	2.30	104.69	113.13	3	1
3	B	389	PX4	C4-N1-C3	2.30	102.94	108.98	15	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	C	342	PX4	C8-C7-C6	2.30	106.43	111.78	11	1
3	C	344	PX4	C4-N1-C2	2.30	119.03	109.91	12	1
3	C	357	PX4	C8-C7-C6	2.30	117.14	111.78	9	2
3	A	626	PX4	C1-C2-N1	2.30	123.19	115.82	13	1
3	B	376	PX4	O5-C8-C7	2.29	115.01	108.40	11	3
3	B	377	PX4	C4-N1-C3	2.29	102.95	108.98	11	3
3	C	307	PX4	O5-C9-C10	2.29	104.84	111.83	15	1
3	C	319	PX4	O7-C7-C6	2.29	116.58	108.34	1	1
3	C	325	PX4	C8-O5-C9	2.29	108.73	117.12	7	2
3	C	355	PX4	O7-C7-C6	2.29	116.58	108.34	4	1
3	A	624	PX4	O5-C8-C7	2.29	115.01	108.40	10	2
3	A	640	PX4	O1-P1-O2	2.29	123.11	112.44	2	1
3	B	346	PX4	O1-P1-O4	2.29	117.96	107.57	8	1
3	C	306	PX4	C17-C16-C15	2.29	102.78	114.37	11	1
3	C	319	PX4	O7-C23-C24	2.29	106.53	111.48	4	2
3	C	331	PX4	C3-N1-C2	2.29	119.02	109.91	4	1
3	C	334	PX4	C5-N1-C2	2.29	119.02	109.91	3	1
3	C	345	PX4	O5-C9-C10	2.29	104.85	111.83	9	1
3	B	325	PX4	O7-C7-C8	2.29	116.56	108.34	9	1
3	B	339	PX4	C5-N1-C4	2.29	102.96	108.98	11	1
3	B	342	PX4	C30-C29-C28	2.29	102.79	114.37	7	1
3	B	344	PX4	C25-C24-C23	2.29	122.09	113.69	5	1
3	B	362	PX4	O5-C9-O6	2.29	129.36	123.63	7	2
3	B	381	PX4	C5-N1-C3	2.29	102.96	108.98	2	2
3	B	393	PX4	C4-N1-C3	2.29	102.96	108.98	2	2
3	C	333	PX4	C26-C25-C24	2.29	121.54	113.13	7	2
3	C	356	PX4	C4-N1-C3	2.29	114.99	108.98	12	1
3	A	612	PX4	O5-C9-C10	2.29	104.86	111.83	11	2
3	A	652	PX4	C19-C18-C17	2.29	102.80	114.37	8	1
3	C	355	PX4	C26-C25-C24	2.29	121.53	113.13	14	1
3	C	357	PX4	O5-C9-C10	2.29	104.86	111.83	4	2
3	A	634	PX4	O1-P1-O2	2.29	123.09	112.44	14	1
3	B	380	PX4	O5-C9-O6	2.29	129.35	123.63	5	3
3	A	613	PX4	O5-C9-O6	2.29	129.35	123.63	7	1
3	A	617	PX4	C33-C32-C31	2.29	102.81	114.37	13	1
3	A	644	PX4	C8-O5-C9	2.29	125.47	117.12	10	1
3	B	303	PX4	C5-N1-C3	2.29	102.97	108.98	6	2
3	B	392	PX4	O5-C9-O6	2.29	129.34	123.63	15	1
3	C	310	PX4	O3-C1-C2	2.29	120.65	109.65	7	1
3	C	342	PX4	C5-N1-C3	2.29	102.97	108.98	5	4
3	B	325	PX4	C5-N1-C3	2.28	102.98	108.98	8	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	340	PX4	C11-C10-C9	2.28	122.06	113.69	4	1
3	C	331	PX4	C26-C25-C24	2.28	104.73	113.13	12	1
3	C	315	PX4	P1-O3-C1	2.28	132.13	121.26	6	1
3	C	364	PX4	C5-N1-C4	2.28	102.98	108.98	3	1
3	A	640	PX4	C16-C15-C14	2.28	102.84	114.37	4	1
3	B	315	PX4	C11-C10-C9	2.28	122.05	113.69	2	1
3	B	368	PX4	O1-P1-O2	2.28	123.06	112.44	1	1
3	B	376	PX4	C5-N1-C2	2.28	118.98	109.91	7	1
3	C	316	PX4	P1-O3-C1	2.28	110.40	121.26	4	2
3	A	632	PX4	C5-N1-C3	2.28	114.96	108.98	11	1
3	A	634	PX4	C26-C25-C24	2.28	104.75	113.13	1	1
3	A	644	PX4	O6-C9-C10	2.28	132.70	123.78	13	1
3	A	645	PX4	O5-C9-O6	2.28	129.33	123.63	11	2
3	B	331	PX4	C8-C7-C6	2.28	106.47	111.78	1	1
3	B	357	PX4	O7-C23-O8	2.28	129.04	123.70	11	3
3	B	338	PX4	O5-C9-C10	2.28	118.78	111.83	1	1
3	B	338	PX4	C7-O7-C23	2.28	112.34	117.80	12	3
3	B	366	PX4	O5-C9-C10	2.28	104.89	111.83	11	1
3	B	372	PX4	C8-C7-C6	2.28	106.47	111.78	4	3
3	C	331	PX4	C12-C11-C10	2.28	104.75	113.13	7	1
3	B	301	PX4	C25-C24-C23	2.28	122.04	113.69	2	1
3	B	363	PX4	O3-C1-C2	2.28	120.61	109.65	10	1
3	C	314	PX4	C26-C25-C24	2.28	104.76	113.13	2	1
3	C	314	PX4	C25-C24-C23	2.28	122.04	113.69	13	1
3	B	322	PX4	C12-C11-C10	2.28	104.76	113.13	13	1
3	A	623	PX4	P1-O4-C6	2.28	108.31	121.35	15	1
3	B	334	PX4	C4-N1-C3	2.28	103.00	108.98	2	1
3	C	361	PX4	C12-C11-C10	2.28	121.49	113.13	5	1
3	A	631	PX4	C3-N1-C2	2.27	100.87	109.91	8	1
3	A	633	PX4	O7-C7-C8	2.27	116.50	108.34	2	2
3	A	633	PX4	O7-C23-O8	2.28	129.02	123.70	10	2
3	B	350	PX4	C29-C28-C27	2.27	102.87	114.37	8	1
3	C	302	PX4	C5-N1-C4	2.27	103.00	108.98	13	2
3	C	322	PX4	C4-N1-C3	2.27	114.95	108.98	13	2
3	C	327	PX4	C4-N1-C2	2.28	118.95	109.91	10	1
3	C	339	PX4	C11-C10-C9	2.28	105.36	113.69	1	1
3	A	619	PX4	O4-P1-O2	2.27	117.94	108.94	15	1
3	A	642	PX4	C1-C2-N1	2.27	123.12	115.82	1	1
3	B	309	PX4	O5-C8-C7	2.27	114.95	108.40	10	2
3	C	333	PX4	O5-C9-C10	2.27	104.90	111.83	4	1
3	B	384	PX4	C5-N1-C4	2.27	114.95	108.98	3	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	C	326	PX4	P1-O4-C6	2.27	108.33	121.35	3	1
3	A	633	PX4	C8-O5-C9	2.27	108.82	117.12	3	1
3	B	397	PX4	C4-N1-C3	2.27	114.94	108.98	10	1
3	C	340	PX4	P1-O3-C1	2.27	110.44	121.26	12	2
3	A	606	PX4	C25-C24-C23	2.27	122.01	113.69	11	1
3	B	324	PX4	C5-N1-C4	2.27	103.01	108.98	15	2
3	A	646	PX4	C25-C24-C23	2.27	105.38	113.69	5	2
3	A	649	PX4	C5-N1-C4	2.27	114.94	108.98	1	1
3	B	308	PX4	C29-C28-C27	2.27	102.90	114.37	2	1
3	B	316	PX4	C4-N1-C3	2.27	103.01	108.98	6	2
3	B	317	PX4	C8-O5-C9	2.27	108.82	117.12	11	2
3	A	651	PX4	C29-C28-C27	2.27	102.91	114.37	2	1
3	B	307	PX4	C4-N1-C3	2.27	103.02	108.98	9	1
3	C	326	PX4	P1-O3-C1	2.27	132.06	121.26	14	1
3	B	314	PX4	C32-C31-C30	2.27	102.91	114.37	5	1
3	B	350	PX4	C12-C11-C10	2.27	104.80	113.13	5	2
3	B	379	PX4	C5-N1-C4	2.27	103.02	108.98	7	1
3	C	344	PX4	O5-C9-C10	2.27	104.92	111.83	7	3
3	A	642	PX4	C4-N1-C2	2.27	118.91	109.91	3	1
3	C	316	PX4	O6-C9-C10	2.27	132.64	123.78	1	1
3	B	307	PX4	O1-P1-O2	2.26	122.97	112.44	10	2
3	B	331	PX4	C5-N1-C2	2.26	118.91	109.91	6	1
3	C	332	PX4	C31-C30-C29	2.26	102.92	114.37	7	1
3	C	337	PX4	C13-C12-C11	2.26	102.92	114.37	11	1
3	A	627	PX4	C33-C32-C31	2.26	102.93	114.37	14	1
3	A	640	PX4	C25-C24-C23	2.26	105.40	113.69	11	1
3	B	382	PX4	C1-C2-N1	2.26	123.08	115.82	8	3
3	B	392	PX4	C5-N1-C3	2.26	103.03	108.98	5	1
3	B	313	PX4	C12-C11-C10	2.26	104.82	113.13	3	1
3	B	391	PX4	O7-C7-C6	2.26	116.46	108.34	2	1
3	B	399	PX4	C32-C31-C30	2.26	102.93	114.37	3	1
3	C	334	PX4	C7-O7-C23	2.26	112.38	117.80	9	2
3	C	346	PX4	C26-C25-C24	2.26	121.44	113.13	15	1
3	C	360	PX4	C25-C24-C23	2.26	105.41	113.69	2	1
3	A	617	PX4	C11-C10-C9	2.26	105.42	113.69	11	2
3	A	647	PX4	C4-N1-C3	2.26	103.04	108.98	6	1
3	A	624	PX4	O3-P1-O2	2.26	99.98	108.94	5	1
3	B	308	PX4	C11-C10-C9	2.26	121.97	113.69	8	1
3	B	362	PX4	O7-C7-C8	2.26	116.45	108.34	12	1
3	B	389	PX4	C5-N1-C3	2.26	103.04	108.98	2	2
3	B	361	PX4	O3-P1-O2	2.26	117.88	108.94	8	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	C	317	PX4	C25-C24-C23	2.26	105.42	113.69	11	2
3	C	322	PX4	O7-C7-C8	2.26	116.45	108.34	3	1
3	C	351	PX4	O7-C7-C8	2.26	116.45	108.34	4	3
3	A	641	PX4	C8-C7-C6	2.26	106.52	111.78	14	1
3	C	330	PX4	C12-C11-C10	2.26	104.83	113.13	14	1
3	C	358	PX4	O6-C9-C10	2.26	132.62	123.78	4	1
3	B	396	PX4	C1-C2-N1	2.26	123.07	115.82	5	1
3	C	361	PX4	C33-C32-C31	2.26	102.95	114.37	4	1
3	C	335	PX4	O1-P1-O2	2.26	122.94	112.44	2	3
3	C	347	PX4	C1-C2-N1	2.26	123.06	115.82	3	2
3	B	319	PX4	C3-N1-C2	2.26	118.88	109.91	7	1
3	B	366	PX4	O7-C23-C24	2.25	106.60	111.48	1	2
3	B	378	PX4	O1-P1-O2	2.25	122.93	112.44	15	1
3	C	339	PX4	O5-C9-O6	2.25	117.99	123.63	6	1
3	C	350	PX4	O8-C23-C24	2.26	114.96	123.78	7	1
3	A	610	PX4	C8-C7-C6	2.25	106.53	111.78	12	1
3	A	613	PX4	O1-P1-O2	2.25	122.92	112.44	5	1
3	A	614	PX4	C8-O5-C9	2.25	108.88	117.12	10	1
3	A	627	PX4	C5-N1-C3	2.25	103.06	108.98	13	1
3	A	631	PX4	C12-C11-C10	2.25	104.85	113.13	14	1
3	A	648	PX4	C26-C25-C24	2.25	104.85	113.13	3	1
3	B	332	PX4	O3-C1-C2	2.25	120.49	109.65	5	2
3	B	343	PX4	C19-C18-C17	2.25	102.97	114.37	5	1
3	C	308	PX4	C5-N1-C4	2.25	103.05	108.98	10	4
3	B	383	PX4	C5-N1-C3	2.25	103.06	108.98	9	2
3	B	341	PX4	P1-O3-C1	2.25	131.98	121.26	13	1
3	C	315	PX4	C8-C7-C6	2.25	106.53	111.78	12	1
3	C	321	PX4	C12-C11-C10	2.25	121.40	113.13	9	1
3	C	331	PX4	O7-C23-O8	2.25	128.97	123.70	14	2
3	B	372	PX4	C13-C12-C11	2.25	102.99	114.37	1	1
3	C	345	PX4	C8-O5-C9	2.25	108.89	117.12	9	1
3	A	605	PX4	O5-C9-O6	2.25	129.26	123.63	5	2
3	A	653	PX4	C5-N1-C4	2.25	103.06	108.98	13	1
3	B	379	PX4	C1-C2-N1	2.25	123.05	115.82	9	2
3	C	319	PX4	C25-C24-C23	2.25	105.45	113.69	5	1
3	C	361	PX4	C18-C17-C16	2.25	102.99	114.37	6	1
3	A	623	PX4	O1-P1-O2	2.25	122.91	112.44	13	1
3	A	640	PX4	O5-C9-O6	2.25	129.25	123.63	8	1
3	B	359	PX4	O1-P1-O2	2.25	122.91	112.44	3	1
3	A	643	PX4	C11-C10-C9	2.25	105.46	113.69	14	1
3	B	375	PX4	O7-C23-O8	2.25	128.96	123.70	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	375	PX4	O8-C23-C24	2.25	132.57	123.78	7	1
3	B	383	PX4	O7-C7-C8	2.25	116.41	108.34	9	1
3	C	349	PX4	C11-C10-C9	2.25	121.93	113.69	4	2
3	A	602	PX4	C8-O5-C9	2.25	108.91	117.12	13	1
3	B	324	PX4	C5-N1-C3	2.25	103.07	108.98	1	3
3	B	337	PX4	C5-N1-C4	2.25	114.88	108.98	1	1
3	A	604	PX4	O1-P1-O2	2.25	122.89	112.44	15	1
3	B	329	PX4	C1-C2-N1	2.25	123.03	115.82	5	1
3	B	340	PX4	C1-C2-N1	2.25	123.03	115.82	2	1
3	A	602	PX4	O1-P1-O2	2.24	122.88	112.44	9	1
3	A	612	PX4	C4-N1-C3	2.24	103.08	108.98	6	1
3	A	619	PX4	C12-C11-C10	2.25	104.88	113.13	4	1
3	A	636	PX4	C5-N1-C3	2.25	103.08	108.98	2	2
3	C	332	PX4	O1-P1-O3	2.25	117.75	107.57	6	1
3	C	333	PX4	C5-N1-C2	2.25	118.84	109.91	7	1
3	C	338	PX4	C4-N1-C3	2.25	103.08	108.98	12	2
3	B	340	PX4	P1-O3-C1	2.24	131.94	121.26	4	1
3	B	303	PX4	O7-C7-C8	2.24	116.39	108.34	12	1
3	A	601	PX4	O5-C9-C10	2.24	105.00	111.83	8	1
3	A	610	PX4	C5-N1-C3	2.24	103.09	108.98	9	1
3	A	627	PX4	C17-C16-C15	2.24	103.04	114.37	14	1
3	A	630	PX4	C29-C28-C27	2.24	103.04	114.37	14	1
3	B	302	PX4	O5-C9-O6	2.24	129.23	123.63	6	1
3	B	338	PX4	O7-C7-C6	2.24	116.38	108.34	5	1
3	B	350	PX4	C16-C15-C14	2.24	103.04	114.37	6	1
3	B	369	PX4	C8-C7-C6	2.24	106.56	111.78	11	1
3	C	318	PX4	C11-C10-C9	2.24	105.48	113.69	9	1
3	C	329	PX4	O5-C9-C10	2.24	105.00	111.83	3	1
3	B	370	PX4	O7-C23-O8	2.24	128.94	123.70	10	2
3	B	385	PX4	C33-C32-C31	2.24	103.05	114.37	2	1
3	C	311	PX4	C5-N1-C4	2.24	103.09	108.98	13	2
3	A	650	PX4	C5-N1-C2	2.24	118.80	109.91	1	1
3	B	323	PX4	O5-C9-C10	2.24	105.01	111.83	3	1
3	B	373	PX4	O5-C9-O6	2.24	129.22	123.63	4	1
3	C	316	PX4	C5-N1-C4	2.24	103.10	108.98	3	1
3	C	330	PX4	C11-C10-C9	2.24	105.49	113.69	15	1
3	A	650	PX4	C1-C2-N1	2.24	123.00	115.82	10	1
3	B	305	PX4	O1-P1-O2	2.24	122.84	112.44	8	2
3	B	310	PX4	P1-O3-C1	2.24	131.90	121.26	5	1
3	B	332	PX4	C4-N1-C3	2.24	114.85	108.98	11	2
3	A	641	PX4	O5-C9-O6	2.23	129.22	123.63	7	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	344	PX4	C1-C2-N1	2.23	122.99	115.82	12	2
3	B	357	PX4	C12-C11-C10	2.24	121.34	113.13	10	1
3	B	371	PX4	C1-C2-N1	2.24	123.00	115.82	7	2
3	C	339	PX4	O5-C8-C7	2.24	114.84	108.40	3	1
3	B	380	PX4	O4-P1-O2	2.23	100.08	108.94	13	1
3	C	350	PX4	C4-N1-C3	2.24	114.85	108.98	5	2
3	B	342	PX4	O5-C9-O6	2.23	129.22	123.63	12	1
3	B	344	PX4	C34-C33-C32	2.23	103.08	114.37	3	1
3	B	376	PX4	C19-C18-C17	2.23	103.08	114.37	14	1
3	C	316	PX4	C25-C24-C23	2.23	121.88	113.69	12	1
3	C	321	PX4	C5-N1-C4	2.23	114.84	108.98	15	1
3	C	335	PX4	C3-N1-C2	2.23	118.79	109.91	15	1
3	B	385	PX4	C26-C25-C24	2.23	121.33	113.13	14	1
3	B	397	PX4	C1-C2-N1	2.23	122.98	115.82	3	2
3	C	333	PX4	C4-N1-C2	2.23	118.78	109.91	5	1
3	B	337	PX4	C22-C21-C20	2.23	128.42	113.36	8	1
3	B	356	PX4	C5-N1-C4	2.23	103.12	108.98	15	1
3	A	642	PX4	C8-C7-C6	2.23	106.59	111.78	6	2
3	B	340	PX4	O7-C23-O8	2.23	128.92	123.70	12	2
3	B	372	PX4	C26-C25-C24	2.23	104.94	113.13	13	2
3	A	626	PX4	C5-N1-C4	2.23	114.83	108.98	7	4
3	B	304	PX4	O5-C9-O6	2.23	129.20	123.63	8	1
3	B	307	PX4	C26-C25-C24	2.23	121.31	113.13	6	1
3	B	381	PX4	C25-C24-C23	2.23	105.53	113.69	4	3
3	C	318	PX4	O7-C7-C6	2.23	100.35	108.34	15	2
3	C	336	PX4	C17-C16-C15	2.23	103.11	114.37	14	1
3	C	339	PX4	C4-N1-C3	2.23	103.12	108.98	13	1
3	C	341	PX4	P1-O3-C1	2.23	131.87	121.26	13	1
3	A	632	PX4	C3-N1-C2	2.23	101.06	109.91	9	1
3	B	314	PX4	O5-C9-C10	2.23	105.05	111.83	4	1
3	C	343	PX4	C20-C19-C18	2.23	125.62	114.37	13	2
3	A	632	PX4	O1-P1-O2	2.22	122.79	112.44	6	1
3	A	614	PX4	C4-N1-C3	2.22	103.14	108.98	3	3
3	A	652	PX4	C5-N1-C3	2.22	114.82	108.98	1	1
3	A	623	PX4	C26-C25-C24	2.22	104.96	113.13	8	1
3	A	646	PX4	O5-C8-C7	2.22	114.80	108.40	12	2
3	B	311	PX4	C31-C30-C29	2.22	125.61	114.37	3	1
3	B	344	PX4	C4-N1-C3	2.22	103.14	108.98	2	1
3	B	364	PX4	C26-C25-C24	2.22	121.29	113.13	11	1
3	B	396	PX4	C5-N1-C4	2.22	103.14	108.98	11	1
3	C	308	PX4	O5-C8-C7	2.22	114.80	108.40	13	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	373	PX4	P1-O3-C1	2.22	131.84	121.26	7	1
3	C	325	PX4	O4-P1-O2	2.22	117.74	108.94	8	1
3	C	328	PX4	C1-C2-N1	2.22	122.95	115.82	11	1
3	A	650	PX4	C26-C25-C24	2.22	104.97	113.13	10	1
3	A	635	PX4	C5-N1-C4	2.22	103.14	108.98	15	3
3	B	344	PX4	O4-P1-O2	2.22	117.73	108.94	1	2
3	C	354	PX4	O1-P1-O2	2.22	122.78	112.44	12	2
3	A	620	PX4	C12-C11-C10	2.22	104.98	113.13	10	2
3	A	644	PX4	C12-C11-C10	2.22	104.98	113.13	8	1
3	B	303	PX4	C26-C25-C24	2.22	104.97	113.13	6	1
3	B	353	PX4	C1-C2-N1	2.22	122.95	115.82	5	1
3	B	366	PX4	C4-N1-C3	2.22	114.81	108.98	2	2
3	C	328	PX4	O8-C23-C24	2.22	132.46	123.78	10	1
3	B	341	PX4	C3-N1-C2	2.22	118.72	109.91	4	1
3	B	367	PX4	C5-N1-C4	2.22	103.15	108.98	12	2
3	B	394	PX4	O1-P1-O2	2.22	122.76	112.44	12	1
3	C	306	PX4	C29-C28-C27	2.22	103.16	114.37	12	1
3	B	312	PX4	C34-C33-C32	2.22	103.17	114.37	10	1
3	B	340	PX4	O5-C8-C7	2.22	114.78	108.40	3	4
3	B	343	PX4	O7-C23-O8	2.22	128.88	123.70	12	2
3	C	334	PX4	C1-C2-N1	2.22	122.93	115.82	7	2
3	C	355	PX4	C16-C15-C14	2.22	103.16	114.37	4	1
3	C	359	PX4	C25-C24-C23	2.22	105.57	113.69	10	2
3	B	394	PX4	C4-N1-C3	2.21	114.79	108.98	12	1
3	C	304	PX4	C4-N1-C2	2.21	118.71	109.91	8	1
3	A	602	PX4	C3-N1-C2	2.21	118.70	109.91	9	1
3	A	609	PX4	C8-O5-C9	2.21	109.03	117.12	1	2
3	A	623	PX4	C5-N1-C4	2.21	114.79	108.98	6	1
3	A	632	PX4	C4-N1-C3	2.21	103.17	108.98	3	1
3	A	634	PX4	O3-P1-O2	2.21	117.70	108.94	3	1
3	A	637	PX4	O7-C23-O8	2.21	128.88	123.70	11	2
3	B	315	PX4	C3-N1-C2	2.21	118.70	109.91	13	1
3	B	378	PX4	O7-C23-O8	2.21	128.88	123.70	6	1
3	B	343	PX4	O4-P1-O2	2.21	100.17	108.94	15	1
3	B	335	PX4	O6-C9-C10	2.21	132.42	123.78	12	1
3	B	369	PX4	C26-C25-C24	2.21	121.25	113.13	14	2
3	C	346	PX4	C31-C30-C29	2.21	103.20	114.37	1	1
3	C	347	PX4	C25-C24-C23	2.21	105.60	113.69	3	2
3	B	315	PX4	O1-P1-O2	2.21	122.72	112.44	10	1
3	C	356	PX4	C11-C10-C9	2.21	105.60	113.69	8	1
3	B	332	PX4	C14-C13-C12	2.21	103.21	114.37	5	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	360	PX4	C12-C11-C10	2.21	105.01	113.13	7	1
3	B	390	PX4	O5-C9-C10	2.21	105.10	111.83	4	2
3	C	328	PX4	O7-C7-C6	2.21	116.27	108.34	2	1
3	A	631	PX4	C8-C7-C6	2.21	106.64	111.78	6	1
3	A	637	PX4	O5-C9-C10	2.21	105.11	111.83	4	1
3	B	384	PX4	C20-C19-C18	2.21	103.22	114.37	5	1
3	B	384	PX4	O5-C9-O6	2.21	129.15	123.63	6	1
3	C	307	PX4	C8-C7-C6	2.21	116.93	111.78	1	2
3	C	352	PX4	C8-C7-C6	2.21	116.93	111.78	3	1
3	A	607	PX4	O7-C7-C8	2.21	116.25	108.34	11	1
3	A	623	PX4	C29-C28-C27	2.21	103.22	114.37	1	1
3	A	640	PX4	C5-N1-C2	2.21	118.68	109.91	15	1
3	C	301	PX4	C11-C10-C9	2.21	105.61	113.69	5	1
3	B	365	PX4	O3-C1-C2	2.20	120.26	109.65	7	1
3	C	307	PX4	O6-C9-C10	2.20	132.40	123.78	8	1
3	C	325	PX4	O1-P1-O3	2.21	117.56	107.57	6	1
3	A	603	PX4	C31-C30-C29	2.20	103.23	114.37	1	1
3	A	618	PX4	O7-C7-C8	2.20	116.25	108.34	15	1
3	A	636	PX4	O7-C7-C6	2.20	116.24	108.34	6	2
3	B	331	PX4	O1-P1-O2	2.20	122.69	112.44	8	1
3	B	346	PX4	O3-P1-O2	2.20	117.67	108.94	1	1
3	B	349	PX4	C12-C11-C10	2.20	121.22	113.13	12	1
3	B	354	PX4	C1-C2-N1	2.20	122.89	115.82	10	2
3	C	333	PX4	C25-C24-C23	2.20	121.77	113.69	9	1
3	C	344	PX4	O3-C1-C2	2.20	120.25	109.65	10	1
3	A	603	PX4	C8-O5-C9	2.20	109.08	117.12	15	1
3	A	644	PX4	C1-C2-N1	2.20	122.88	115.82	7	1
3	A	647	PX4	C25-C24-C23	2.20	105.63	113.69	12	3
3	B	308	PX4	O7-C7-C8	2.20	116.24	108.34	7	2
3	B	332	PX4	C11-C10-C9	2.20	105.63	113.69	6	3
3	B	391	PX4	O8-C23-C24	2.20	115.17	123.78	13	1
3	C	302	PX4	C26-C25-C24	2.20	105.04	113.13	1	1
3	C	313	PX4	C8-C7-C6	2.20	106.65	111.78	2	2
3	A	622	PX4	O3-C1-C2	2.20	120.23	109.65	1	1
3	A	622	PX4	C32-C31-C30	2.20	103.25	114.37	5	1
3	A	649	PX4	C12-C11-C10	2.20	121.21	113.13	3	1
3	B	325	PX4	C12-C11-C10	2.20	105.05	113.13	13	2
3	B	392	PX4	O7-C7-C6	2.20	116.23	108.34	13	1
3	C	323	PX4	O7-C7-C8	2.20	116.24	108.34	2	1
3	C	335	PX4	C31-C30-C29	2.20	103.25	114.37	9	1
3	C	340	PX4	O1-P1-O2	2.20	122.68	112.44	11	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	A	612	PX4	C12-C11-C10	2.20	105.05	113.13	5	1
3	B	358	PX4	C13-C12-C11	2.20	125.48	114.37	15	1
3	B	364	PX4	O1-P1-O4	2.20	117.53	107.57	12	1
3	C	312	PX4	C5-N1-C3	2.20	103.20	108.98	7	1
3	C	332	PX4	C13-C12-C11	2.20	103.26	114.37	9	1
3	C	359	PX4	O7-C23-C24	2.20	106.72	111.48	15	1
3	C	307	PX4	C26-C25-C24	2.20	121.20	113.13	8	1
3	C	327	PX4	O5-C9-O6	2.20	129.12	123.63	5	1
3	C	336	PX4	O7-C7-C8	2.20	116.23	108.34	3	1
3	A	638	PX4	O5-C9-C10	2.20	105.14	111.83	9	1
3	B	325	PX4	O5-C9-O6	2.20	129.12	123.63	2	1
3	C	312	PX4	C1-C2-N1	2.20	122.87	115.82	12	1
3	B	357	PX4	C26-C25-C24	2.19	105.06	113.13	13	1
3	B	369	PX4	C5-N1-C4	2.19	103.21	108.98	3	1
3	B	374	PX4	C15-C14-C13	2.19	103.28	114.37	12	1
3	C	303	PX4	C8-O5-C9	2.19	109.10	117.12	5	1
3	C	354	PX4	O5-C9-O6	2.19	129.12	123.63	13	2
3	A	652	PX4	O7-C23-O8	2.19	128.83	123.70	7	3
3	A	612	PX4	O8-C23-C24	2.19	132.35	123.78	4	1
3	B	382	PX4	O1-P1-O2	2.19	122.64	112.44	15	1
3	B	387	PX4	O6-C9-C10	2.19	132.35	123.78	7	1
3	C	352	PX4	C1-C2-N1	2.19	122.86	115.82	5	1
3	B	319	PX4	C5-N1-C3	2.19	114.73	108.98	14	2
3	B	334	PX4	O5-C9-O6	2.19	129.10	123.63	11	1
3	B	338	PX4	C8-O5-C9	2.19	109.12	117.12	1	3
3	B	387	PX4	C5-N1-C3	2.19	114.73	108.98	4	1
3	C	317	PX4	C18-C17-C16	2.19	103.30	114.37	1	1
3	A	604	PX4	O5-C9-O6	2.19	129.10	123.63	5	1
3	B	324	PX4	O5-C9-C10	2.19	105.17	111.83	11	2
3	C	320	PX4	O7-C23-O8	2.19	128.82	123.70	9	2
3	A	628	PX4	C33-C32-C31	2.19	103.32	114.37	7	1
3	C	329	PX4	O1-P1-O4	2.19	117.47	107.57	6	1
3	C	352	PX4	C11-C10-C9	2.19	105.68	113.69	12	3
3	A	629	PX4	O7-C23-O8	2.19	128.81	123.70	6	1
3	A	617	PX4	C1-C2-N1	2.18	122.83	115.82	4	2
3	A	618	PX4	C19-C18-C17	2.18	103.33	114.37	12	1
3	B	320	PX4	O7-C7-C6	2.18	116.18	108.34	5	2
3	C	313	PX4	C8-O5-C9	2.19	125.11	117.12	4	1
3	C	340	PX4	C26-C25-C24	2.19	121.16	113.13	10	1
3	A	646	PX4	C1-C2-N1	2.18	122.83	115.82	9	1
3	A	654	PX4	C5-N1-C4	2.18	114.71	108.98	10	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	336	PX4	C8-C7-C6	2.18	106.69	111.78	7	1
3	B	363	PX4	O4-P1-O2	2.18	117.59	108.94	9	1
3	C	337	PX4	O5-C9-O6	2.18	129.09	123.63	3	1
3	C	350	PX4	C5-N1-C2	2.18	118.59	109.91	7	1
3	B	336	PX4	C5-N1-C3	2.18	114.71	108.98	13	1
3	A	625	PX4	O5-C9-C10	2.18	105.18	111.83	13	2
3	A	628	PX4	C11-C10-C9	2.18	105.70	113.69	2	2
3	B	386	PX4	O8-C23-C24	2.18	132.32	123.78	14	1
3	B	388	PX4	O7-C7-C6	2.18	116.17	108.34	3	2
3	B	369	PX4	O4-P1-O2	2.18	100.29	108.94	3	1
3	B	377	PX4	C12-C11-C10	2.18	121.14	113.13	12	1
3	C	325	PX4	C15-C14-C13	2.18	103.34	114.37	15	1
3	C	340	PX4	C5-N1-C3	2.18	103.24	108.98	2	2
3	B	347	PX4	C31-C30-C29	2.18	103.34	114.37	7	1
3	A	606	PX4	C4-N1-C2	2.18	118.57	109.91	6	1
3	A	619	PX4	O5-C9-O6	2.18	129.08	123.63	9	3
3	B	308	PX4	C17-C16-C15	2.18	103.35	114.37	11	1
3	B	318	PX4	O7-C23-O8	2.18	128.80	123.70	1	1
3	B	329	PX4	C5-N1-C2	2.18	101.25	109.91	9	1
3	B	336	PX4	C5-N1-C4	2.18	103.25	108.98	4	2
3	B	375	PX4	C5-N1-C4	2.18	114.70	108.98	11	2
3	B	382	PX4	C4-N1-C3	2.18	103.25	108.98	1	3
3	B	397	PX4	C33-C32-C31	2.18	103.35	114.37	3	1
3	C	308	PX4	C1-C2-N1	2.18	122.82	115.82	2	1
3	C	310	PX4	O7-C7-C8	2.18	116.16	108.34	9	1
3	C	311	PX4	C25-C24-C23	2.18	105.70	113.69	5	2
3	B	302	PX4	C4-N1-C2	2.18	118.56	109.91	7	1
3	B	364	PX4	C4-N1-C2	2.18	118.56	109.91	3	1
3	B	392	PX4	C3-N1-C2	2.18	101.25	109.91	10	1
3	A	626	PX4	O7-C7-C8	2.18	116.15	108.34	14	2
3	A	626	PX4	C4-N1-C3	2.18	103.26	108.98	3	1
3	B	303	PX4	O7-C7-C6	2.18	116.15	108.34	1	1
3	B	382	PX4	O7-C23-O8	2.18	118.62	123.70	6	1
3	C	351	PX4	O8-C23-C24	2.18	132.29	123.78	4	1
3	C	352	PX4	C4-N1-C3	2.18	114.69	108.98	14	1
3	A	648	PX4	C5-N1-C4	2.17	103.27	108.98	6	1
3	B	331	PX4	C32-C31-C30	2.18	103.37	114.37	1	1
3	B	315	PX4	C25-C24-C23	2.17	121.66	113.69	4	2
3	B	320	PX4	C28-C27-C26	2.17	103.37	114.37	12	2
3	B	374	PX4	C11-C10-C9	2.17	121.66	113.69	14	1
3	C	358	PX4	P1-O3-C1	2.18	131.62	121.26	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	310	PX4	O1-P1-O2	2.17	122.55	112.44	15	1
3	A	602	PX4	O7-C23-C24	2.17	106.78	111.48	11	1
3	A	602	PX4	O3-P1-O2	2.17	117.54	108.94	13	1
3	B	327	PX4	C28-C27-C26	2.17	125.35	114.37	3	1
3	B	359	PX4	O7-C7-C8	2.17	116.14	108.34	3	3
3	B	381	PX4	P1-O3-C1	2.17	131.60	121.26	13	1
3	C	314	PX4	C8-O5-C9	2.17	109.18	117.12	15	1
3	A	643	PX4	O7-C23-C24	2.17	106.78	111.48	12	1
3	A	646	PX4	O1-P1-O2	2.17	122.55	112.44	2	2
3	A	644	PX4	C5-N1-C3	2.17	103.28	108.98	4	2
3	B	340	PX4	O8-C23-C24	2.17	132.27	123.78	9	1
3	C	347	PX4	O8-C23-C24	2.17	132.27	123.78	11	1
3	B	370	PX4	C19-C18-C17	2.17	125.33	114.37	15	1
3	C	356	PX4	C14-C13-C12	2.17	103.40	114.37	13	1
3	A	610	PX4	C26-C25-C24	2.17	105.16	113.13	10	1
3	C	358	PX4	C5-N1-C4	2.17	114.67	108.98	13	1
3	C	361	PX4	C5-N1-C2	2.17	118.53	109.91	9	1
3	B	304	PX4	C5-N1-C4	2.17	114.67	108.98	13	1
3	B	364	PX4	C32-C31-C30	2.17	103.42	114.37	10	1
3	B	386	PX4	O4-P1-O2	2.17	100.35	108.94	13	1
3	C	322	PX4	C8-O5-C9	2.17	109.20	117.12	8	1
3	A	601	PX4	C33-C32-C31	2.16	103.43	114.37	11	1
3	B	309	PX4	C27-C26-C25	2.16	103.42	114.37	10	1
3	B	310	PX4	O7-C7-C6	2.16	116.11	108.34	4	1
3	B	340	PX4	C4-N1-C2	2.17	118.52	109.91	13	1
3	B	393	PX4	O5-C9-O6	2.17	129.05	123.63	4	4
3	B	393	PX4	C5-N1-C4	2.17	114.66	108.98	13	1
3	C	334	PX4	C25-C24-C23	2.16	105.77	113.69	7	1
3	C	346	PX4	C5-N1-C4	2.16	103.30	108.98	6	2
3	C	348	PX4	O5-C9-O6	2.16	129.04	123.63	9	1
3	A	605	PX4	O7-C7-C8	2.16	100.59	108.34	1	1
3	A	627	PX4	C1-C2-N1	2.16	122.76	115.82	13	2
3	B	375	PX4	C33-C32-C31	2.16	103.44	114.37	4	1
3	C	306	PX4	C34-C33-C32	2.16	125.30	114.37	15	1
3	B	334	PX4	C11-C10-C9	2.16	105.78	113.69	4	1
3	B	374	PX4	O7-C7-C6	2.16	116.09	108.34	1	1
3	B	388	PX4	C34-C33-C32	2.16	103.45	114.37	13	1
3	C	303	PX4	C32-C31-C30	2.16	103.45	114.37	2	1
3	C	344	PX4	C4-N1-C3	2.16	103.30	108.98	4	1
3	B	334	PX4	C1-C2-N1	2.16	122.75	115.82	15	1
3	C	351	PX4	C11-C10-C9	2.16	121.61	113.69	10	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	A	604	PX4	C30-C29-C28	2.16	103.46	114.37	13	1
3	B	342	PX4	C5-N1-C3	2.16	114.65	108.98	5	1
3	B	346	PX4	P1-O4-C6	2.16	133.72	121.35	4	1
3	B	347	PX4	O3-C1-C2	2.16	120.04	109.65	2	1
3	B	323	PX4	C8-O5-C9	2.16	125.00	117.12	8	1
3	B	393	PX4	C14-C13-C12	2.16	125.28	114.37	12	1
3	B	394	PX4	C18-C17-C16	2.16	103.46	114.37	7	1
3	C	322	PX4	O5-C9-C10	2.16	105.25	111.83	12	1
3	B	355	PX4	O5-C9-O6	2.16	129.03	123.63	6	1
3	C	330	PX4	C5-N1-C2	2.16	118.49	109.91	5	1
3	B	385	PX4	O6-C9-C10	2.16	132.22	123.78	5	1
3	B	398	PX4	C12-C11-C10	2.16	121.05	113.13	10	1
3	C	343	PX4	P1-O3-C1	2.16	131.53	121.26	6	1
3	A	622	PX4	C5-N1-C2	2.16	118.48	109.91	4	1
3	A	636	PX4	C27-C26-C25	2.16	103.47	114.37	7	1
3	B	341	PX4	C29-C28-C27	2.16	125.27	114.37	5	1
3	B	356	PX4	C20-C19-C18	2.16	103.47	114.37	3	1
3	B	363	PX4	O7-C7-C8	2.15	116.07	108.34	2	1
3	C	309	PX4	C4-N1-C2	2.16	118.48	109.91	11	1
3	C	312	PX4	C4-N1-C3	2.16	103.31	108.98	9	4
3	C	349	PX4	O1-P1-O2	2.16	122.48	112.44	4	1
3	B	356	PX4	C8-O5-C9	2.15	109.24	117.12	13	1
3	B	372	PX4	C5-N1-C2	2.15	118.47	109.91	15	1
3	B	389	PX4	O7-C23-O8	2.15	128.74	123.70	3	1
3	B	399	PX4	O4-P1-O2	2.15	117.47	108.94	11	1
3	C	335	PX4	C28-C27-C26	2.15	125.26	114.37	7	1
3	C	347	PX4	O5-C8-C7	2.15	114.61	108.40	10	2
3	C	349	PX4	O7-C7-C8	2.15	116.07	108.34	6	3
3	B	357	PX4	C34-C33-C32	2.15	103.48	114.37	14	1
3	C	332	PX4	C16-C15-C14	2.15	103.48	114.37	4	1
3	C	344	PX4	O8-C23-C24	2.15	132.20	123.78	9	1
3	C	358	PX4	C31-C30-C29	2.15	103.48	114.37	15	1
3	A	615	PX4	C11-C10-C9	2.15	105.81	113.69	6	1
3	A	621	PX4	C4-N1-C2	2.15	118.46	109.91	12	1
3	B	312	PX4	O3-C1-C2	2.15	120.00	109.65	7	1
3	B	340	PX4	C14-C13-C12	2.15	103.50	114.37	1	1
3	B	354	PX4	O5-C9-C10	2.15	105.27	111.83	3	2
3	C	354	PX4	C4-N1-C3	2.15	103.32	108.98	5	1
3	B	384	PX4	C1-C2-N1	2.15	122.72	115.82	6	1
3	C	303	PX4	C4-N1-C2	2.15	118.46	109.91	3	1
3	A	632	PX4	C26-C25-C24	2.15	105.23	113.13	3	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	314	PX4	C25-C24-C23	2.15	105.82	113.69	6	1
3	C	347	PX4	C8-O5-C9	2.15	124.97	117.12	9	1
3	C	348	PX4	O7-C7-C8	2.15	116.06	108.34	4	1
3	C	358	PX4	C12-C11-C10	2.15	105.23	113.13	14	1
3	B	341	PX4	C28-C27-C26	2.15	103.51	114.37	7	1
3	B	396	PX4	P1-O4-C6	2.15	109.04	121.35	6	1
3	C	301	PX4	C5-N1-C4	2.15	114.62	108.98	8	1
3	C	304	PX4	C8-O5-C9	2.15	109.26	117.12	6	2
3	C	310	PX4	O5-C9-O6	2.15	129.00	123.63	7	1
3	C	316	PX4	C17-C16-C15	2.15	103.51	114.37	2	1
3	C	343	PX4	O7-C7-C6	2.15	116.05	108.34	2	2
3	C	358	PX4	O8-C23-C24	2.15	132.19	123.78	1	1
3	A	605	PX4	C5-N1-C4	2.15	103.34	108.98	13	1
3	B	366	PX4	O7-C23-O8	2.15	128.72	123.70	8	1
3	A	609	PX4	O4-P1-O2	2.14	100.44	108.94	15	1
3	A	642	PX4	O7-C7-C6	2.15	116.04	108.34	10	1
3	C	302	PX4	P1-O4-C6	2.15	133.65	121.35	9	2
3	C	355	PX4	C5-N1-C3	2.15	103.34	108.98	2	3
3	A	623	PX4	O7-C7-C8	2.14	116.03	108.34	11	1
3	B	309	PX4	O1-P1-O2	2.14	122.42	112.44	15	1
3	B	342	PX4	O1-P1-O2	2.14	122.42	112.44	13	1
3	B	357	PX4	C5-N1-C2	2.14	118.43	109.91	8	1
3	B	371	PX4	C13-C12-C11	2.14	103.53	114.37	3	1
3	A	609	PX4	C4-N1-C3	2.14	114.60	108.98	3	1
3	A	616	PX4	C20-C19-C18	2.14	103.54	114.37	2	1
3	A	638	PX4	O1-P1-O2	2.14	122.41	112.44	2	1
3	B	383	PX4	O6-C9-C10	2.14	132.17	123.78	1	2
3	C	321	PX4	C1-C2-N1	2.14	122.70	115.82	9	2
3	C	325	PX4	C11-C10-C9	2.14	121.55	113.69	4	2
3	A	636	PX4	C25-C24-C23	2.14	105.85	113.69	10	1
3	A	644	PX4	C32-C31-C30	2.14	103.54	114.37	14	1
3	B	309	PX4	C5-N1-C2	2.14	118.42	109.91	2	1
3	B	327	PX4	C8-C7-C6	2.14	106.79	111.78	3	1
3	B	357	PX4	O7-C7-C6	2.14	116.03	108.34	11	1
3	C	328	PX4	C19-C18-C17	2.14	103.53	114.37	13	1
3	C	310	PX4	C12-C11-C10	2.14	105.26	113.13	12	1
3	C	337	PX4	C8-C7-C6	2.14	106.79	111.78	2	1
3	C	352	PX4	O1-P1-O2	2.14	122.41	112.44	7	2
3	A	629	PX4	O7-C7-C6	2.14	116.02	108.34	9	2
3	A	642	PX4	C15-C14-C13	2.14	125.18	114.37	5	1
3	B	324	PX4	C26-C25-C24	2.14	120.99	113.13	12	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	348	PX4	O1-P1-O2	2.14	122.40	112.44	1	1
3	B	359	PX4	C7-O7-C23	2.14	112.67	117.80	2	2
3	B	360	PX4	O1-P1-O2	2.14	122.40	112.44	14	1
3	B	384	PX4	C19-C18-C17	2.14	103.55	114.37	14	1
3	B	386	PX4	C33-C32-C31	2.14	103.55	114.37	4	1
3	C	310	PX4	O1-P1-O3	2.14	117.27	107.57	12	1
3	B	305	PX4	C8-C7-C6	2.14	106.80	111.78	4	1
3	C	323	PX4	C4-N1-C2	2.14	101.41	109.91	2	1
3	B	391	PX4	C12-C11-C10	2.14	105.28	113.13	13	1
3	C	310	PX4	C28-C27-C26	2.14	103.56	114.37	8	1
3	C	327	PX4	C25-C24-C23	2.14	105.87	113.69	1	1
3	C	333	PX4	C8-O5-C9	2.14	124.93	117.12	12	1
3	A	604	PX4	C33-C32-C31	2.14	103.57	114.37	8	1
3	A	605	PX4	C28-C27-C26	2.14	125.16	114.37	6	1
3	A	622	PX4	O7-C7-C8	2.13	116.00	108.34	13	1
3	B	307	PX4	O3-C1-C2	2.14	119.92	109.65	11	2
3	B	351	PX4	C8-C7-C6	2.14	106.81	111.78	4	3
3	B	374	PX4	O7-C23-O8	2.14	128.70	123.70	9	2
3	A	634	PX4	P1-O4-C6	2.13	109.12	121.35	2	1
3	C	311	PX4	C26-C25-C24	2.13	120.97	113.13	2	1
3	C	313	PX4	O5-C9-C10	2.13	105.33	111.83	10	1
3	C	328	PX4	O3-C1-C2	2.13	119.92	109.65	9	1
3	A	614	PX4	C5-N1-C3	2.13	103.38	108.98	3	1
3	A	625	PX4	O7-C23-O8	2.13	118.72	123.70	8	2
3	A	635	PX4	C26-C25-C24	2.13	120.96	113.13	12	1
3	A	653	PX4	C11-C10-C9	2.13	105.89	113.69	2	1
3	B	319	PX4	O1-P1-O2	2.13	122.36	112.44	14	1
3	B	341	PX4	C8-O5-C9	2.13	109.33	117.12	12	1
3	B	349	PX4	O3-C1-C2	2.13	119.90	109.65	14	1
3	B	371	PX4	C8-O5-C9	2.13	109.33	117.12	7	1
3	C	312	PX4	C26-C25-C24	2.13	105.30	113.13	13	1
3	A	603	PX4	C5-N1-C3	2.13	103.38	108.98	2	1
3	B	356	PX4	P1-O3-C1	2.13	131.40	121.26	2	1
3	A	609	PX4	C11-C10-C9	2.13	105.90	113.69	6	2
3	A	611	PX4	C5-N1-C4	2.13	114.56	108.98	15	2
3	A	622	PX4	O5-C9-O6	2.13	128.95	123.63	5	2
3	B	322	PX4	C11-C10-C9	2.13	105.90	113.69	1	1
3	B	323	PX4	C4-N1-C3	2.13	103.39	108.98	6	1
3	B	352	PX4	O6-C9-C10	2.13	132.11	123.78	1	1
3	B	354	PX4	O1-P1-O4	2.13	117.21	107.57	9	1
3	B	381	PX4	C7-O7-C23	2.13	122.89	117.80	14	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	388	PX4	C18-C17-C16	2.13	103.62	114.37	2	1
3	C	346	PX4	O5-C9-C10	2.13	105.35	111.83	9	1
3	C	353	PX4	C33-C32-C31	2.13	103.62	114.37	13	1
3	C	360	PX4	C11-C10-C9	2.13	105.90	113.69	12	1
3	A	643	PX4	C33-C32-C31	2.13	103.62	114.37	2	1
3	A	652	PX4	C14-C13-C12	2.13	103.62	114.37	8	1
3	B	309	PX4	C4-N1-C3	2.13	114.56	108.98	11	2
3	A	635	PX4	O7-C23-C24	2.12	106.89	111.48	6	1
3	B	321	PX4	O1-P1-O2	2.13	122.33	112.44	6	1
3	B	368	PX4	O6-C9-C10	2.13	132.10	123.78	4	1
3	B	378	PX4	C36-C35-C34	2.13	127.72	113.36	9	1
3	B	378	PX4	C30-C29-C28	2.13	103.62	114.37	13	1
3	C	324	PX4	O7-C7-C6	2.13	100.72	108.34	11	1
3	C	331	PX4	O3-C1-C2	2.13	119.88	109.65	13	2
3	C	336	PX4	O7-C7-C6	2.13	100.72	108.34	11	1
3	C	340	PX4	O6-C9-C10	2.13	132.10	123.78	12	1
3	C	356	PX4	O7-C7-C8	2.13	115.97	108.34	14	1
3	A	606	PX4	C1-C2-N1	2.12	122.64	115.82	5	1
3	A	650	PX4	C8-C7-C6	2.12	106.83	111.78	11	1
3	B	307	PX4	O7-C7-C8	2.12	100.72	108.34	8	2
3	B	338	PX4	C1-C2-N1	2.12	122.64	115.82	13	1
3	B	353	PX4	C26-C25-C24	2.12	120.93	113.13	6	1
3	C	305	PX4	C19-C18-C17	2.12	125.11	114.37	7	1
3	C	311	PX4	C12-C11-C10	2.12	105.32	113.13	10	1
3	C	323	PX4	O1-P1-O2	2.12	122.33	112.44	15	1
3	C	340	PX4	C5-N1-C2	2.12	118.35	109.91	11	1
3	C	343	PX4	C11-C10-C9	2.12	105.92	113.69	12	1
3	C	354	PX4	C8-O5-C9	2.12	124.88	117.12	8	2
3	A	629	PX4	O5-C9-O6	2.12	128.94	123.63	9	2
3	B	341	PX4	C31-C30-C29	2.12	103.64	114.37	11	2
3	B	347	PX4	C29-C28-C27	2.12	103.64	114.37	11	1
3	B	349	PX4	C27-C26-C25	2.12	103.64	114.37	12	1
3	B	352	PX4	C27-C26-C25	2.12	125.09	114.37	15	1
3	B	397	PX4	C5-N1-C2	2.12	118.35	109.91	15	1
3	B	374	PX4	C5-N1-C3	2.12	103.40	108.98	3	1
3	B	375	PX4	C8-C7-C6	2.12	106.84	111.78	15	1
3	A	618	PX4	C27-C26-C25	2.12	103.65	114.37	12	1
3	C	361	PX4	C5-N1-C4	2.12	103.41	108.98	4	1
3	A	606	PX4	C8-O5-C9	2.12	109.37	117.12	14	1
3	A	643	PX4	O1-P1-O2	2.12	122.30	112.44	14	1
3	B	363	PX4	C5-N1-C3	2.12	103.41	108.98	15	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	386	PX4	C12-C11-C10	2.12	120.92	113.13	4	1
3	C	361	PX4	O1-P1-O2	2.12	122.31	112.44	2	1
3	A	649	PX4	P1-O3-C1	2.12	131.34	121.26	4	1
3	B	319	PX4	C4-N1-C3	2.12	114.54	108.98	3	1
3	B	383	PX4	O7-C7-C6	2.12	115.94	108.34	9	2
3	B	395	PX4	C4-N1-C3	2.12	114.54	108.98	2	1
3	B	333	PX4	O7-C7-C8	2.12	100.75	108.34	13	2
3	A	613	PX4	C28-C27-C26	2.12	103.67	114.37	14	1
3	A	616	PX4	O7-C7-C6	2.12	115.94	108.34	3	1
3	A	624	PX4	C28-C27-C26	2.12	103.67	114.37	13	1
3	A	631	PX4	P1-O3-C1	2.12	131.33	121.26	12	1
3	A	651	PX4	C32-C31-C30	2.12	103.67	114.37	3	1
3	B	301	PX4	P1-O4-C6	2.12	133.48	121.35	15	1
3	C	301	PX4	C15-C14-C13	2.12	103.67	114.37	11	1
3	C	328	PX4	C25-C24-C23	2.12	105.94	113.69	13	1
3	C	353	PX4	C26-C25-C24	2.12	105.35	113.13	13	1
3	B	352	PX4	O7-C23-O8	2.12	128.65	123.70	7	1
3	C	341	PX4	C5-N1-C4	2.12	114.53	108.98	7	1
3	B	304	PX4	O4-P1-O2	2.11	100.56	108.94	2	1
3	B	317	PX4	O7-C23-O8	2.11	128.65	123.70	12	2
3	B	343	PX4	O5-C9-C10	2.11	105.39	111.83	11	1
3	C	347	PX4	C5-N1-C2	2.12	101.50	109.91	5	1
3	C	348	PX4	C15-C14-C13	2.12	103.68	114.37	4	1
3	C	348	PX4	C26-C25-C24	2.11	105.36	113.13	14	1
3	C	361	PX4	C14-C13-C12	2.12	103.67	114.37	10	1
3	B	385	PX4	C5-N1-C3	2.11	103.42	108.98	2	2
3	C	324	PX4	O5-C9-O6	2.11	128.92	123.63	8	2
3	A	616	PX4	C8-C7-C6	2.11	116.71	111.78	5	1
3	C	335	PX4	C5-N1-C4	2.11	114.53	108.98	3	1
3	A	636	PX4	C15-C14-C13	2.11	103.69	114.37	8	1
3	B	363	PX4	C4-N1-C3	2.11	114.52	108.98	1	1
3	B	366	PX4	O1-P1-O3	2.11	117.14	107.57	15	1
3	B	386	PX4	C11-C10-C9	2.11	105.96	113.69	8	1
3	C	312	PX4	O3-C1-C2	2.11	119.81	109.65	13	1
3	C	323	PX4	O6-C9-C10	2.11	132.04	123.78	3	1
3	C	344	PX4	O7-C7-C8	2.11	115.92	108.34	4	1
3	A	628	PX4	C1-C2-N1	2.11	122.60	115.82	3	1
3	B	342	PX4	O3-C1-C2	2.11	119.81	109.65	15	1
3	C	355	PX4	O1-P1-O2	2.11	122.27	112.44	8	1
3	C	363	PX4	O3-P1-O2	2.11	117.31	108.94	6	1
3	B	319	PX4	C8-O5-C9	2.11	109.41	117.12	5	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	330	PX4	O1-P1-O2	2.11	122.27	112.44	11	1
3	B	352	PX4	O3-C1-C2	2.11	119.80	109.65	3	1
3	C	318	PX4	O7-C23-O8	2.11	128.64	123.70	6	3
3	C	362	PX4	O7-C7-C8	2.11	115.91	108.34	7	1
3	C	362	PX4	O5-C9-O6	2.11	128.91	123.63	14	1
3	B	352	PX4	C14-C13-C12	2.11	125.03	114.37	7	1
3	B	363	PX4	O1-P1-O2	2.11	122.25	112.44	11	1
3	B	380	PX4	C36-C35-C34	2.11	127.60	113.36	2	1
3	B	395	PX4	P1-O3-C1	2.11	131.29	121.26	3	1
3	C	304	PX4	C5-N1-C3	2.11	103.44	108.98	2	2
3	C	357	PX4	O7-C7-C8	2.11	115.91	108.34	2	1
3	A	605	PX4	C5-N1-C3	2.11	103.44	108.98	5	1
3	A	624	PX4	C25-C24-C23	2.11	121.41	113.69	15	1
3	A	628	PX4	C17-C16-C15	2.11	103.72	114.37	7	1
3	A	633	PX4	O7-C7-C6	2.11	115.90	108.34	6	1
3	B	319	PX4	C5-N1-C4	2.11	103.44	108.98	13	1
3	B	341	PX4	C15-C14-C13	2.11	125.01	114.37	15	1
3	B	382	PX4	C16-C15-C14	2.11	103.72	114.37	1	1
3	B	395	PX4	C17-C16-C15	2.11	125.02	114.37	6	1
3	C	321	PX4	O5-C9-C10	2.11	105.41	111.83	8	1
3	C	326	PX4	O1-P1-O2	2.11	122.24	112.44	10	1
3	C	338	PX4	C5-N1-C3	2.11	114.51	108.98	13	1
3	C	344	PX4	C3-N1-C2	2.11	118.28	109.91	4	1
3	A	637	PX4	C1-C2-N1	2.10	122.58	115.82	2	1
3	B	317	PX4	O7-C23-C24	2.11	106.93	111.48	13	1
3	C	359	PX4	O5-C9-O6	2.11	128.89	123.63	6	1
3	A	605	PX4	C20-C19-C18	2.10	103.73	114.37	2	1
3	A	611	PX4	C12-C11-C10	2.10	120.86	113.13	12	1
3	B	318	PX4	C4-N1-C3	2.10	103.45	108.98	14	1
3	B	396	PX4	O1-P1-O4	2.10	117.10	107.57	10	1
3	C	313	PX4	C32-C31-C30	2.10	125.00	114.37	2	1
3	C	344	PX4	O1-P1-O2	2.10	122.23	112.44	15	1
3	C	348	PX4	C29-C28-C27	2.10	103.74	114.37	3	1
3	A	626	PX4	O3-C1-C2	2.10	119.76	109.65	8	2
3	A	640	PX4	C8-O5-C9	2.10	109.44	117.12	8	1
3	A	644	PX4	O3-C1-C2	2.10	119.76	109.65	12	1
3	B	302	PX4	C12-C11-C10	2.10	105.41	113.13	7	1
3	B	312	PX4	C8-O5-C9	2.10	109.44	117.12	15	1
3	B	359	PX4	C26-C25-C24	2.10	105.41	113.13	12	1
3	B	384	PX4	C29-C28-C27	2.10	124.99	114.37	12	1
3	B	389	PX4	O1-P1-O4	2.10	117.09	107.57	3	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	A	651	PX4	C26-C25-C24	2.10	120.84	113.13	12	1
3	C	327	PX4	C8-O5-C9	2.10	124.79	117.12	10	1
3	C	330	PX4	O7-C7-C8	2.10	115.88	108.34	4	1
3	C	359	PX4	C7-O7-C23	2.10	112.77	117.80	8	1
3	C	306	PX4	O3-C1-C2	2.10	119.75	109.65	11	1
3	A	632	PX4	O5-C9-O6	2.10	128.88	123.63	6	1
3	B	312	PX4	C31-C30-C29	2.10	103.76	114.37	1	1
3	B	368	PX4	O3-C1-C2	2.10	119.74	109.65	6	1
3	C	363	PX4	C5-N1-C4	2.10	103.46	108.98	3	1
3	A	644	PX4	O4-P1-O2	2.10	100.62	108.94	2	1
3	B	393	PX4	O7-C7-C6	2.10	115.87	108.34	8	1
3	B	394	PX4	C26-C25-C24	2.10	120.83	113.13	13	1
3	B	321	PX4	C1-C2-N1	2.10	122.55	115.82	11	1
3	C	350	PX4	O6-C9-C10	2.10	131.98	123.78	8	1
3	A	603	PX4	O1-P1-O2	2.09	122.19	112.44	14	1
3	A	629	PX4	C25-C24-C23	2.10	121.37	113.69	5	1
3	B	314	PX4	C36-C35-C34	2.09	99.22	113.36	10	1
3	B	329	PX4	O7-C7-C8	2.10	115.86	108.34	15	2
3	B	387	PX4	C5-N1-C4	2.10	114.48	108.98	15	1
3	C	351	PX4	C30-C29-C28	2.10	103.78	114.37	1	1
3	C	352	PX4	C25-C24-C23	2.10	106.02	113.69	12	1
3	A	620	PX4	C8-O5-C9	2.09	124.77	117.12	10	1
3	B	333	PX4	O7-C7-C6	2.09	100.83	108.34	7	1
3	B	338	PX4	C11-C10-C9	2.09	121.37	113.69	11	1
3	C	353	PX4	C4-N1-C3	2.09	114.48	108.98	6	1
3	A	651	PX4	O7-C7-C6	2.09	115.85	108.34	3	1
3	A	652	PX4	O7-C7-C8	2.09	115.85	108.34	8	1
3	B	306	PX4	O7-C7-C8	2.09	115.85	108.34	13	2
3	B	329	PX4	O5-C9-C10	2.09	105.45	111.83	8	1
3	C	301	PX4	P1-O4-C6	2.09	133.34	121.35	6	1
3	C	313	PX4	O1-P1-O2	2.09	122.18	112.44	2	1
3	C	313	PX4	C19-C18-C17	2.09	103.79	114.37	10	1
3	C	355	PX4	P1-O3-C1	2.09	131.22	121.26	2	1
3	A	643	PX4	O3-C1-C2	2.09	119.71	109.65	13	1
3	A	645	PX4	O5-C9-C10	2.09	105.46	111.83	8	1
3	C	350	PX4	C25-C24-C23	2.09	106.03	113.69	12	1
3	A	601	PX4	C19-C18-C17	2.09	103.81	114.37	3	1
3	B	343	PX4	C14-C13-C12	2.09	103.80	114.37	5	1
3	B	382	PX4	C5-N1-C3	2.09	103.49	108.98	8	1
3	A	627	PX4	O5-C9-O6	2.09	128.85	123.63	7	1
3	A	647	PX4	C15-C14-C13	2.09	103.81	114.37	14	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	307	PX4	C8-O5-C9	2.09	109.48	117.12	14	1
3	B	339	PX4	C4-N1-C3	2.09	114.46	108.98	10	1
3	A	630	PX4	C12-C11-C10	2.09	105.46	113.13	11	1
3	B	335	PX4	C25-C24-C23	2.09	106.05	113.69	4	1
3	A	604	PX4	C19-C18-C17	2.09	103.82	114.37	11	1
3	A	642	PX4	C26-C25-C24	2.09	105.46	113.13	15	1
3	B	337	PX4	P1-O3-C1	2.09	111.33	121.26	3	1
3	B	337	PX4	O1-P1-O2	2.09	122.15	112.44	12	1
3	B	341	PX4	O7-C7-C6	2.09	115.83	108.34	13	1
3	B	380	PX4	O7-C7-C8	2.09	115.83	108.34	9	1
3	B	343	PX4	O5-C9-O6	2.09	128.85	123.63	1	2
3	B	399	PX4	C5-N1-C3	2.09	114.46	108.98	6	1
3	B	333	PX4	C27-C26-C25	2.09	103.83	114.37	15	1
3	B	359	PX4	O3-C1-C2	2.09	119.68	109.65	4	1
3	C	309	PX4	O7-C7-C6	2.09	100.86	108.34	3	1
3	C	342	PX4	O1-P1-O2	2.09	122.15	112.44	7	1
3	B	365	PX4	O7-C7-C8	2.08	115.82	108.34	13	1
3	C	342	PX4	O4-P1-O2	2.09	100.67	108.94	12	1
3	A	603	PX4	C8-C7-C6	2.08	106.93	111.78	8	1
3	A	619	PX4	O7-C7-C8	2.08	115.82	108.34	4	1
3	B	395	PX4	C1-C2-N1	2.08	122.51	115.82	13	1
3	C	348	PX4	C12-C11-C10	2.08	120.79	113.13	7	1
3	A	619	PX4	C5-N1-C2	2.08	118.19	109.91	5	1
3	B	334	PX4	C26-C25-C24	2.08	105.47	113.13	2	1
3	B	353	PX4	O7-C7-C6	2.08	115.81	108.34	11	1
3	B	356	PX4	O5-C9-O6	2.08	128.84	123.63	8	1
3	B	400	PX4	C11-C10-C9	2.08	121.33	113.69	15	1
3	C	309	PX4	C4-N1-C3	2.08	103.50	108.98	11	1
3	C	356	PX4	C8-O5-C9	2.08	109.50	117.12	1	1
3	A	604	PX4	O8-C23-C24	2.08	131.92	123.78	3	1
3	A	620	PX4	O8-C23-C24	2.08	131.92	123.78	13	1
3	B	306	PX4	C26-C25-C24	2.08	120.77	113.13	1	1
3	B	307	PX4	C3-N1-C2	2.08	118.18	109.91	9	1
3	B	352	PX4	O5-C9-O6	2.08	128.83	123.63	2	1
3	B	388	PX4	O8-C23-C24	2.08	131.93	123.78	3	1
3	B	362	PX4	C5-N1-C3	2.08	103.51	108.98	10	1
3	A	628	PX4	C4-N1-C3	2.08	114.44	108.98	11	2
3	B	380	PX4	C18-C17-C16	2.08	103.85	114.37	2	1
3	C	320	PX4	O4-P1-O2	2.08	100.69	108.94	3	1
3	C	332	PX4	C25-C24-C23	2.08	106.07	113.69	15	1
3	C	340	PX4	O4-P1-O2	2.08	100.69	108.94	6	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	C	358	PX4	P1-O4-C6	2.08	109.43	121.35	3	1
3	A	624	PX4	C11-C10-C9	2.08	106.08	113.69	1	1
3	B	301	PX4	O8-C23-C24	2.08	115.65	123.78	13	1
3	A	633	PX4	C13-C12-C11	2.08	103.86	114.37	7	1
3	B	305	PX4	C5-N1-C2	2.08	118.17	109.91	15	1
3	B	314	PX4	C5-N1-C2	2.08	118.17	109.91	12	1
3	C	311	PX4	C1-C2-N1	2.08	122.49	115.82	9	1
3	C	313	PX4	C30-C29-C28	2.08	103.87	114.37	3	1
3	C	321	PX4	C26-C25-C24	2.08	105.49	113.13	1	1
3	C	325	PX4	C25-C24-C23	2.08	106.08	113.69	2	2
3	C	343	PX4	C4-N1-C2	2.08	118.17	109.91	5	1
3	A	624	PX4	O7-C7-C8	2.08	115.79	108.34	10	1
3	A	628	PX4	C26-C25-C24	2.08	120.75	113.13	6	1
3	B	351	PX4	C4-N1-C3	2.08	103.52	108.98	7	1
3	B	356	PX4	O4-P1-O2	2.08	100.70	108.94	15	1
3	C	354	PX4	C16-C15-C14	2.08	103.87	114.37	15	1
3	A	608	PX4	O6-C9-C10	2.07	131.90	123.78	4	1
3	A	647	PX4	C8-O5-C9	2.08	109.53	117.12	6	1
3	B	369	PX4	C12-C11-C10	2.08	105.50	113.13	5	2
3	B	397	PX4	C12-C11-C10	2.08	105.50	113.13	15	1
3	B	304	PX4	O3-P1-O2	2.07	117.16	108.94	3	1
3	B	399	PX4	C14-C13-C12	2.07	103.88	114.37	10	1
3	C	336	PX4	C30-C29-C28	2.08	103.88	114.37	4	1
3	C	328	PX4	C8-O5-C9	2.07	109.54	117.12	7	1
3	C	338	PX4	C8-O5-C9	2.07	124.70	117.12	15	3
3	C	360	PX4	C5-N1-C4	2.08	103.53	108.98	3	1
3	C	362	PX4	C8-O5-C9	2.08	109.53	117.12	4	1
3	A	618	PX4	O1-P1-O2	2.07	122.09	112.44	11	1
3	A	629	PX4	C1-C2-N1	2.07	122.48	115.82	8	1
3	B	310	PX4	C4-N1-C2	2.07	118.15	109.91	3	1
3	B	318	PX4	C8-O5-C9	2.07	109.54	117.12	7	1
3	A	621	PX4	C32-C31-C30	2.07	124.84	114.37	9	1
3	A	631	PX4	O5-C9-C10	2.07	105.51	111.83	10	2
3	C	357	PX4	C8-O5-C9	2.07	109.54	117.12	6	1
3	A	634	PX4	O7-C7-C8	2.07	115.78	108.34	15	1
3	A	654	PX4	C11-C10-C9	2.07	121.29	113.69	11	1
3	C	302	PX4	C8-O5-C9	2.07	109.54	117.12	13	1
3	A	606	PX4	O5-C9-O6	2.07	128.81	123.63	14	1
3	B	341	PX4	O1-P1-O2	2.07	122.08	112.44	9	1
3	B	351	PX4	C3-N1-C2	2.07	101.68	109.91	1	1
3	B	366	PX4	O7-C7-C6	2.07	100.91	108.34	9	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	377	PX4	C27-C26-C25	2.07	103.89	114.37	11	1
3	B	356	PX4	C16-C15-C14	2.07	103.90	114.37	3	1
3	B	371	PX4	C4-N1-C2	2.07	118.14	109.91	1	1
3	C	312	PX4	C11-C10-C9	2.07	121.28	113.69	10	1
3	C	320	PX4	C26-C25-C24	2.07	120.74	113.13	6	1
3	C	334	PX4	O7-C23-C24	2.07	107.00	111.48	4	1
3	A	618	PX4	O5-C9-O6	2.07	128.80	123.63	1	1
3	A	619	PX4	C8-C7-C6	2.07	106.96	111.78	11	1
3	A	625	PX4	C4-N1-C2	2.07	118.14	109.91	2	1
3	A	629	PX4	O7-C23-C24	2.07	107.00	111.48	7	1
3	A	642	PX4	C31-C30-C29	2.07	103.91	114.37	9	1
3	A	638	PX4	C25-C24-C23	2.07	106.11	113.69	5	1
3	B	302	PX4	O7-C7-C8	2.07	115.77	108.34	14	1
3	B	317	PX4	O5-C8-C7	2.07	114.36	108.40	11	2
3	B	369	PX4	C19-C18-C17	2.07	124.83	114.37	1	1
3	B	369	PX4	O7-C7-C6	2.07	115.77	108.34	3	1
3	B	374	PX4	O7-C23-C24	2.07	107.00	111.48	8	2
3	C	307	PX4	C18-C17-C16	2.07	103.91	114.37	12	1
3	C	327	PX4	C16-C15-C14	2.07	103.91	114.37	15	1
3	B	325	PX4	C15-C14-C13	2.07	103.91	114.37	12	1
3	B	344	PX4	O7-C7-C6	2.07	115.77	108.34	14	1
3	C	320	PX4	C4-N1-C3	2.07	103.54	108.98	11	1
3	C	322	PX4	O4-P1-O2	2.07	100.73	108.94	2	1
3	A	606	PX4	C11-C10-C9	2.07	121.27	113.69	6	1
3	B	304	PX4	C3-N1-C2	2.07	118.13	109.91	10	1
3	B	308	PX4	C31-C30-C29	2.07	103.92	114.37	8	2
3	A	616	PX4	C8-O5-C9	2.07	109.56	117.12	15	1
3	B	301	PX4	C34-C33-C32	2.07	103.92	114.37	10	1
3	A	632	PX4	C8-O5-C9	2.07	124.67	117.12	15	1
3	B	302	PX4	C11-C10-C9	2.07	106.12	113.69	2	1
3	B	349	PX4	O6-C9-C10	2.07	131.87	123.78	3	1
3	A	610	PX4	P1-O3-C1	2.06	111.43	121.26	6	2
3	A	618	PX4	C13-C12-C11	2.06	103.93	114.37	11	1
3	B	308	PX4	C32-C31-C30	2.07	103.93	114.37	10	1
3	B	325	PX4	C5-N1-C4	2.07	103.55	108.98	11	1
3	B	382	PX4	C12-C11-C10	2.07	105.53	113.13	9	1
3	C	325	PX4	C5-N1-C4	2.07	103.55	108.98	11	1
3	C	337	PX4	C5-N1-C3	2.07	114.40	108.98	8	1
3	C	343	PX4	O5-C9-O6	2.07	128.80	123.63	13	1
3	B	390	PX4	C11-C10-C9	2.07	121.26	113.69	3	1
3	B	346	PX4	O7-C23-O8	2.06	128.53	123.70	15	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	A	601	PX4	C25-C24-C23	2.06	106.13	113.69	15	1
3	A	651	PX4	C16-C15-C14	2.06	103.93	114.37	11	1
3	C	326	PX4	C25-C24-C23	2.06	106.13	113.69	4	1
3	B	302	PX4	C26-C25-C24	2.06	105.55	113.13	15	1
3	B	313	PX4	O1-P1-O2	2.06	122.04	112.44	11	1
3	B	330	PX4	C5-N1-C2	2.06	118.11	109.91	4	1
3	B	372	PX4	C20-C19-C18	2.06	124.80	114.37	6	1
3	C	359	PX4	C1-C2-N1	2.06	122.45	115.82	15	1
3	A	613	PX4	C5-N1-C4	2.06	114.39	108.98	9	1
3	A	616	PX4	C3-N1-C2	2.06	118.10	109.91	3	1
3	B	324	PX4	O1-P1-O2	2.06	122.04	112.44	8	1
3	B	375	PX4	O5-C8-C7	2.06	114.34	108.40	14	1
3	B	376	PX4	C30-C29-C28	2.06	103.95	114.37	5	2
3	C	341	PX4	C4-N1-C3	2.06	114.39	108.98	5	1
3	A	605	PX4	C3-N1-C2	2.06	118.10	109.91	4	1
3	A	608	PX4	C4-N1-C3	2.06	103.57	108.98	15	1
3	A	653	PX4	P1-O4-C6	2.06	133.15	121.35	3	1
3	B	371	PX4	C12-C11-C10	2.06	105.56	113.13	4	1
3	C	304	PX4	O1-P1-O2	2.06	122.03	112.44	7	1
3	C	305	PX4	C5-N1-C4	2.06	103.56	108.98	1	2
3	C	354	PX4	C1-C2-N1	2.06	122.44	115.82	12	1
3	A	610	PX4	O8-C23-C24	2.06	131.83	123.78	5	1
3	B	379	PX4	O6-C9-C10	2.06	131.83	123.78	9	1
3	C	304	PX4	P1-O3-C1	2.06	111.46	121.26	8	1
3	B	386	PX4	C1-C2-N1	2.06	122.42	115.82	9	1
3	C	359	PX4	C4-N1-C3	2.06	103.57	108.98	6	1
3	A	607	PX4	O3-C1-C2	2.05	119.54	109.65	1	1
3	A	607	PX4	C33-C32-C31	2.05	103.98	114.37	1	1
3	A	629	PX4	C18-C17-C16	2.06	103.98	114.37	8	1
3	A	627	PX4	C5-N1-C4	2.05	103.58	108.98	9	1
3	A	630	PX4	O1-P1-O2	2.05	122.00	112.44	12	1
3	B	318	PX4	C16-C15-C14	2.05	124.75	114.37	10	1
3	B	320	PX4	O7-C7-C8	2.05	115.71	108.34	3	1
3	B	323	PX4	P1-O3-C1	2.05	131.04	121.26	6	1
3	B	325	PX4	C5-N1-C2	2.05	118.07	109.91	8	1
3	B	332	PX4	O5-C9-C10	2.05	105.57	111.83	11	1
3	B	372	PX4	C25-C24-C23	2.05	106.17	113.69	2	2
3	B	376	PX4	C34-C33-C32	2.05	103.99	114.37	4	1
3	B	398	PX4	O7-C7-C8	2.05	115.71	108.34	14	2
3	C	302	PX4	O7-C7-C6	2.05	100.98	108.34	8	2
3	A	604	PX4	C5-N1-C4	2.05	114.37	108.98	14	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	A	637	PX4	C5-N1-C4	2.05	103.59	108.98	14	2
3	A	639	PX4	C11-C10-C9	2.05	106.17	113.69	8	1
3	B	305	PX4	C25-C24-C23	2.05	106.17	113.69	2	1
3	B	376	PX4	C5-N1-C3	2.05	103.58	108.98	11	1
3	B	378	PX4	C13-C12-C11	2.05	103.99	114.37	9	1
3	C	319	PX4	O7-C7-C8	2.05	115.71	108.34	6	1
3	C	320	PX4	C11-C10-C9	2.05	106.18	113.69	9	1
3	B	306	PX4	O1-P1-O2	2.05	121.98	112.44	4	1
3	B	375	PX4	P1-O3-C1	2.05	131.02	121.26	6	1
3	B	386	PX4	C15-C14-C13	2.05	124.73	114.37	15	1
3	C	310	PX4	O1-P1-O2	2.05	121.98	112.44	3	1
3	C	327	PX4	C1-C2-N1	2.05	122.40	115.82	5	1
3	A	615	PX4	C8-O5-C9	2.05	109.63	117.12	11	1
3	A	618	PX4	C1-C2-N1	2.05	122.39	115.82	7	1
3	A	636	PX4	O5-C9-O6	2.05	128.75	123.63	4	1
3	C	301	PX4	C30-C29-C28	2.05	104.01	114.37	4	1
3	C	305	PX4	C16-C15-C14	2.05	104.01	114.37	6	1
3	C	344	PX4	C25-C24-C23	2.05	106.19	113.69	11	1
3	C	352	PX4	O4-P1-O2	2.05	117.06	108.94	10	1
3	A	624	PX4	C20-C19-C18	2.05	104.02	114.37	11	1
3	A	638	PX4	O7-C23-O8	2.05	118.92	123.70	4	1
3	B	303	PX4	C31-C30-C29	2.05	104.02	114.37	11	1
3	B	310	PX4	C4-N1-C3	2.05	103.60	108.98	5	1
3	B	349	PX4	C3-N1-C2	2.05	118.05	109.91	5	1
3	B	362	PX4	C14-C13-C12	2.05	104.03	114.37	7	1
3	B	376	PX4	O1-P1-O2	2.05	121.97	112.44	6	1
3	B	386	PX4	C4-N1-C2	2.05	118.05	109.91	4	1
3	C	325	PX4	O1-P1-O2	2.05	121.97	112.44	11	1
3	C	351	PX4	C5-N1-C4	2.05	114.35	108.98	11	1
3	A	604	PX4	C5-N1-C3	2.05	103.60	108.98	7	1
3	A	613	PX4	C29-C28-C27	2.05	104.03	114.37	7	1
3	A	615	PX4	O7-C7-C6	2.05	115.68	108.34	14	1
3	C	352	PX4	C4-N1-C2	2.05	118.04	109.91	11	1
3	C	359	PX4	O7-C7-C8	2.05	115.69	108.34	4	1
3	B	322	PX4	O5-C9-O6	2.05	128.75	123.63	1	1
3	A	642	PX4	P1-O4-C6	2.04	133.06	121.35	6	1
3	A	649	PX4	C8-O5-C9	2.04	109.64	117.12	13	1
3	B	317	PX4	C12-C11-C10	2.04	120.64	113.13	8	1
3	B	335	PX4	C19-C18-C17	2.05	104.03	114.37	8	1
3	B	369	PX4	O6-C9-C10	2.05	131.78	123.78	15	1
3	C	359	PX4	O3-P1-O2	2.05	117.04	108.94	8	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	C	363	PX4	P1-O3-C1	2.05	131.00	121.26	8	1
3	C	337	PX4	C3-N1-C2	2.05	101.78	109.91	6	2
3	B	327	PX4	C31-C30-C29	2.04	104.04	114.37	12	1
3	B	379	PX4	C20-C19-C18	2.04	124.70	114.37	13	1
3	C	330	PX4	C1-C2-N1	2.04	122.38	115.82	3	1
3	C	363	PX4	O1-P1-O4	2.04	116.83	107.57	9	1
3	A	609	PX4	C3-N1-C2	2.04	101.79	109.91	3	1
3	B	387	PX4	O5-C8-C7	2.04	114.28	108.40	9	2
3	B	395	PX4	C25-C24-C23	2.04	106.21	113.69	1	1
3	C	314	PX4	O8-C23-C24	2.04	131.77	123.78	13	1
3	A	629	PX4	C5-N1-C3	2.04	103.61	108.98	13	1
3	B	369	PX4	O5-C9-C10	2.04	105.61	111.83	1	2
3	B	374	PX4	C4-N1-C3	2.04	103.62	108.98	8	1
3	B	394	PX4	C8-O5-C9	2.04	109.66	117.12	6	1
3	C	312	PX4	C16-C15-C14	2.04	104.05	114.37	9	2
3	C	315	PX4	C4-N1-C3	2.04	114.34	108.98	1	1
3	A	626	PX4	C11-C10-C9	2.04	106.22	113.69	3	1
3	A	632	PX4	C17-C16-C15	2.04	104.06	114.37	12	1
3	A	639	PX4	C25-C24-C23	2.04	106.22	113.69	1	1
3	C	336	PX4	C5-N1-C4	2.04	103.62	108.98	12	1
3	C	351	PX4	C19-C18-C17	2.04	104.05	114.37	9	1
3	C	364	PX4	C18-C17-C16	2.04	104.05	114.37	7	1
3	A	607	PX4	O7-C23-O8	2.04	128.47	123.70	6	1
3	A	622	PX4	C1-C2-N1	2.04	122.36	115.82	14	1
3	B	313	PX4	O5-C9-C10	2.04	105.62	111.83	7	2
3	B	364	PX4	O4-P1-O2	2.04	100.85	108.94	7	1
3	C	310	PX4	C25-C24-C23	2.04	106.22	113.69	1	1
3	B	366	PX4	C8-O5-C9	2.04	109.67	117.12	6	1
3	C	327	PX4	C4-N1-C3	2.04	114.33	108.98	10	1
3	C	338	PX4	O1-P1-O4	2.04	116.81	107.57	14	1
3	A	630	PX4	C5-N1-C3	2.04	103.63	108.98	11	1
3	B	307	PX4	O7-C23-O8	2.04	128.47	123.70	8	1
3	B	316	PX4	C25-C24-C23	2.04	121.15	113.69	9	1
3	A	608	PX4	C1-C2-N1	2.03	122.35	115.82	4	1
3	A	610	PX4	C5-N1-C2	2.03	101.82	109.91	13	1
3	A	622	PX4	P1-O3-C1	2.03	111.57	121.26	7	1
3	A	624	PX4	P1-O3-C1	2.03	130.94	121.26	15	1
3	A	653	PX4	C12-C11-C10	2.03	105.65	113.13	1	1
3	B	307	PX4	C16-C15-C14	2.03	104.08	114.37	6	1
3	B	331	PX4	O7-C7-C8	2.04	115.64	108.34	3	1
3	B	336	PX4	O7-C7-C6	2.04	115.65	108.34	2	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	338	PX4	C5-N1-C3	2.04	103.63	108.98	7	1
3	B	355	PX4	C11-C10-C9	2.04	121.15	113.69	9	1
3	C	323	PX4	C12-C11-C10	2.04	105.64	113.13	8	2
3	C	342	PX4	O8-C23-C24	2.04	131.74	123.78	3	1
3	C	348	PX4	O1-P1-O2	2.04	121.92	112.44	4	1
3	C	356	PX4	O5-C8-C7	2.04	114.27	108.40	7	1
3	B	332	PX4	P1-O3-C1	2.03	130.94	121.26	5	1
3	B	336	PX4	P1-O4-C6	2.03	133.00	121.35	8	1
3	B	380	PX4	C11-C10-C9	2.03	106.24	113.69	2	1
3	C	330	PX4	C14-C13-C12	2.03	104.09	114.37	7	1
3	C	333	PX4	O5-C8-C7	2.03	114.26	108.40	1	1
3	C	345	PX4	O1-P1-O2	2.03	121.91	112.44	7	1
3	C	356	PX4	C27-C26-C25	2.03	104.08	114.37	14	1
3	B	312	PX4	C33-C32-C31	2.03	104.09	114.37	12	1
3	B	323	PX4	O3-C1-C2	2.03	119.43	109.65	9	1
3	B	377	PX4	O7-C23-C24	2.03	107.08	111.48	14	2
3	C	364	PX4	O7-C7-C8	2.03	101.05	108.34	7	1
3	B	319	PX4	C28-C27-C26	2.03	104.10	114.37	1	1
3	C	311	PX4	C14-C13-C12	2.03	104.10	114.37	12	1
3	C	333	PX4	C3-N1-C2	2.03	117.98	109.91	14	1
3	C	336	PX4	C1-C2-N1	2.03	122.33	115.82	10	1
3	C	338	PX4	C3-N1-C2	2.03	117.98	109.91	12	1
3	C	339	PX4	O7-C7-C8	2.03	115.63	108.34	3	1
3	A	635	PX4	O1-P1-O4	2.03	116.76	107.57	7	1
3	A	648	PX4	C3-N1-C2	2.03	101.84	109.91	11	1
3	A	606	PX4	O1-P1-O2	2.03	121.88	112.44	5	1
3	A	645	PX4	C25-C24-C23	2.03	121.12	113.69	7	1
3	B	328	PX4	O1-P1-O4	2.03	116.76	107.57	15	1
3	B	371	PX4	C11-C10-C9	2.03	106.26	113.69	12	1
3	B	373	PX4	C5-N1-C2	2.03	117.97	109.91	8	1
3	C	339	PX4	C4-N1-C2	2.03	117.98	109.91	15	1
3	C	302	PX4	C13-C12-C11	2.03	104.11	114.37	12	1
3	B	377	PX4	C8-O5-C9	2.03	109.71	117.12	2	1
3	B	379	PX4	O8-C23-C24	2.03	131.71	123.78	1	1
3	C	304	PX4	O8-C23-C24	2.03	131.71	123.78	12	1
3	C	311	PX4	C4-N1-C3	2.03	103.65	108.98	4	1
3	C	327	PX4	C5-N1-C2	2.03	101.85	109.91	11	1
3	C	351	PX4	C27-C26-C25	2.03	104.12	114.37	6	1
3	C	360	PX4	C26-C25-C24	2.03	105.67	113.13	12	1
3	A	615	PX4	C4-N1-C3	2.03	103.65	108.98	11	1
3	B	379	PX4	O1-P1-O2	2.02	121.86	112.44	5	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	B	390	PX4	O7-C23-O8	2.03	128.44	123.70	6	2
3	C	314	PX4	O5-C9-O6	2.03	128.70	123.63	4	1
3	C	362	PX4	C20-C19-C18	2.03	104.12	114.37	3	1
3	B	306	PX4	O1-P1-O3	2.03	116.75	107.57	11	1
3	A	617	PX4	C13-C12-C11	2.02	104.14	114.37	11	1
3	A	644	PX4	O1-P1-O2	2.02	121.86	112.44	12	1
3	A	623	PX4	C20-C19-C18	2.02	104.14	114.37	14	1
3	C	316	PX4	O7-C7-C8	2.02	115.61	108.34	5	1
3	B	384	PX4	C26-C25-C24	2.02	105.69	113.13	3	1
3	C	322	PX4	C31-C30-C29	2.02	104.14	114.37	10	1
3	A	641	PX4	C5-N1-C3	2.02	114.29	108.98	5	1
3	A	632	PX4	C13-C12-C11	2.02	104.15	114.37	12	1
3	B	306	PX4	P1-O3-C1	2.02	130.88	121.26	14	1
3	B	321	PX4	C28-C27-C26	2.02	104.15	114.37	9	1
3	B	358	PX4	O7-C7-C8	2.02	101.09	108.34	9	1
3	C	305	PX4	O3-P1-O2	2.02	116.95	108.94	5	1
3	C	347	PX4	O3-C1-C2	2.02	119.38	109.65	9	1
3	C	362	PX4	C32-C31-C30	2.02	104.14	114.37	10	1
3	B	378	PX4	O7-C7-C6	2.02	101.09	108.34	3	1
3	C	364	PX4	C26-C25-C24	2.02	105.70	113.13	5	1
3	A	639	PX4	O3-C1-C2	2.02	119.37	109.65	6	1
3	A	618	PX4	O7-C7-C6	2.02	115.59	108.34	14	1
3	B	312	PX4	O1-P1-O2	2.02	121.84	112.44	2	1
3	B	358	PX4	O7-C7-C6	2.02	115.59	108.34	9	1
3	B	397	PX4	C11-C10-C9	2.02	121.09	113.69	12	1
3	C	305	PX4	O7-C7-C8	2.02	115.59	108.34	3	1
3	C	312	PX4	O7-C7-C8	2.02	115.59	108.34	8	1
3	C	312	PX4	C15-C14-C13	2.02	104.16	114.37	13	1
3	C	327	PX4	C20-C19-C18	2.02	104.16	114.37	8	1
3	C	332	PX4	C33-C32-C31	2.02	104.16	114.37	9	1
3	B	306	PX4	O3-C1-C2	2.02	119.36	109.65	6	1
3	B	316	PX4	O1-P1-O2	2.02	121.83	112.44	14	1
3	A	603	PX4	C5-N1-C2	2.02	117.92	109.91	2	1
3	A	615	PX4	O1-P1-O2	2.02	121.82	112.44	12	1
3	B	308	PX4	C8-C7-C6	2.02	107.08	111.78	11	1
3	B	363	PX4	O8-C23-C24	2.02	131.67	123.78	7	1
3	C	305	PX4	O1-P1-O4	2.02	116.70	107.57	1	1
3	C	322	PX4	P1-O3-C1	2.02	111.67	121.26	3	1
3	C	337	PX4	C4-N1-C3	2.02	114.27	108.98	5	1
3	C	339	PX4	C26-C25-C24	2.02	105.72	113.13	12	1
3	C	361	PX4	C4-N1-C3	2.02	103.68	108.98	7	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	A	613	PX4	C25-C24-C23	2.01	121.07	113.69	8	1
3	A	622	PX4	C8-O5-C9	2.01	124.48	117.12	14	1
3	A	632	PX4	C19-C18-C17	2.01	104.19	114.37	6	1
3	C	314	PX4	C18-C17-C16	2.02	104.18	114.37	2	1
3	A	646	PX4	C27-C26-C25	2.01	104.19	114.37	6	1
3	A	652	PX4	O8-C23-C24	2.01	131.66	123.78	6	1
3	B	336	PX4	C12-C11-C10	2.01	105.73	113.13	2	1
3	C	343	PX4	O3-C1-C2	2.01	119.34	109.65	14	1
3	B	384	PX4	O1-P1-O4	2.01	116.69	107.57	8	1
3	C	321	PX4	C8-O5-C9	2.01	109.76	117.12	4	1
3	C	354	PX4	O3-C1-C2	2.01	119.33	109.65	1	1
3	A	620	PX4	C33-C32-C31	2.01	104.20	114.37	2	1
3	A	629	PX4	O3-C1-C2	2.01	99.97	109.65	3	1
3	B	334	PX4	C5-N1-C4	2.01	114.26	108.98	9	1
3	B	360	PX4	O7-C7-C8	2.01	115.56	108.34	7	1
3	B	362	PX4	O1-P1-O2	2.01	121.80	112.44	7	1
3	B	370	PX4	C12-C11-C10	2.01	105.74	113.13	10	1
3	B	385	PX4	O7-C7-C8	2.01	115.56	108.34	10	1
3	C	312	PX4	O5-C9-O6	2.01	128.66	123.63	5	1
3	B	372	PX4	C27-C26-C25	2.01	104.21	114.37	13	1
3	C	341	PX4	C19-C18-C17	2.01	104.20	114.37	9	1
3	A	608	PX4	C17-C16-C15	2.01	124.53	114.37	10	1
3	A	614	PX4	C27-C26-C25	2.01	104.22	114.37	10	1
3	B	305	PX4	C5-N1-C3	2.01	114.25	108.98	1	1
3	B	358	PX4	O5-C8-C7	2.01	114.19	108.40	15	1
3	B	322	PX4	C25-C24-C23	2.01	106.33	113.69	1	1
3	B	370	PX4	C25-C24-C23	2.01	106.33	113.69	9	1
3	C	332	PX4	C5-N1-C3	2.01	114.25	108.98	11	1
3	C	337	PX4	O3-P1-O2	2.01	116.89	108.94	10	1
3	C	348	PX4	O4-P1-O2	2.01	100.97	108.94	14	1
3	A	610	PX4	O6-C9-C10	2.01	115.93	123.78	7	1
3	A	647	PX4	O1-P1-O2	2.01	121.78	112.44	12	1
3	B	350	PX4	O3-P1-O2	2.01	100.98	108.94	2	1
3	B	381	PX4	C14-C13-C12	2.01	104.22	114.37	12	1
3	B	358	PX4	P1-O3-C1	2.01	130.81	121.26	12	1
3	C	340	PX4	C5-N1-C4	2.01	103.70	108.98	9	1
3	B	350	PX4	C25-C24-C23	2.01	106.35	113.69	11	1
3	A	630	PX4	O5-C8-C7	2.00	114.17	108.40	12	1
3	A	643	PX4	C5-N1-C3	2.00	103.71	108.98	7	1
3	A	651	PX4	C11-C10-C9	2.01	121.04	113.69	9	1
3	B	390	PX4	O1-P1-O4	2.01	116.66	107.57	11	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
3	A	654	PX4	C15-C14-C13	2.00	104.24	114.37	9	1
3	B	301	PX4	C8-O5-C9	2.00	109.79	117.12	10	1
3	C	328	PX4	O4-P1-O2	2.00	100.99	108.94	8	1
3	C	333	PX4	C28-C27-C26	2.00	124.50	114.37	14	1
3	B	367	PX4	O1-P1-O2	2.00	121.77	112.44	8	1
3	C	335	PX4	O5-C9-C10	2.00	105.72	111.83	7	1
3	C	343	PX4	C25-C24-C23	2.00	121.04	113.69	14	1
3	C	355	PX4	C4-N1-C3	2.00	103.71	108.98	14	1
3	C	356	PX4	C26-C25-C24	2.00	105.76	113.13	15	1
3	C	361	PX4	C27-C26-C25	2.00	104.24	114.37	11	1
3	A	618	PX4	C26-C25-C24	2.00	105.77	113.13	11	1
3	B	320	PX4	C8-O5-C9	2.00	109.80	117.12	11	1
3	B	330	PX4	O5-C9-C10	2.00	105.73	111.83	13	1
3	B	342	PX4	C1-C2-N1	2.00	122.25	115.82	10	1
3	A	624	PX4	C8-O5-C9	2.00	109.80	117.12	5	1
3	A	647	PX4	O5-C9-O6	2.00	128.64	123.63	12	1
3	B	369	PX4	O1-P1-O3	2.00	116.64	107.57	3	1
3	C	311	PX4	O7-C7-C6	2.00	101.16	108.34	15	1
3	C	319	PX4	O1-P1-O2	2.00	121.76	112.44	11	1
3	B	301	PX4	O6-C9-C10	2.00	131.61	123.78	10	1
3	A	630	PX4	C5-N1-C4	2.00	103.72	108.98	15	1
3	B	302	PX4	C31-C30-C29	2.00	104.26	114.37	8	1
3	B	361	PX4	C30-C29-C28	2.00	124.48	114.37	12	1
3	C	326	PX4	O3-P1-O2	2.00	116.86	108.94	13	1

There are no chirality outliers.

All unique torsion outliers are listed below.

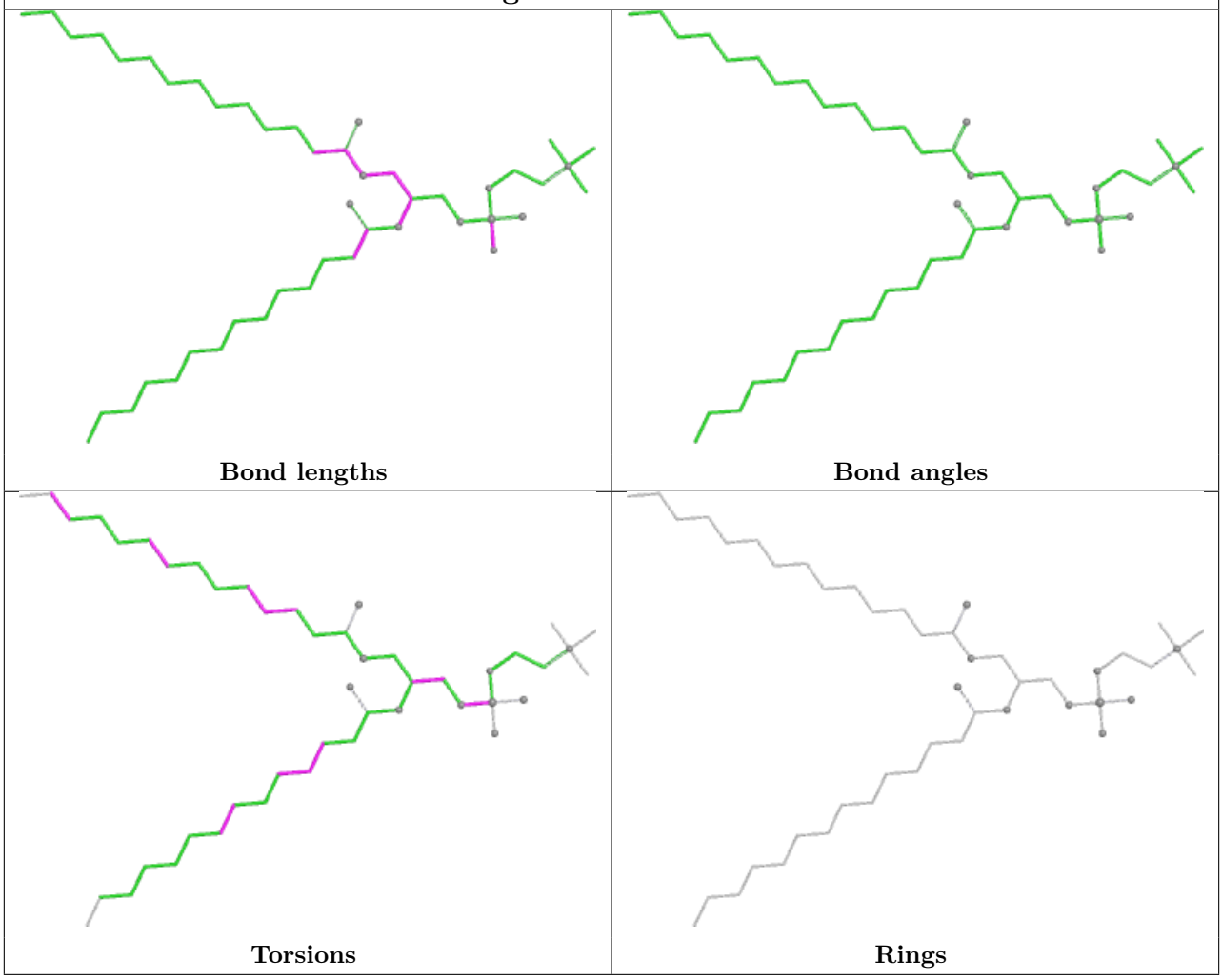
Mol	Chain	Res	Type	Atoms	Models (Total)
3	C	320	PX4	C7-C6-O4-P1	1

There are no ring outliers.

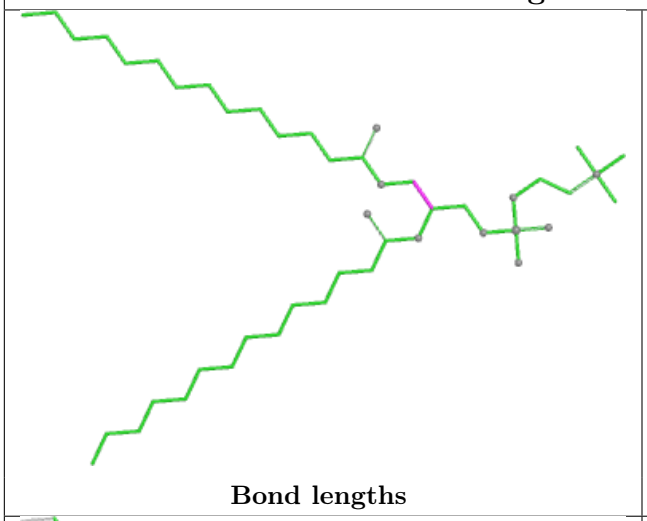
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

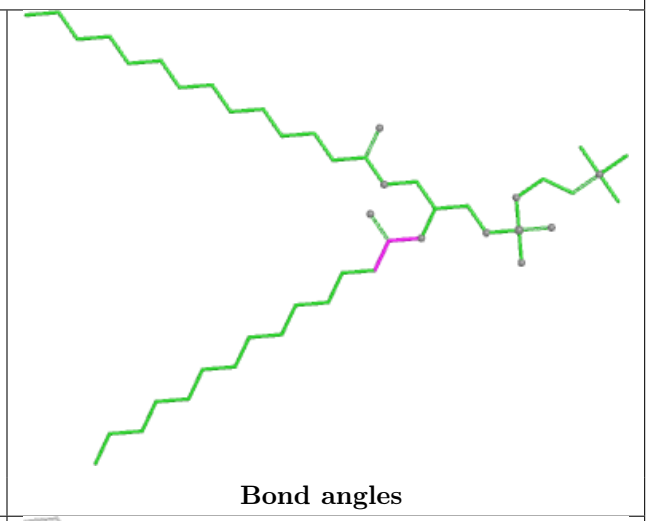
Ligand PX4 C 308



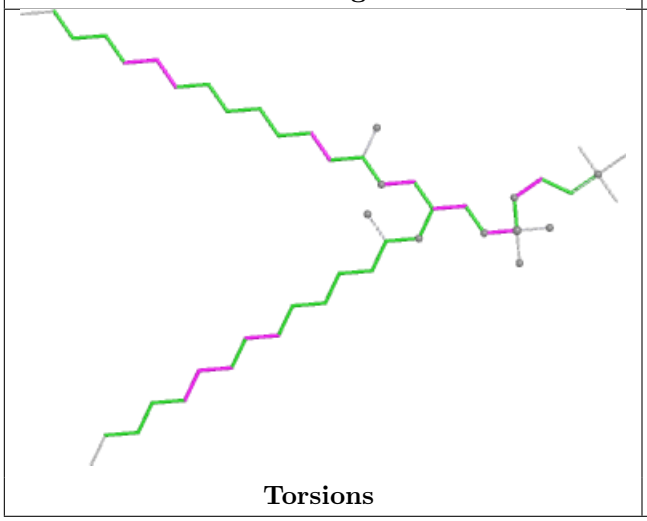
Ligand PX4 C 335



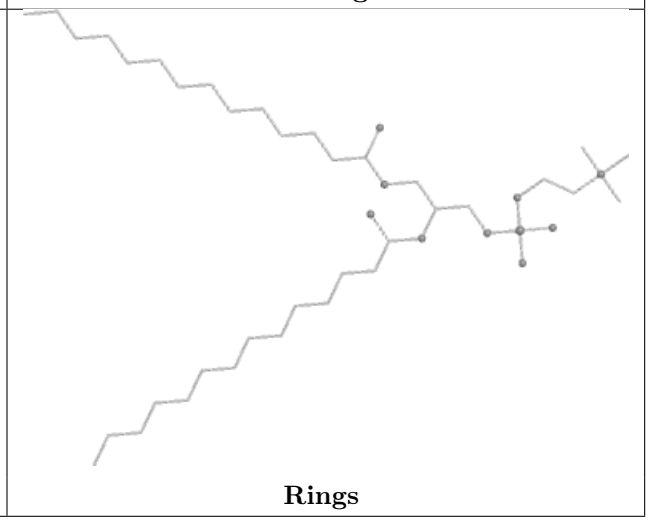
Bond lengths



Bond angles

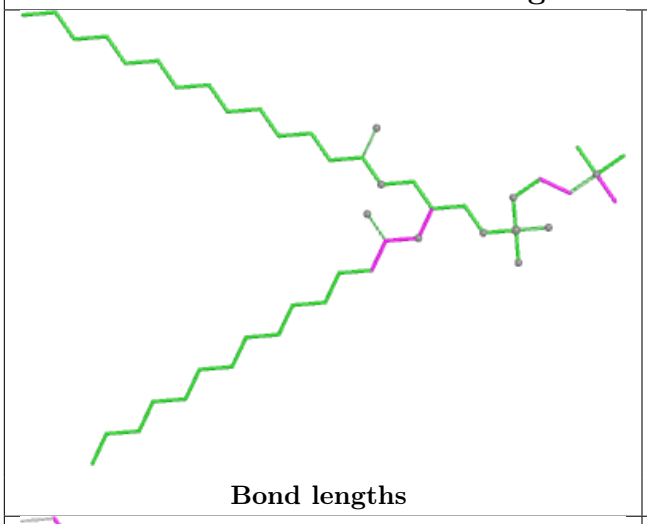


Torsions

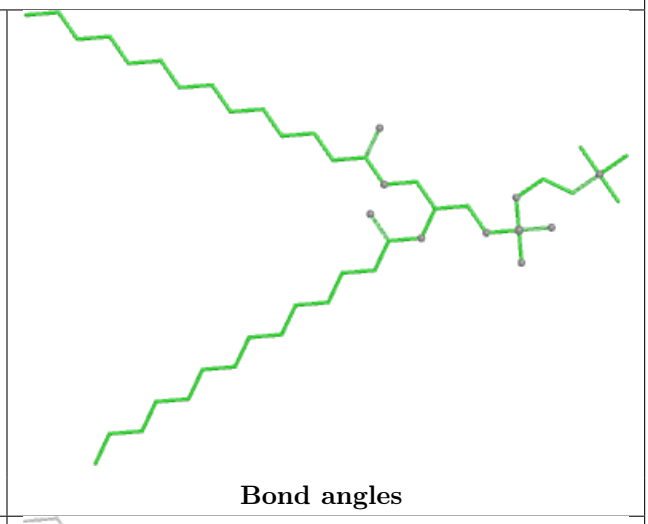


Rings

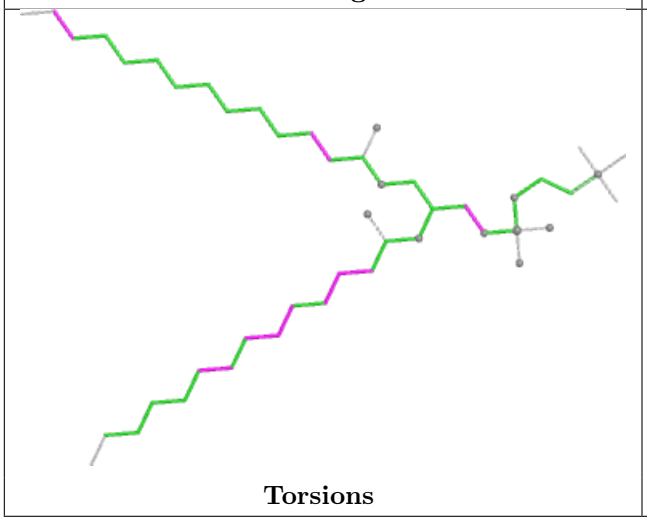
Ligand PX4 B 330



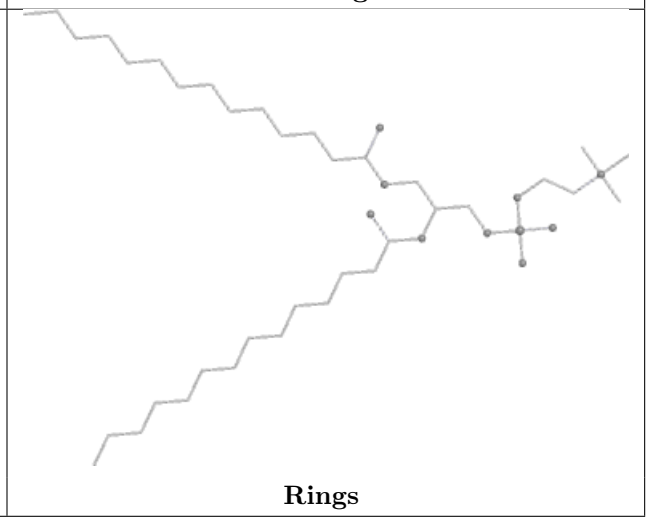
Bond lengths



Bond angles

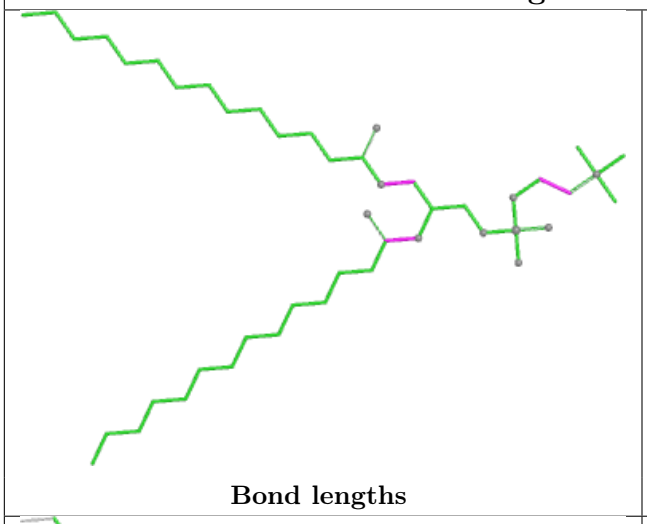


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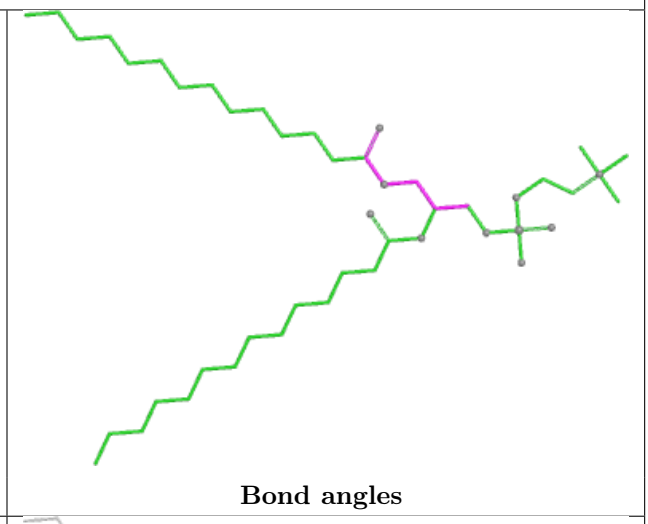


Rings

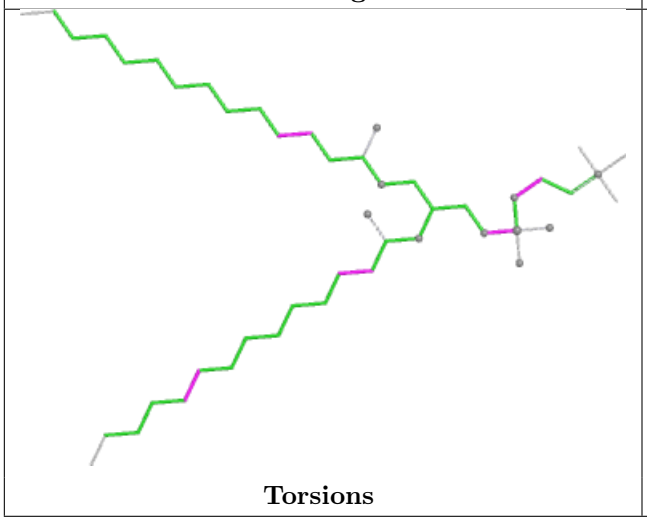
Ligand PX4 B 396



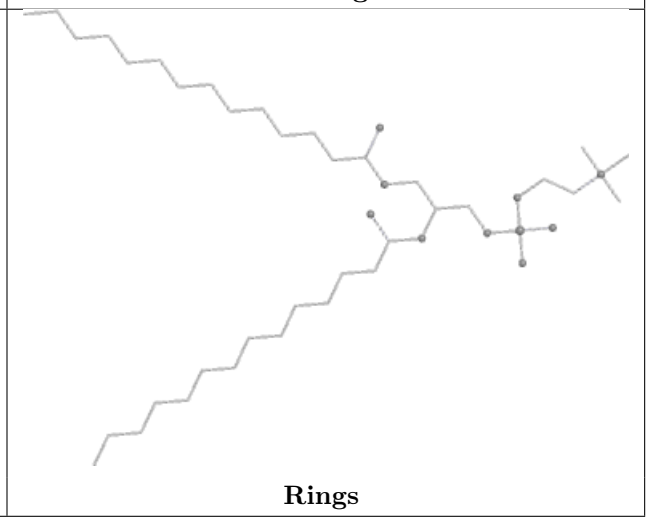
Bond lengths



Bond angles

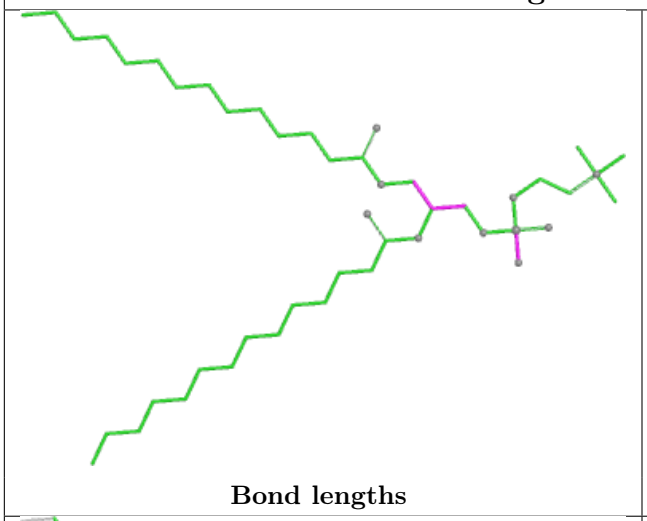


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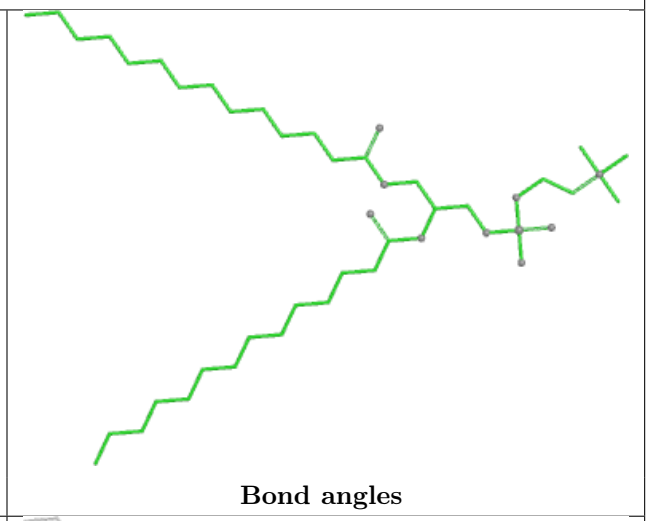


Rings

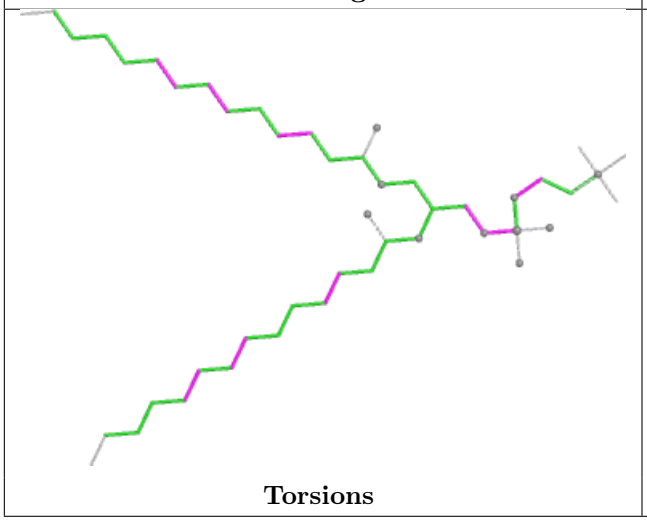
Ligand PX4 C 309



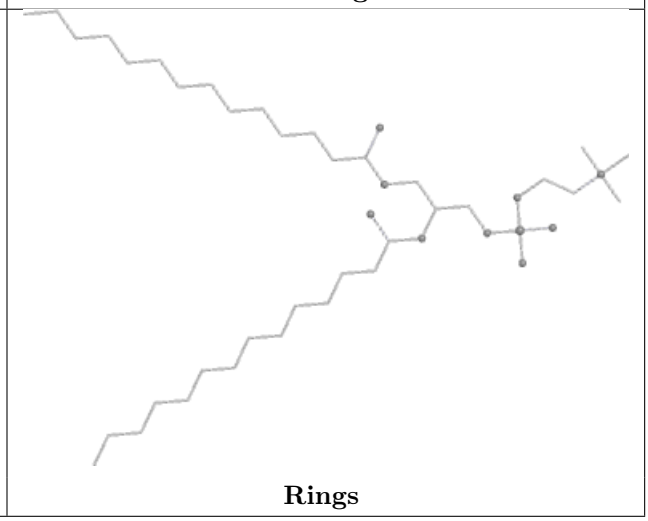
Bond lengths



Bond angles

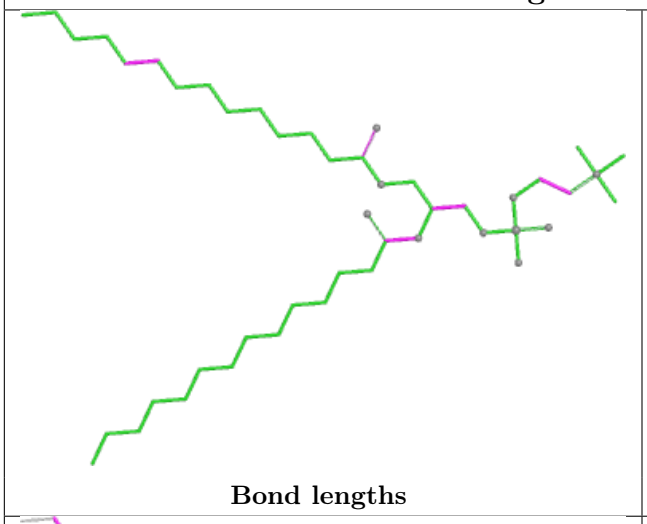


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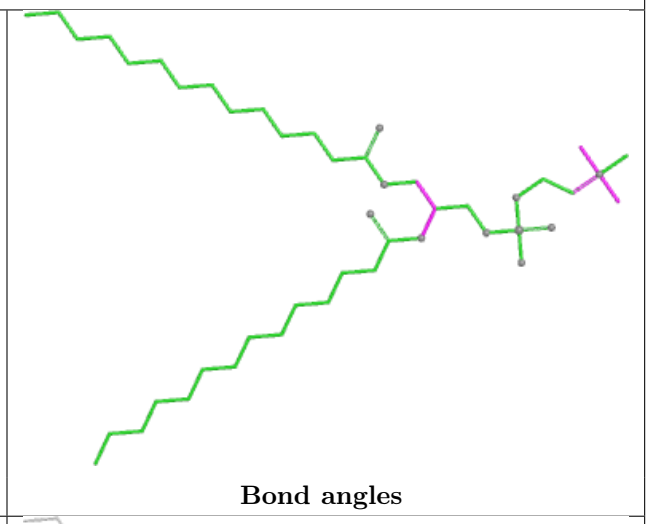


Rings

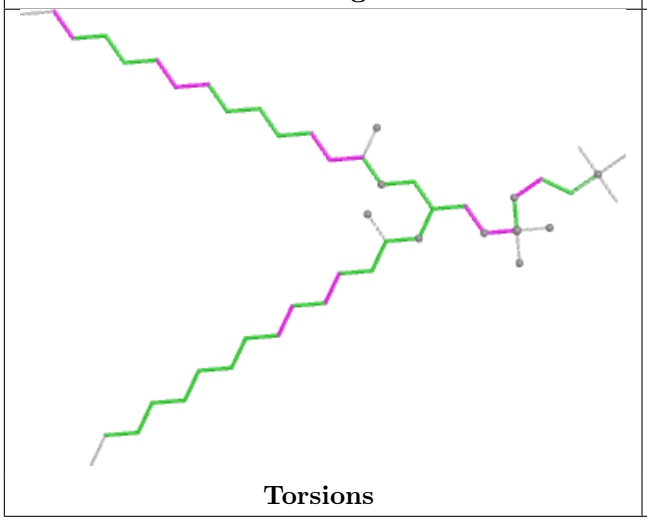
Ligand PX4 C 347



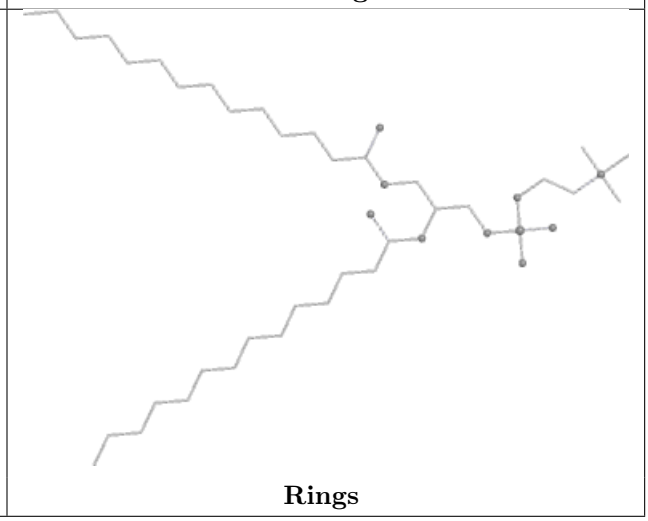
Bond lengths



Bond angles

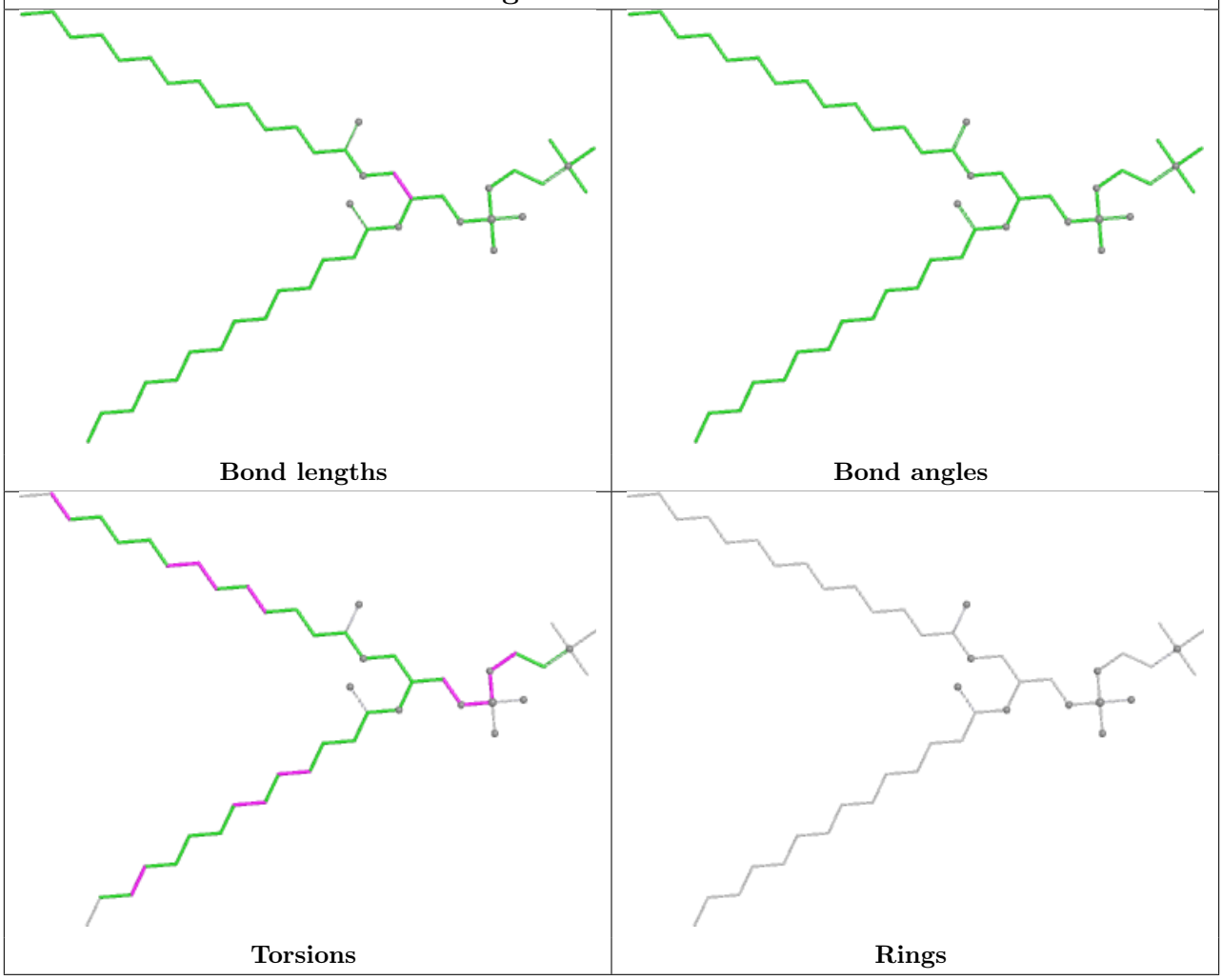


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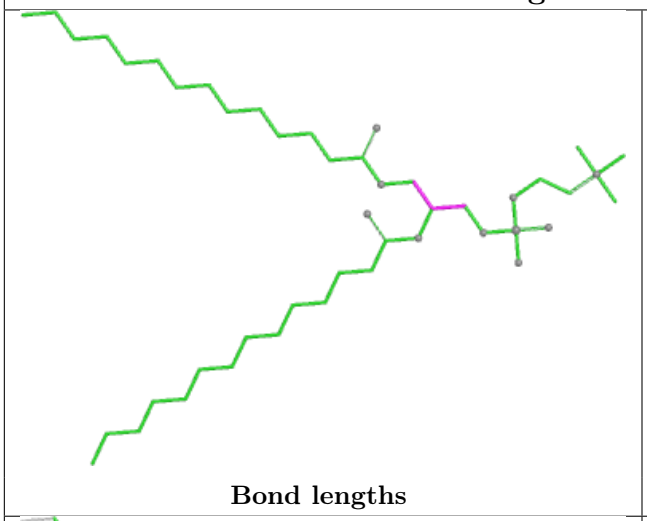


Rings

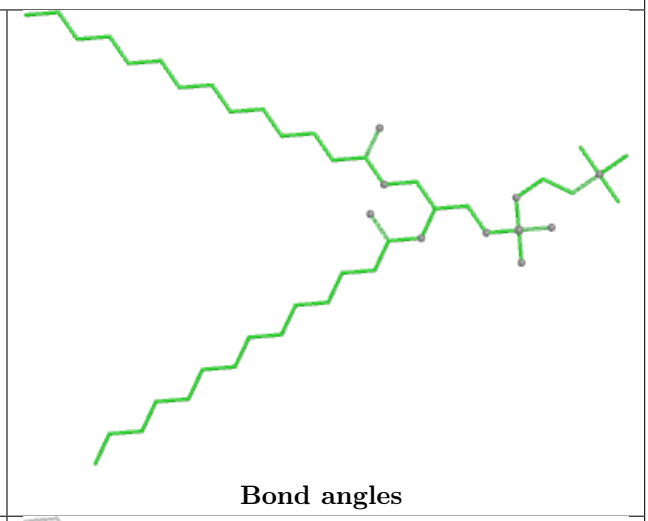
Ligand PX4 A 654



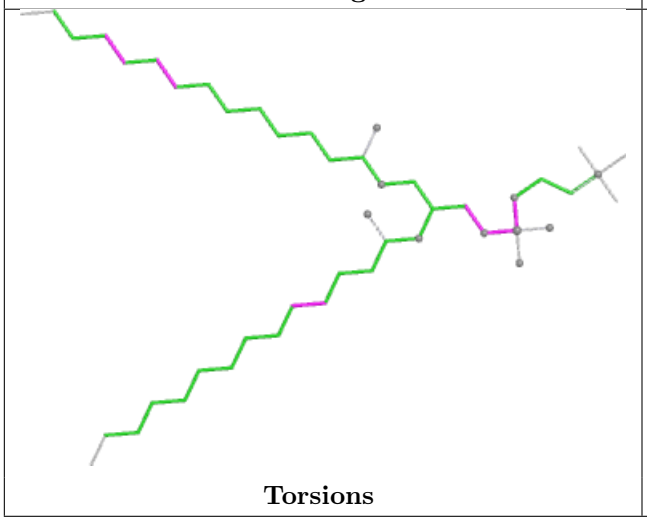
Ligand PX4 B 386



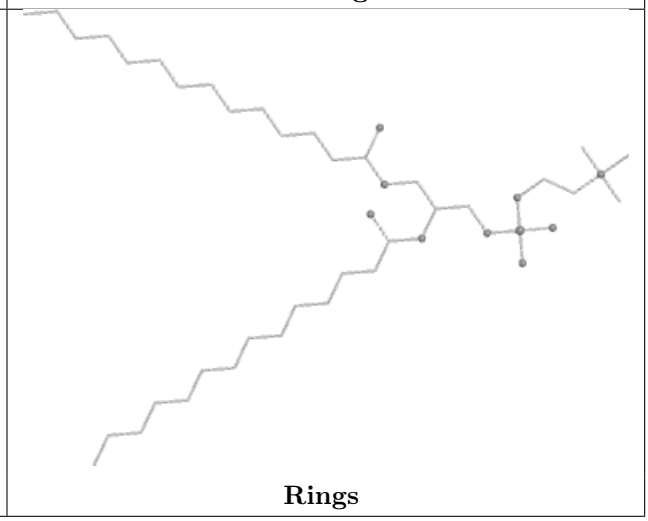
Bond lengths



Bond angles

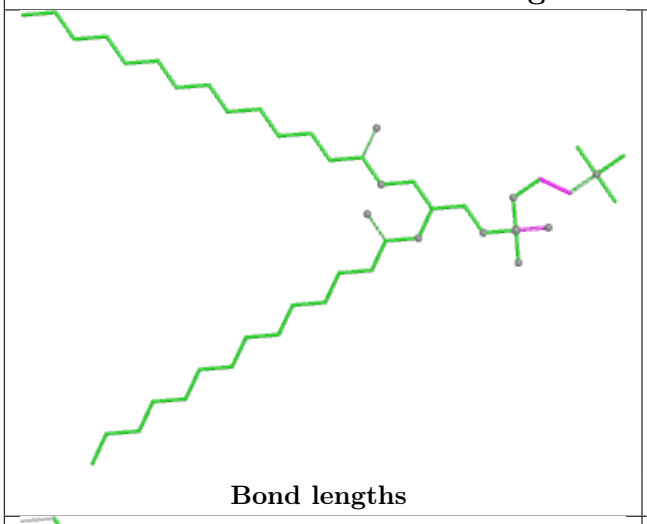


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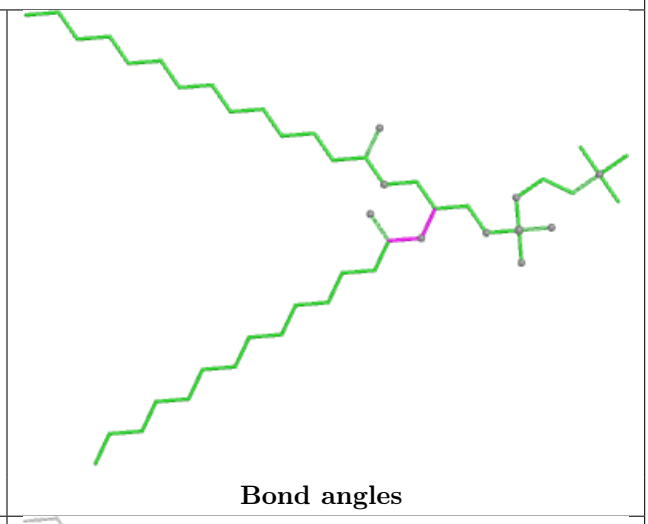


Rings

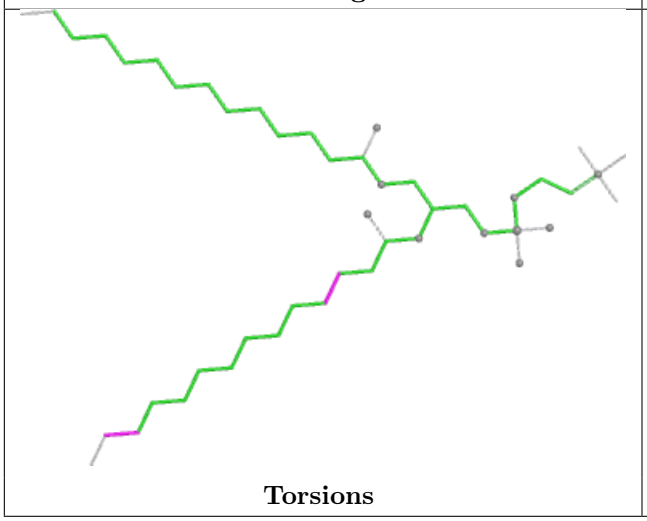
Ligand PX4 B 381



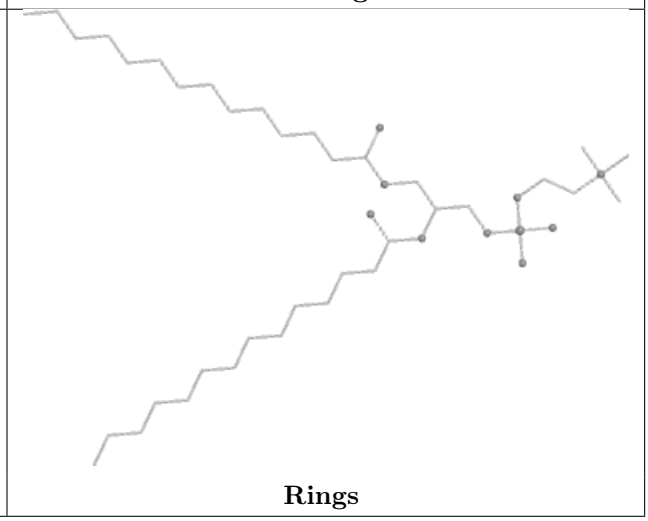
Bond lengths



Bond angles

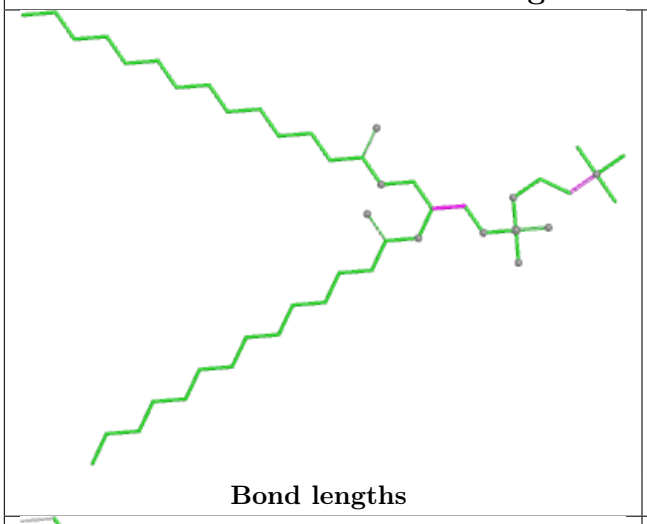


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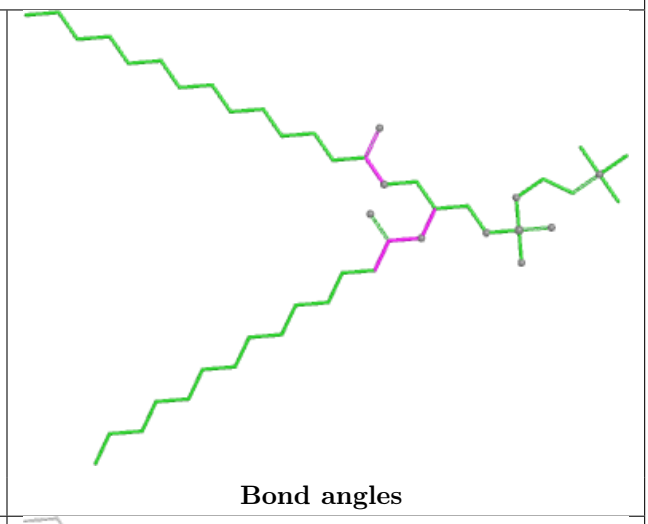


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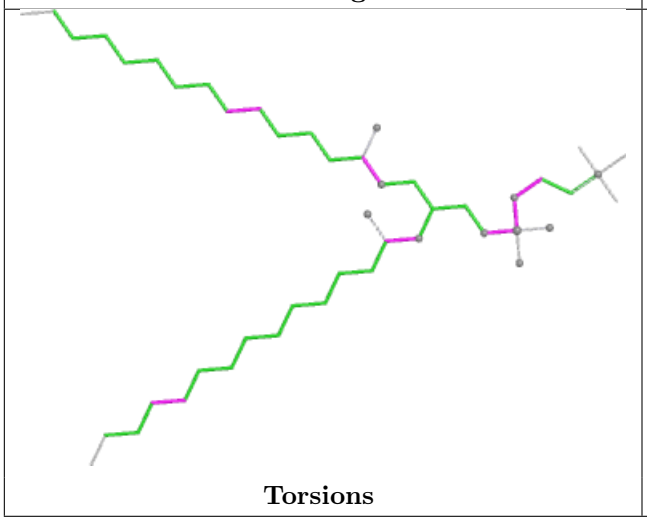
Ligand PX4 C 330



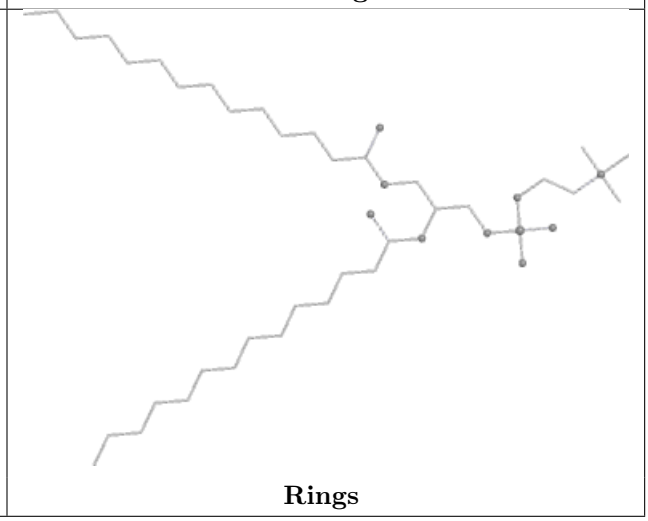
Bond lengths



Bond angles

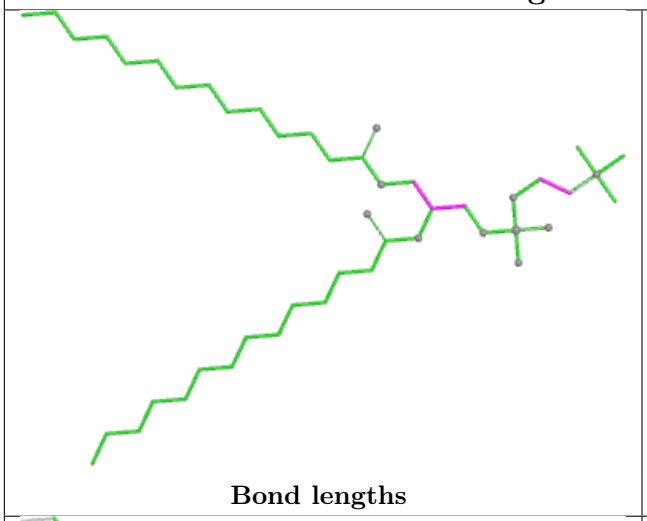


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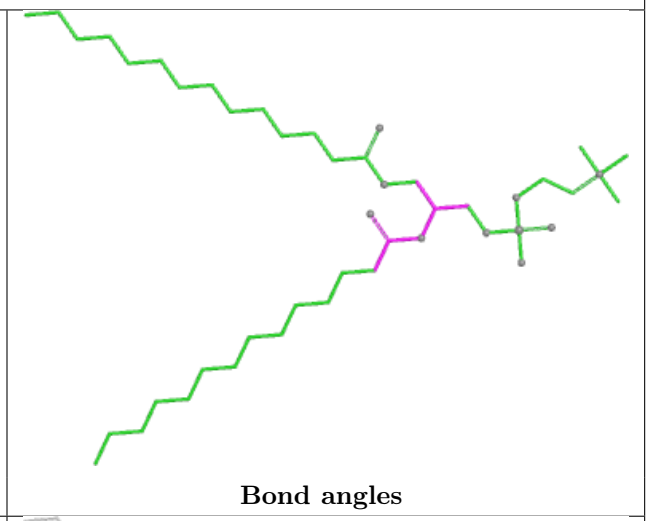


Rings

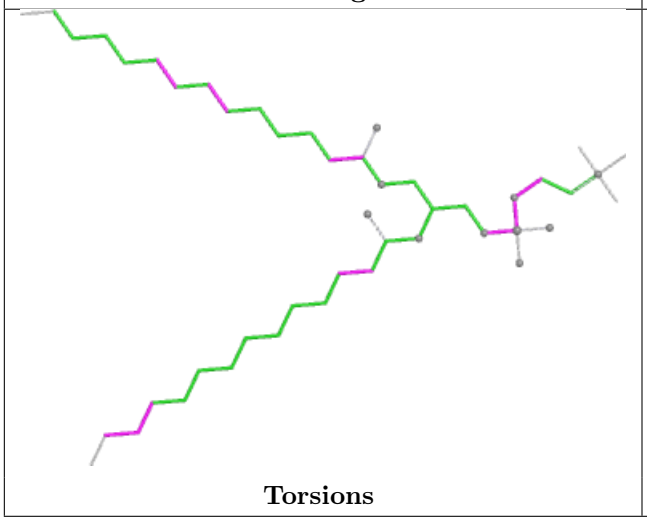
Ligand PX4 B 339



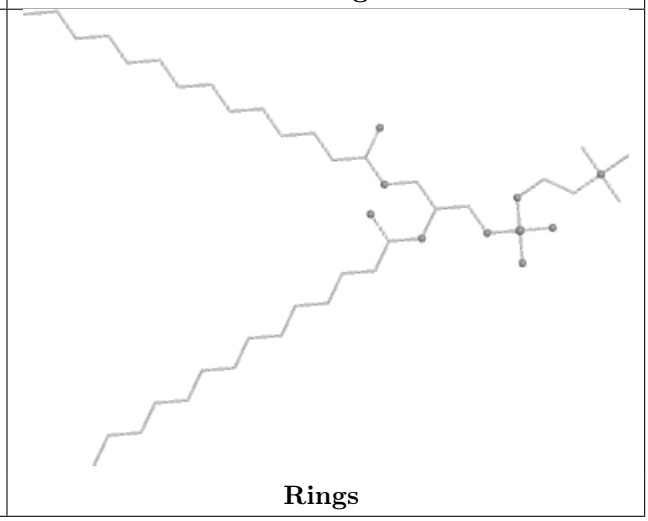
Bond lengths



Bond angles

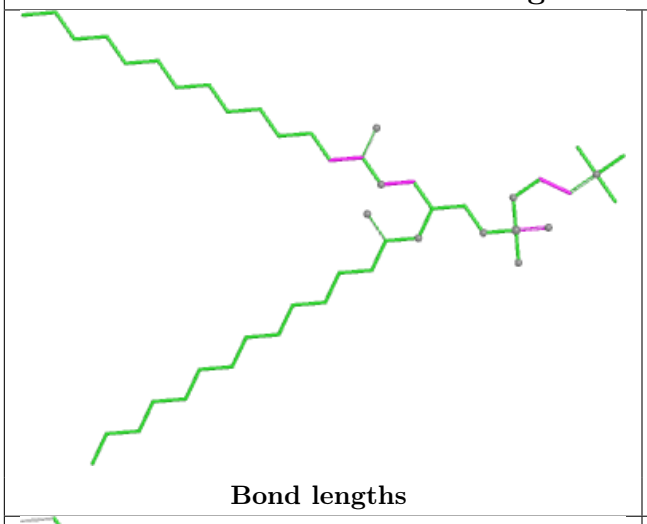


Torsions

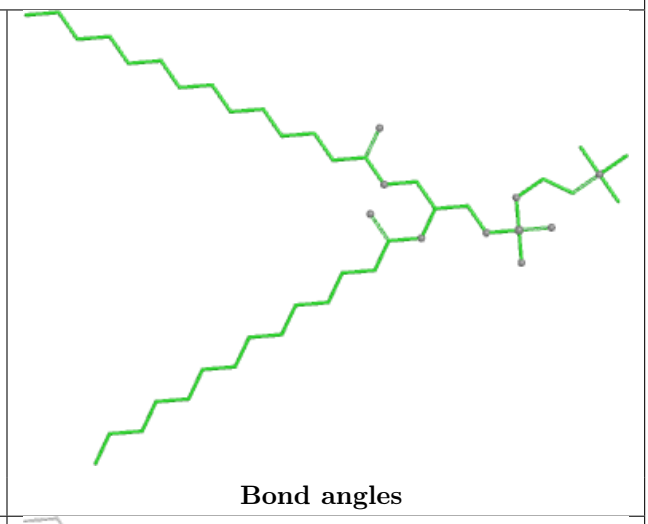


Rings

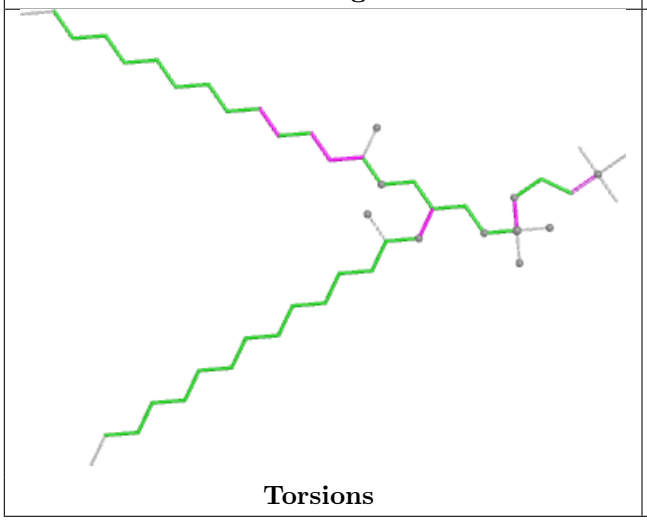
Ligand PX4 C 337



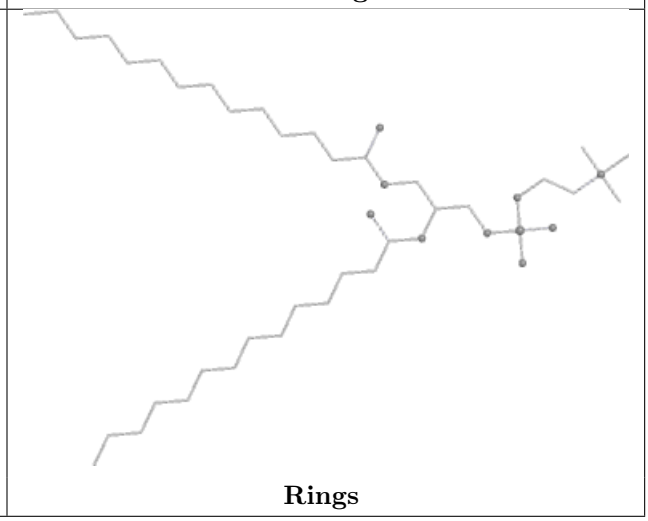
Bond lengths



Bond angles

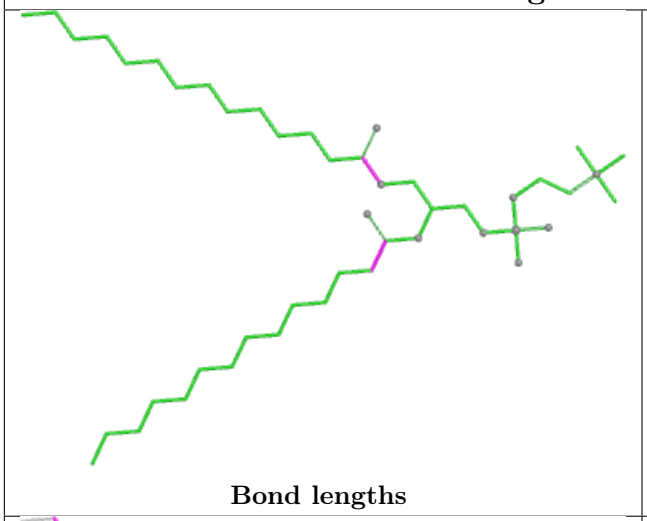


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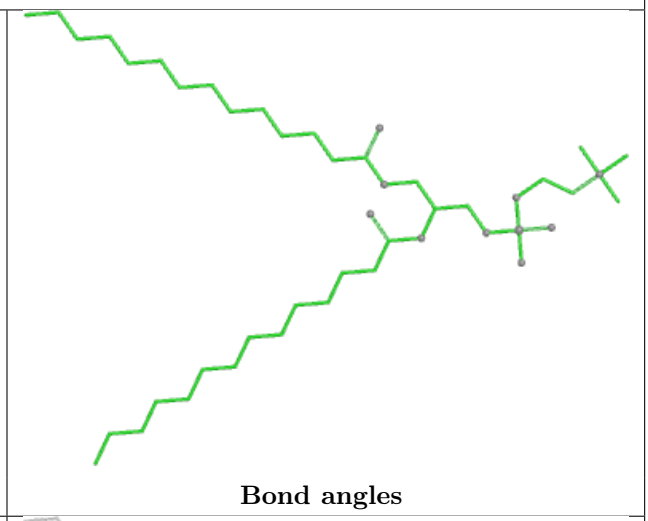


Rings

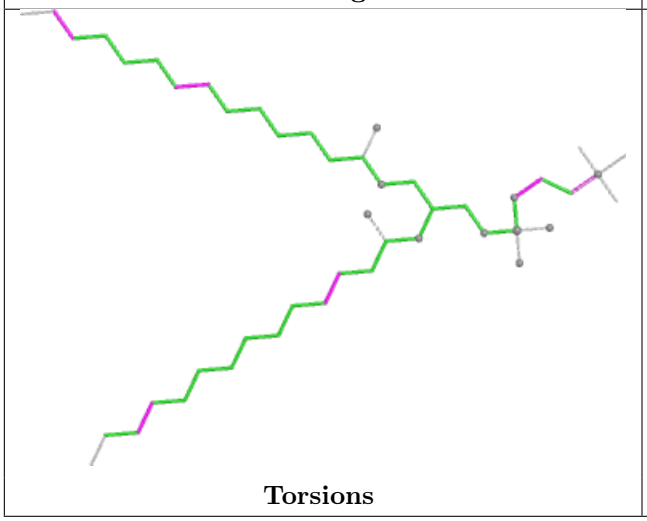
Ligand PX4 C 332



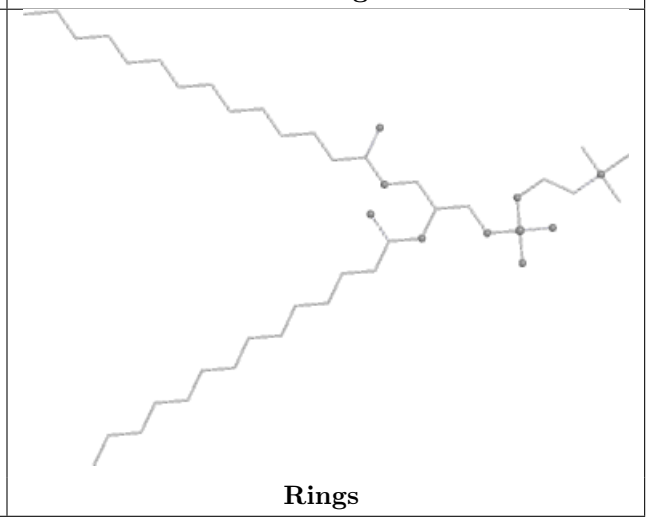
Bond lengths



Bond angles

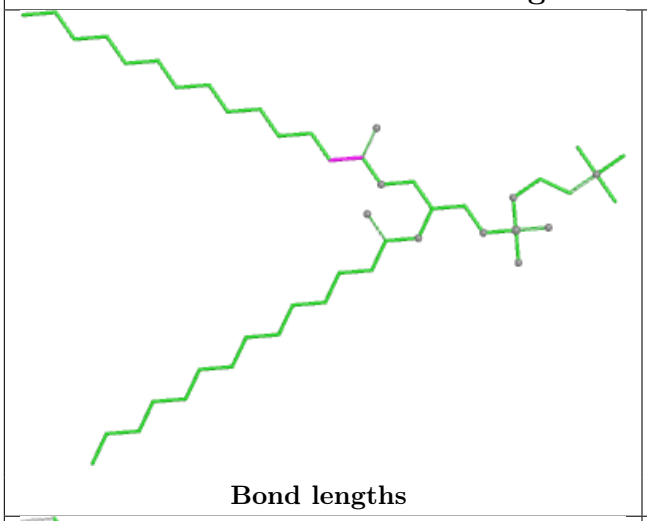


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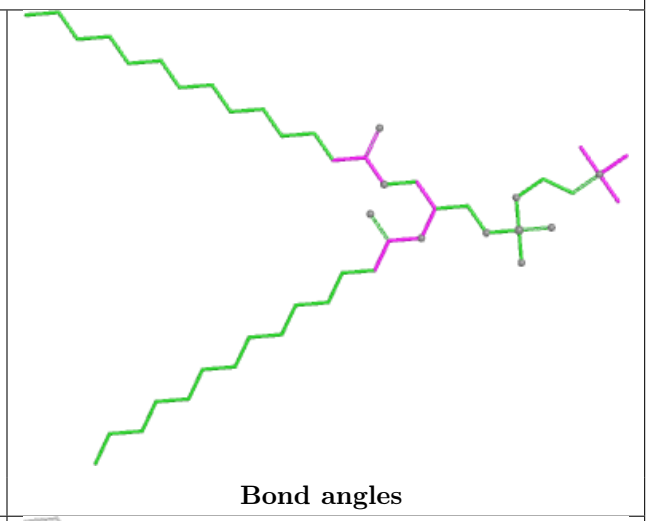


Rings

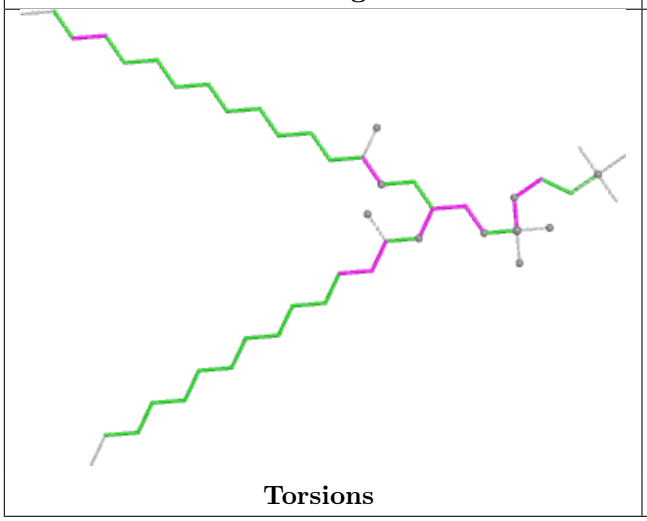
Ligand PX4 B 359



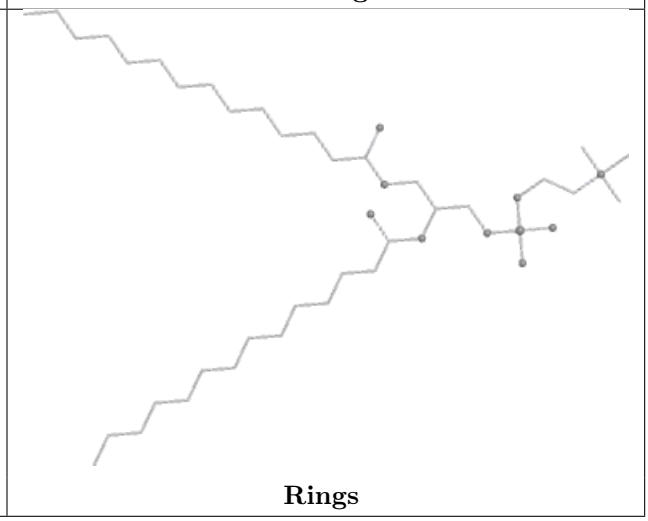
Bond lengths



Bond angles

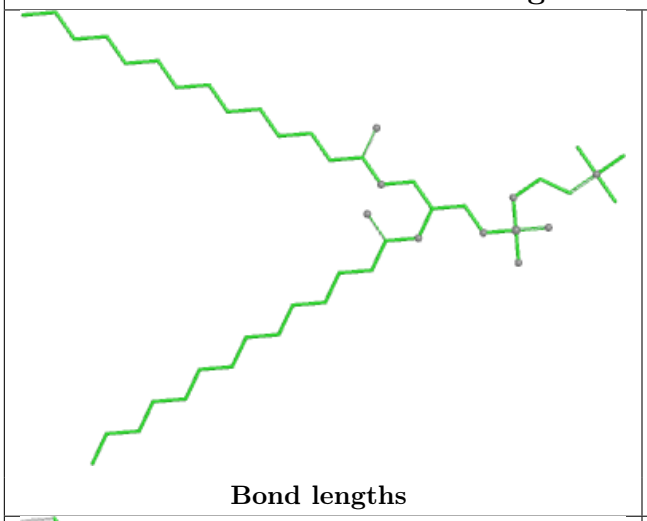


Torsions

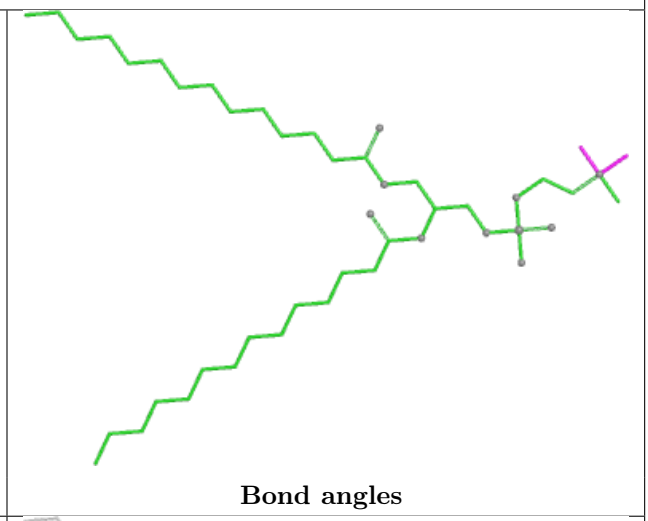


Rings

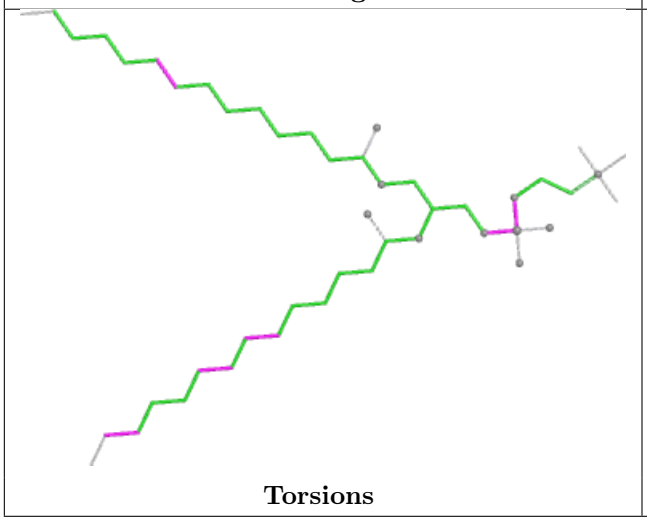
Ligand PX4 C 338



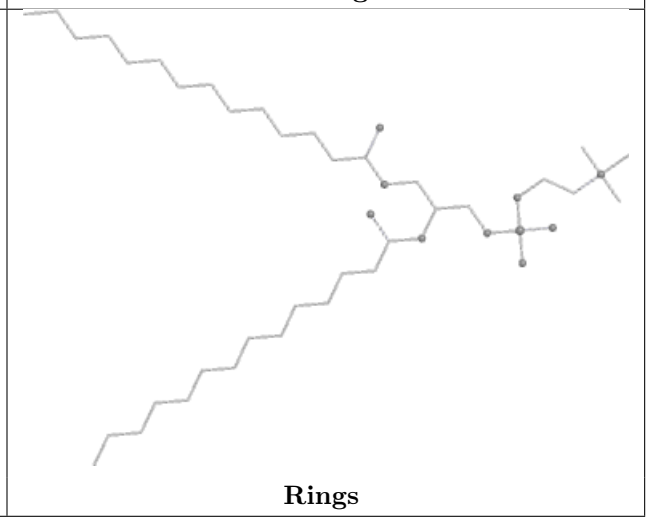
Bond lengths



Bond angles

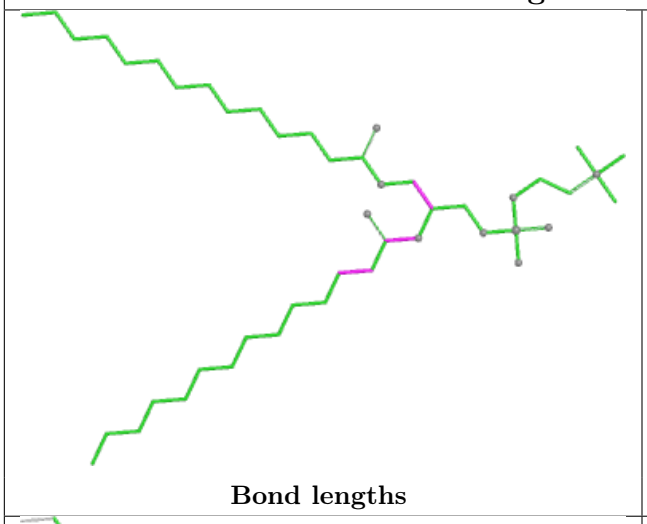


Torsions

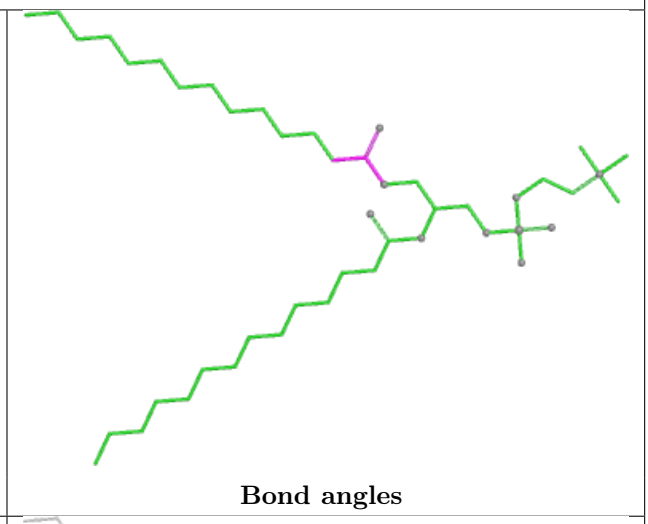


Rings

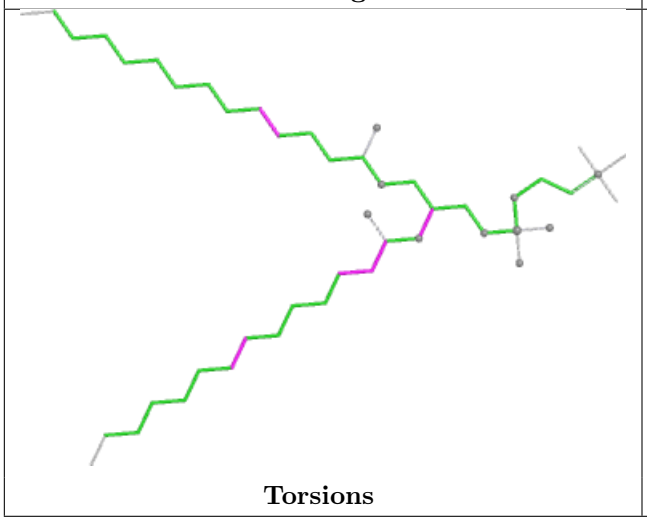
Ligand PX4 C 316



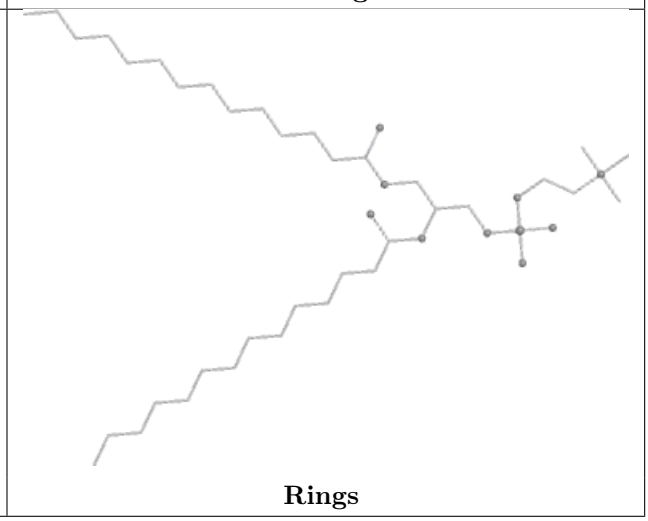
Bond lengths



Bond angles

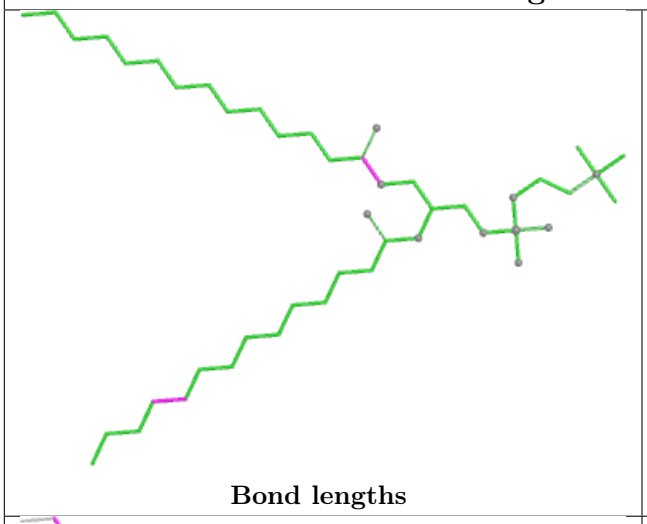


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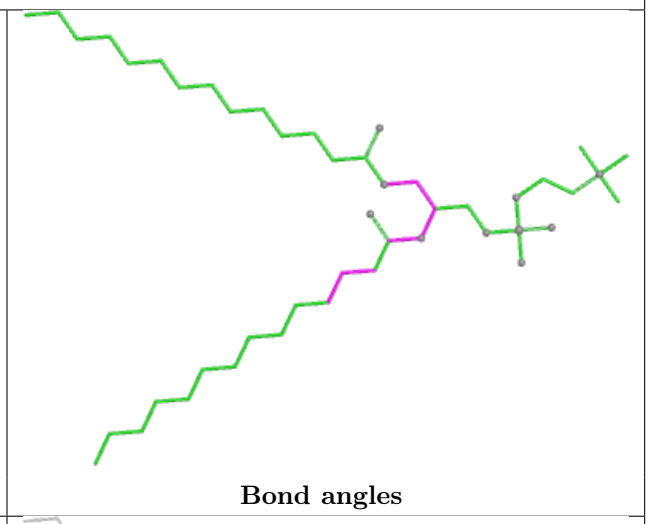


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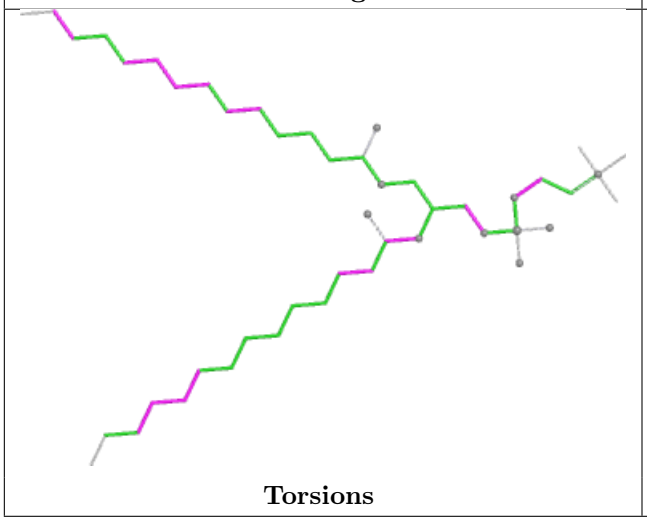
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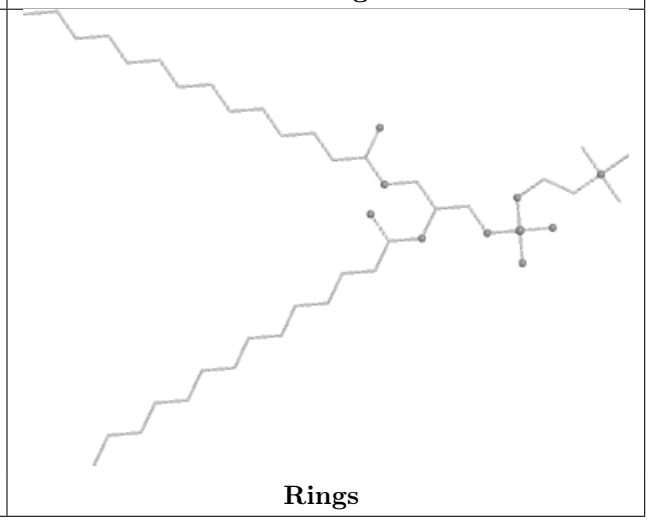
Bond lengths



Bond angles

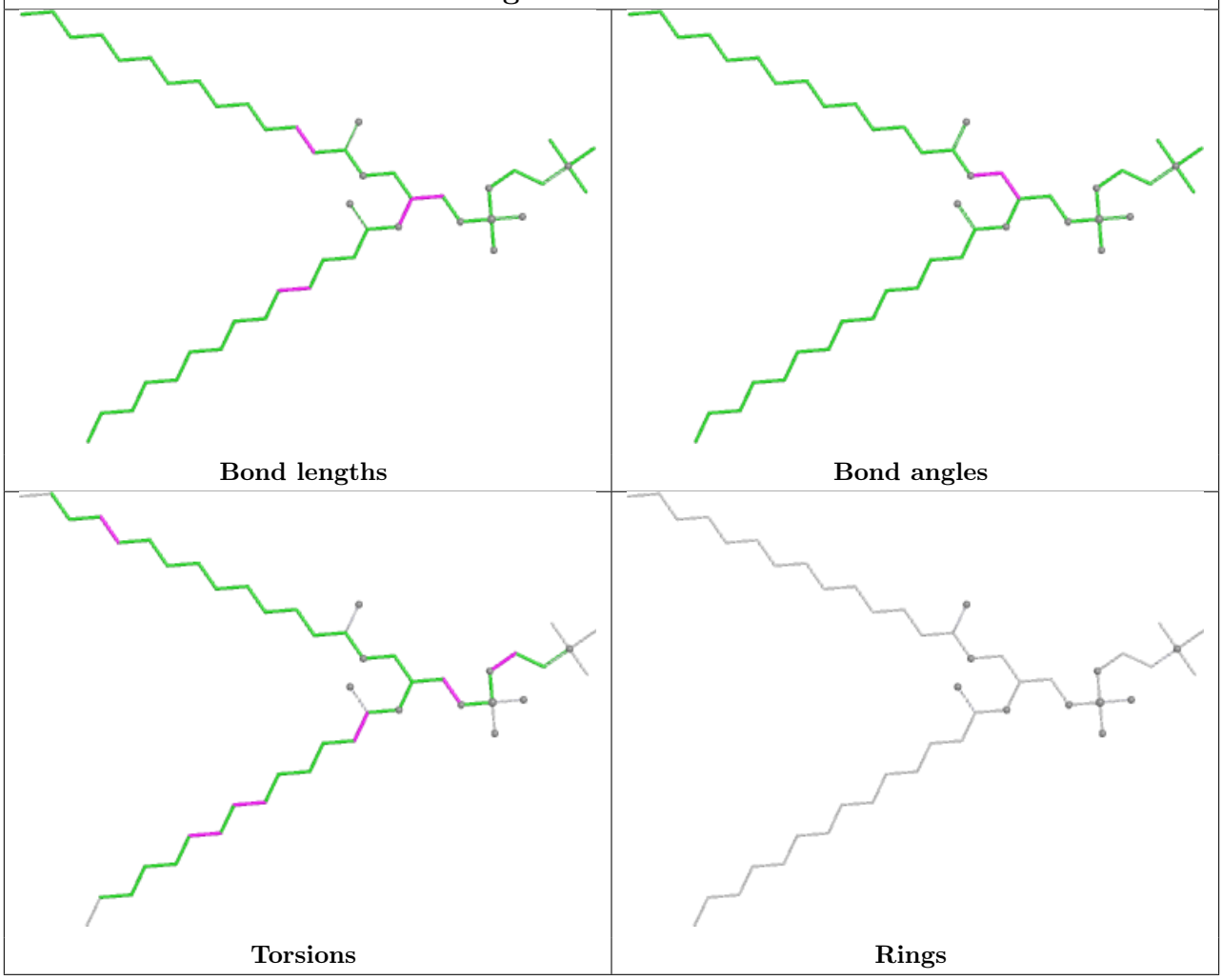


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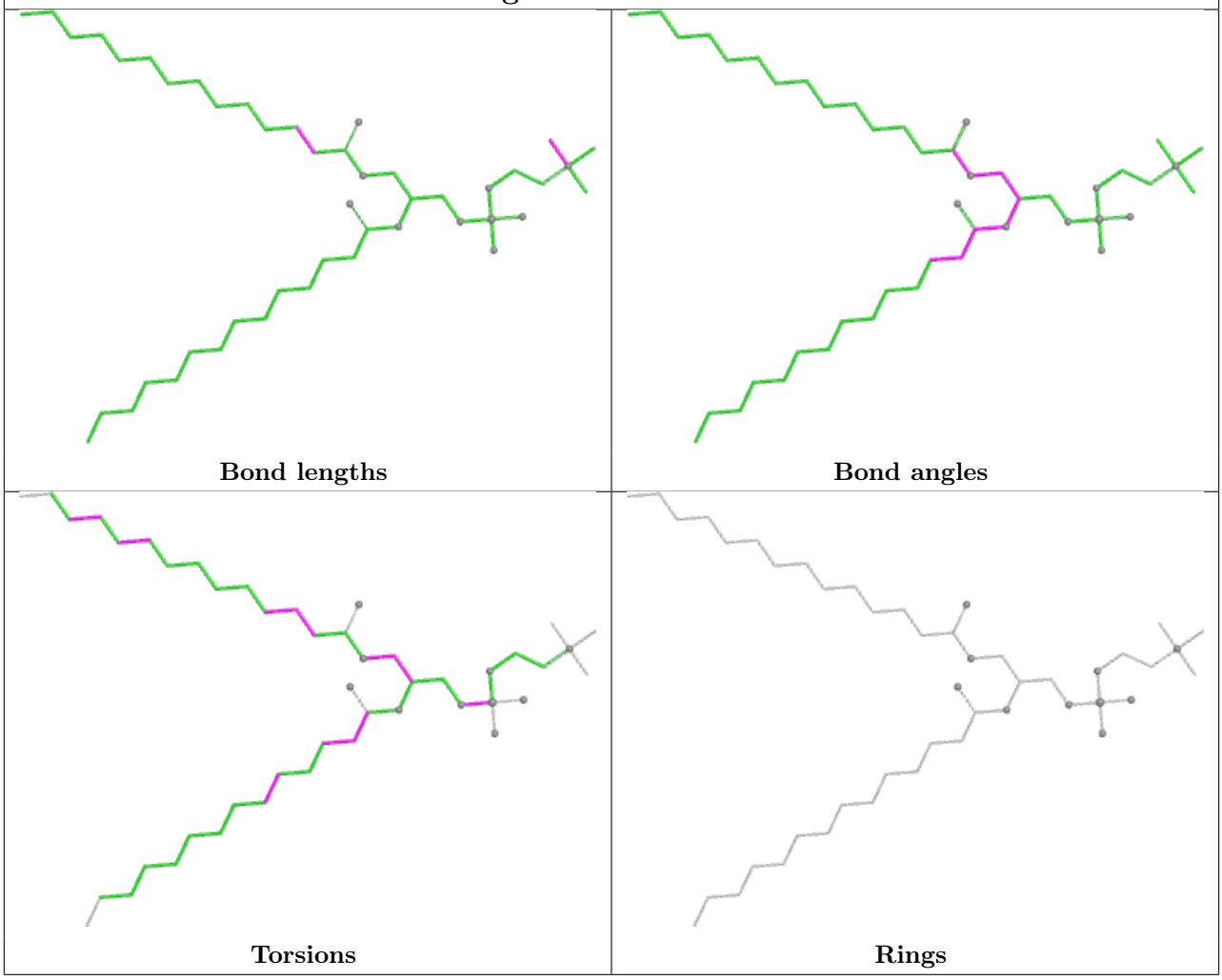


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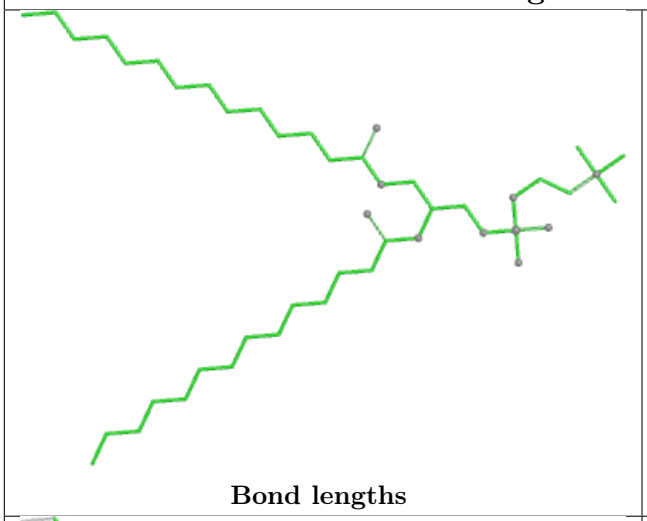
Ligand PX4 B 393



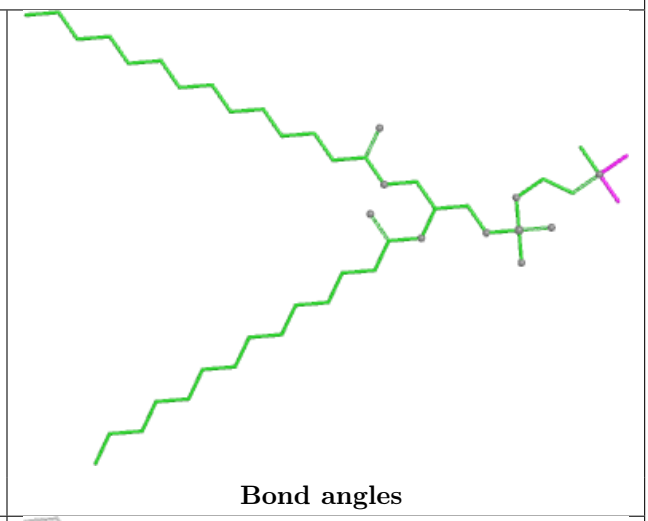
Ligand PX4 A 609



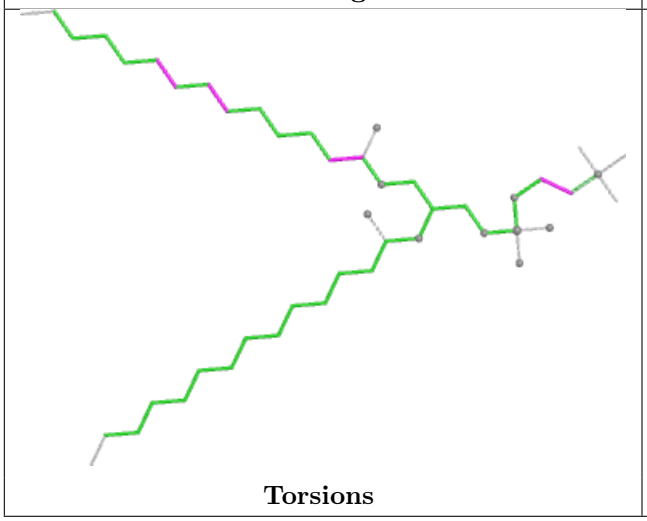
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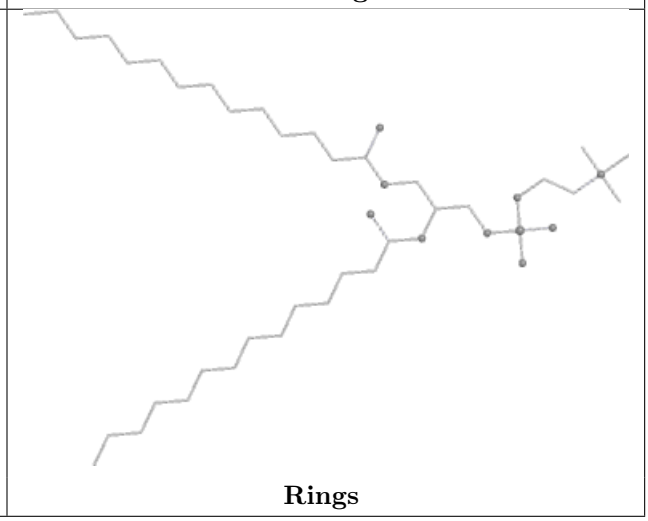
Bond lengths



Bond angles

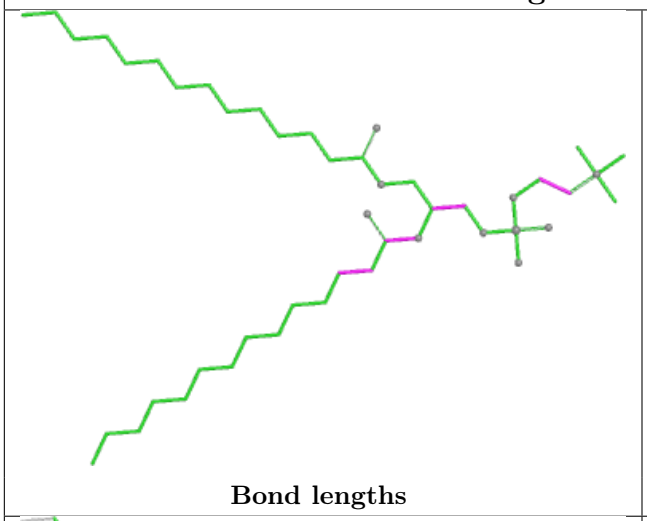


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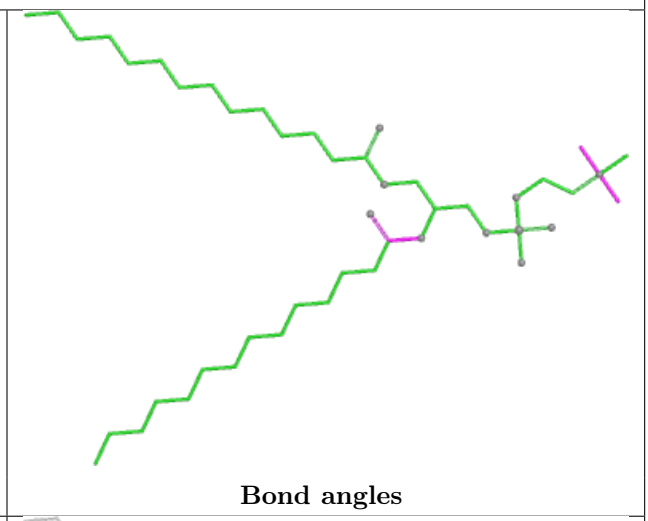


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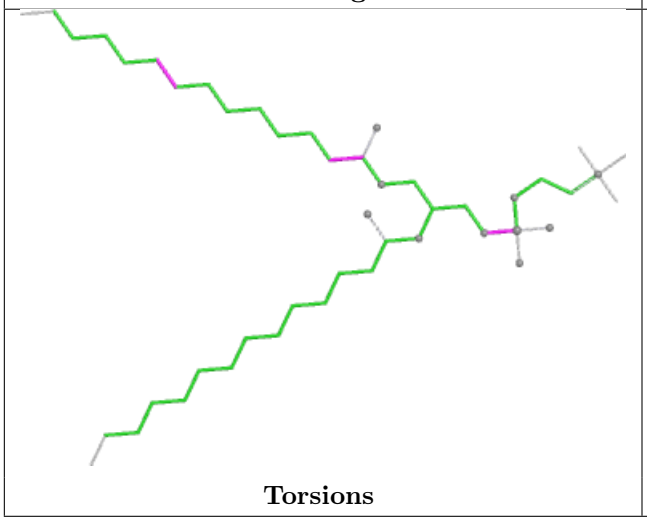
Ligand PX4 B 347



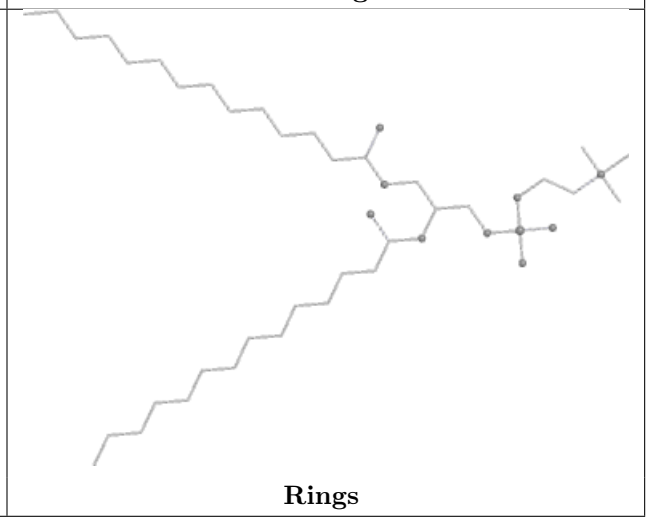
Bond lengths



Bond angles

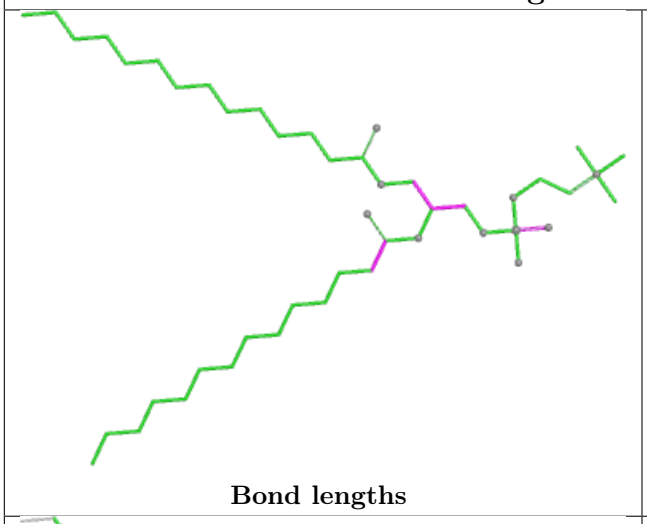


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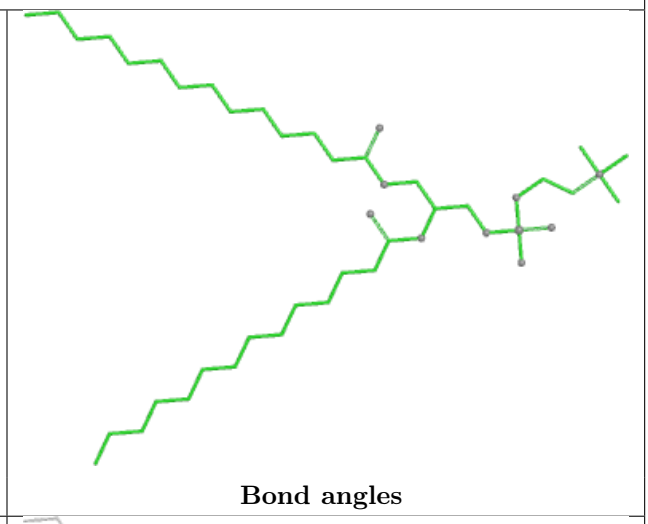


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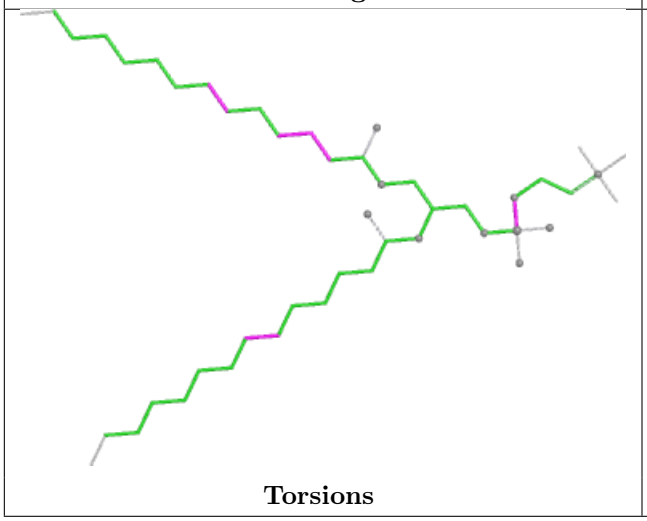
Ligand PX4 A 601



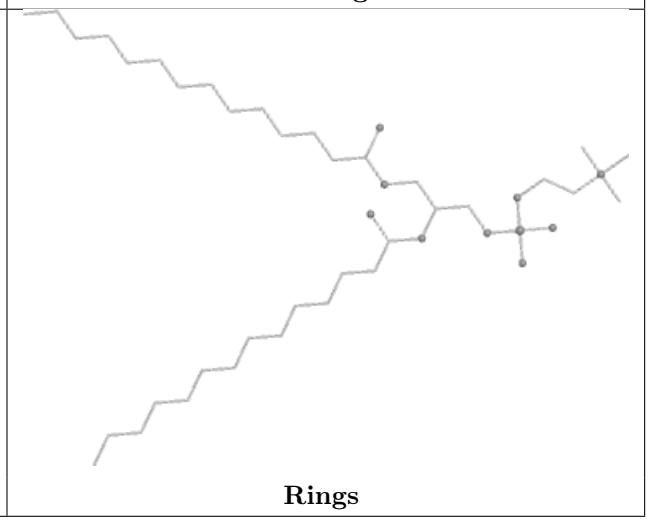
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Bond angles

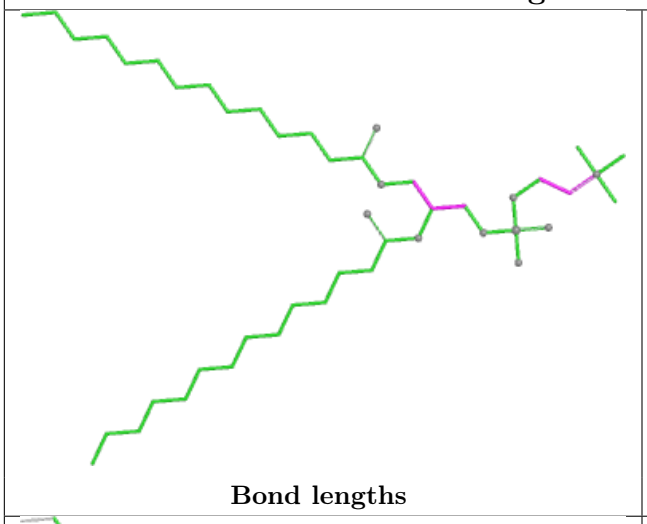


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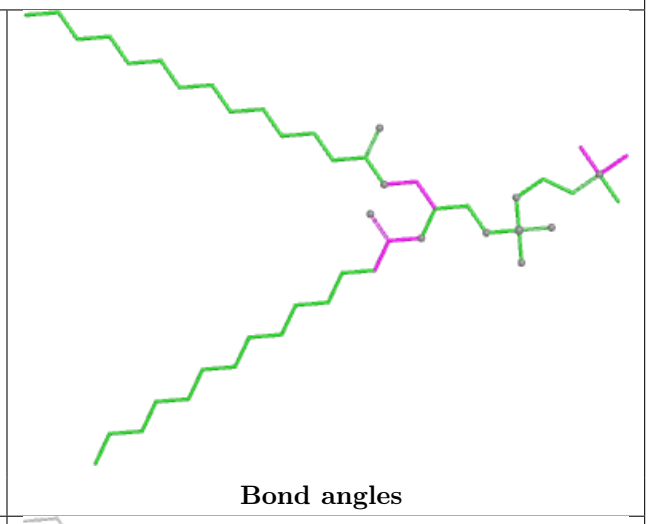


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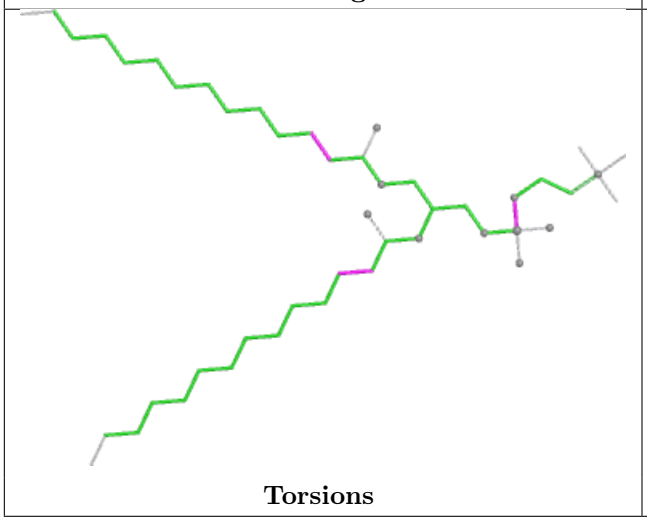
Ligand PX4 B 342



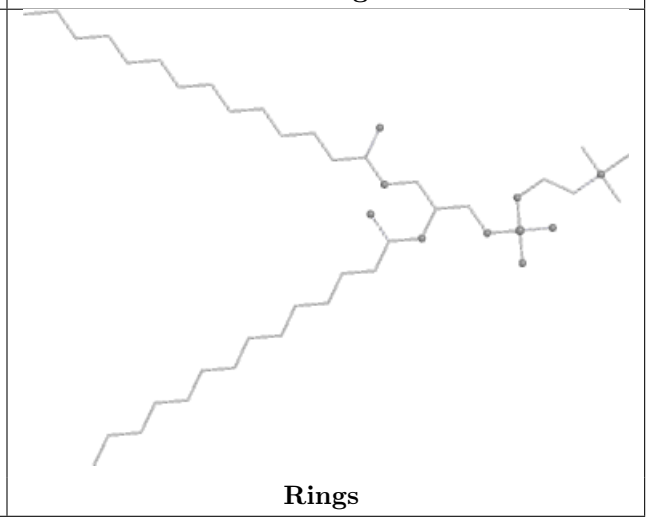
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Bond angles

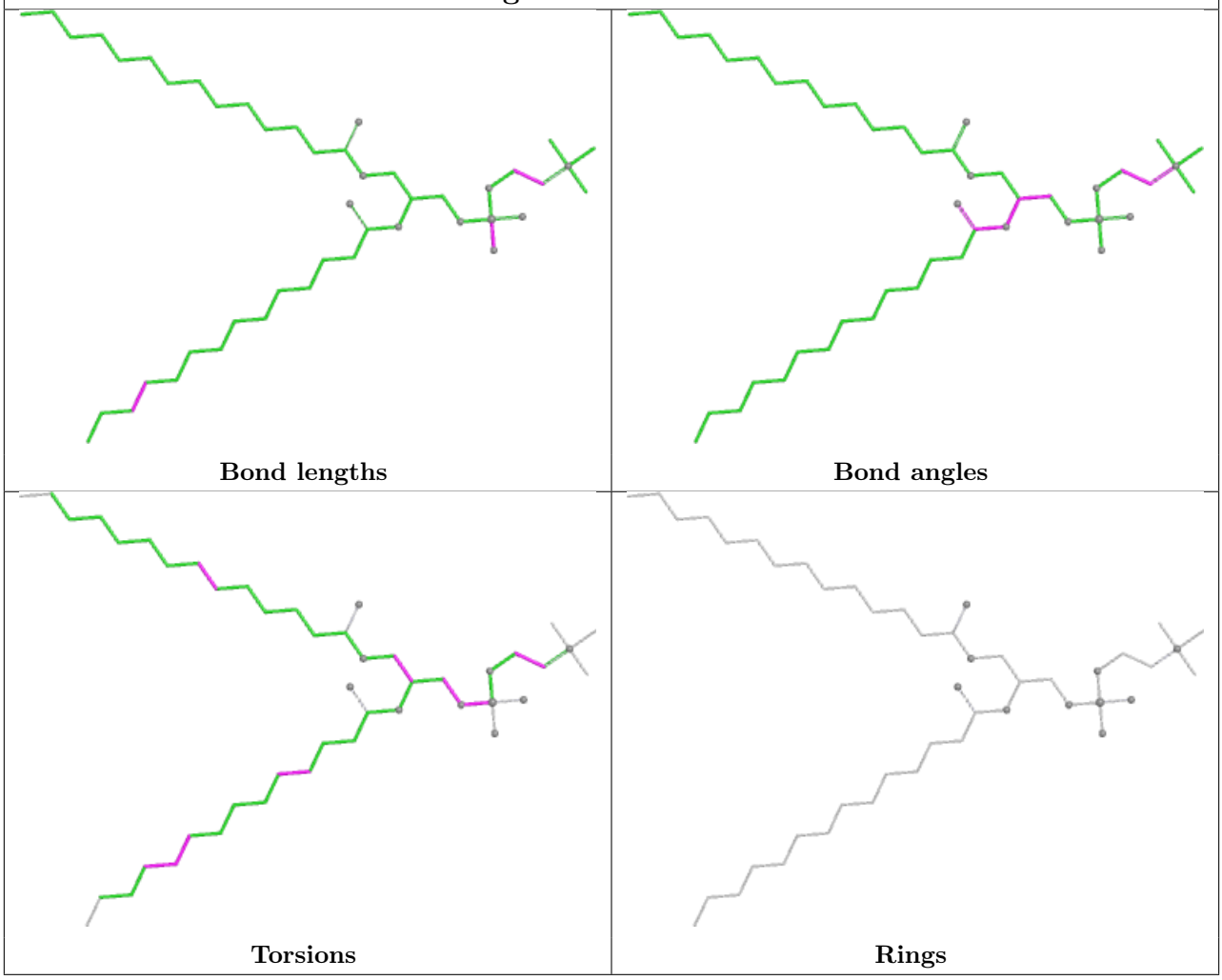


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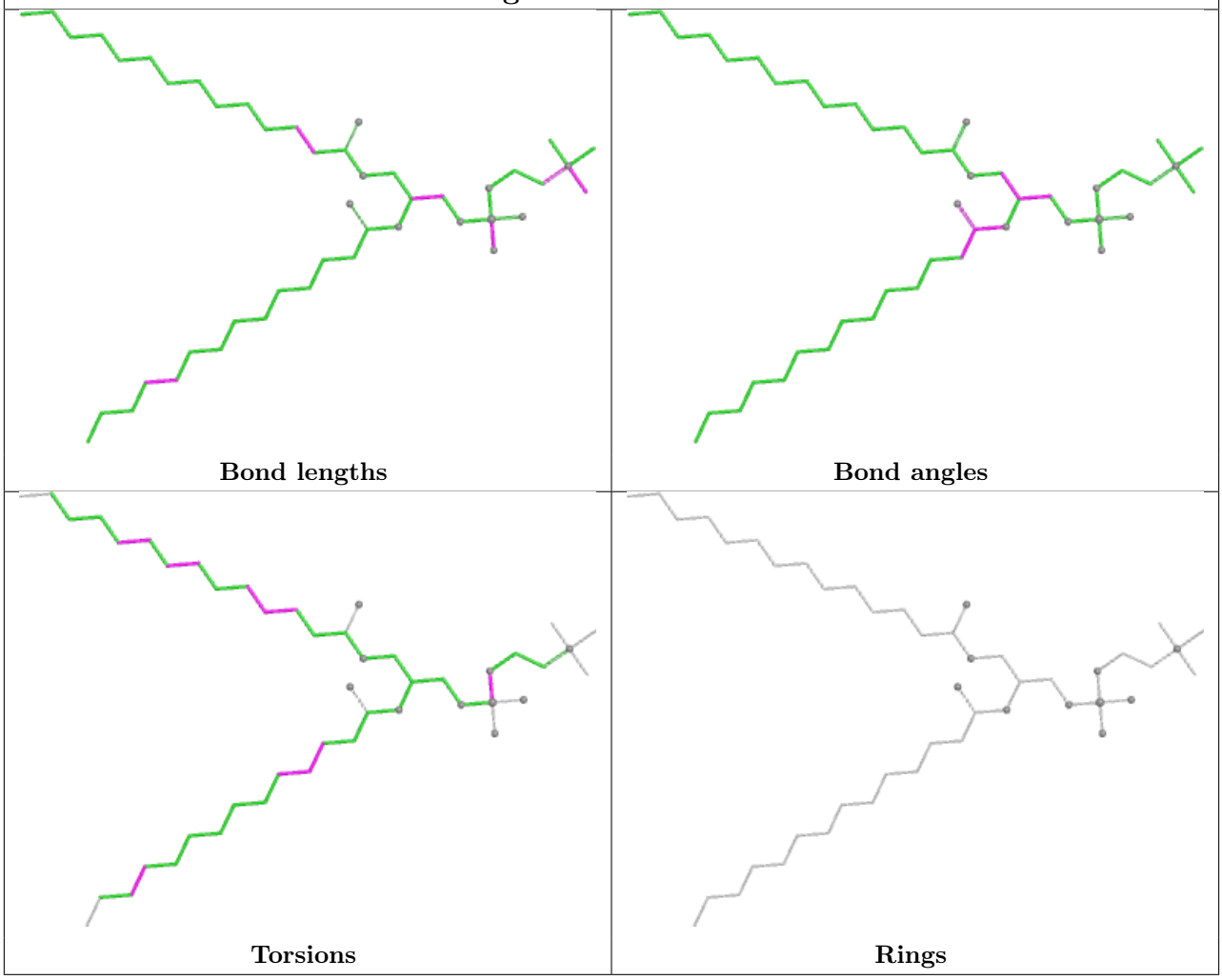


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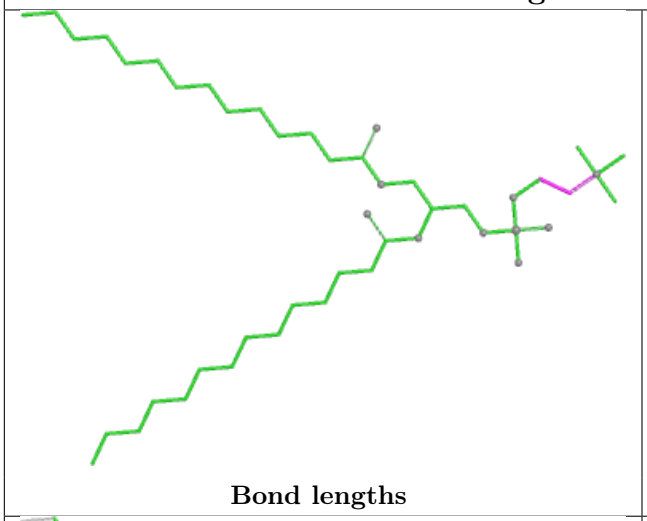
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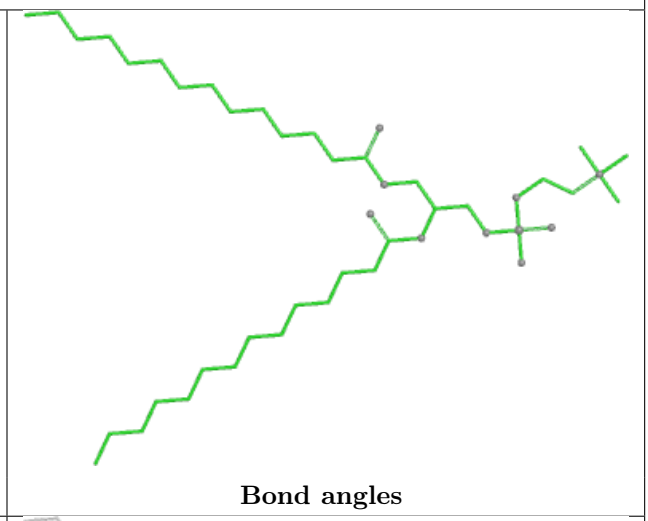
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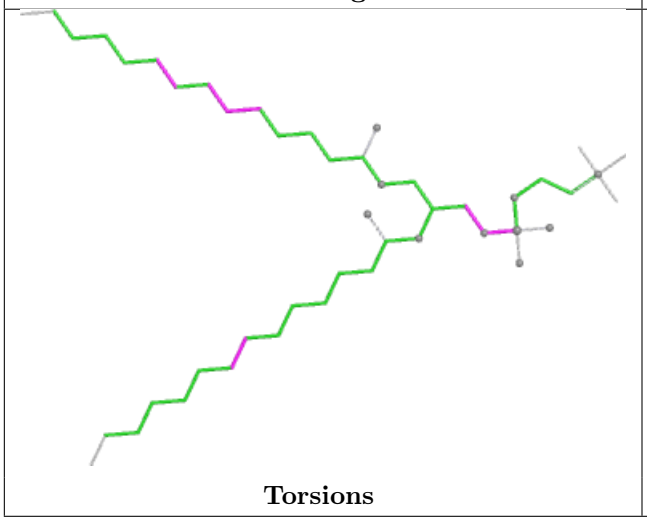
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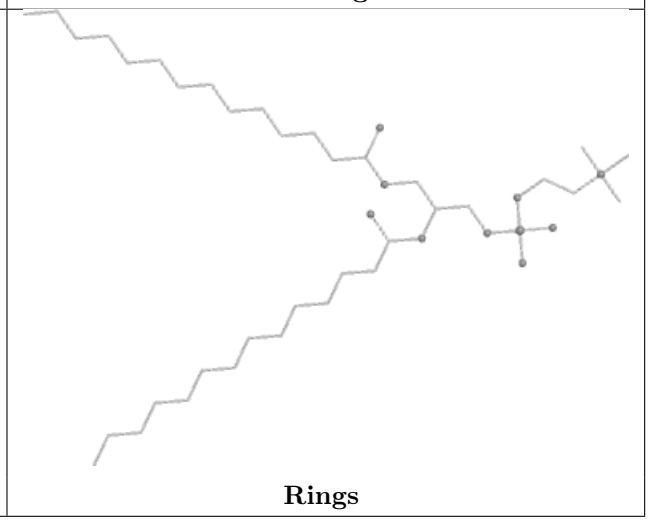
Bond lengths



Bond angles

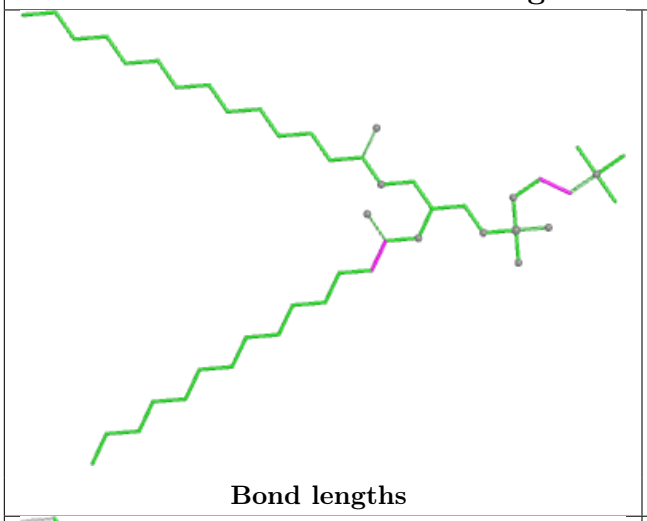


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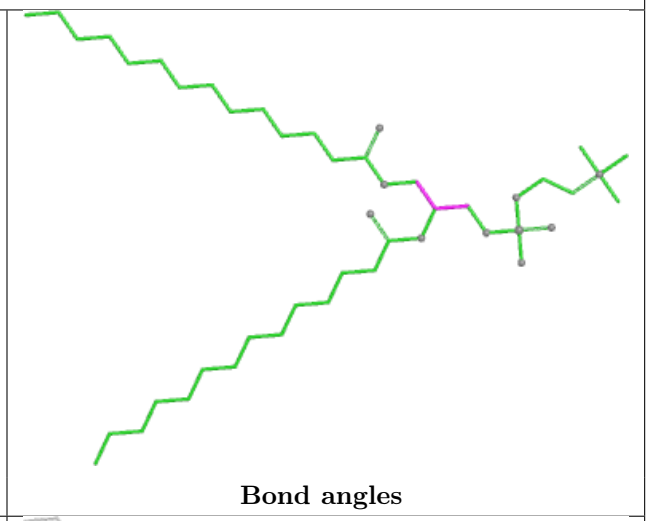


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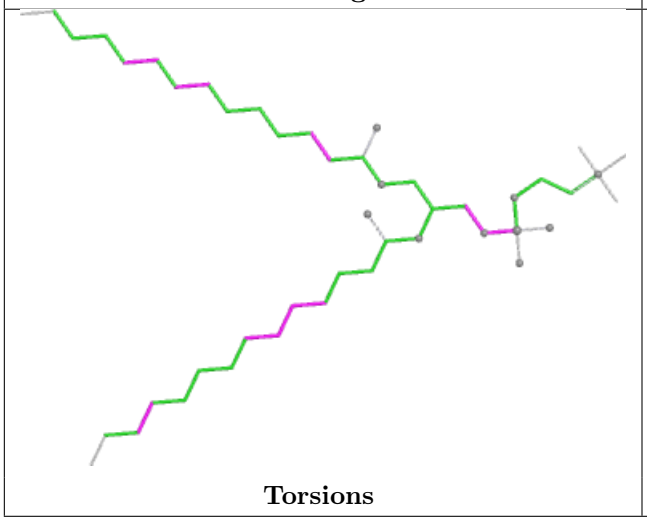
Ligand PX4 C 360



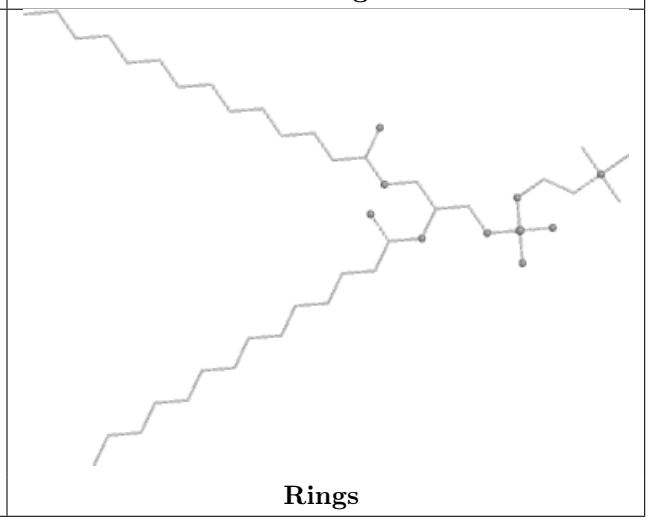
Bond lengths



Bond angles

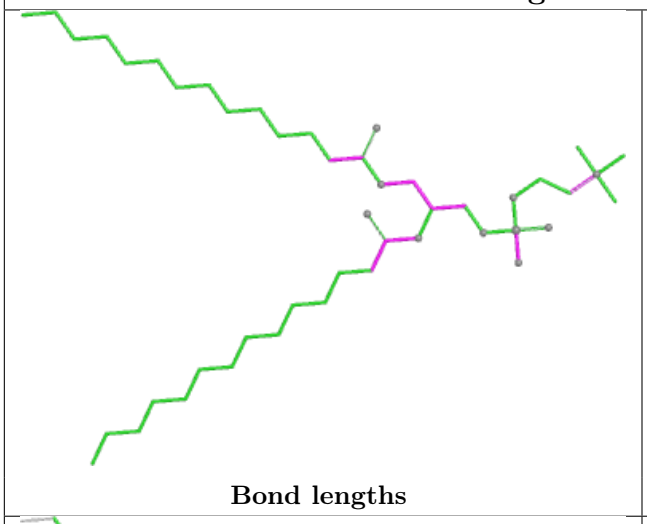


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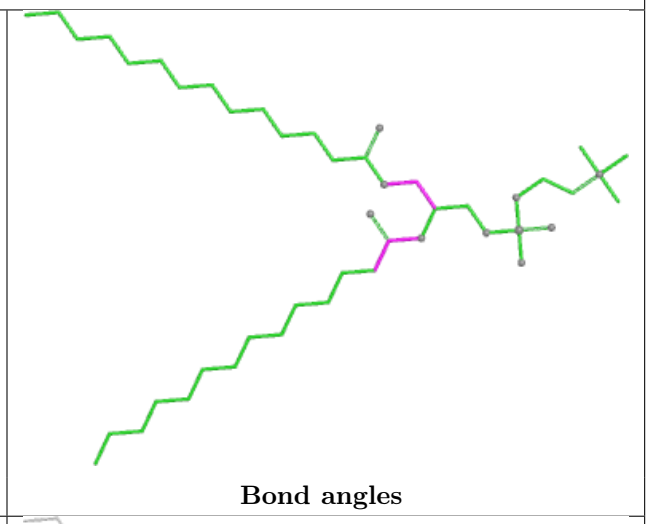


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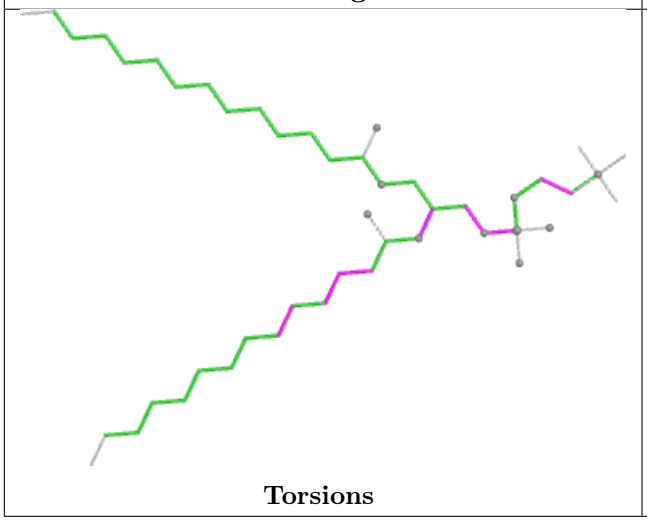
Ligand PX4 B 355



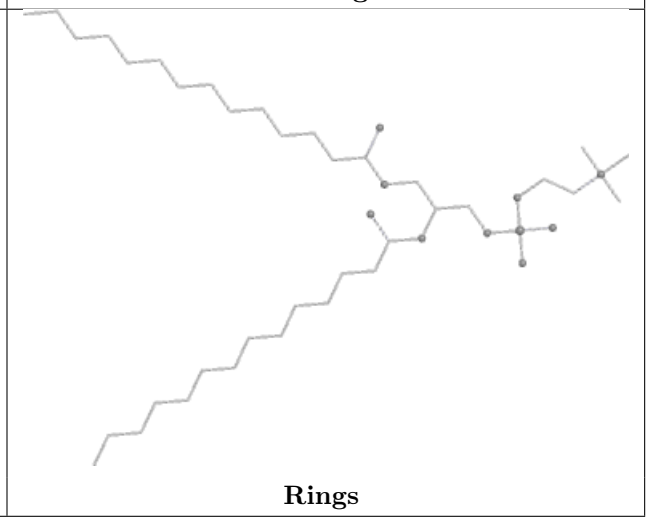
Bond lengths



Bond angles

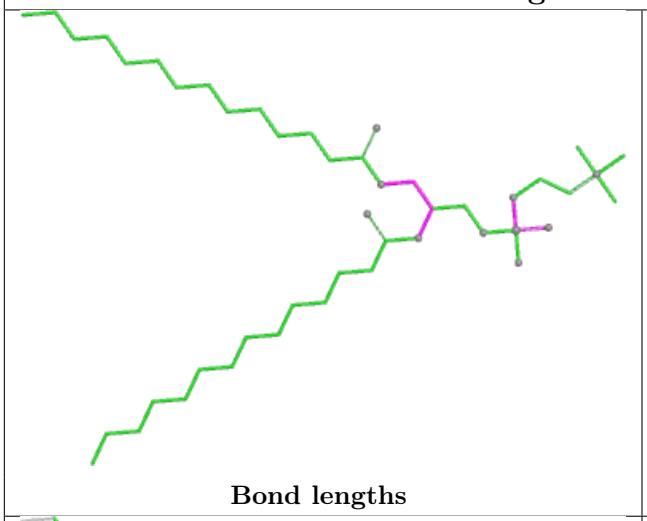


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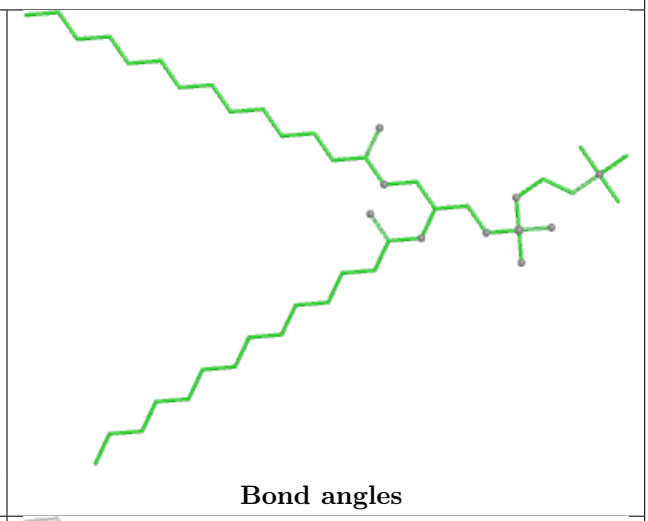


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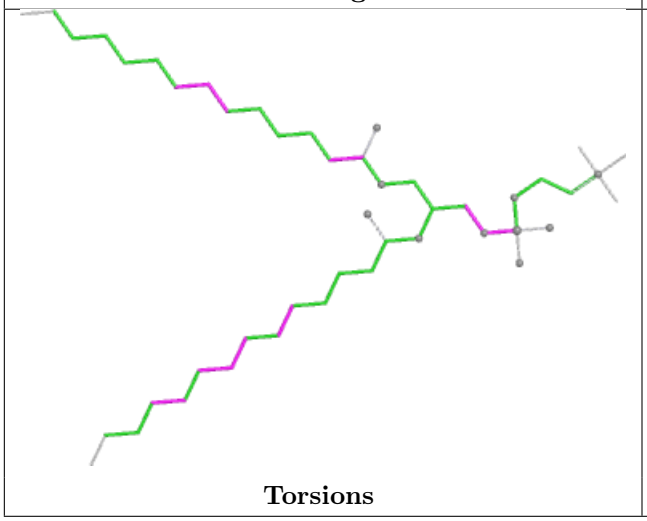
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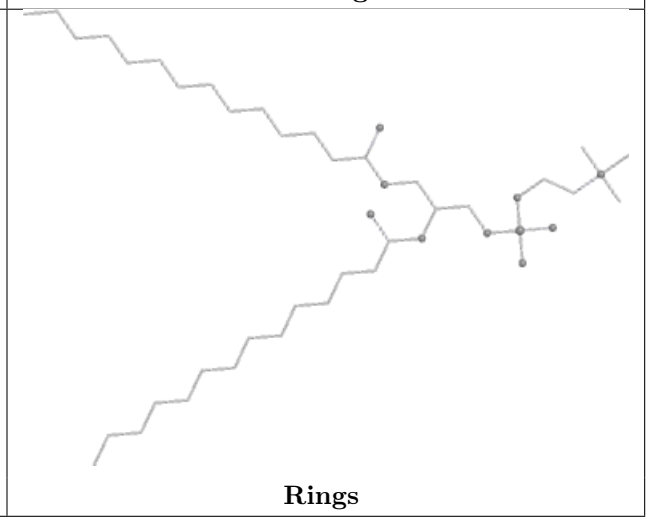
Bond lengths



Bond angles

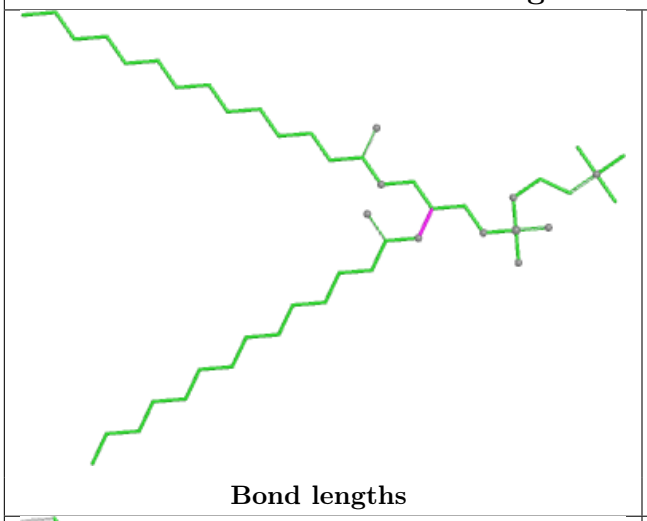


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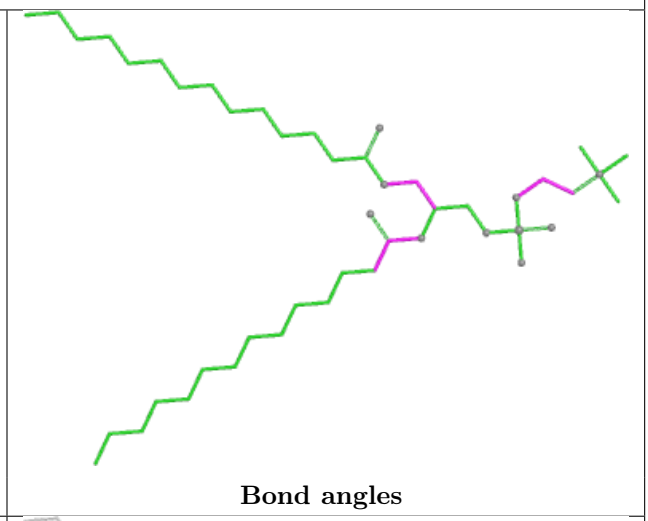


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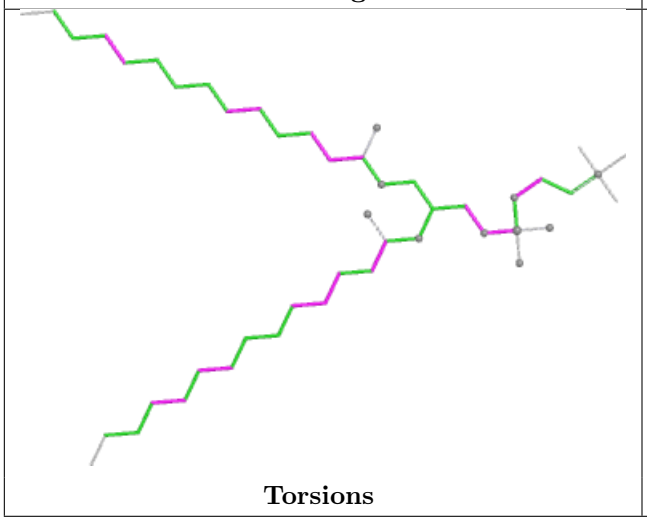
Ligand PX4 A 622



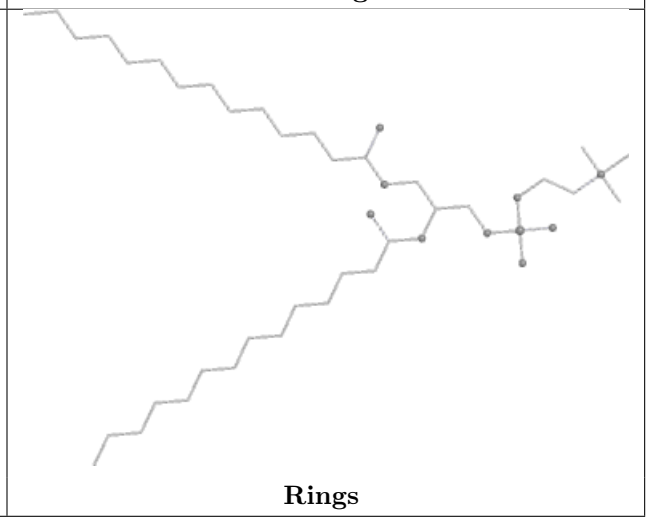
Bond lengths



Bond angles

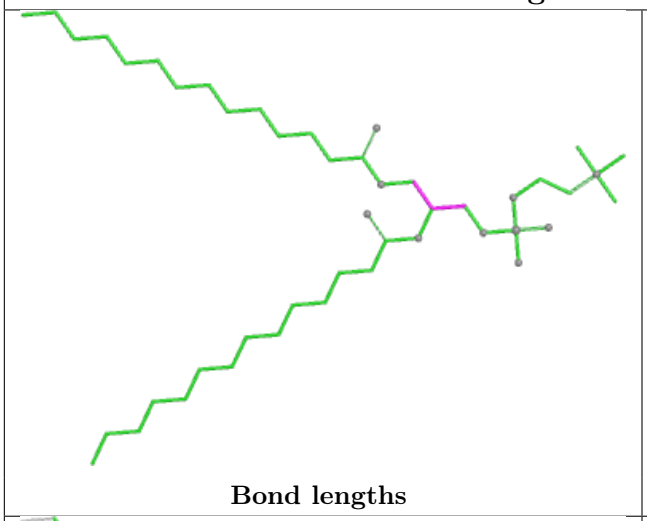


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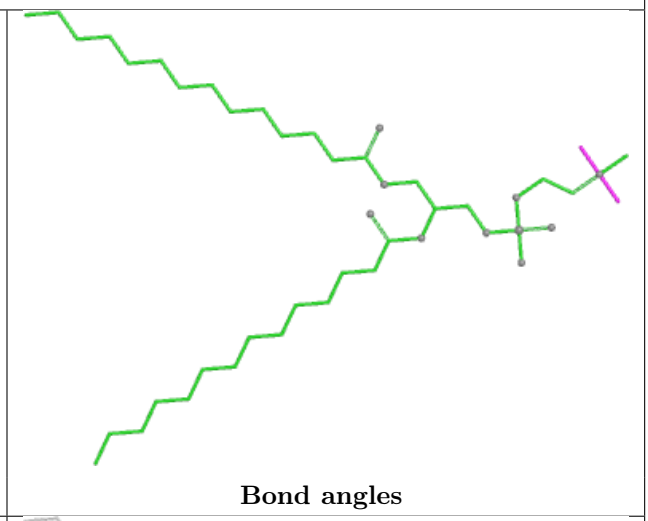


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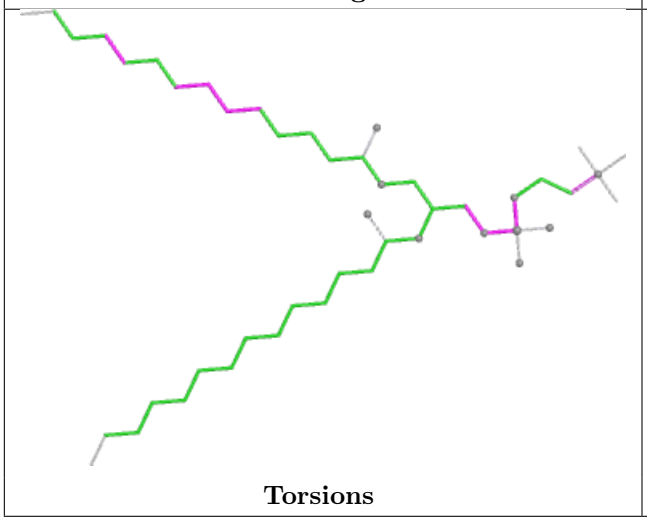
Ligand PX4 C 313



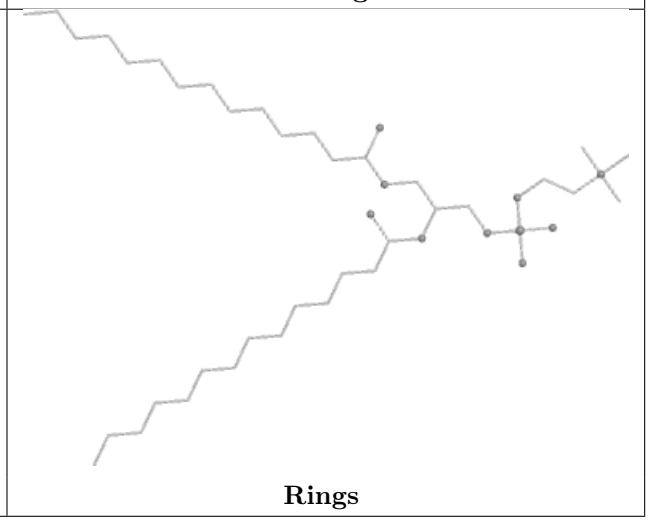
Bond lengths



Bond angles

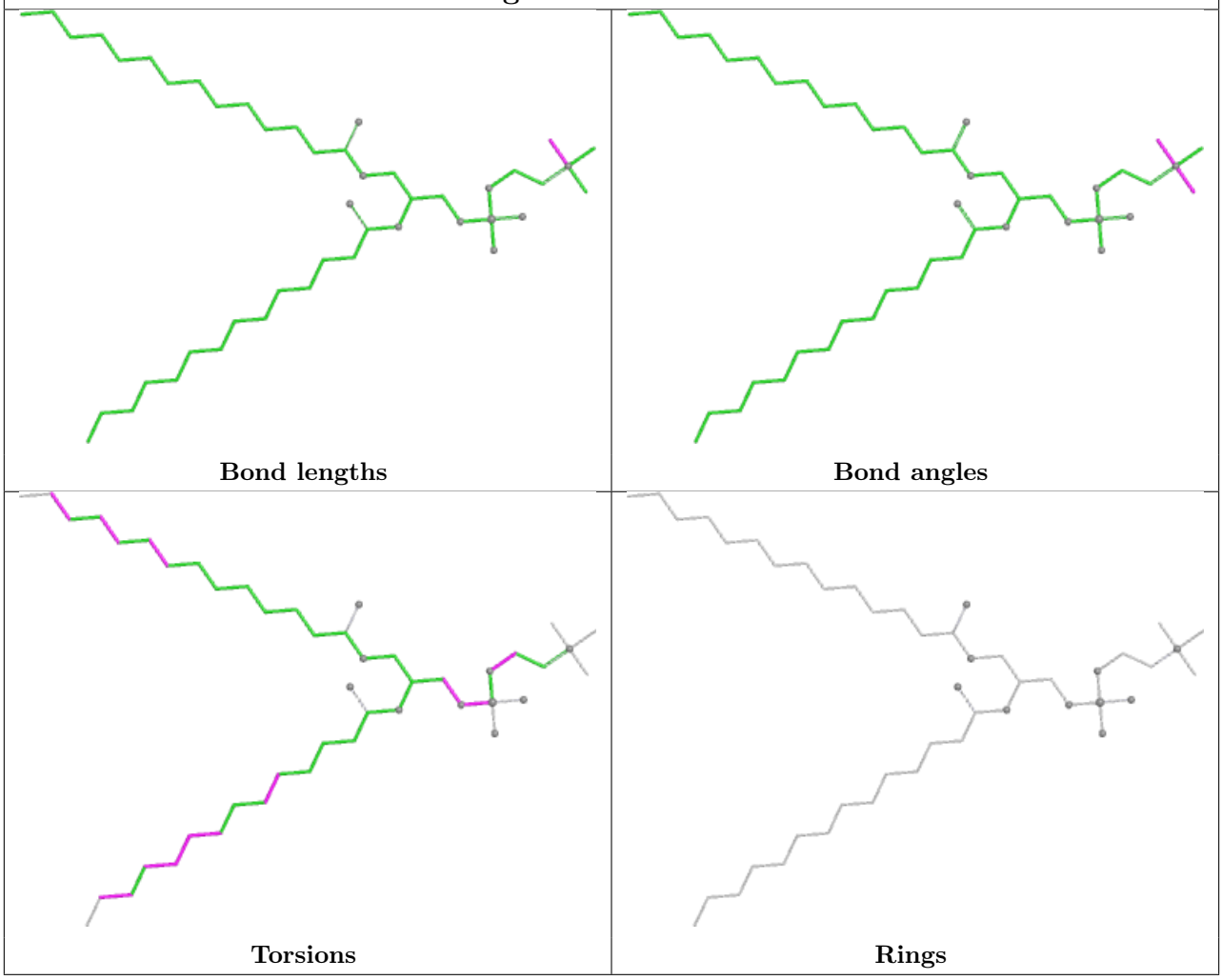


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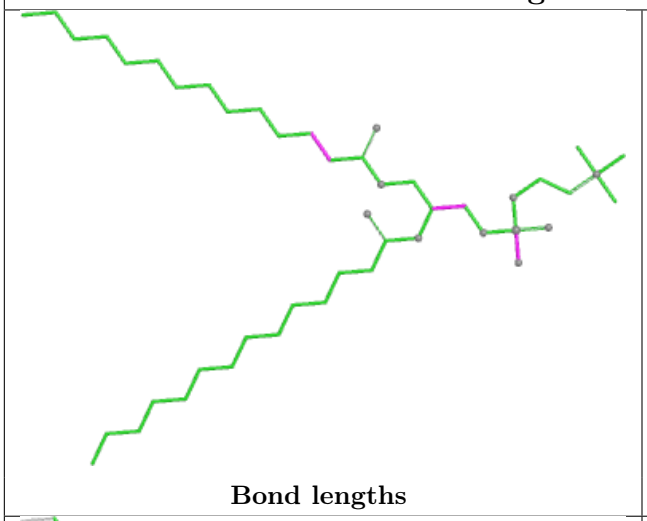


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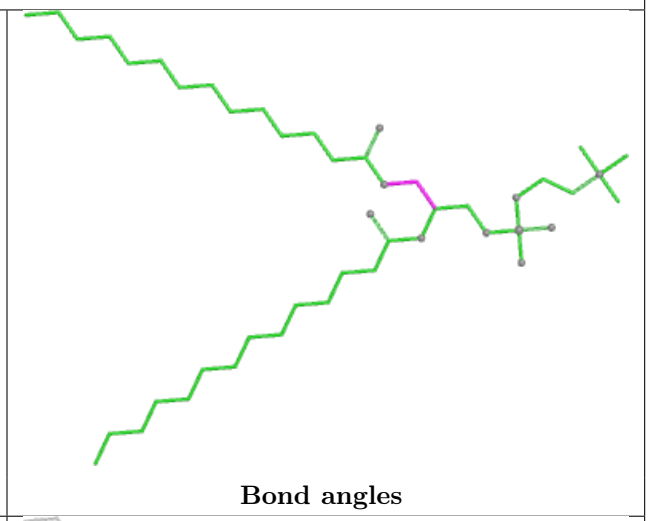
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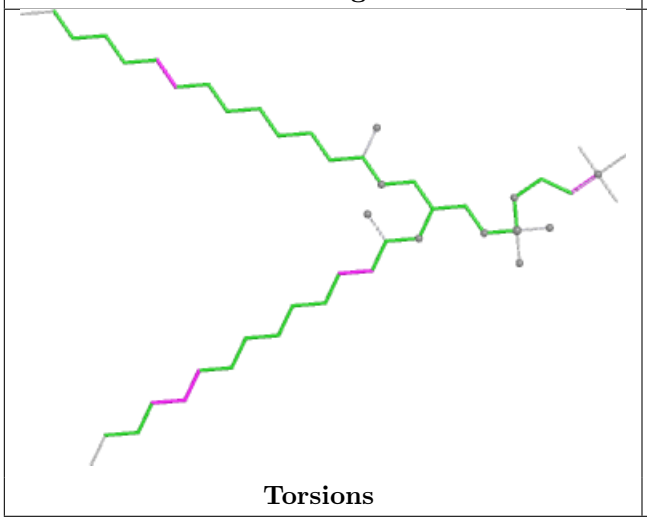
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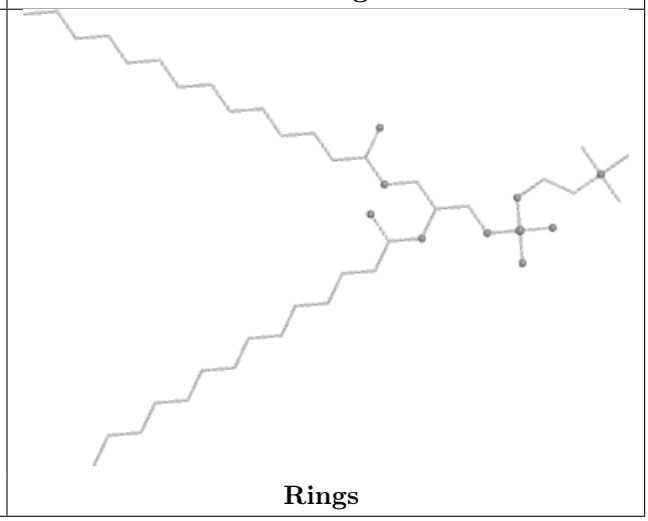
Bond lengths



Bond angles

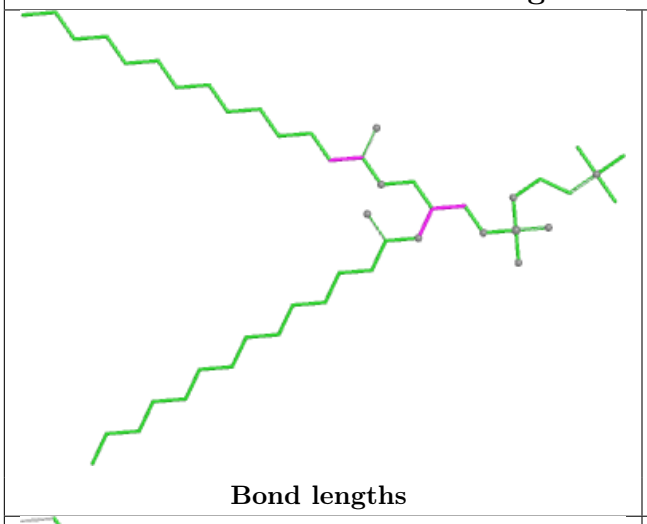


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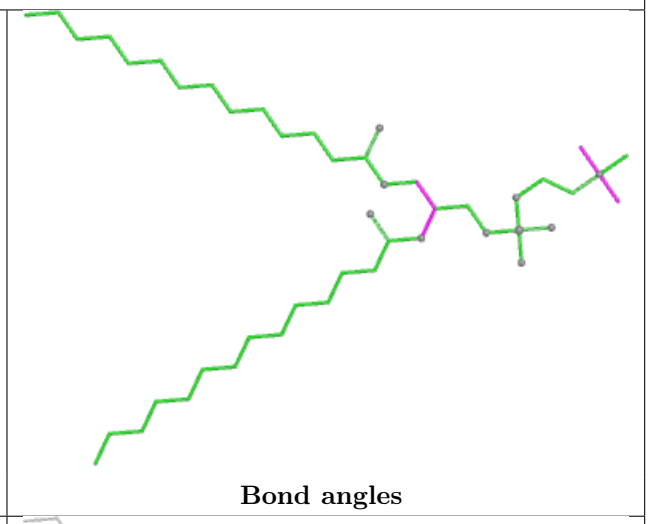


Rings

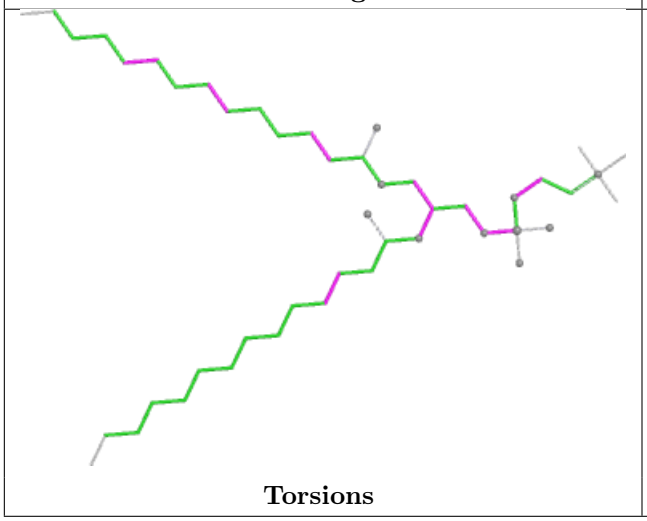
Ligand PX4 C 306



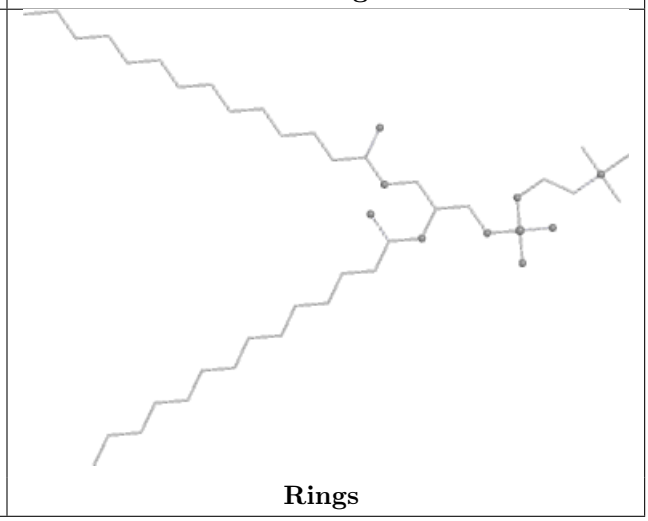
Bond lengths



Bond angles

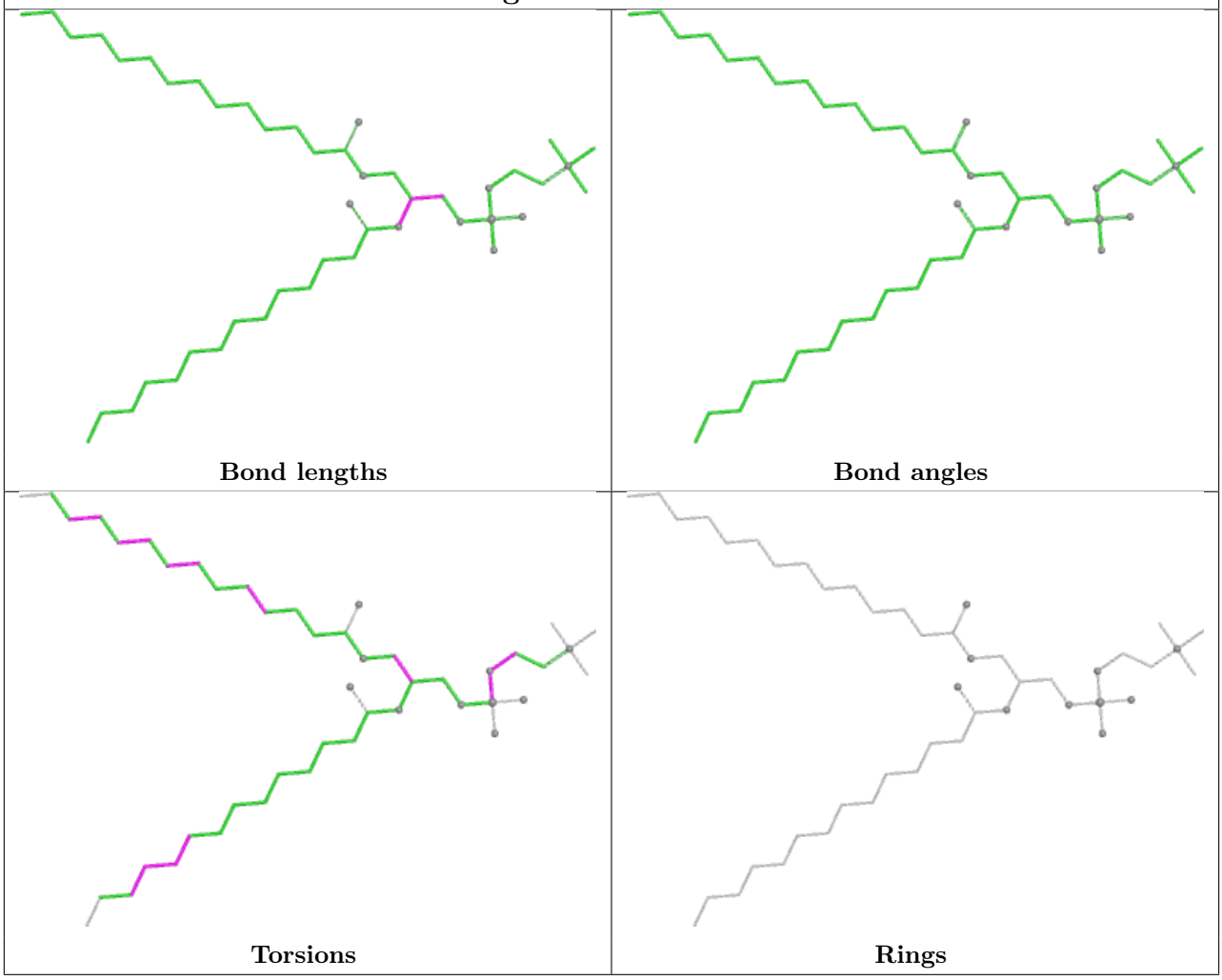


Torsions

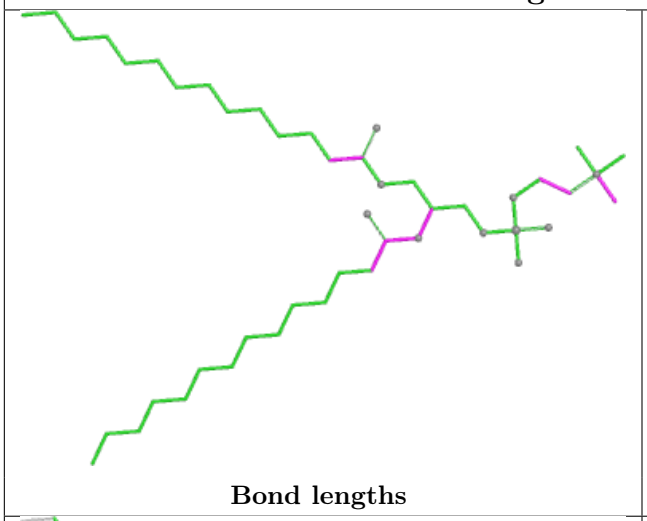


Rings

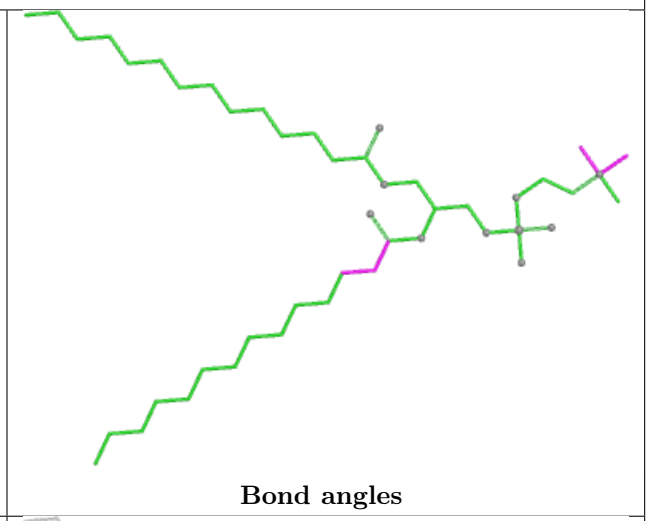
Ligand PX4 B 361



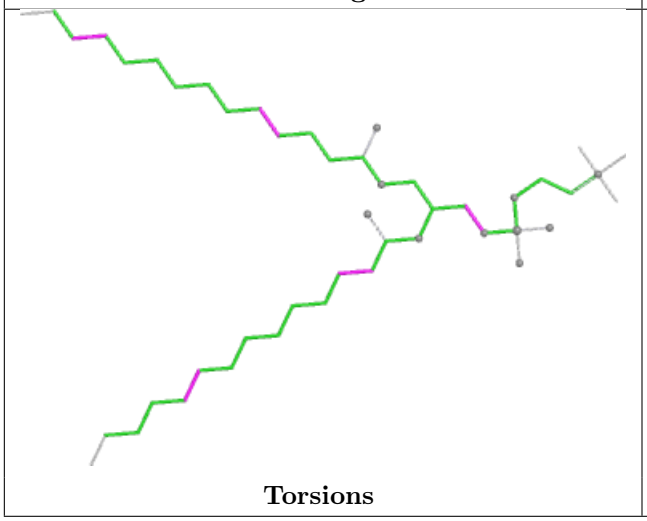
Ligand PX4 A 639



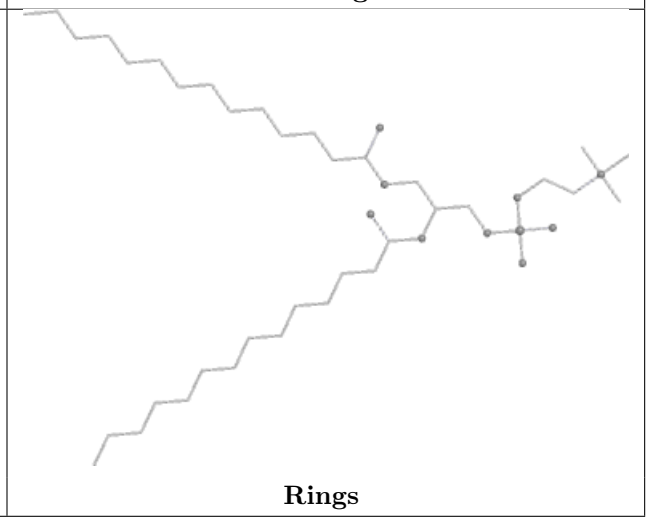
Bond lengths



Bond angles

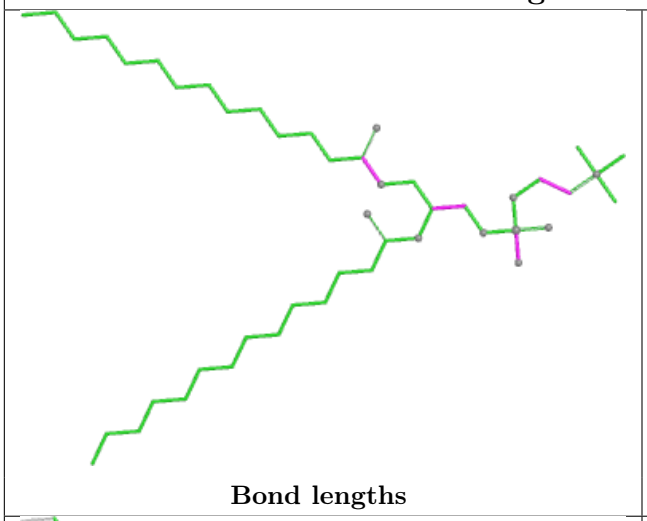


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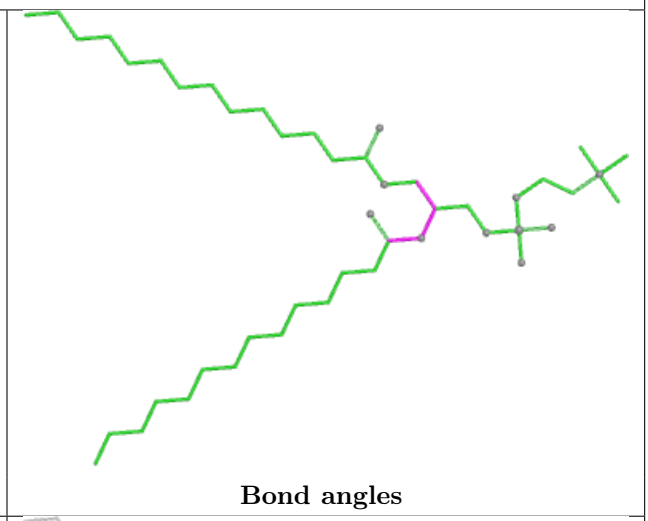


Rings

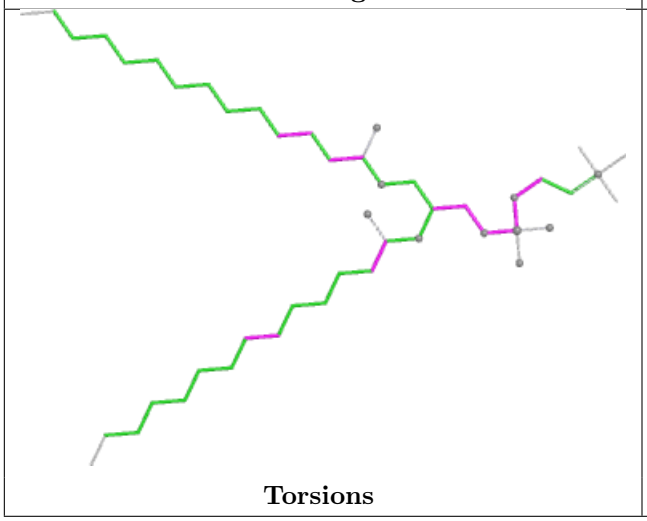
Ligand PX4 C 345



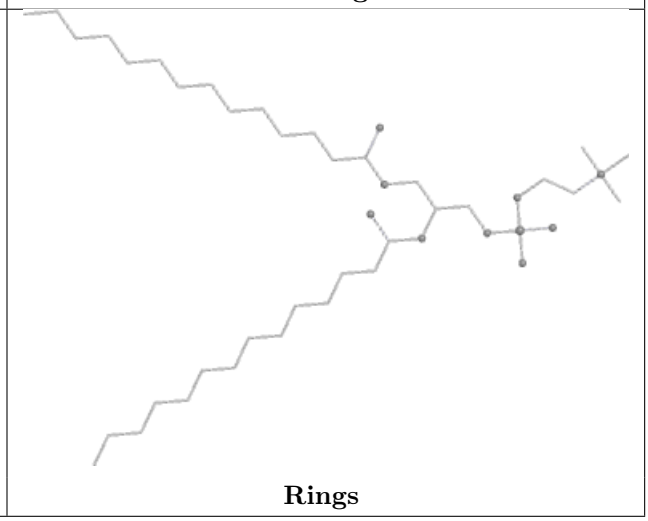
Bond lengths



Bond angles

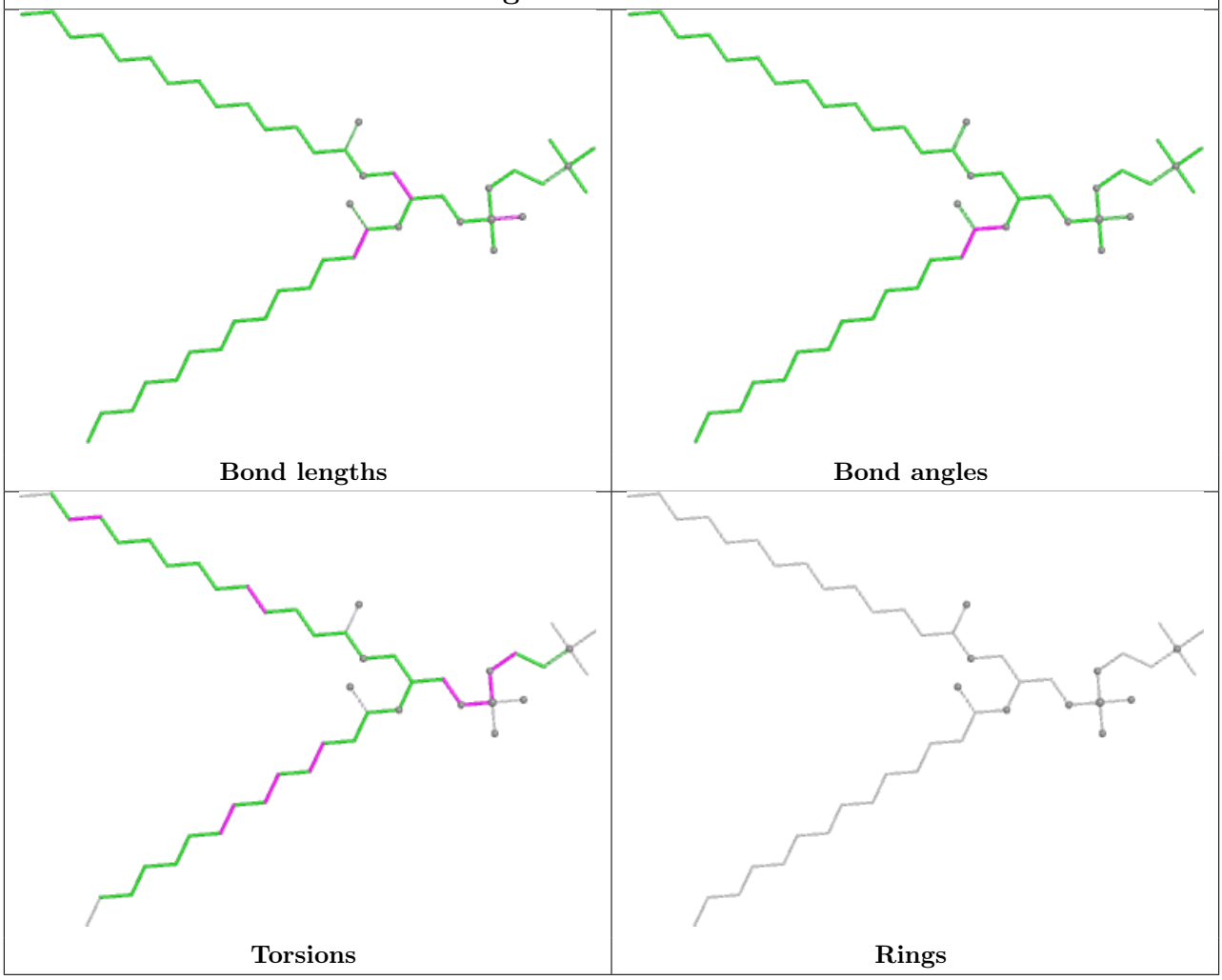


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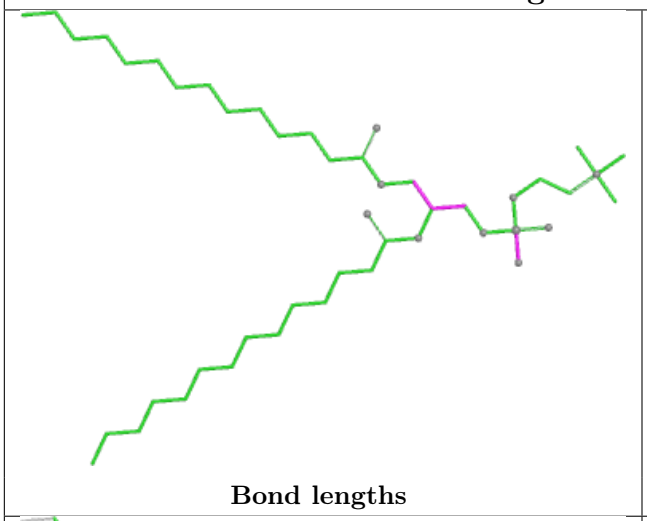


Rings

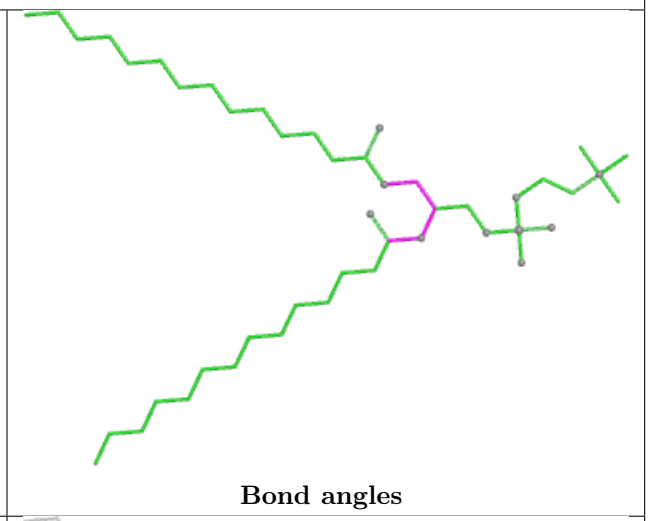
Ligand PX4 B 311



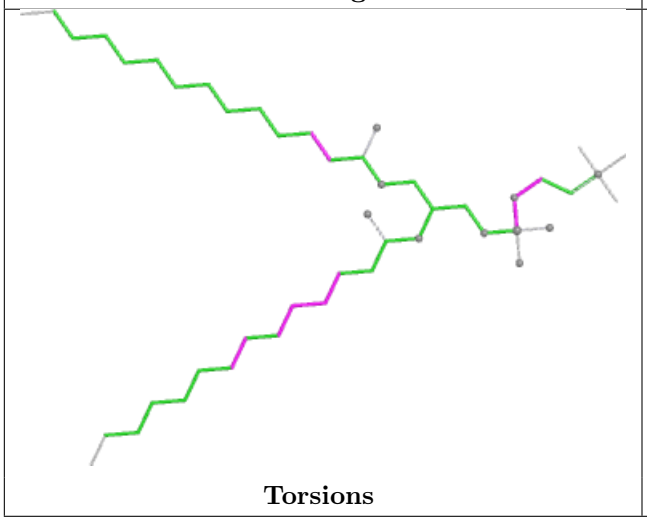
Ligand PX4 A 615



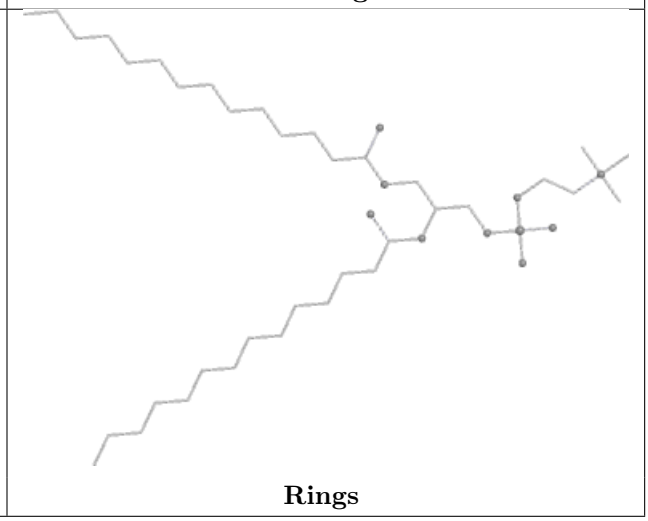
Bond lengths



Bond angles

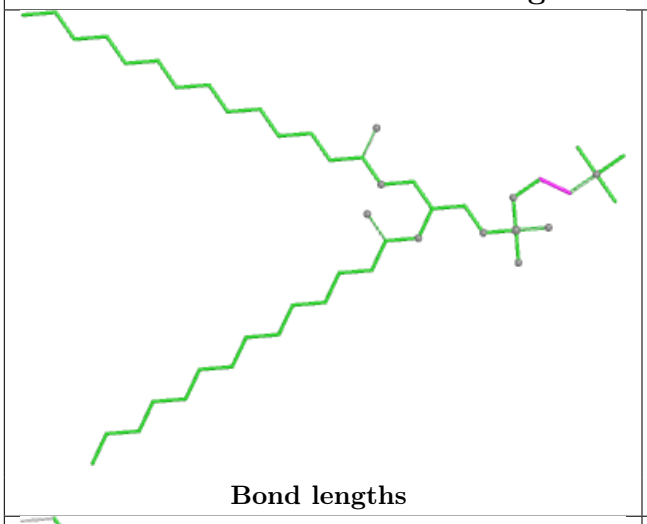


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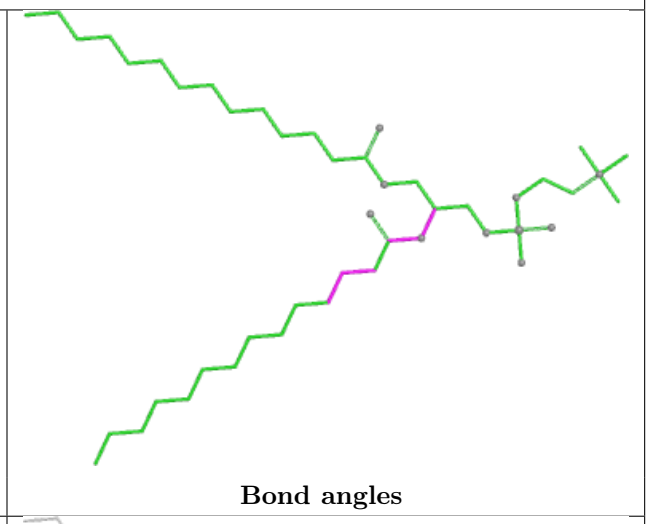


Rings

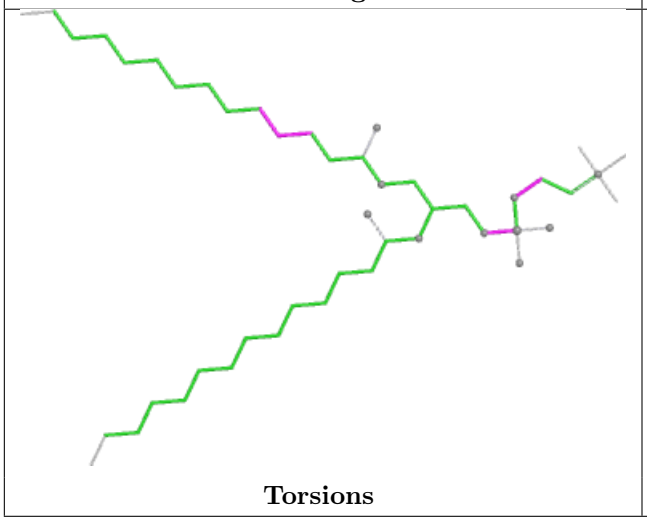
Ligand PX4 B 335



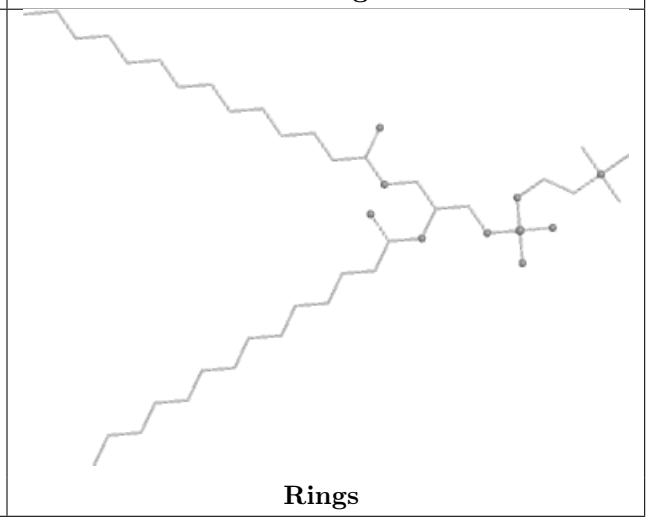
Bond lengths



Bond angles

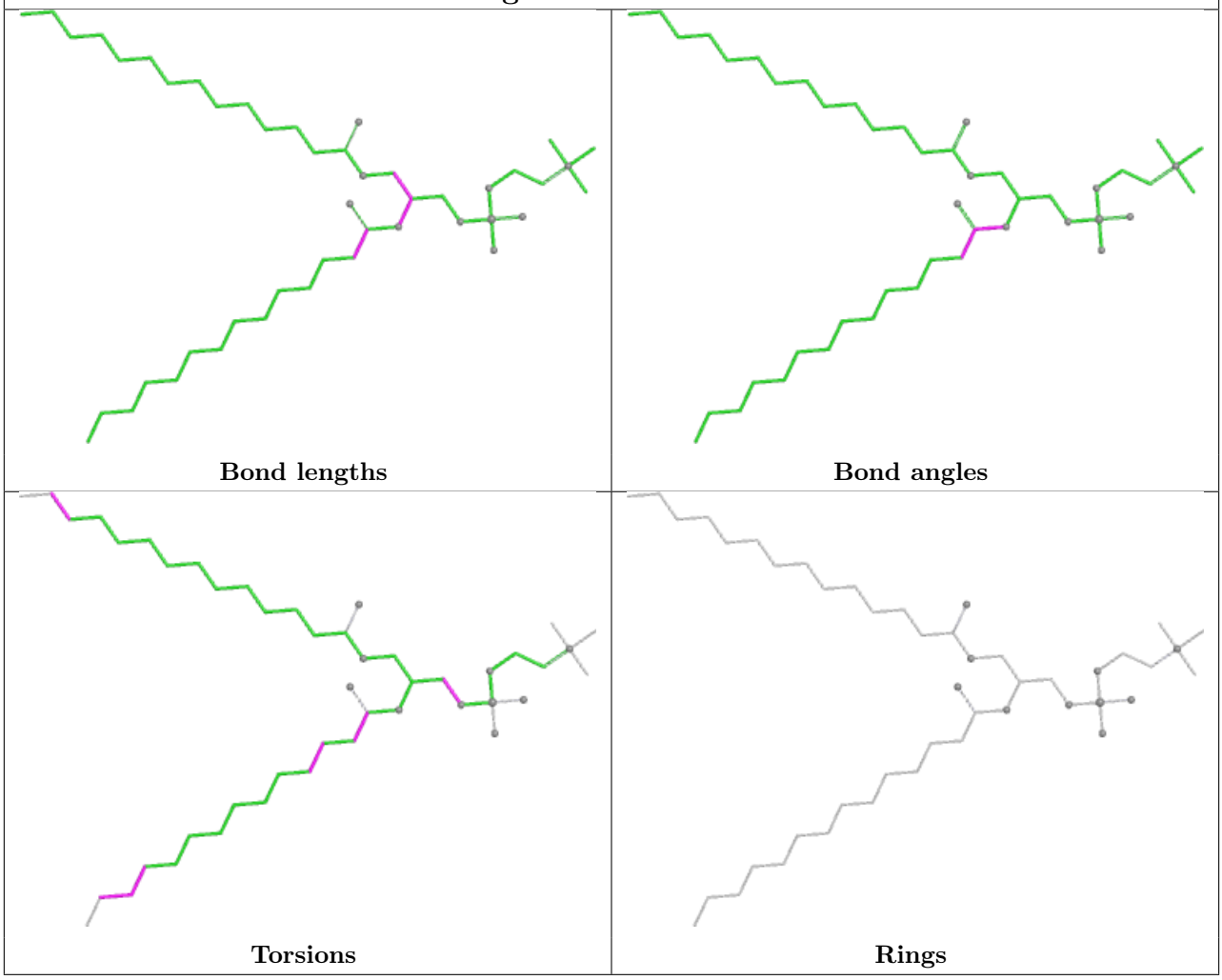


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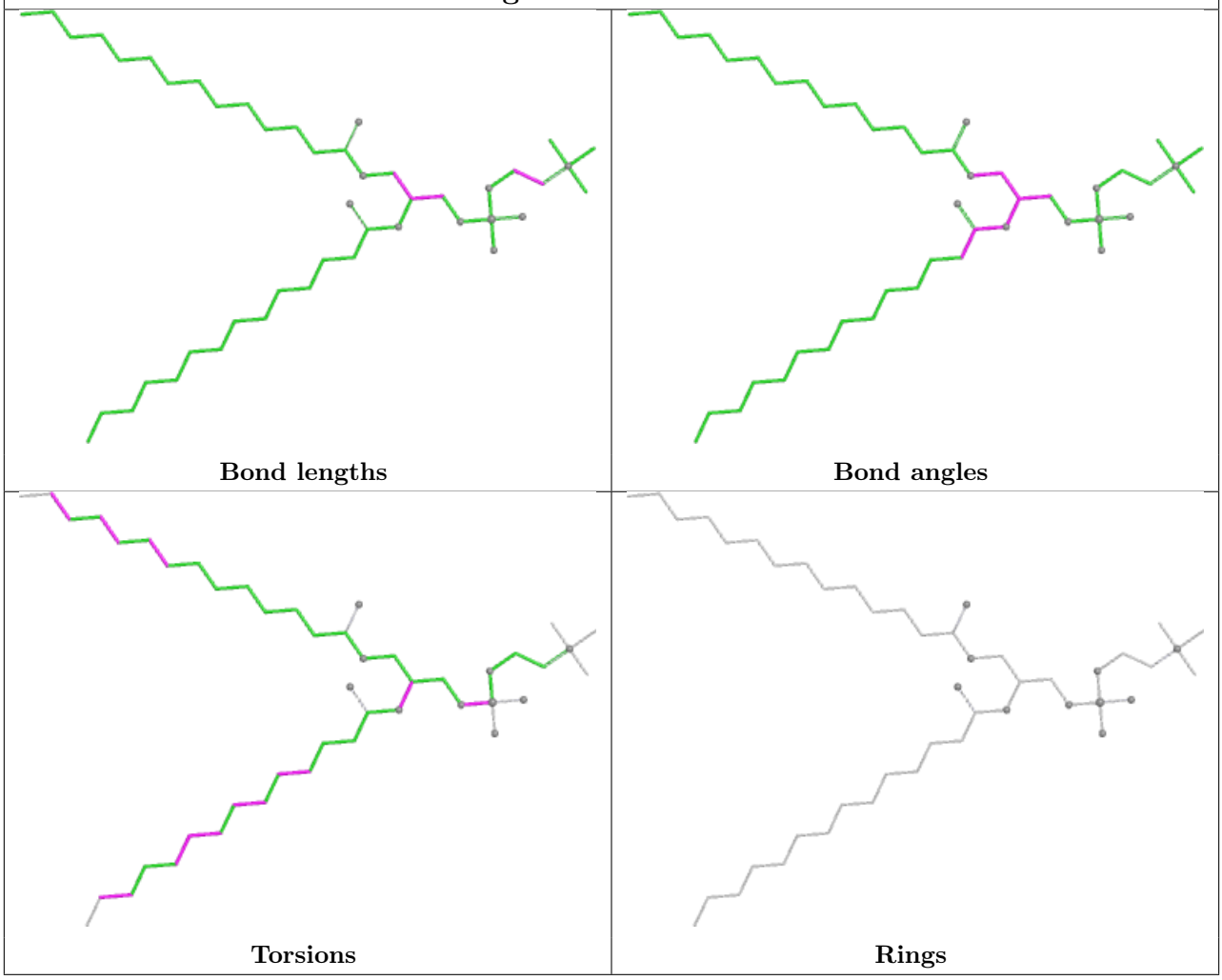


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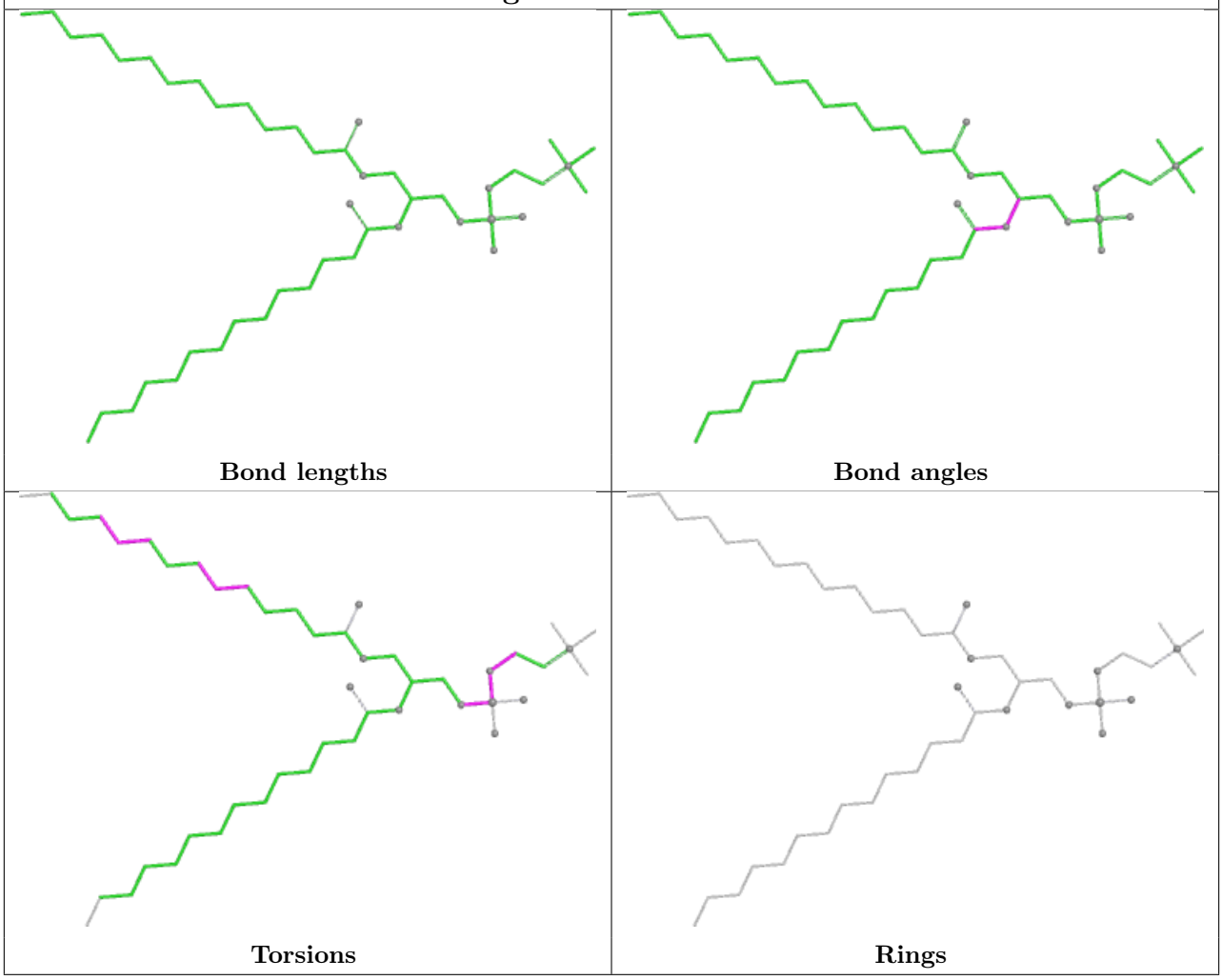
Ligand PX4 A 632



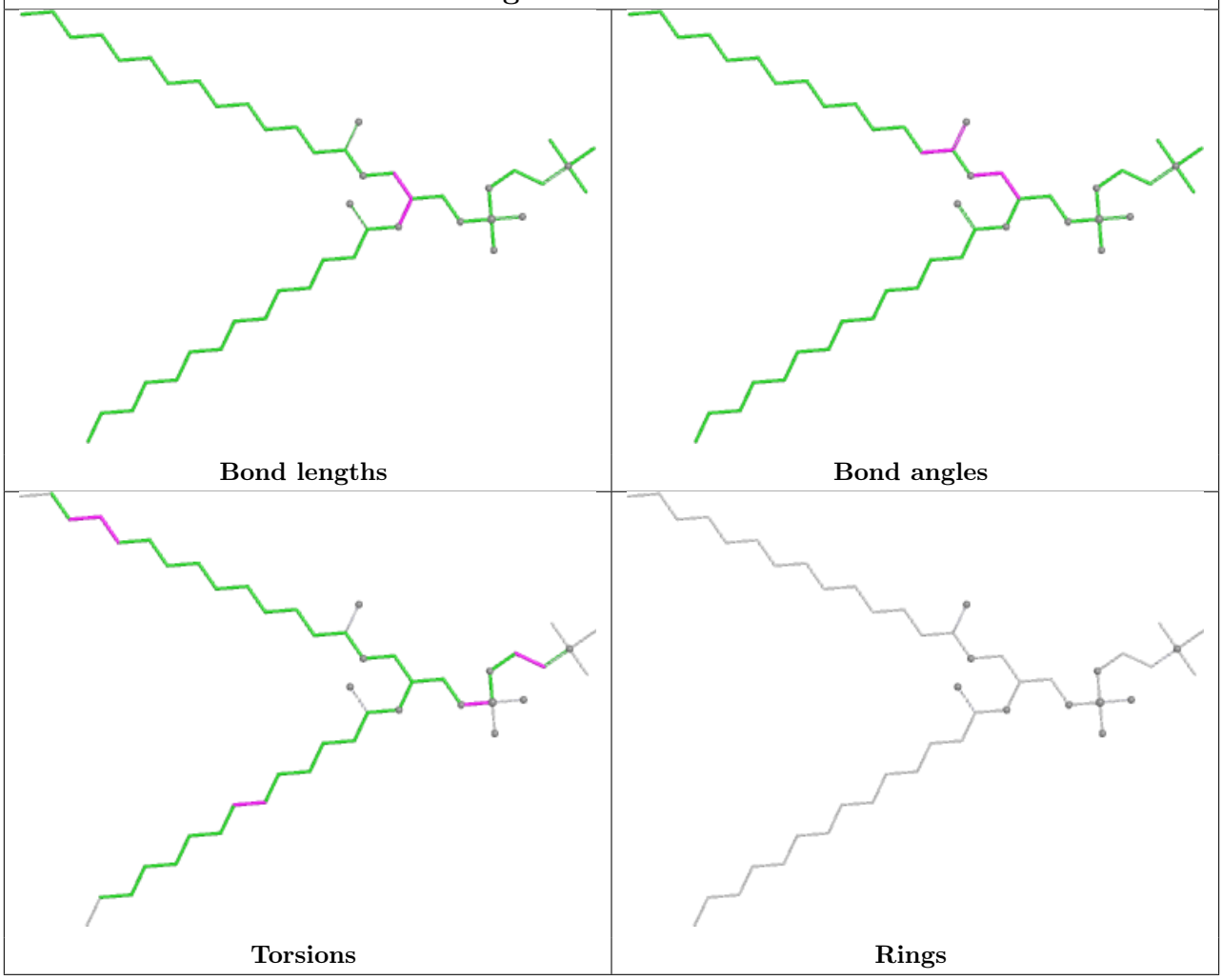
Ligand PX4 C 350



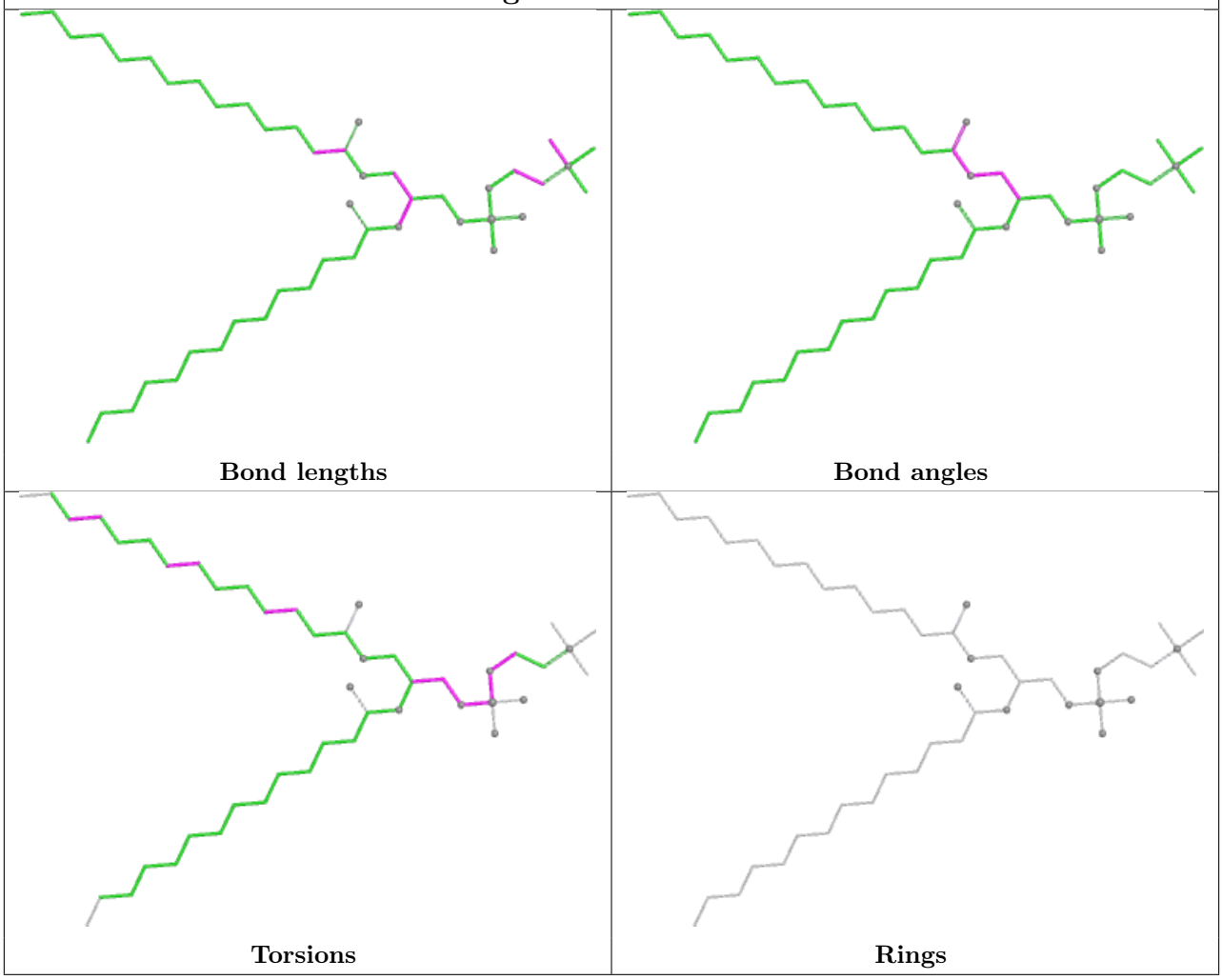
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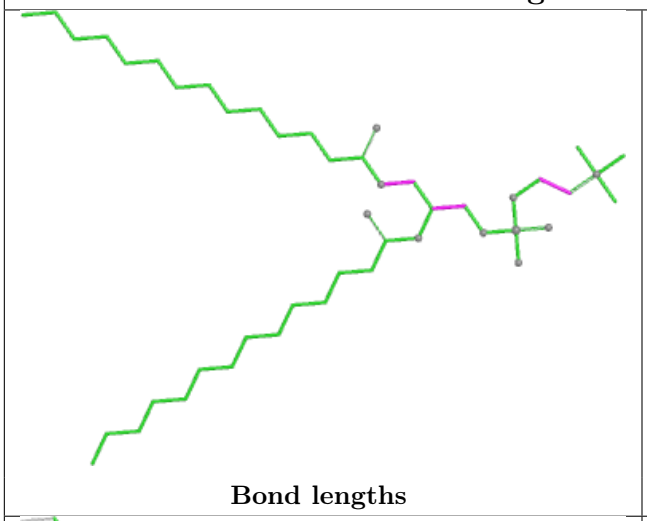
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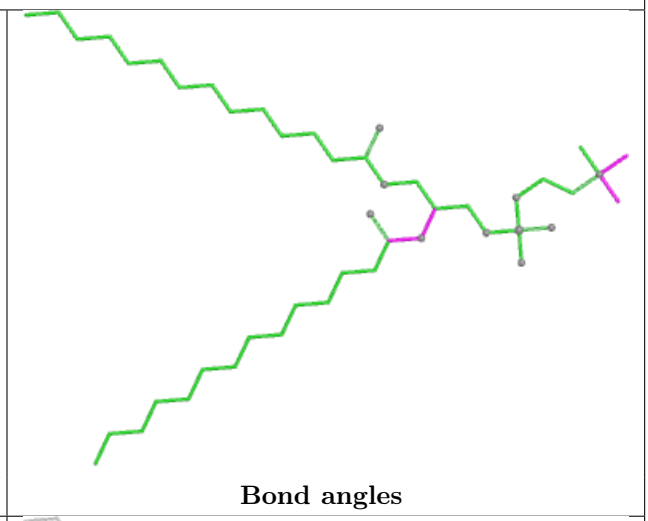
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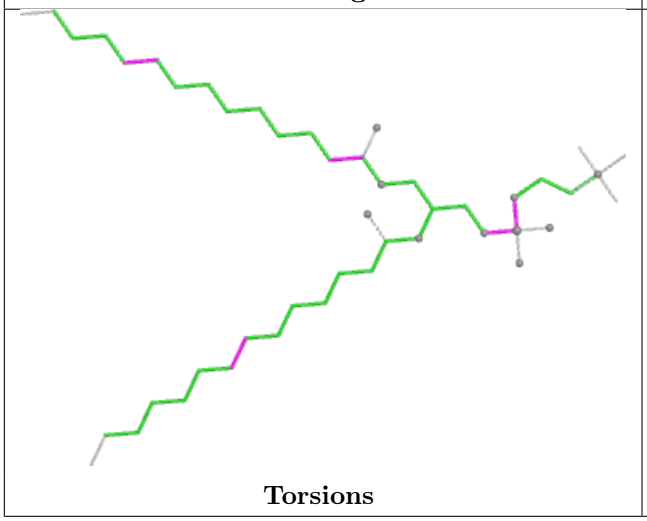
Ligand PX4 A 610



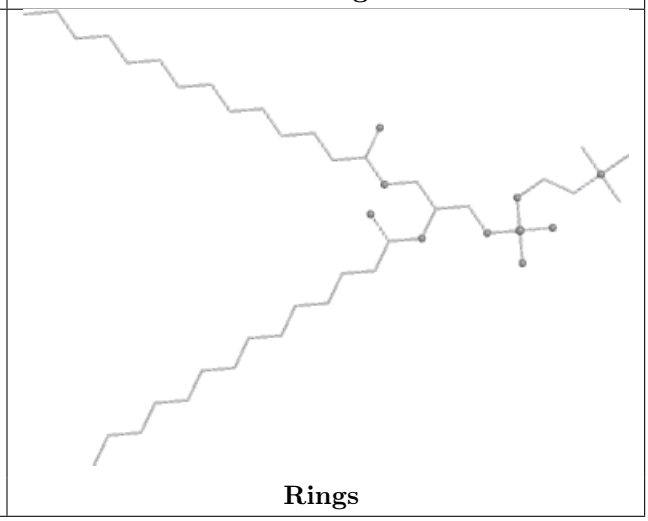
Bond lengths



Bond angles

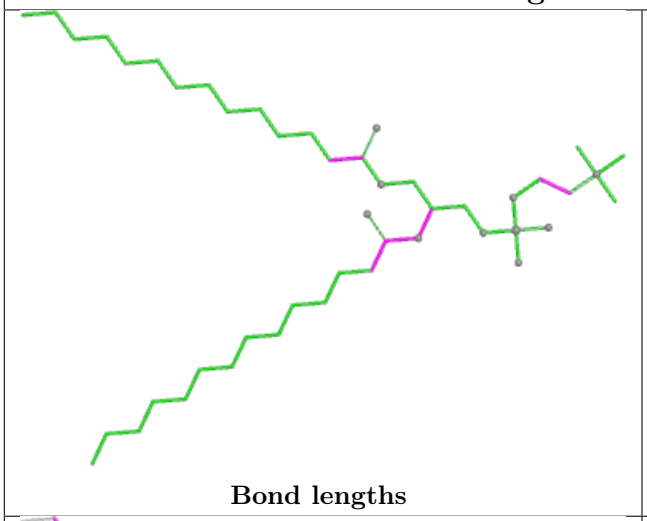


Torsions

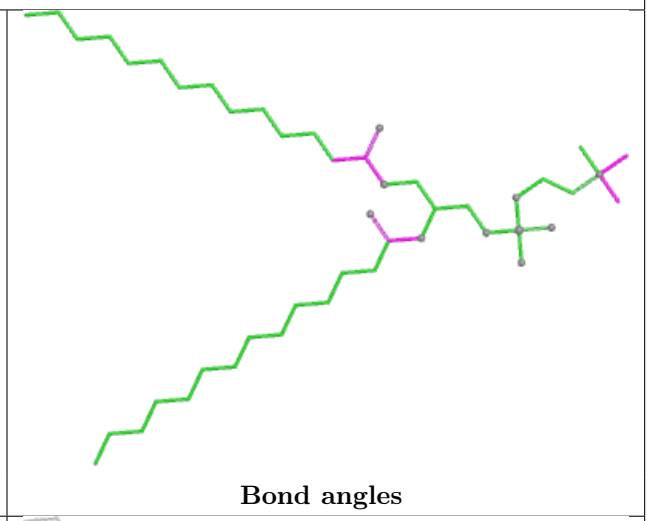


Rings

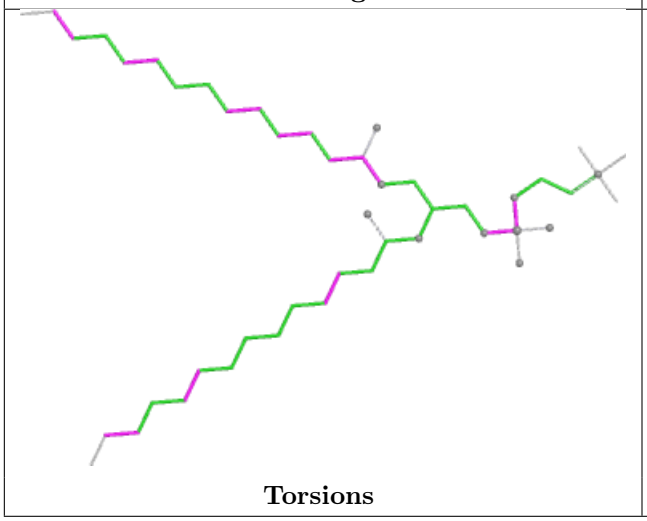
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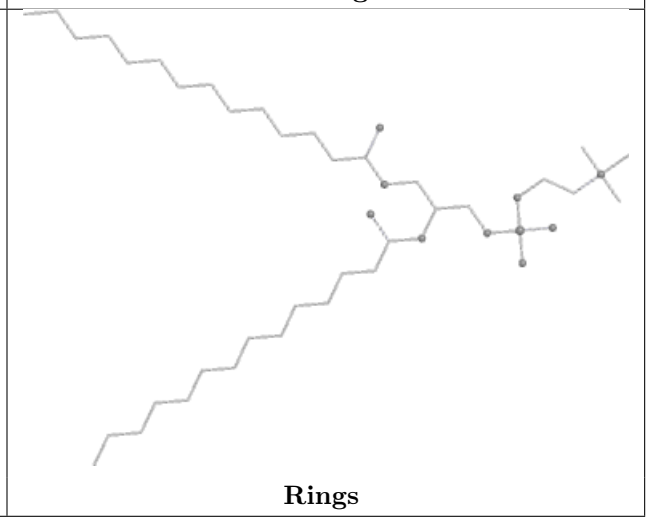
Bond lengths



Bond angles

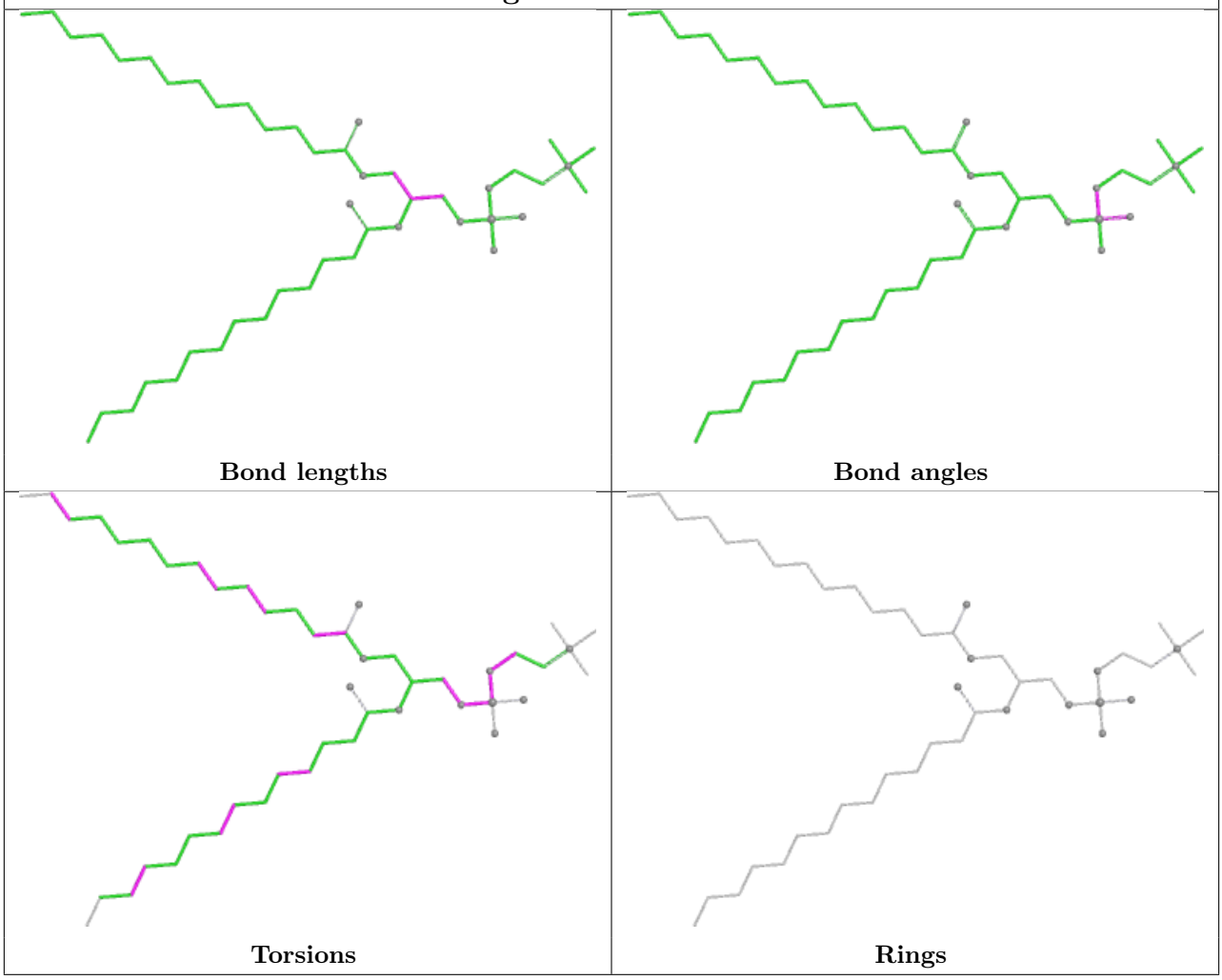


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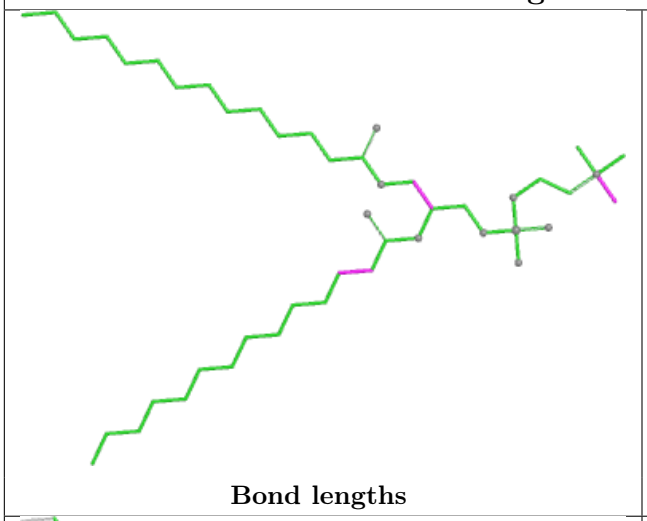


Rings

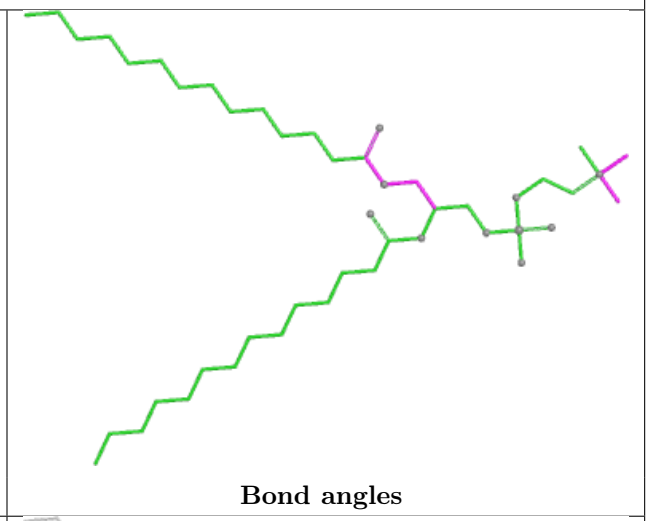
Ligand PX4 B 326



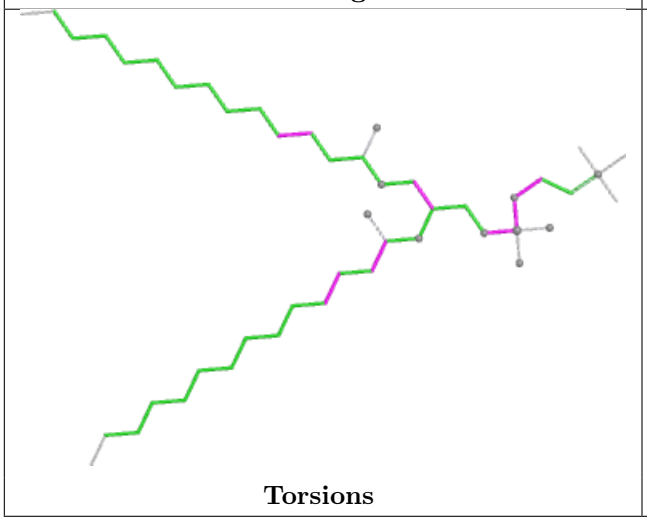
Ligand PX4 A 618



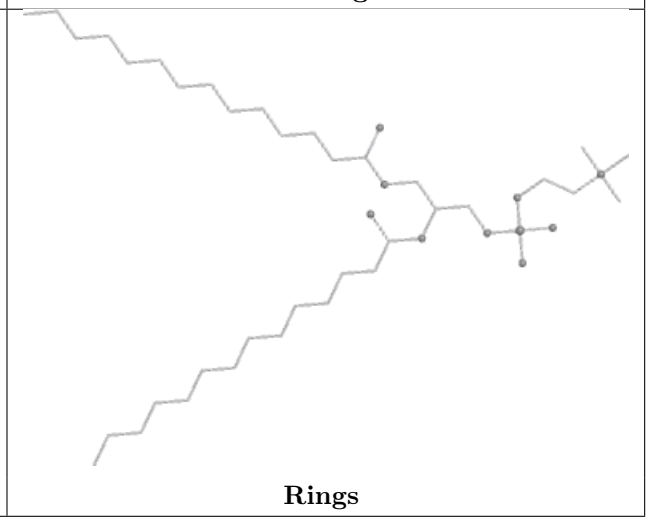
Bond lengths



Bond angles

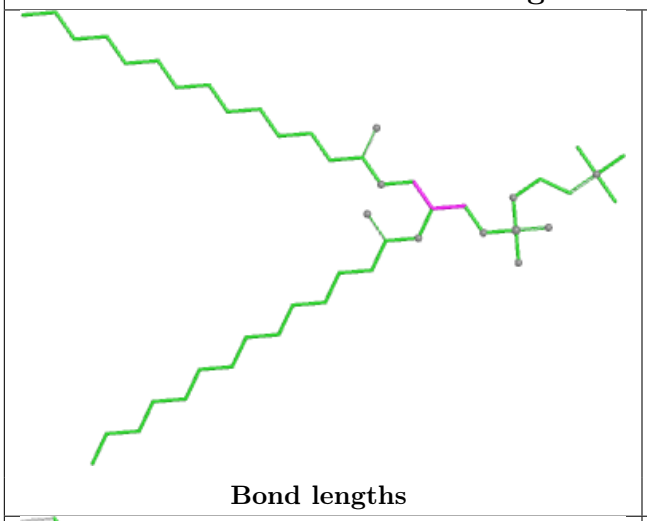


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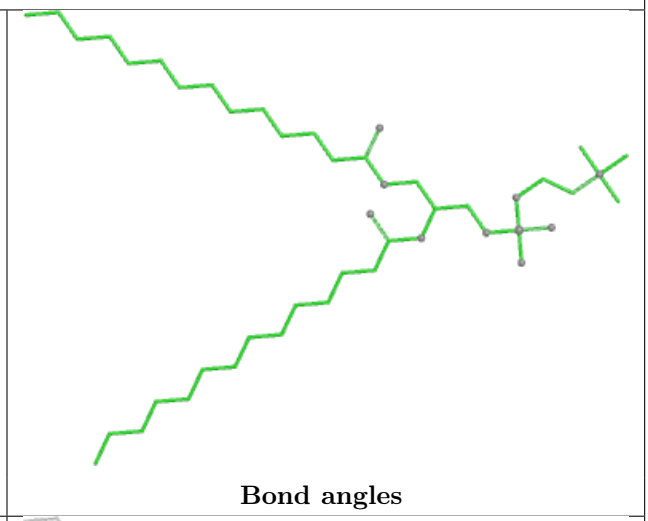


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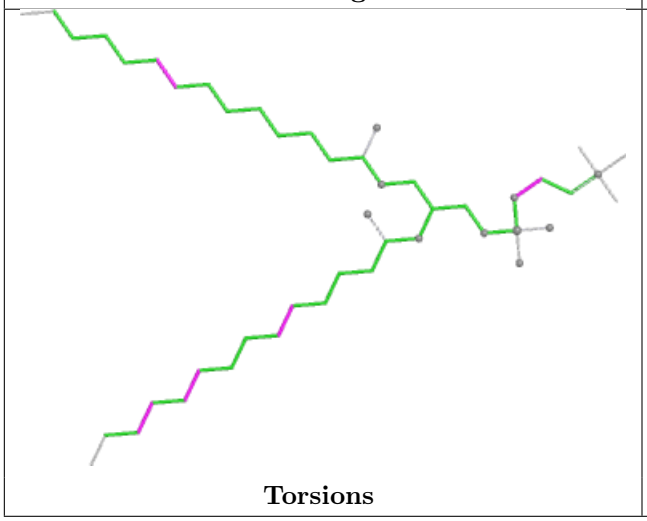
Ligand PX4 A 638



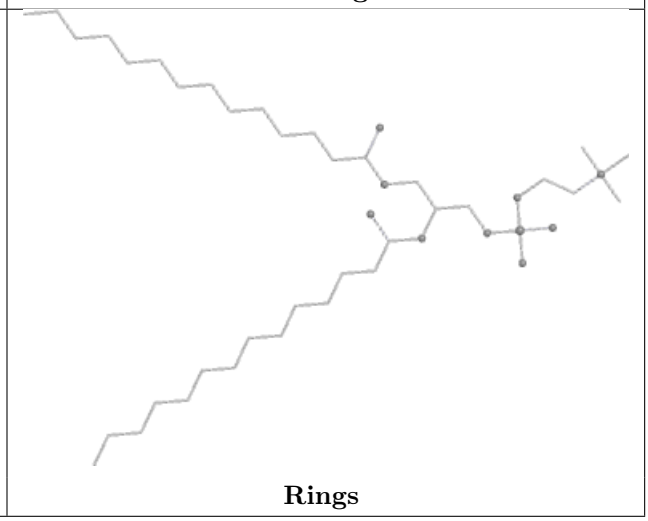
Bond lengths



Bond angles

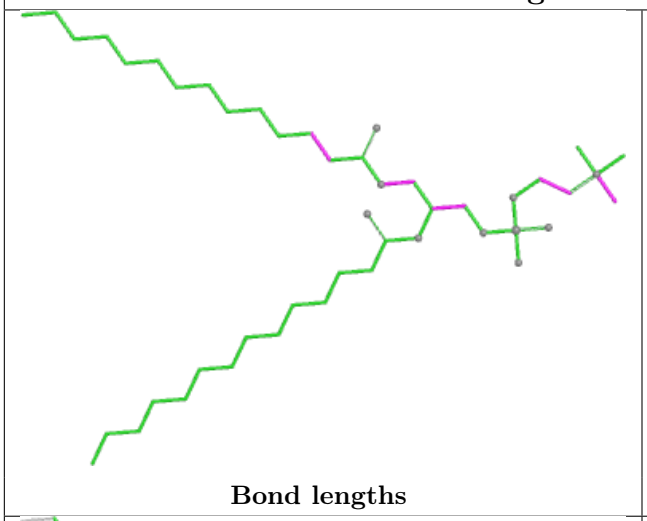


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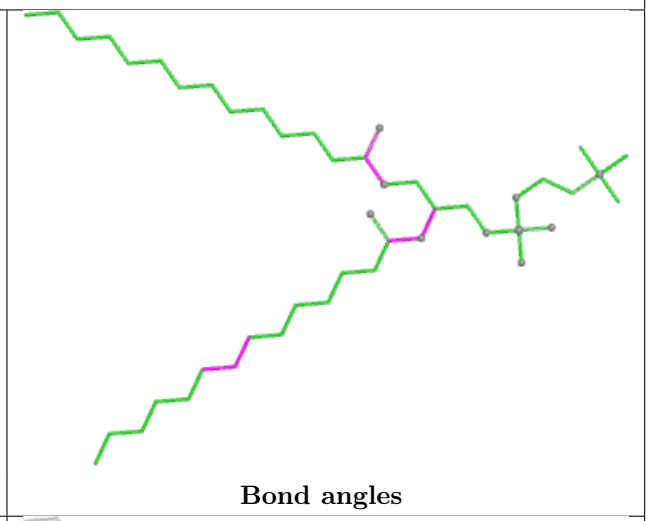


Rings

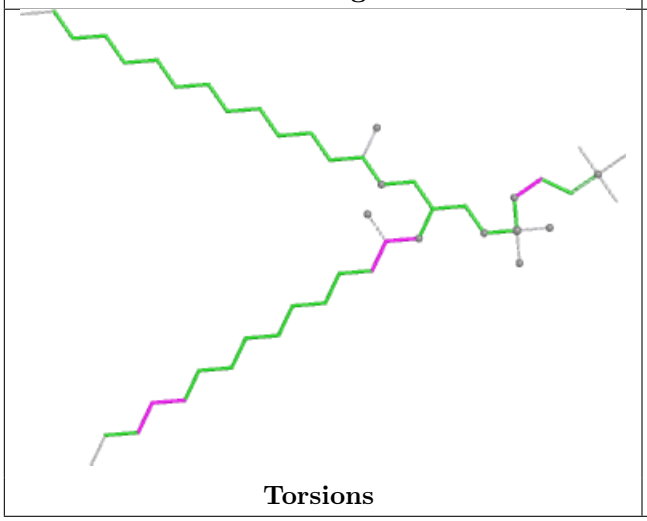
Ligand PX4 A 603



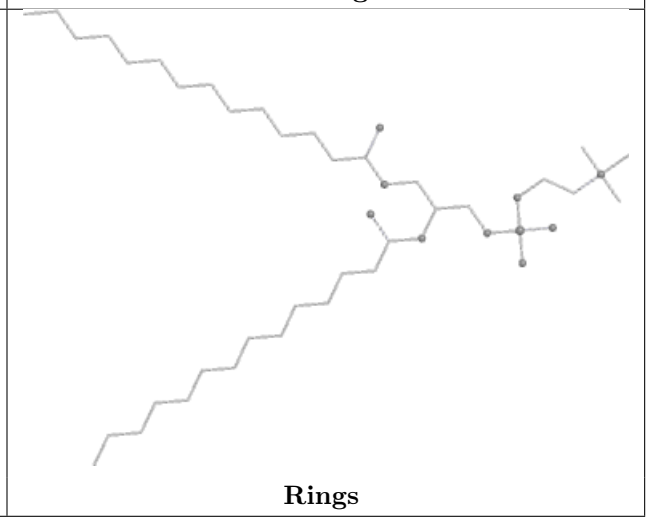
Bond lengths



Bond angles

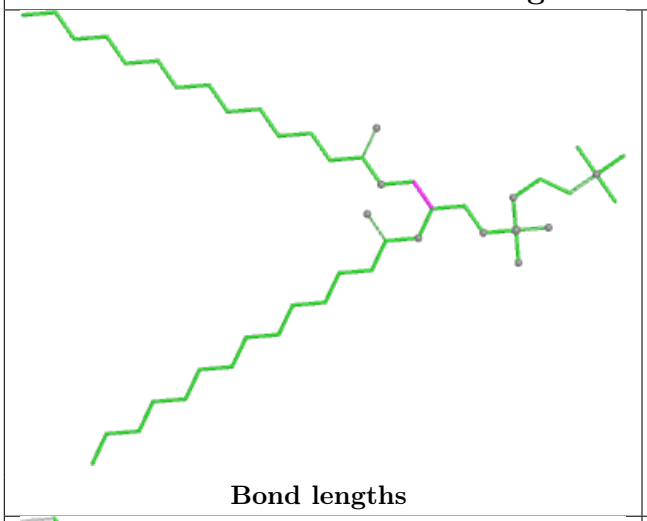


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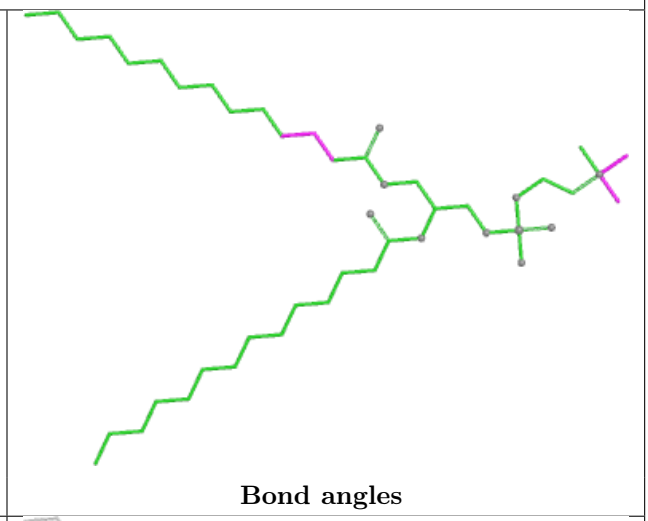


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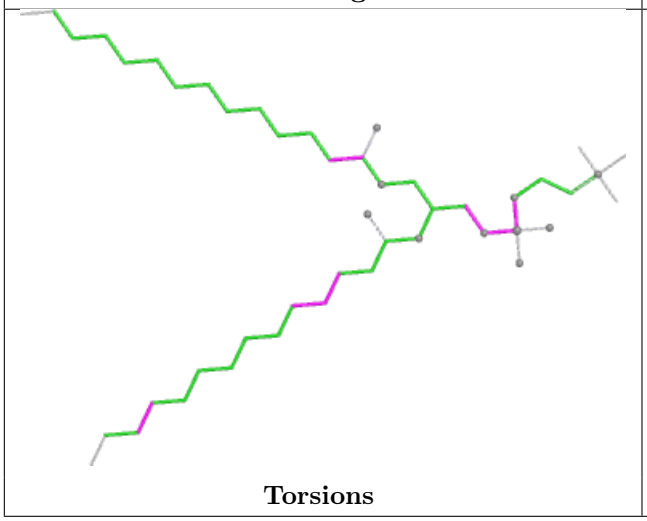
Ligand PX4 A 628



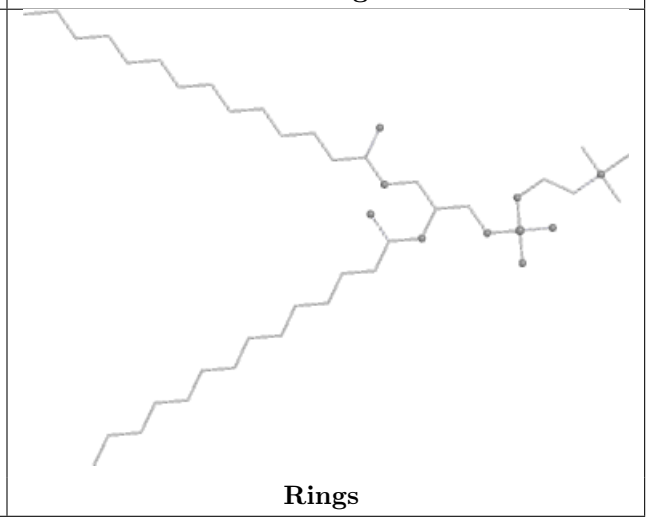
Bond lengths



Bond angles

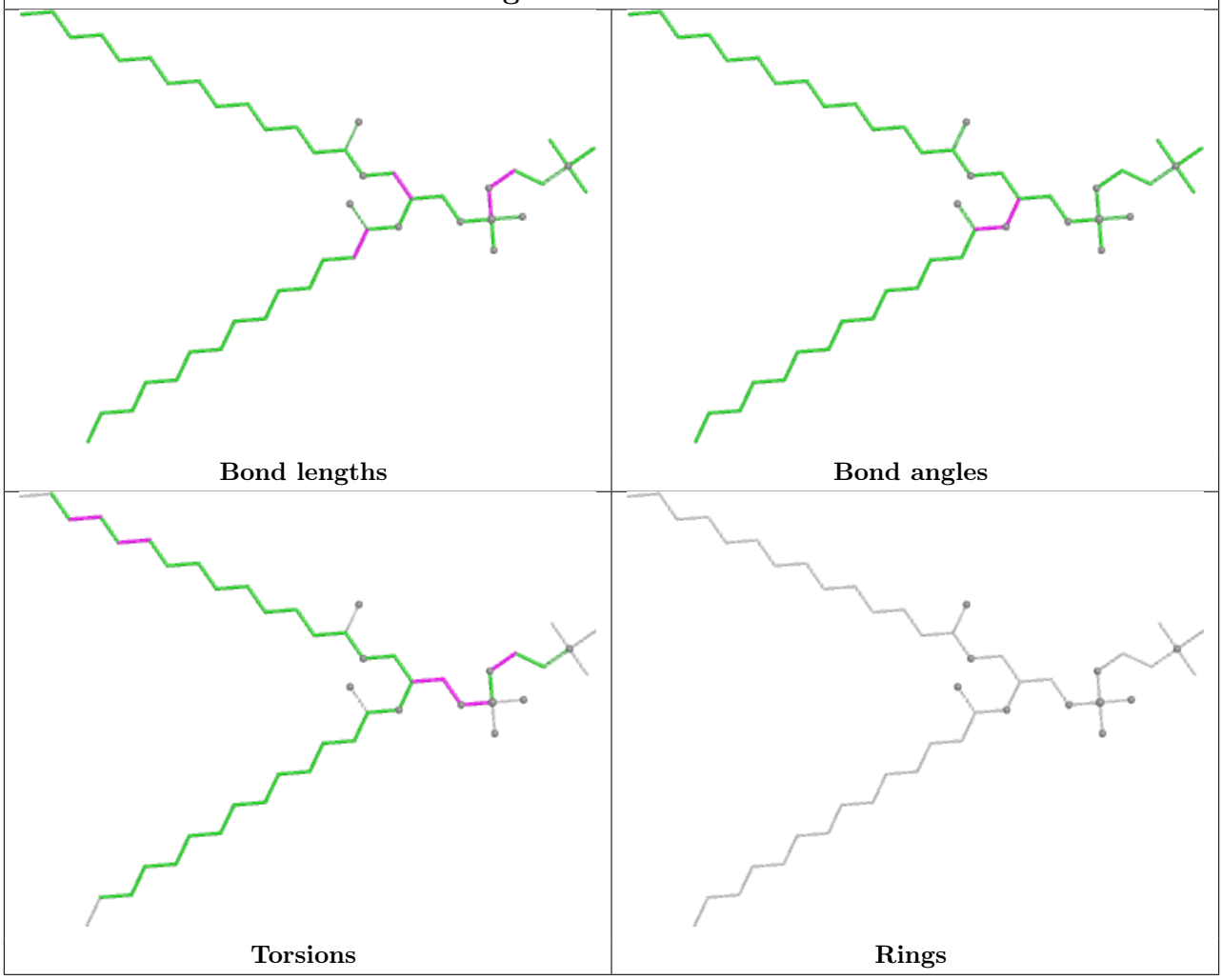


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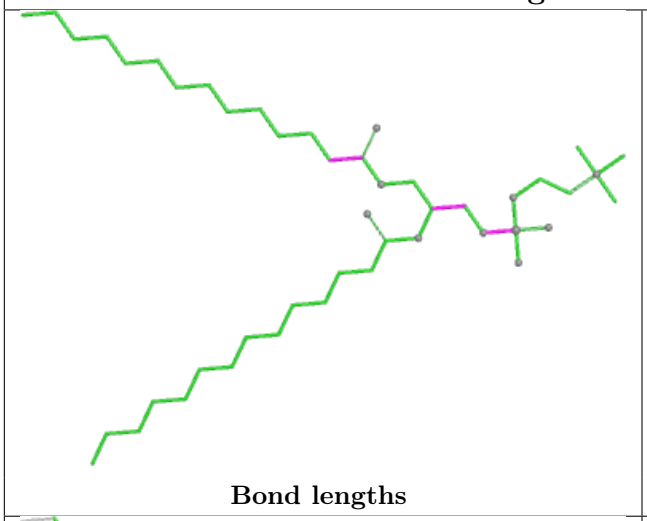


Rings

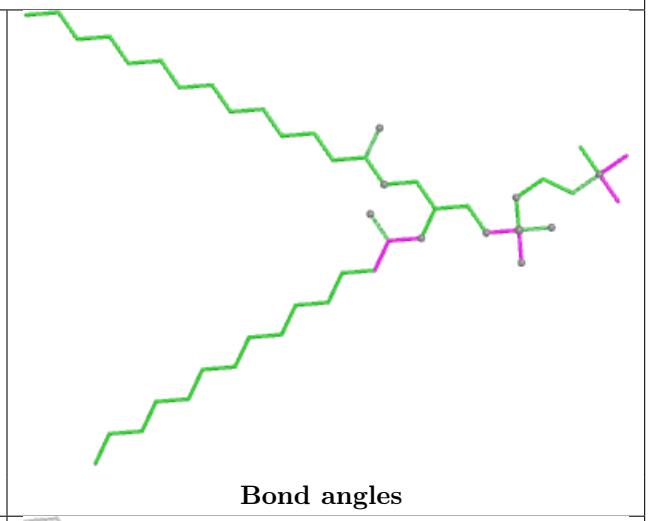
Ligand PX4 B 384



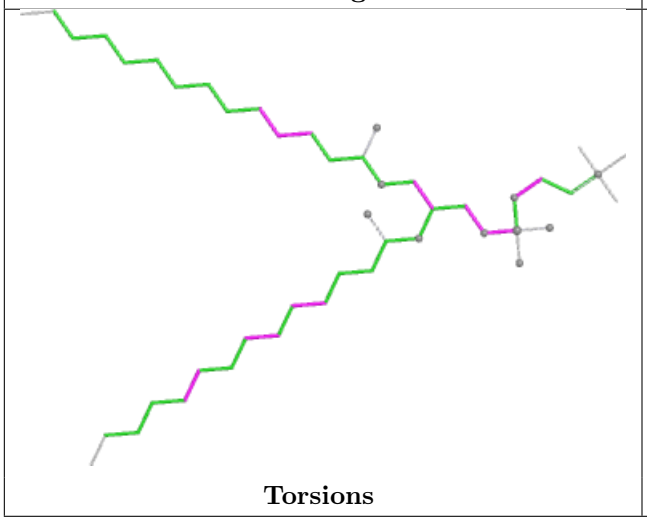
Ligand PX4 C 305



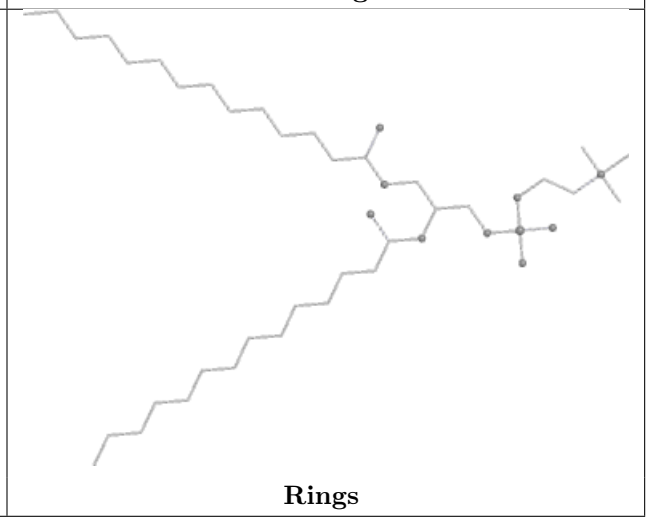
Bond lengths



Bond angles

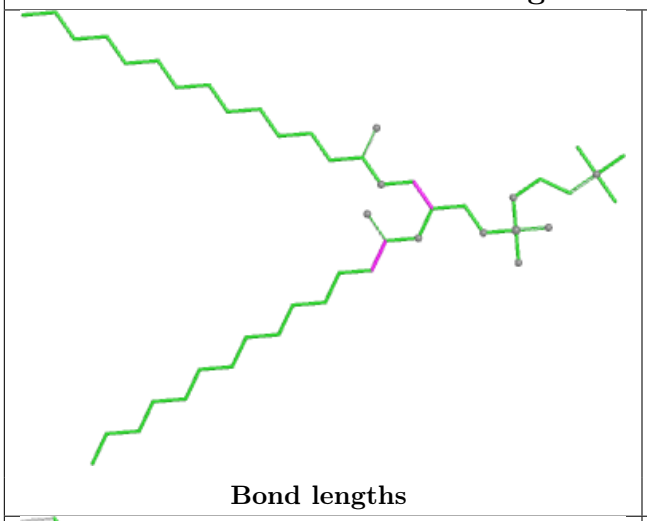


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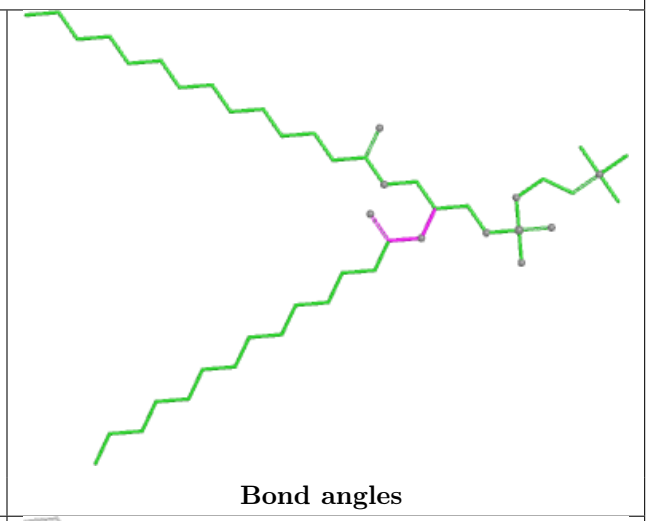


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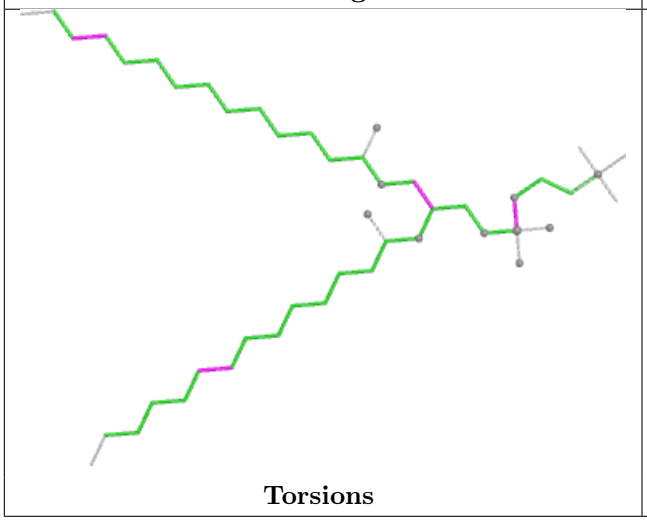
Ligand PX4 C 357



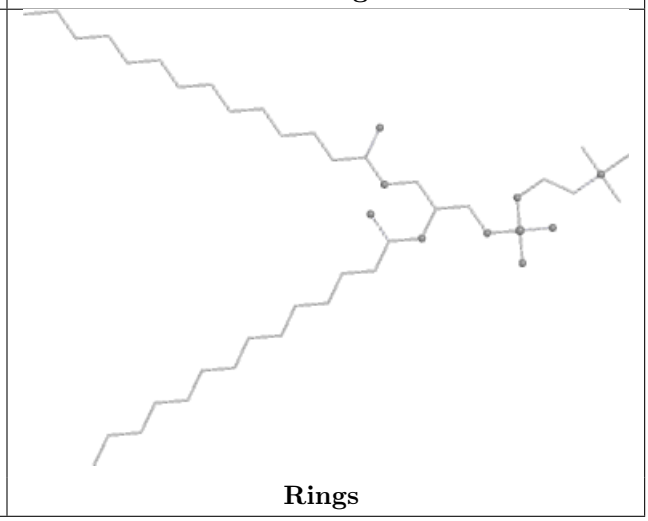
Bond lengths



Bond angles

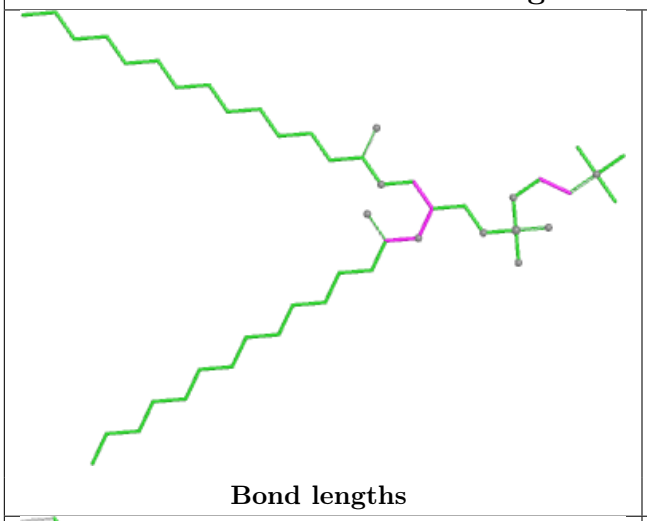


Torsions

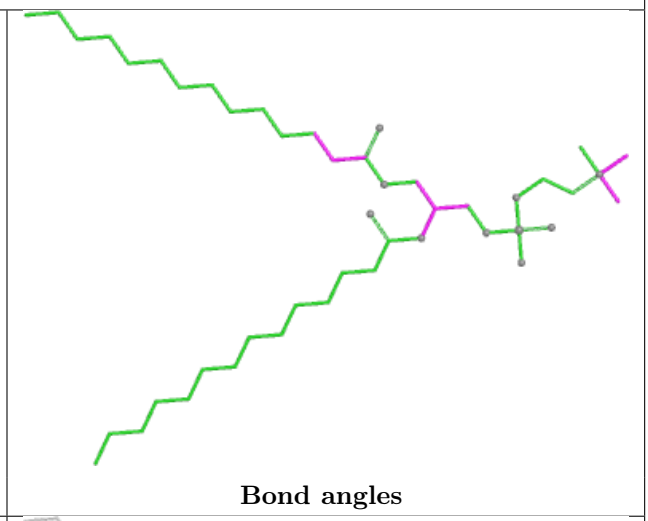


Rings

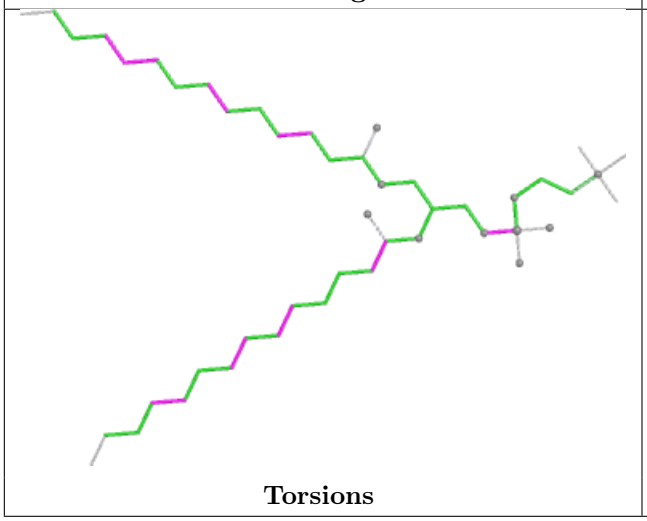
Ligand PX4 C 339



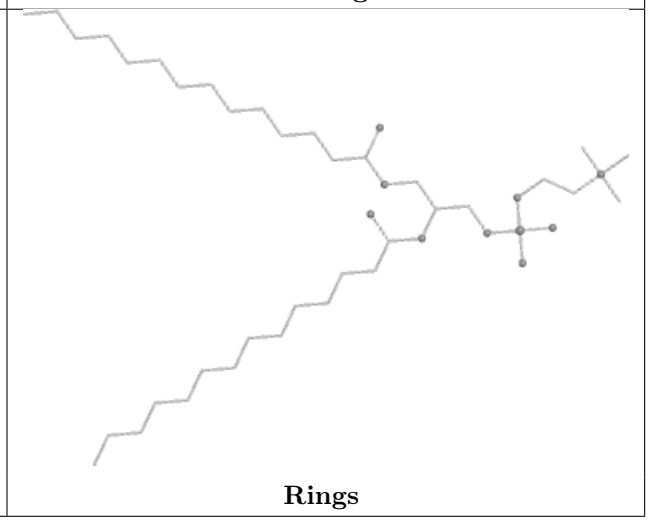
Bond lengths



Bond angles

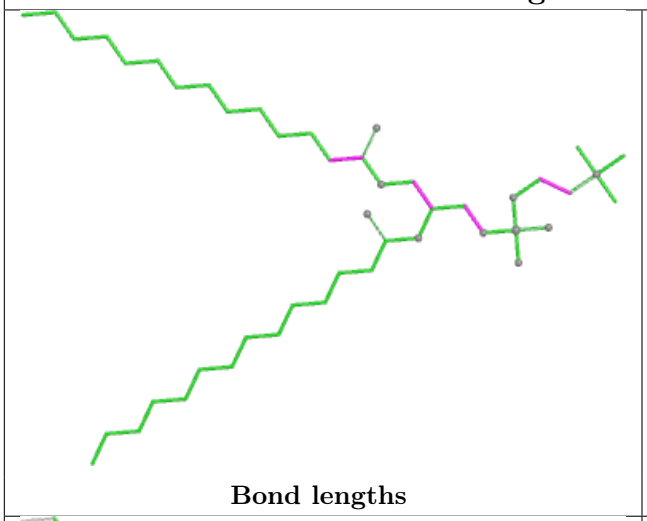


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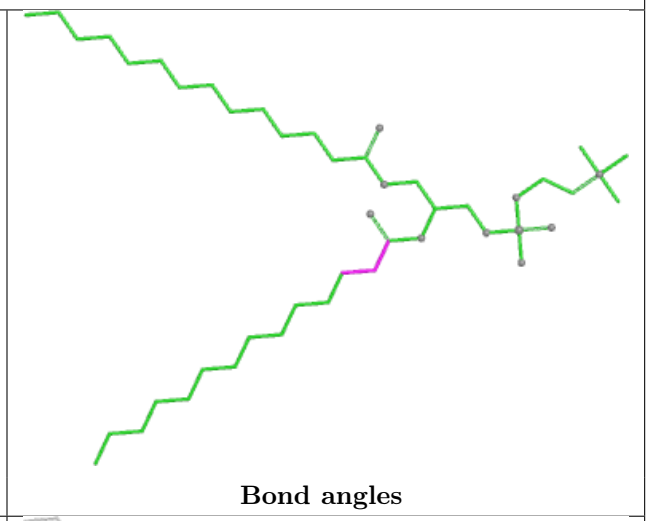


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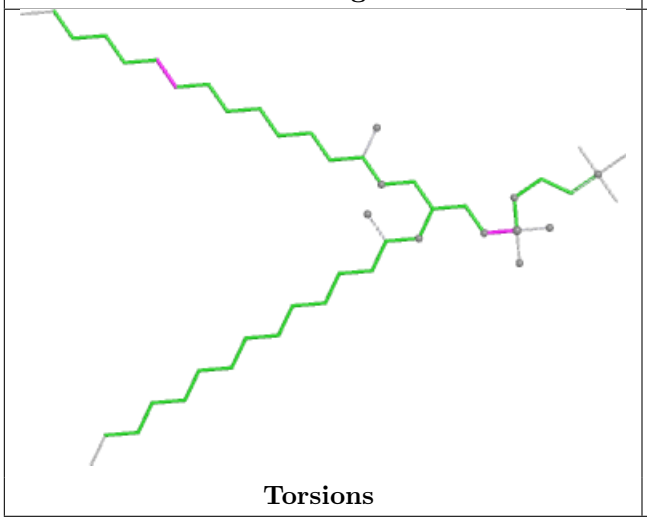
Ligand PX4 B 395



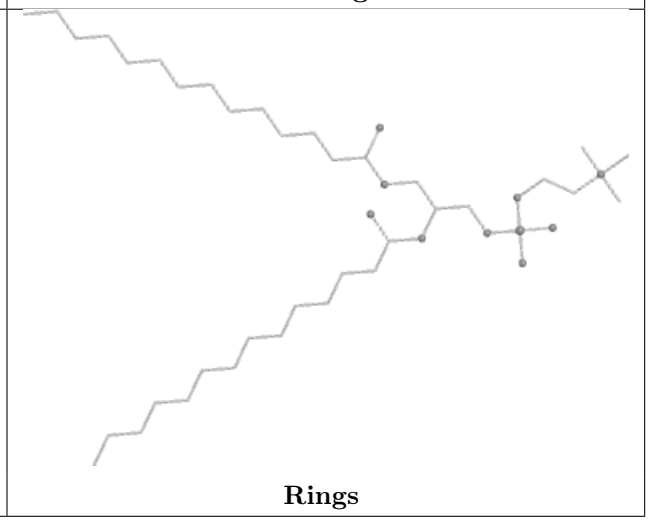
Bond lengths



Bond angles

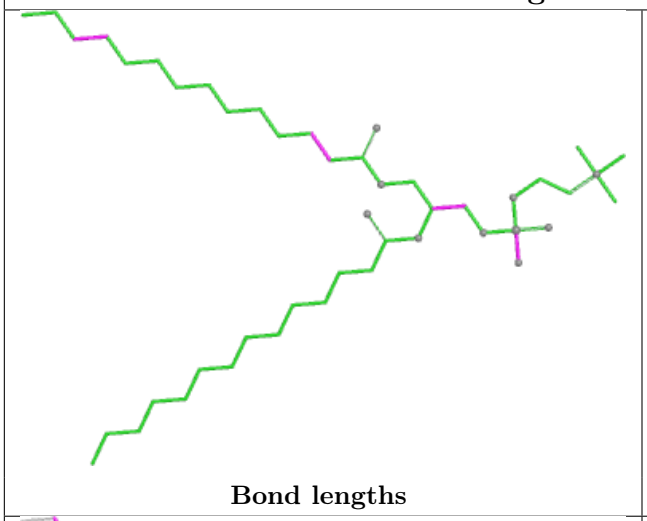


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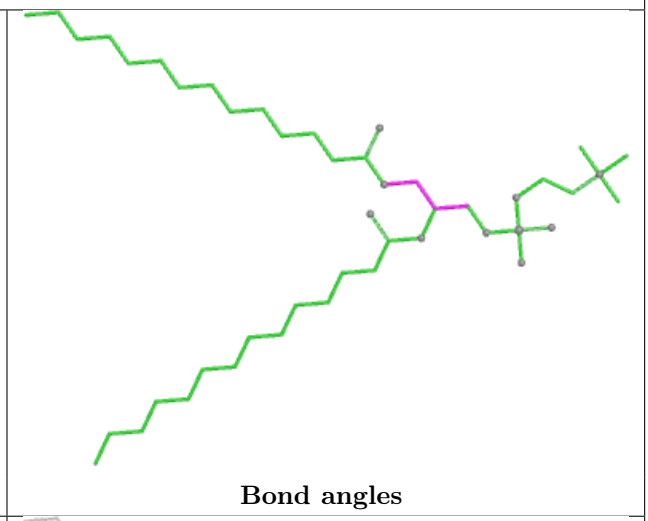


Rings

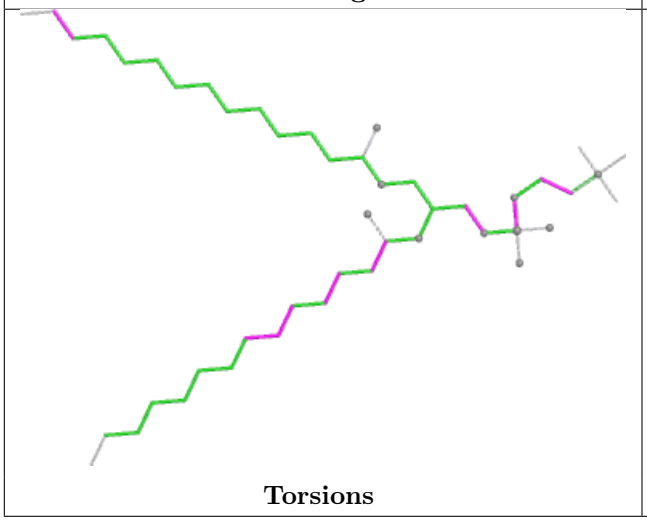
Ligand PX4 C 307



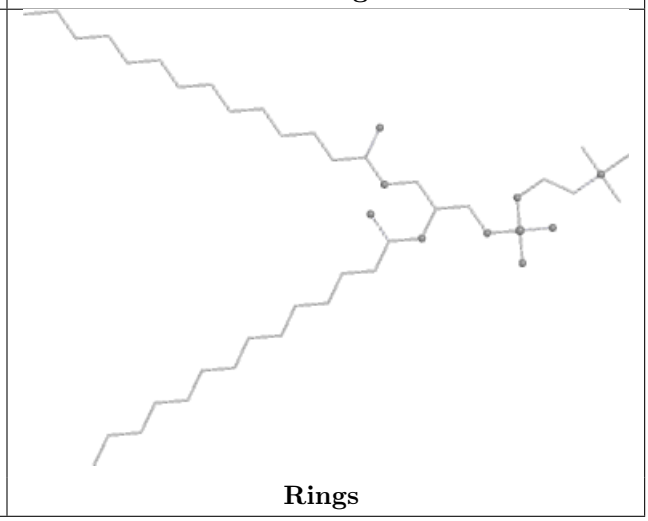
Bond lengths



Bond angles

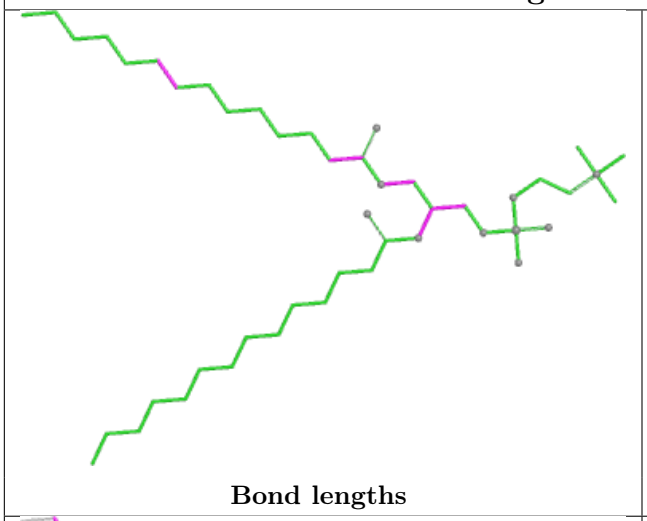


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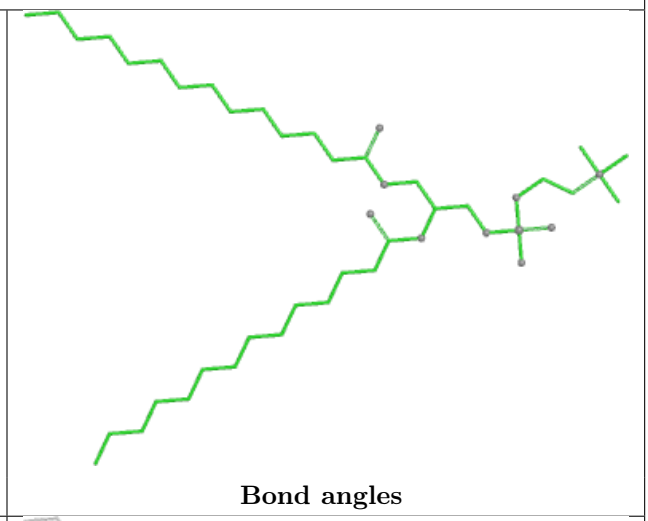


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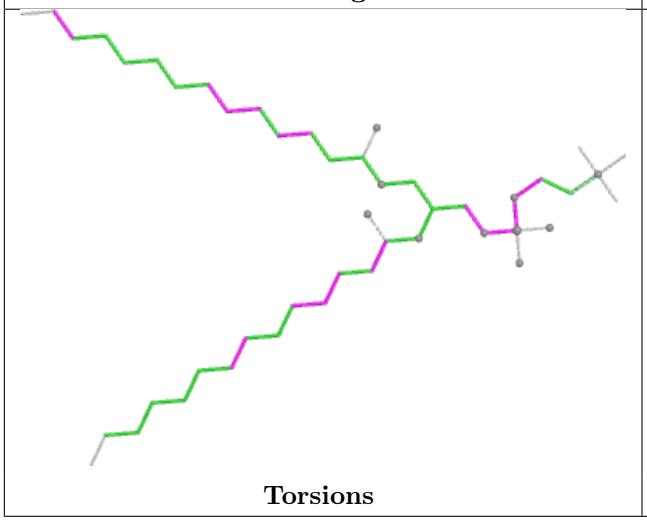
Ligand PX4 A 619



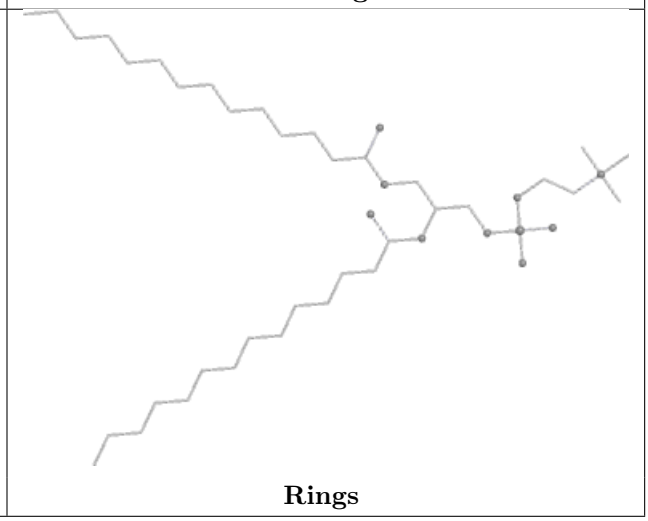
Bond lengths



Bond angles

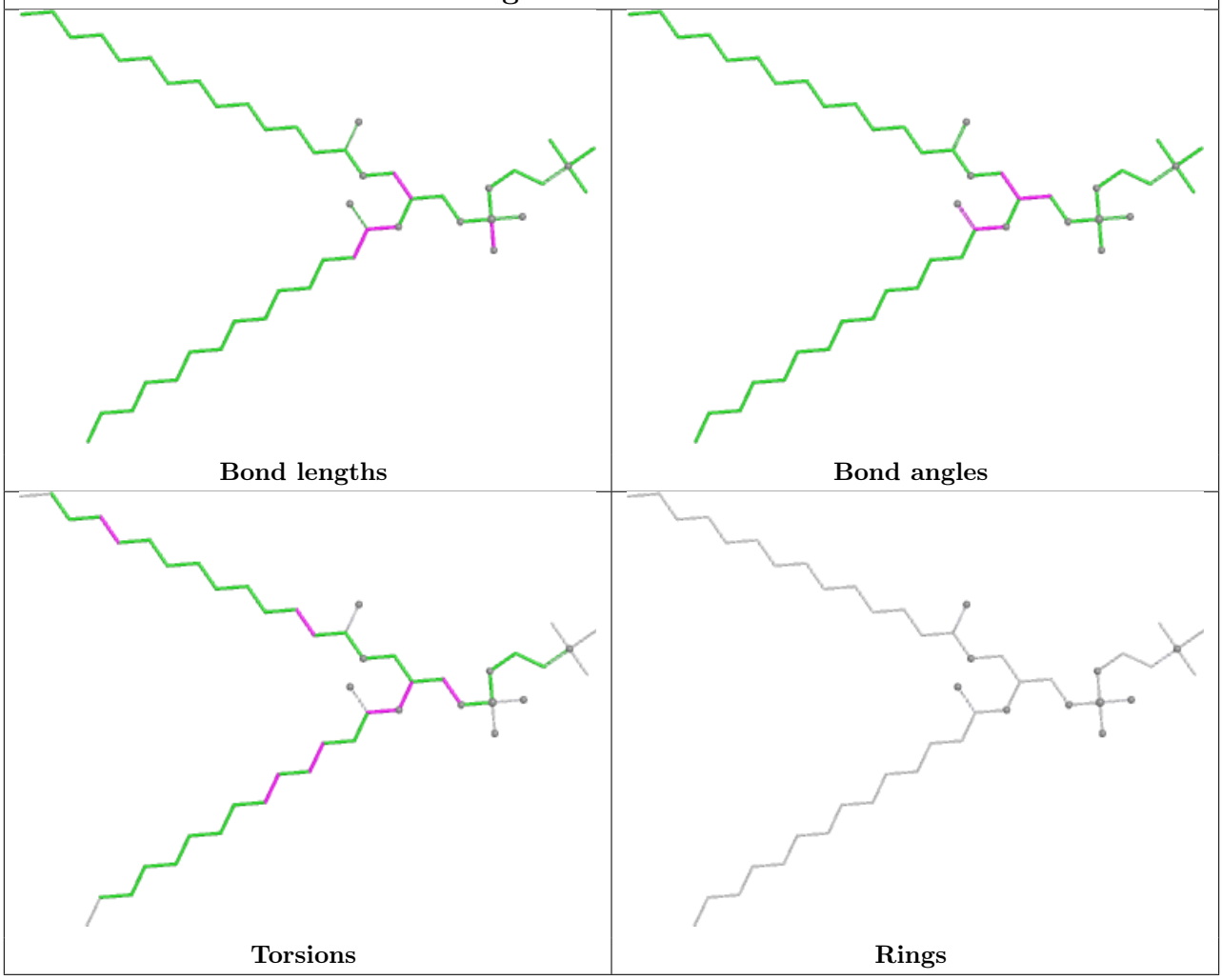


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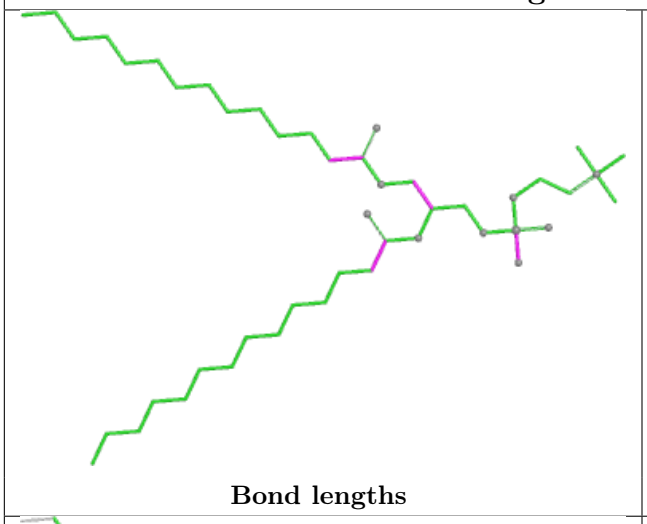


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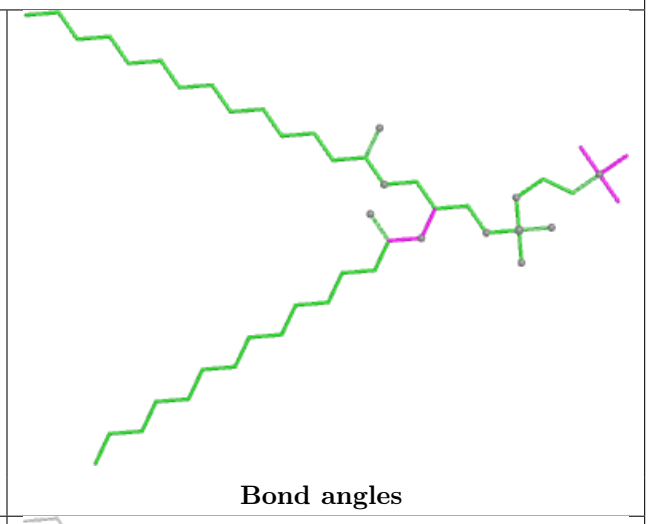
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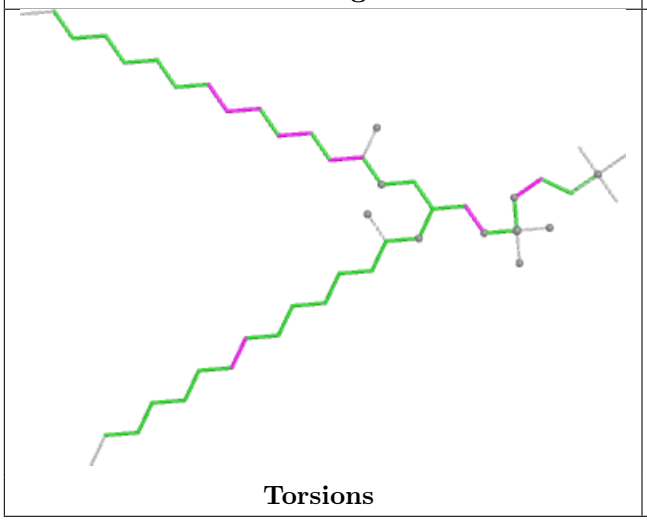
Ligand PX4 B 305



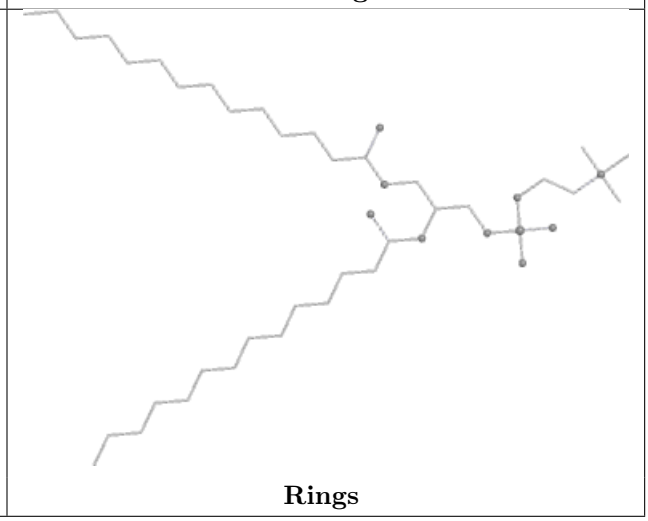
Bond lengths



Bond angles

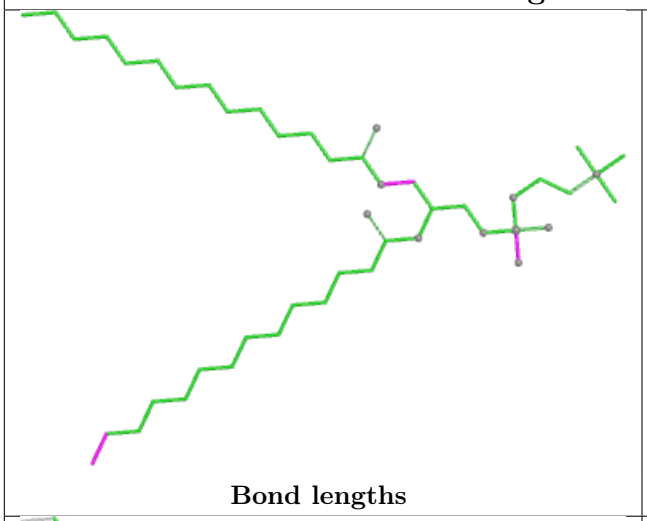


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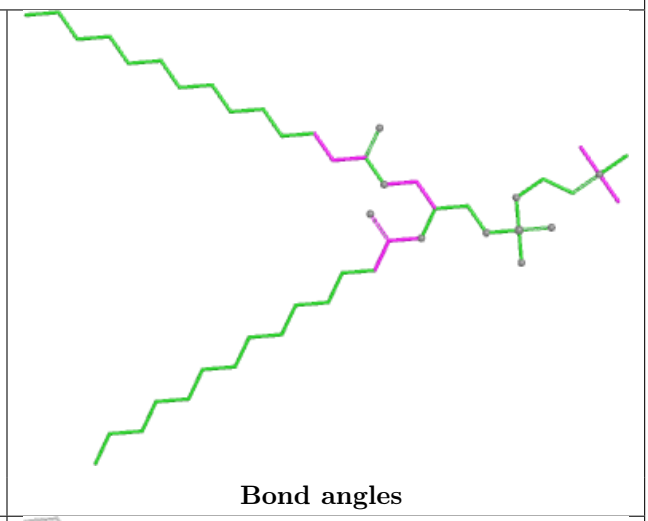


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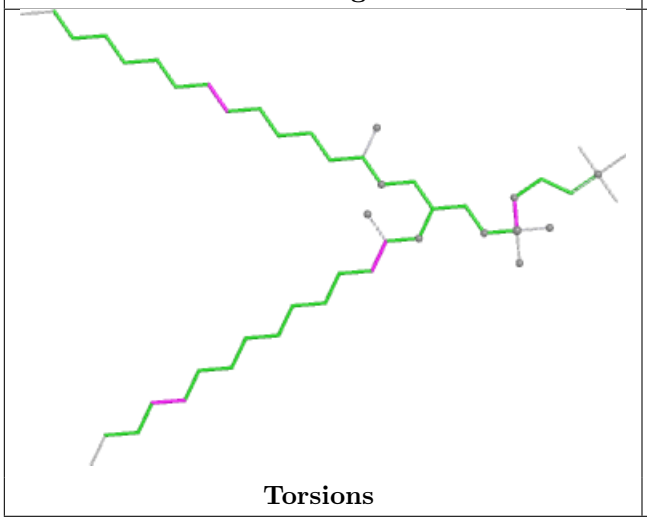
Ligand PX4 C 329



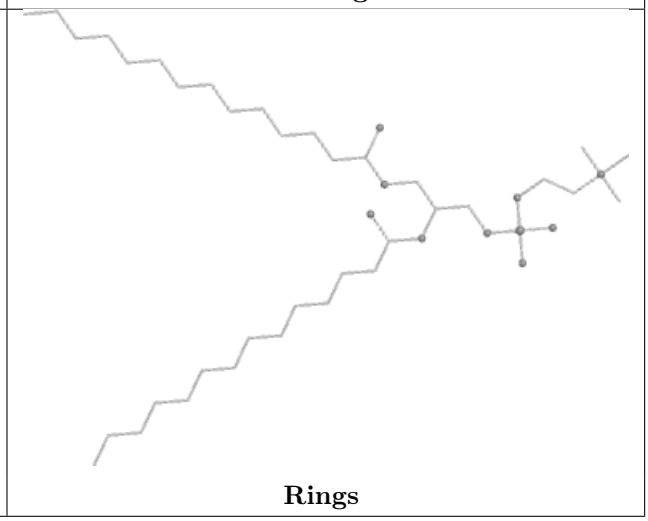
Bond lengths



Bond angles

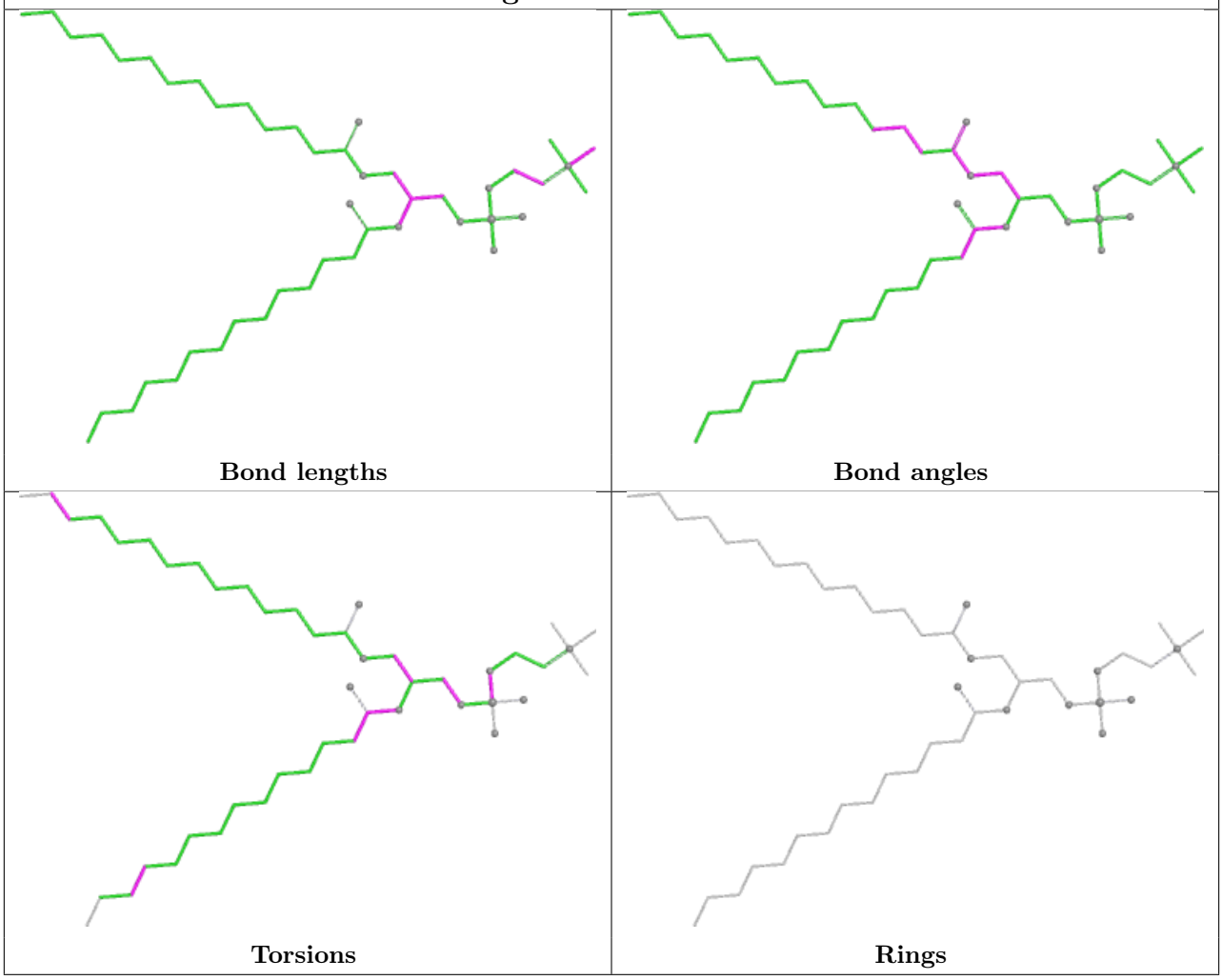


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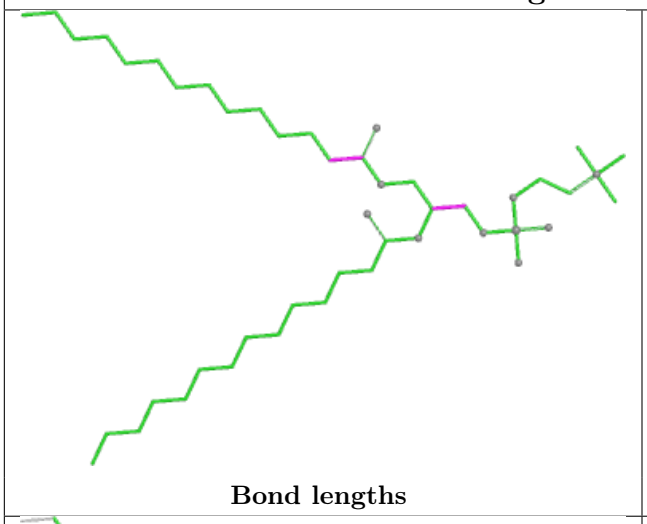


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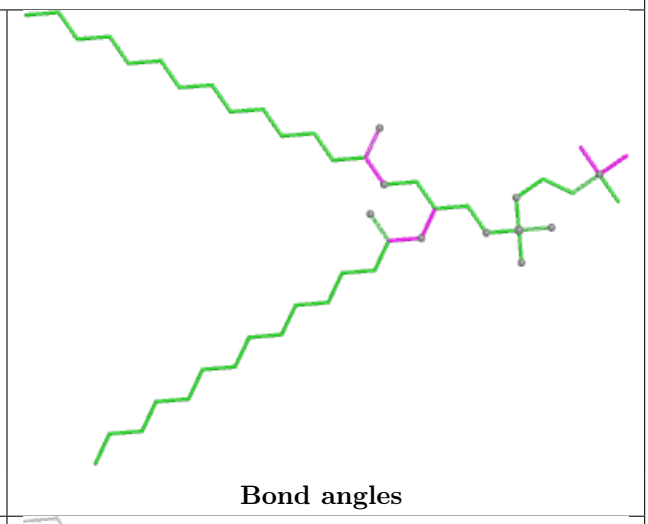
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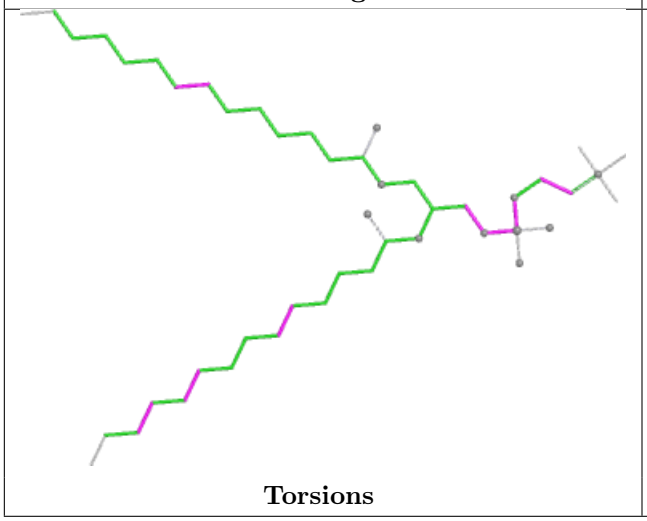
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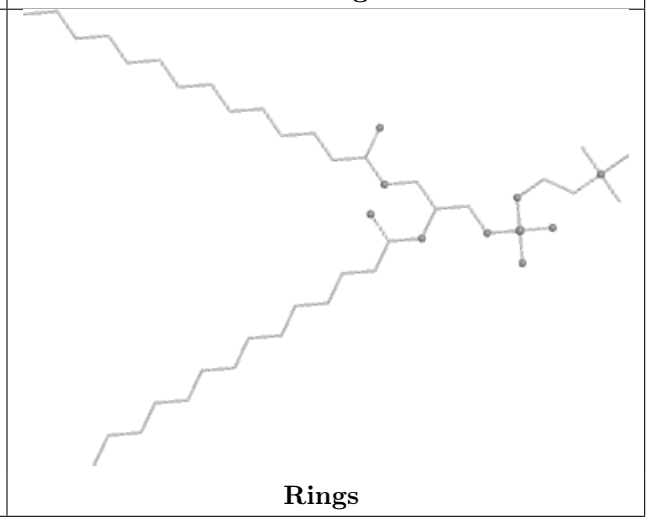
Bond lengths



Bond angles

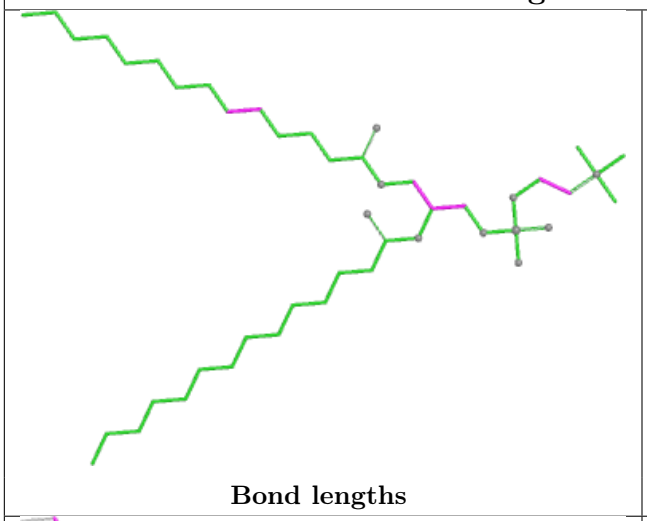


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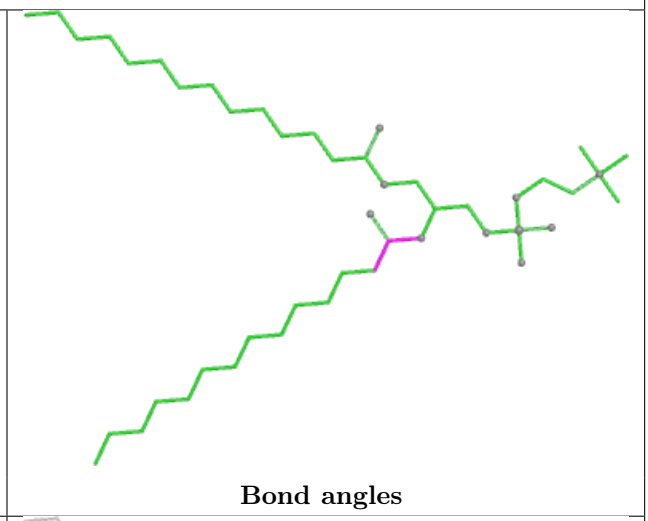


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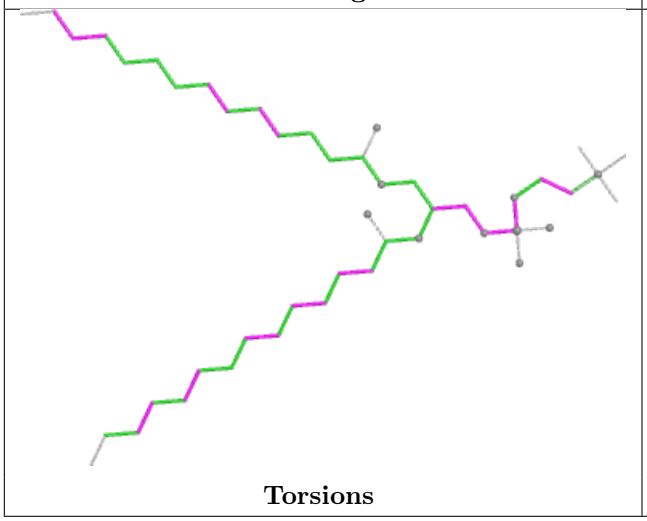
Ligand PX4 B 385



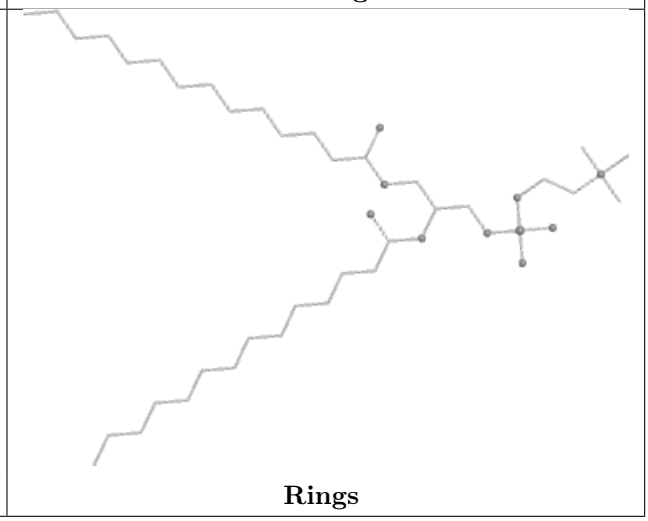
Bond lengths



Bond angles

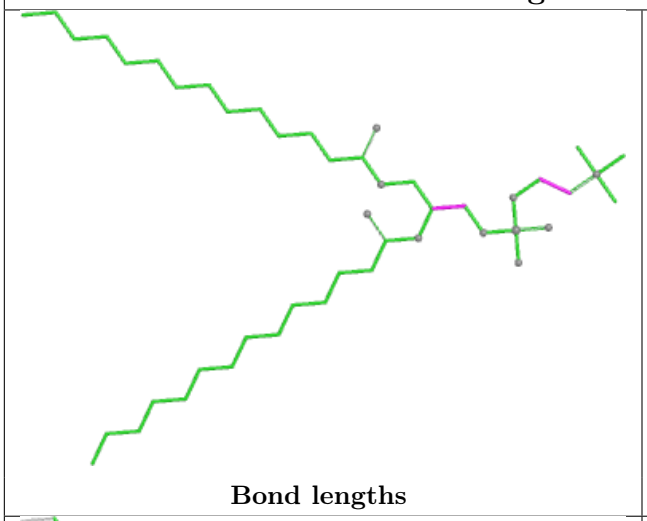


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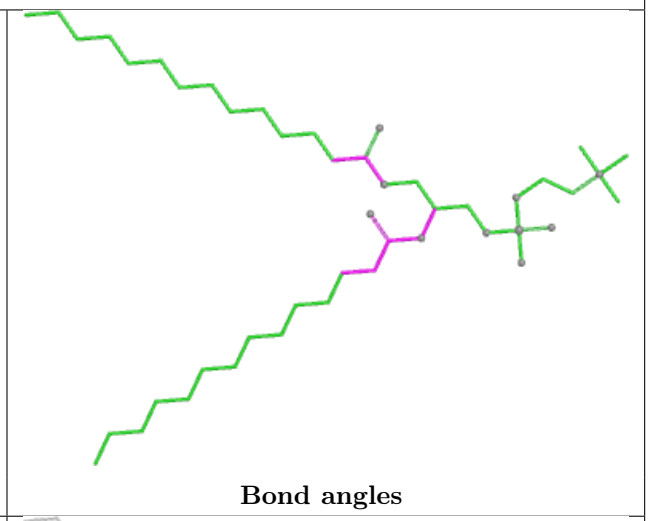


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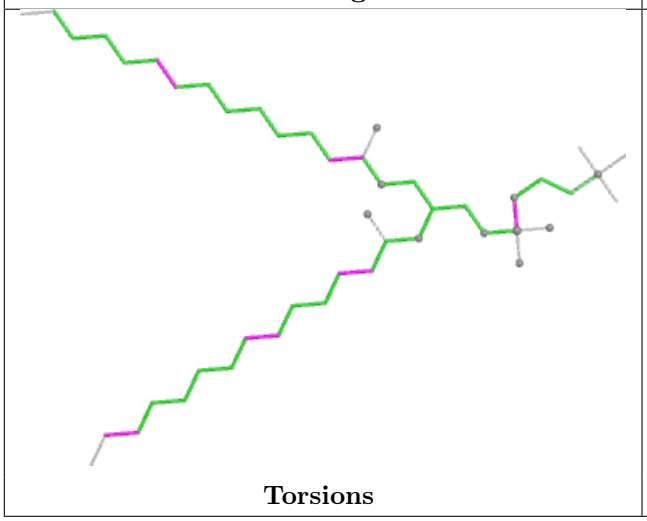
Ligand PX4 C 310



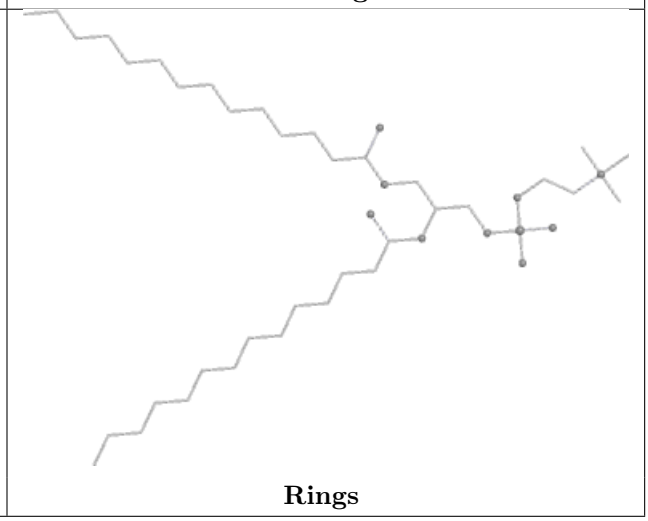
Bond lengths



Bond angles

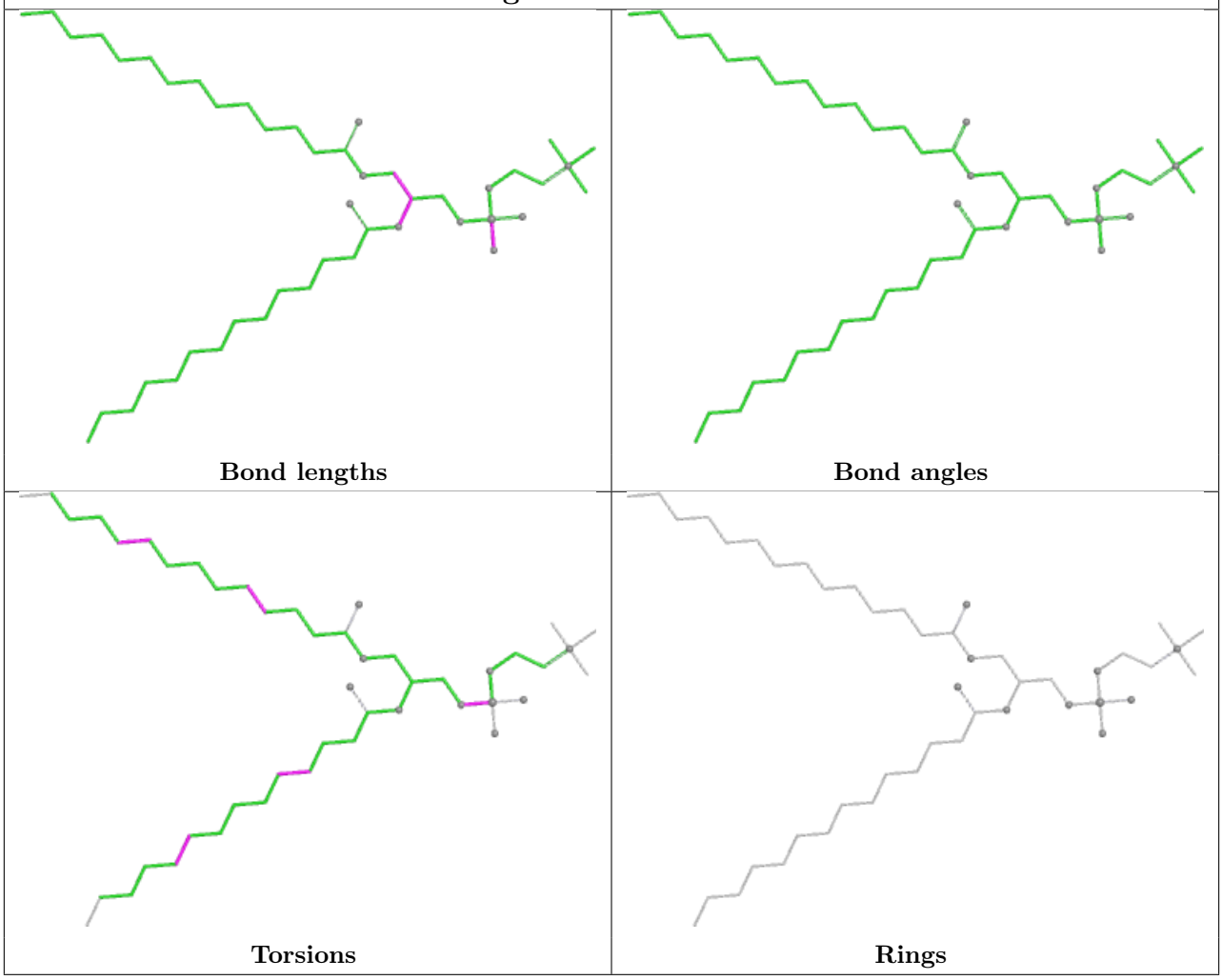


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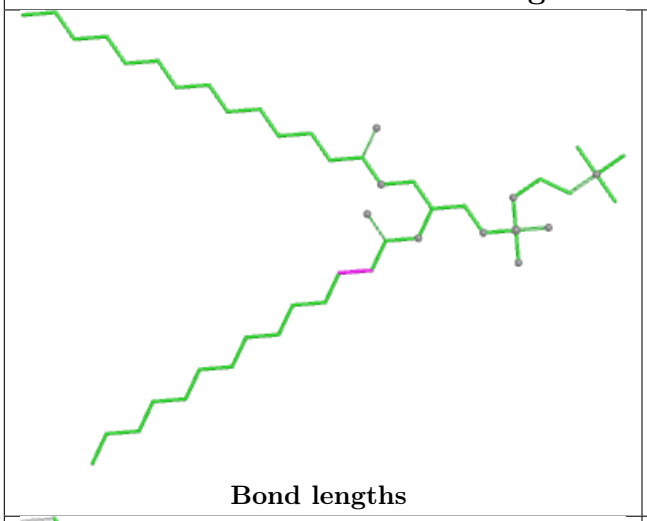


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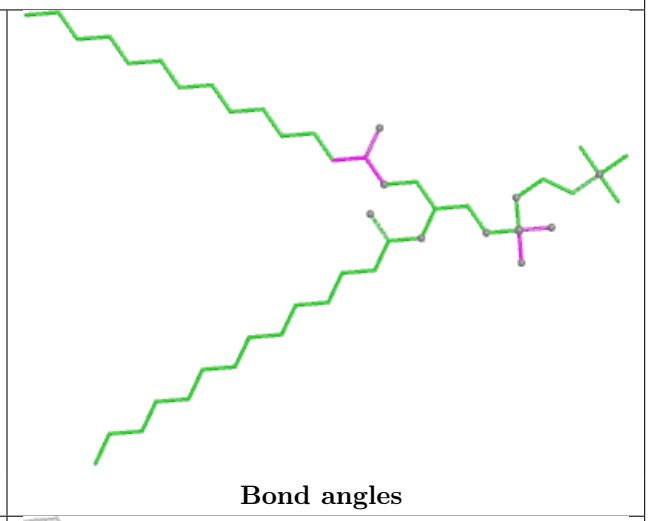
Ligand PX4 B 399



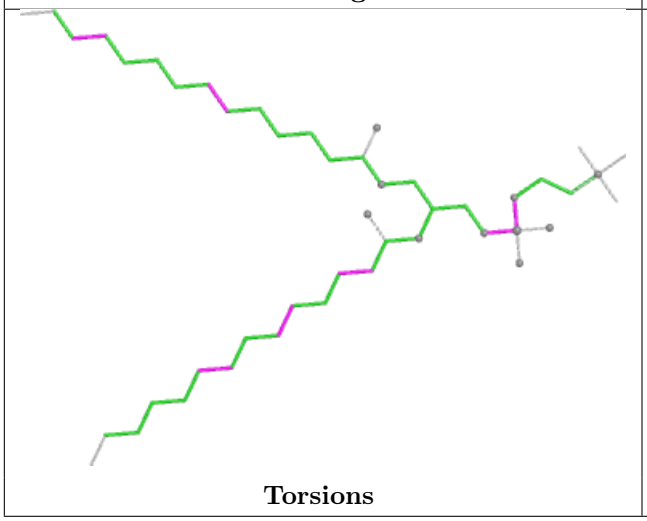
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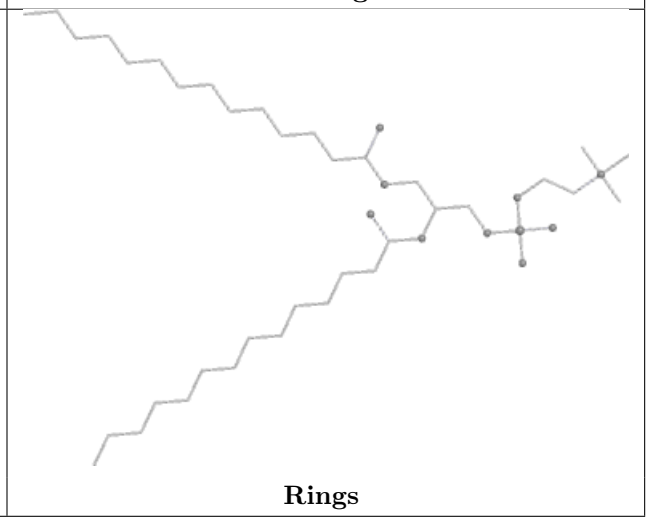
Bond lengths



Bond angles

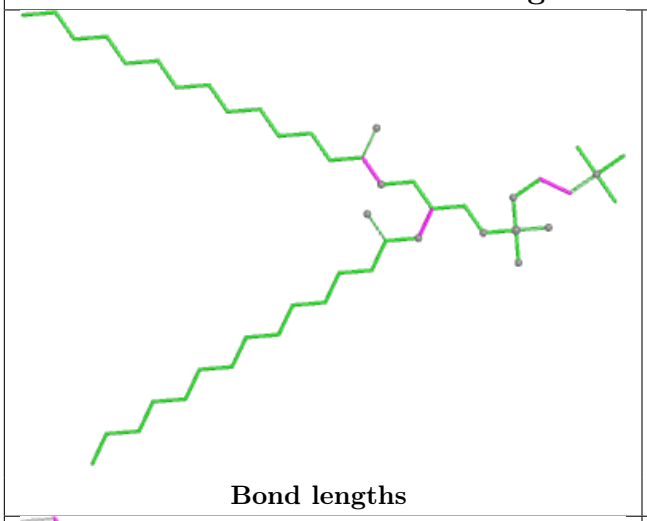


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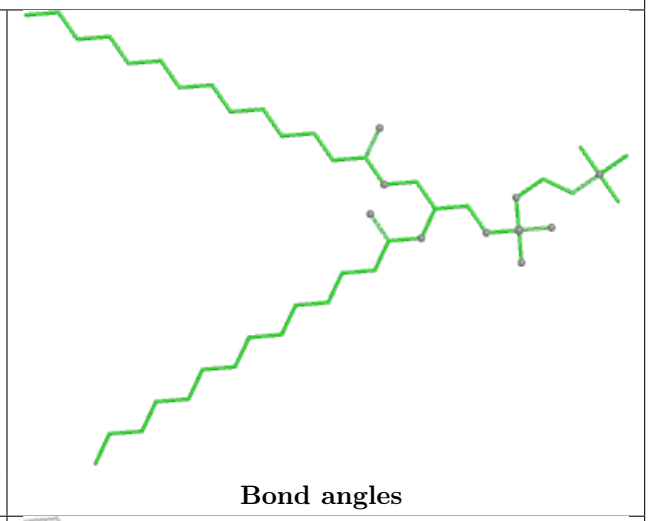


Rings

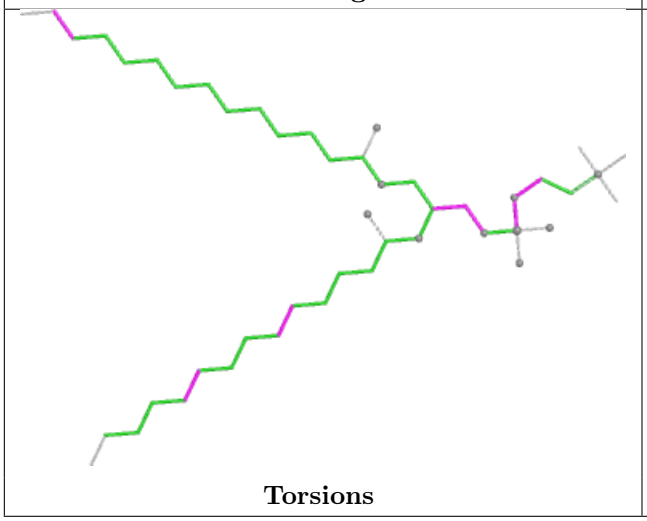
Ligand PX4 C 359



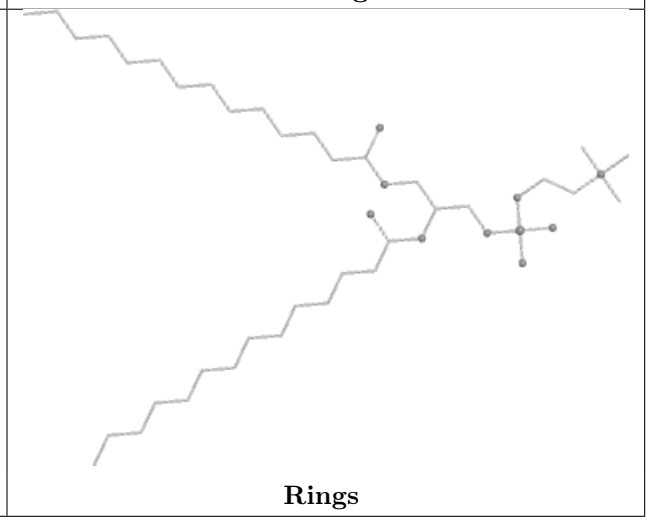
Bond lengths



Bond angles

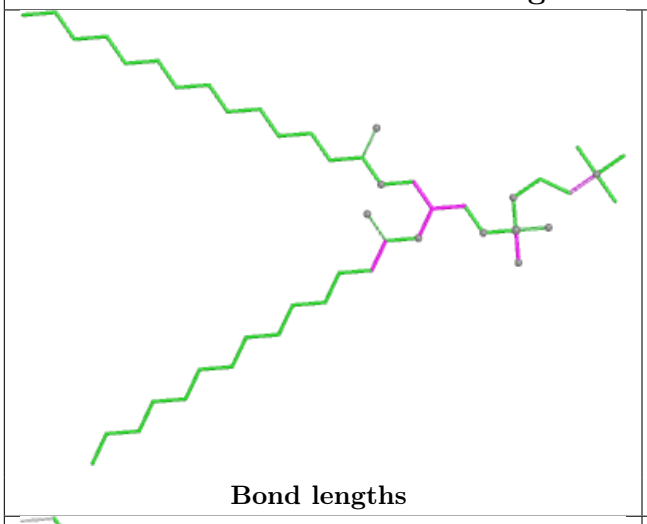


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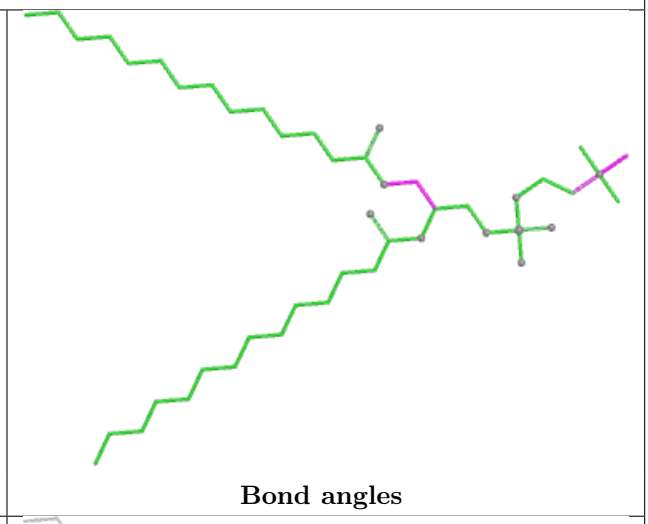


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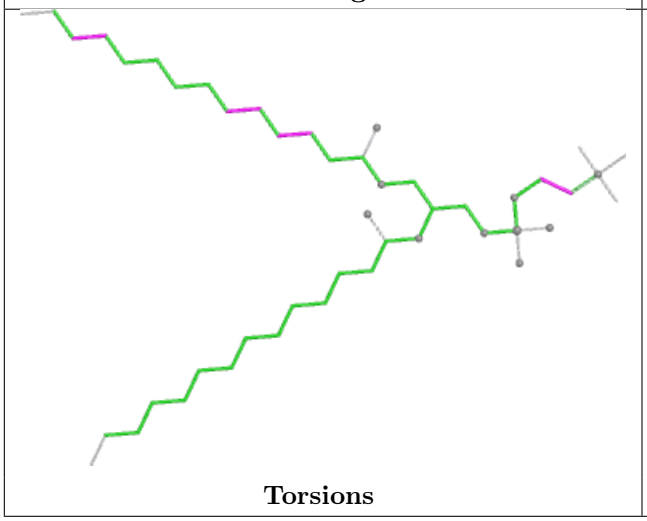
Ligand PX4 B 371



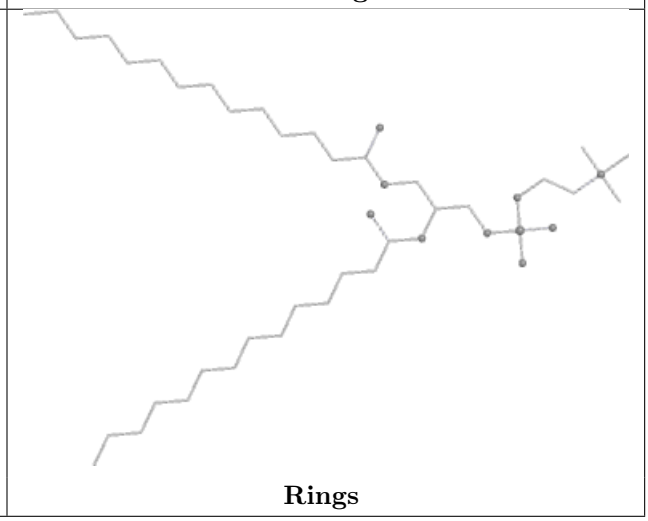
Bond lengths



Bond angles

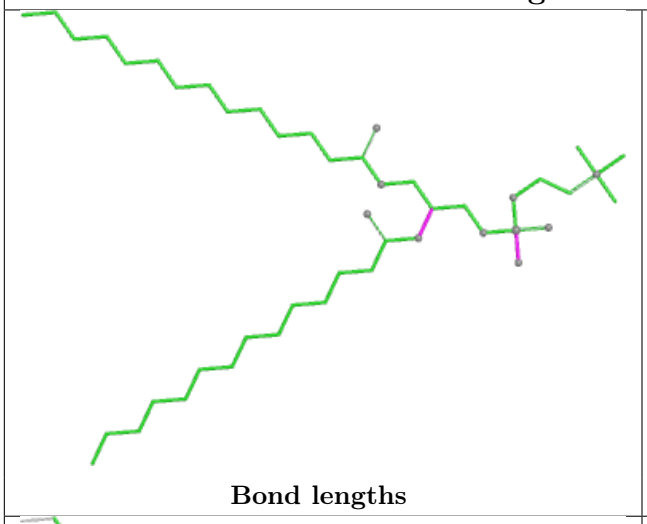


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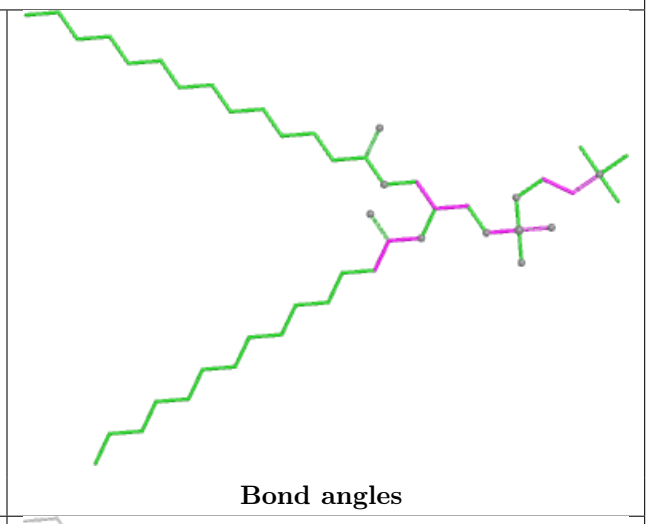


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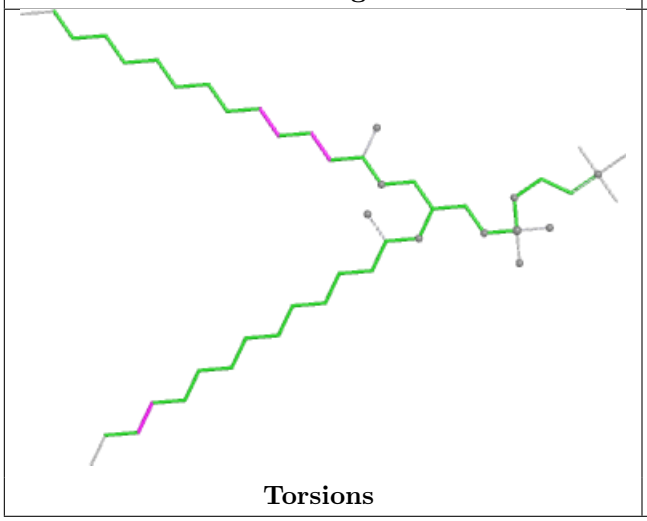
Ligand PX4 B 309



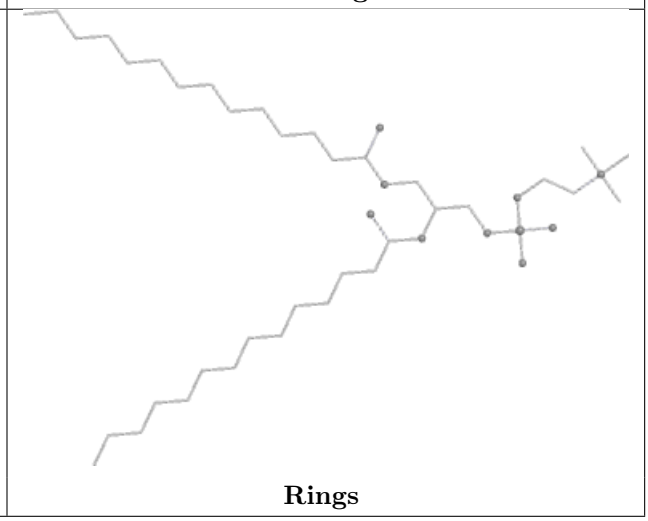
Bond lengths



Bond angles

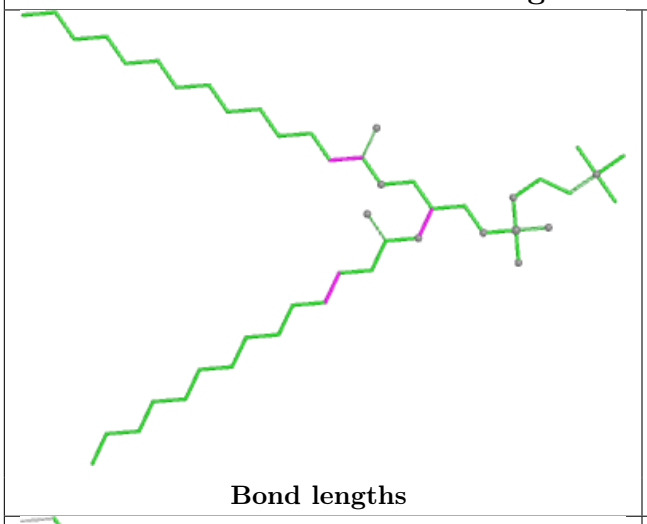


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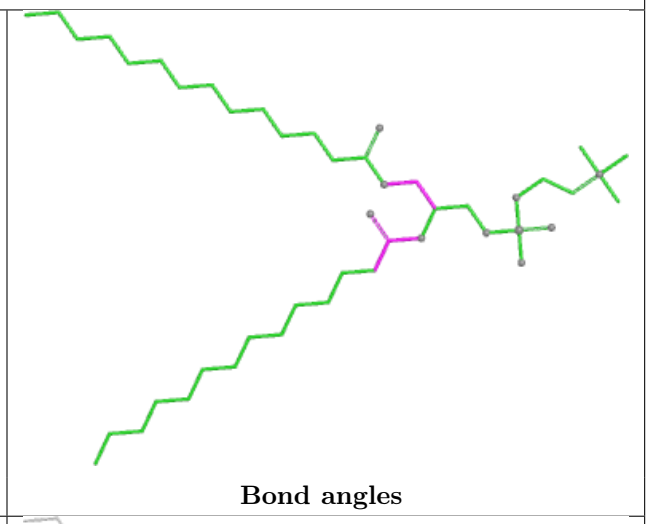


Rings

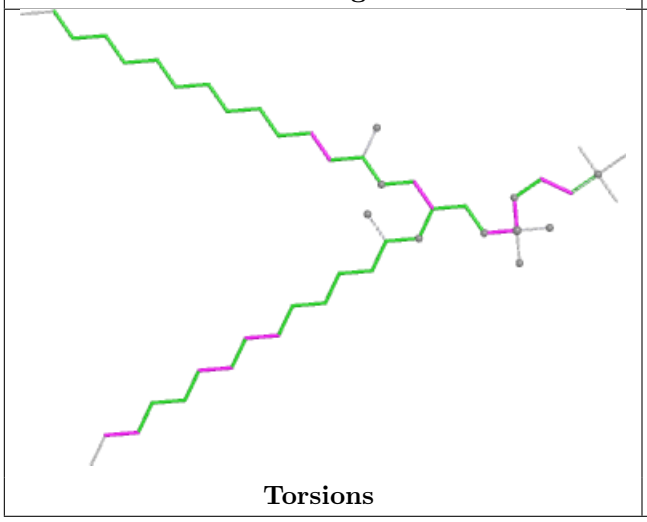
Ligand PX4 C 328



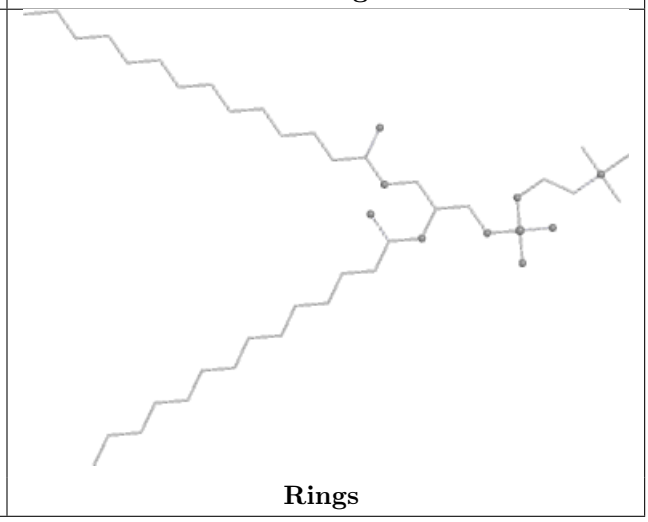
Bond lengths



Bond angles

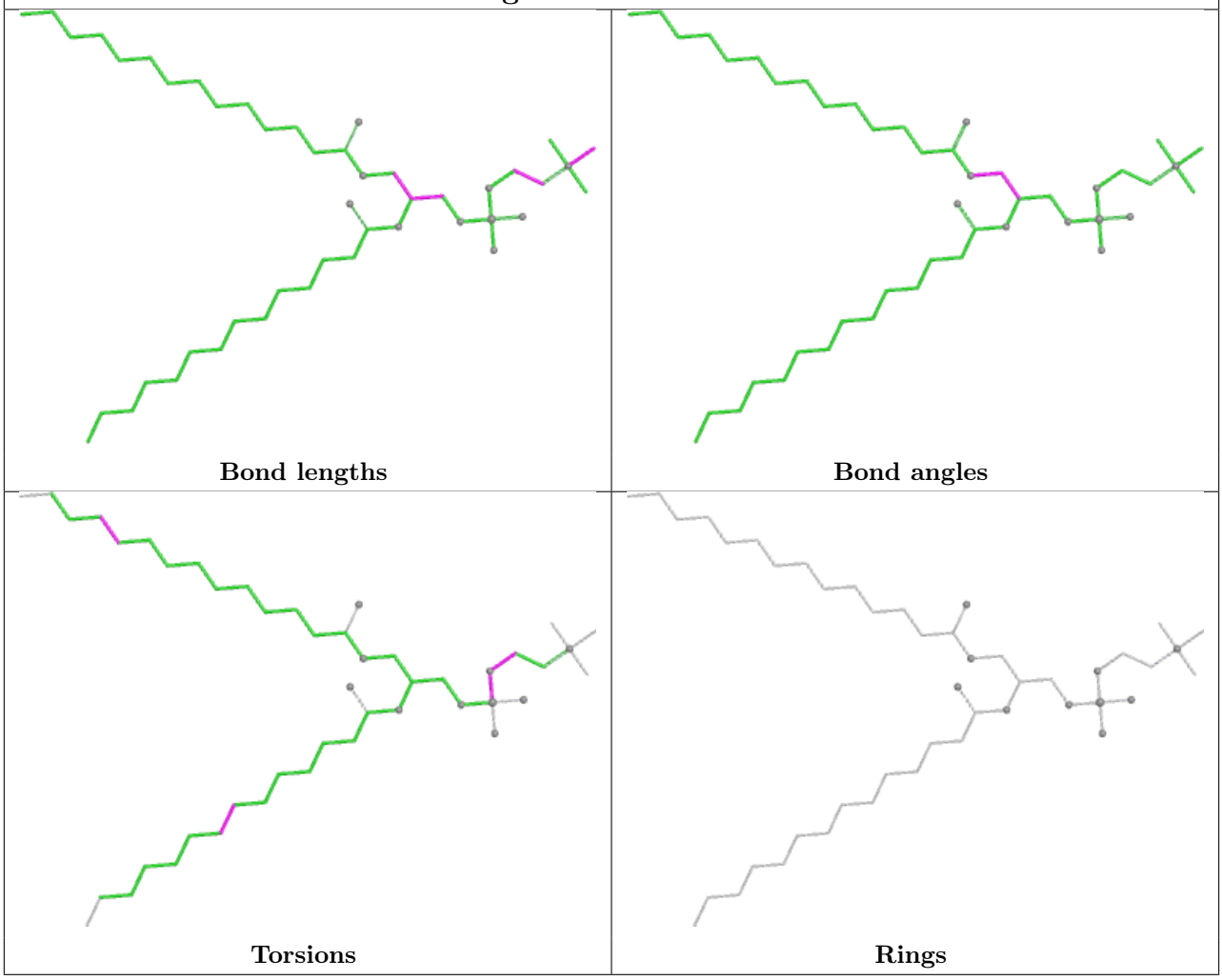


Torsions

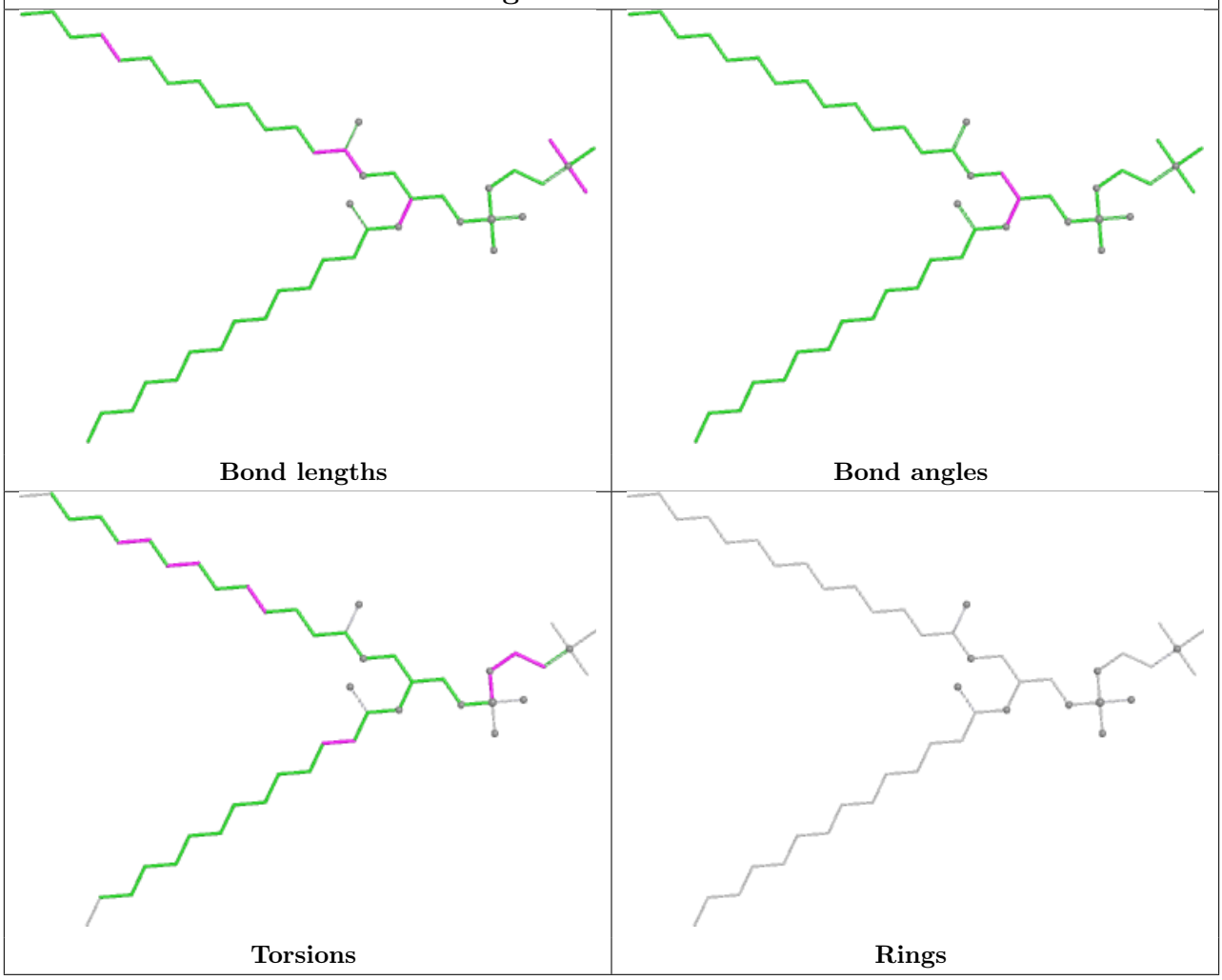


Rings

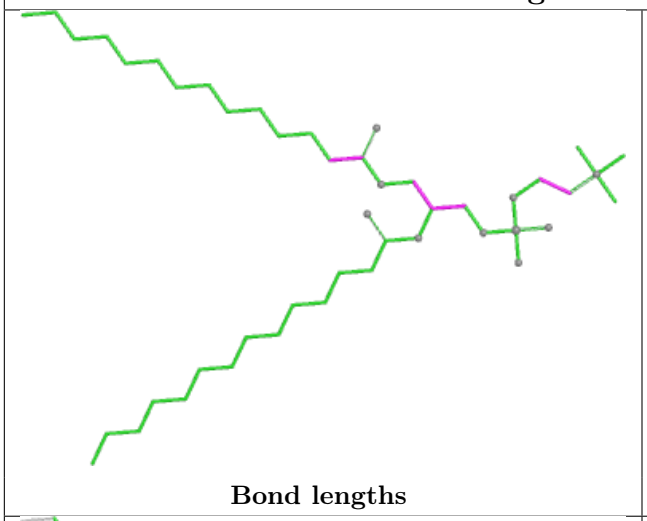
Ligand PX4 A 637



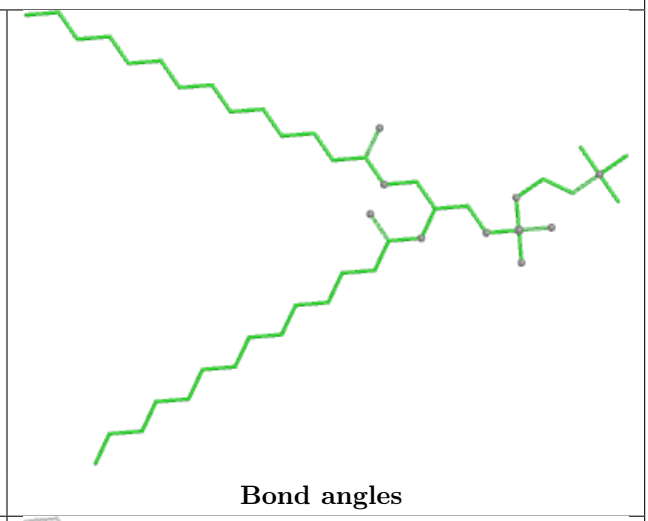
Ligand PX4 C 361



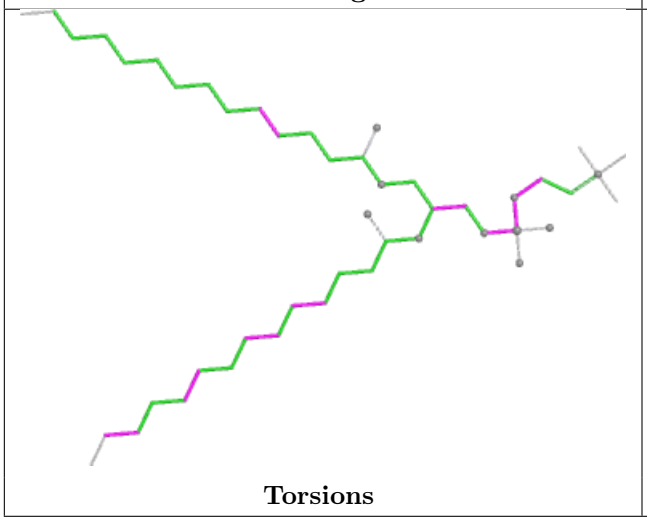
Ligand PX4 C 301



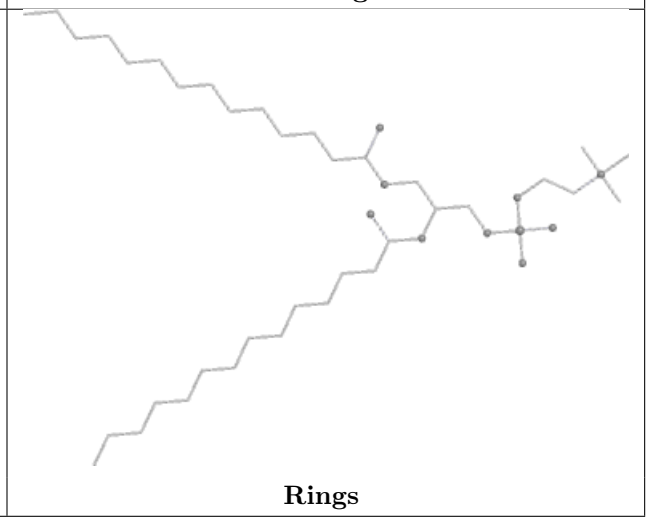
Bond lengths



Bond angles

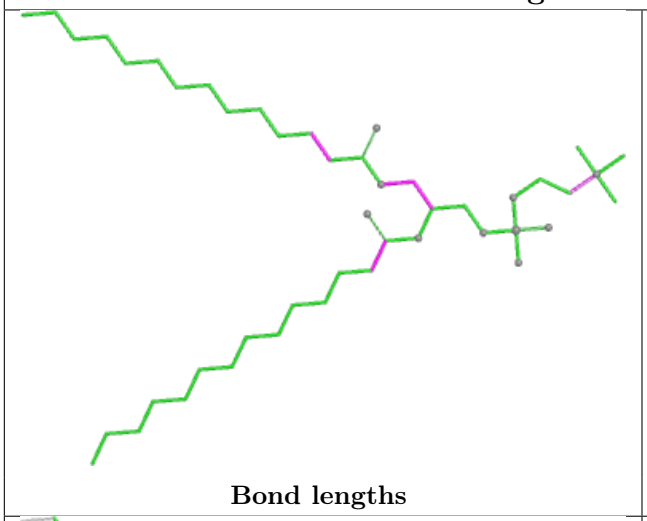


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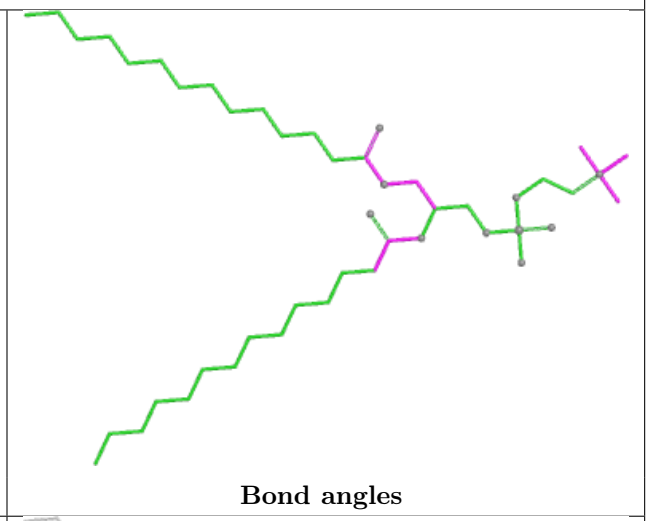


Rings

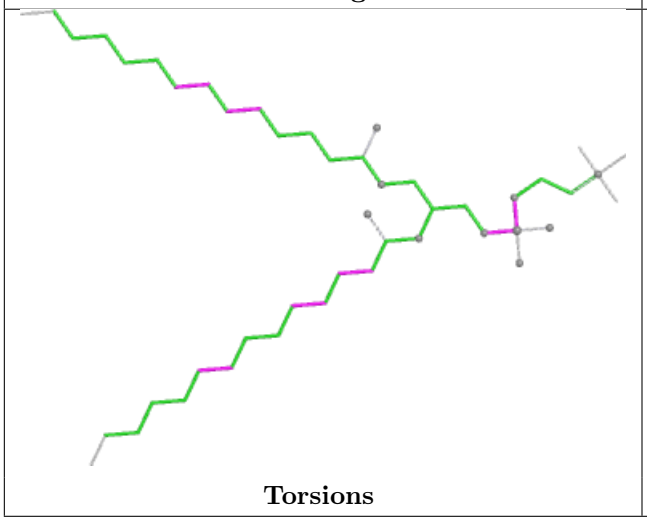
Ligand PX4 A 651



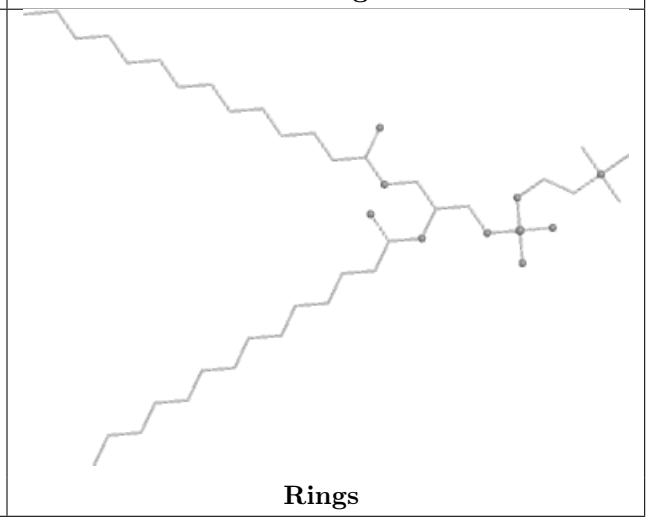
Bond lengths



Bond angles

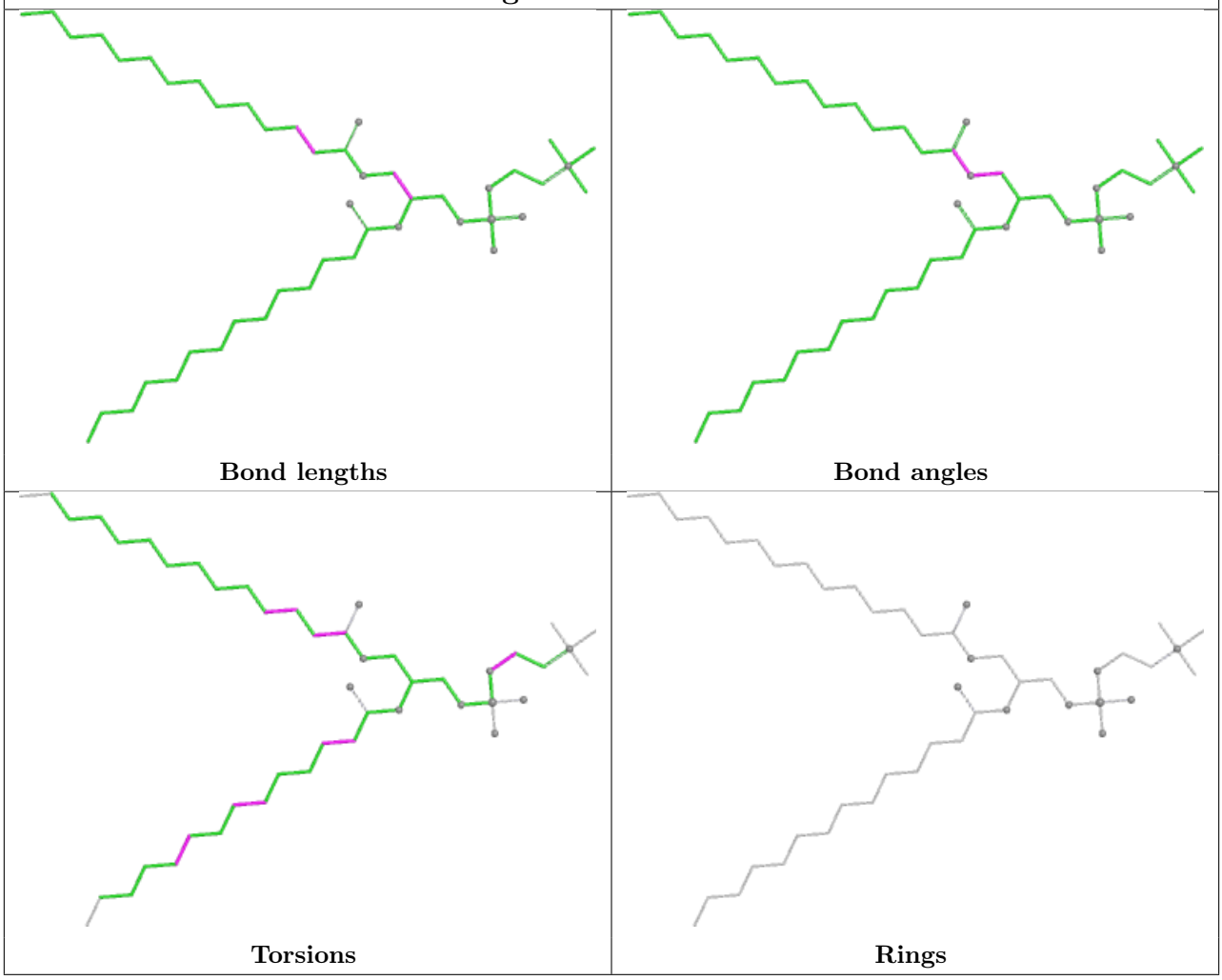


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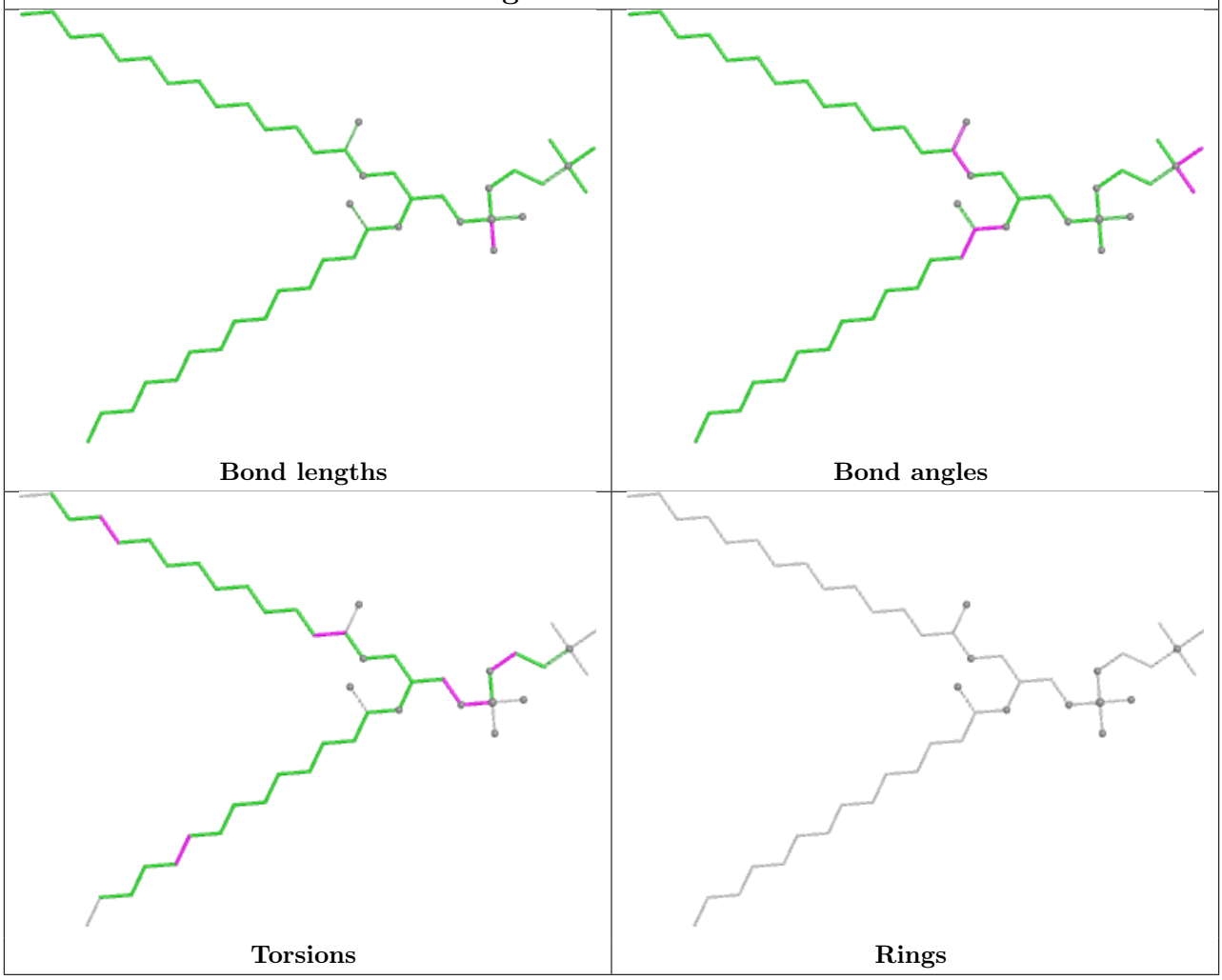


Rings

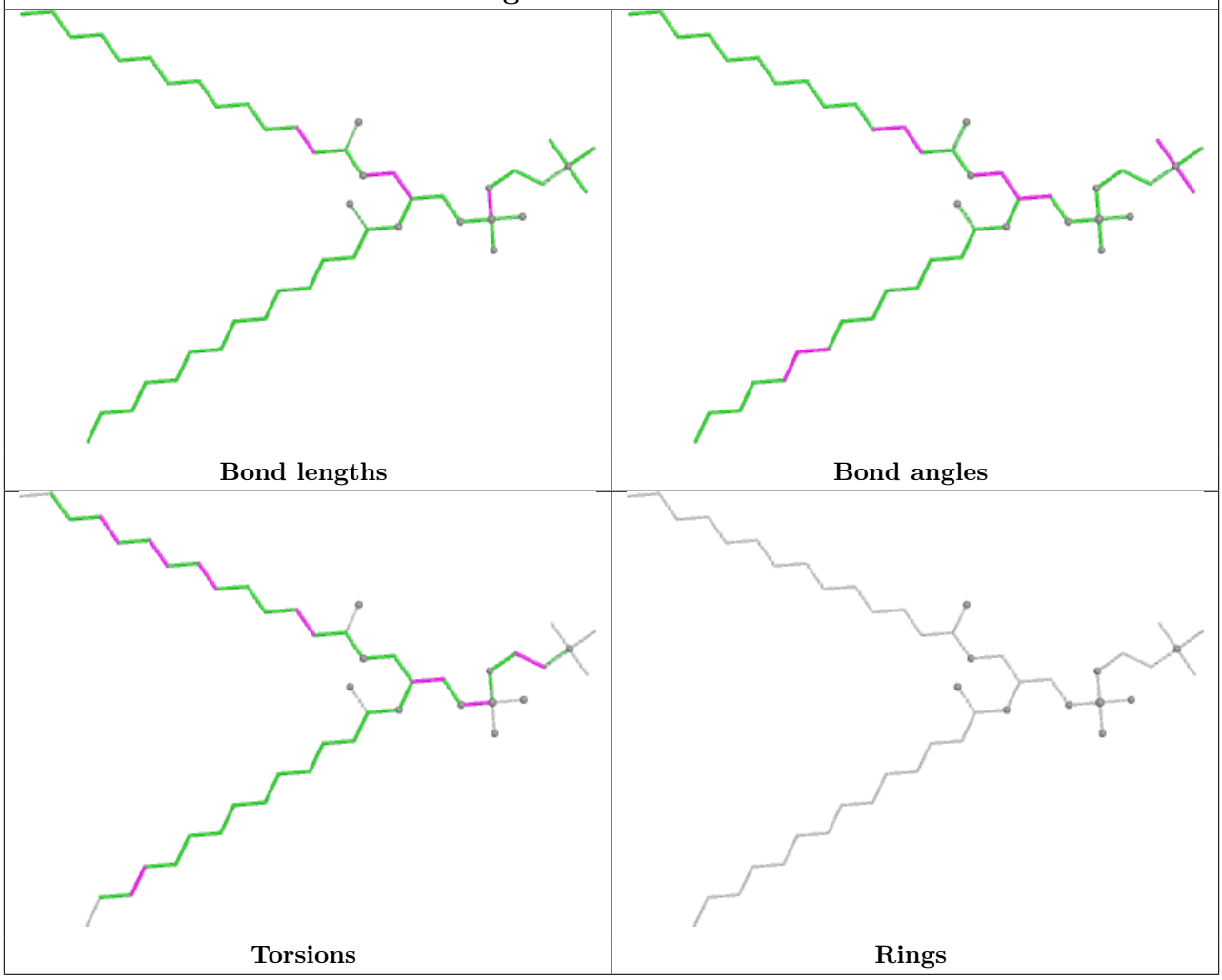
Ligand PX4 A 645



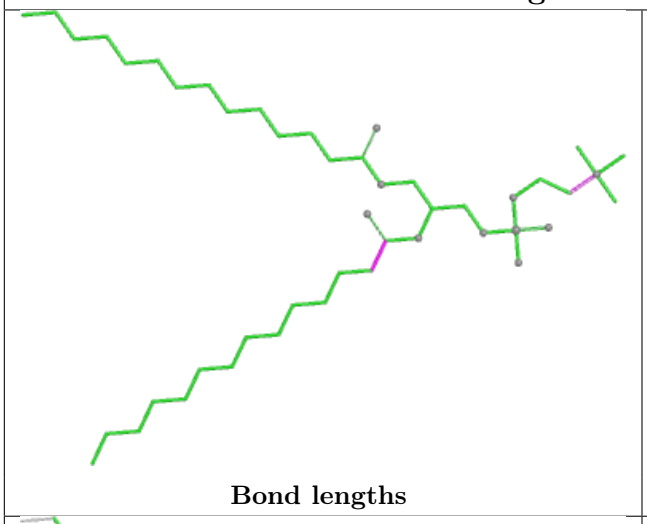
Ligand PX4 A 616



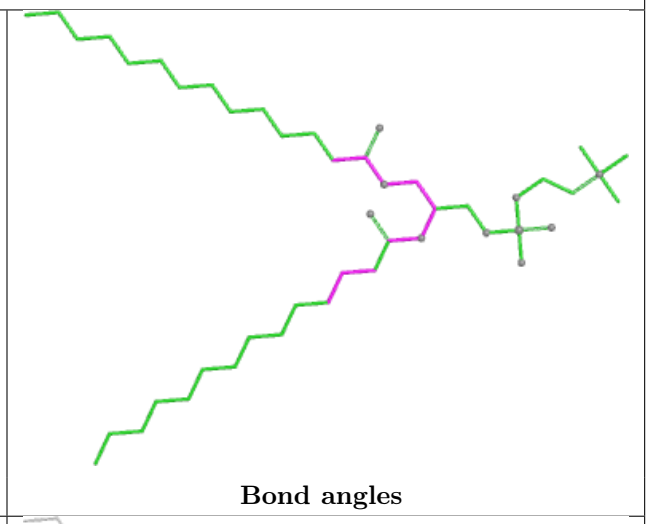
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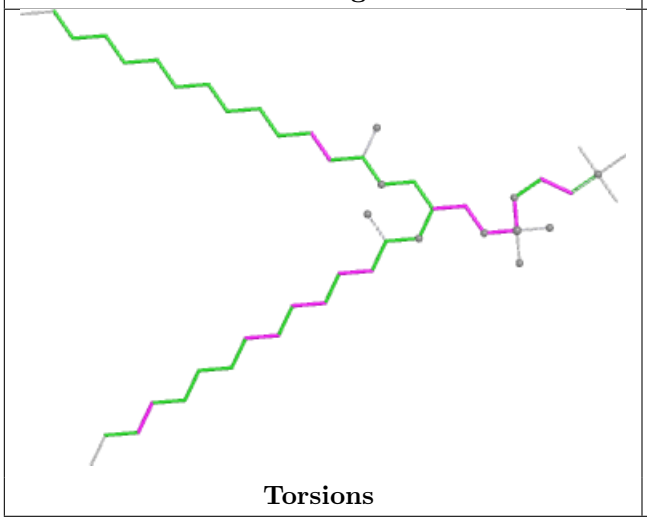
Ligand PX4 B 306



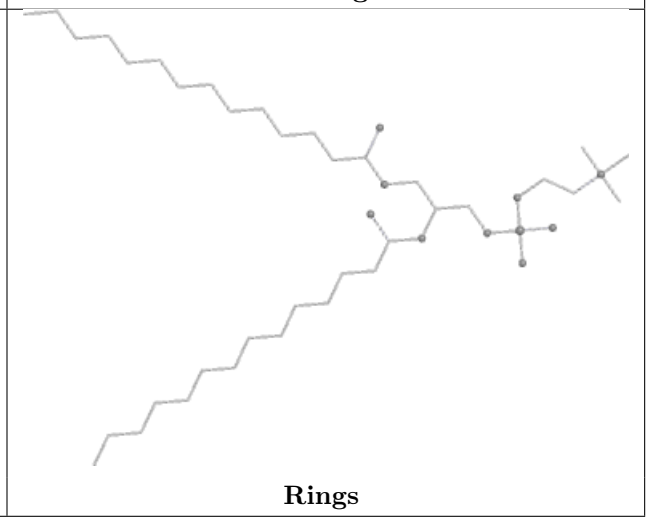
Bond lengths



Bond angles

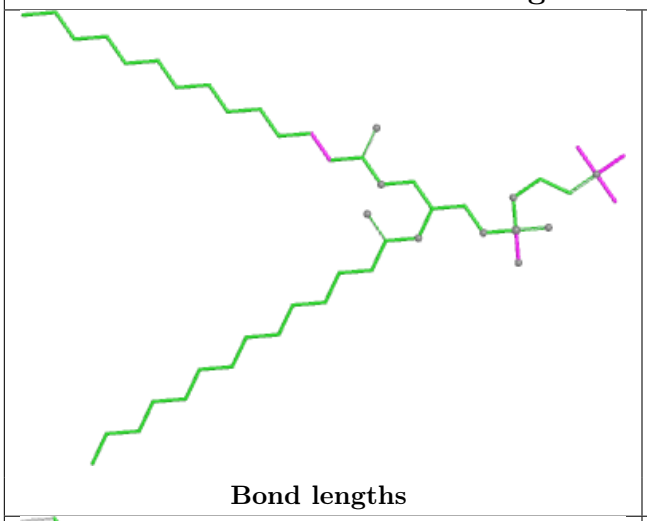


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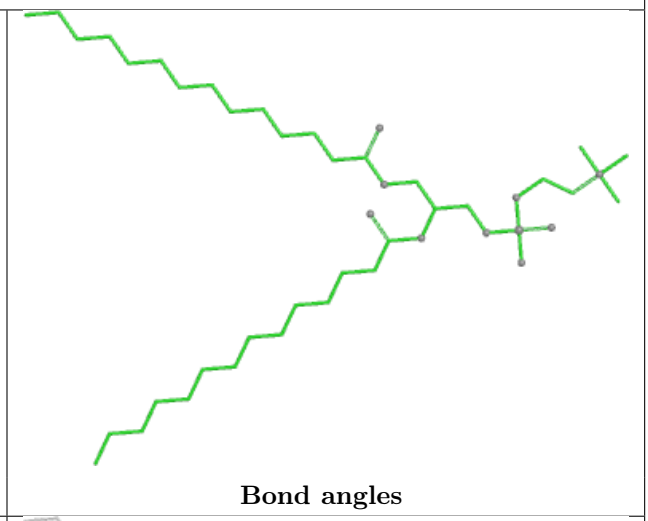


Rings

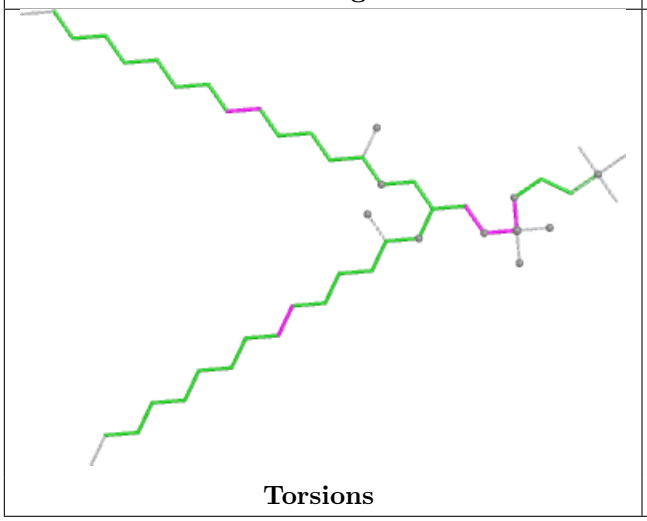
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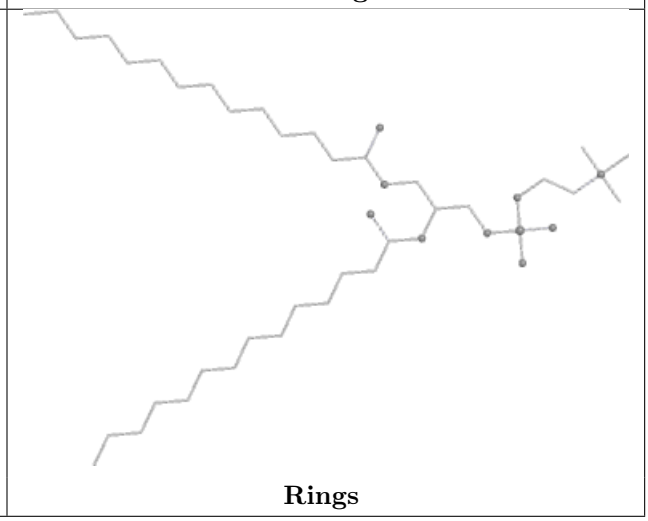
Bond lengths



Bond angles

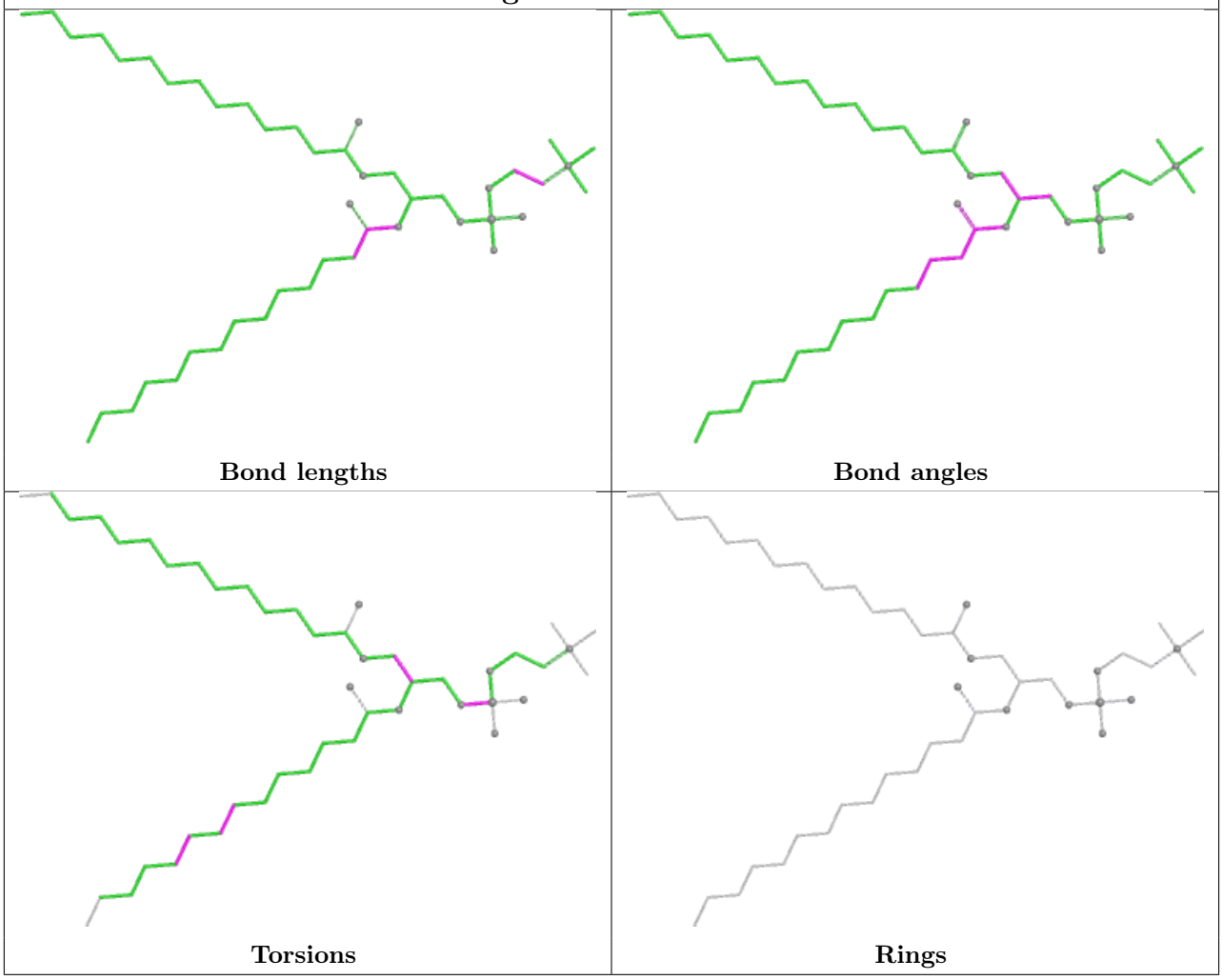


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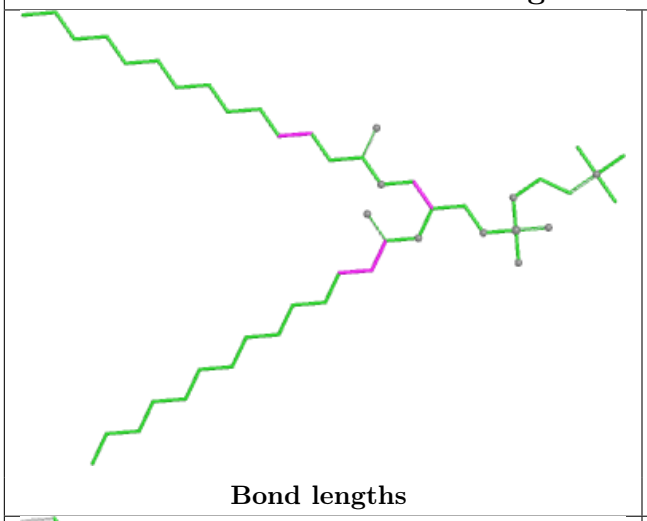


Rings

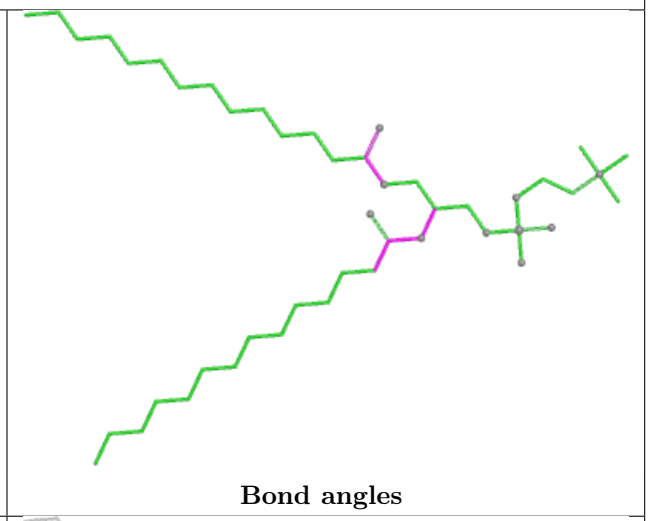
Ligand PX4 A 613



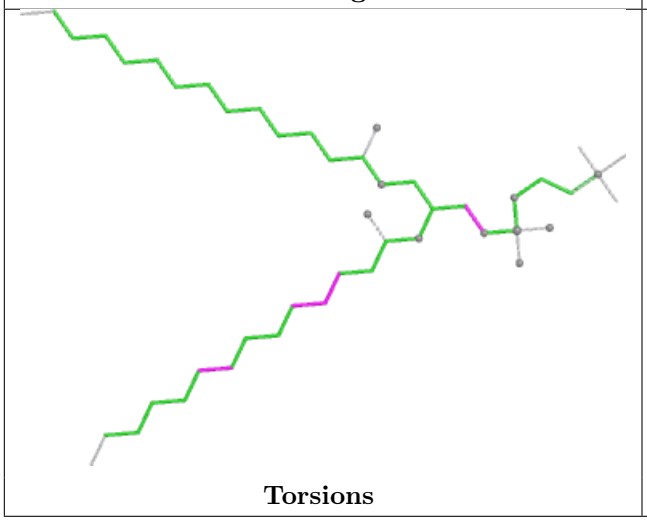
Ligand PX4 C 311



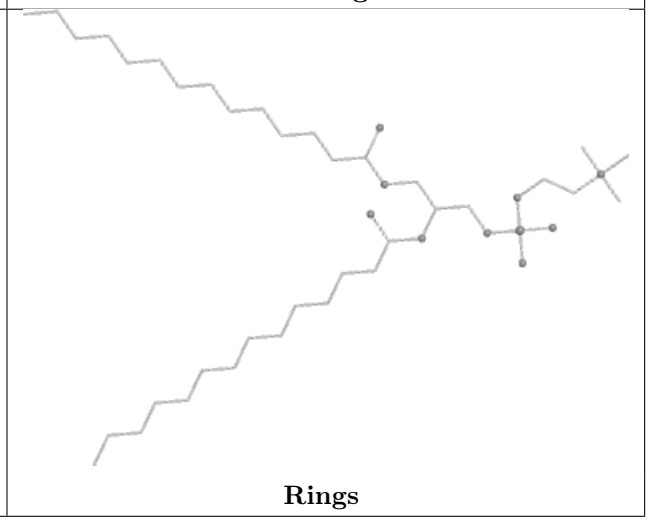
Bond lengths



Bond angles

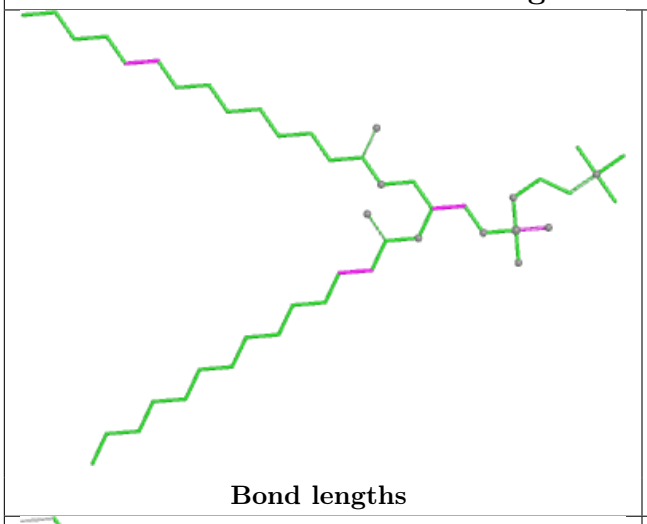


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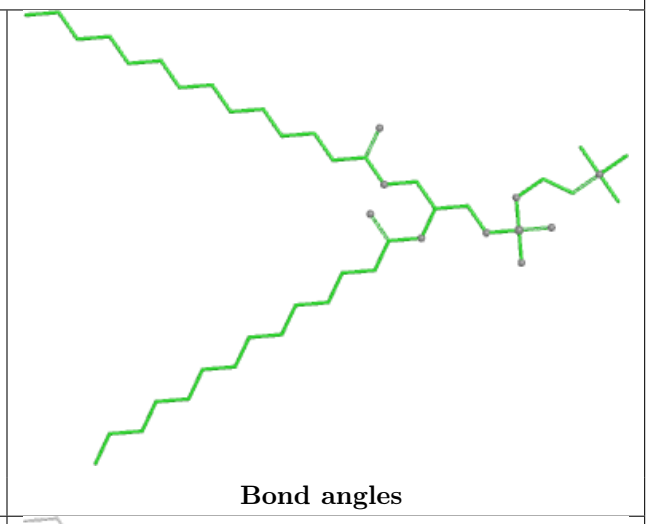


Rings

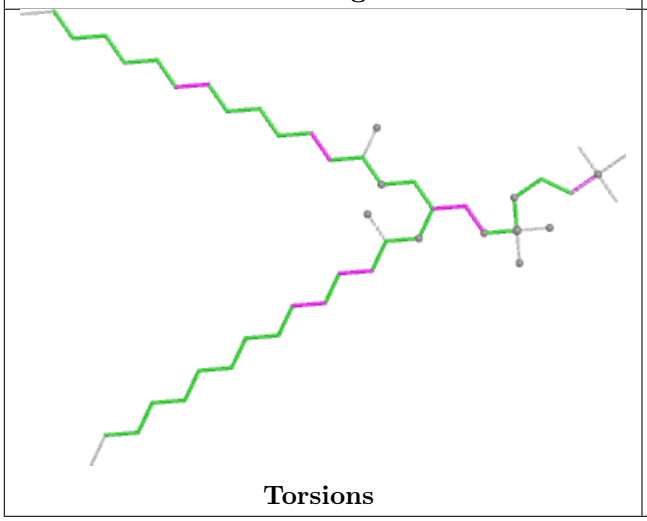
Ligand PX4 B 349



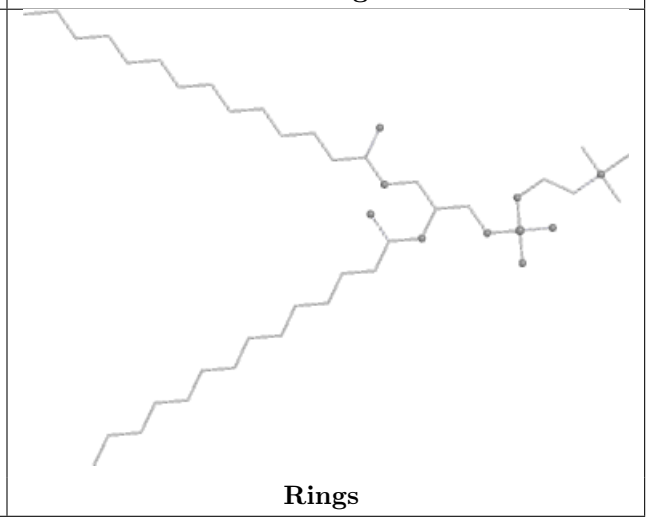
Bond lengths



Bond angles

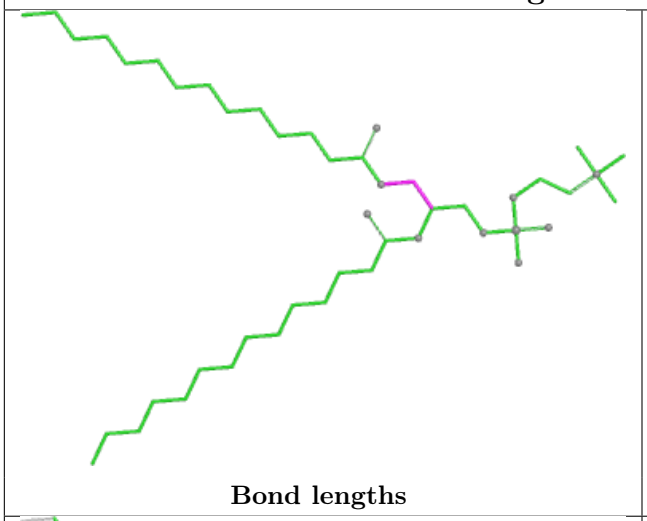


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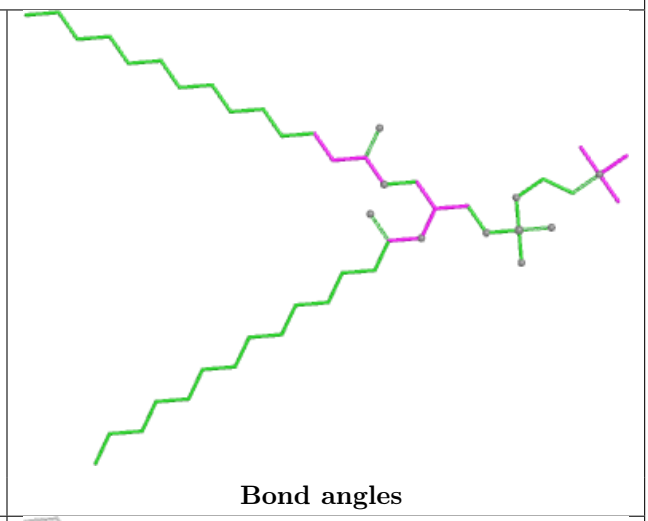


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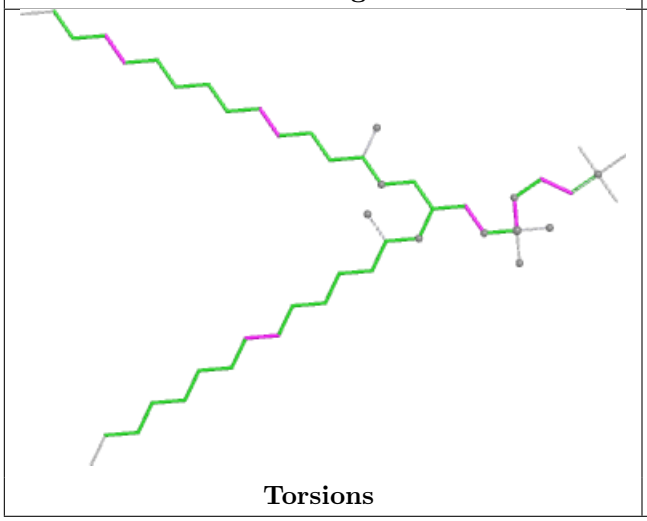
Ligand PX4 A 652



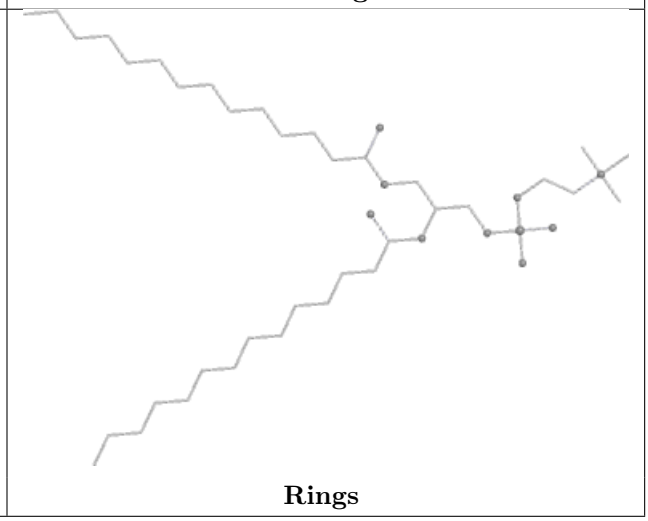
Bond lengths



Bond angles

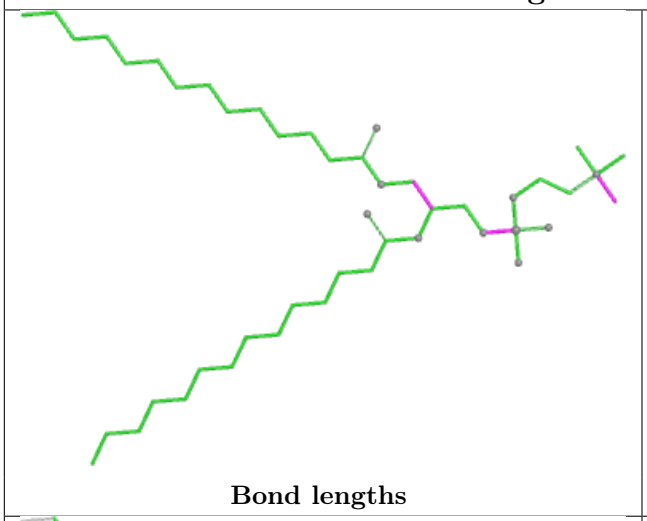


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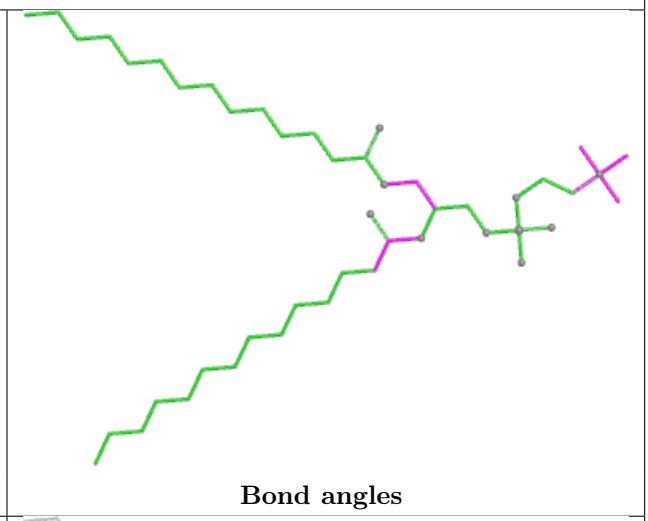


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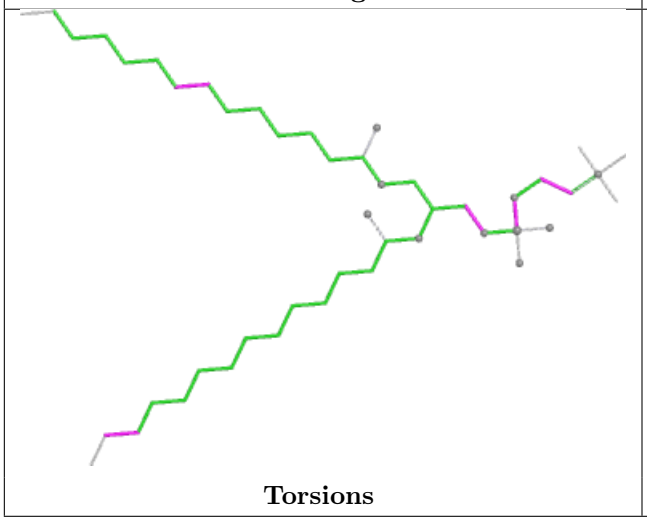
Ligand PX4 C 363



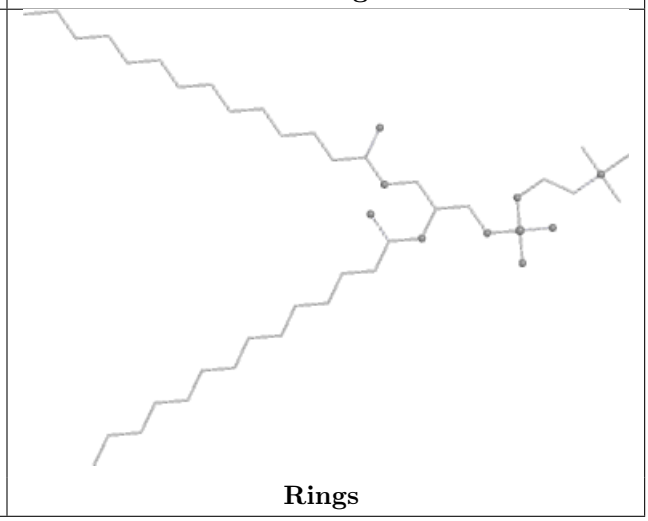
Bond lengths



Bond angles

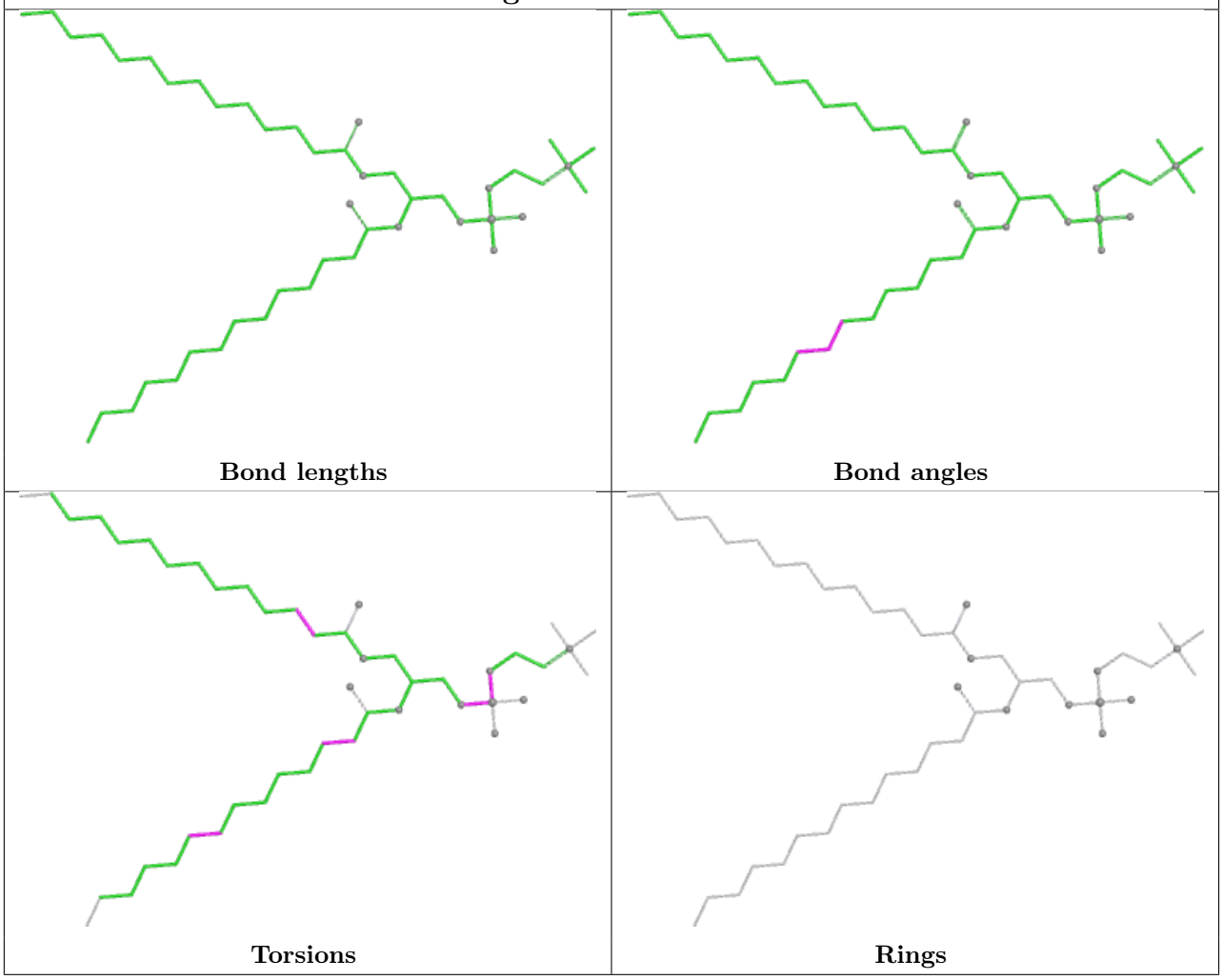


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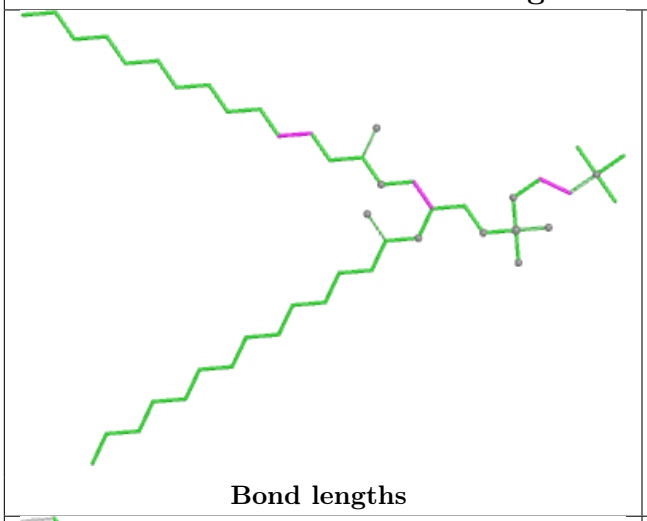


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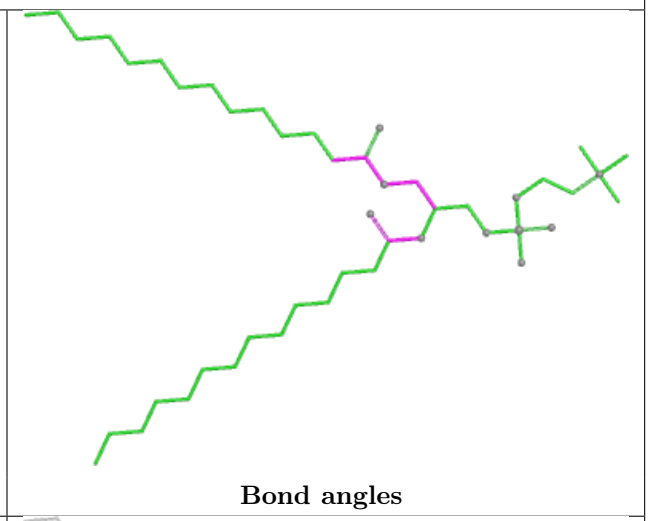
Ligand PX4 B 312



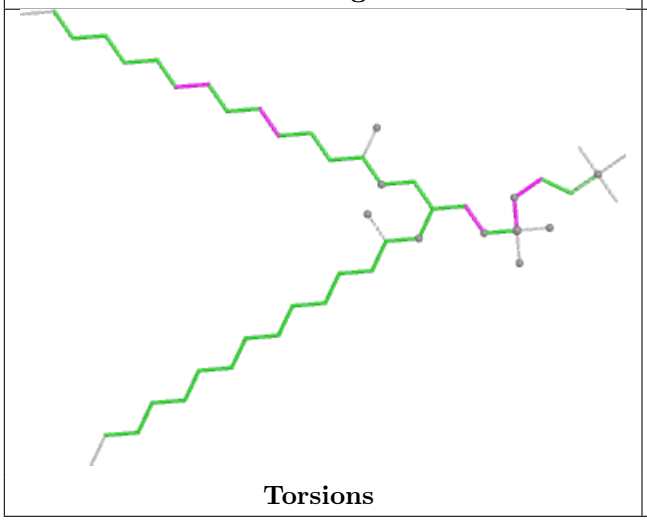
Ligand PX4 A 643



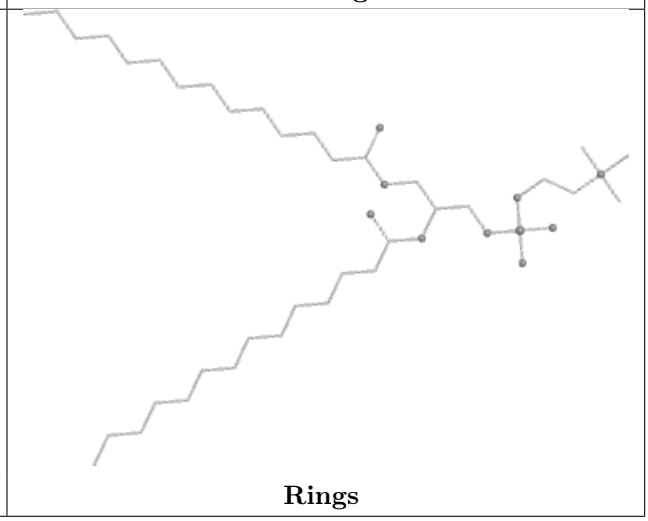
Bond lengths



Bond angles

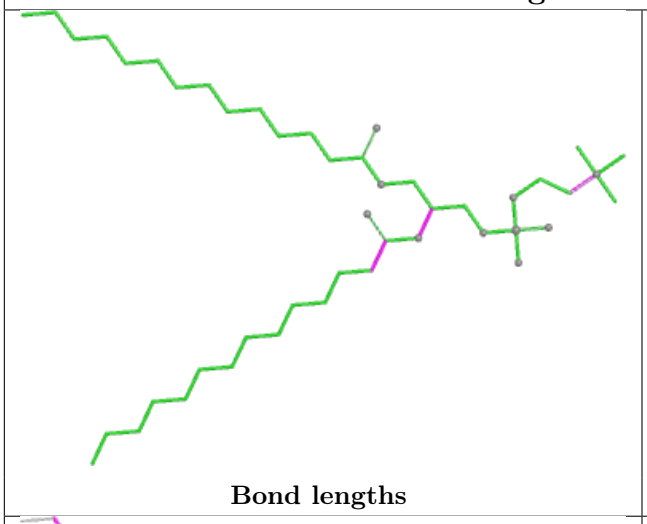


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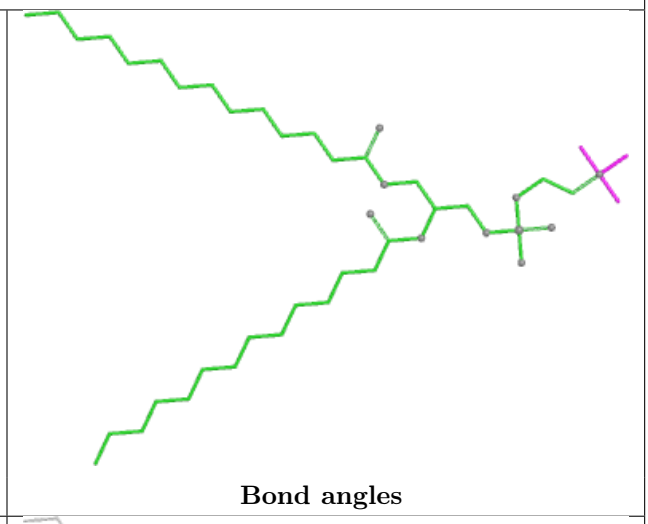


Rings

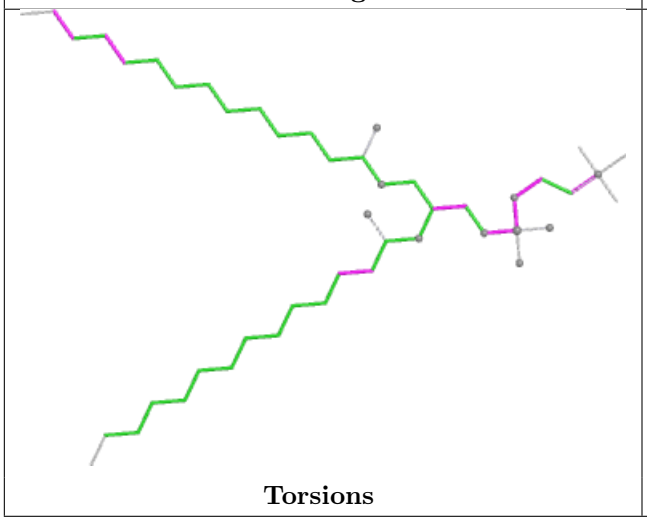
Ligand PX4 B 391



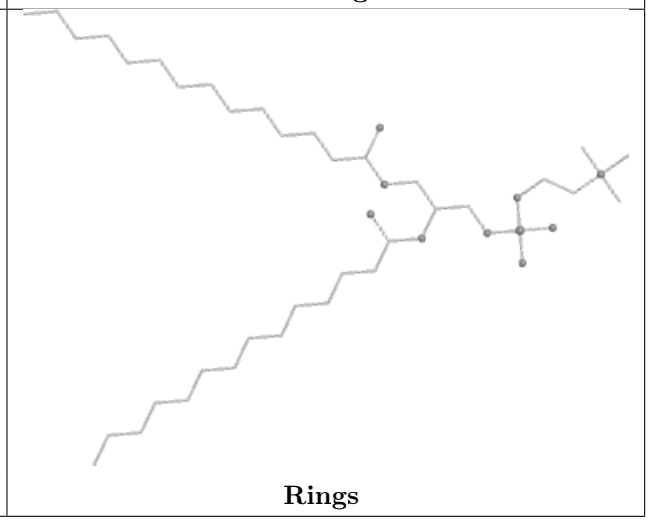
Bond lengths



Bond angles

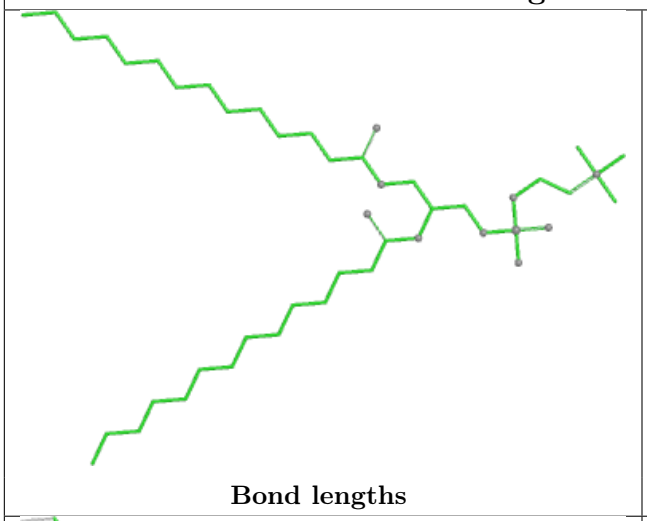


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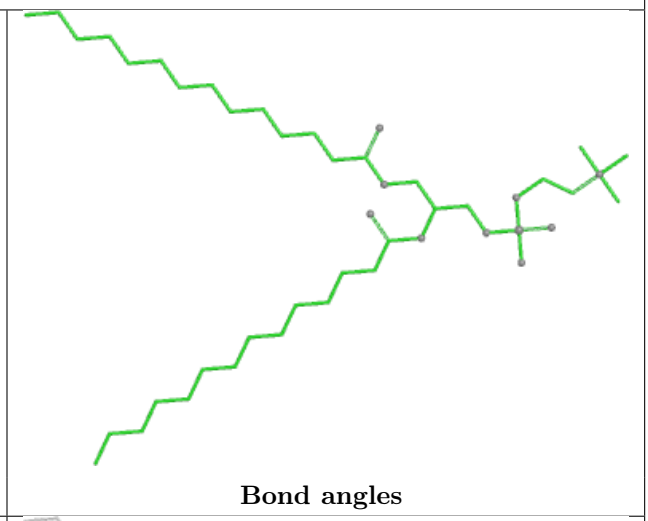


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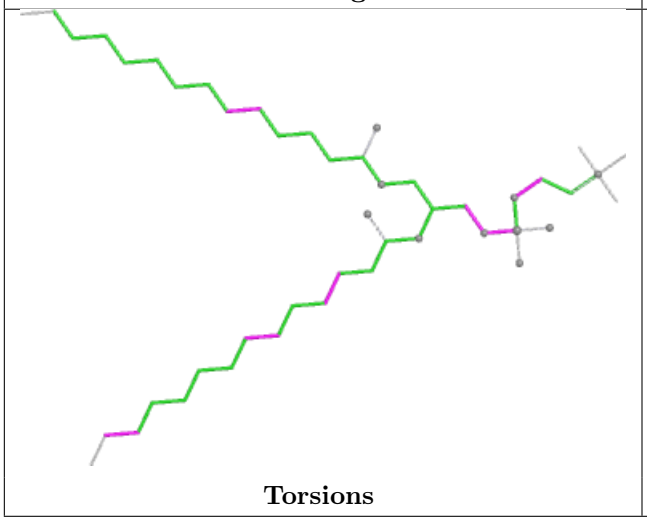
Ligand PX4 B 356



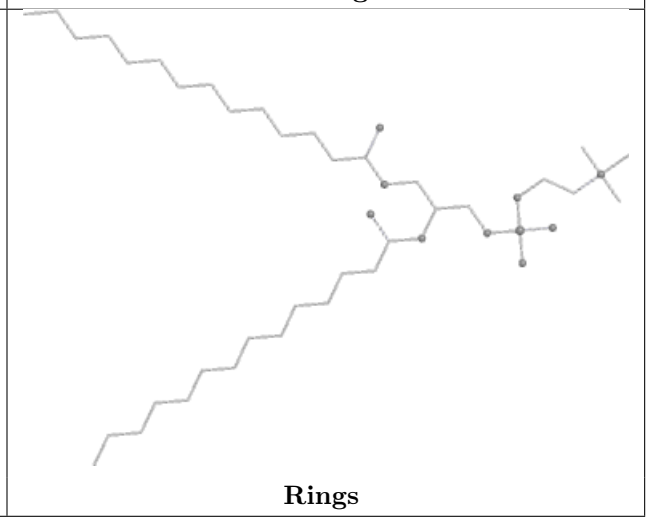
Bond lengths



Bond angles

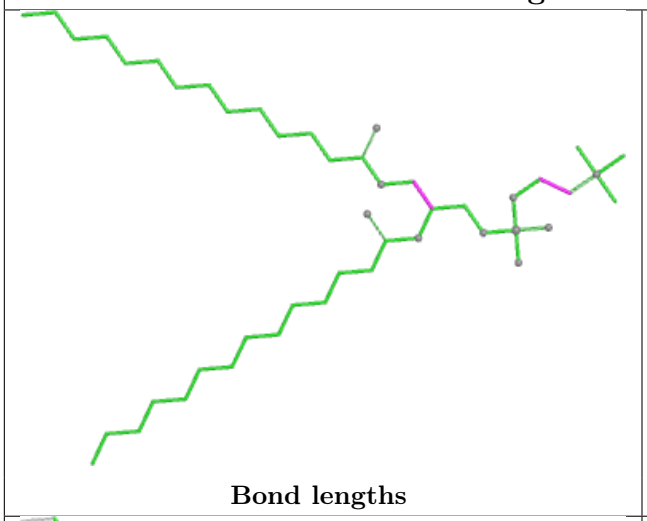


Torsions

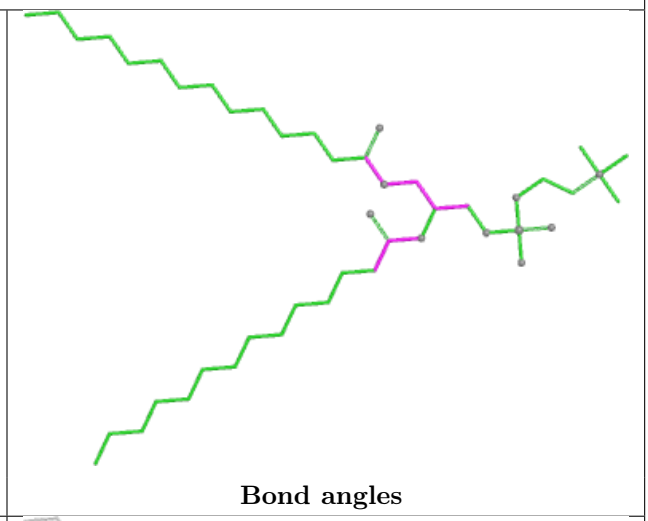


Rings

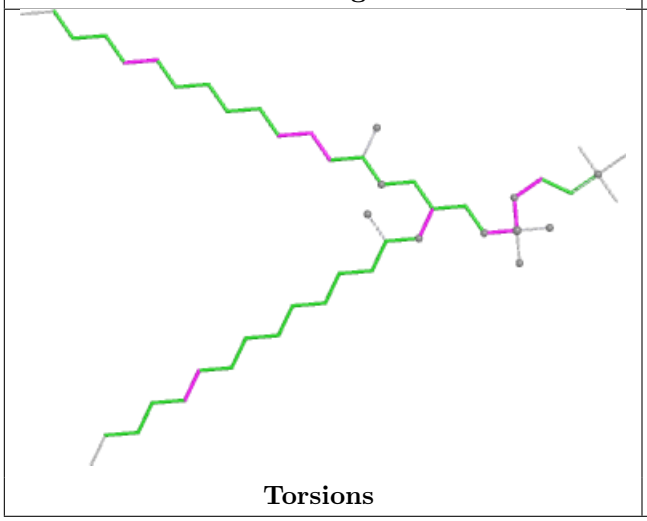
Ligand PX4 C 356



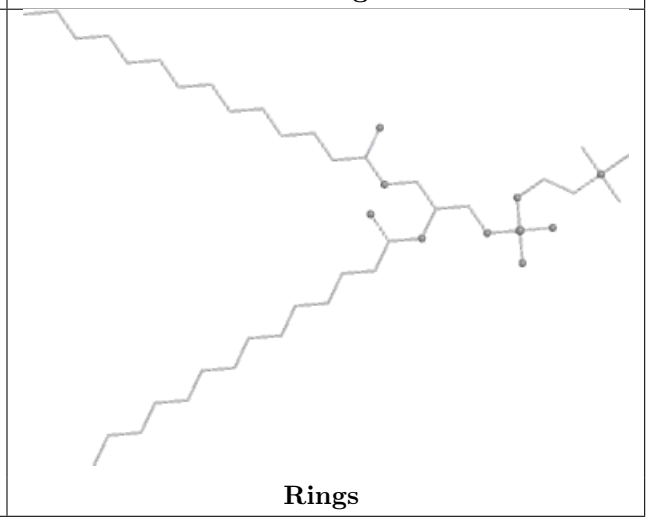
Bond lengths



Bond angles

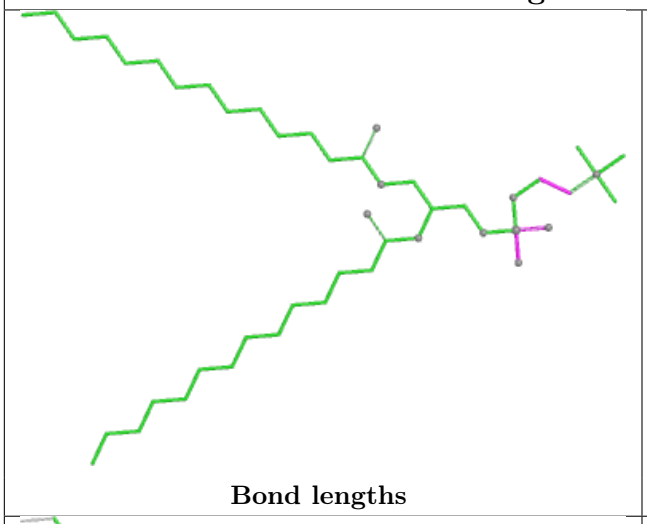


Torsions

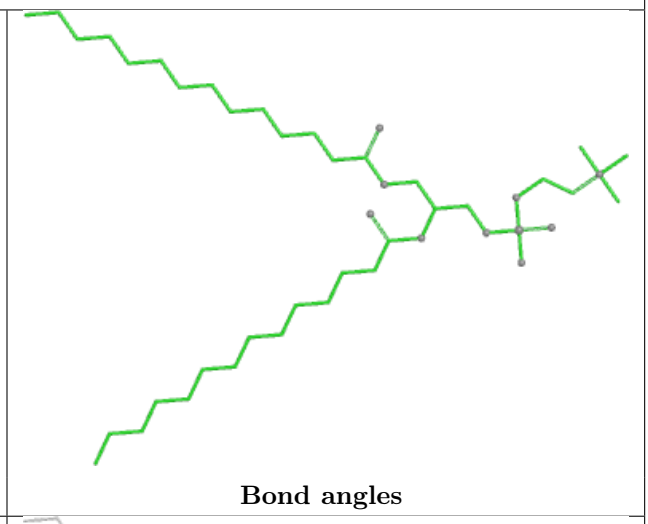


Rings

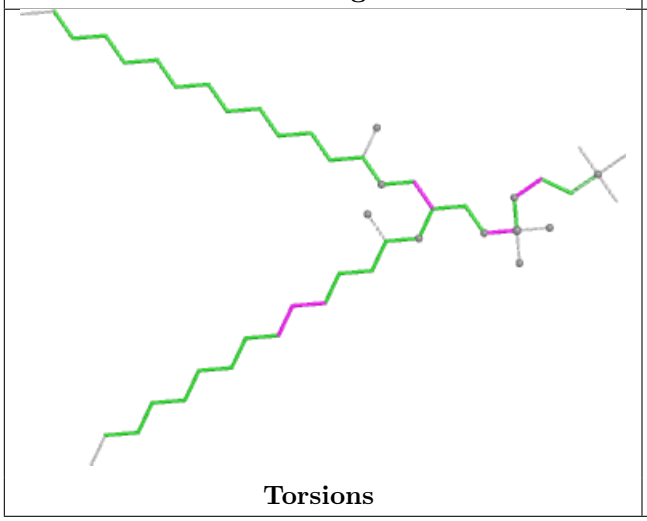
Ligand PX4 C 318



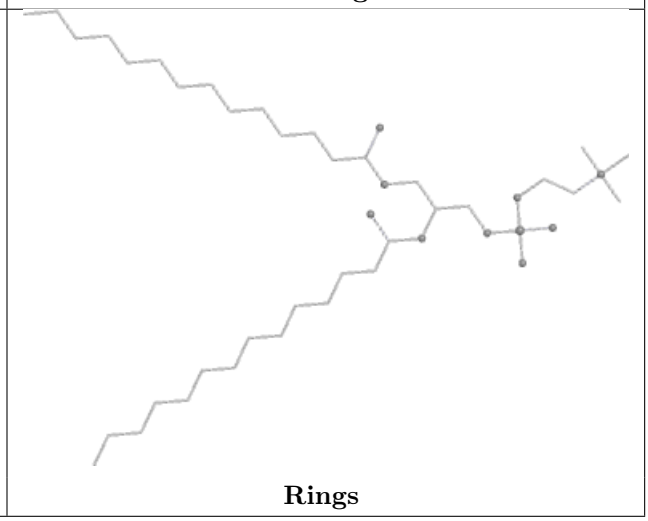
Bond lengths



Bond angles

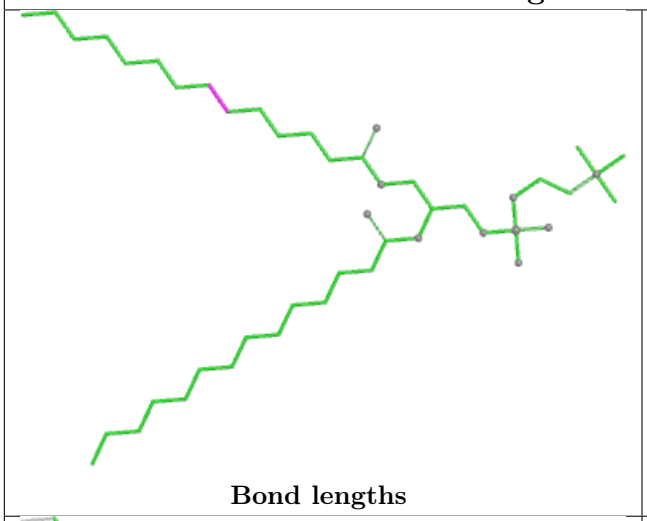


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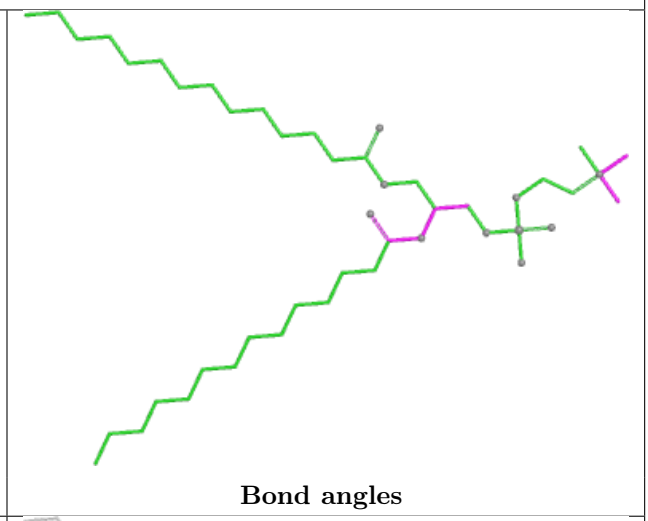


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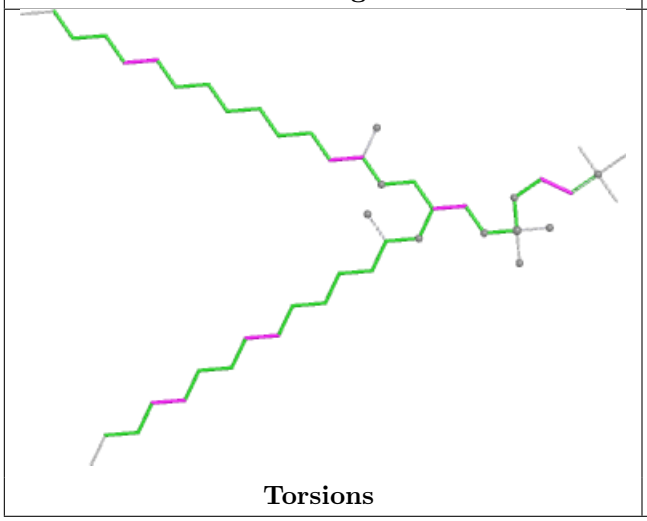
Ligand PX4 A 604



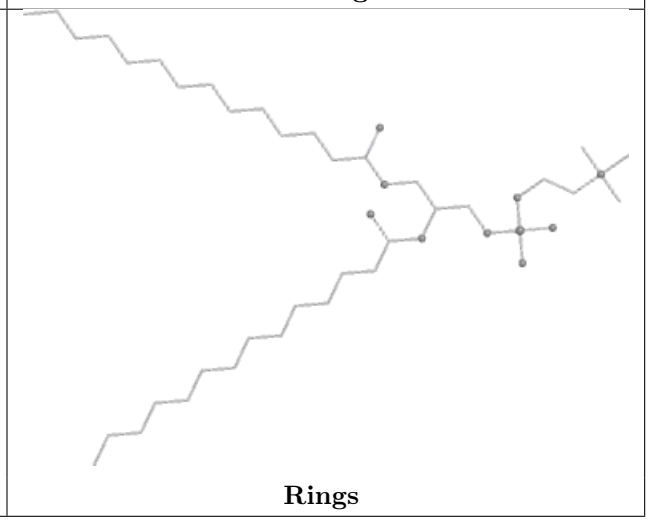
Bond lengths



Bond angles

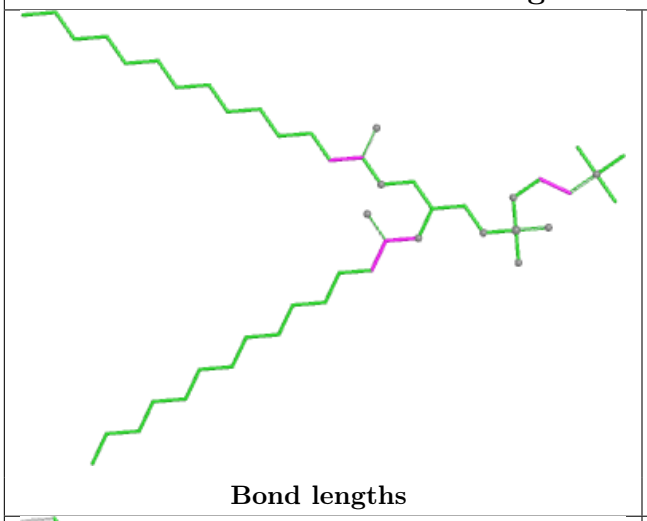


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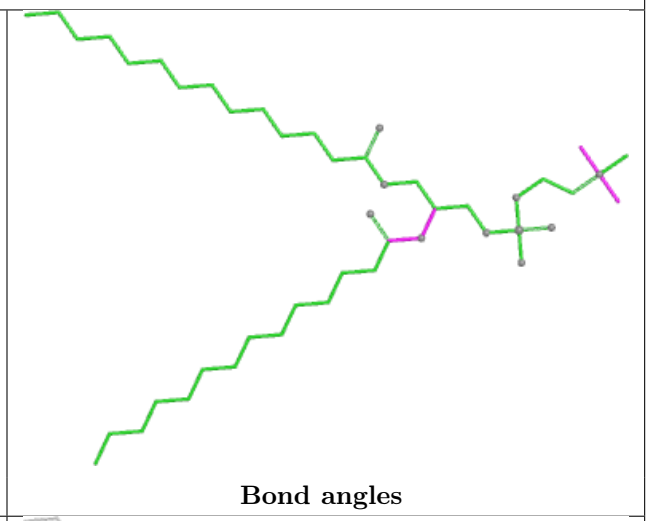


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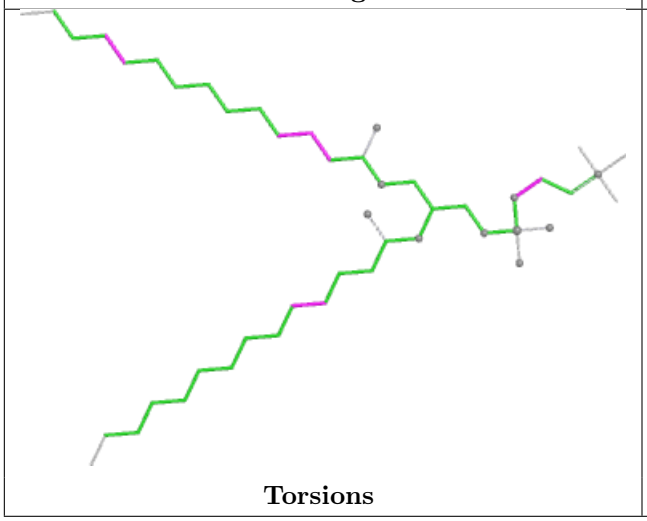
Ligand PX4 C 349



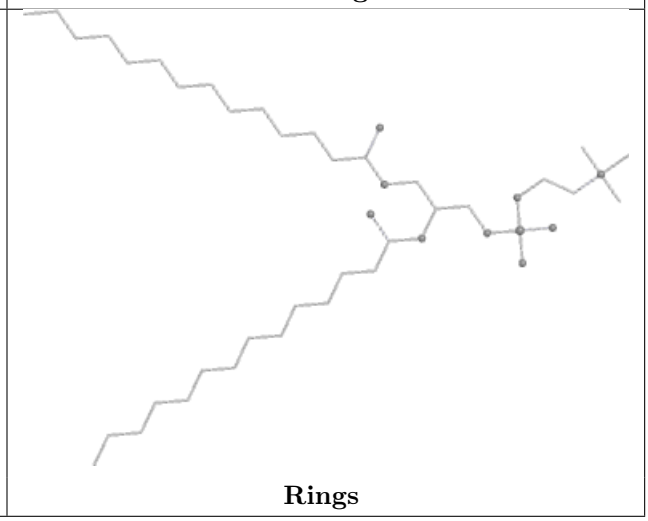
Bond lengths



Bond angles

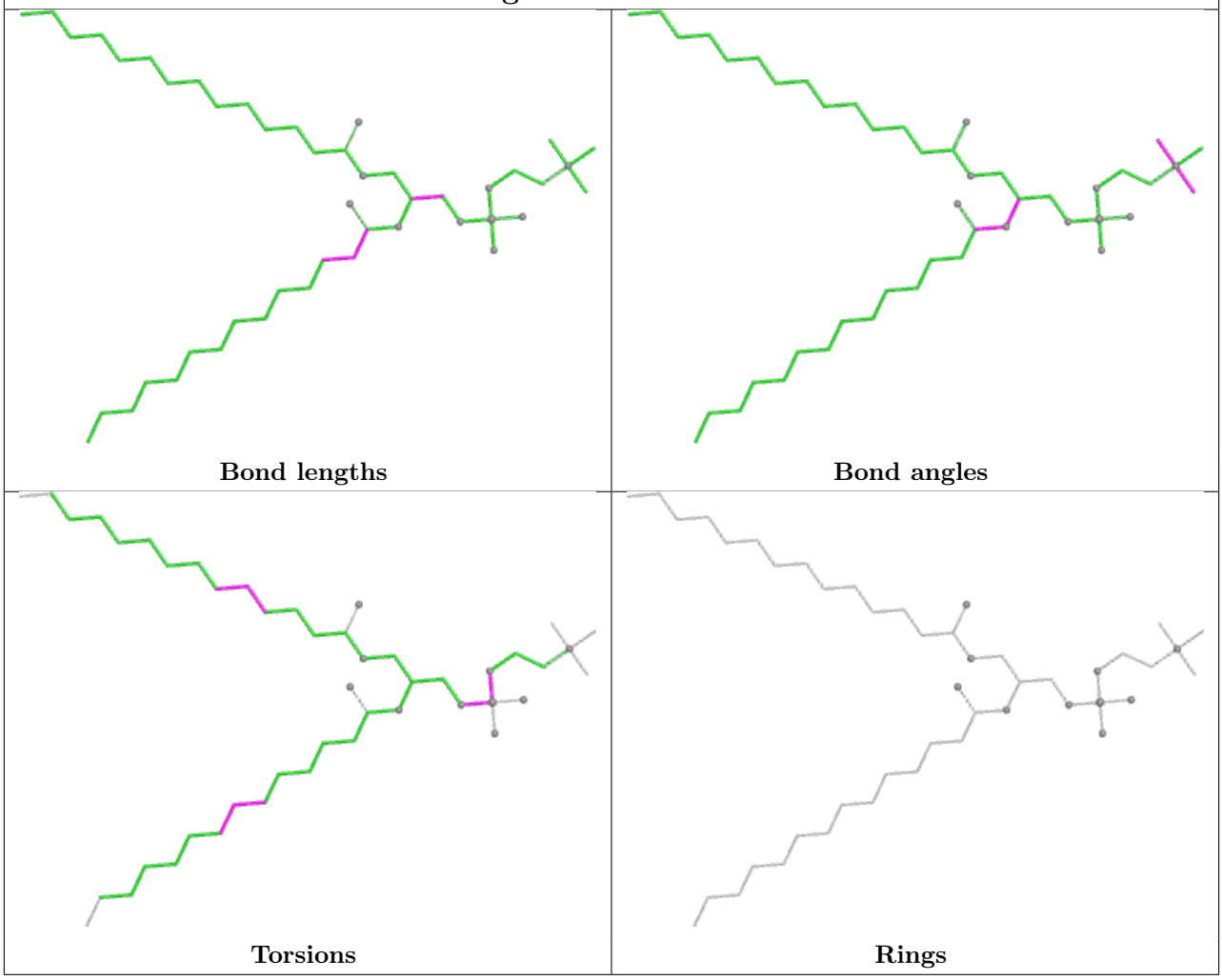


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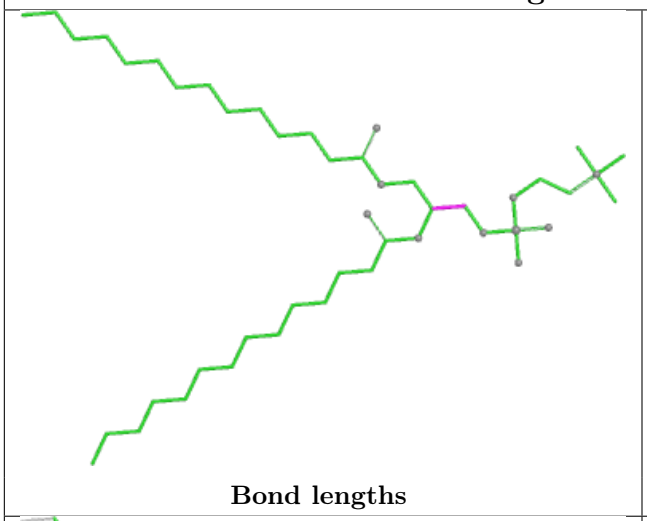


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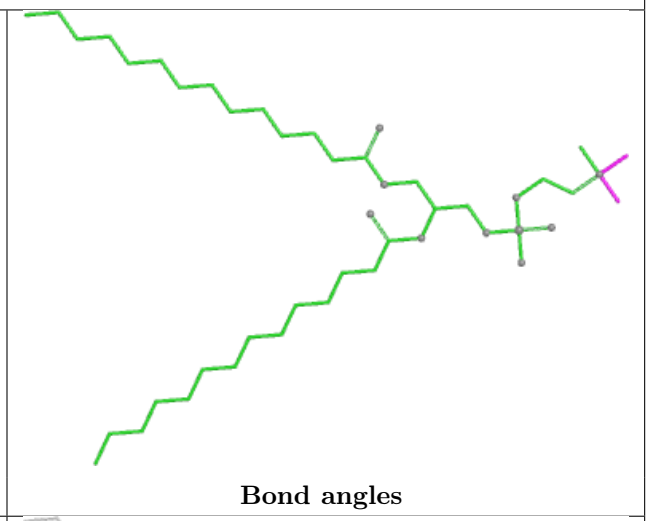
Ligand PX4 A 635



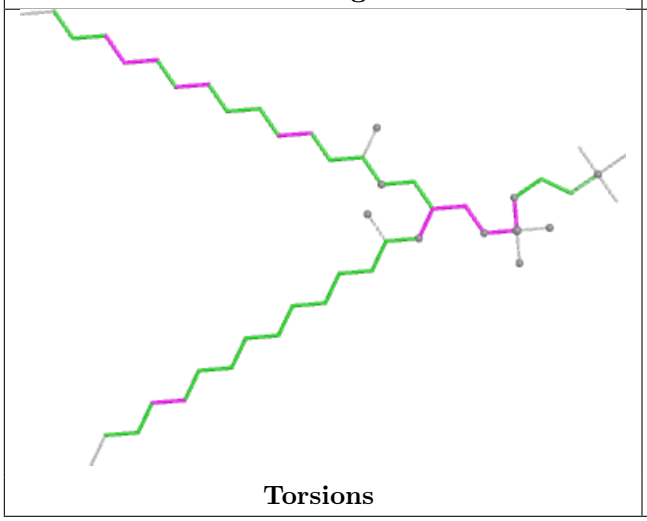
Ligand PX4 A 612



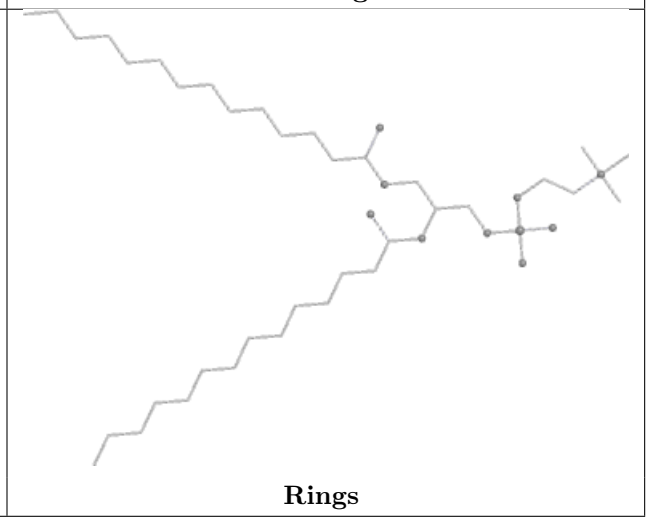
Bond lengths



Bond angles

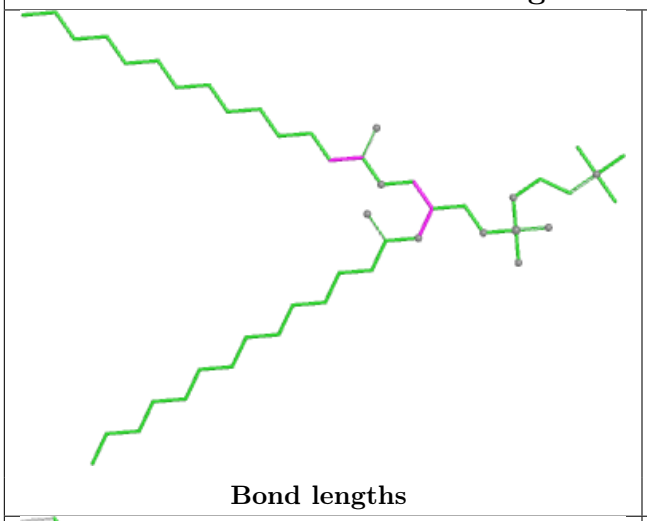


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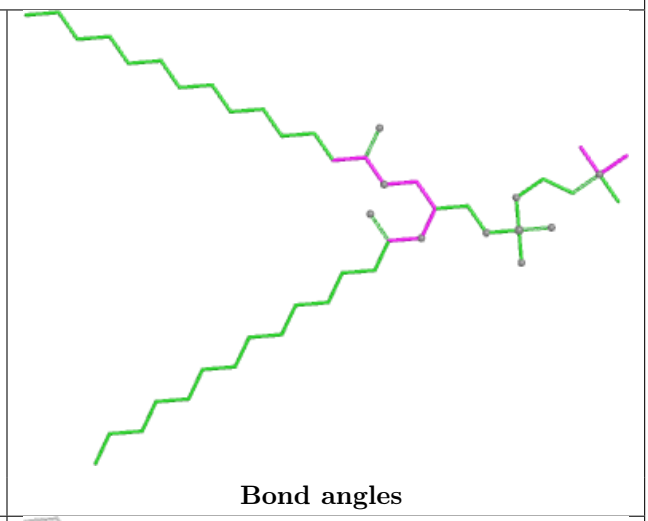


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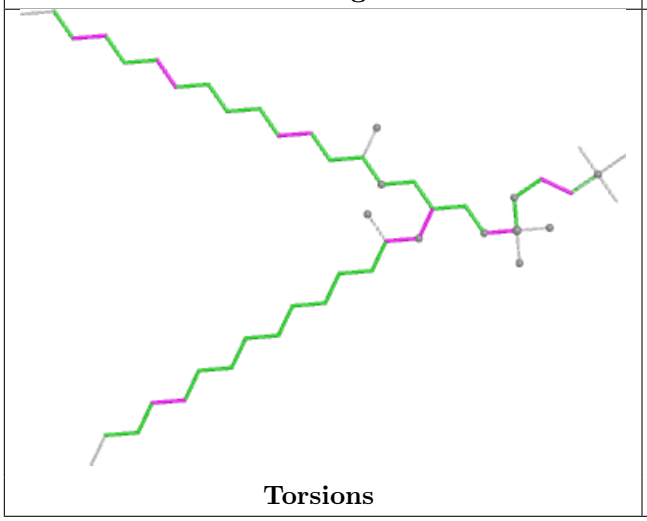
Ligand PX4 B 392



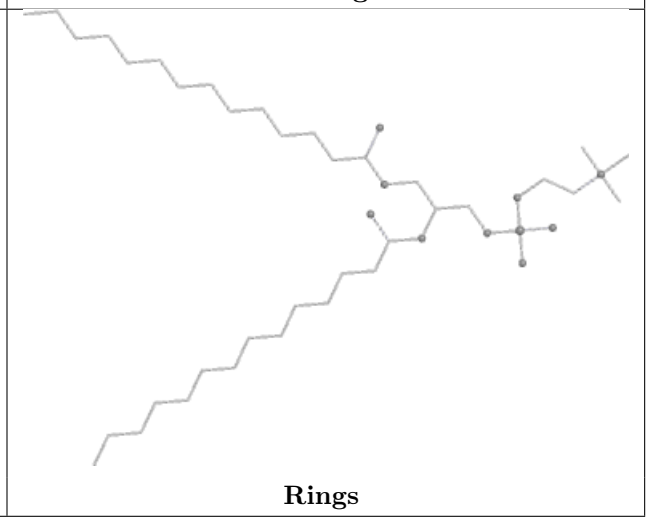
Bond lengths



Bond angles

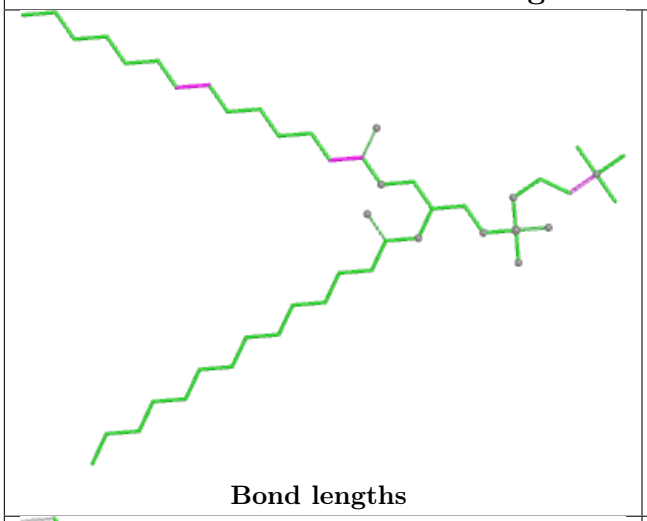


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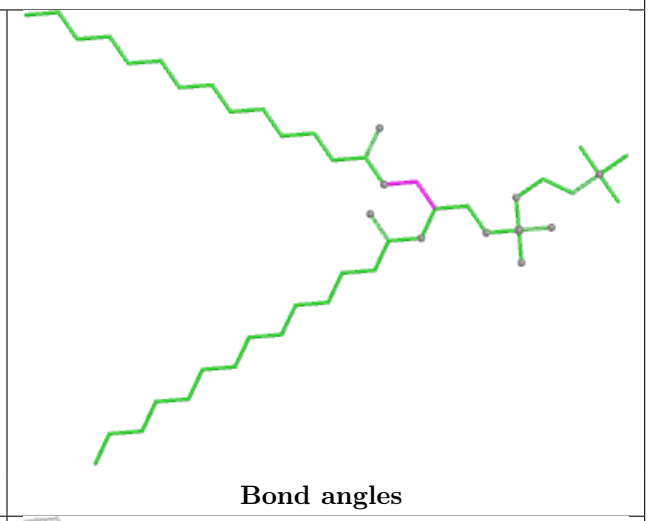


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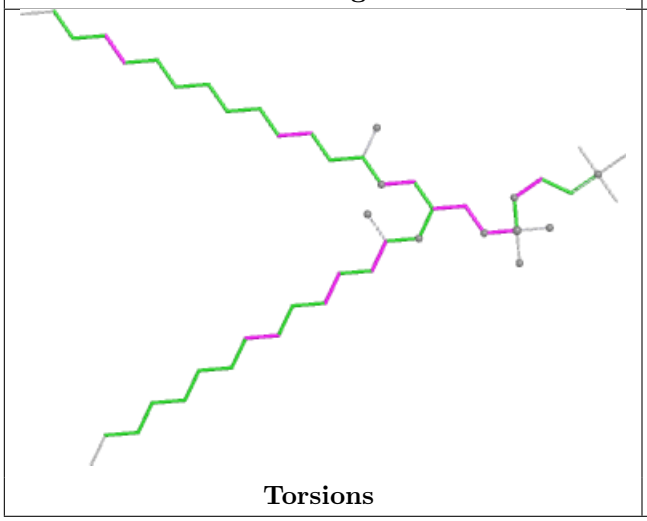
Ligand PX4 C 320



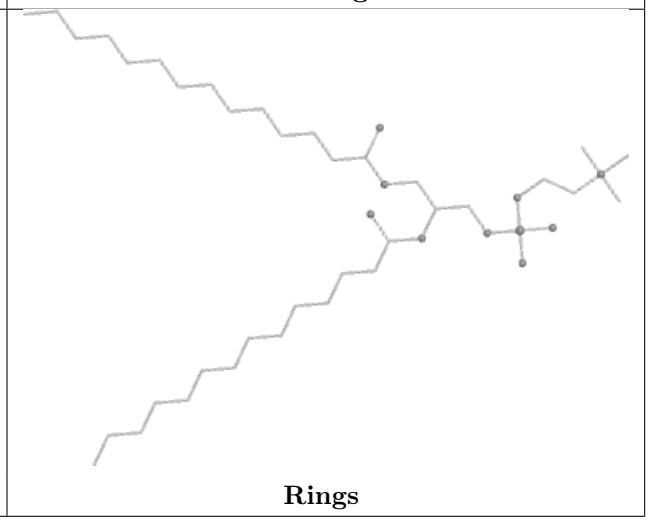
Bond lengths



Bond angles

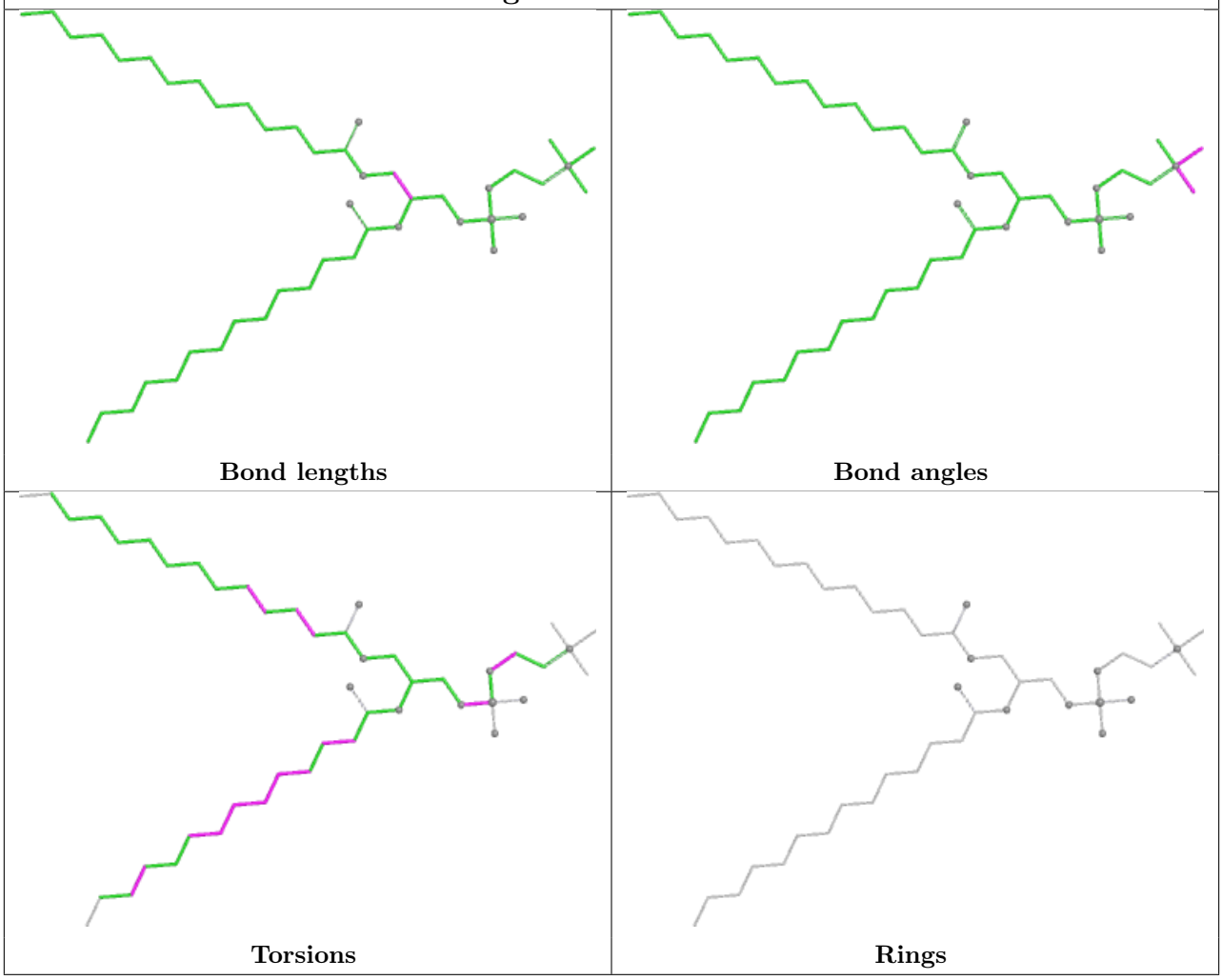


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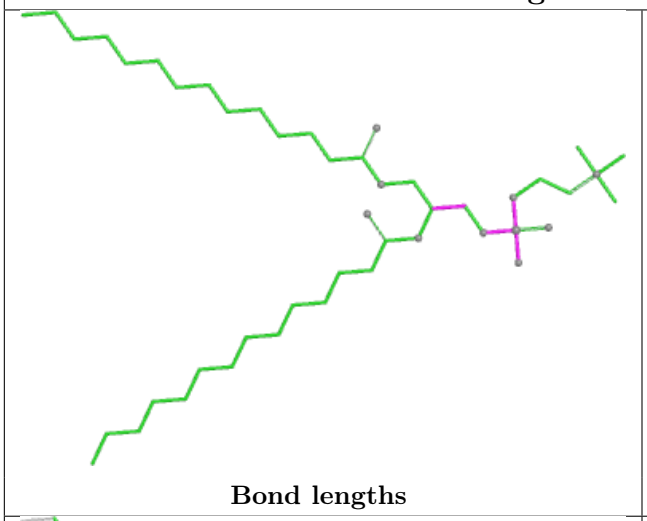


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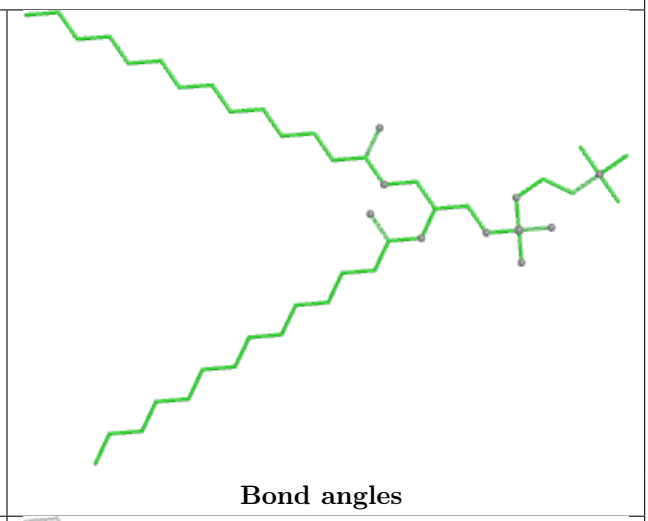
Ligand PX4 B 337



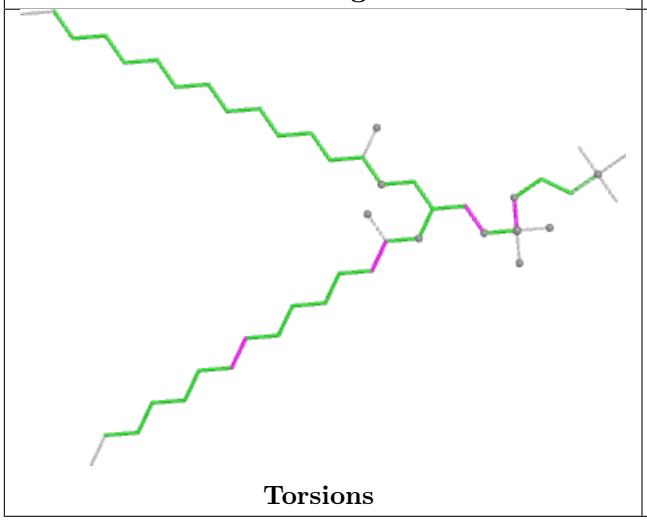
Ligand PX4 C 312



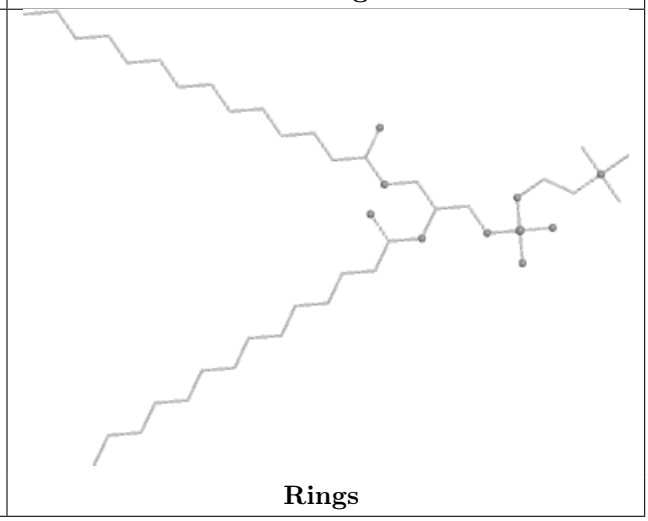
Bond lengths



Bond angles

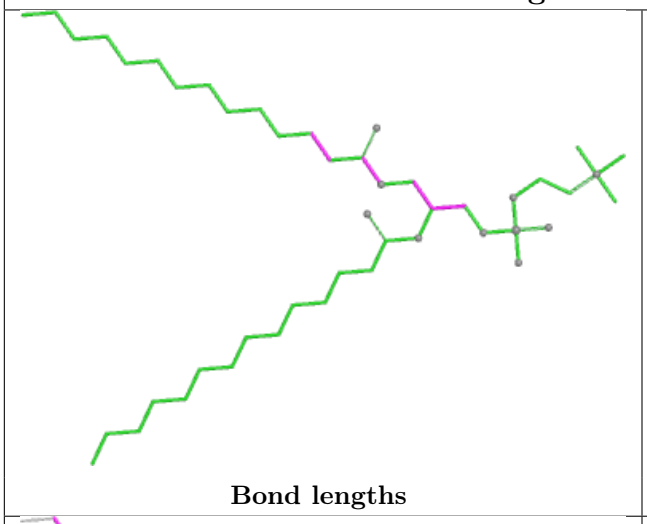


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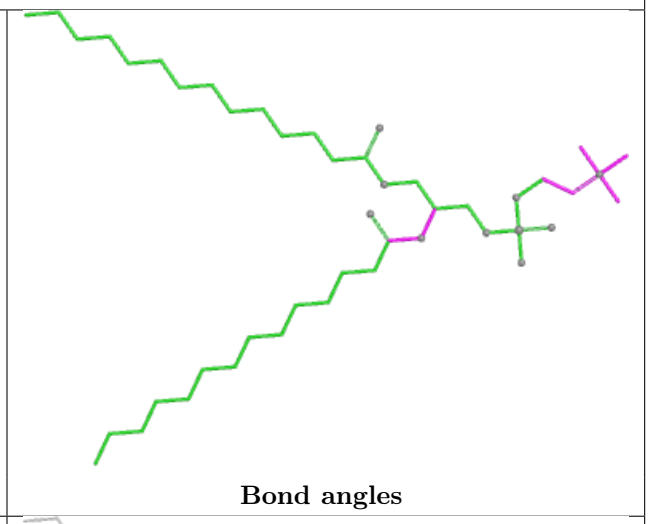


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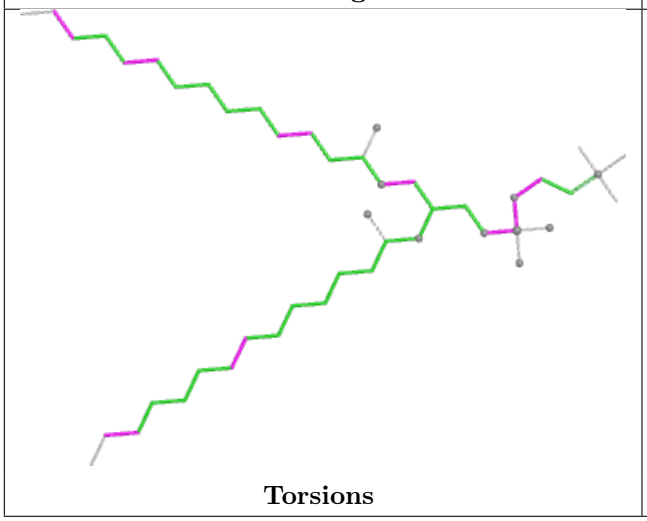
Ligand PX4 B 332



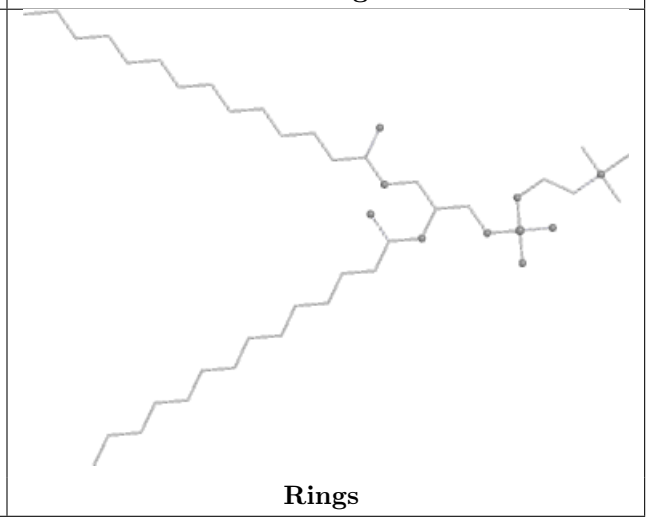
Bond lengths



Bond angles

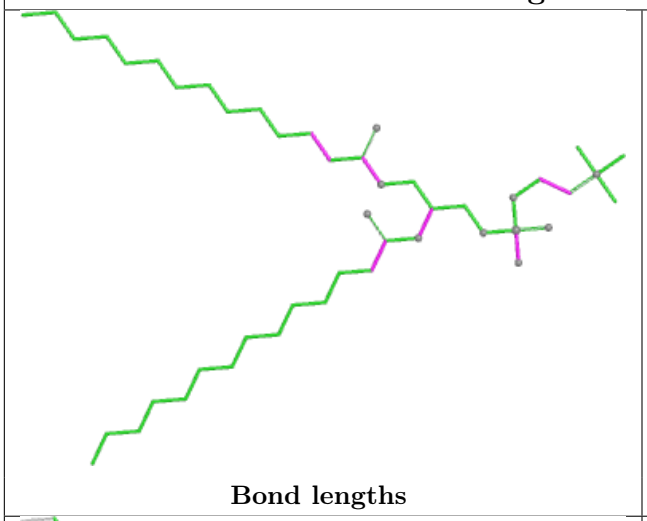


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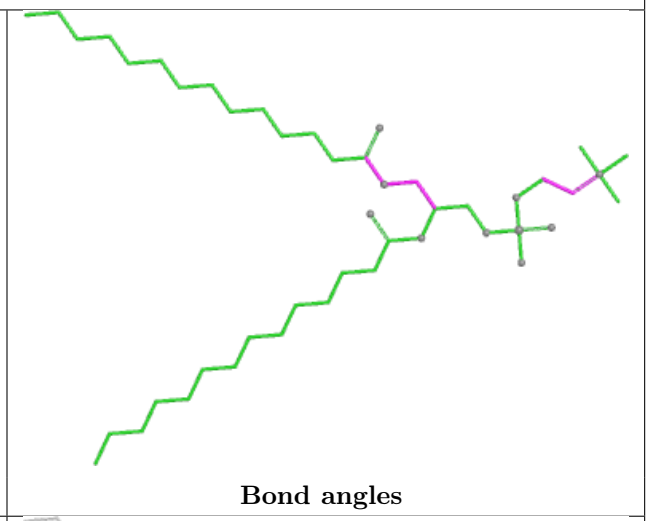


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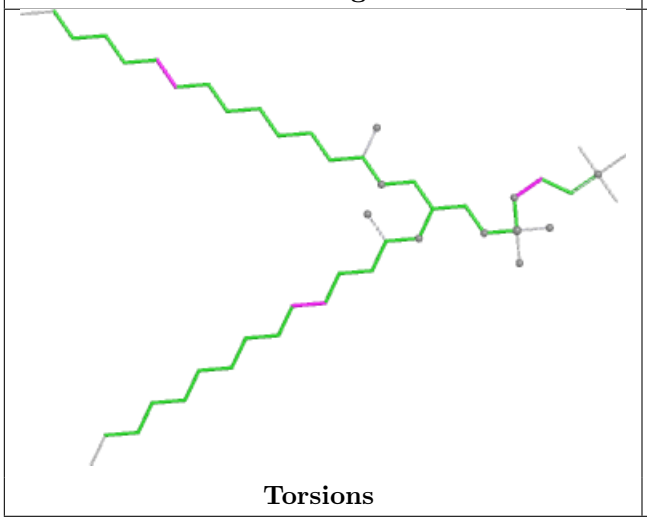
Ligand PX4 C 353



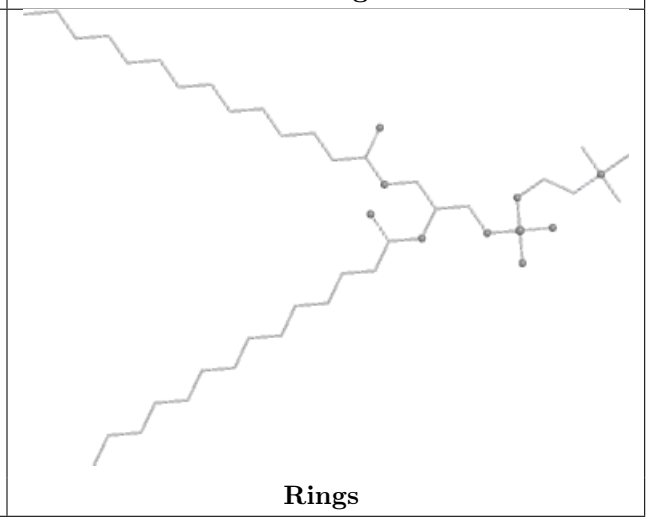
Bond lengths



Bond angles

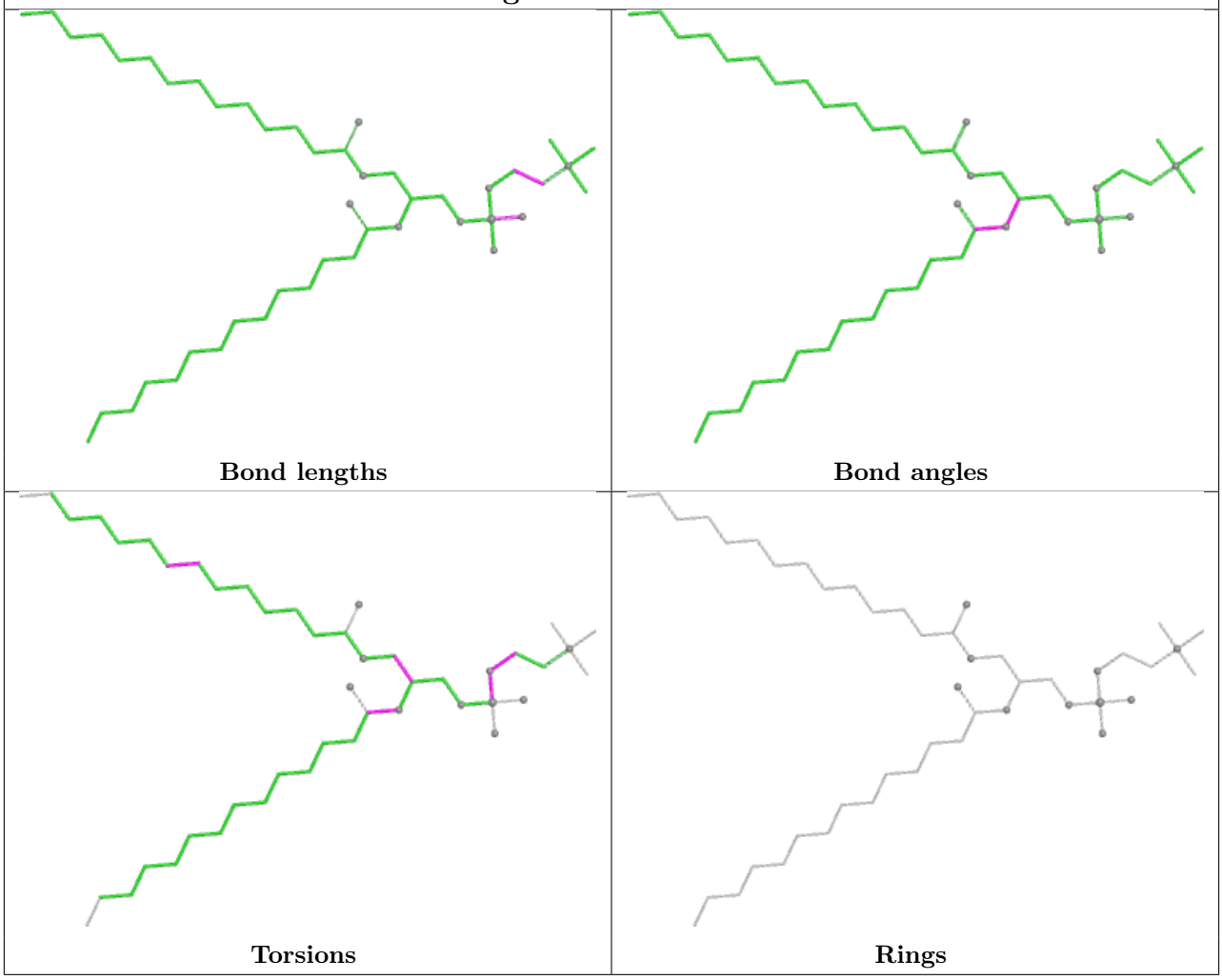


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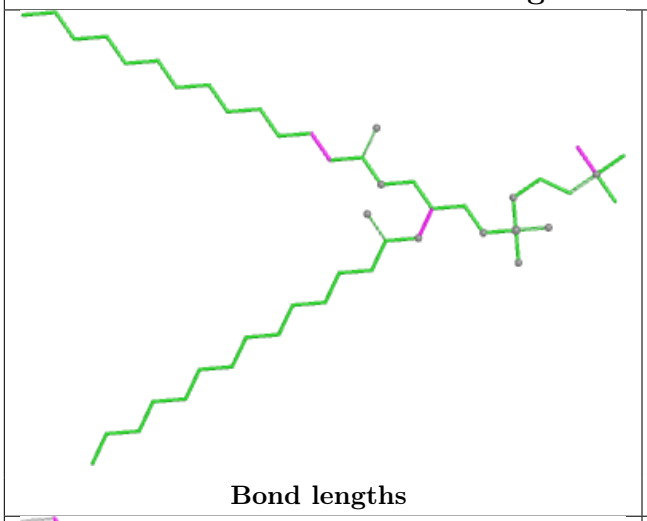


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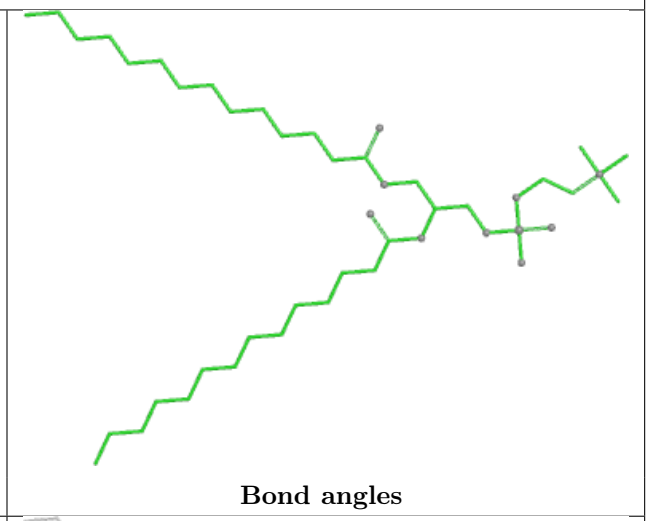
Ligand PX4 B 367



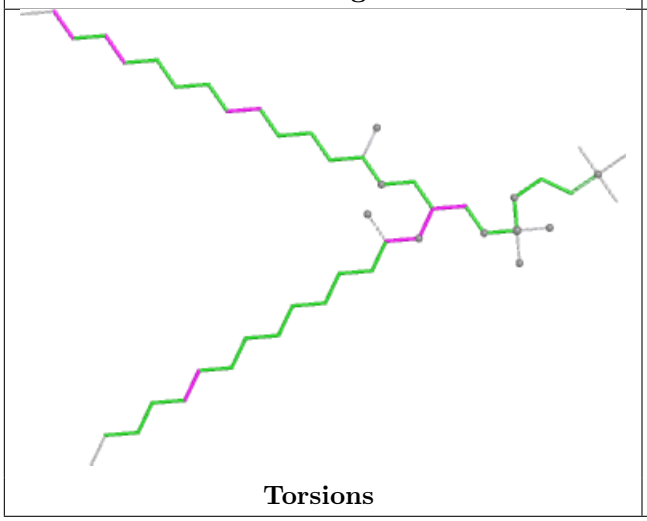
Ligand PX4 A 629



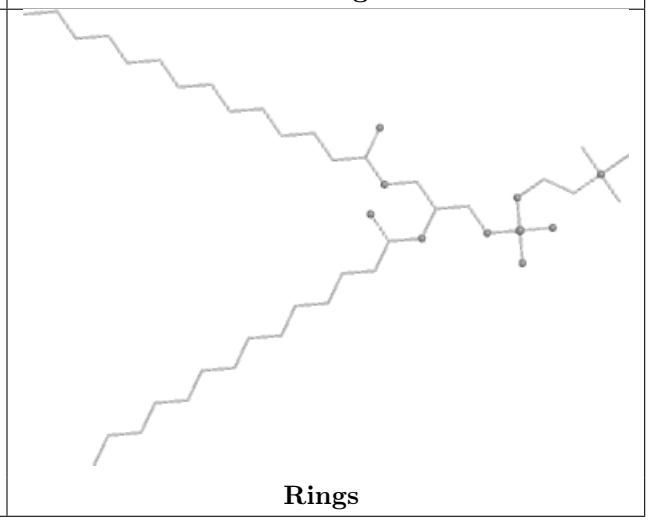
Bond lengths



Bond angles

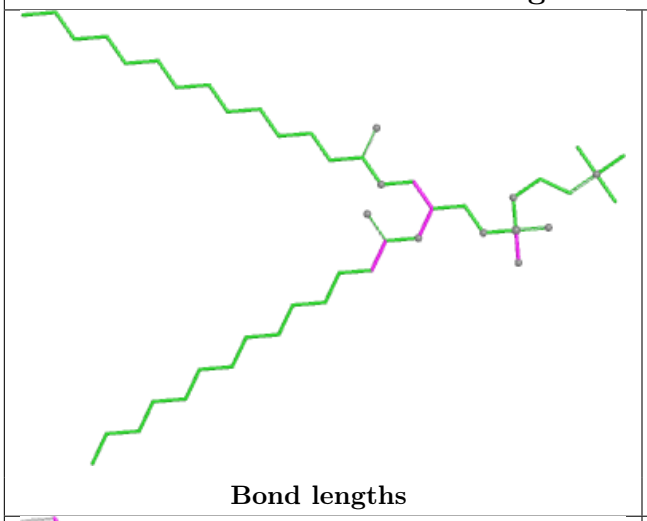


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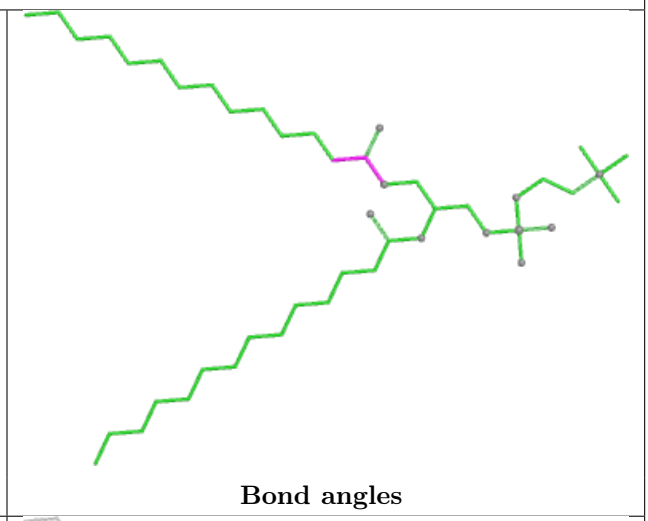


Rings

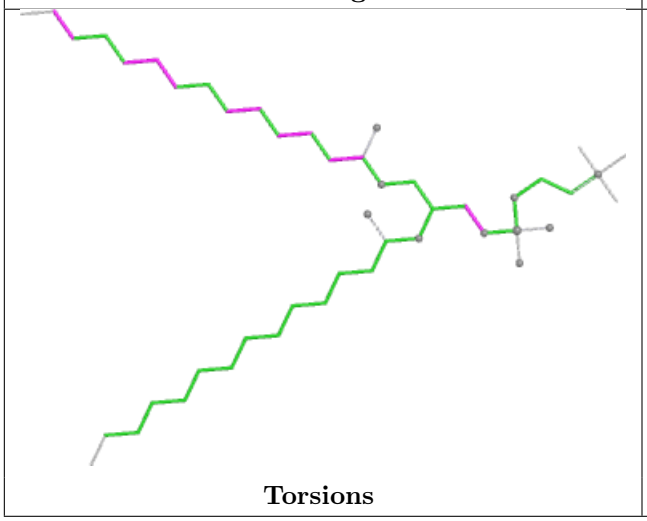
Ligand PX4 B 333



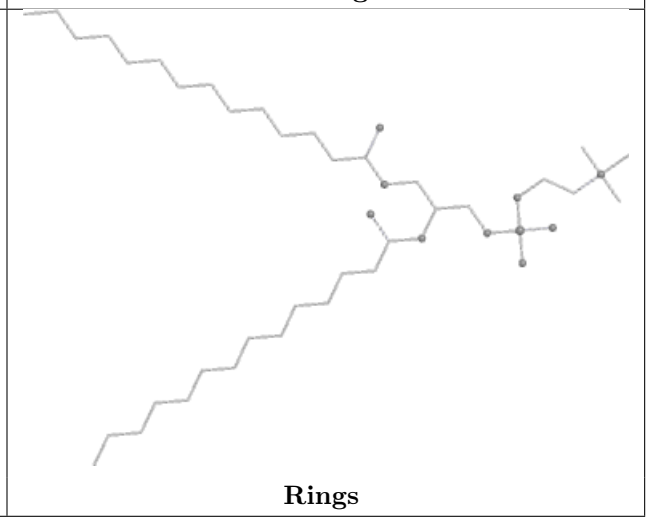
Bond lengths



Bond angles

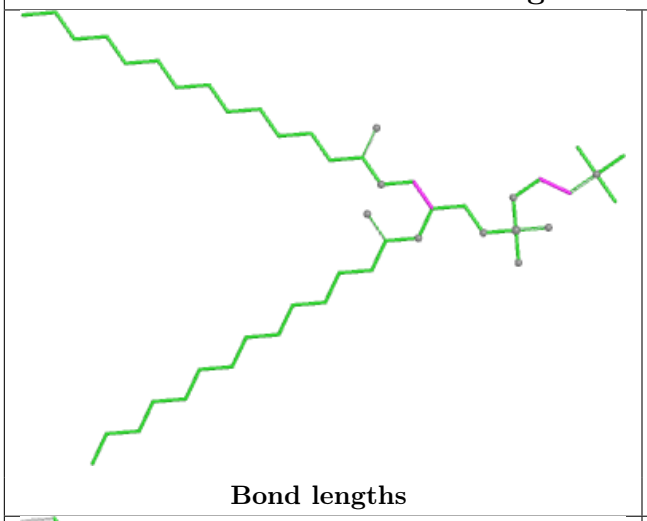


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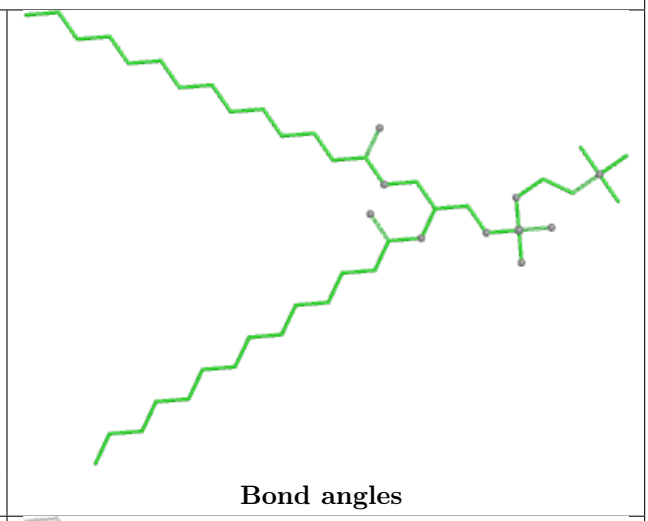


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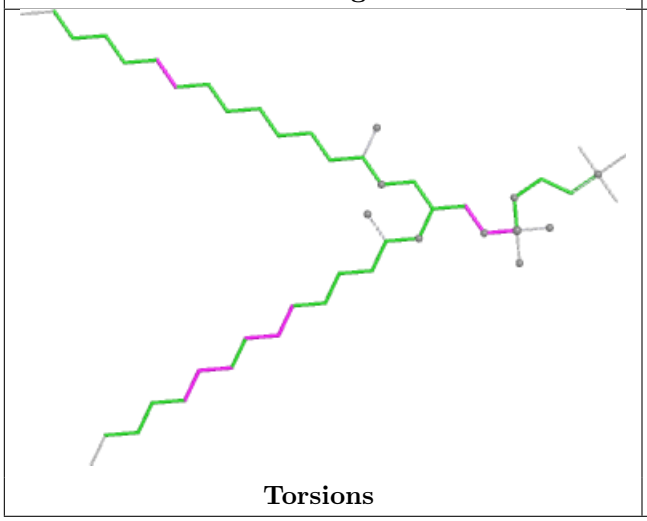
Ligand PX4 A 608



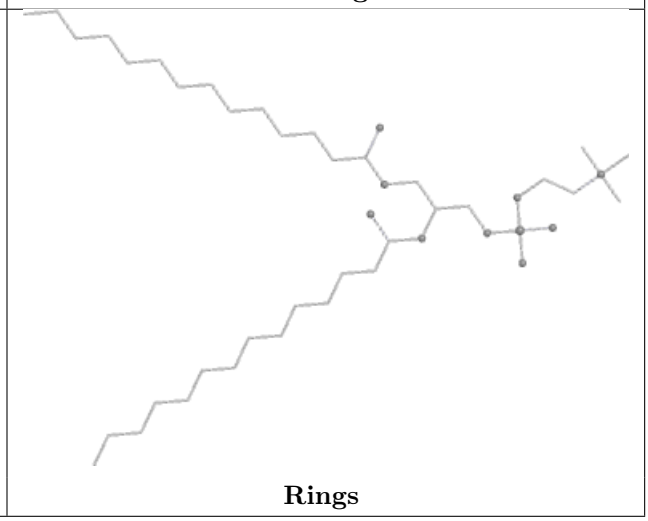
Bond lengths



Bond angles

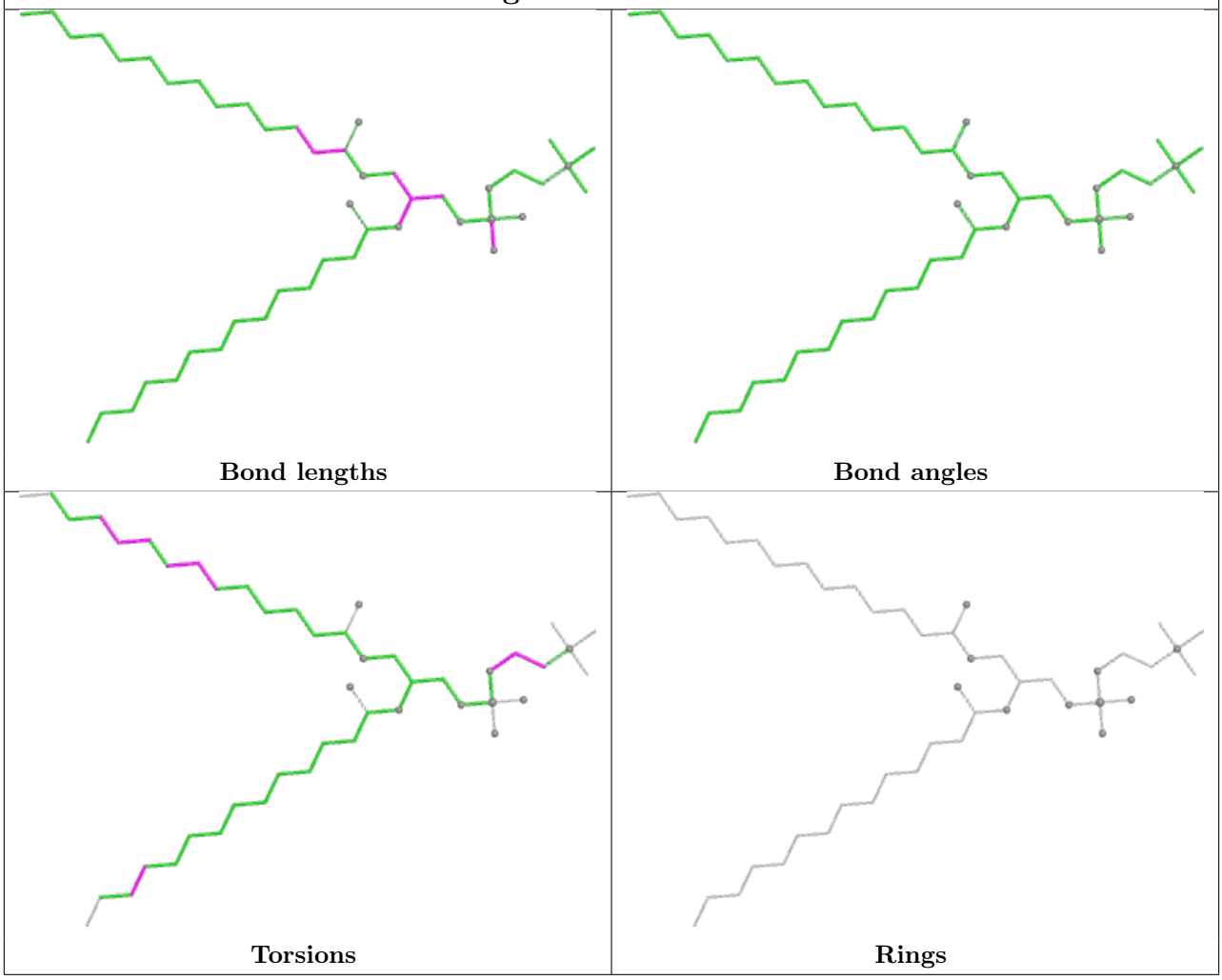


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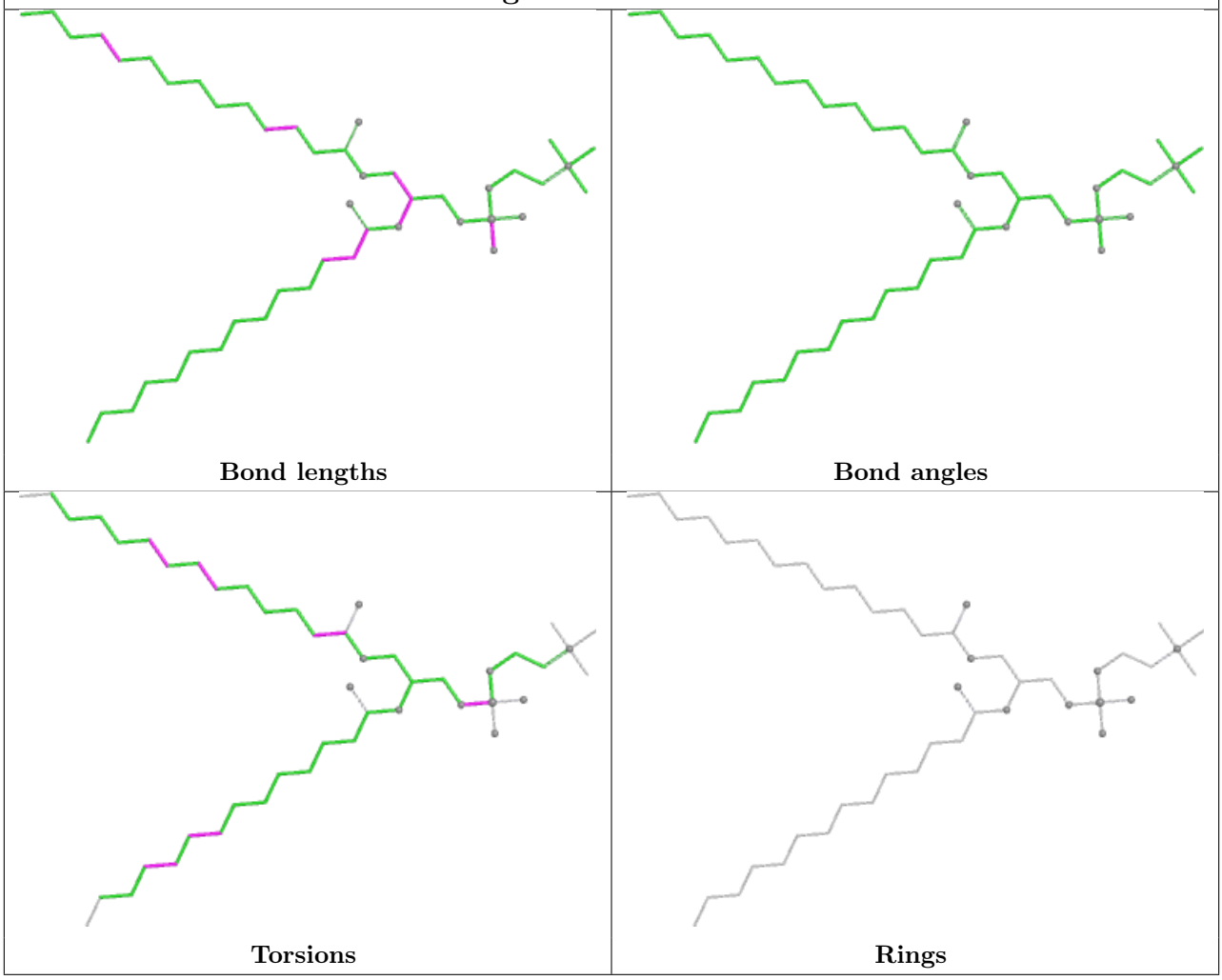


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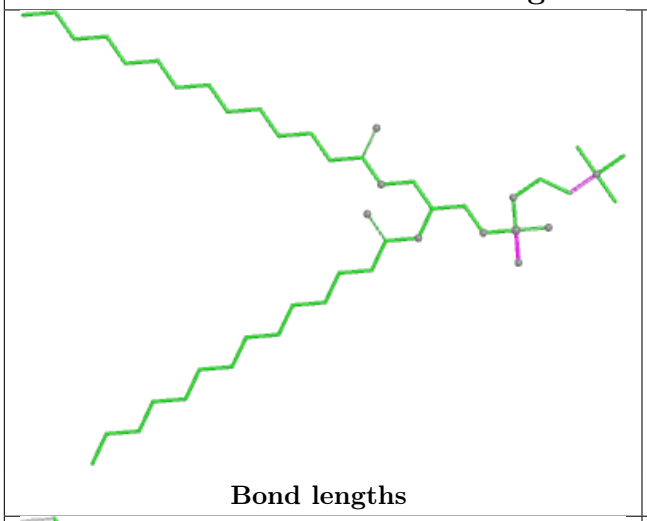
Ligand PX4 B 350



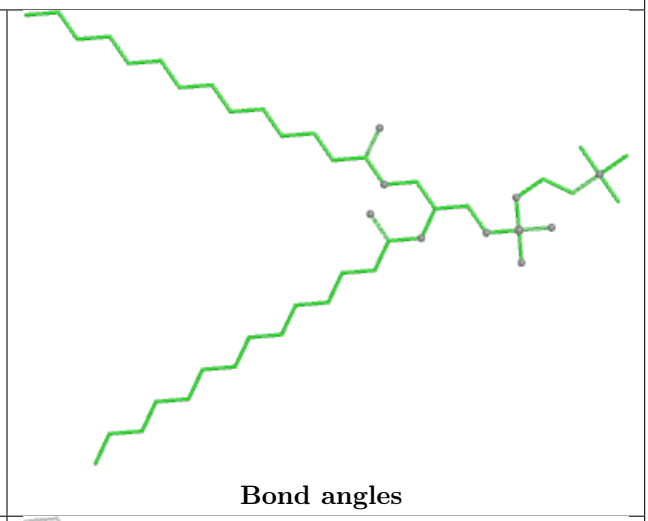
Ligand PX4 C 362



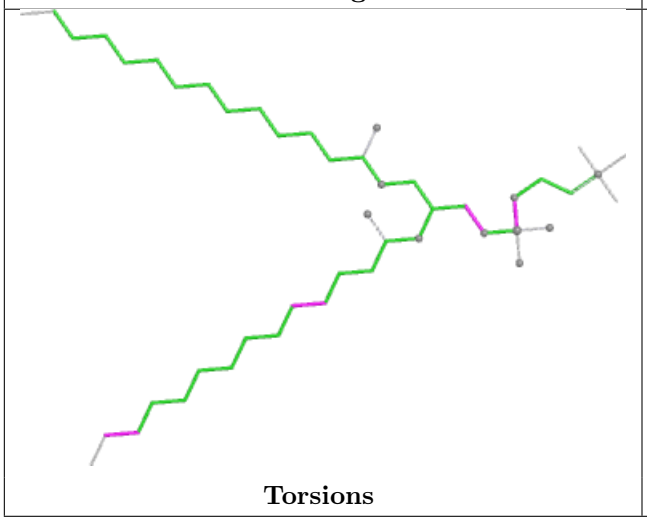
Ligand PX4 C 336



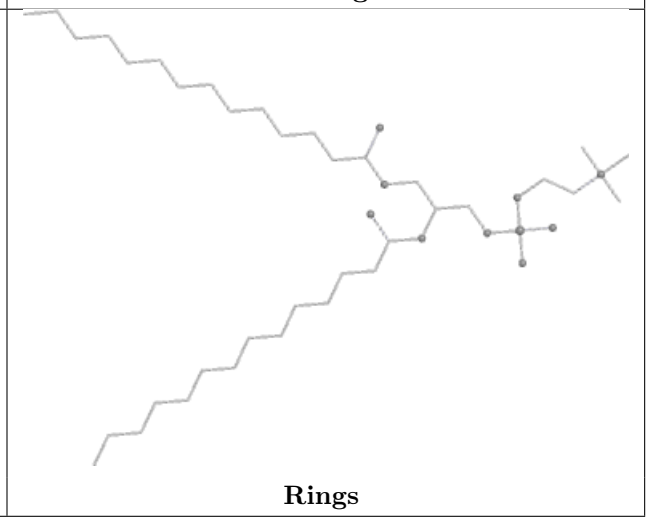
Bond lengths



Bond angles

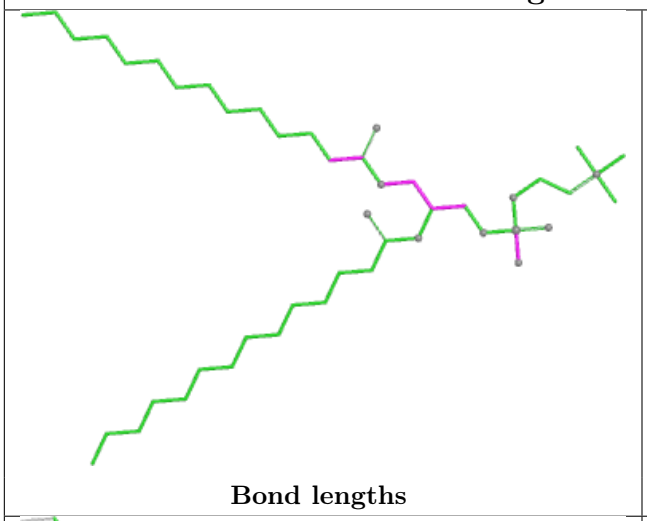


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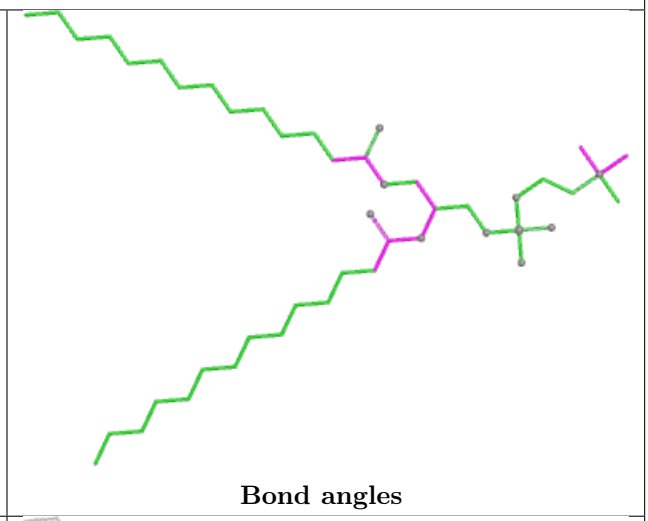


Rings

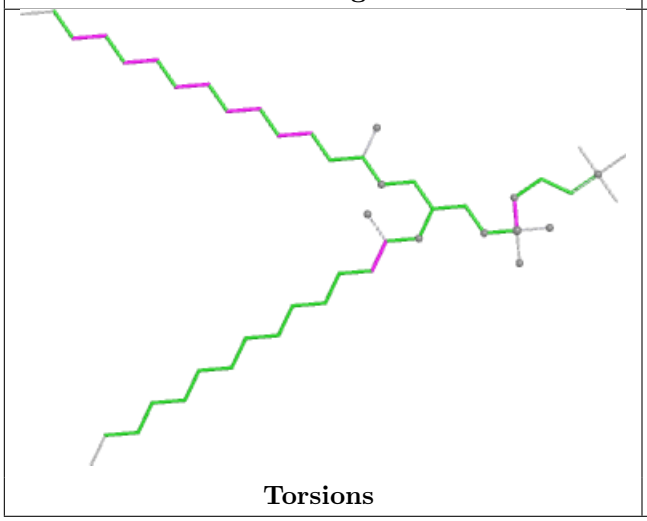
Ligand PX4 A 605



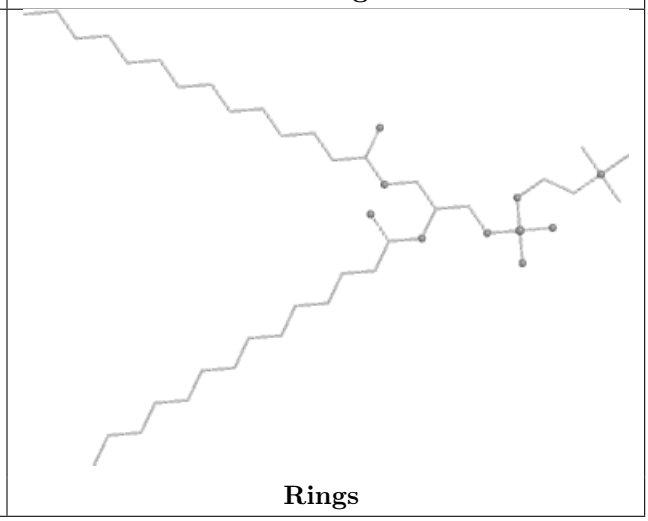
Bond lengths



Bond angles

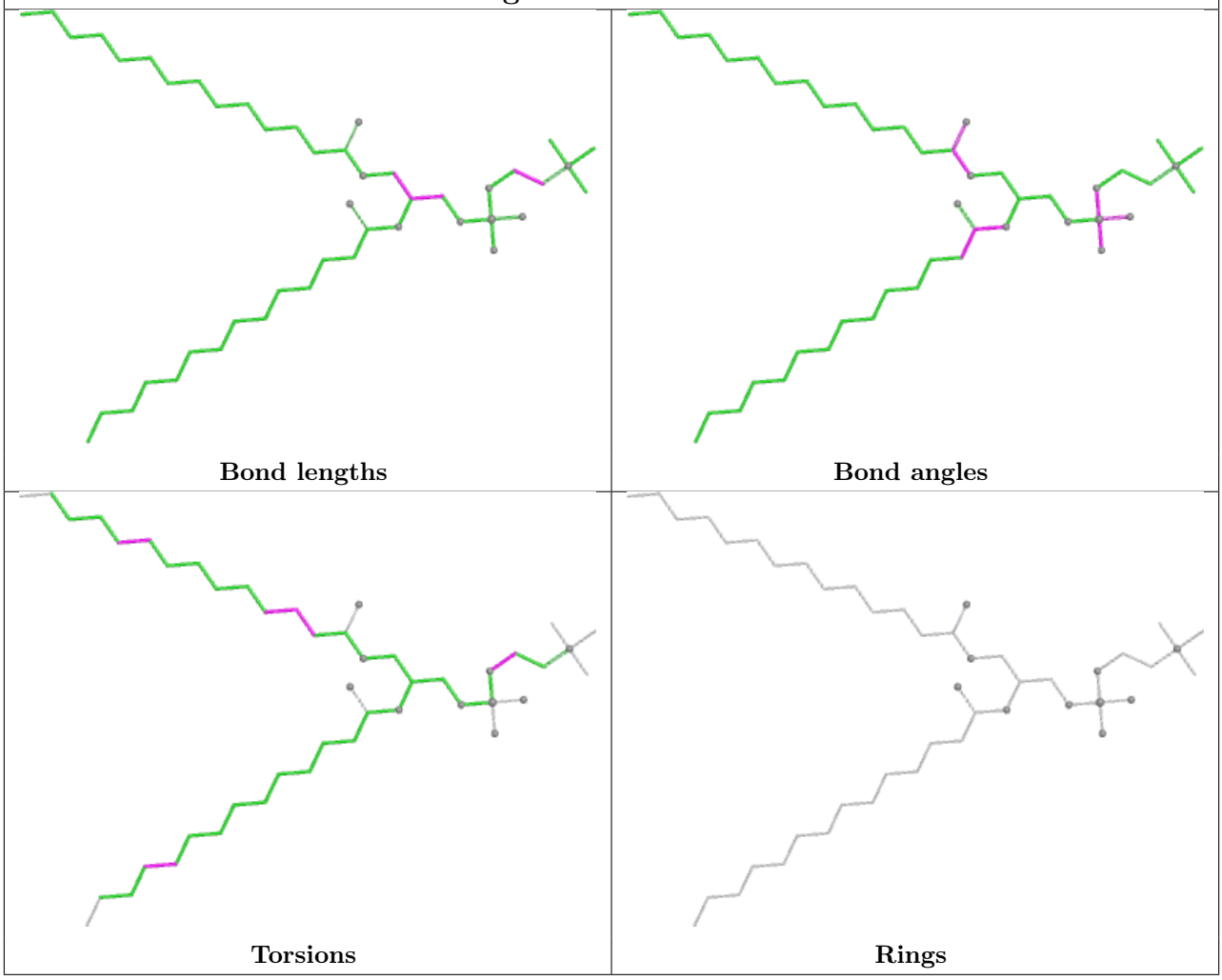


Torsions

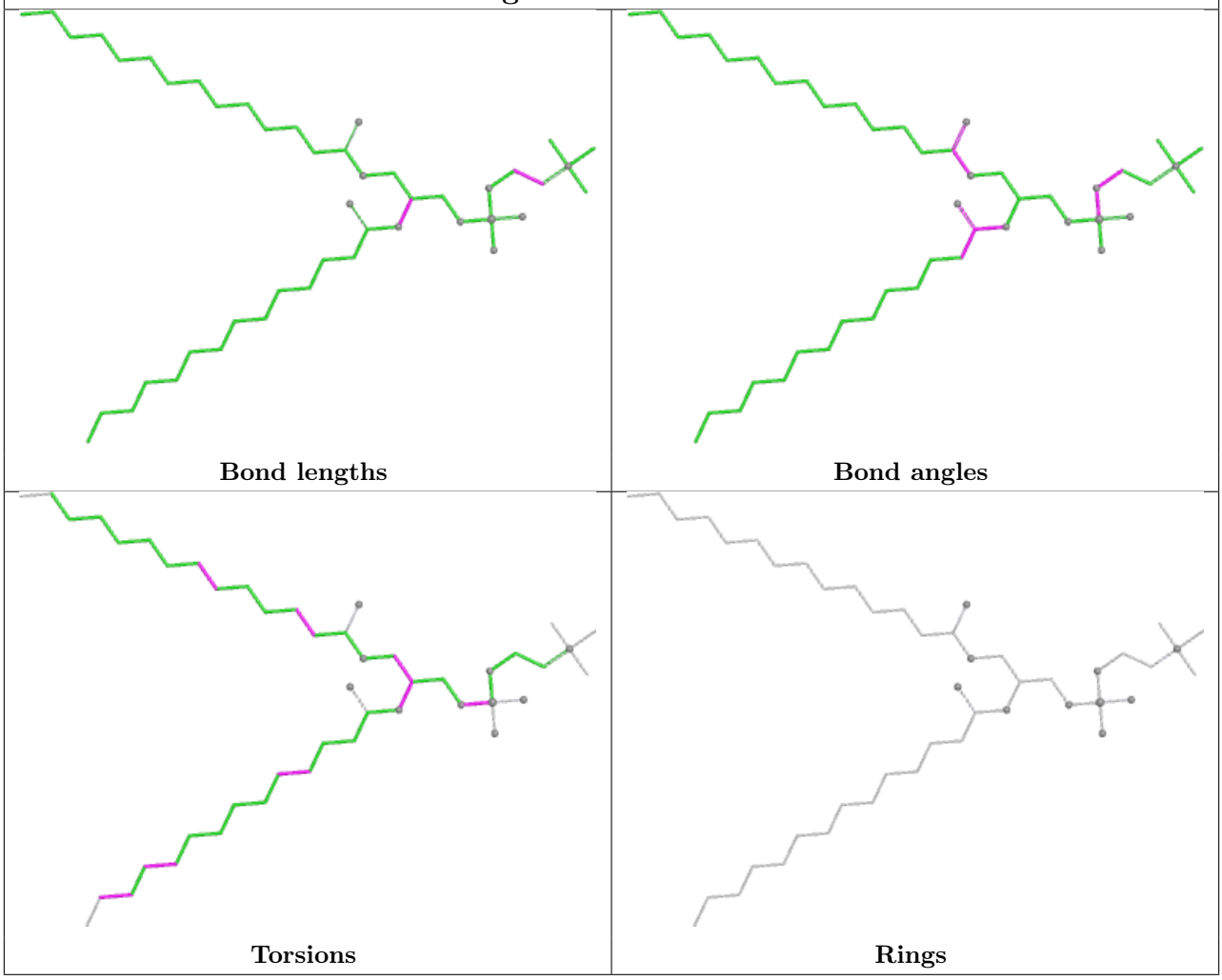


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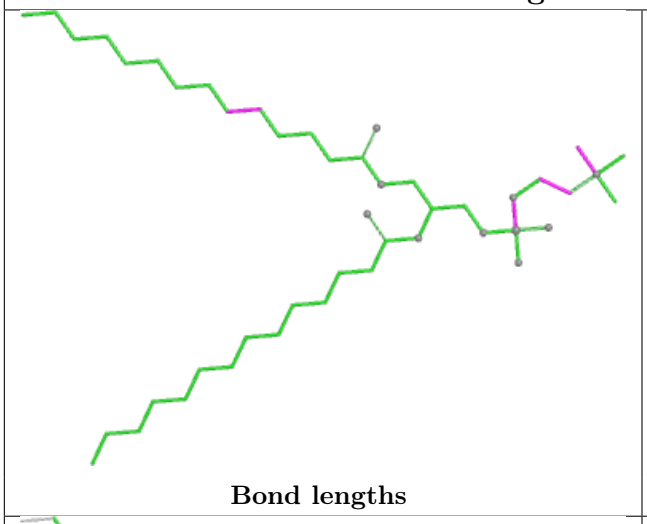
Ligand PX4 B 368



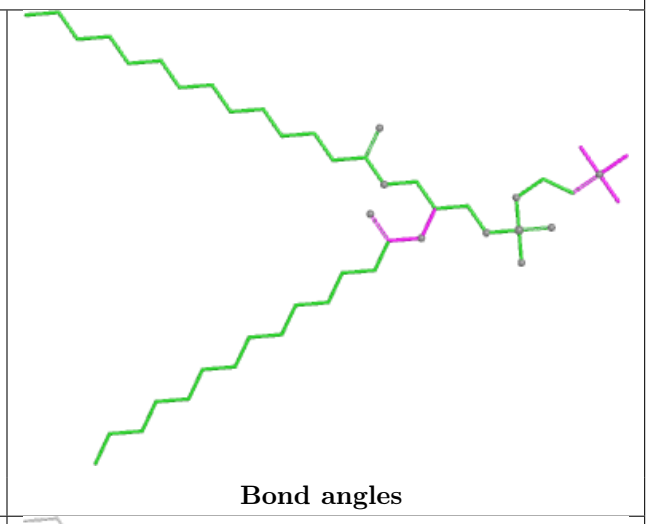
Ligand PX4 A 644



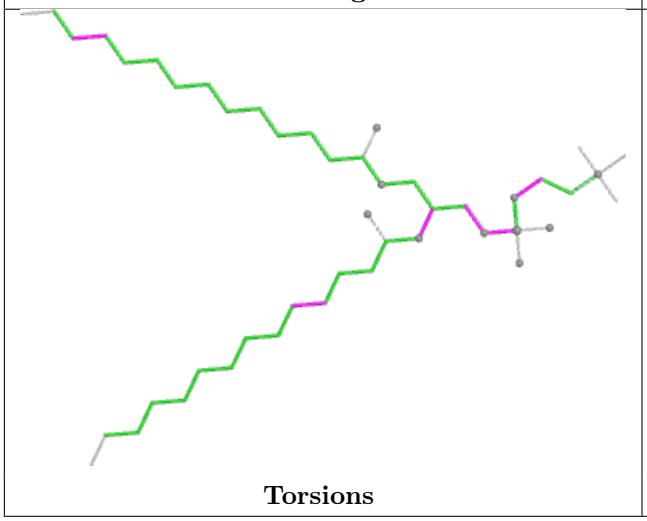
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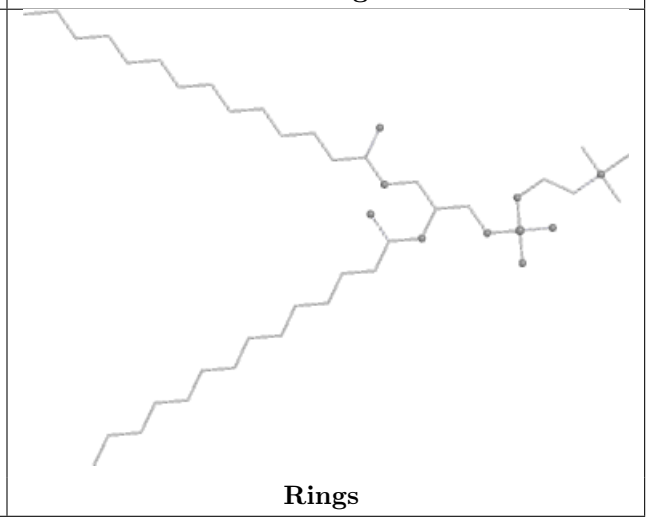
Bond lengths



Bond angles

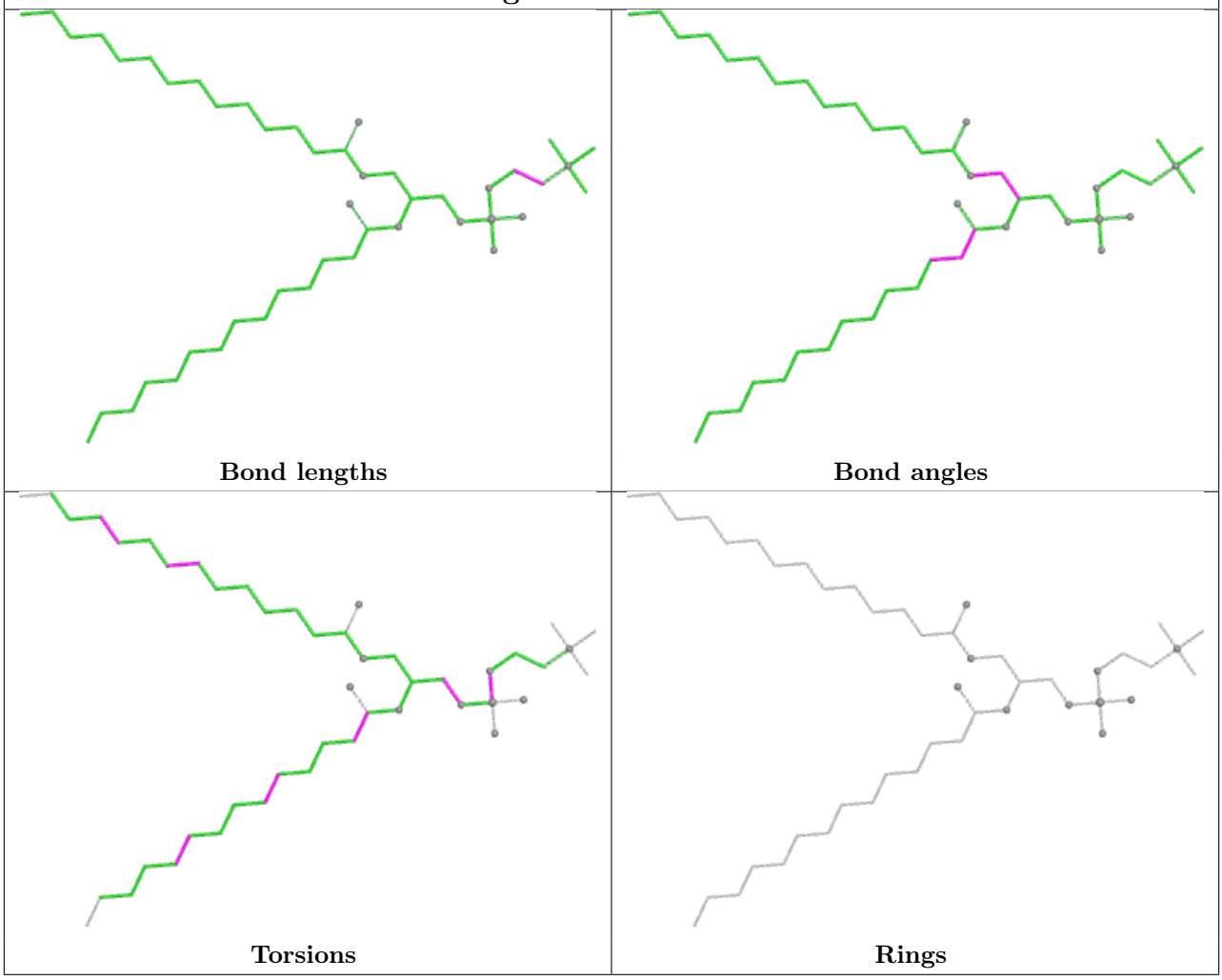


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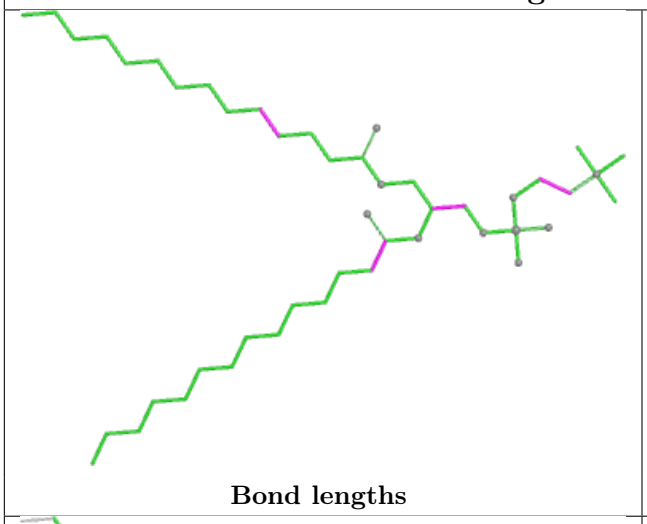


Rings

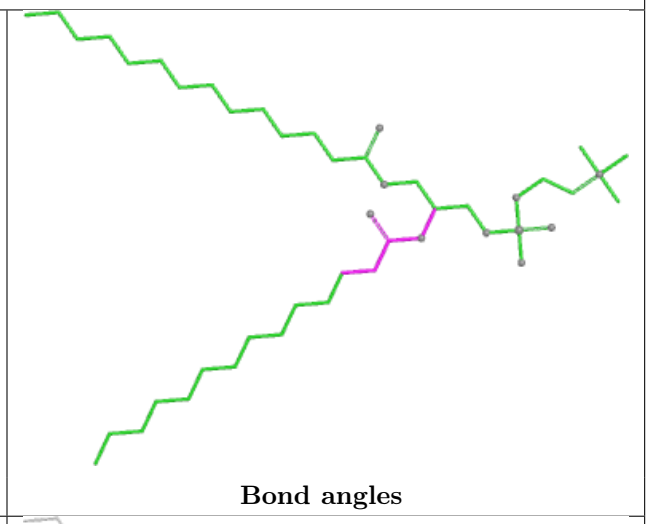
Ligand PX4 B 325



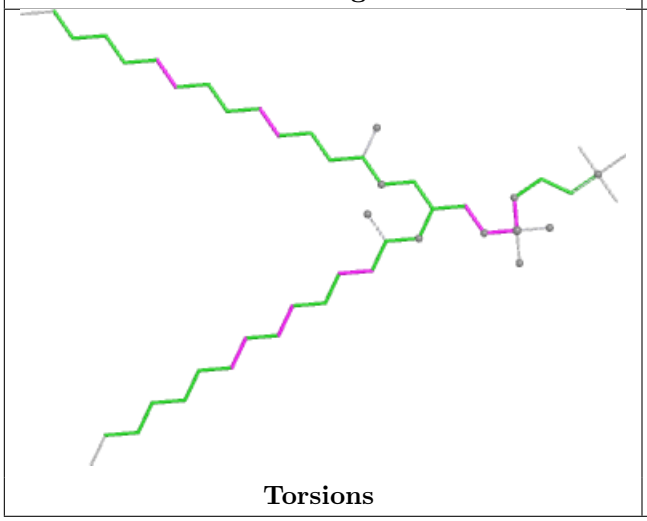
Ligand PX4 C 325



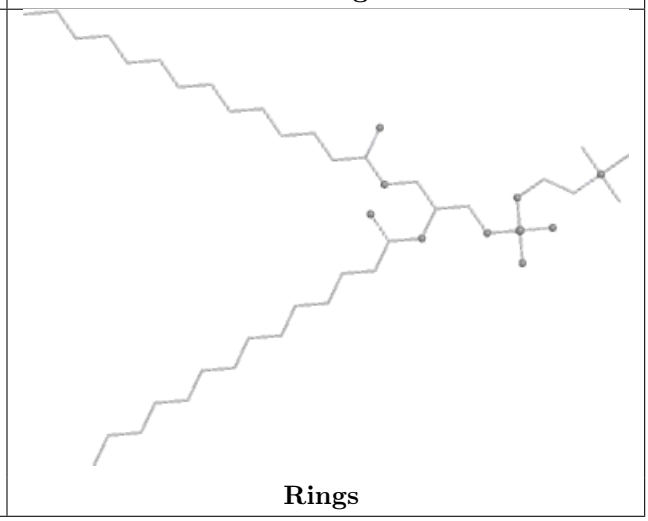
Bond lengths



Bond angles

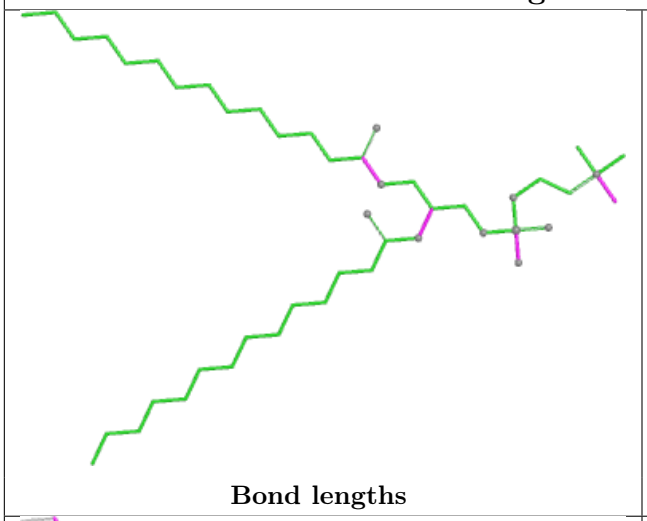


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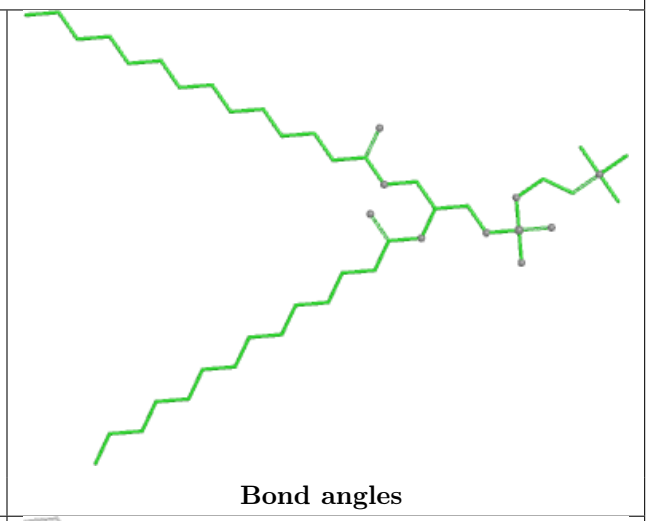


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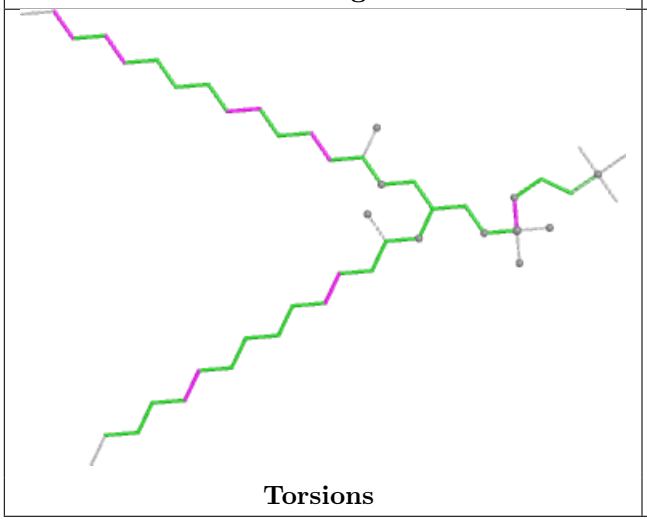
Ligand PX4 B 323



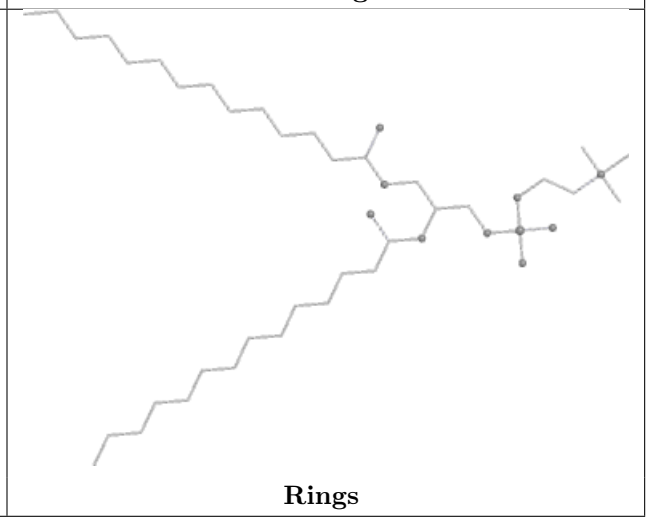
Bond lengths



Bond angles

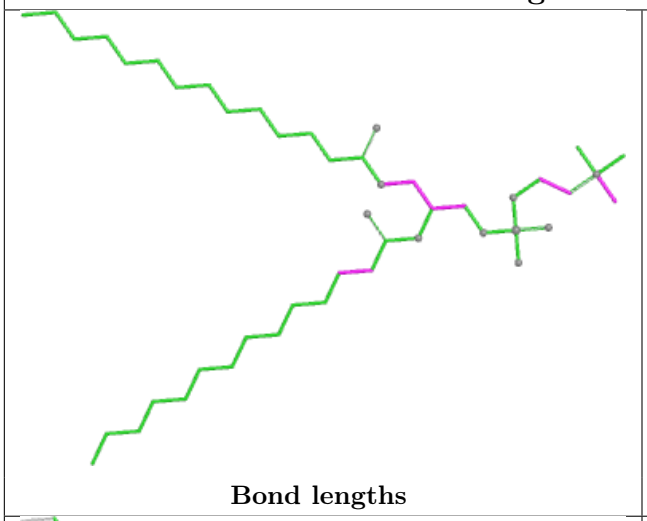


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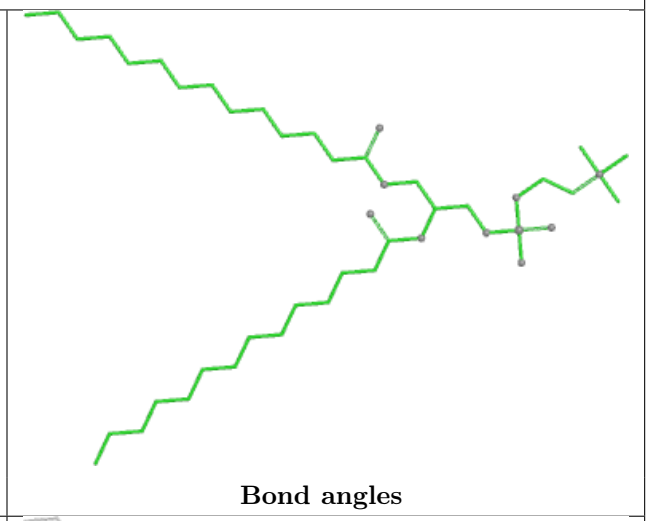


Rings

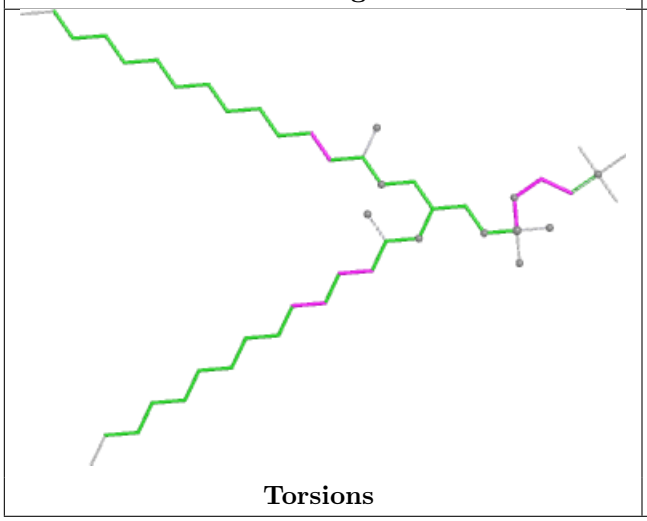
Ligand PX4 C 303



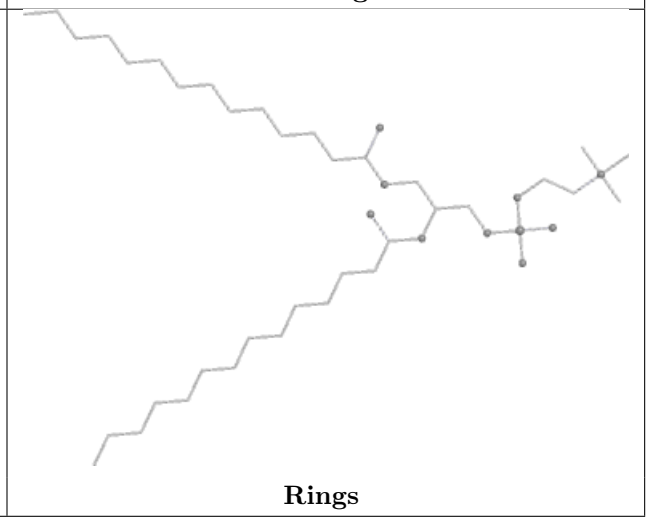
Bond lengths



Bond angles

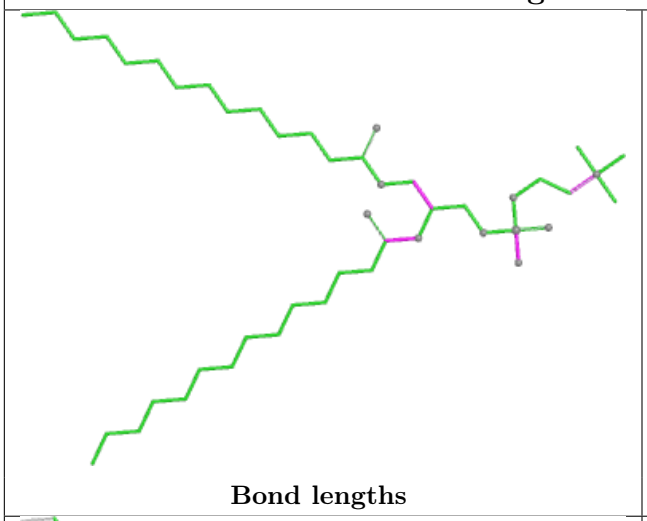


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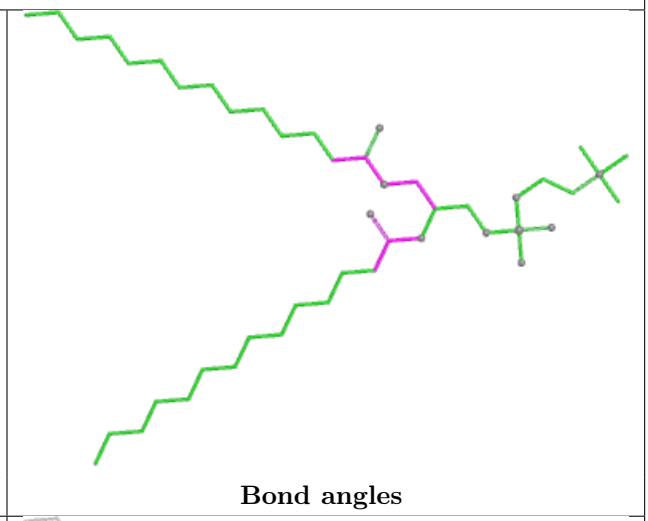


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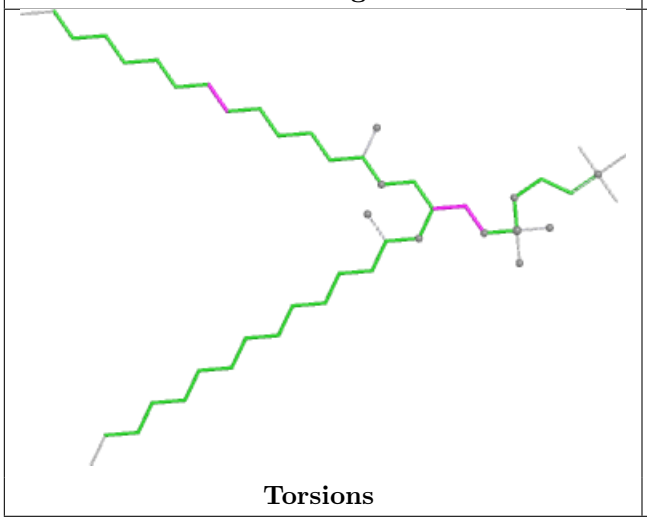
Ligand PX4 A 631



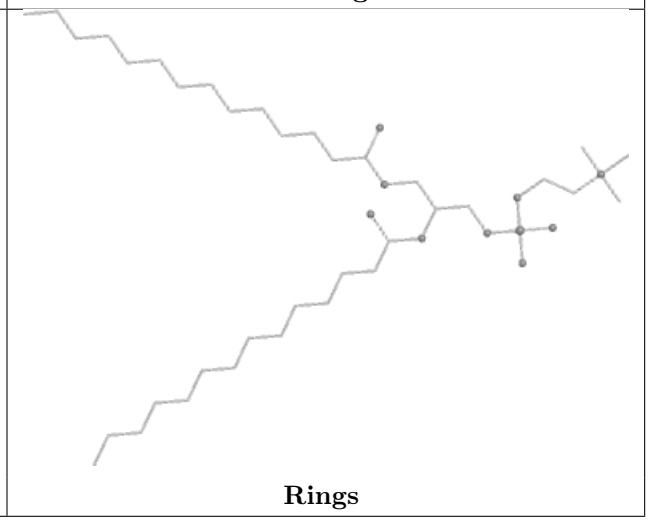
Bond lengths



Bond angles

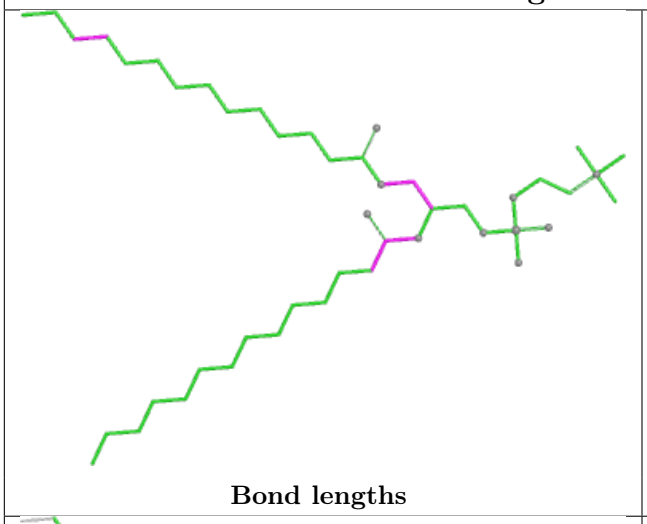


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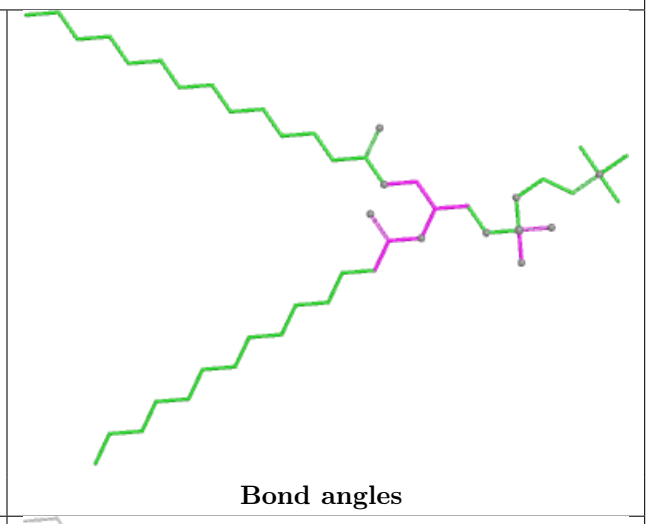


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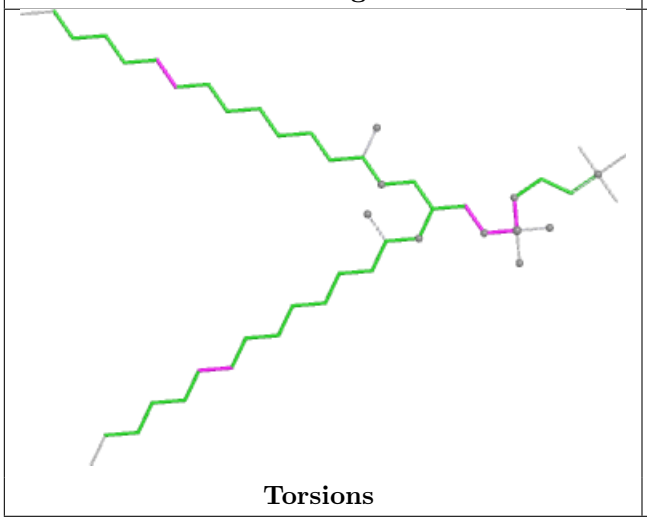
Ligand PX4 C 333



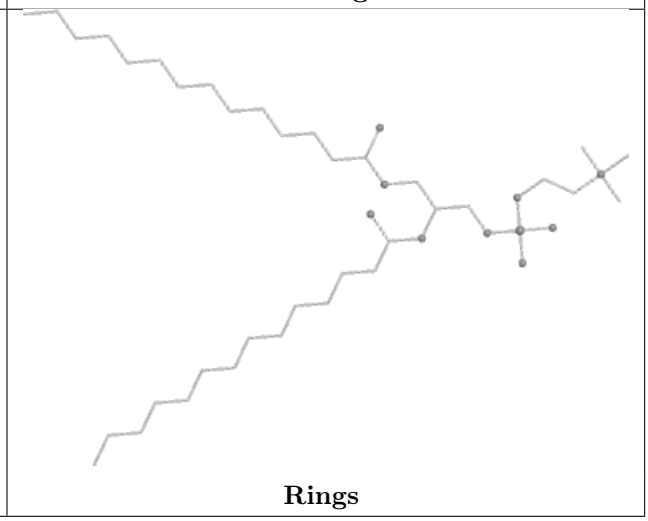
Bond lengths



Bond angles

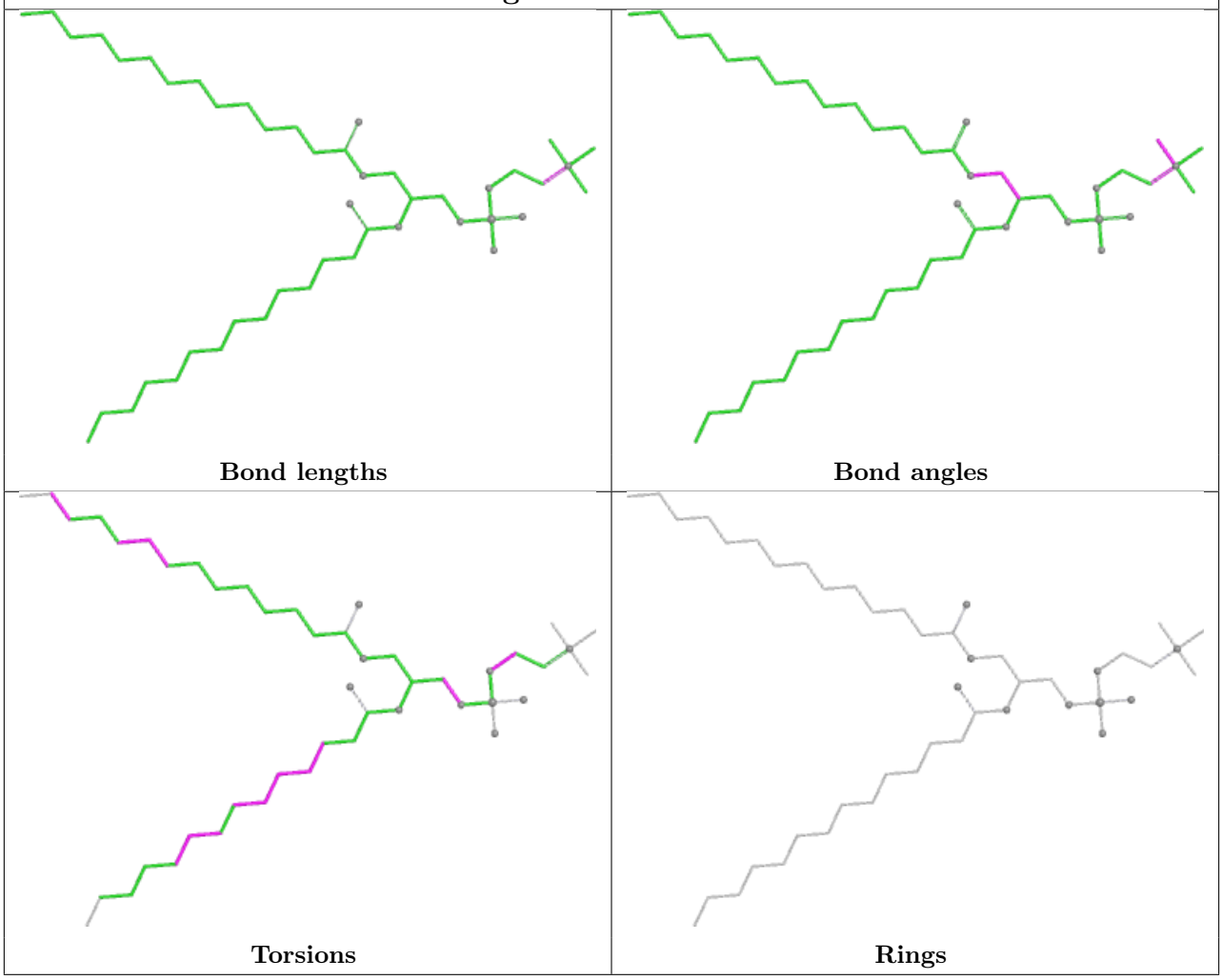


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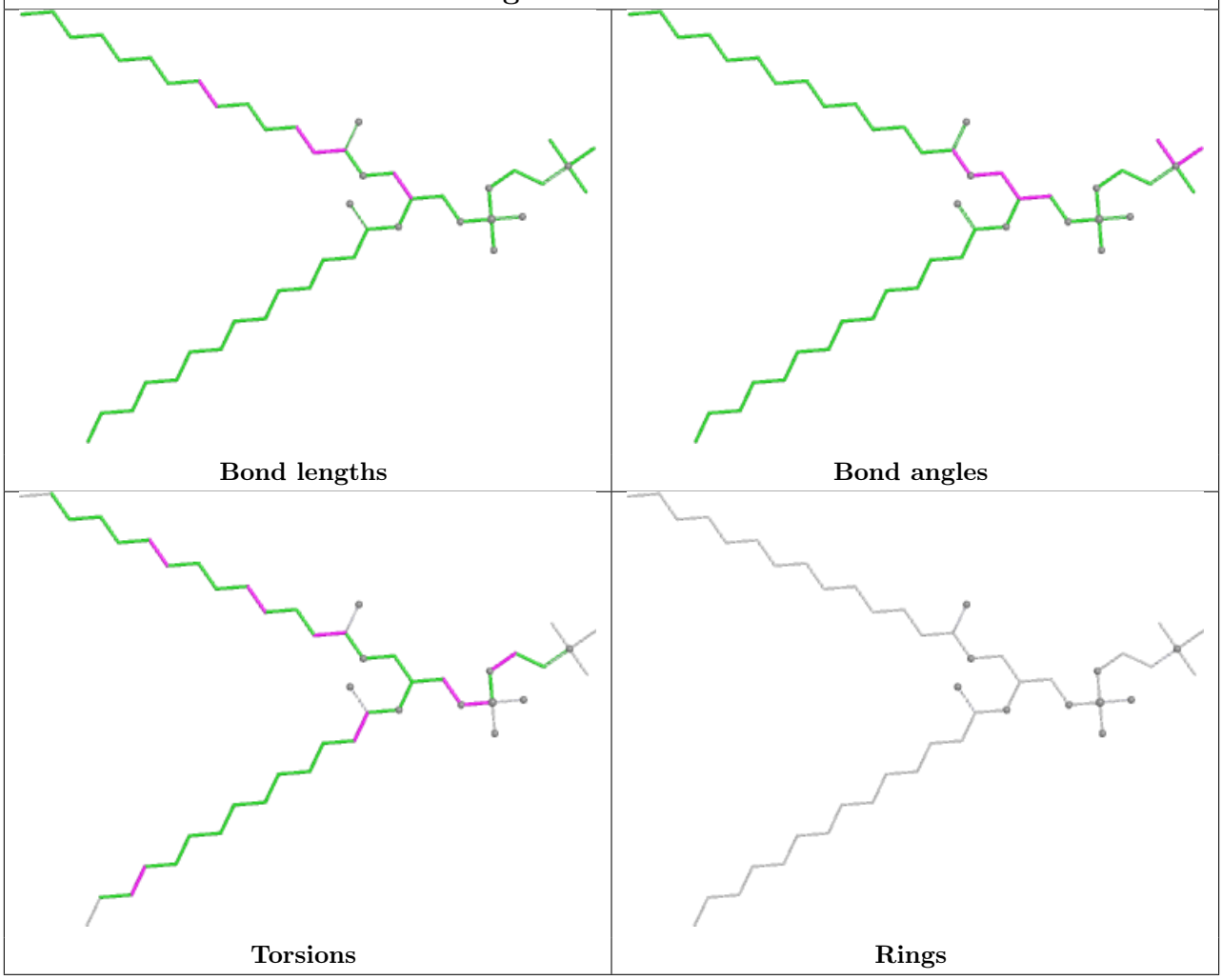


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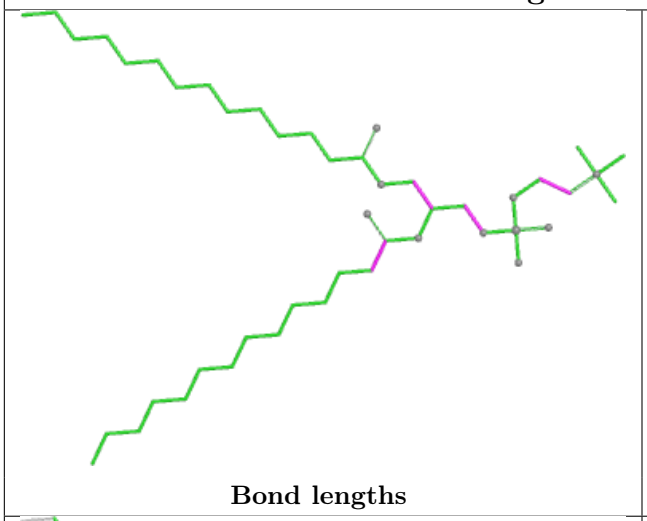
Ligand PX4 B 351



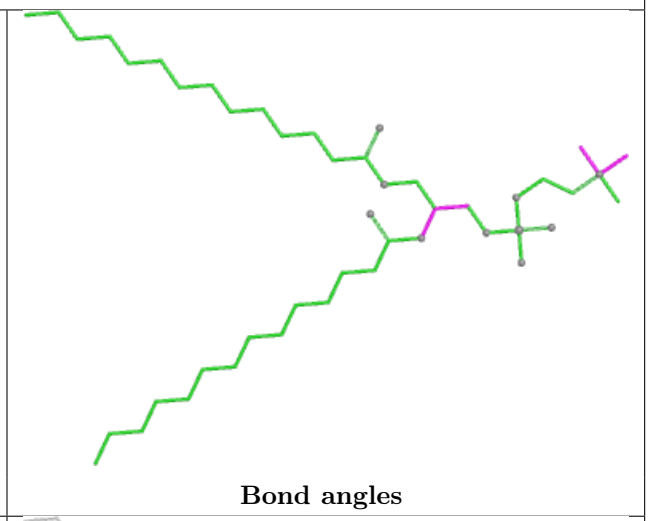
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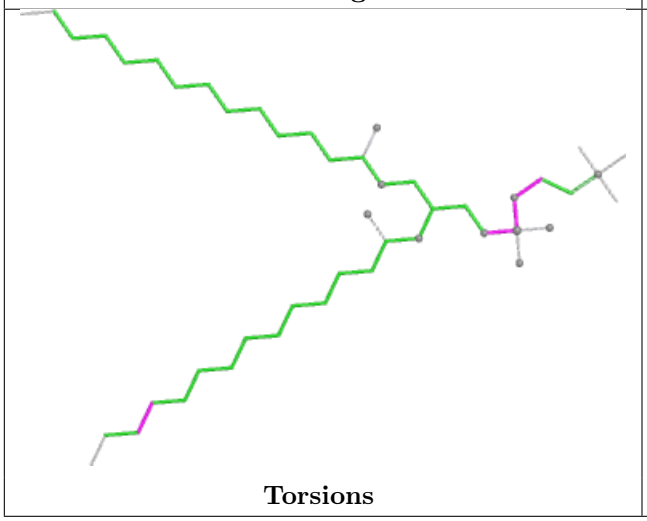
Ligand PX4 A 602



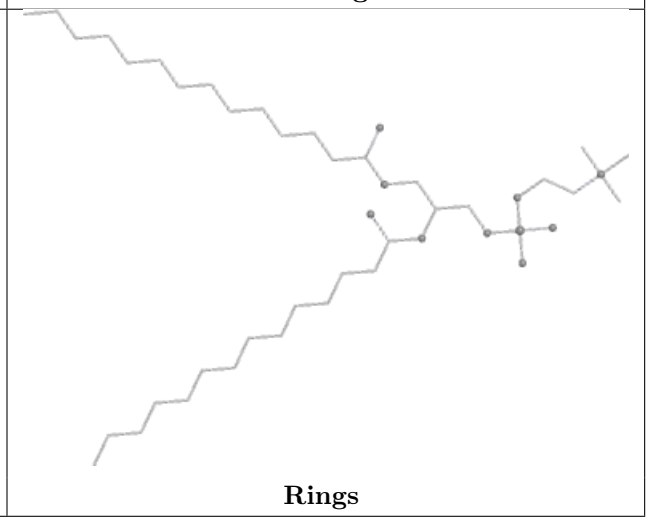
Bond lengths



Bond angles

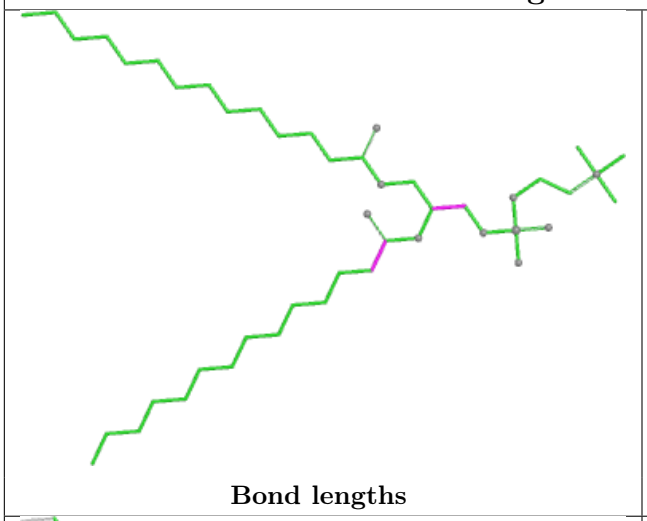


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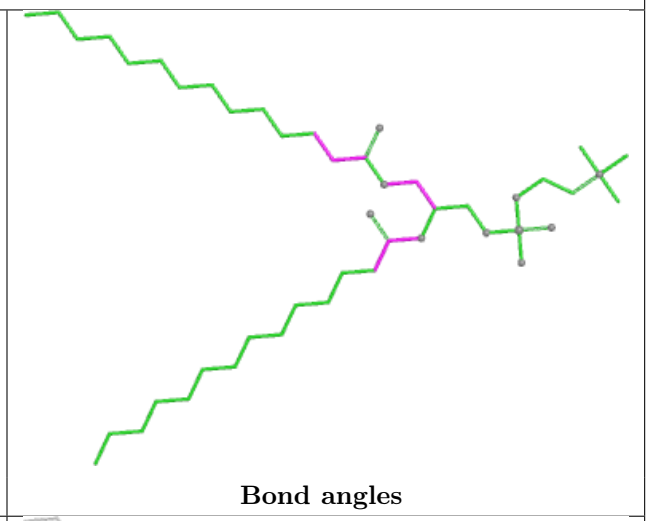


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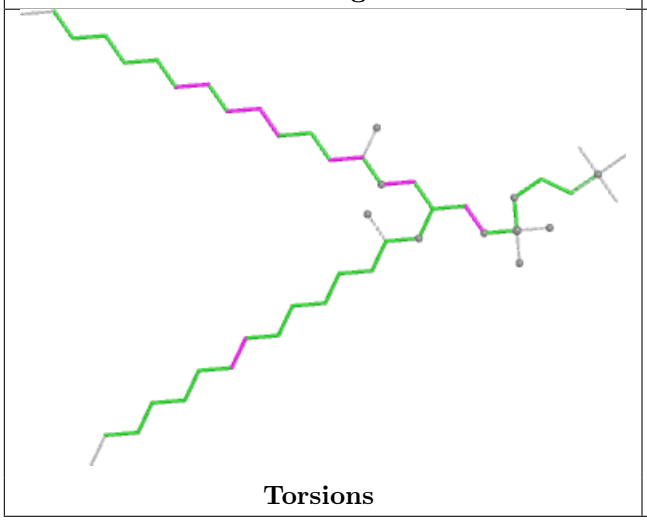
Ligand PX4 A 620



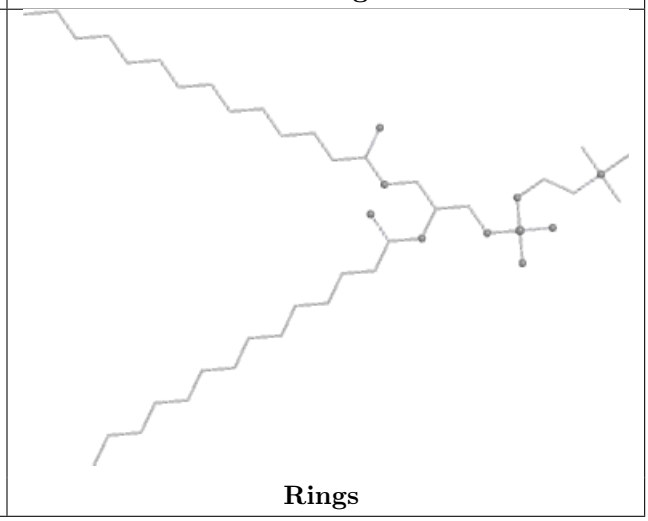
Bond lengths



Bond angles

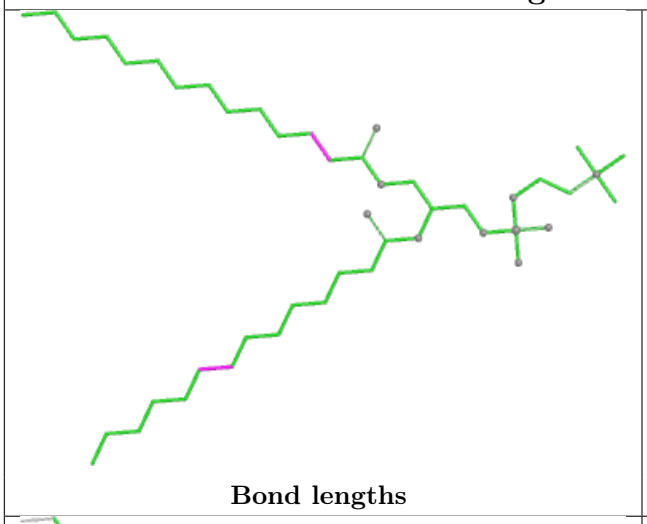


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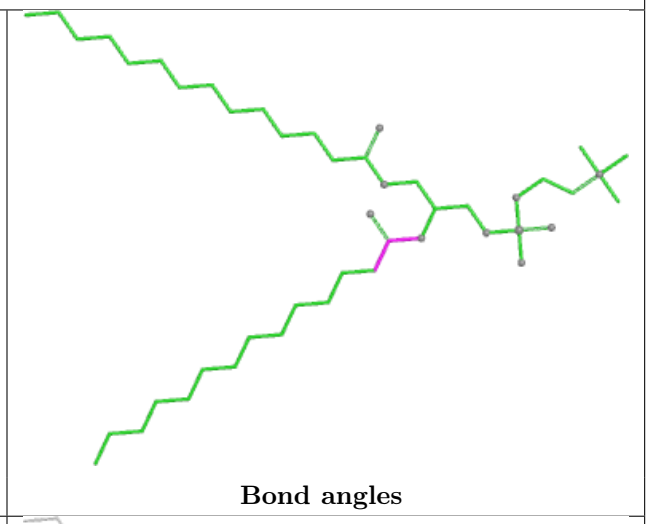


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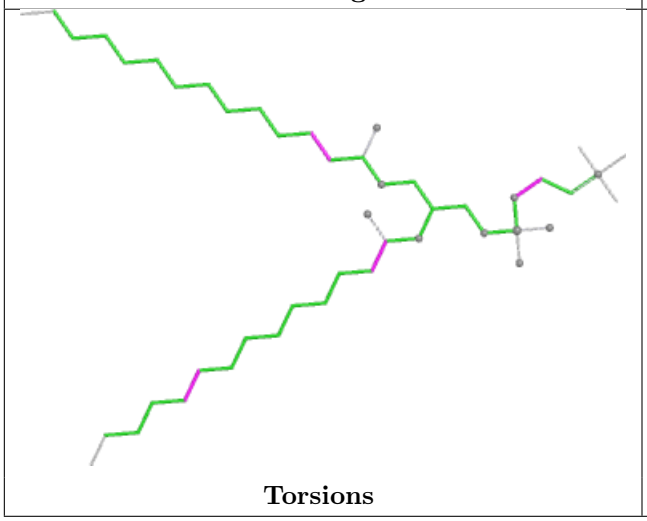
Ligand PX4 B 364



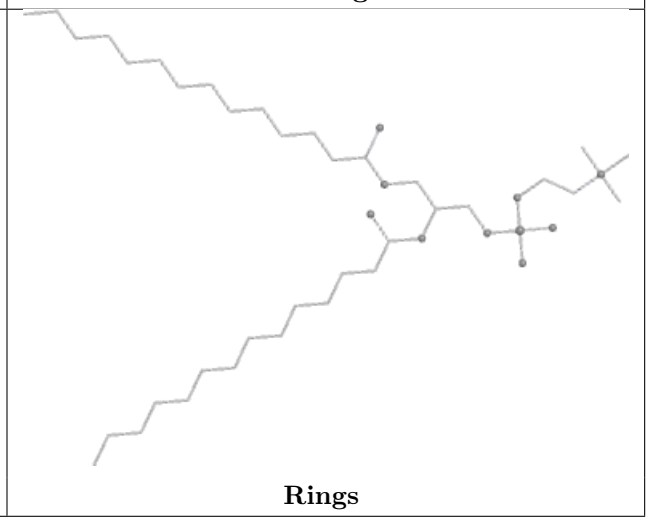
Bond lengths



Bond angles

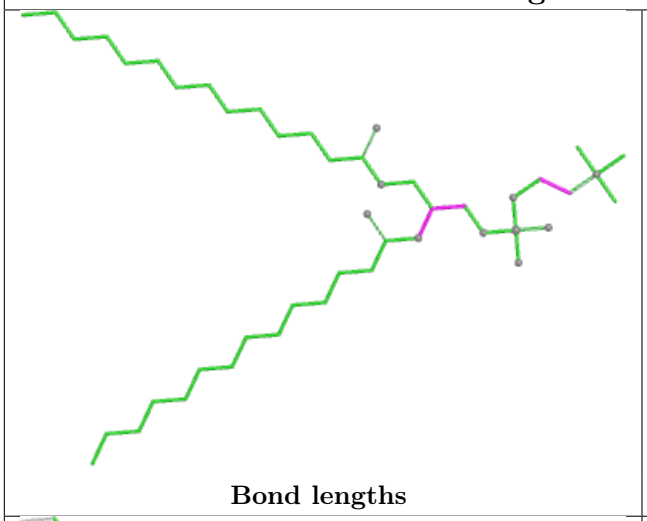


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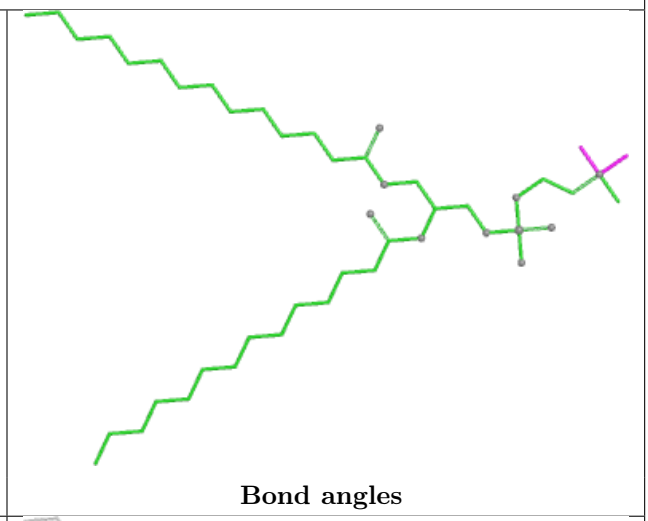


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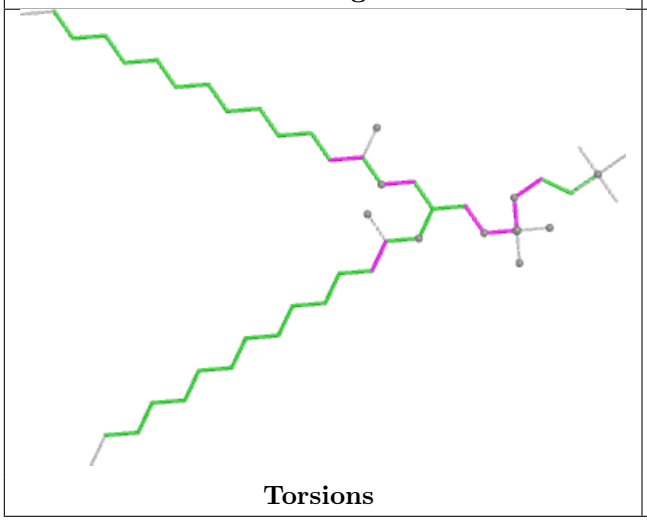
Ligand PX4 B 363



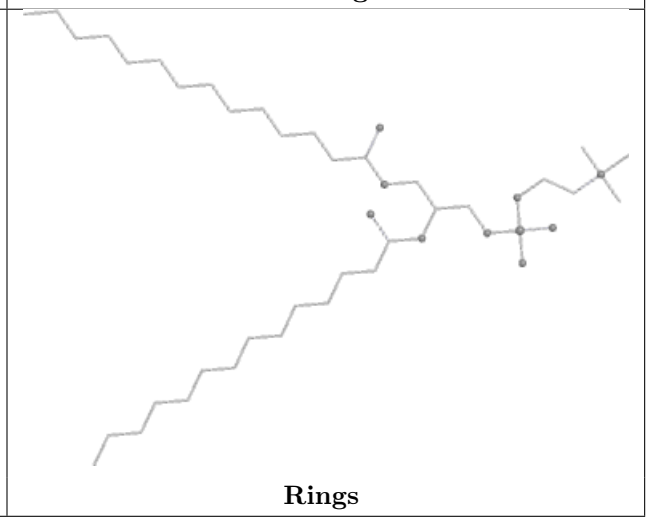
Bond lengths



Bond angles

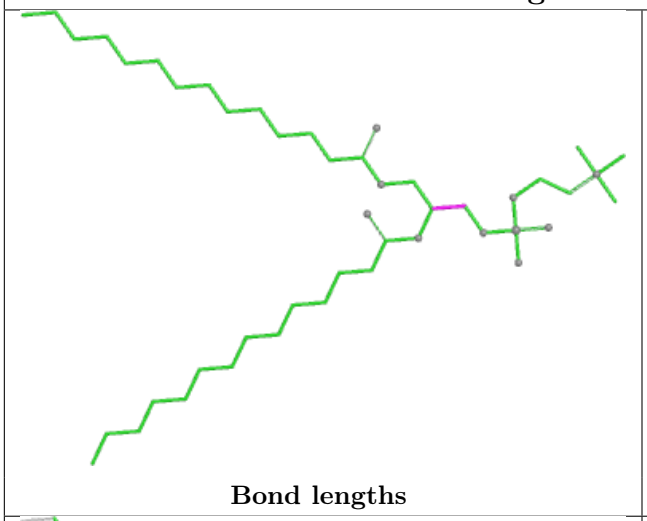


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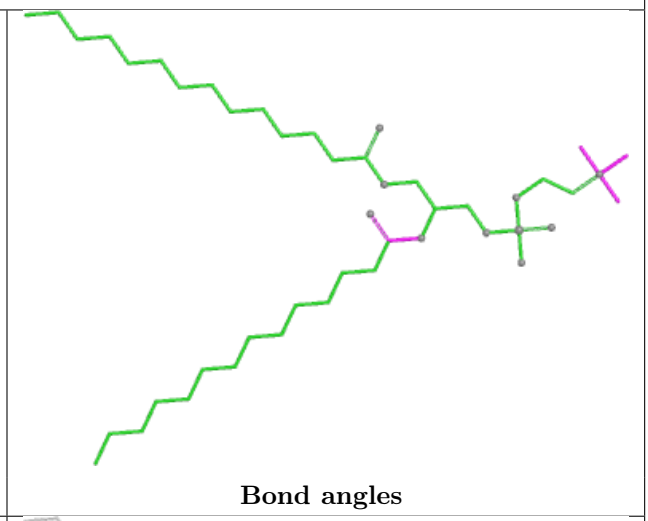


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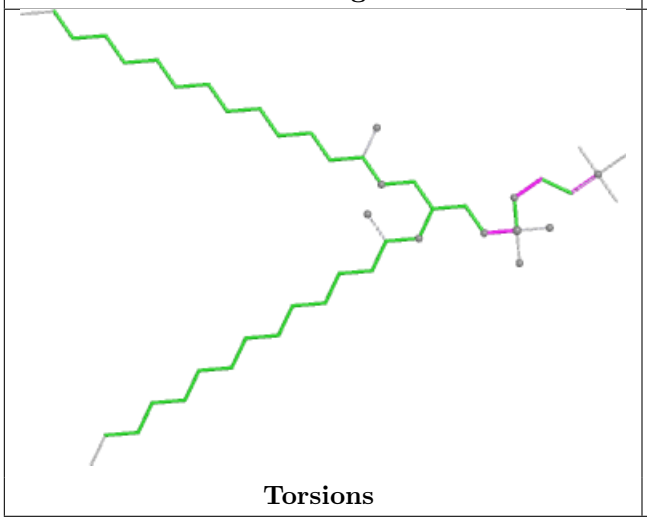
Ligand PX4 C 344



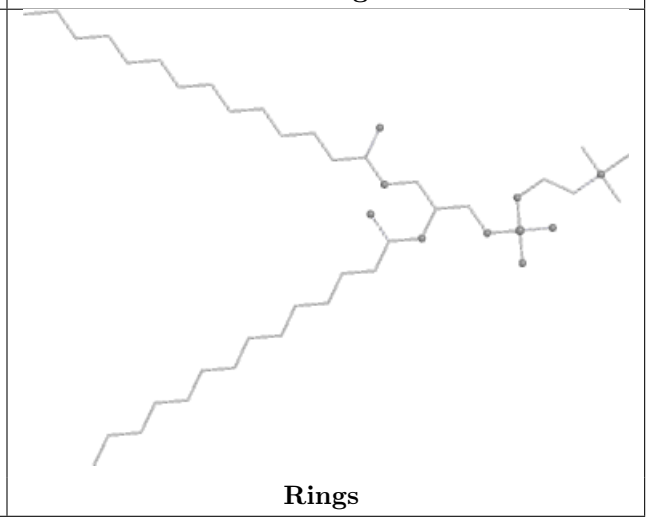
Bond lengths



Bond angles

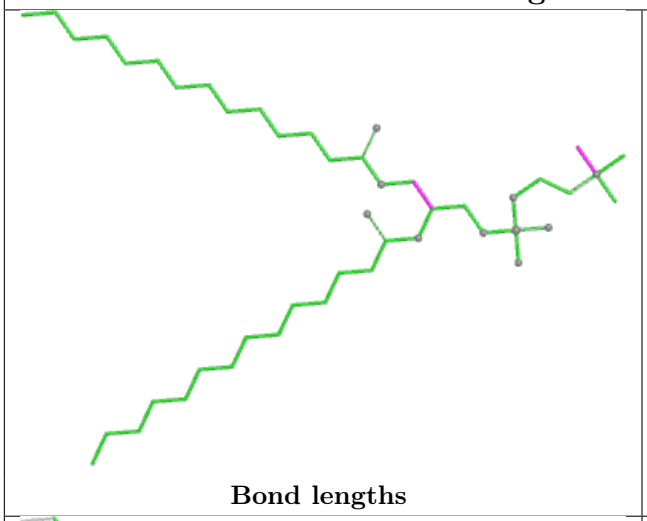


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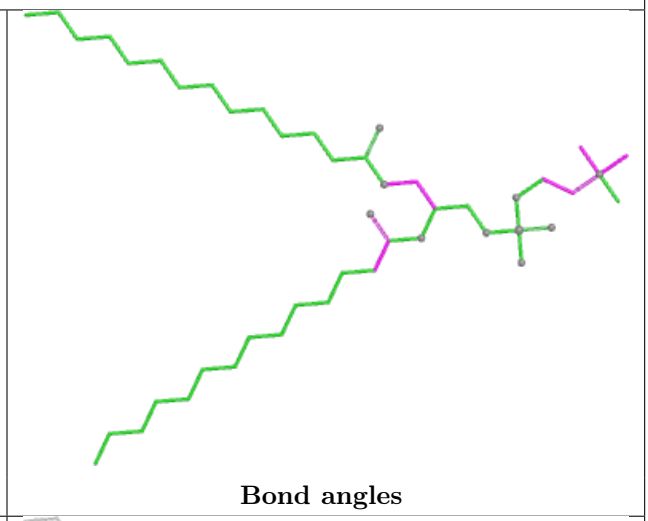


Rings

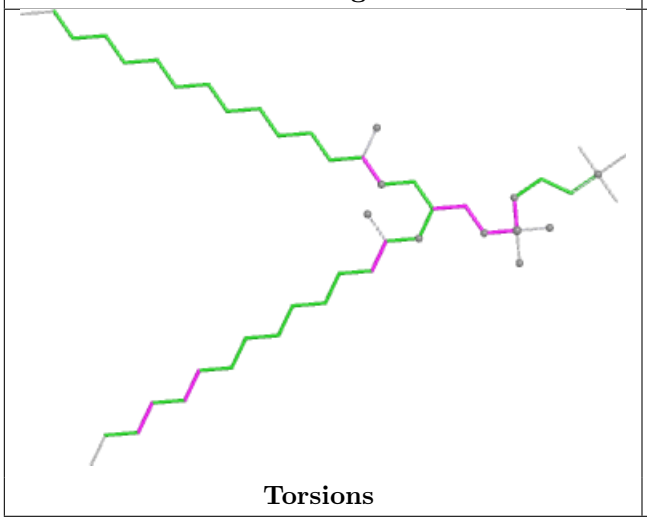
Ligand PX4 B 379



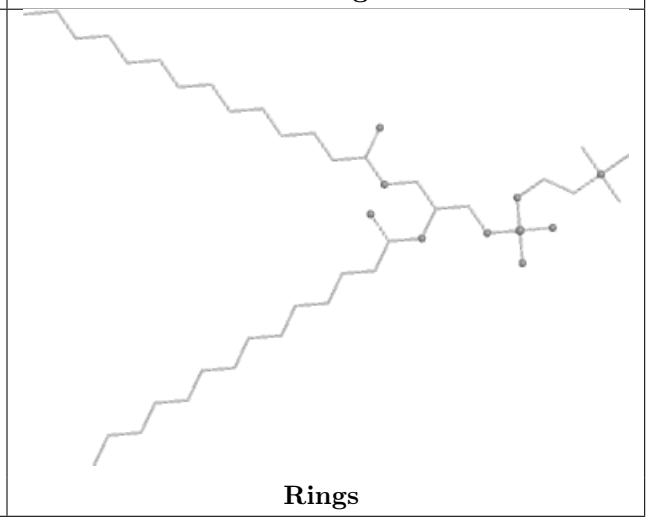
Bond lengths



Bond angles

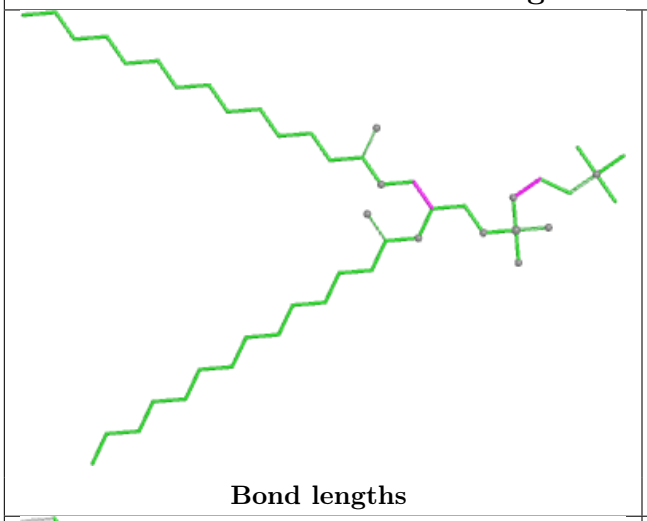


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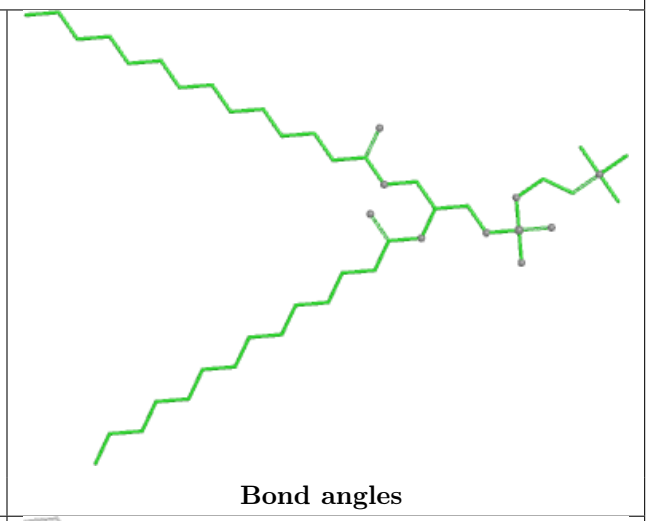


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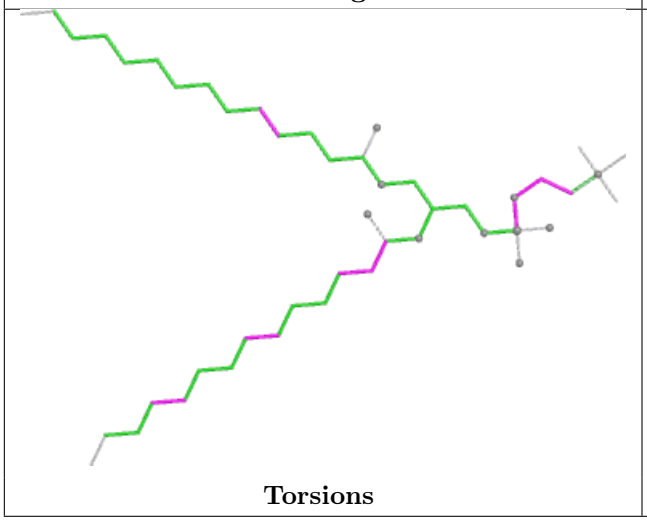
Ligand PX4 A 647



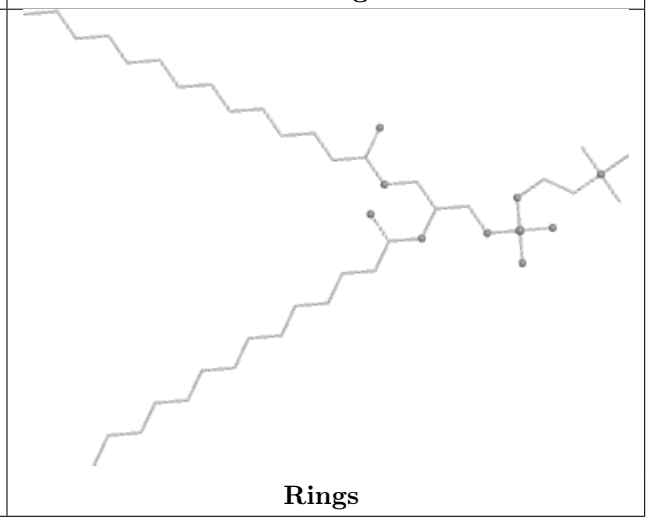
Bond lengths



Bond angles

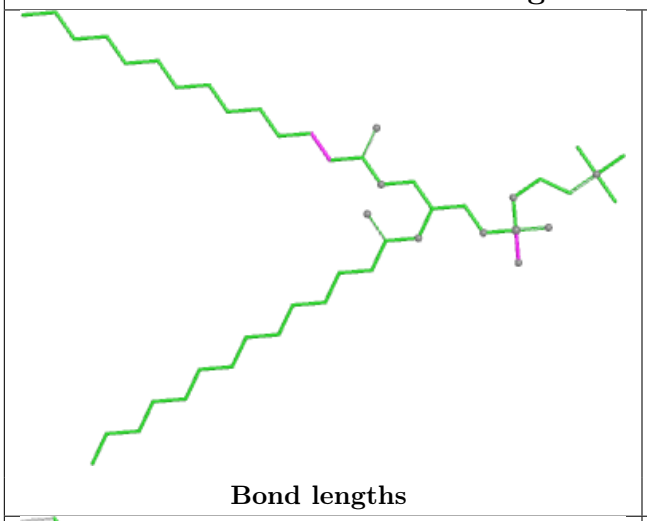


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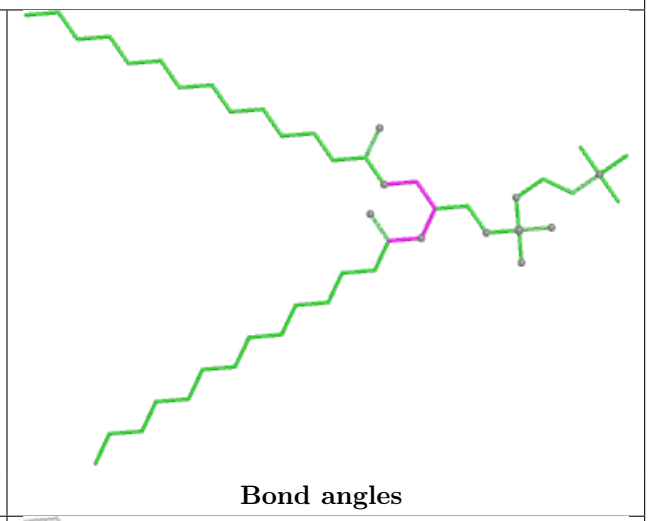


Rings

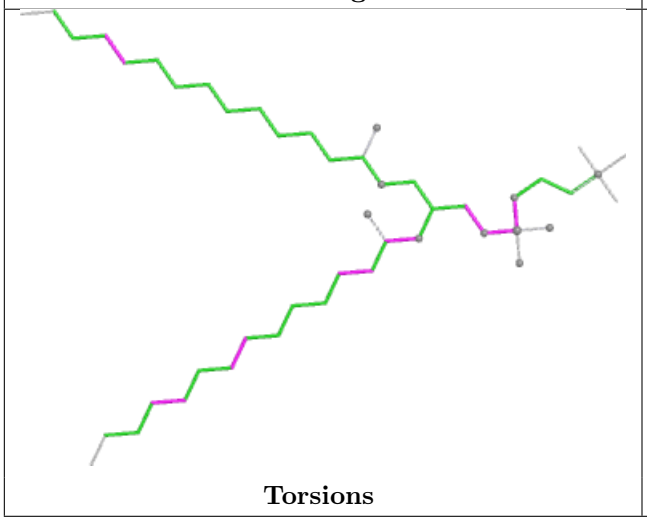
Ligand PX4 C 348



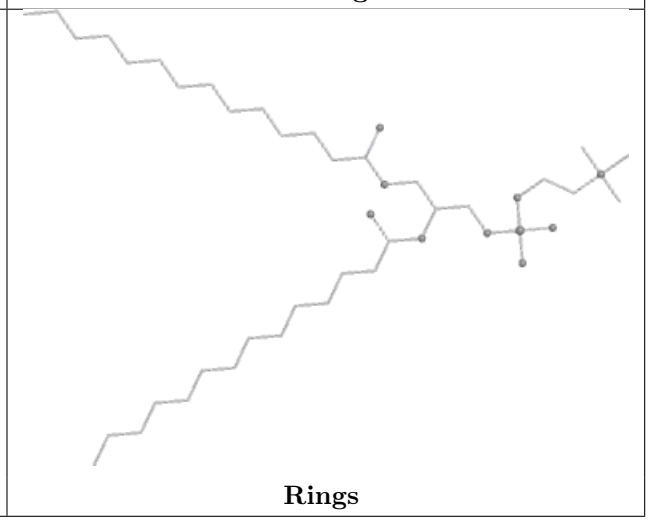
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Bond angles

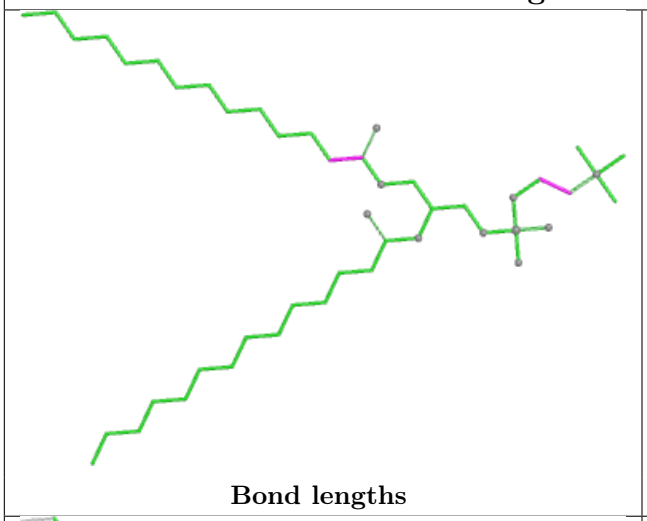


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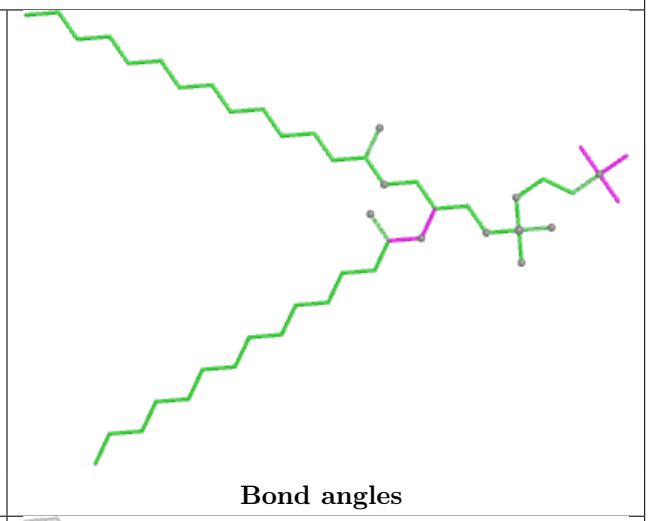


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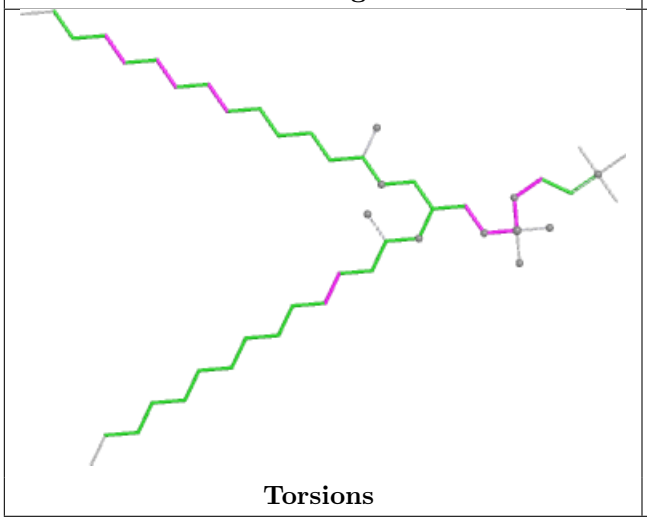
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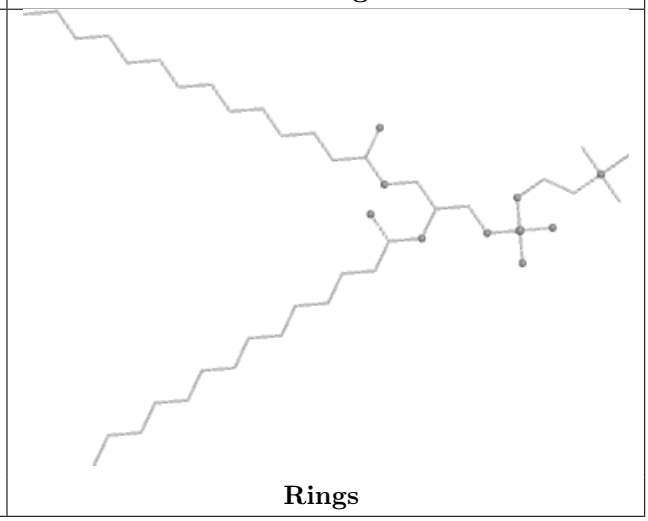
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Bond angles

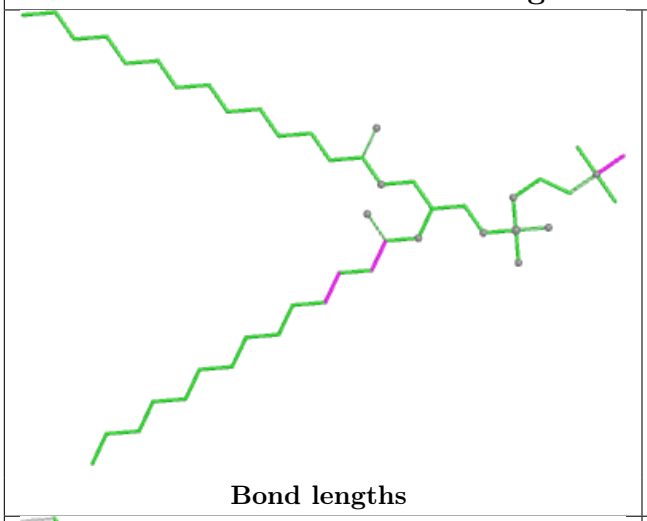


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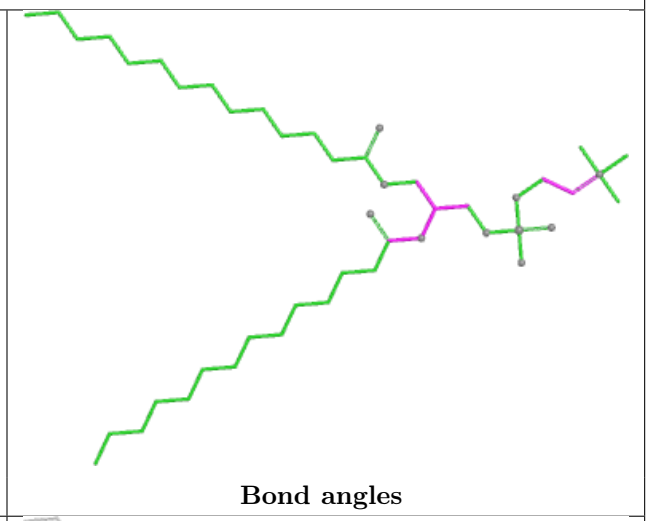


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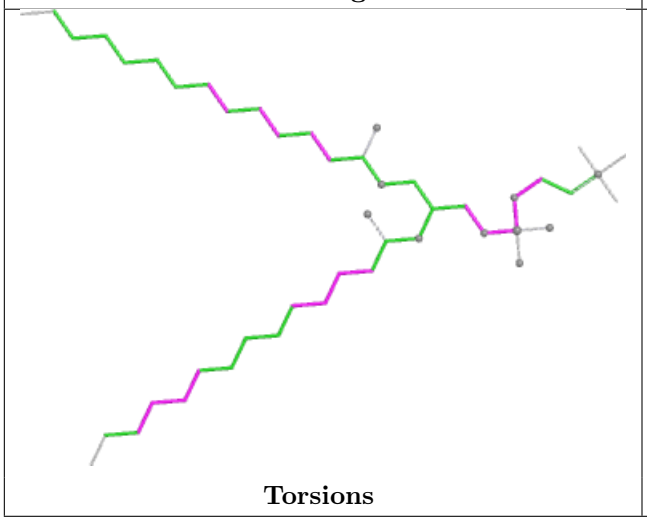
Ligand PX4 C 334



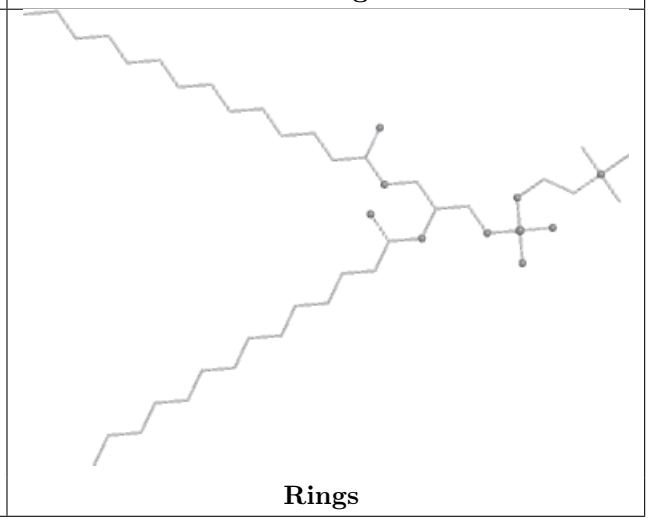
Bond lengths



Bond angles

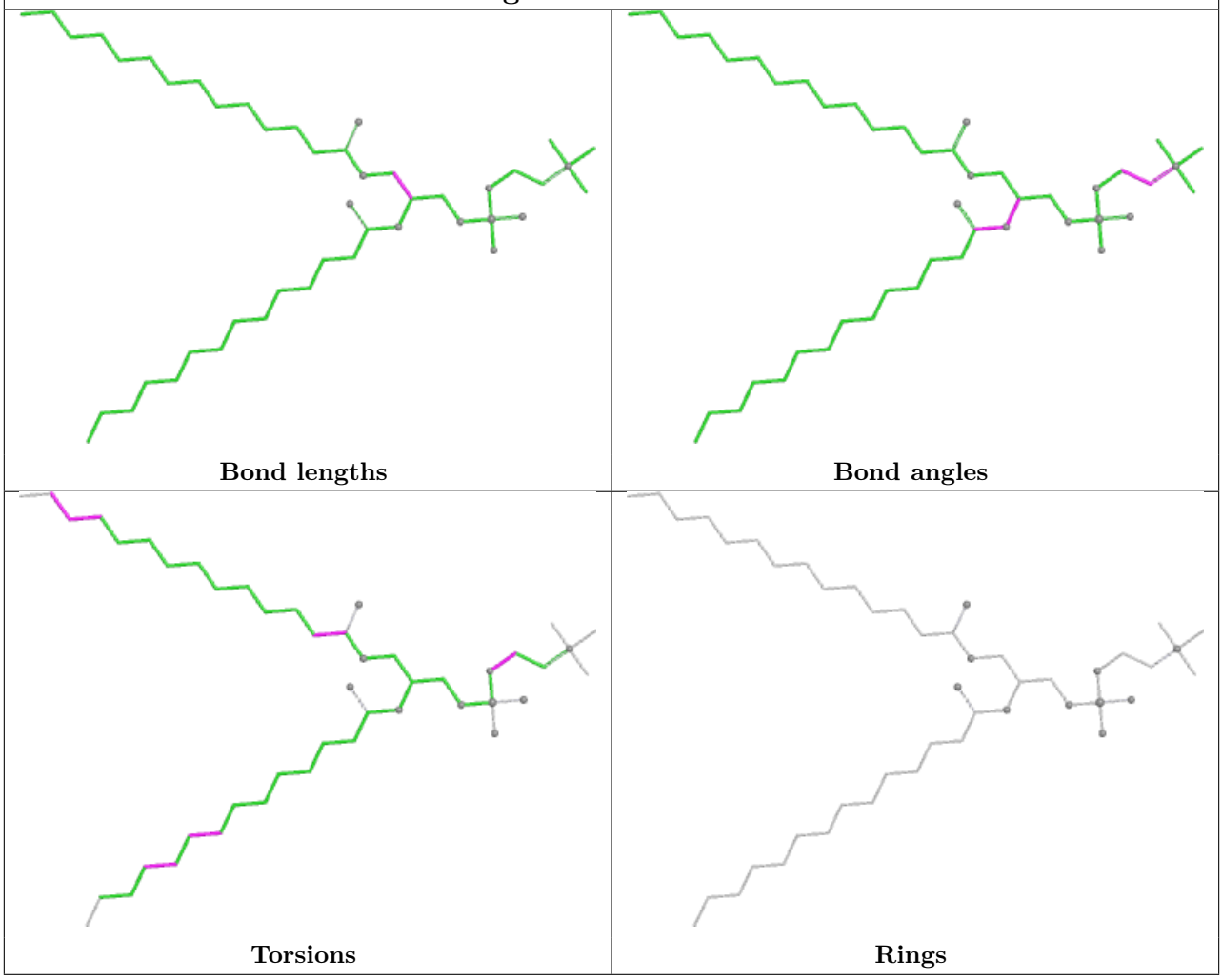


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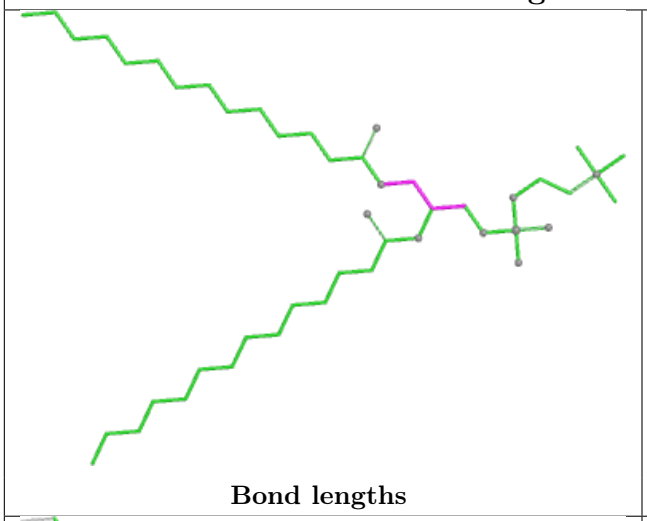


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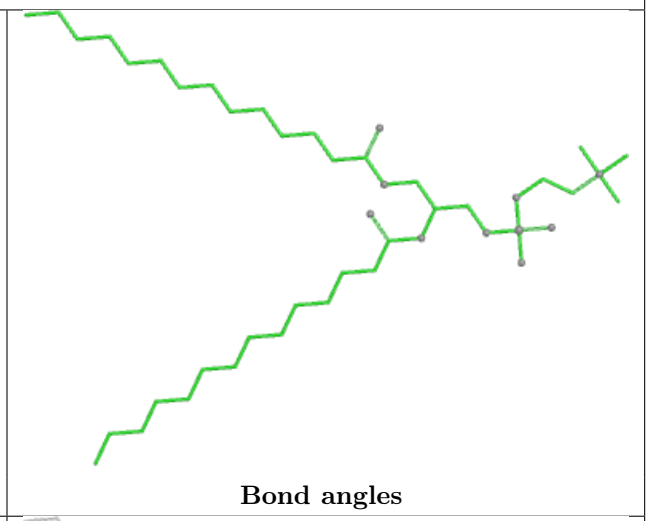
Ligand PX4 B 370



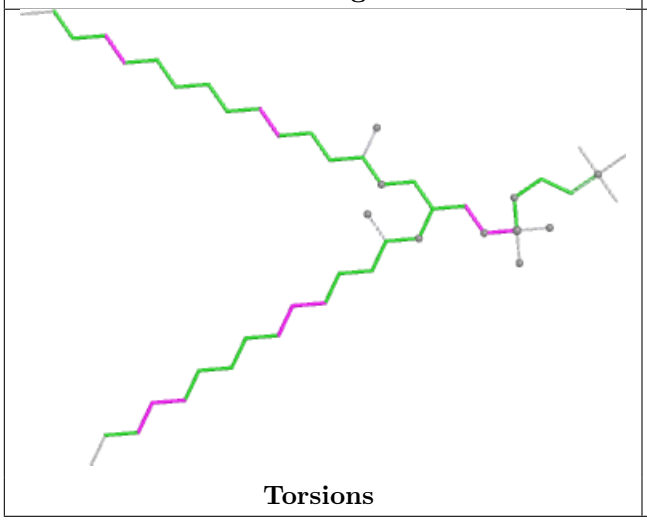
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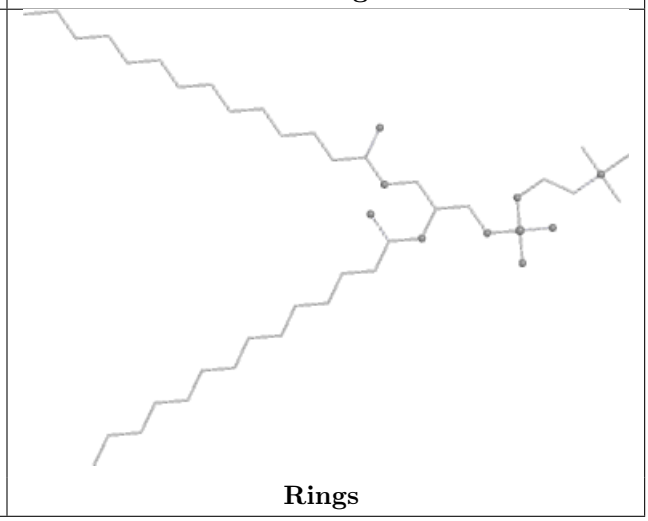
Bond lengths



Bond angles

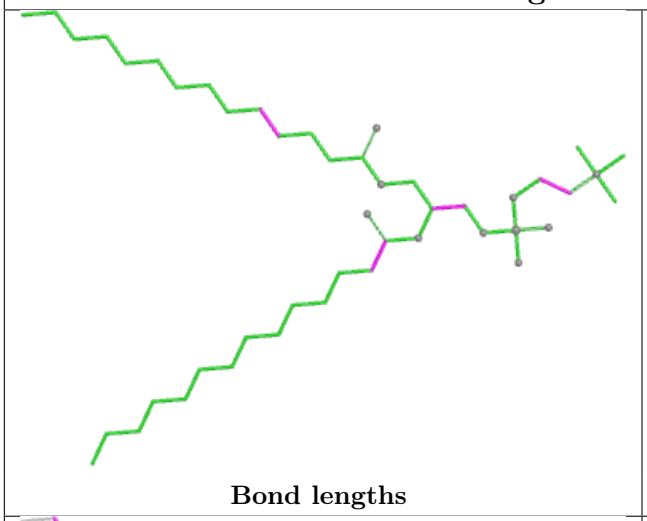


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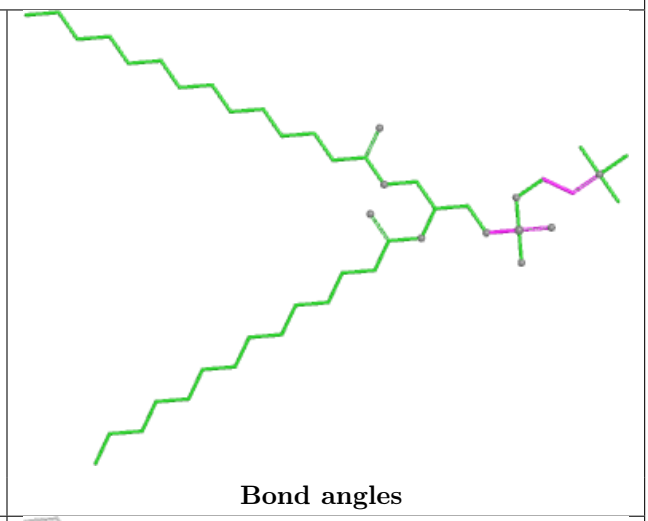


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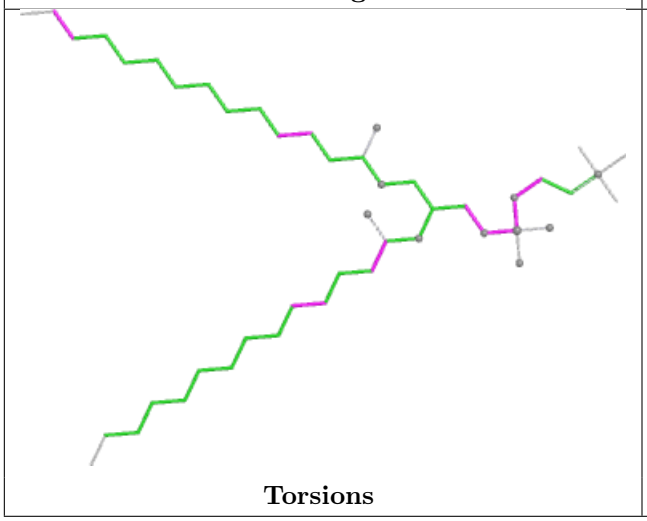
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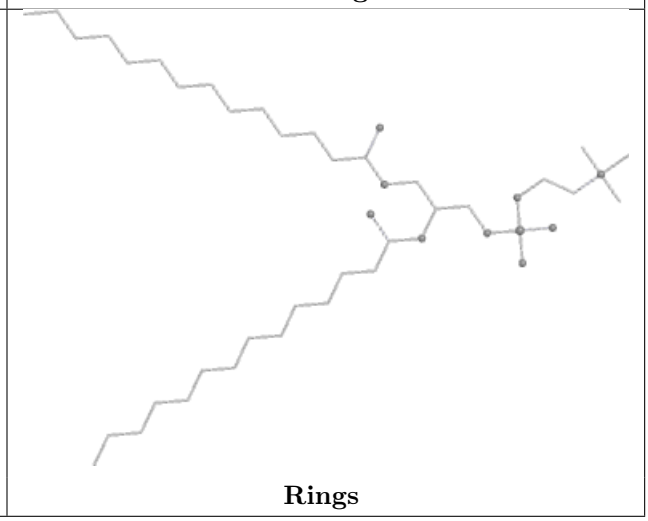
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Bond angles

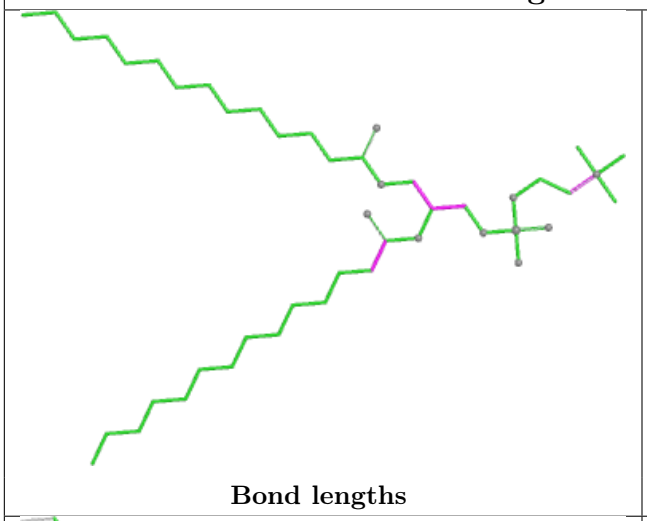


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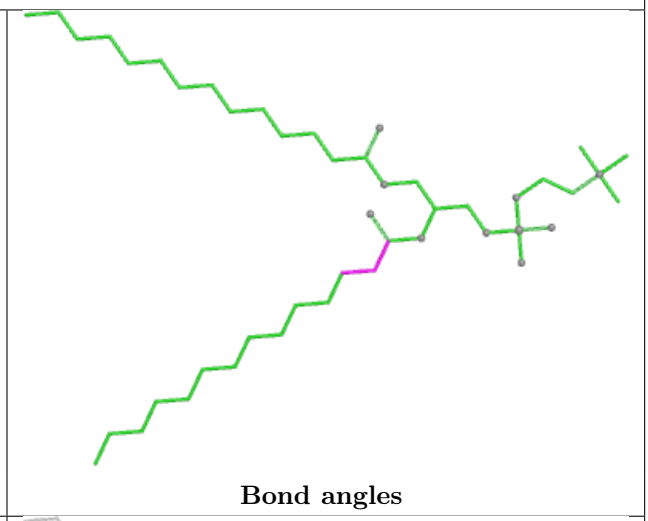


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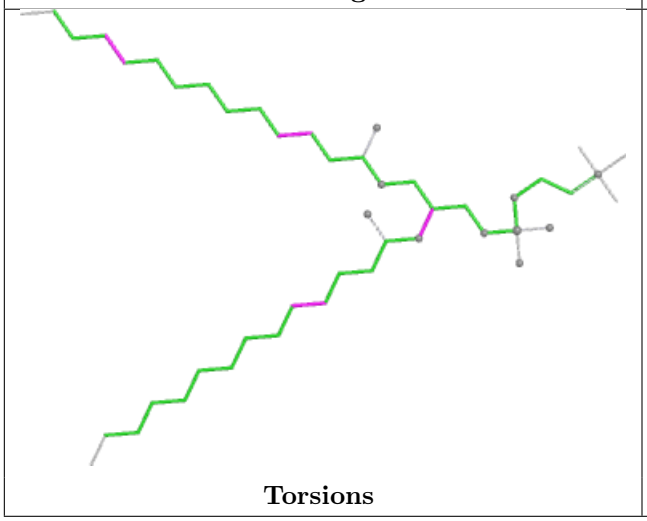
Ligand PX4 C 327



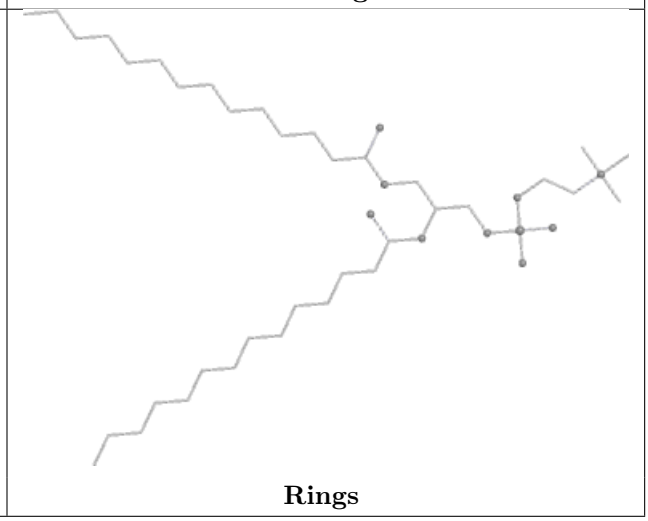
Bond lengths



Bond angles

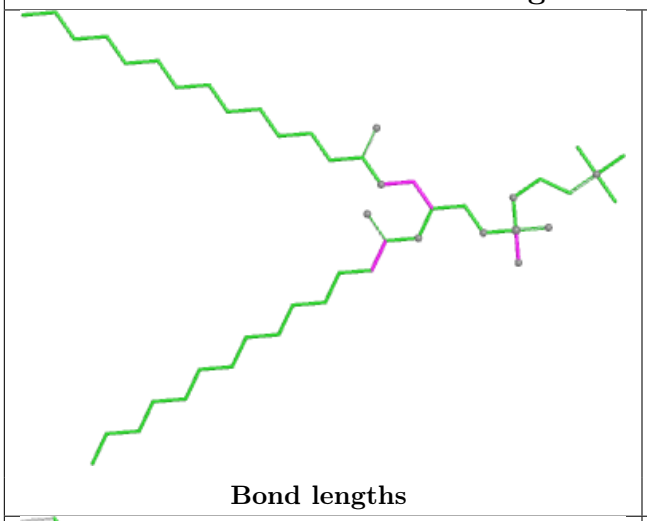


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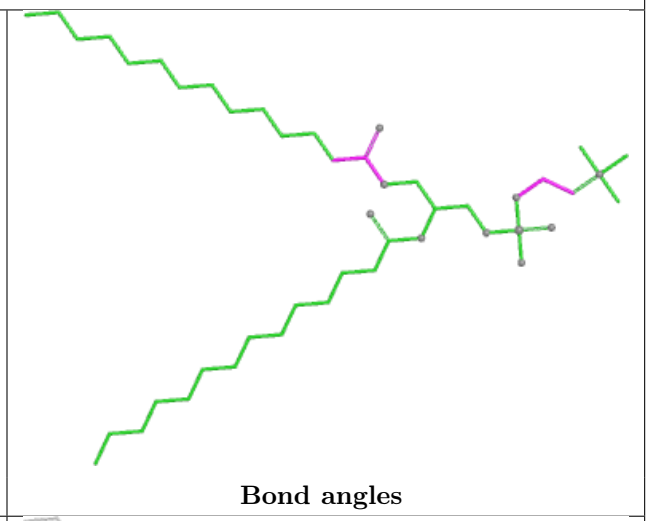


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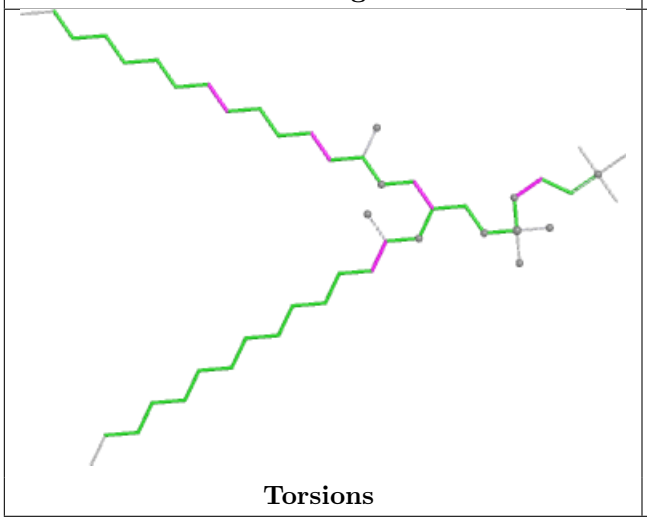
Ligand PX4 B 383



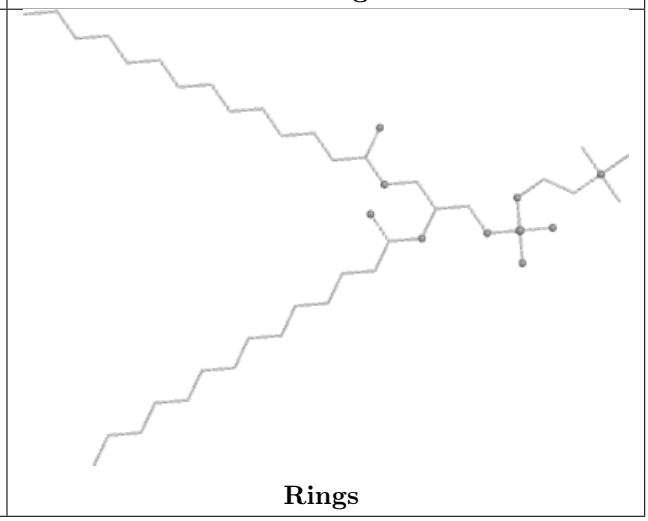
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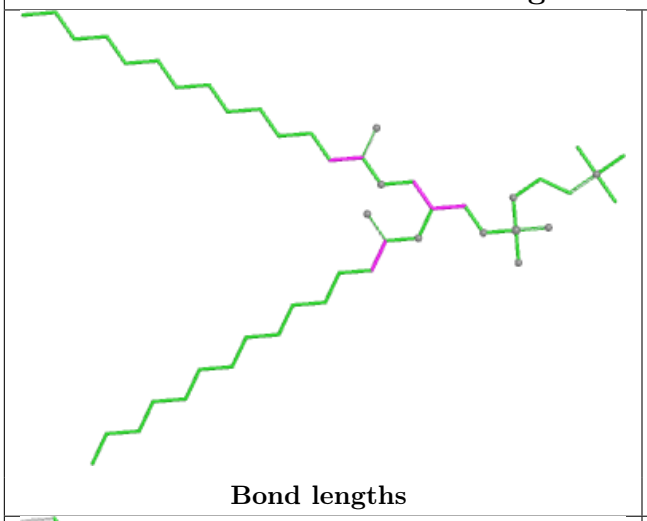


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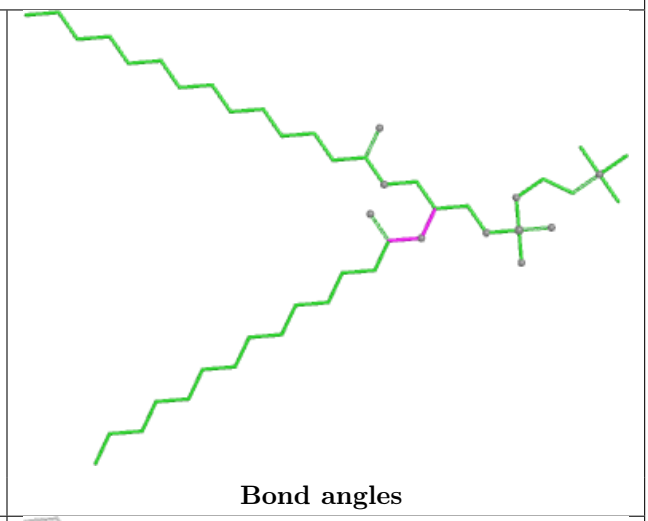


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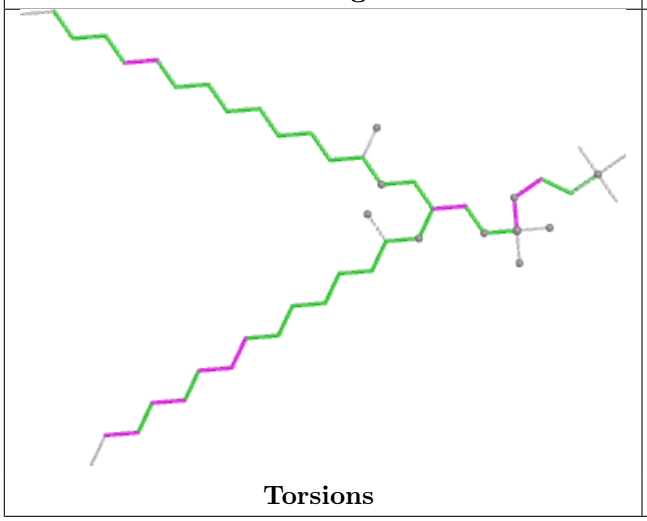
Ligand PX4 B 307



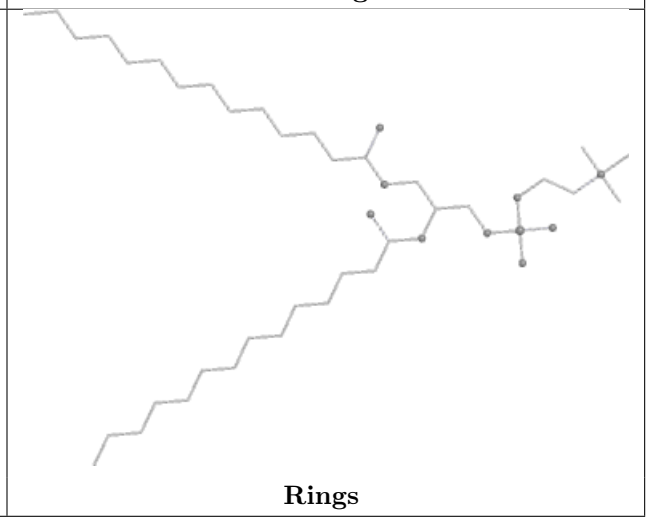
Bond lengths



Bond angles

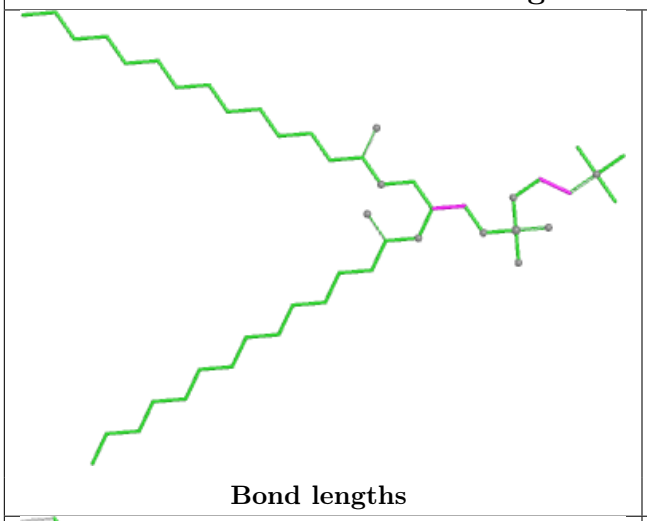


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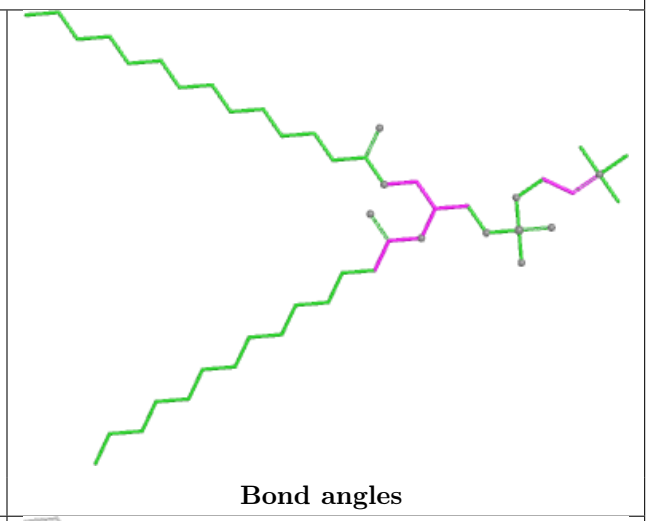


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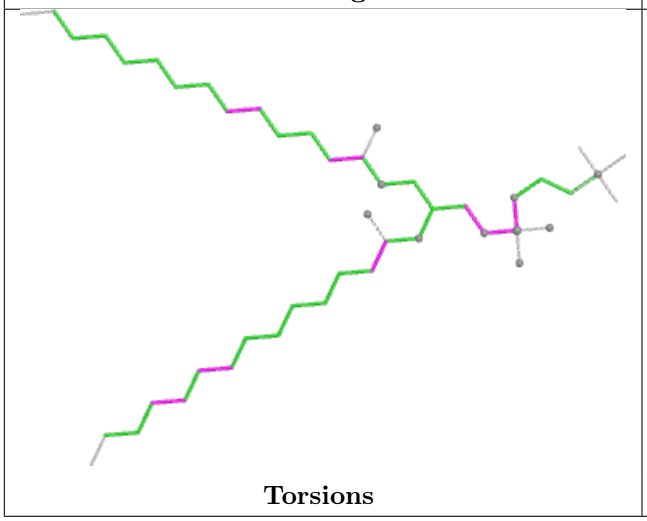
Ligand PX4 C 319



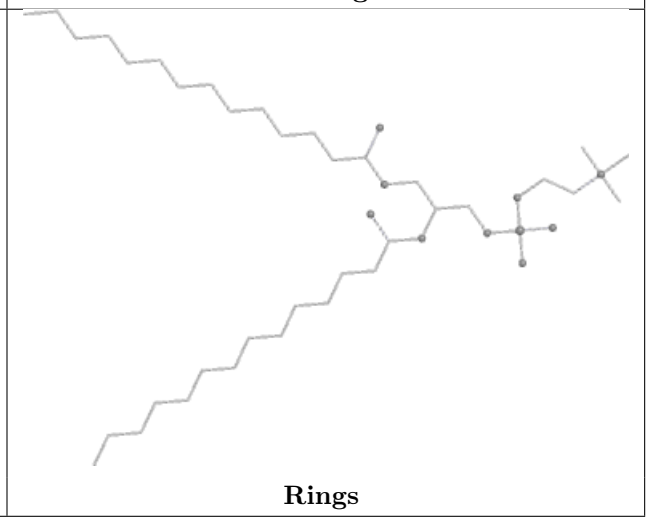
Bond lengths



Bond angles

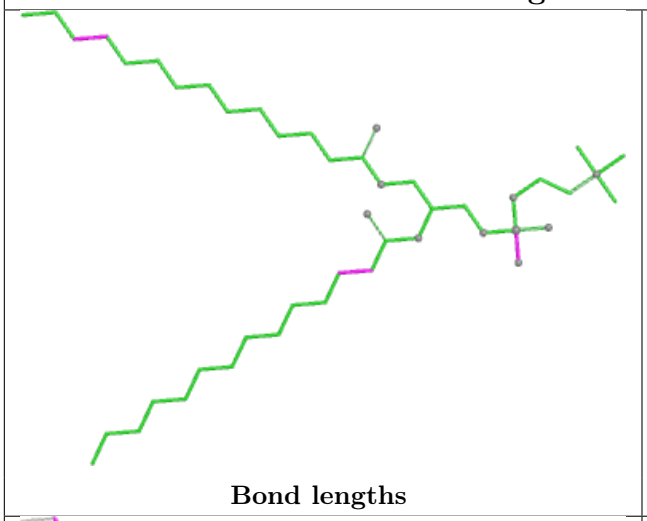


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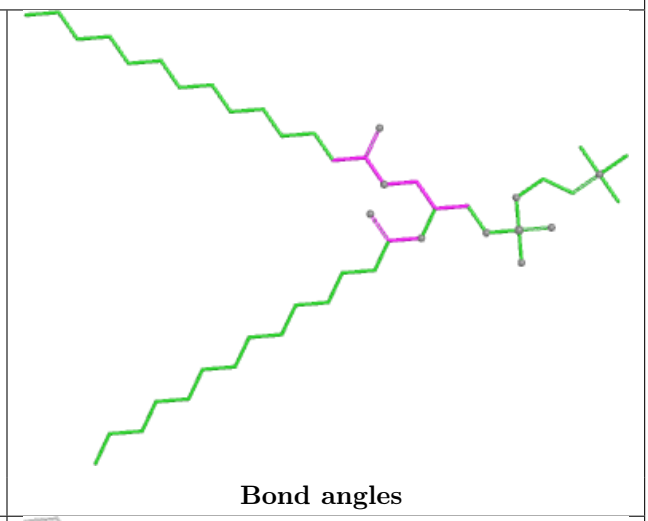


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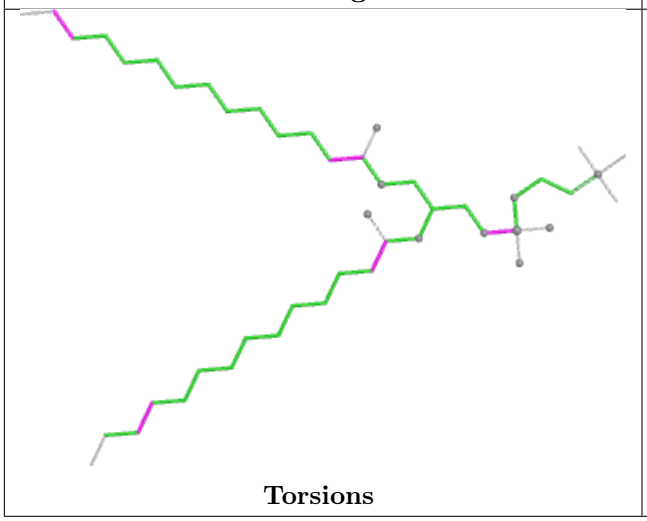
Ligand PX4 B 338



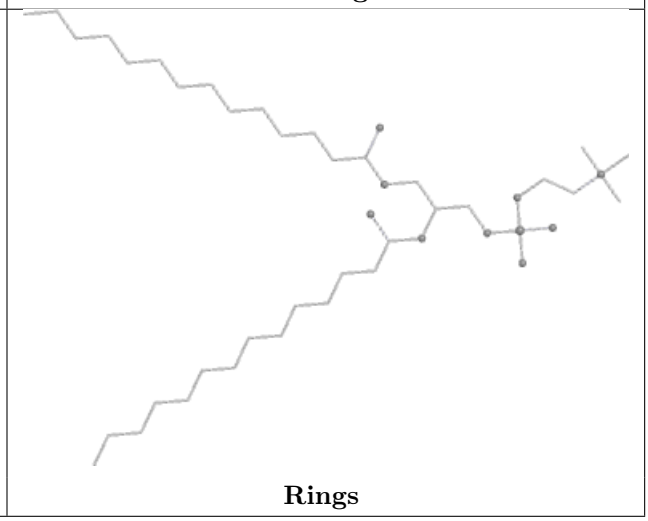
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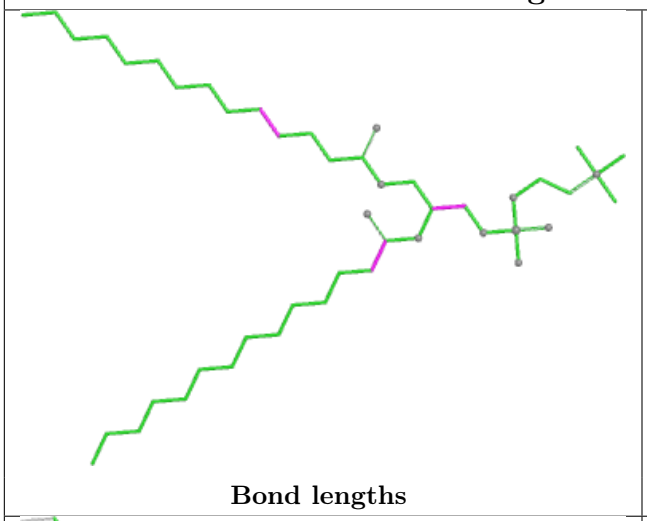


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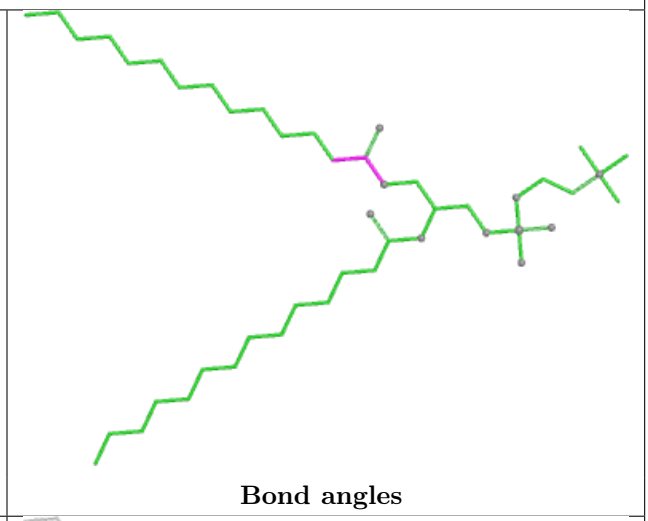


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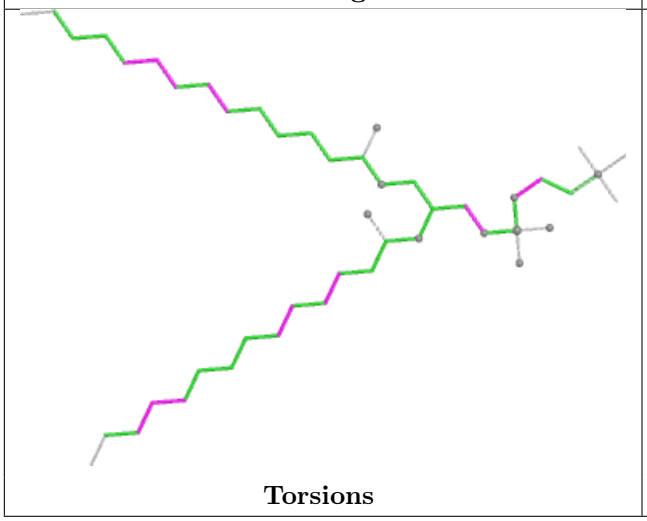
Ligand PX4 C 341



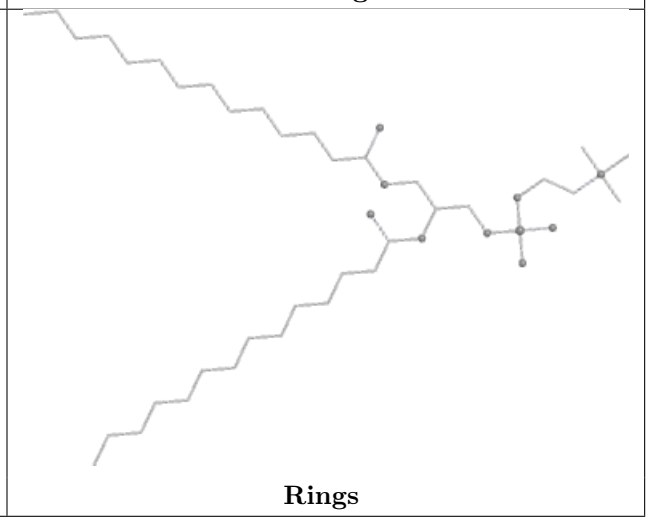
Bond lengths



Bond angles

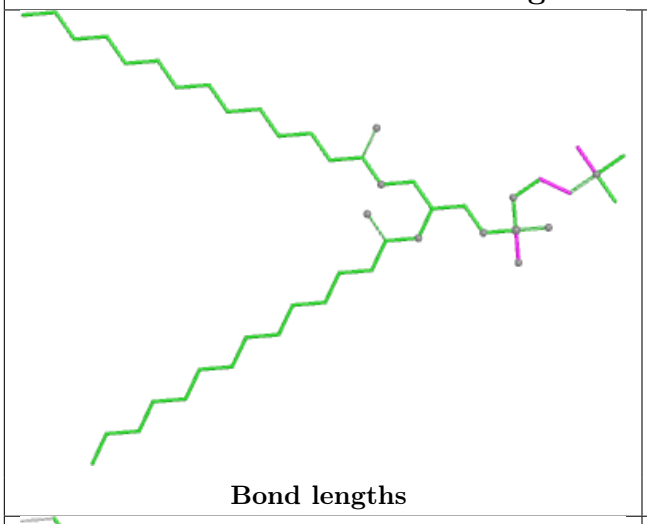


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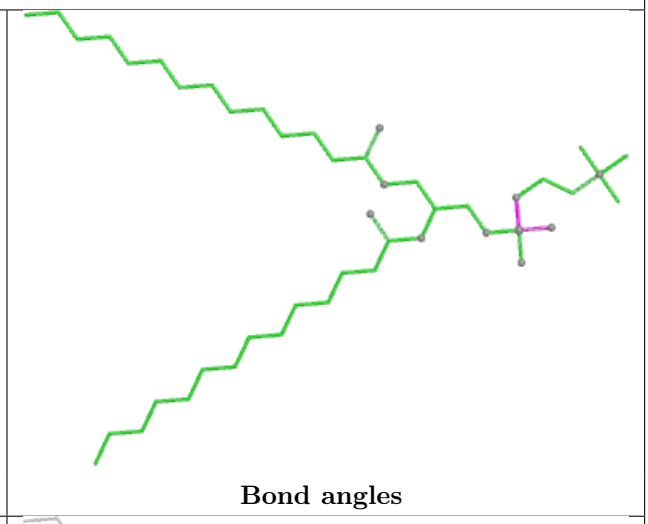


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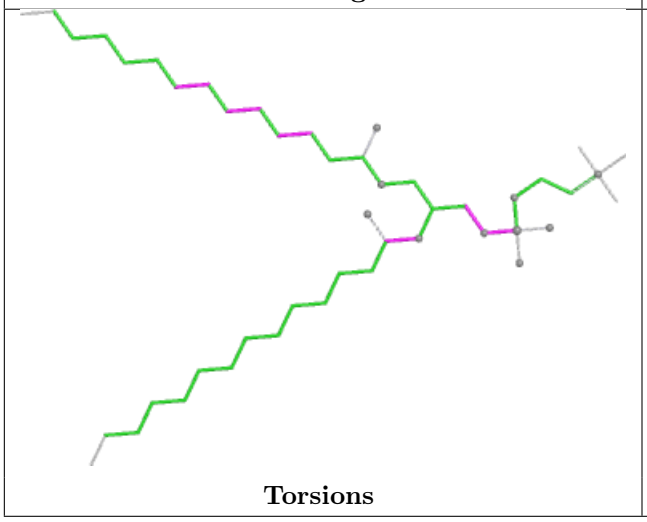
Ligand PX4 B 346



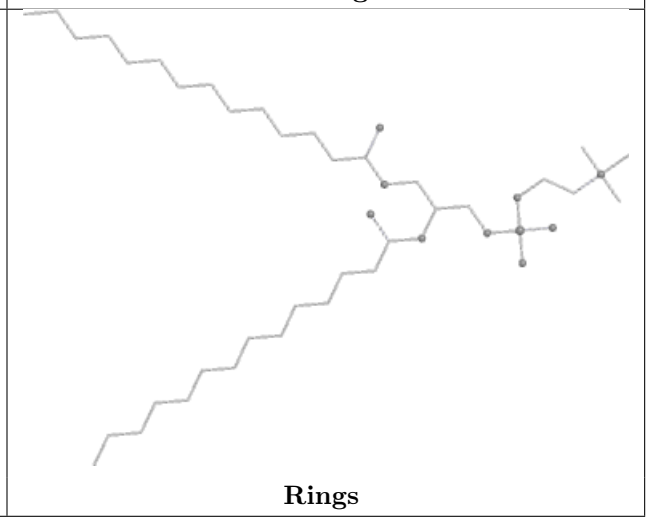
Bond lengths



Bond angles

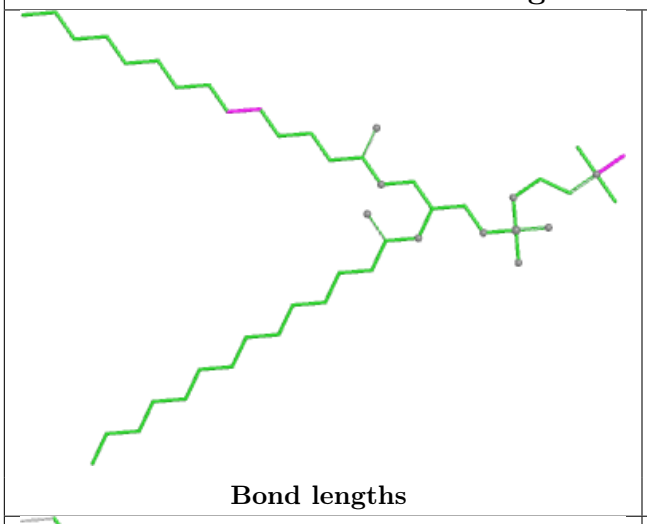


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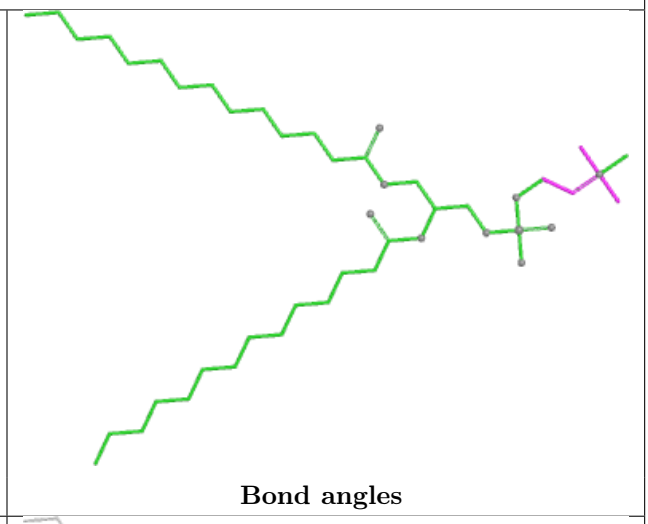


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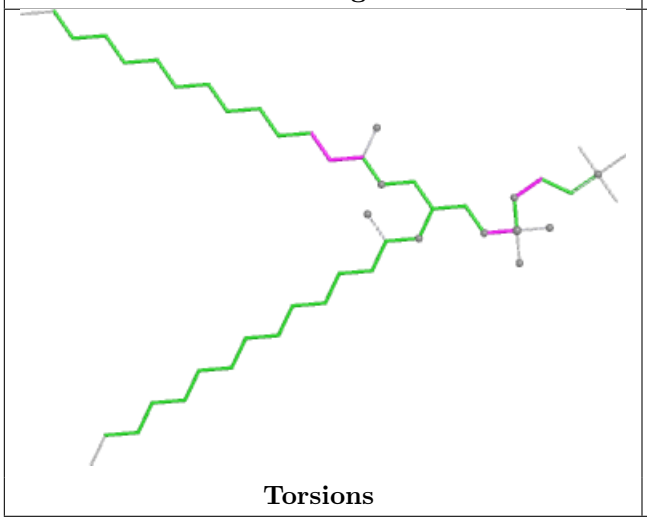
Ligand PX4 B 324



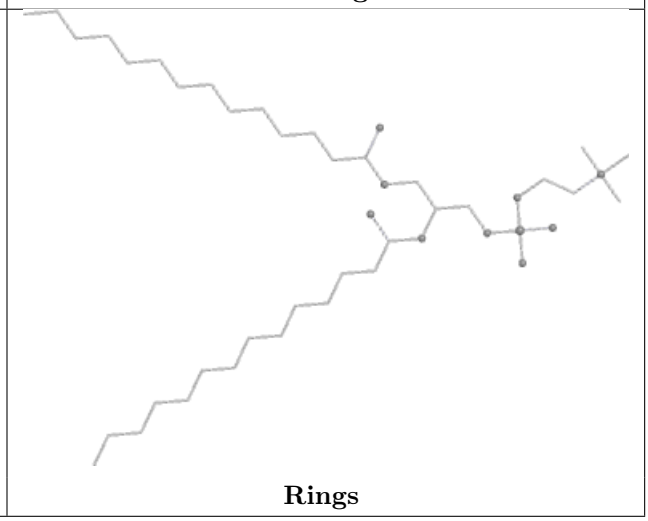
Bond lengths



Bond angles

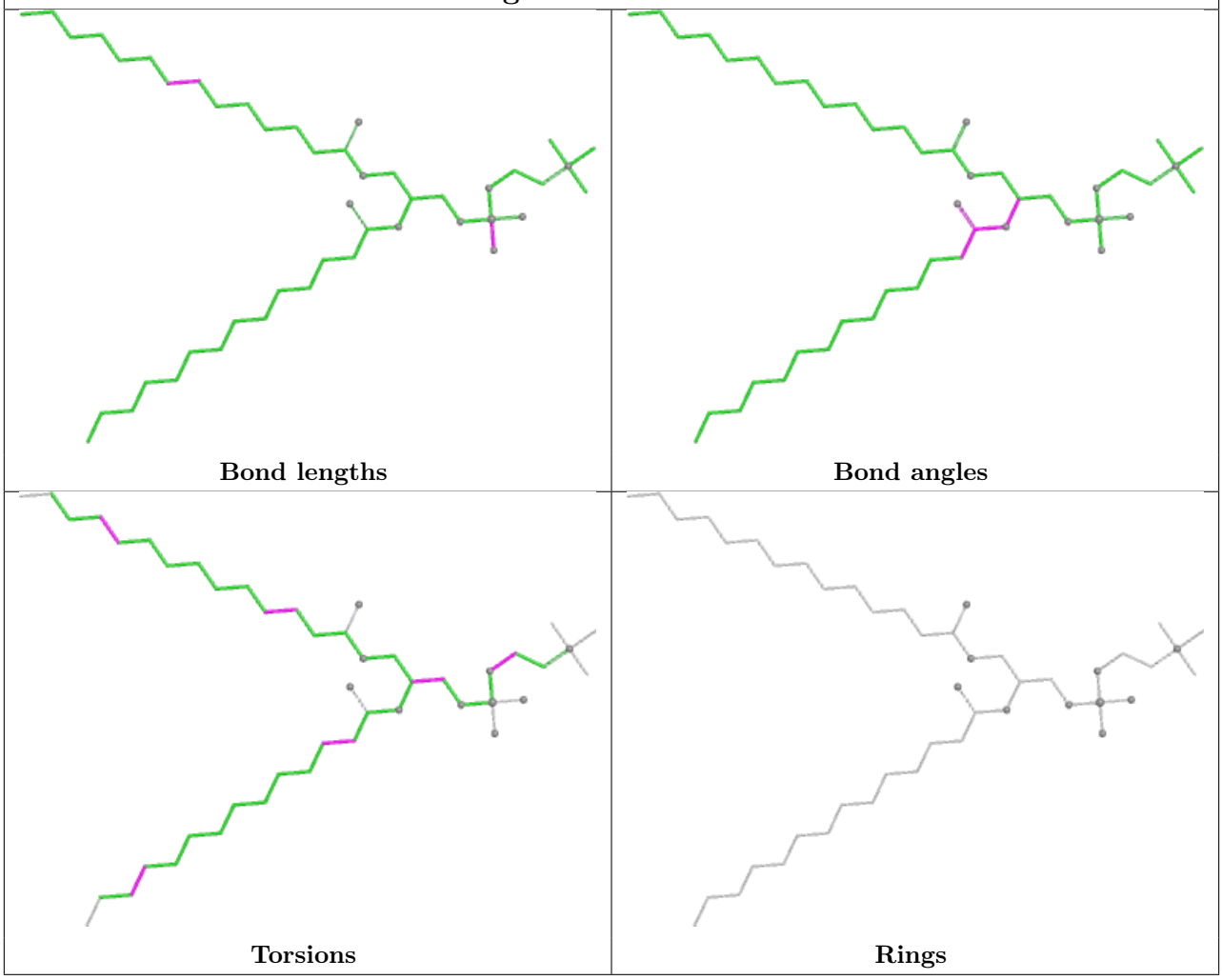


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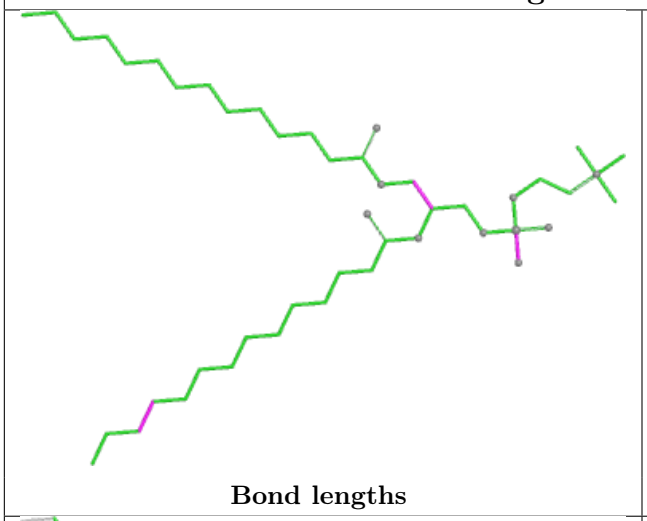


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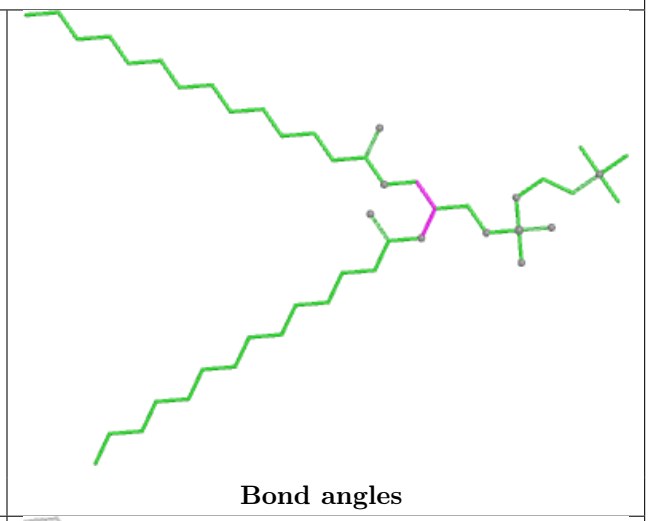
Ligand PX4 B 336



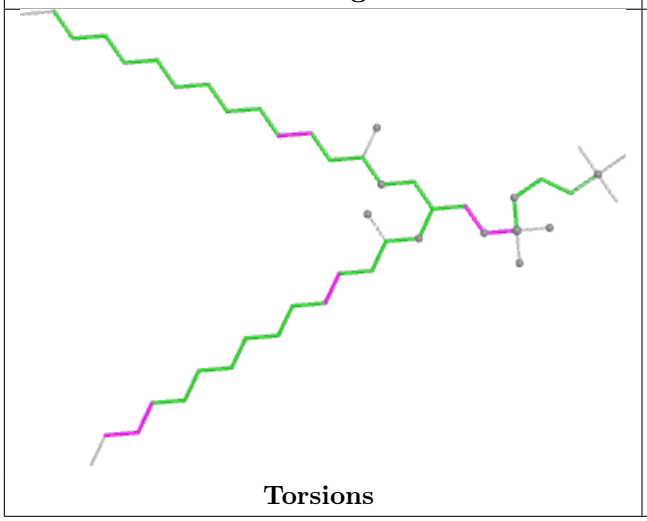
Ligand PX4 A 626



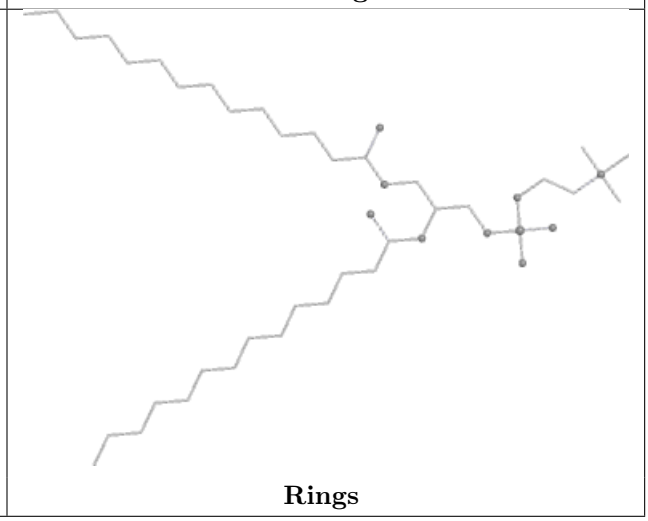
Bond lengths



Bond angles

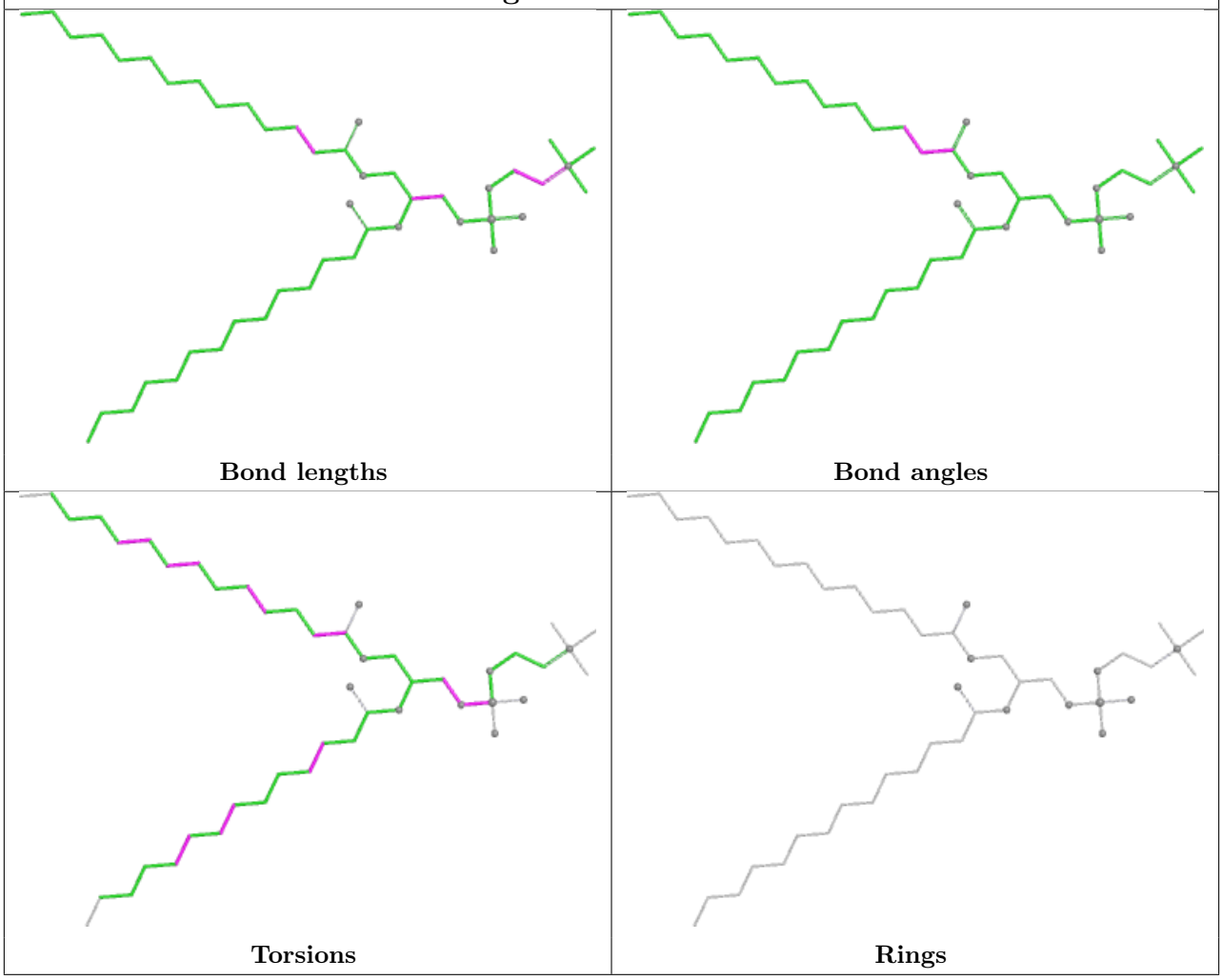


Torsions

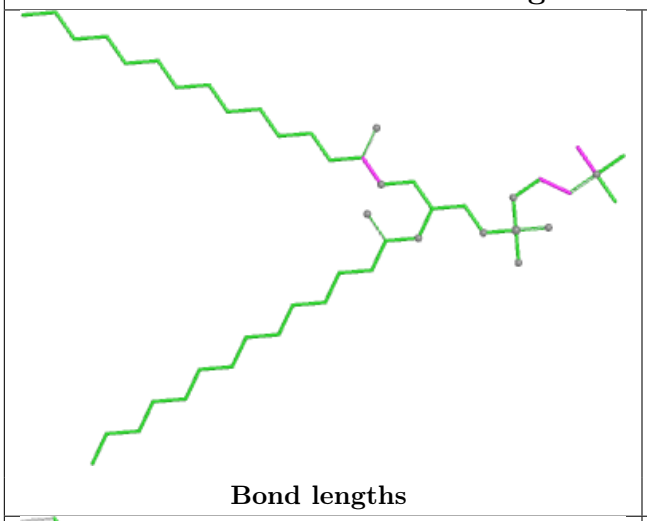


Rings

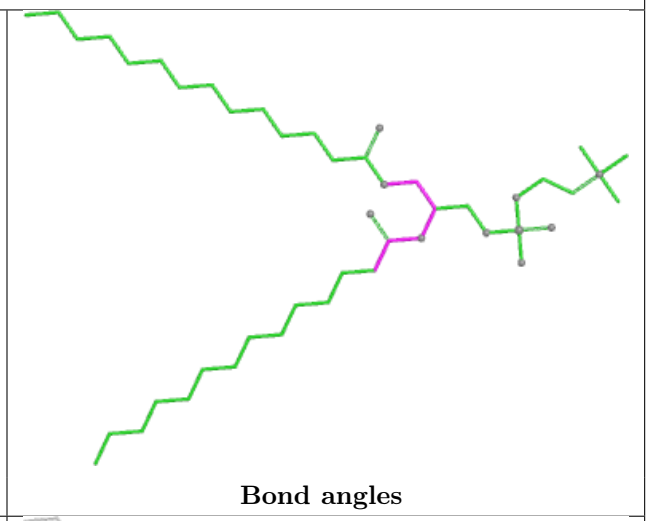
Ligand PX4 B 389



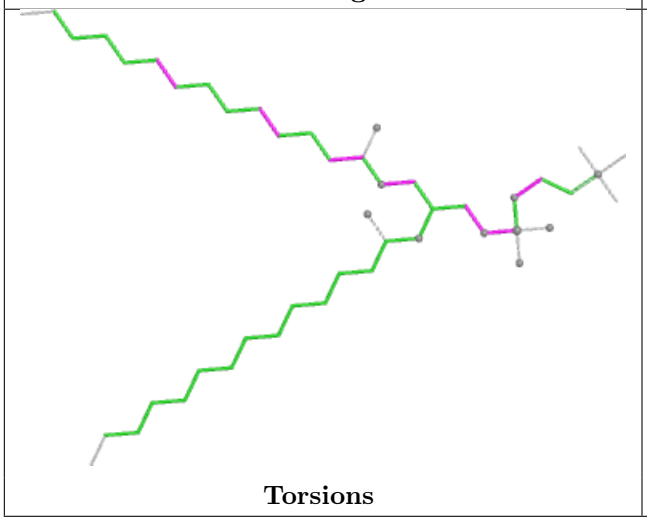
Ligand PX4 B 380



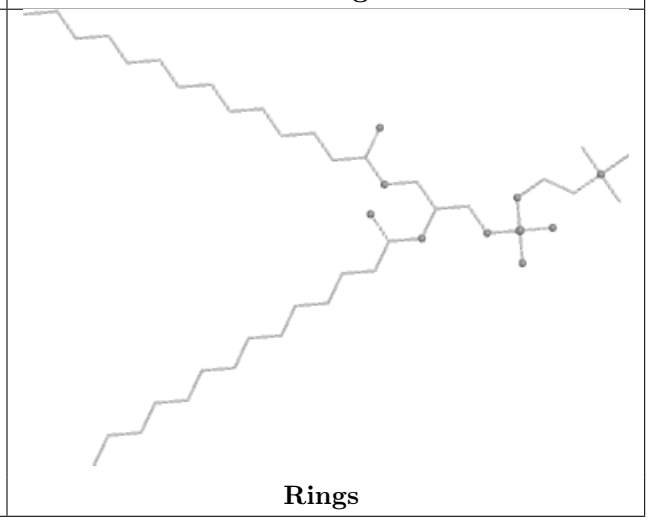
Bond lengths



Bond angles

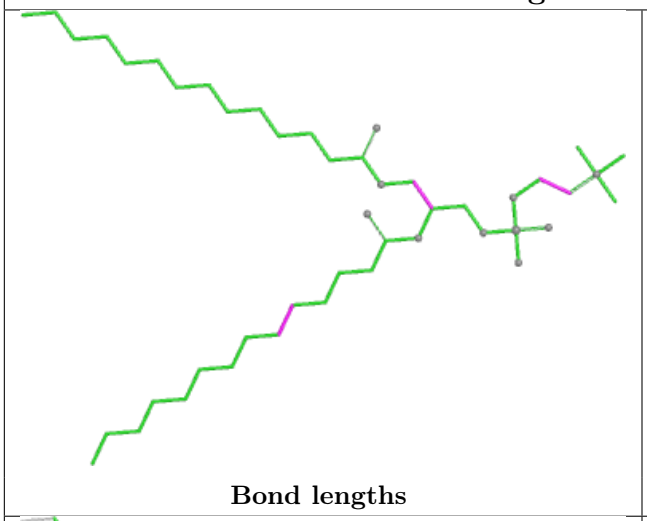


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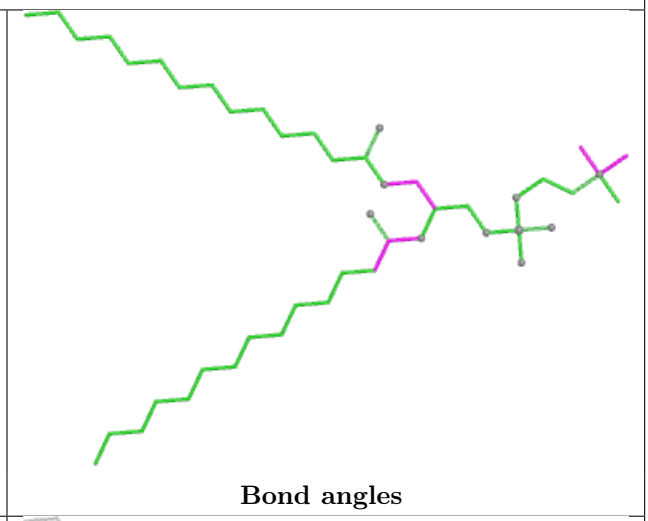


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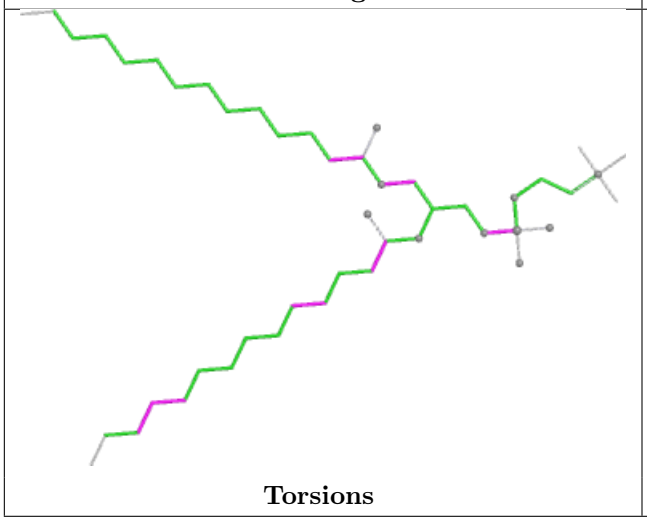
Ligand PX4 B 366



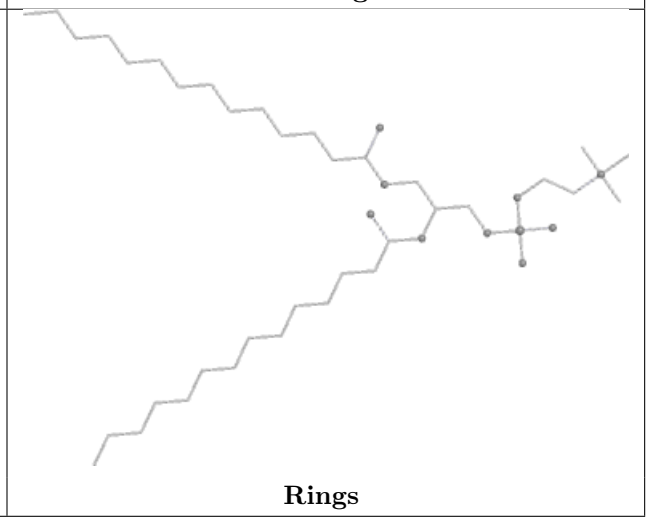
Bond lengths



Bond angles

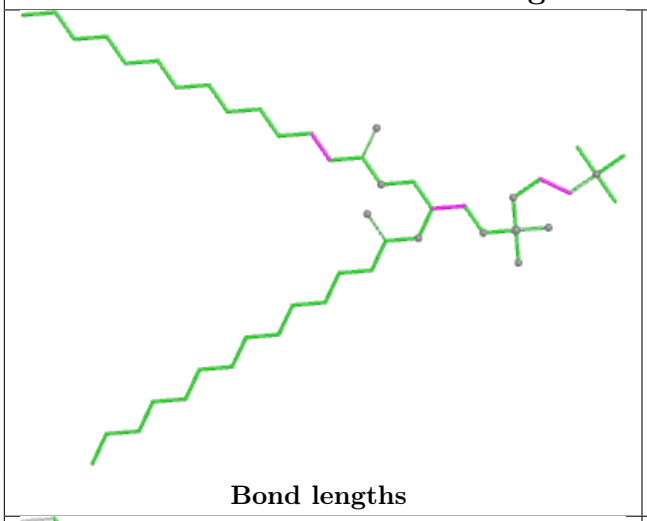


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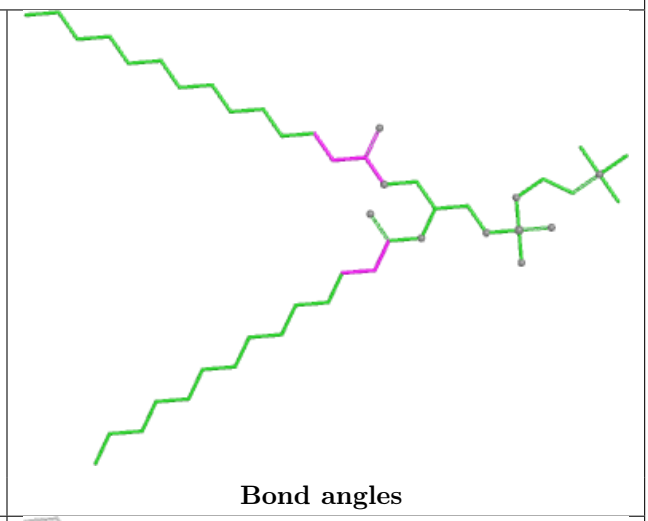


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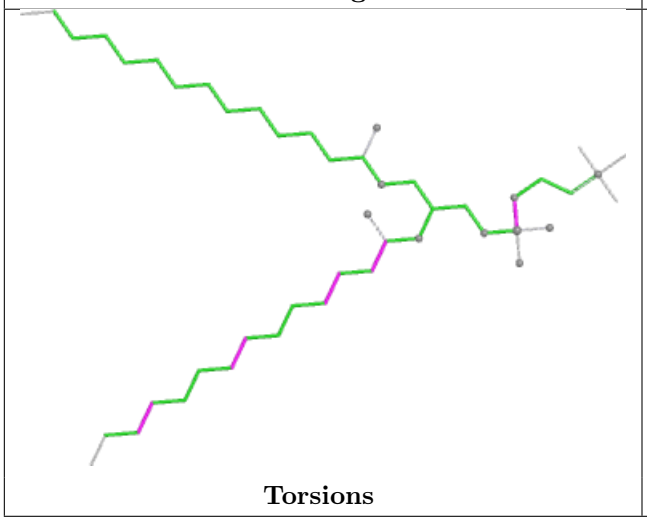
Ligand PX4 B 322



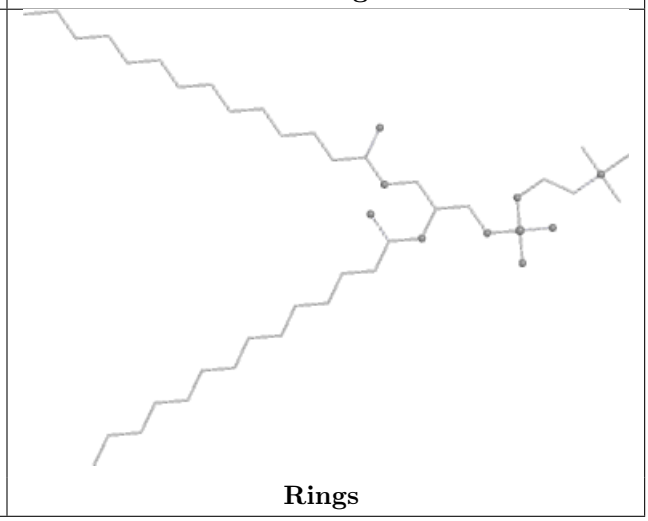
Bond lengths



Bond angles

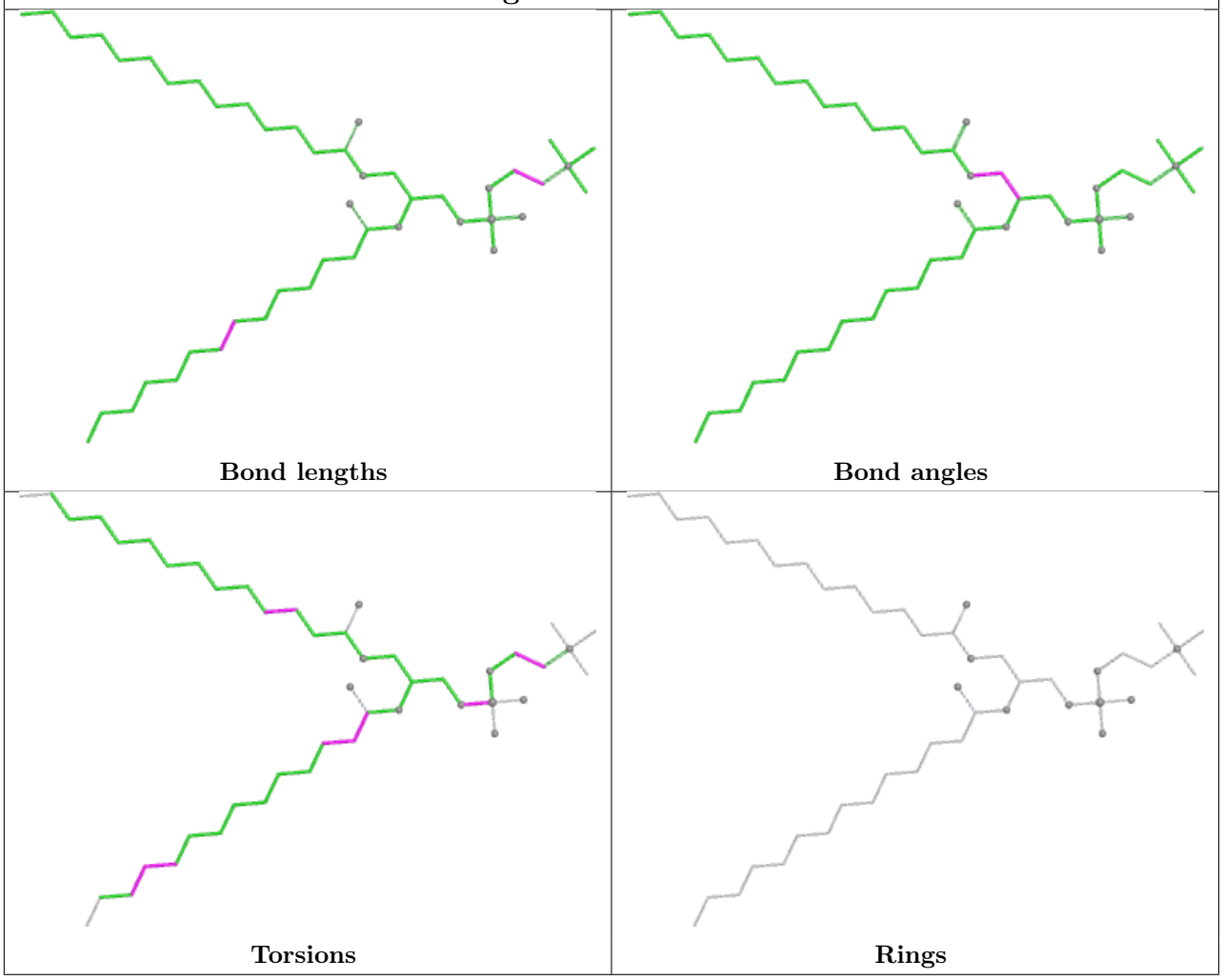


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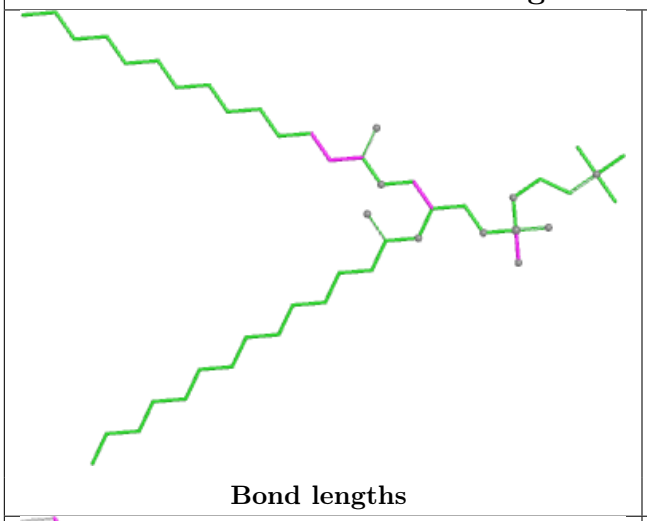


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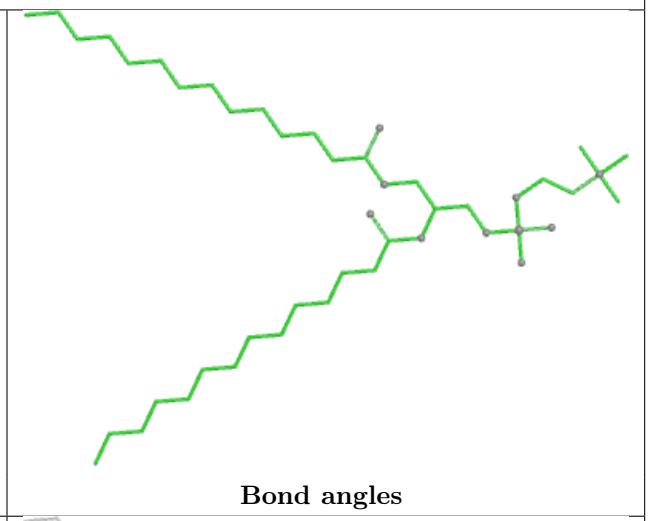
Ligand PX4 B 398



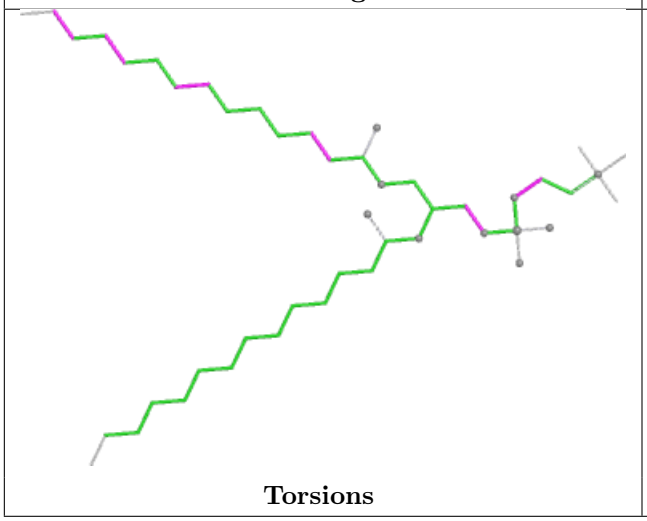
Ligand PX4 C 326



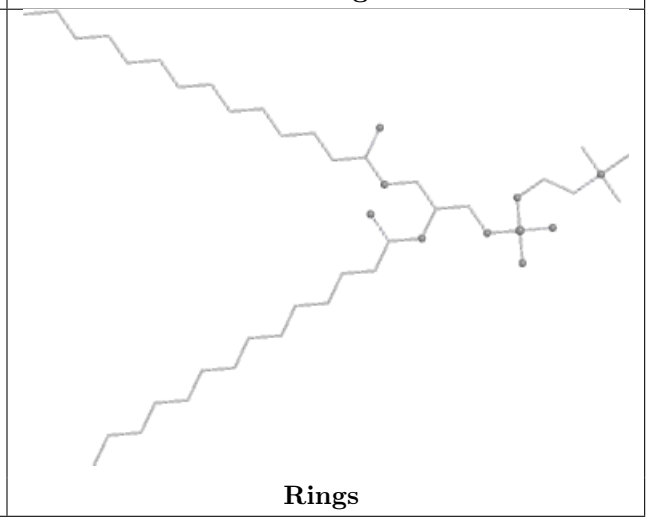
Bond lengths



Bond angles

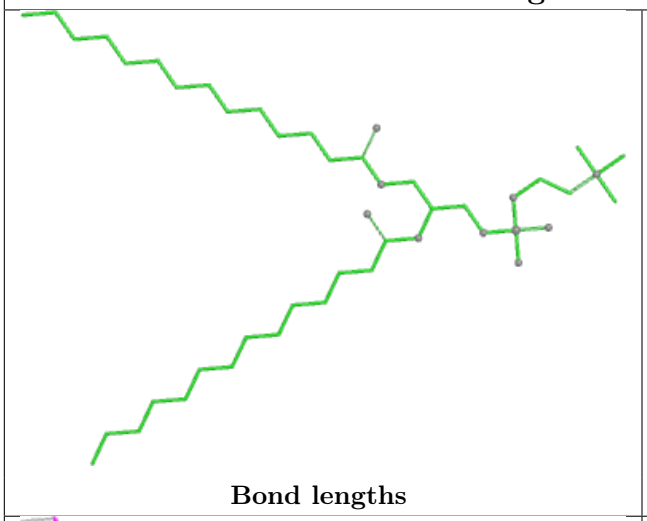


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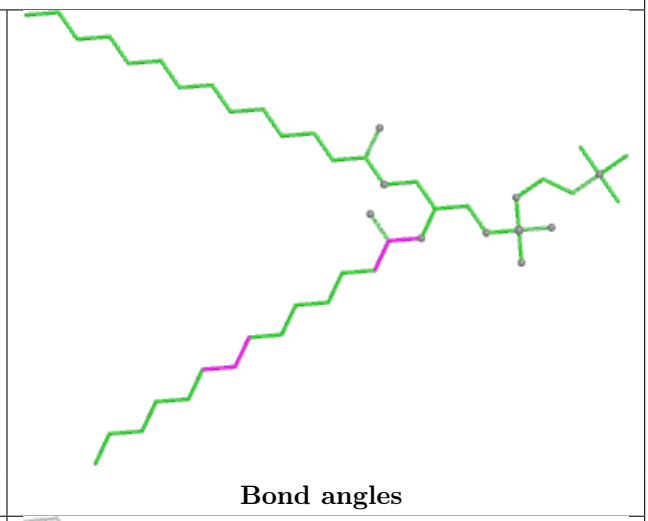


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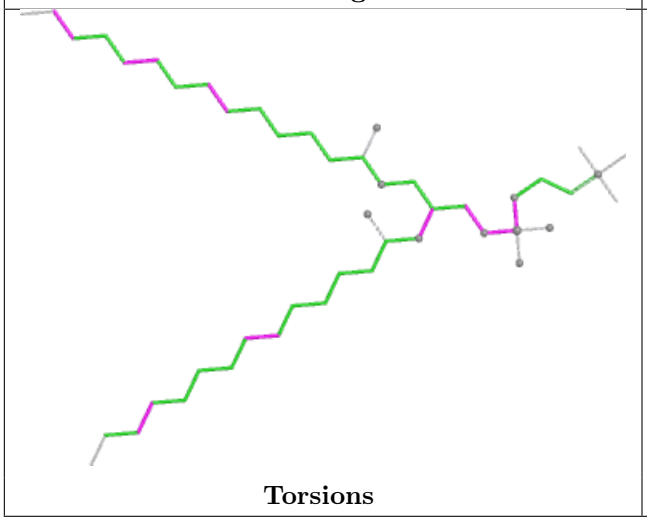
Ligand PX4 C 346



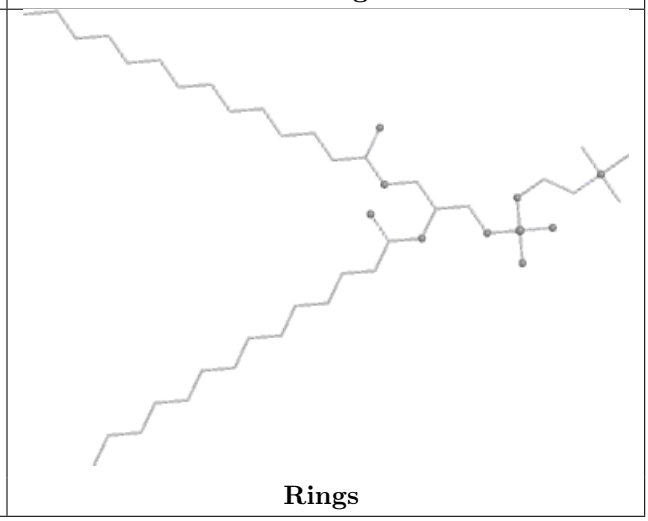
Bond lengths



Bond angles

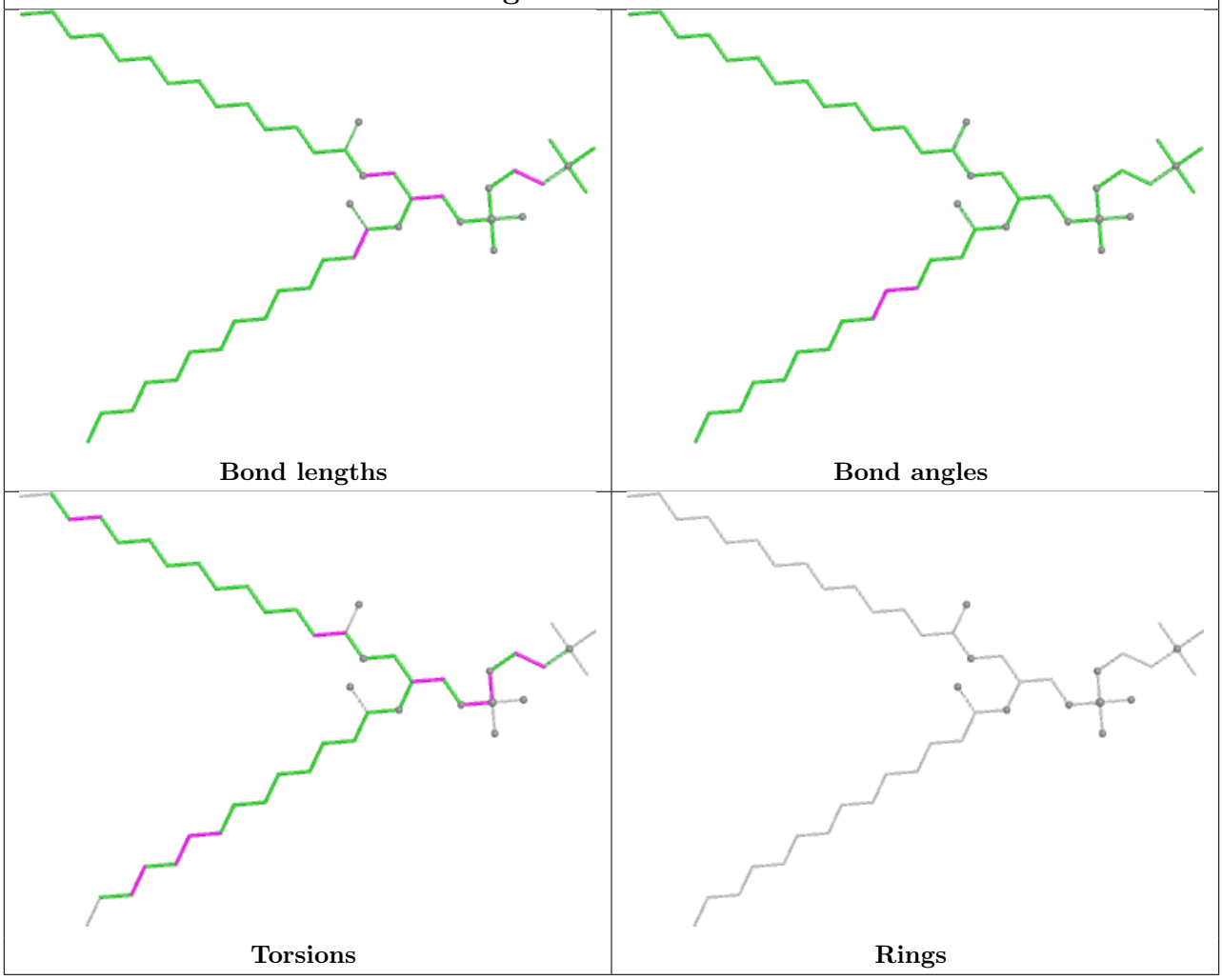


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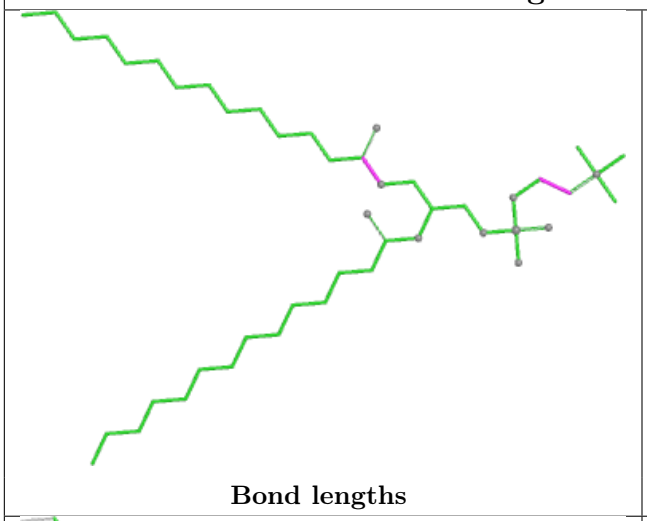


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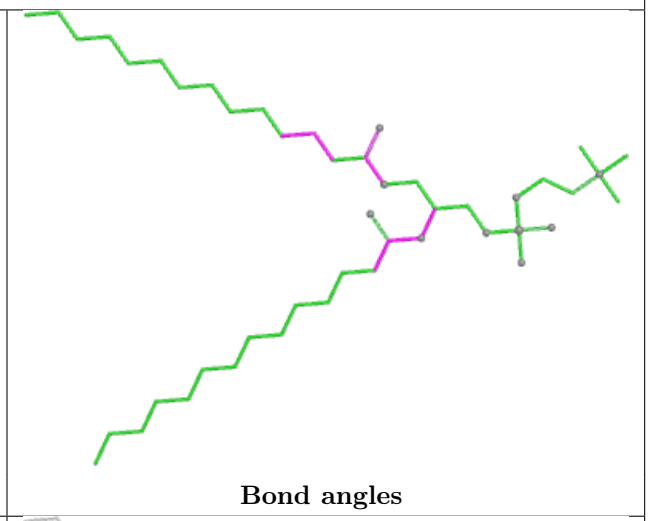
Ligand PX4 B 397



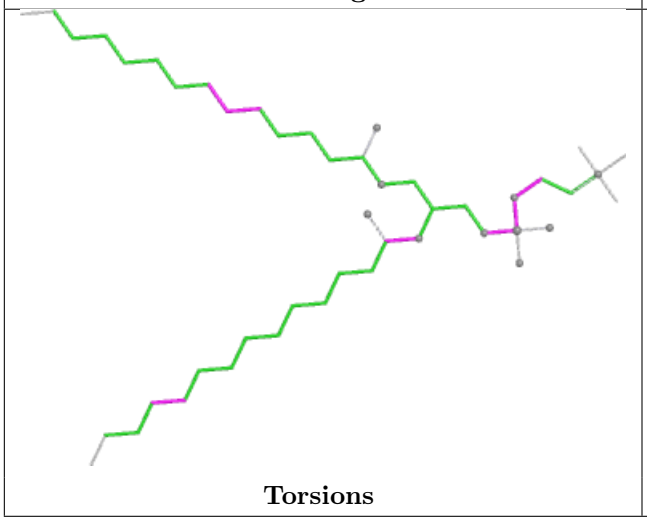
Ligand PX4 A 648



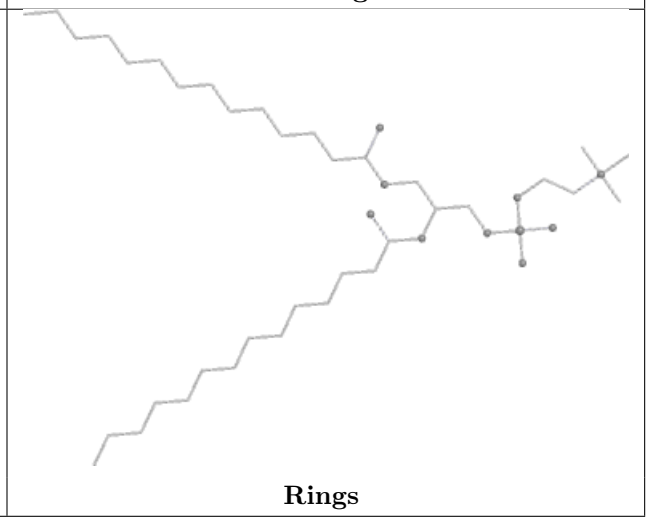
Bond lengths



Bond angles

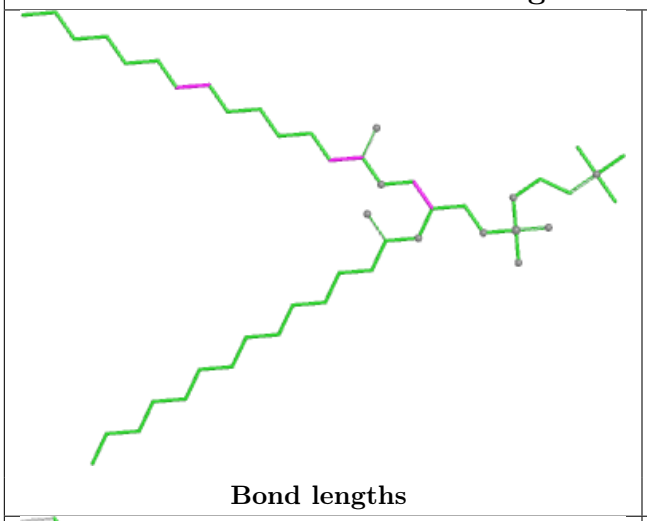


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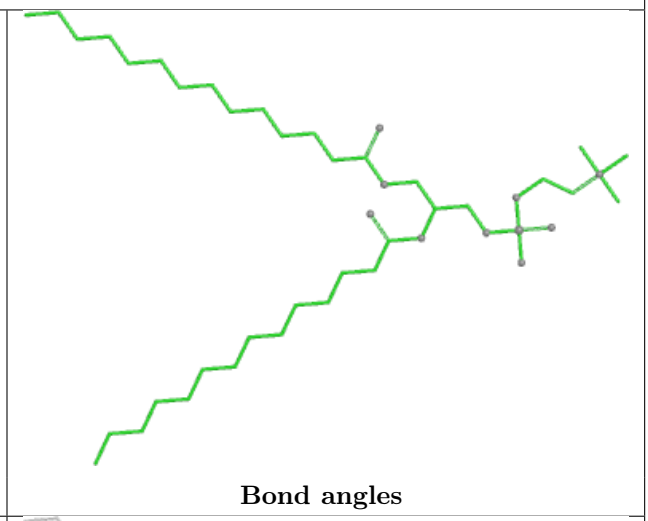


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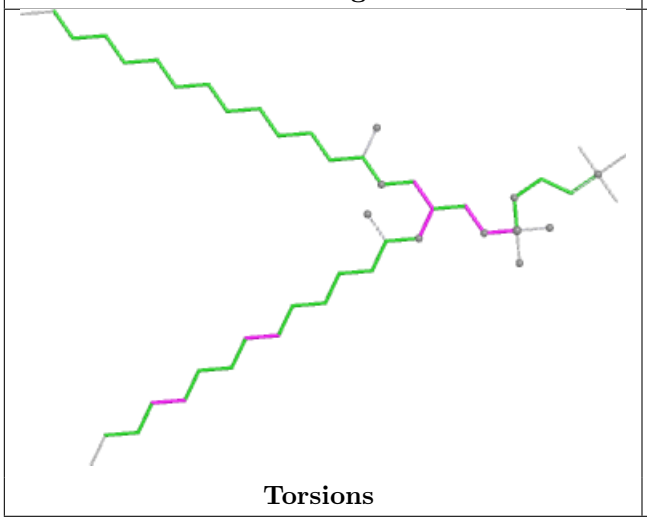
Ligand PX4 B 362



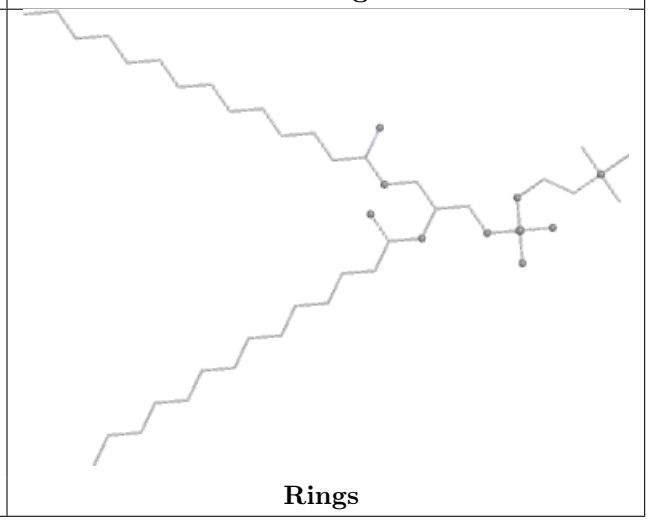
Bond lengths



Bond angles

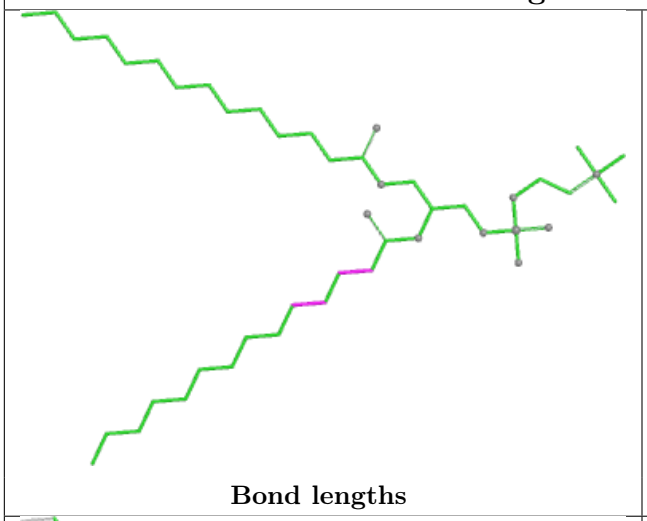


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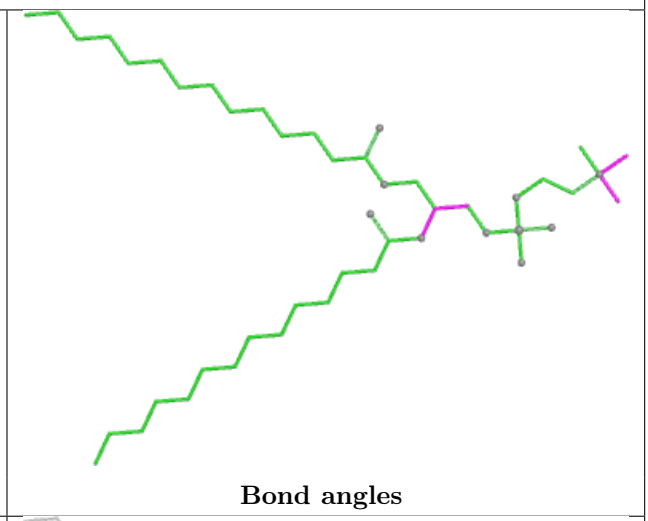


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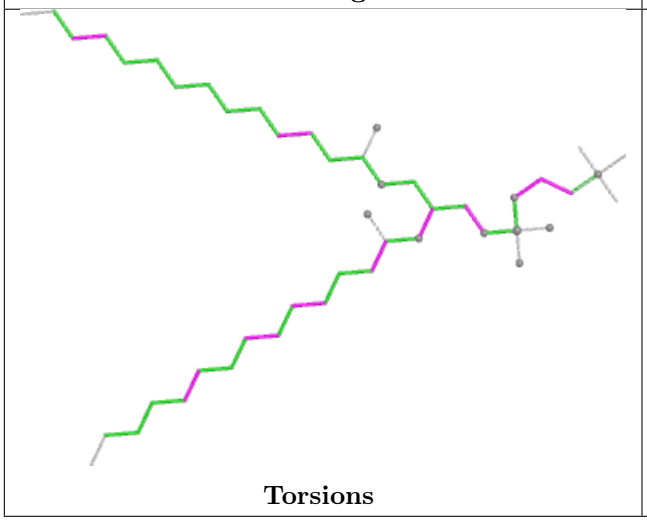
Ligand PX4 B 313



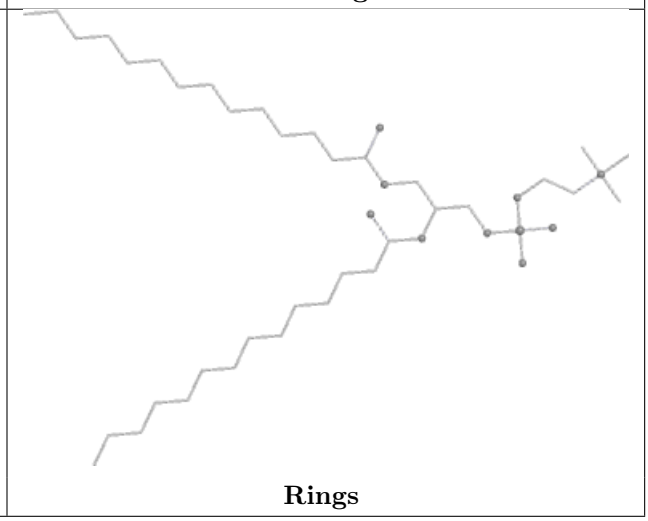
Bond lengths



Bond angles

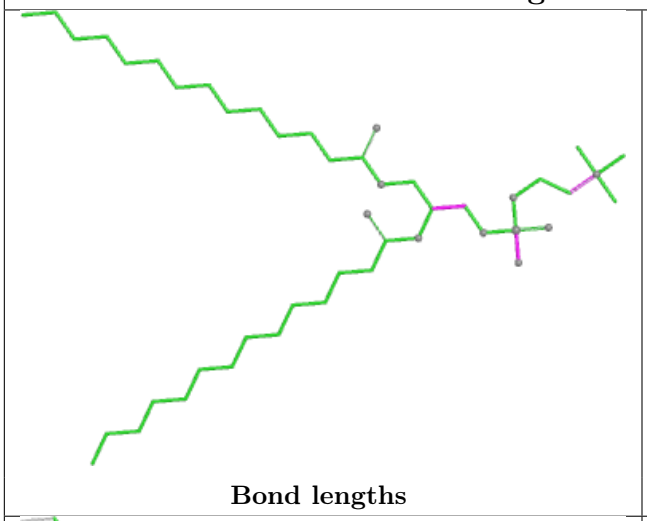


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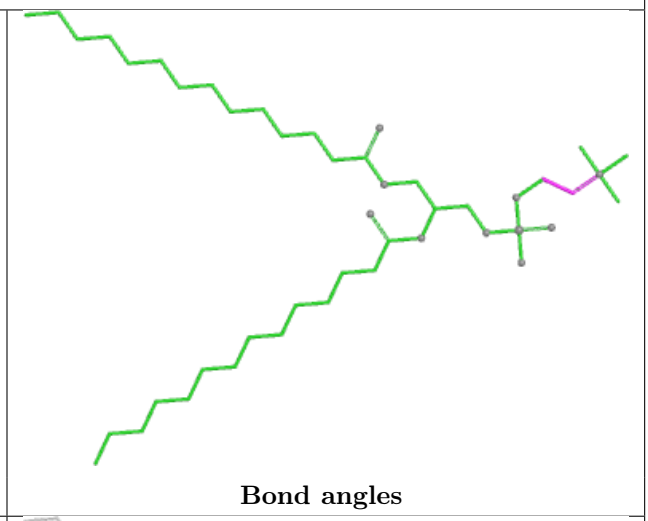


Rings

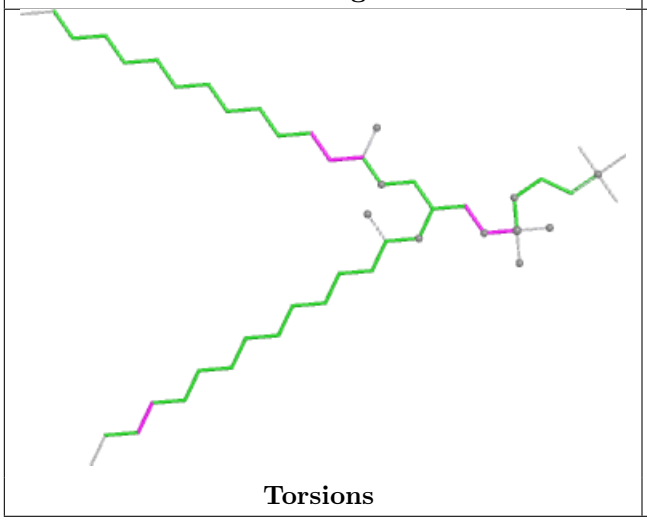
Ligand PX4 C 343



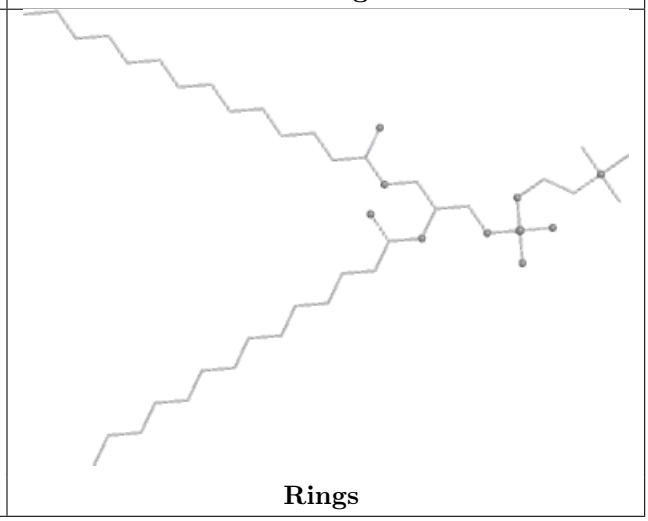
Bond lengths



Bond angles

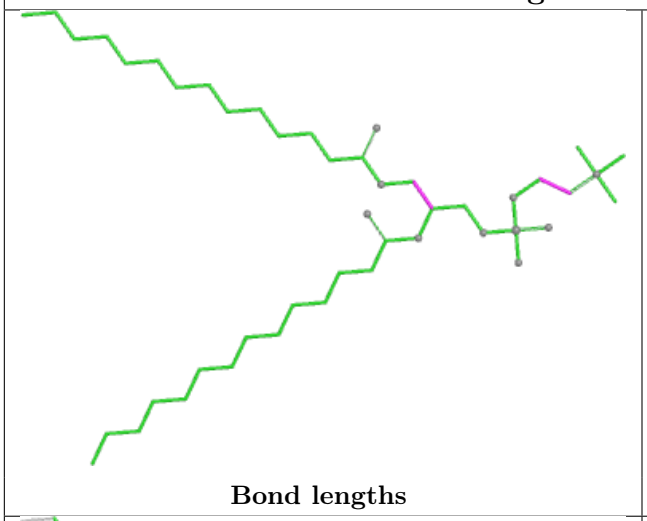


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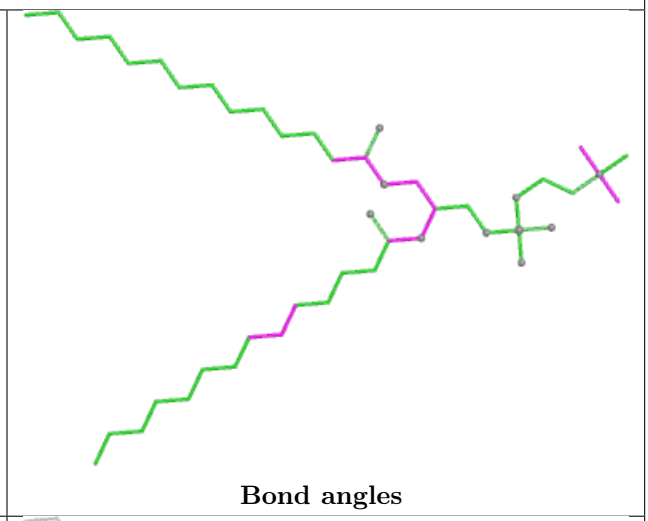


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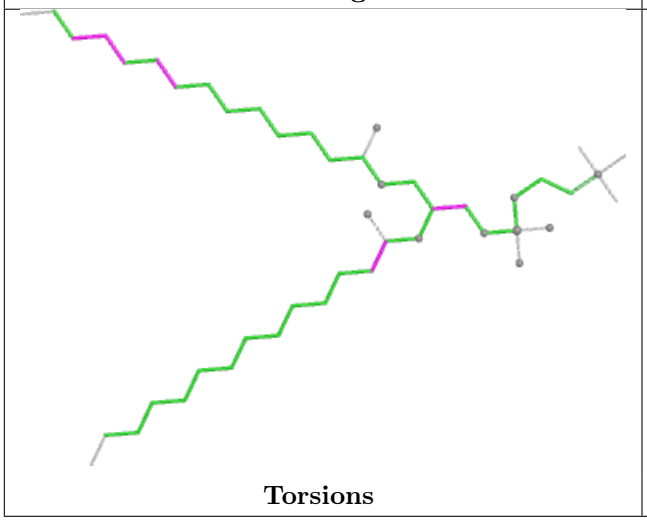
Ligand PX4 A 623



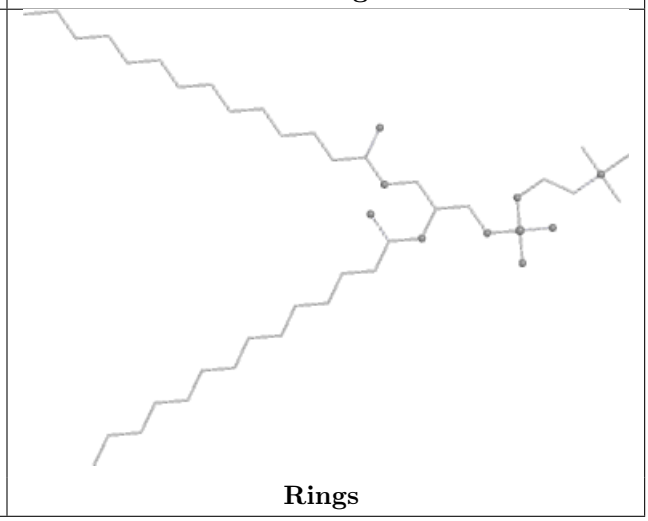
Bond lengths



Bond angles

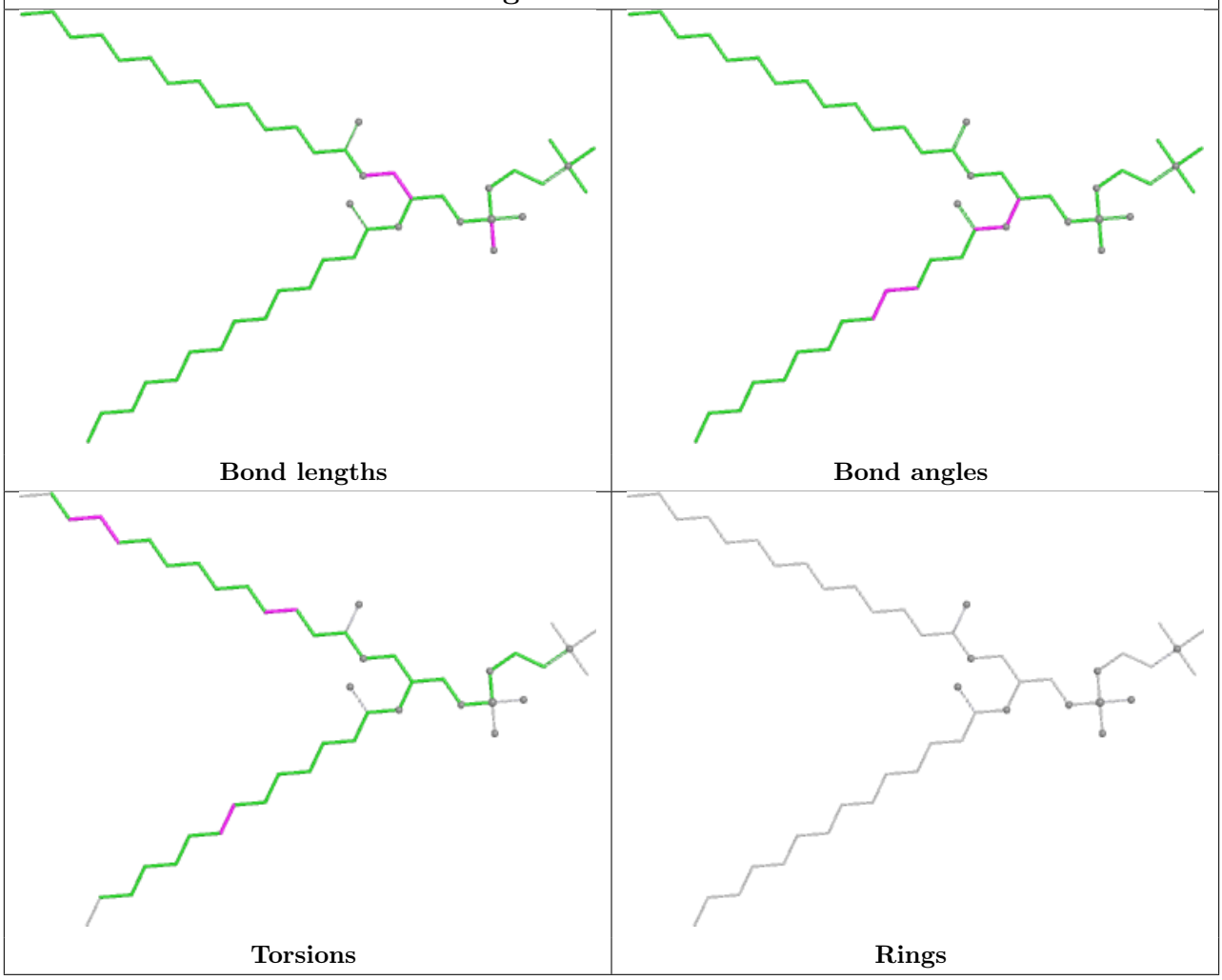


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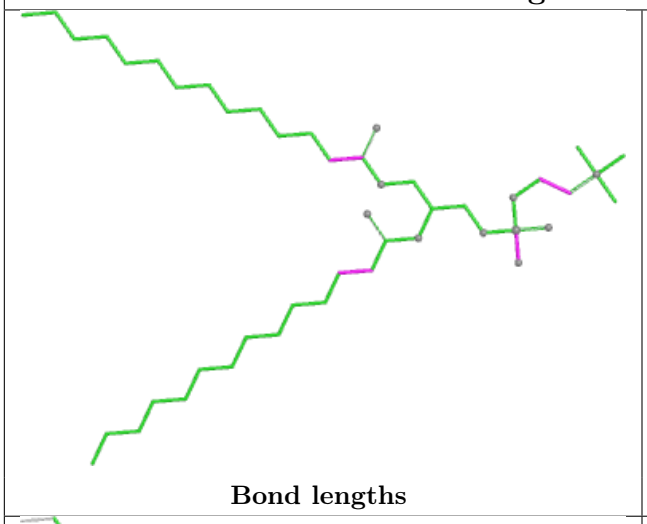


Rings

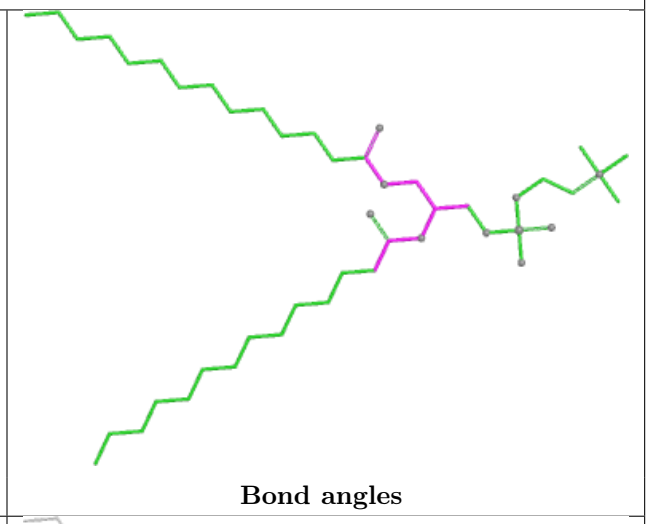
Ligand PX4 B 319



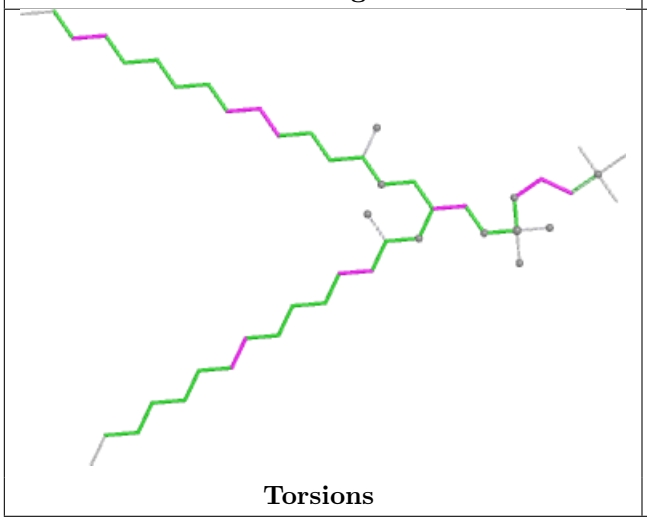
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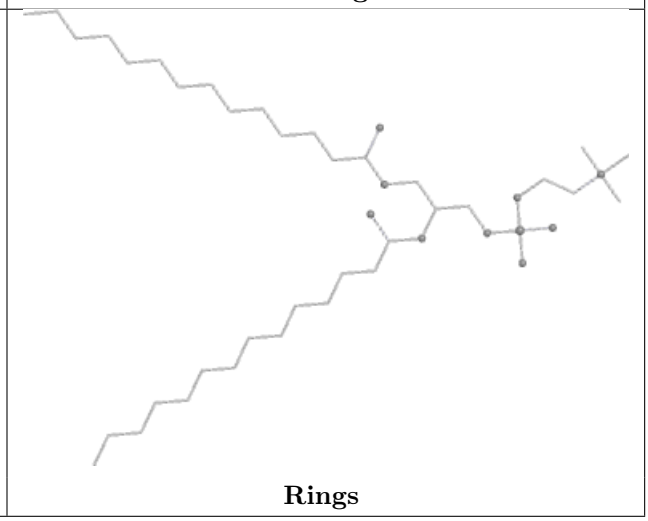
Bond lengths



Bond angles

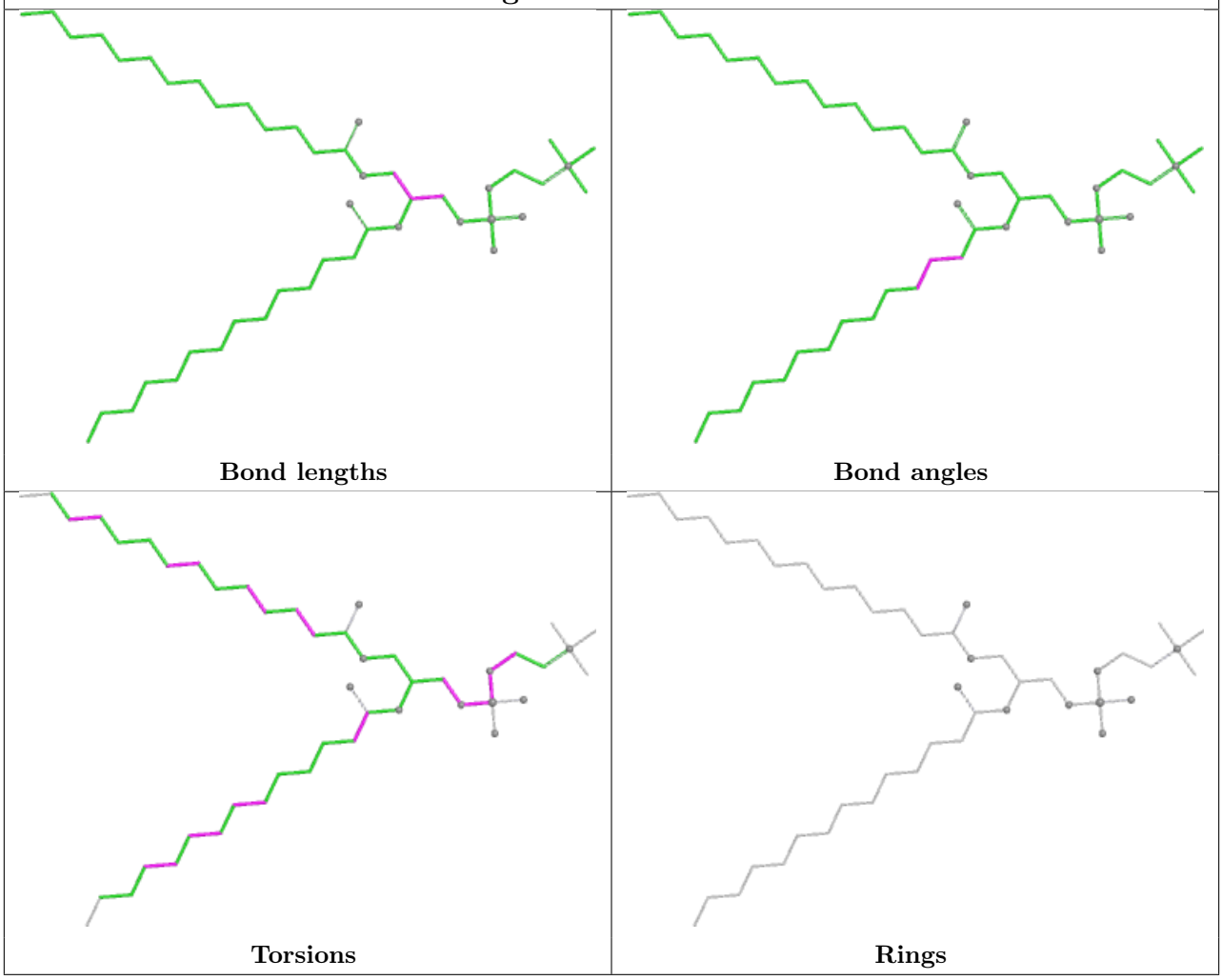


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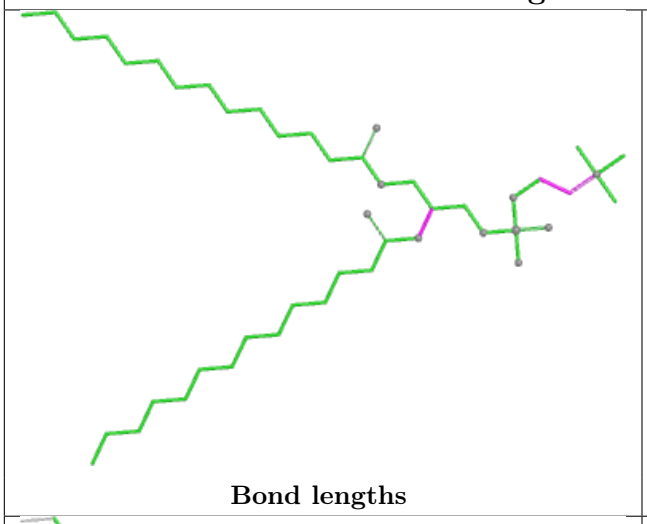


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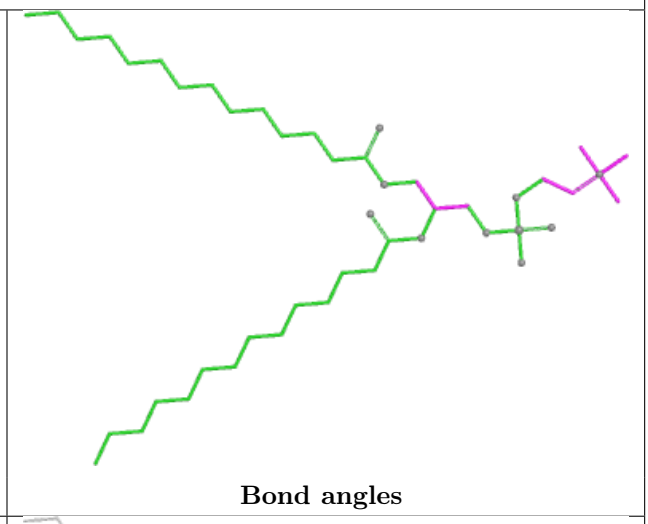
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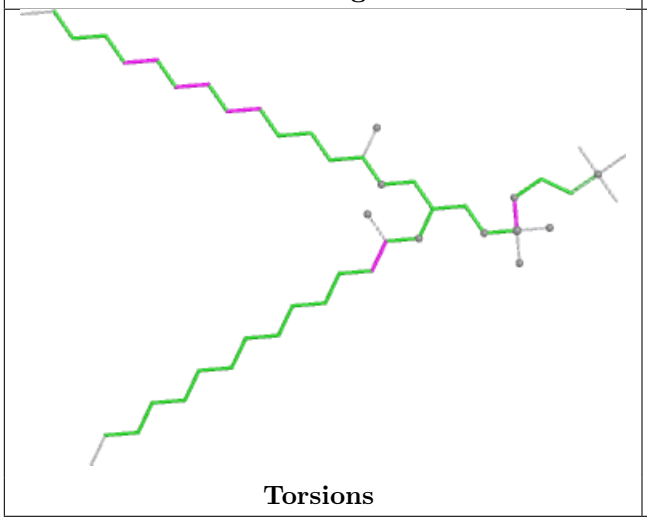
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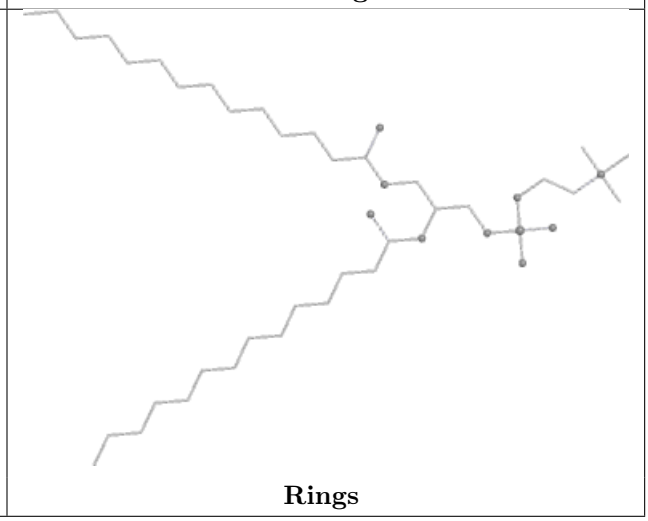
Bond lengths



Bond angles

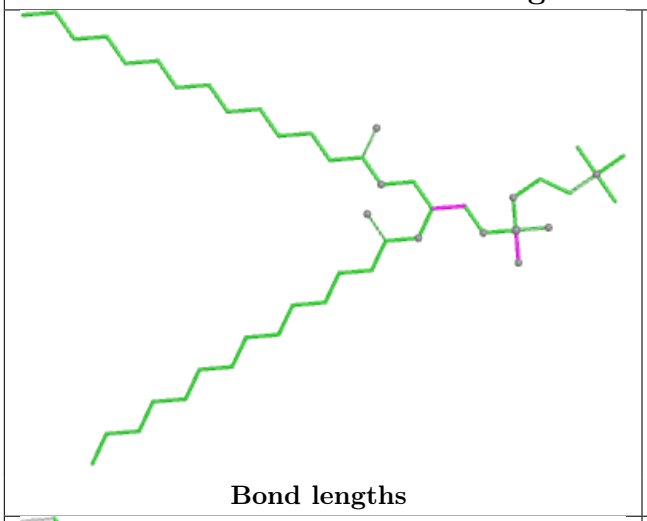


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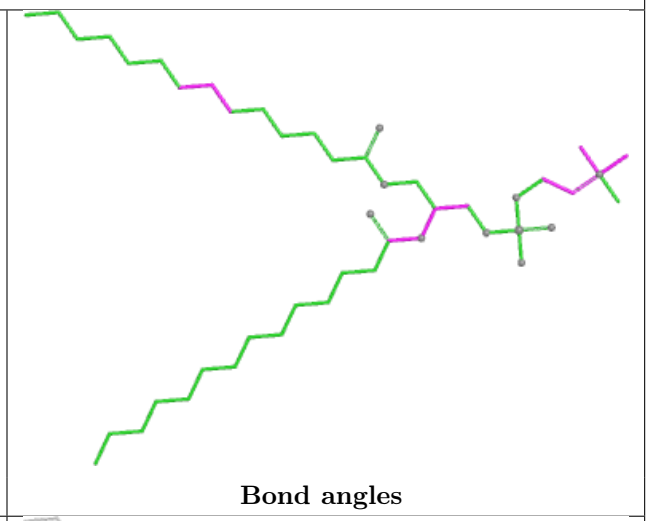


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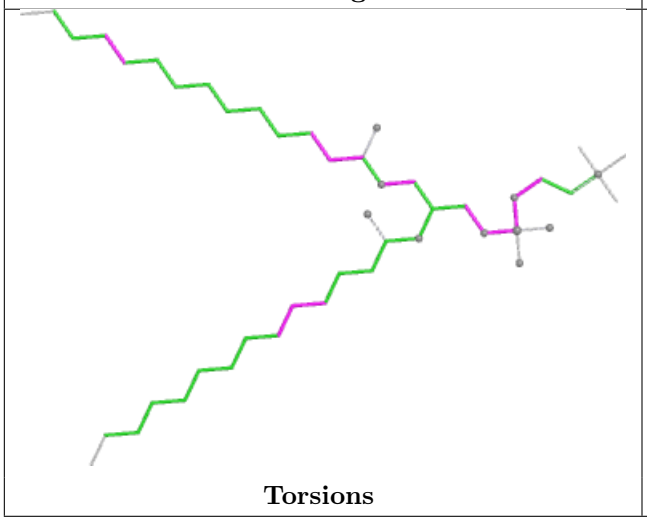
Ligand PX4 B 382



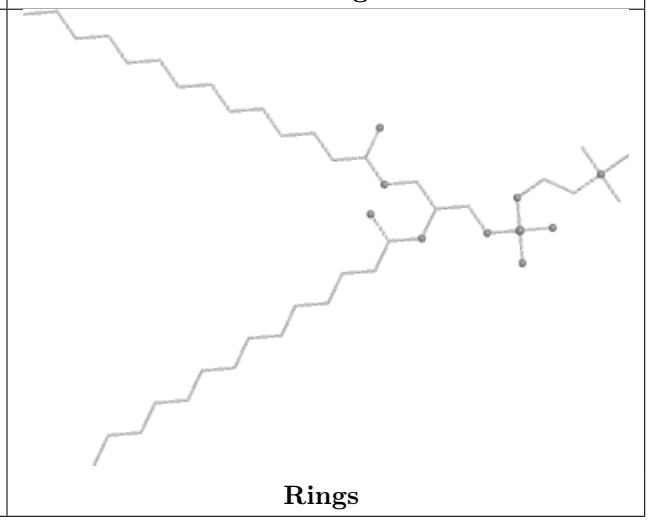
Bond lengths



Bond angles

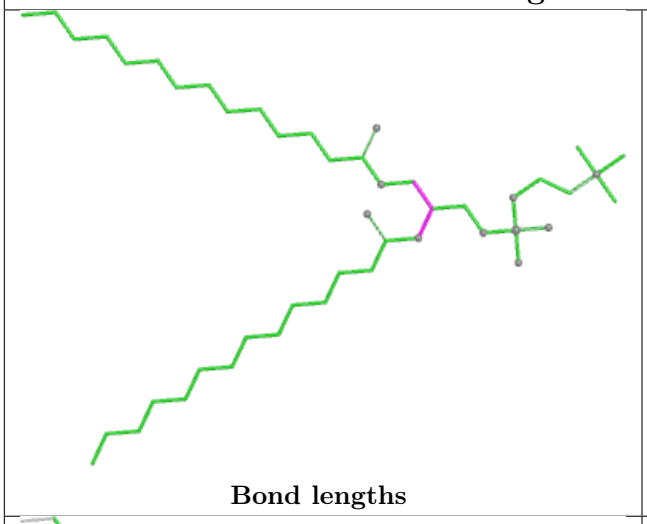


Torsions

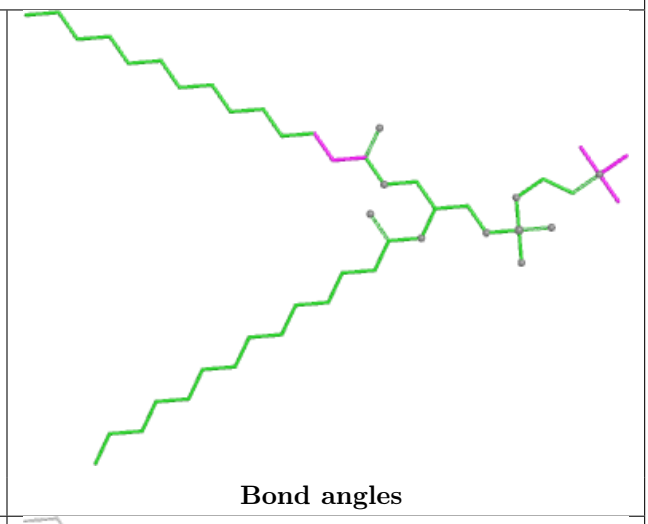


Rings

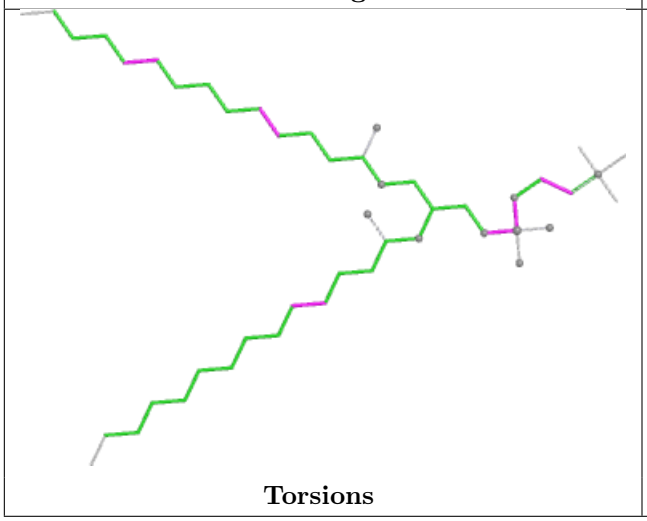
Ligand PX4 A 624



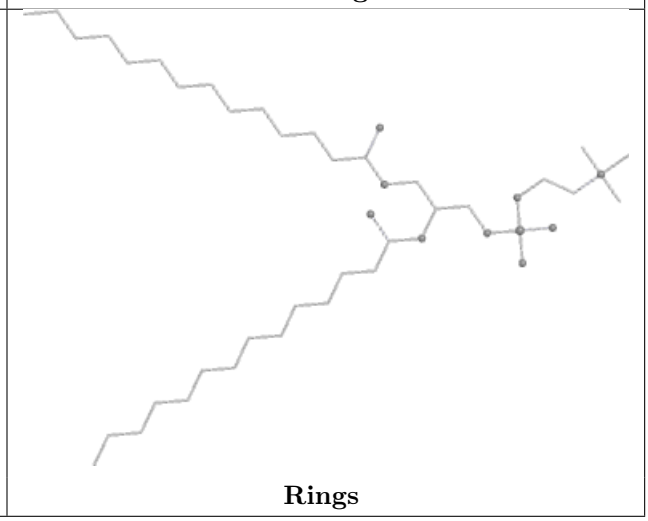
Bond lengths



Bond angles

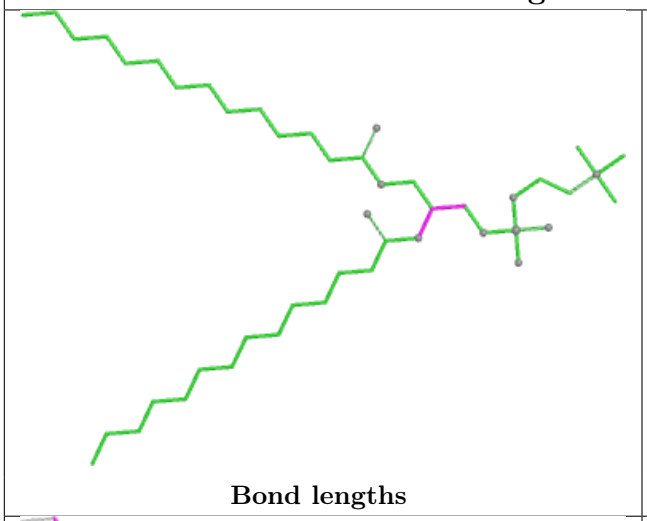


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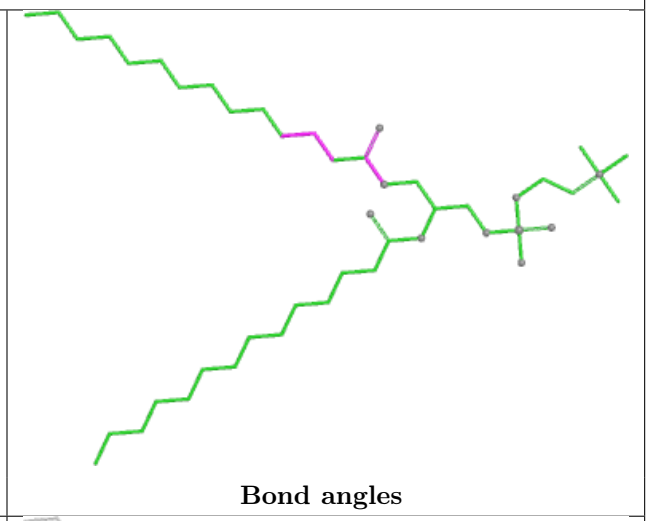


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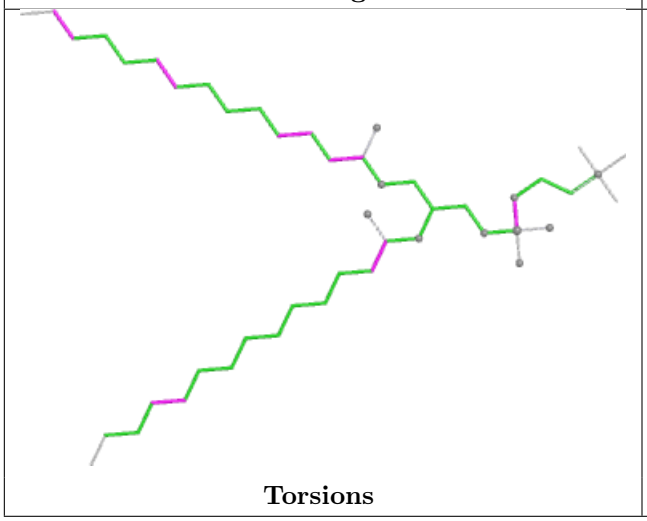
Ligand PX4 B 394



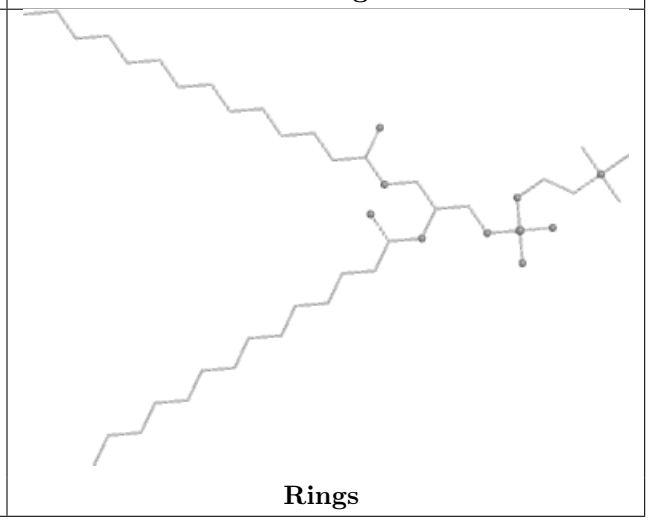
Bond lengths



Bond angles

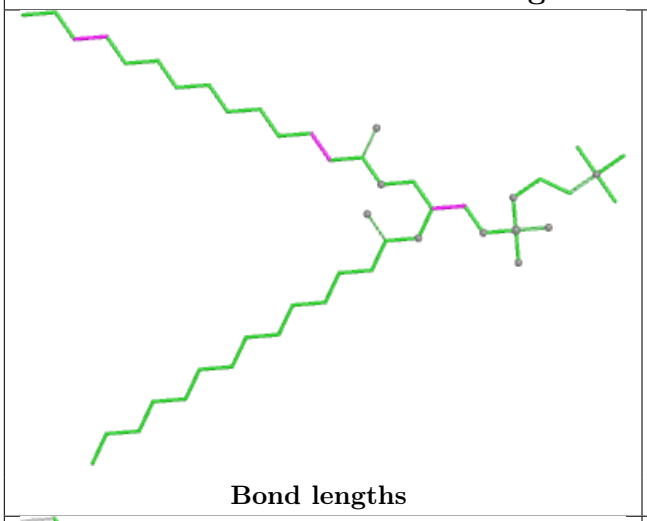


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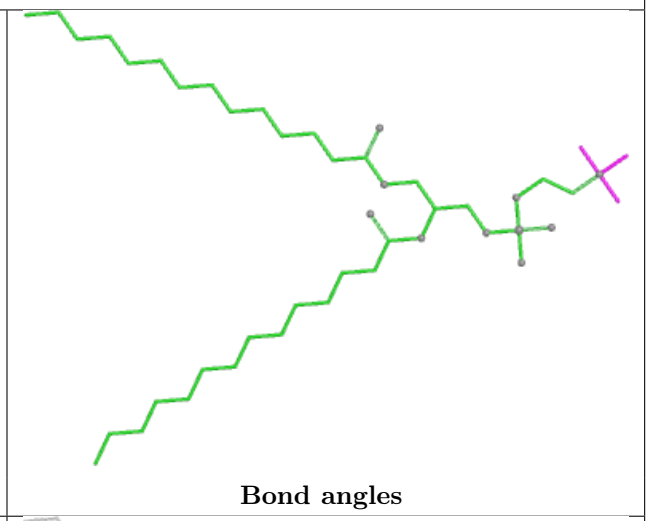


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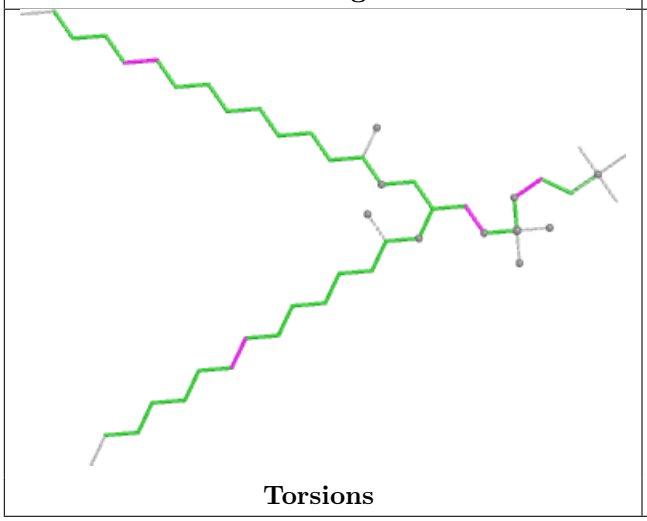
Ligand PX4 B 327



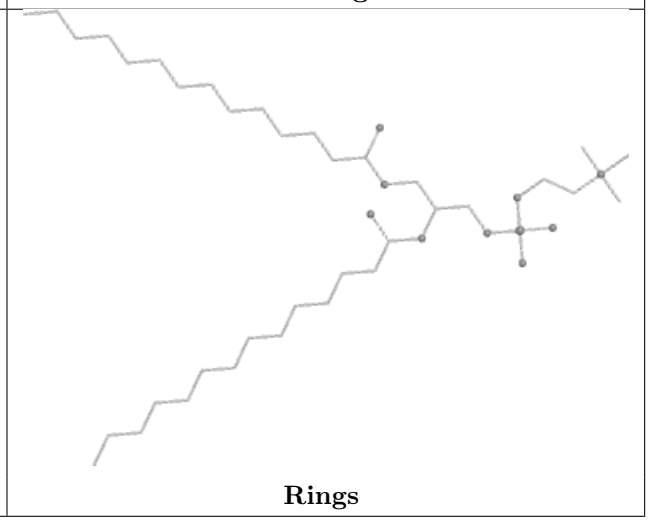
Bond lengths



Bond angles

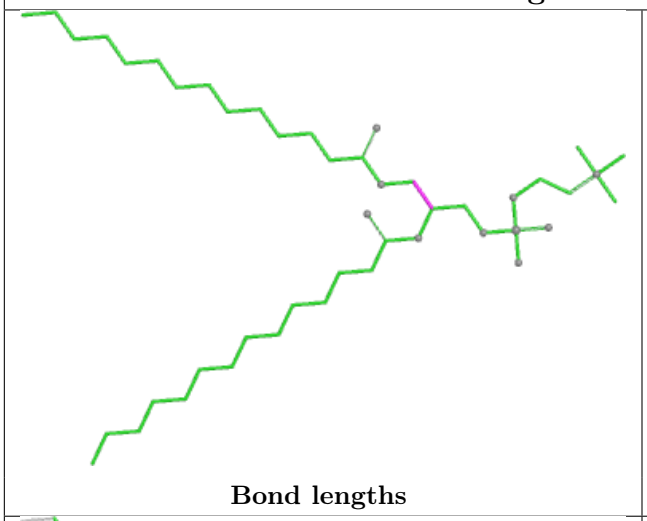


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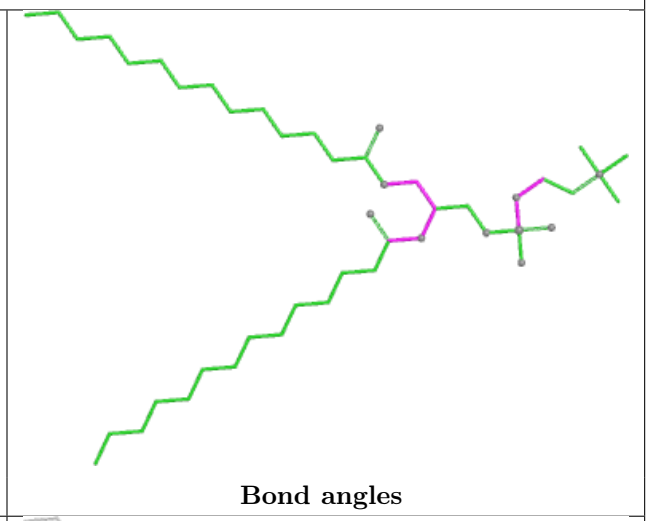


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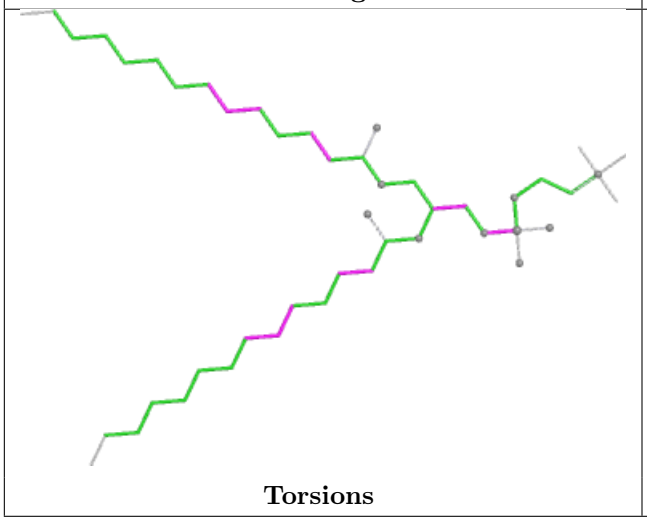
Ligand PX4 C 340



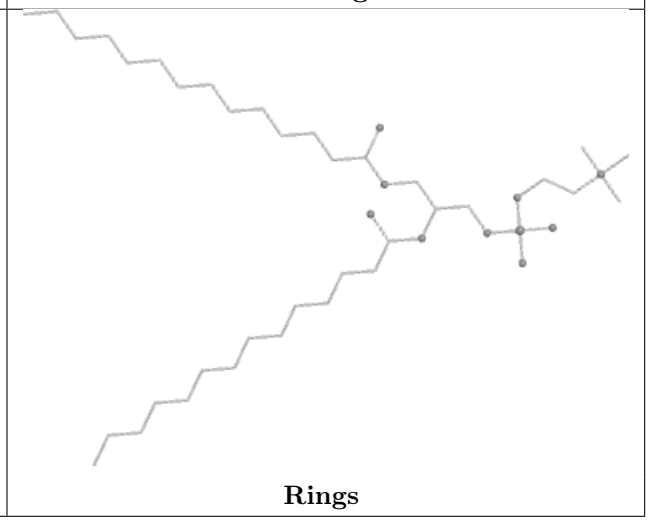
Bond lengths



Bond angles

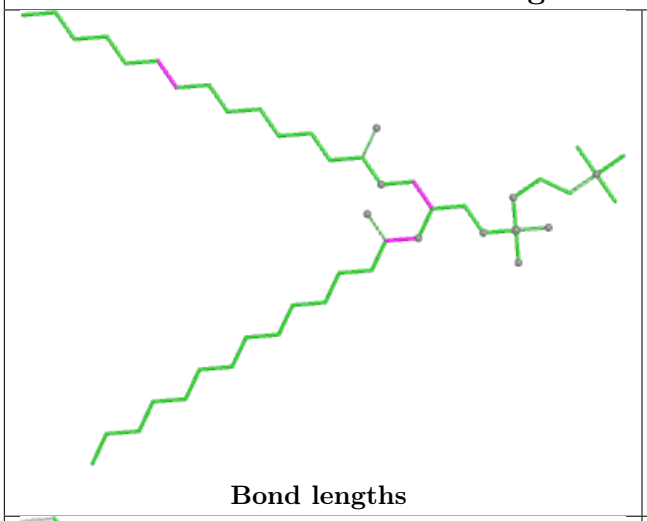


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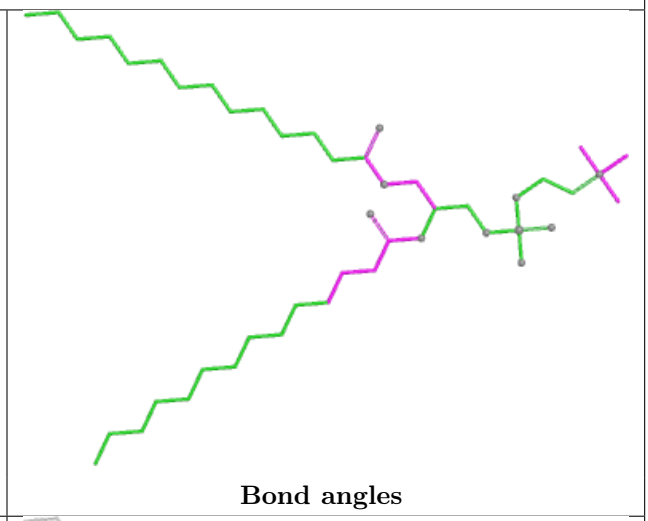


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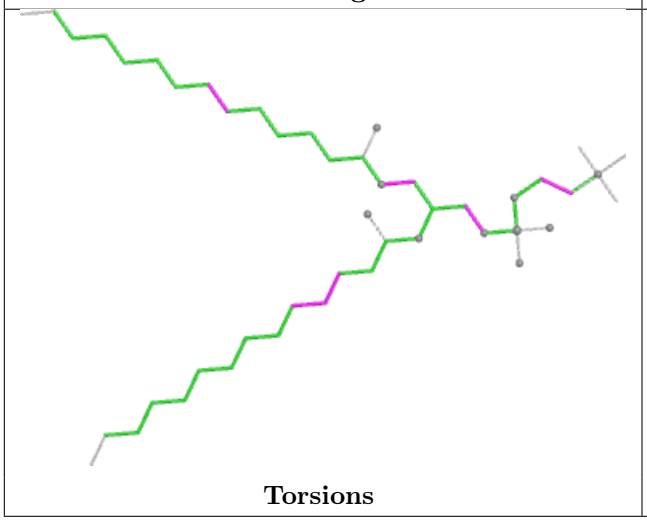
Ligand PX4 C 302



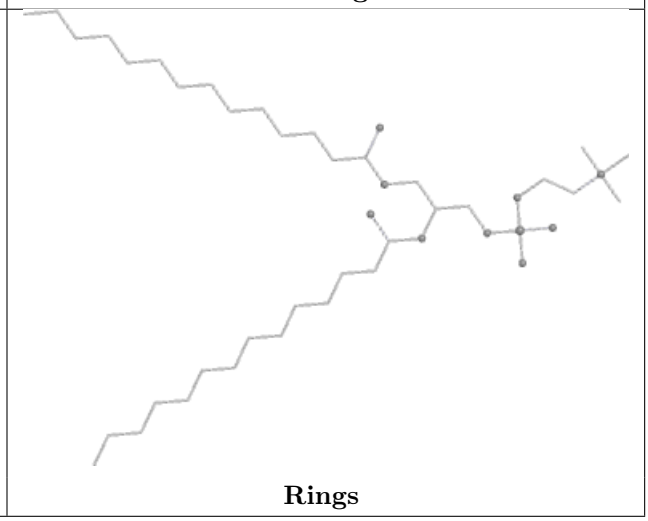
Bond lengths



Bond angles

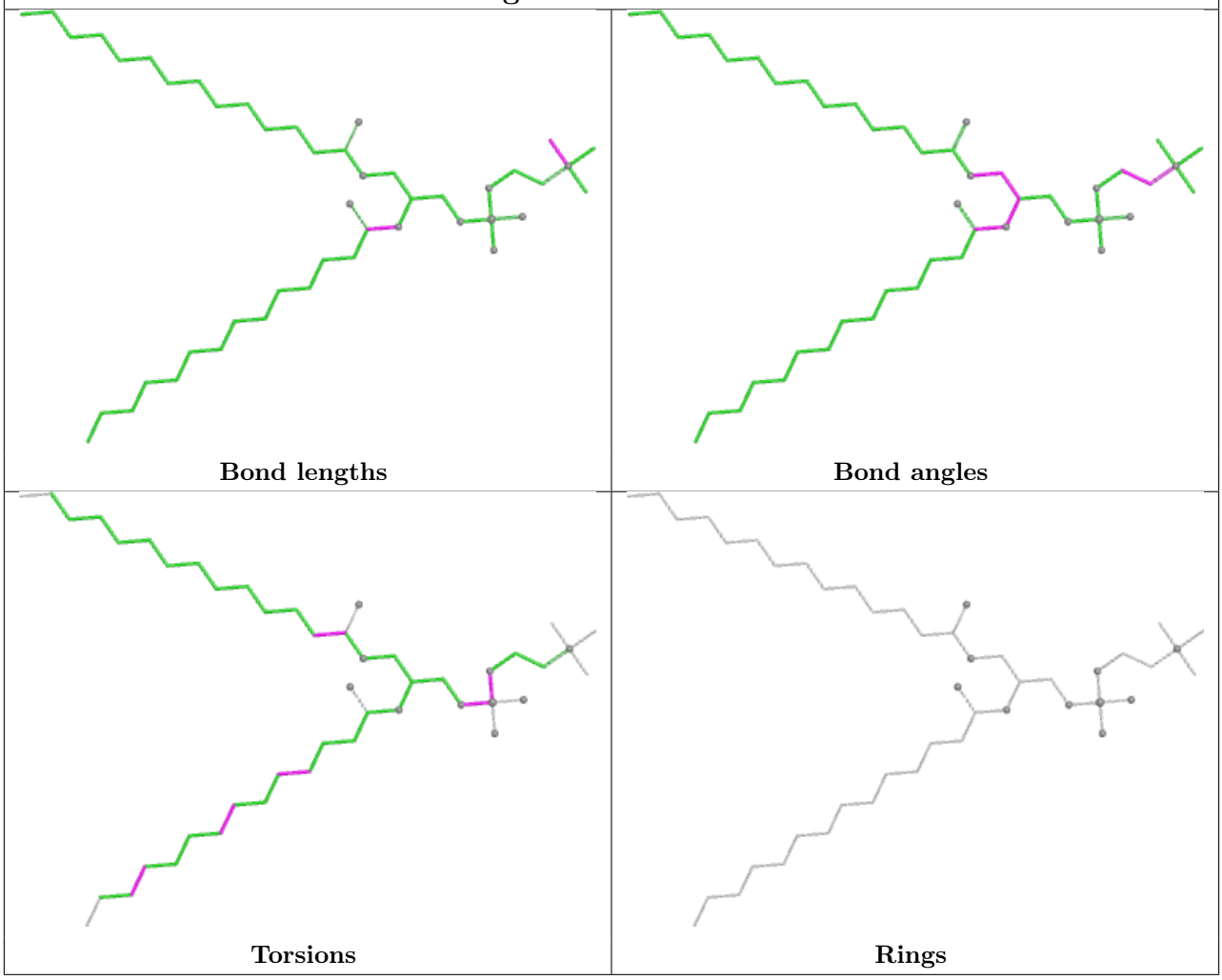


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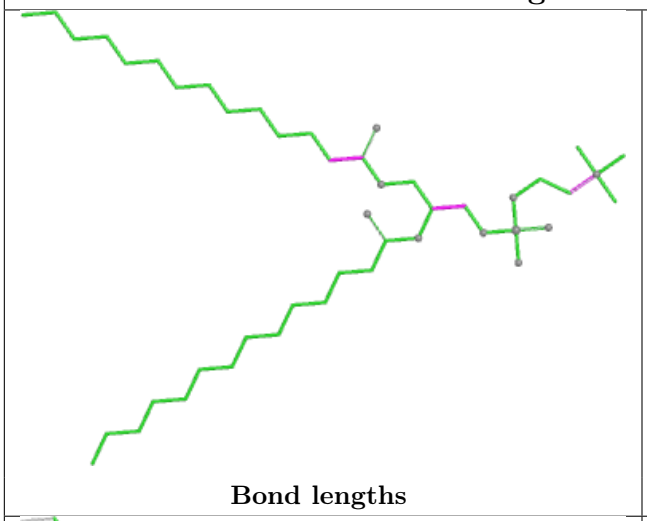


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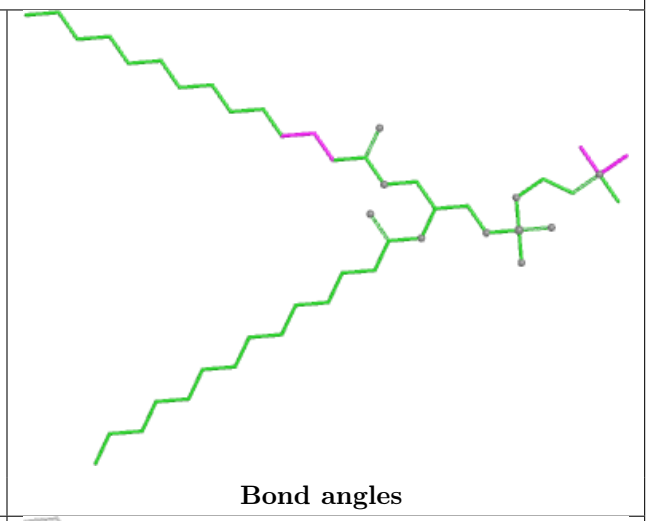
Ligand PX4 B 390



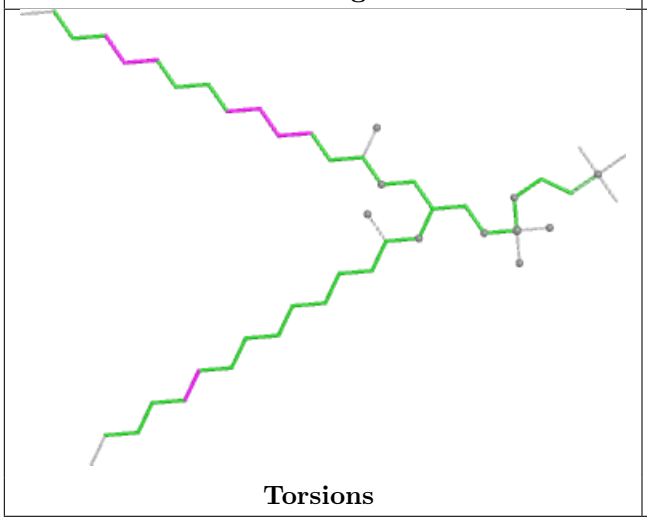
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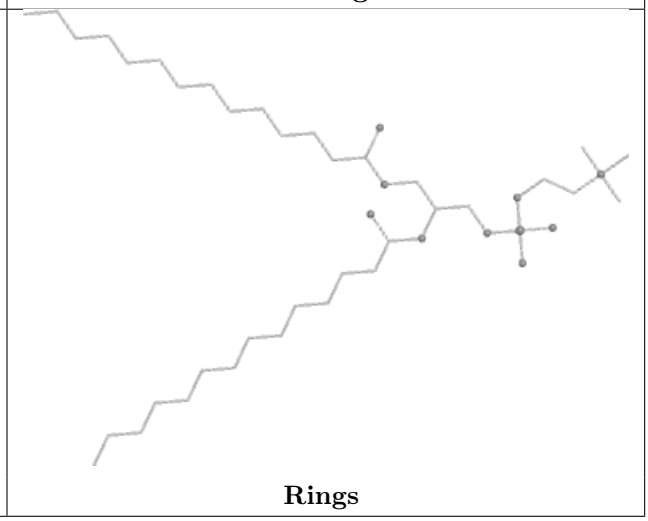
Bond lengths



Bond angles

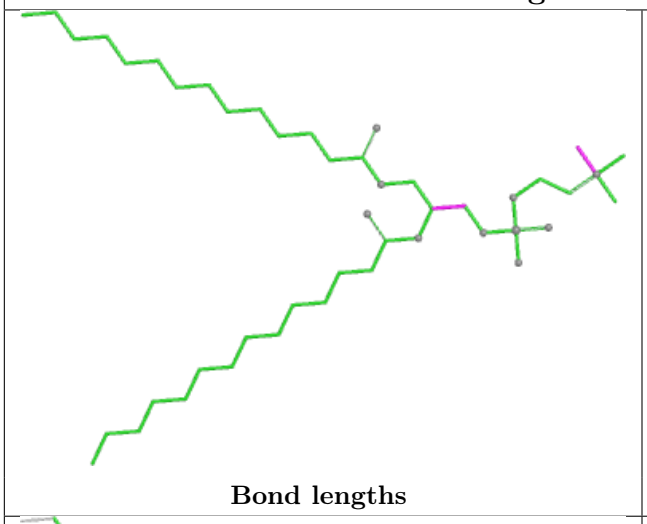


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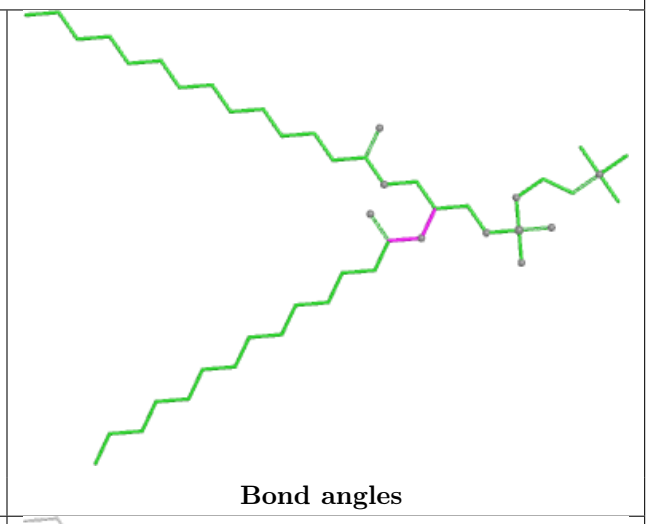


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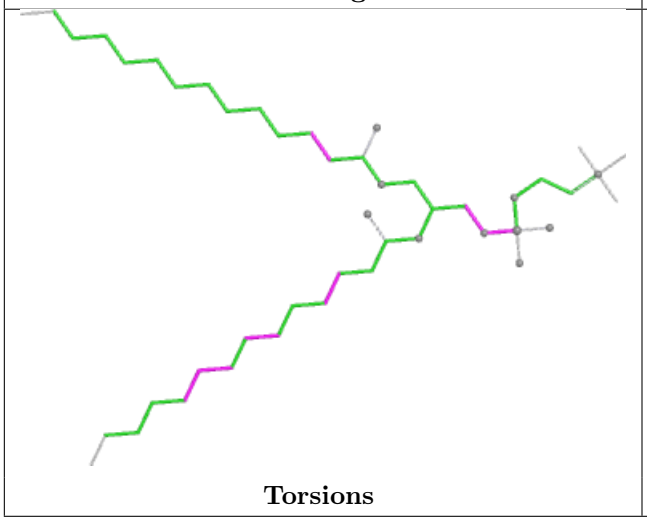
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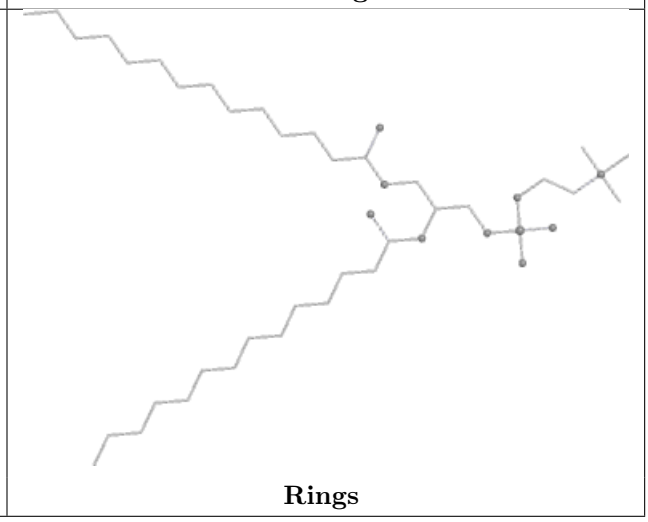
Bond lengths



Bond angles

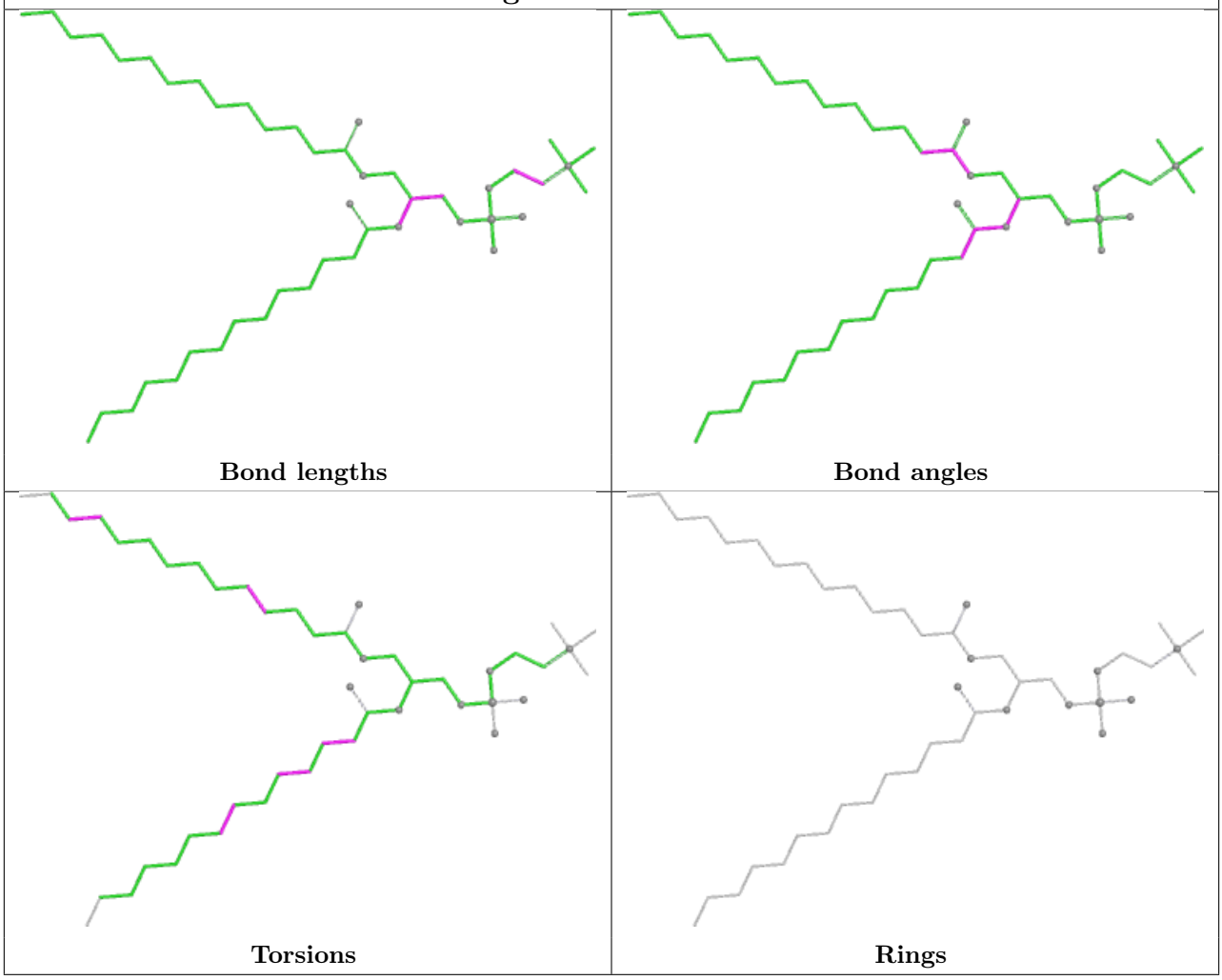


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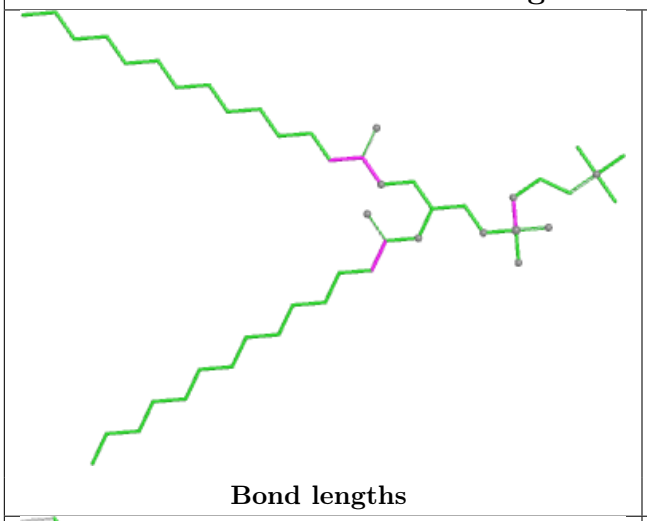


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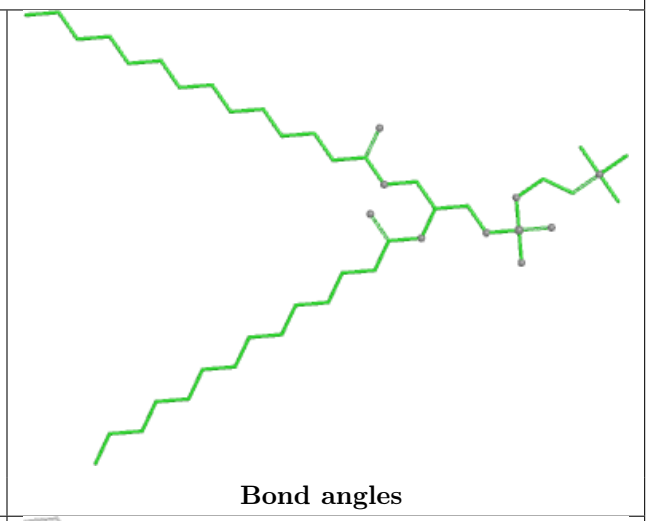
Ligand PX4 B 387



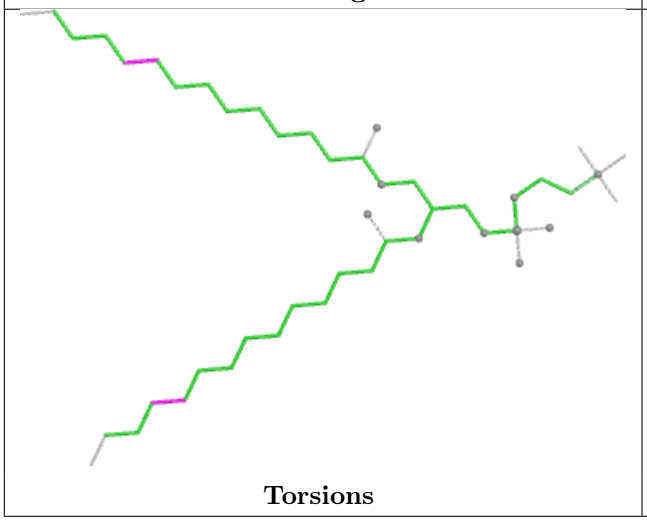
Ligand PX4 C 324



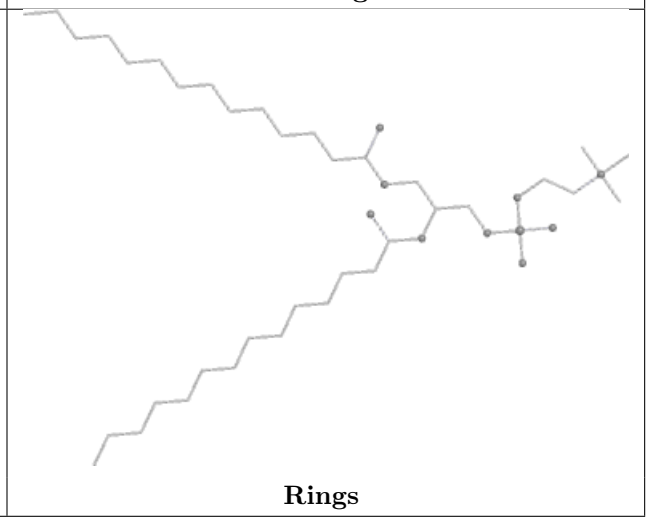
Bond lengths



Bond angles

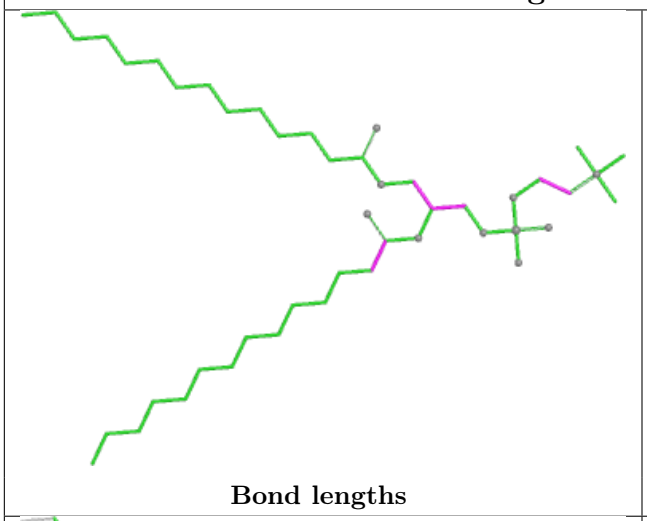


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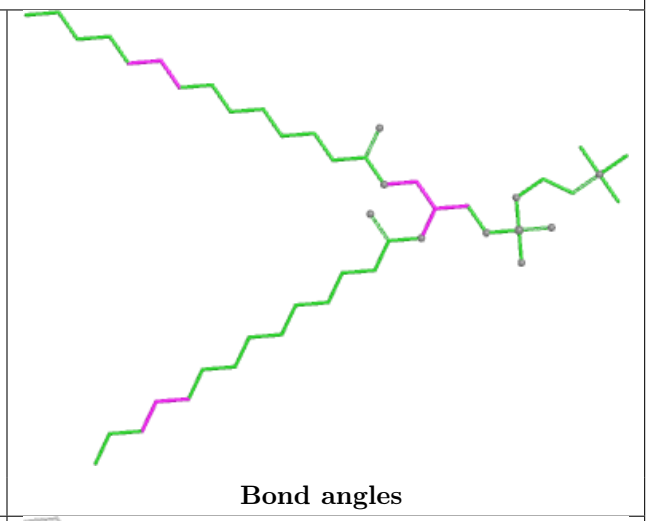


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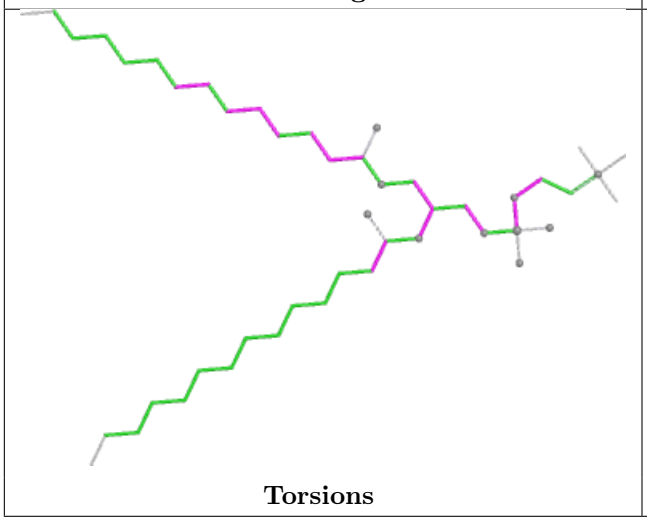
Ligand PX4 C 317



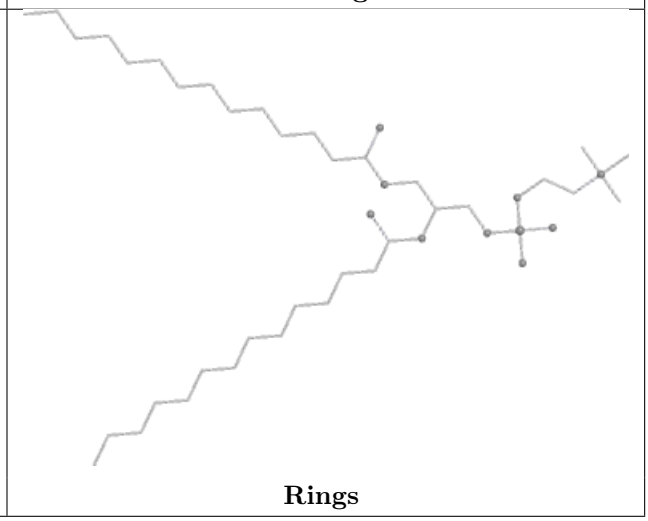
Bond lengths



Bond angles

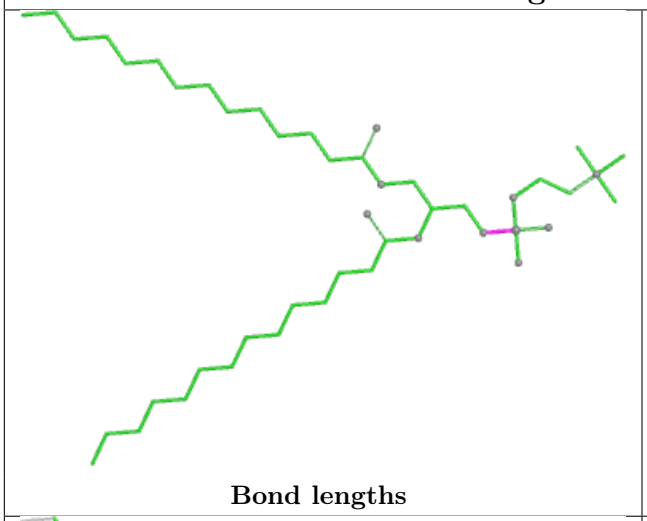


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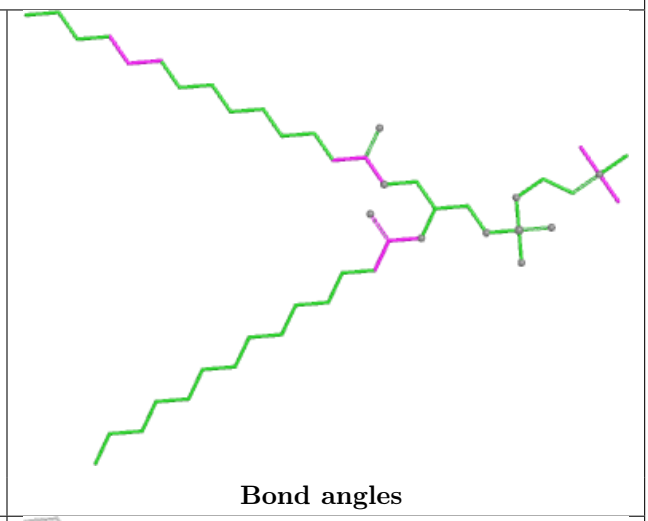


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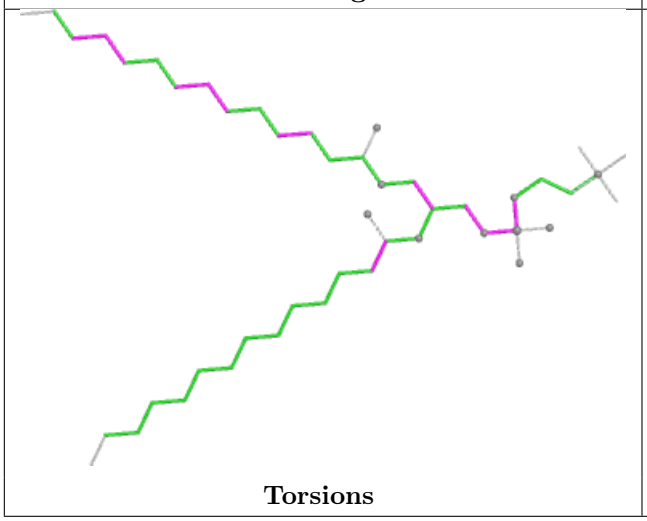
Ligand PX4 B 369



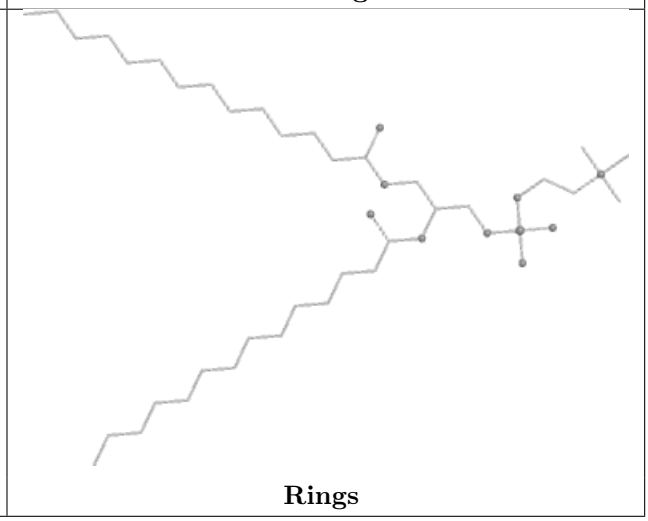
Bond lengths



Bond angles

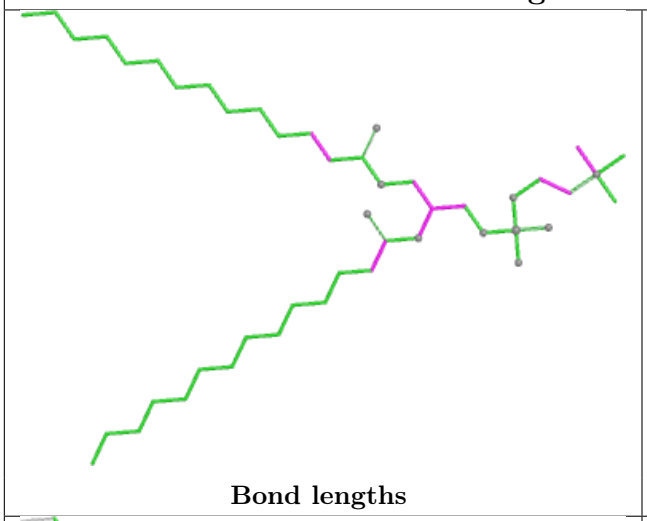


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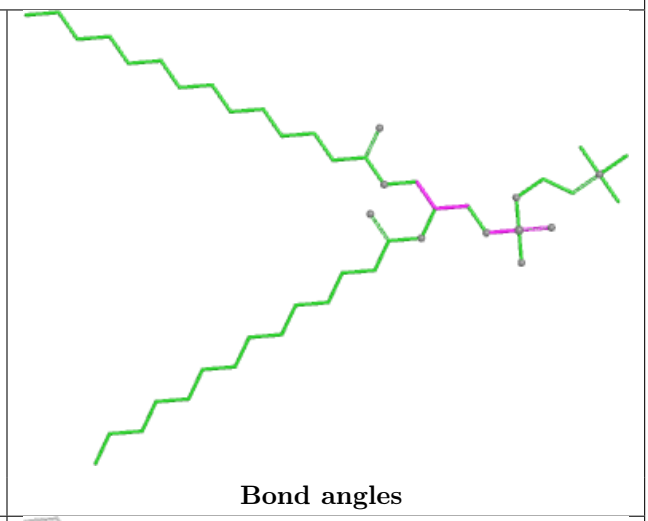


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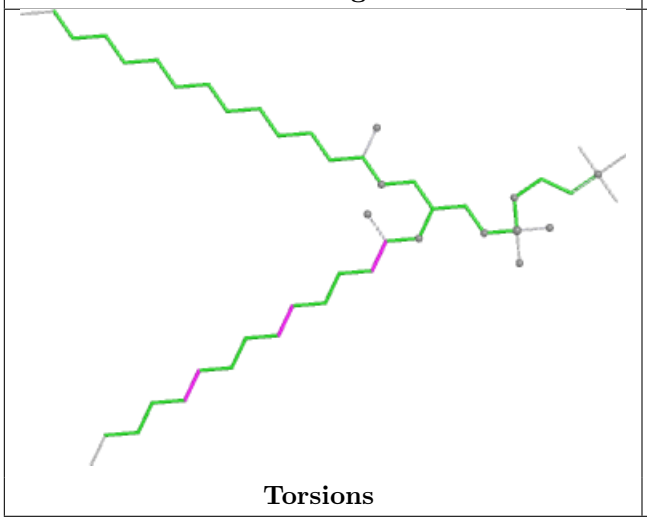
Ligand PX4 B 344



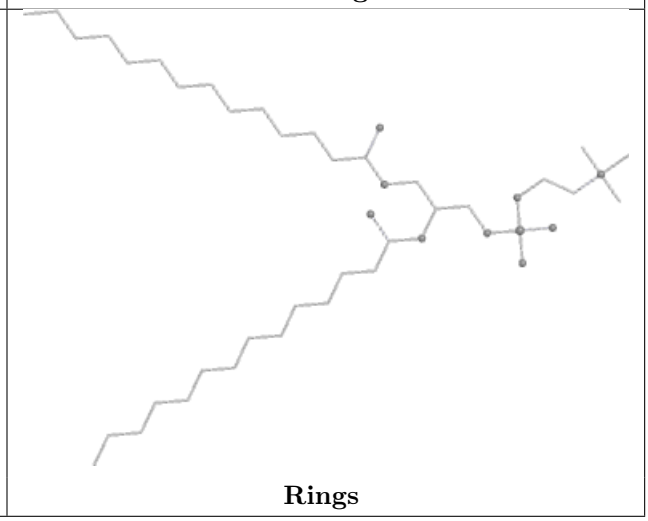
Bond lengths



Bond angles

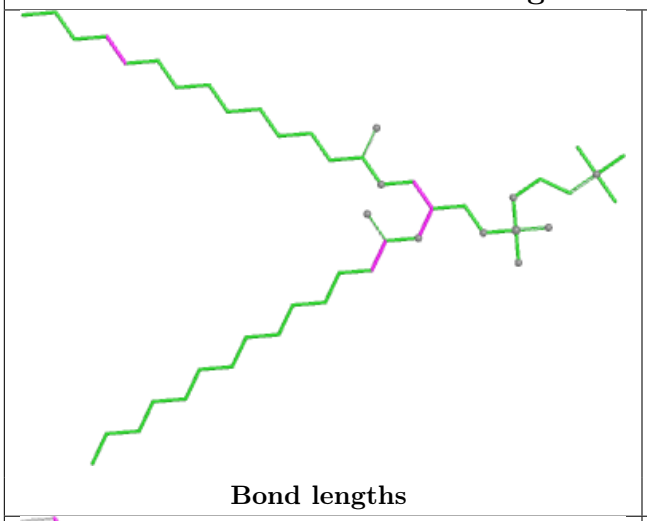


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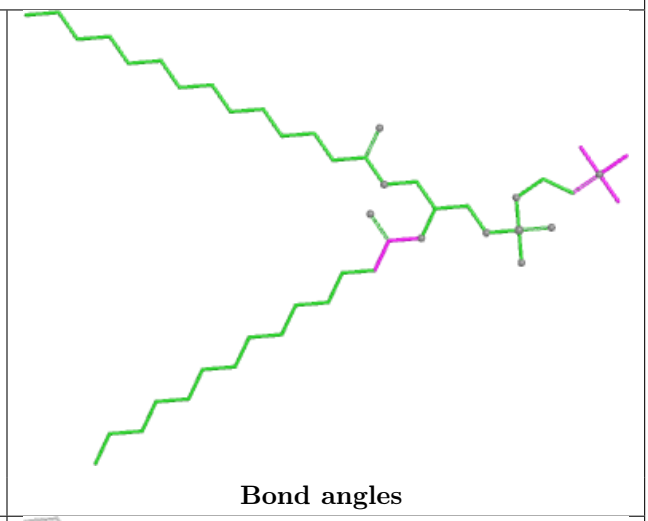


Rings

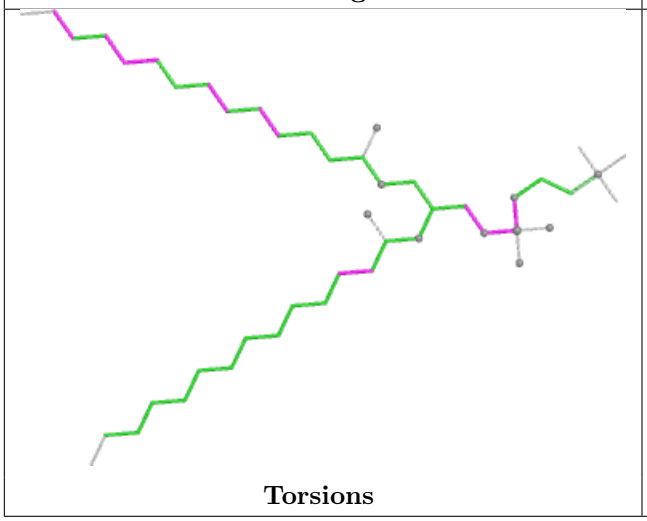
Ligand PX4 A 650



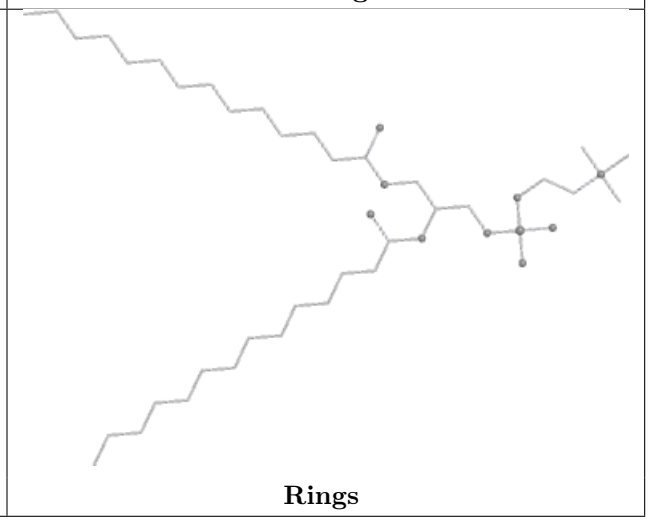
Bond lengths



Bond angles

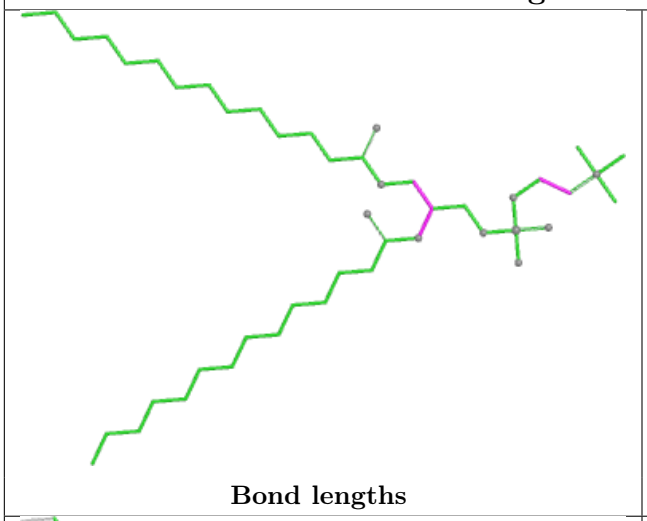


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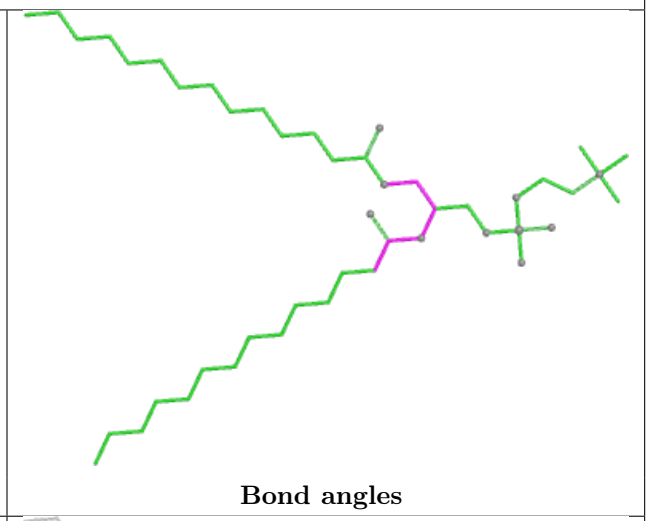


Rings

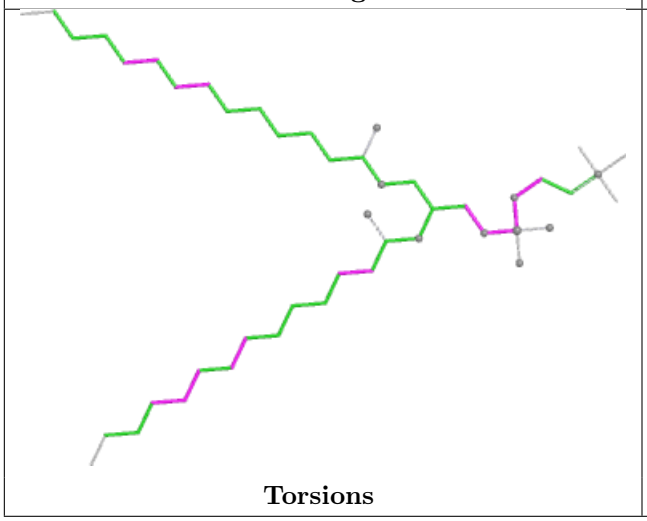
Ligand PX4 B 302



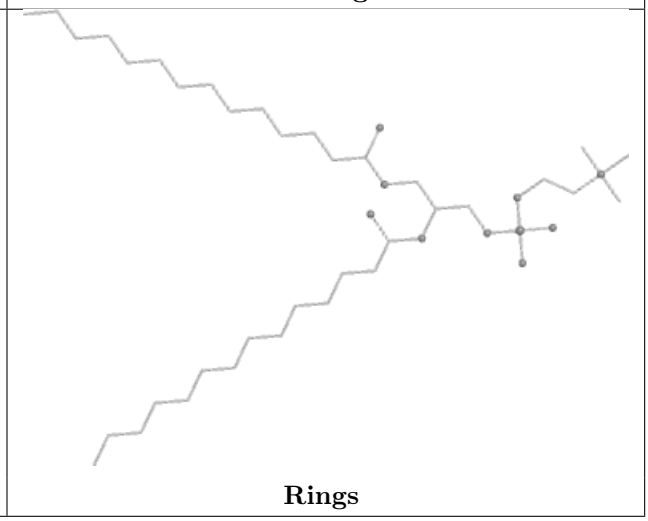
Bond lengths



Bond angles

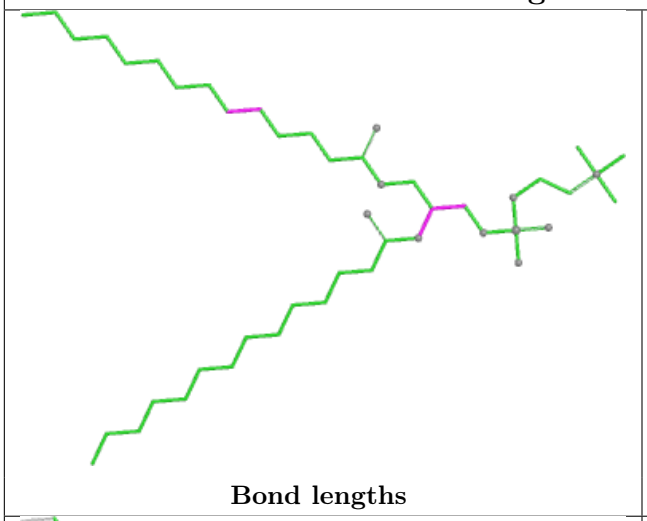


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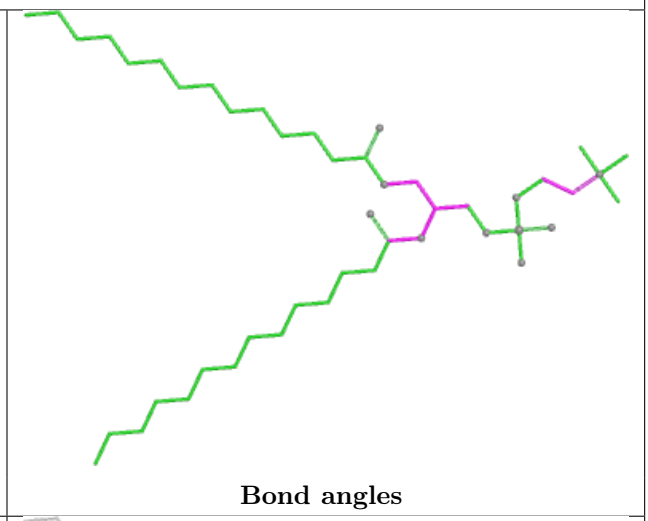


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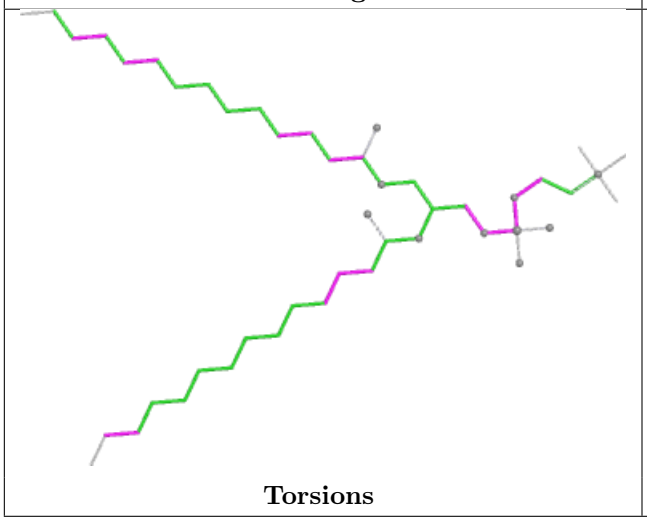
Ligand PX4 B 357



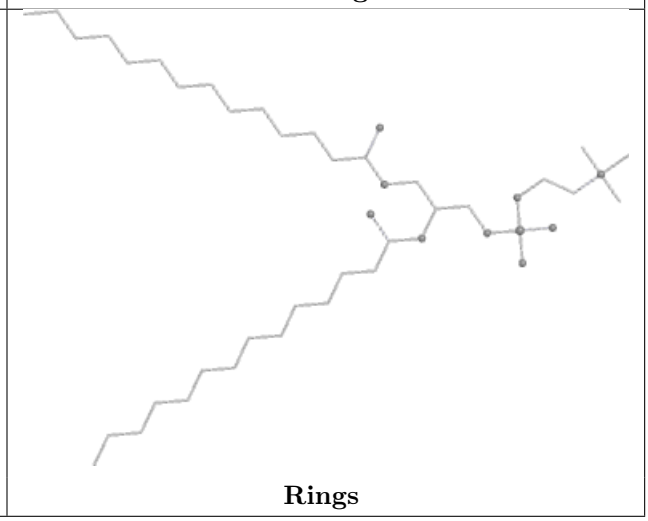
Bond lengths



Bond angles

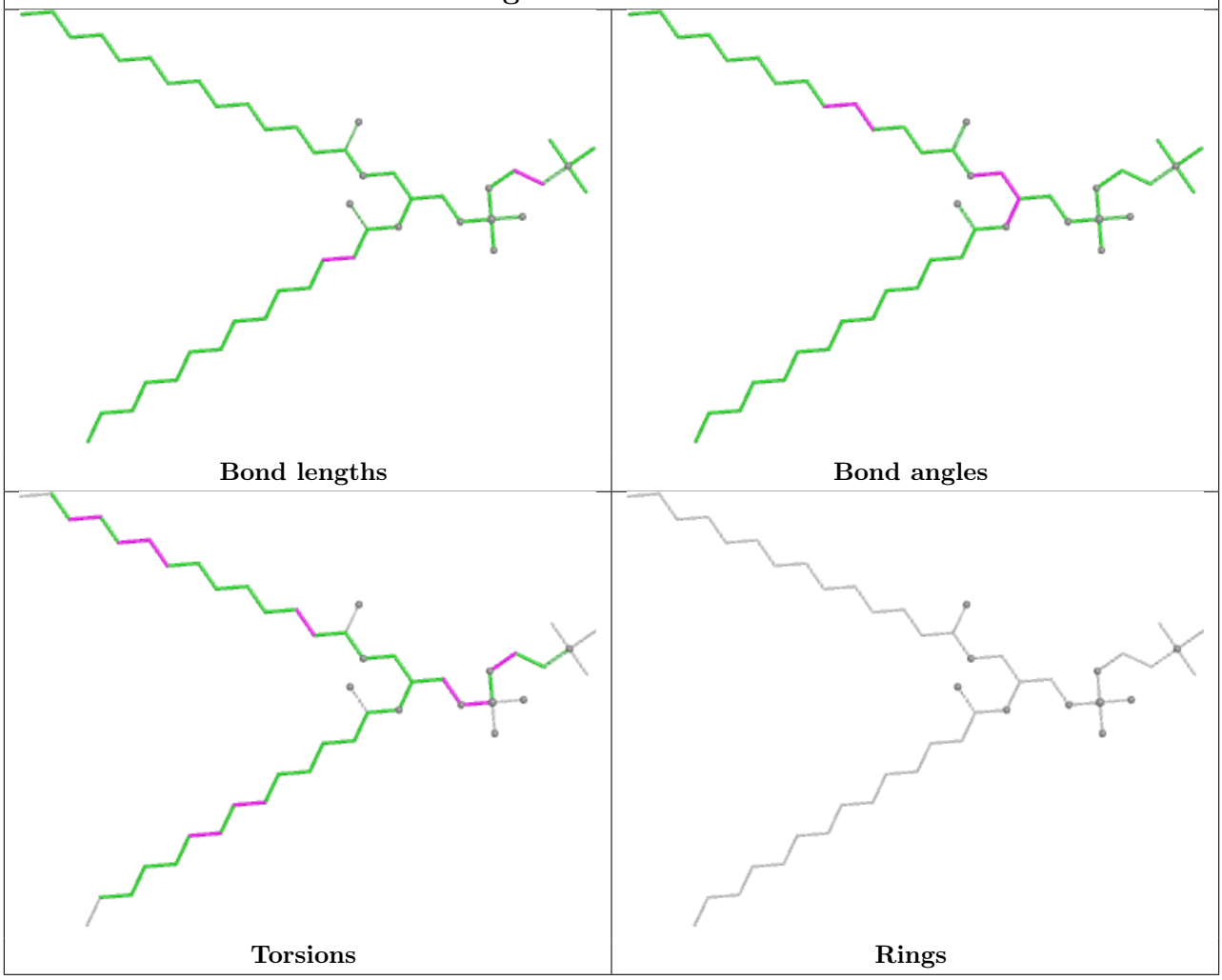


Torsions

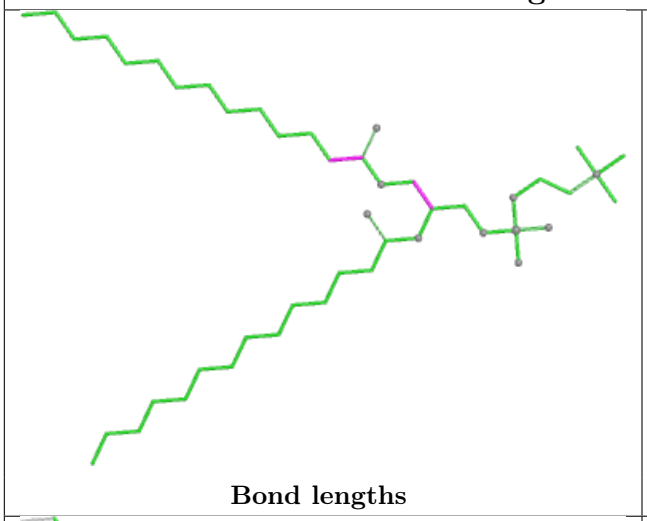


Rings

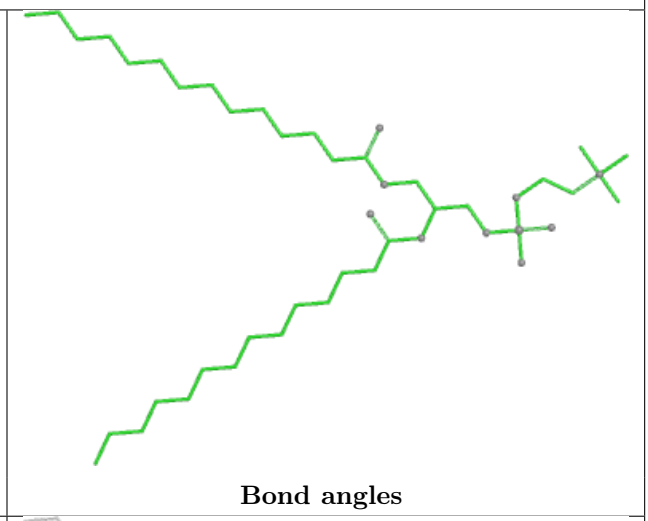
Ligand PX4 B 340



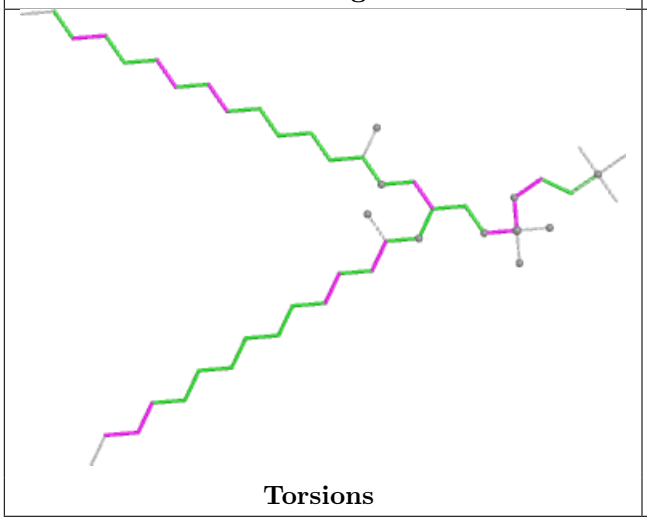
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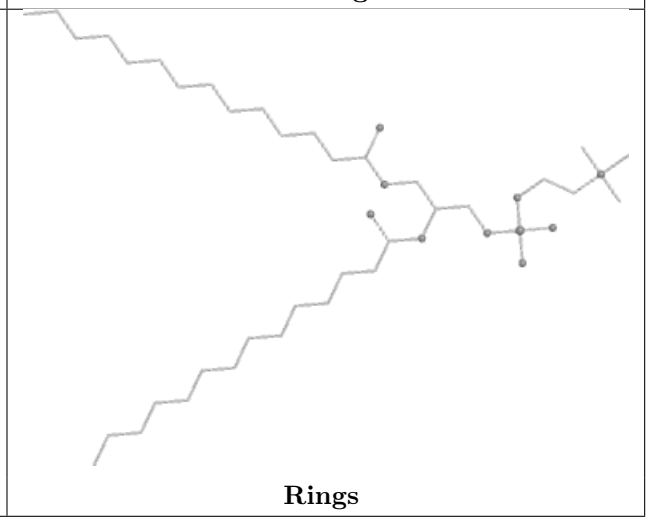
Bond lengths



Bond angles

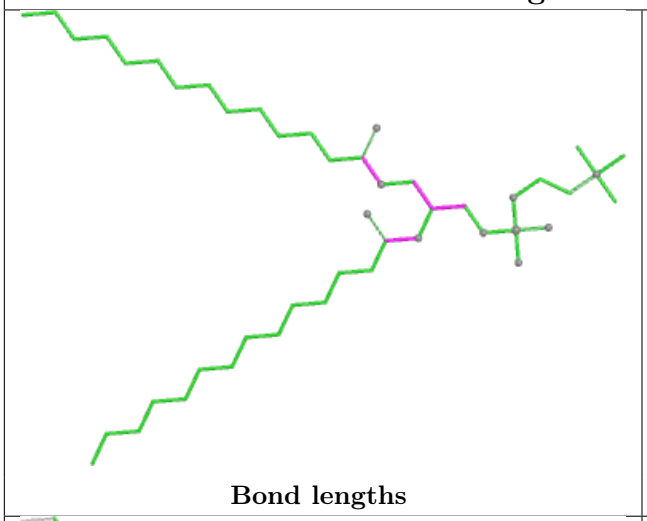


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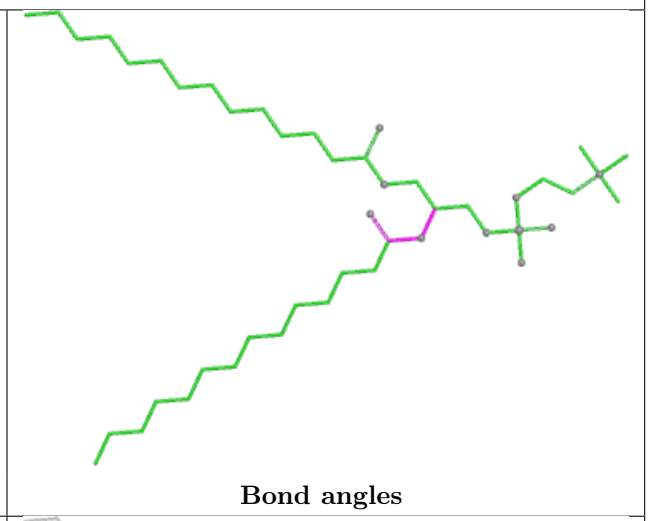


Rings

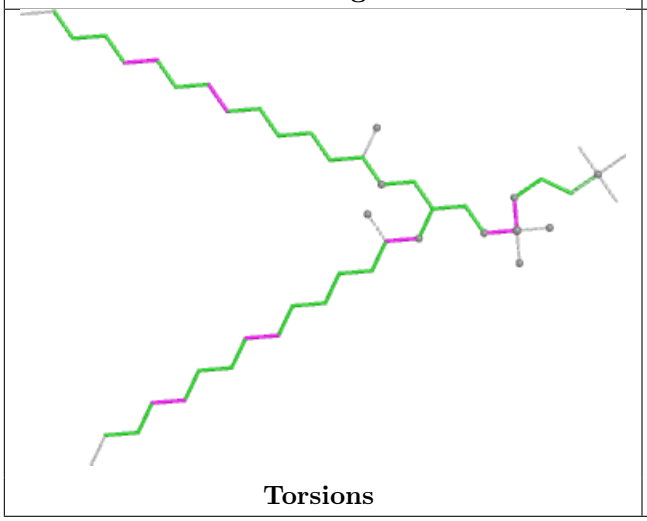
Ligand PX4 C 314



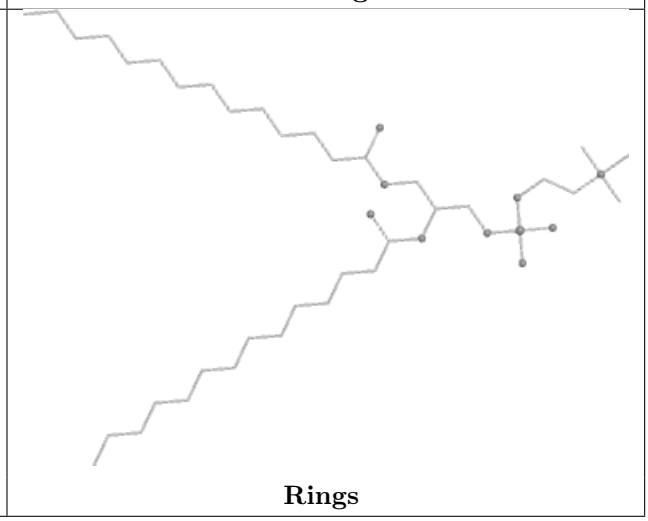
Bond lengths



Bond angles

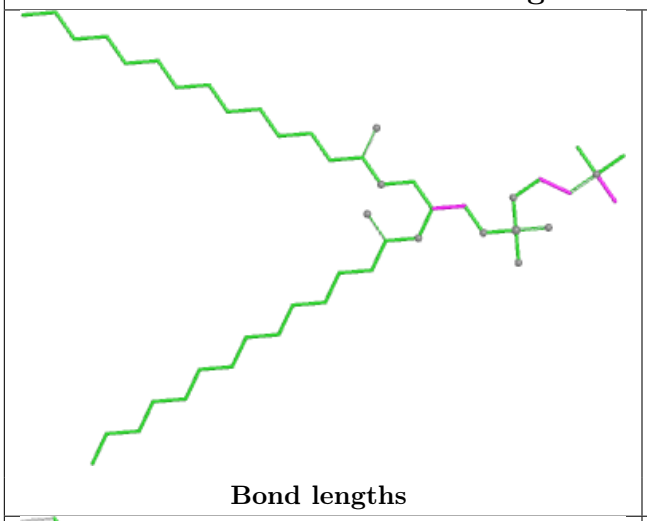


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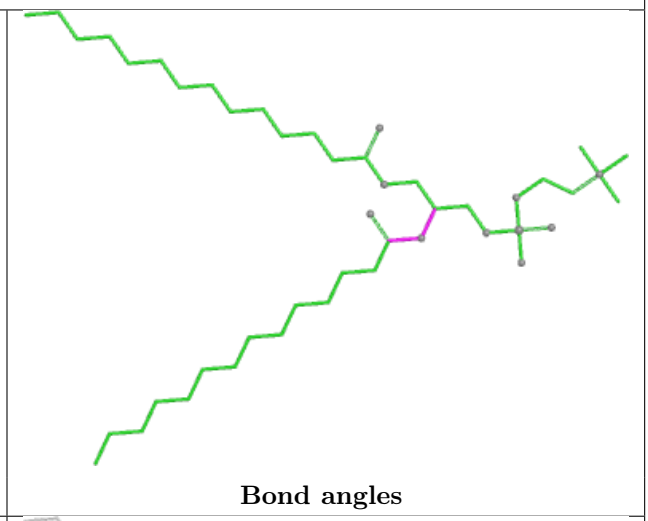


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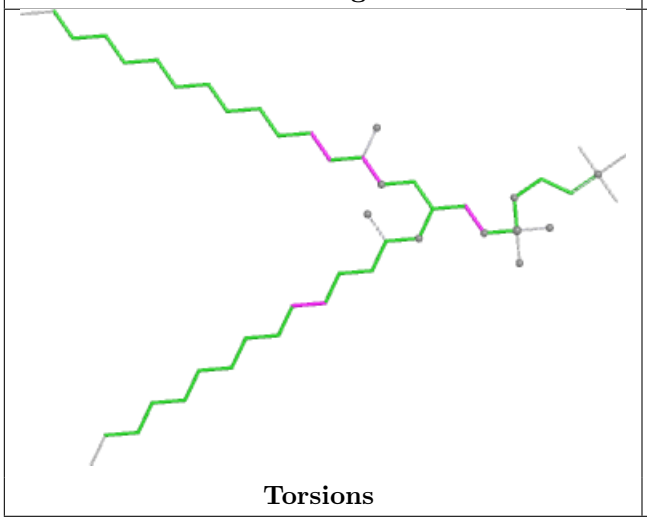
Ligand PX4 A 646



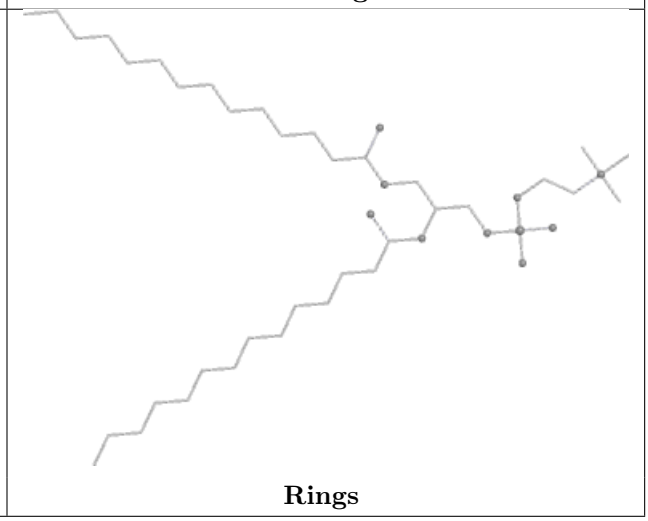
Bond lengths



Bond angles

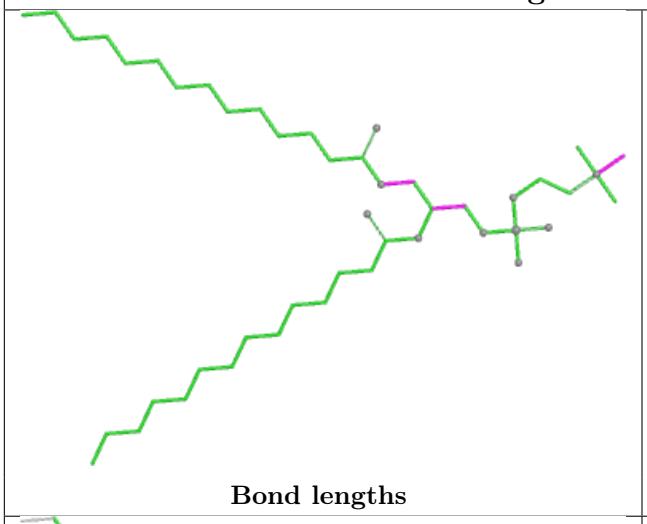


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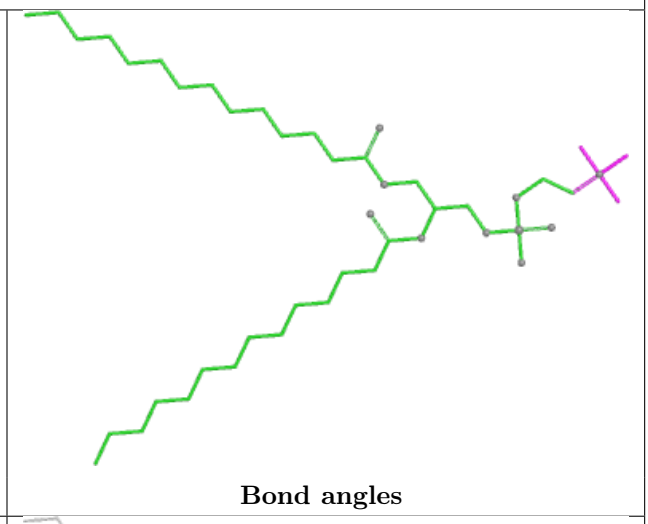


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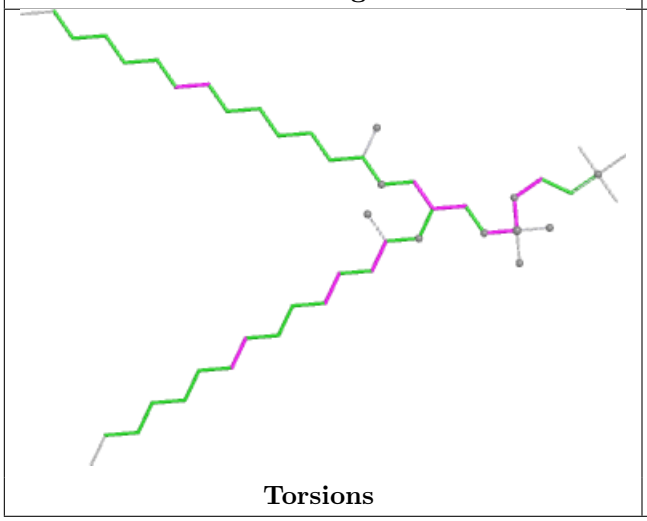
Ligand PX4 C 304



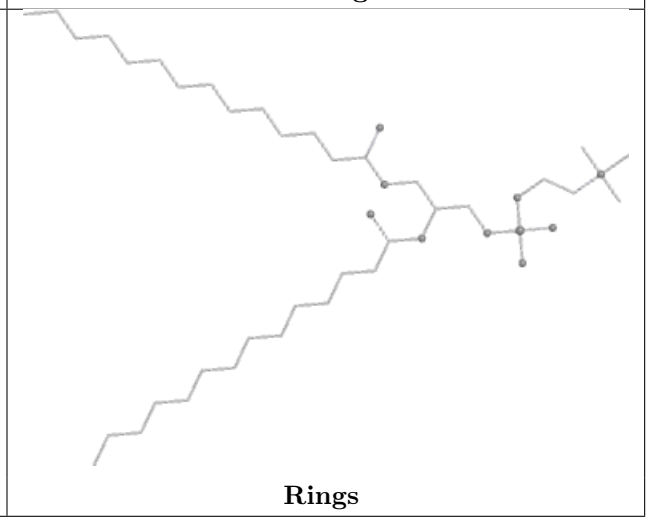
Bond lengths



Bond angles

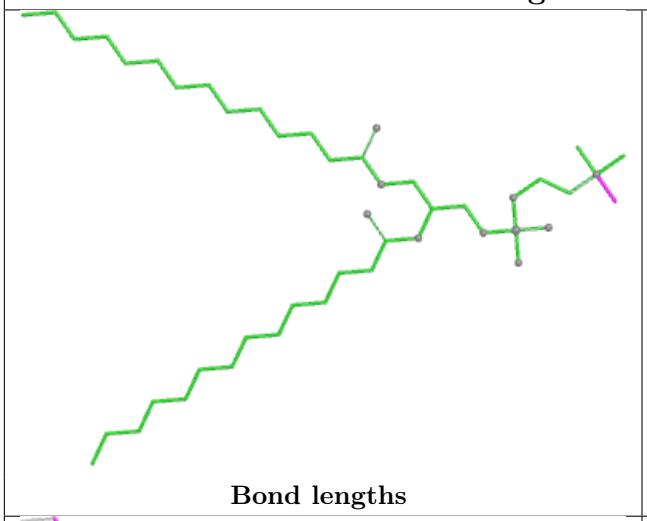


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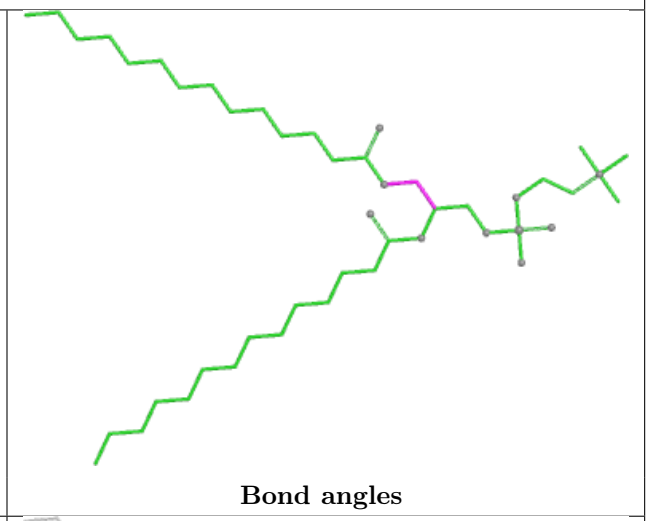


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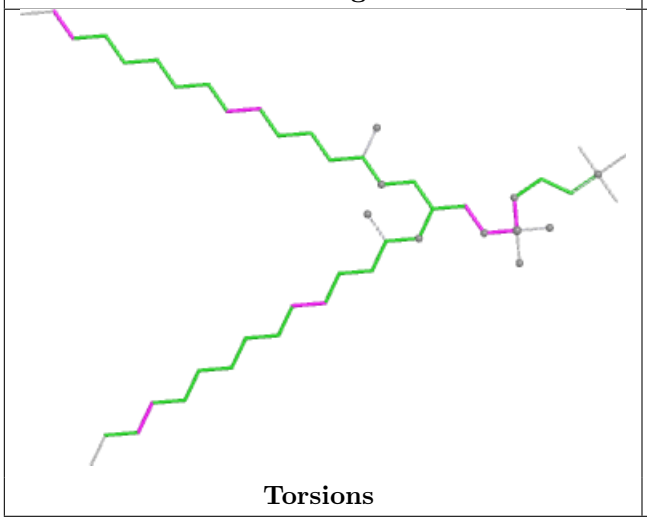
Ligand PX4 B 365



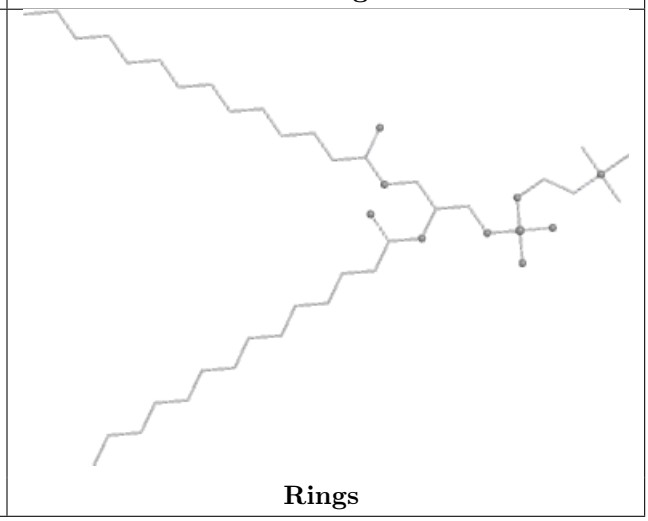
Bond lengths



Bond angles

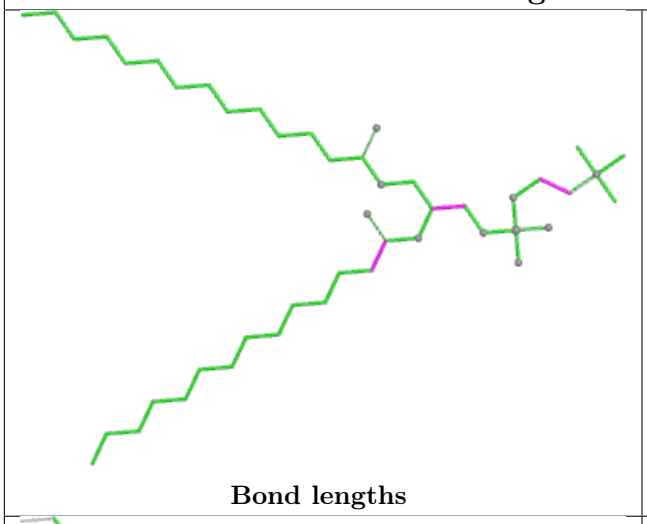


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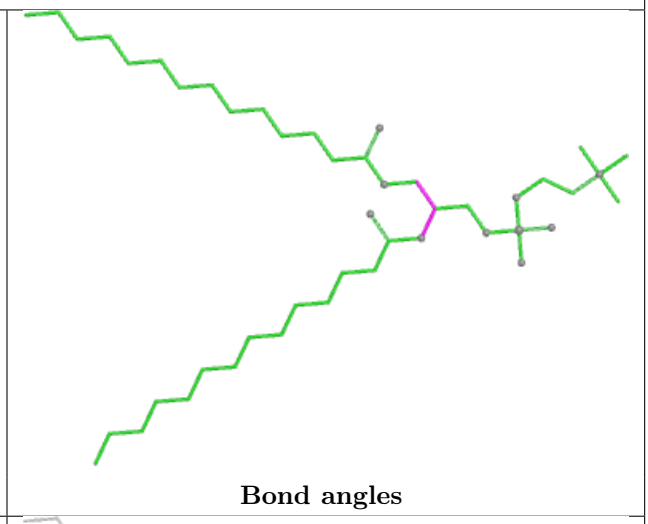


Rings

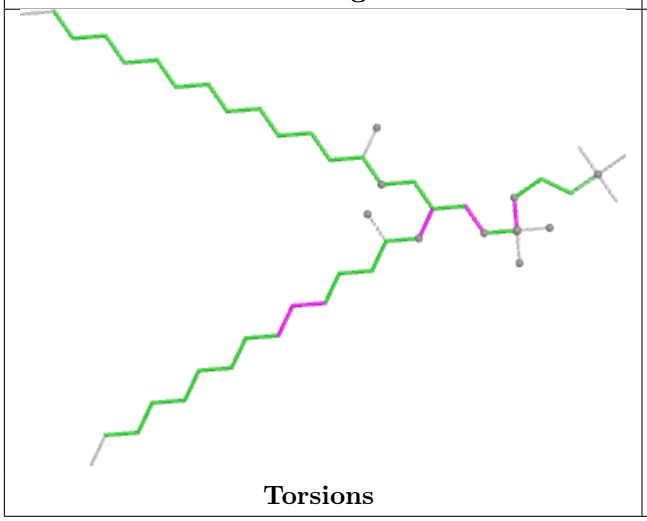
Ligand PX4 B 316



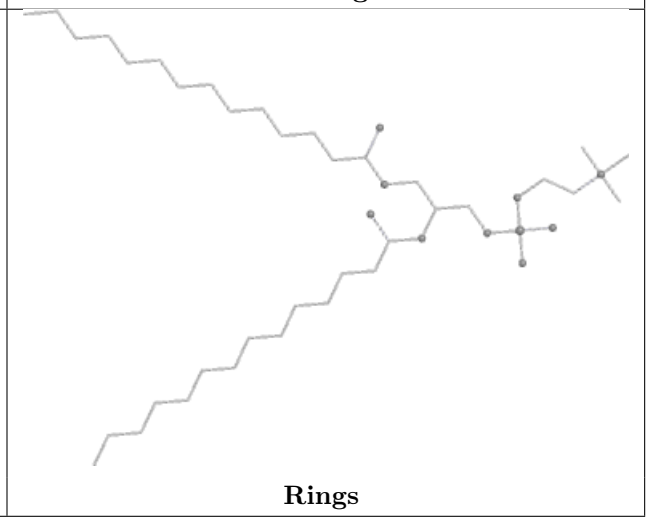
Bond lengths



Bond angles

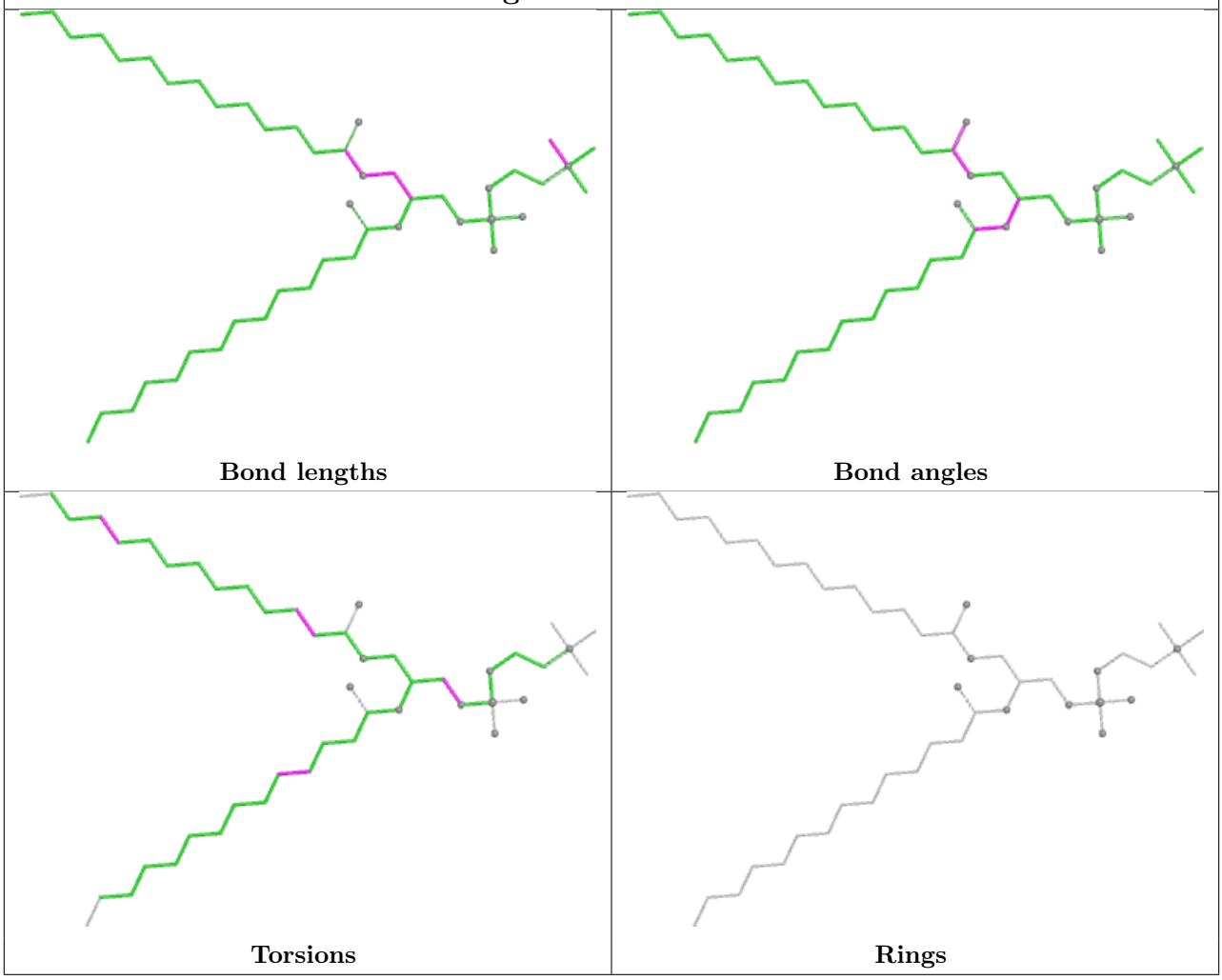


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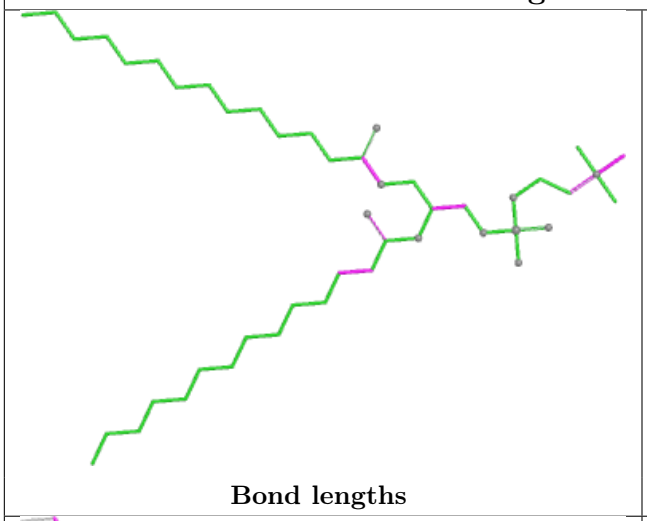


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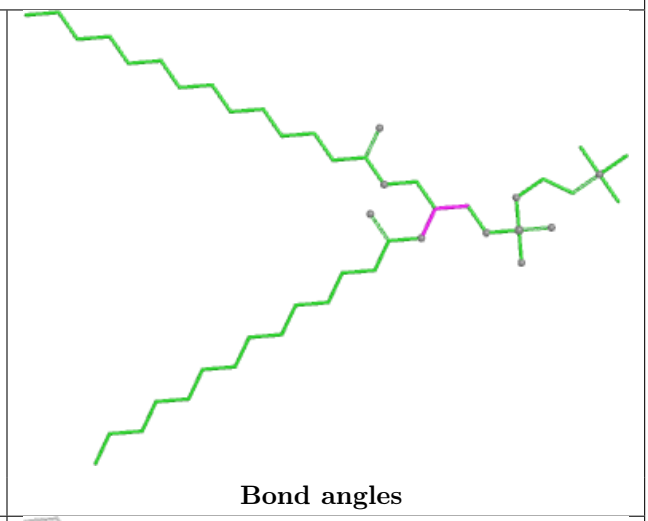
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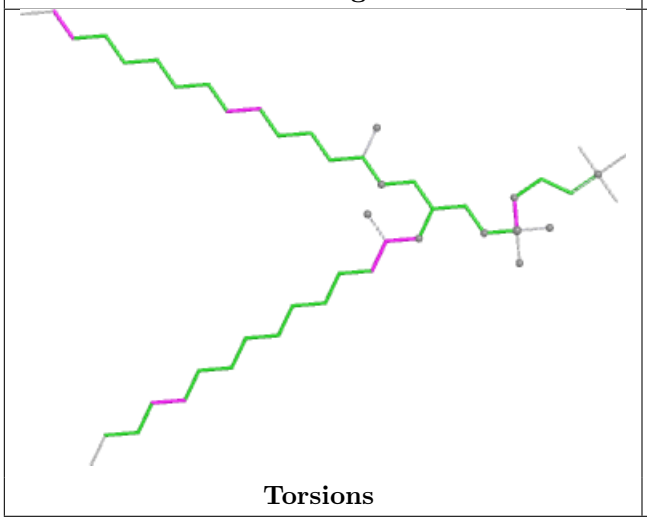
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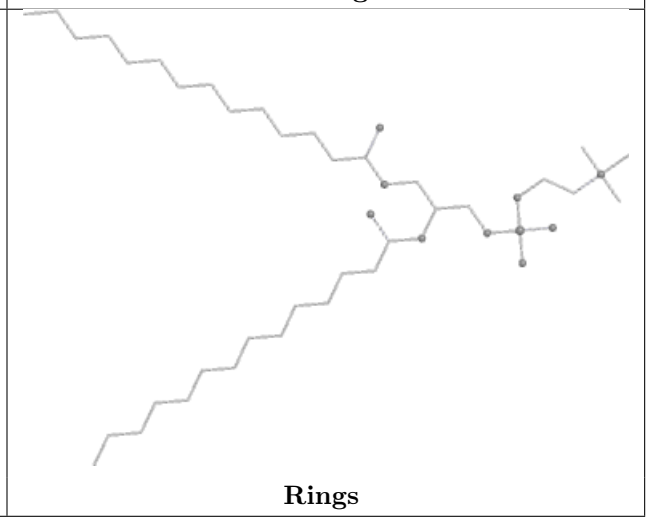
Bond lengths



Bond angles

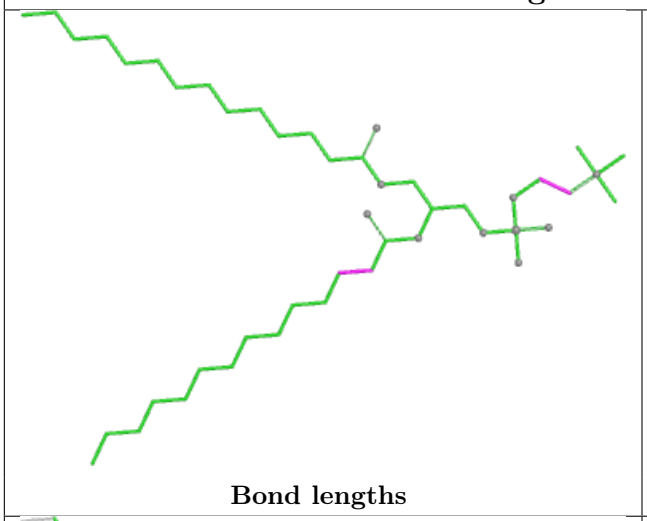


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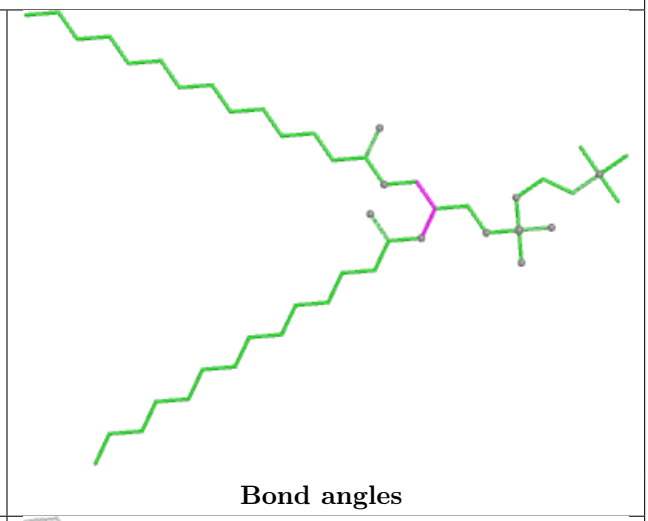


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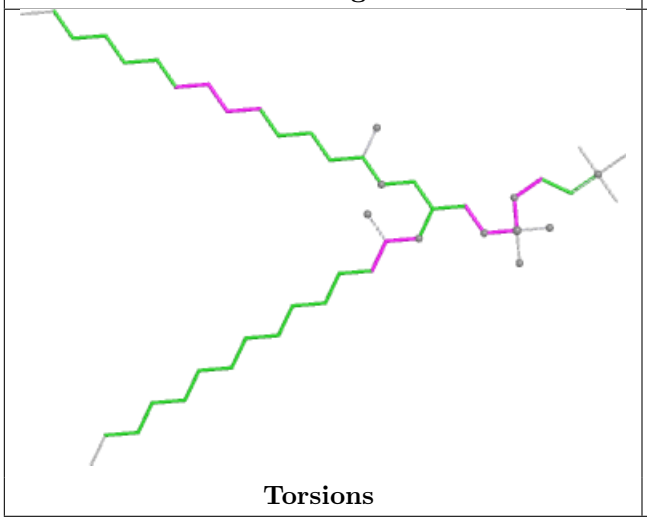
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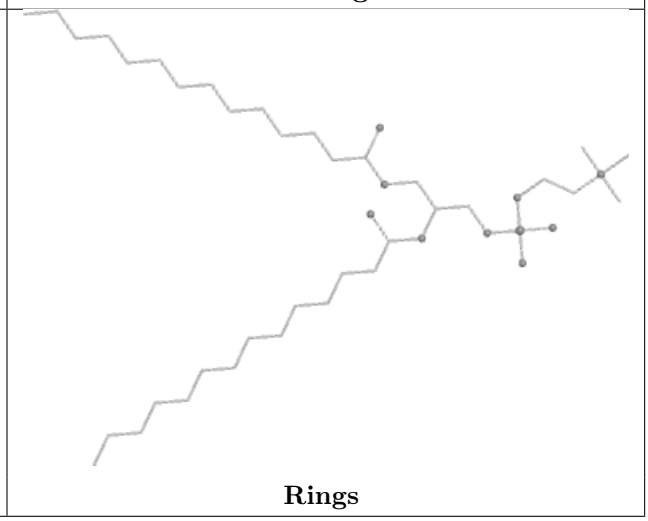
Bond lengths



Bond angles

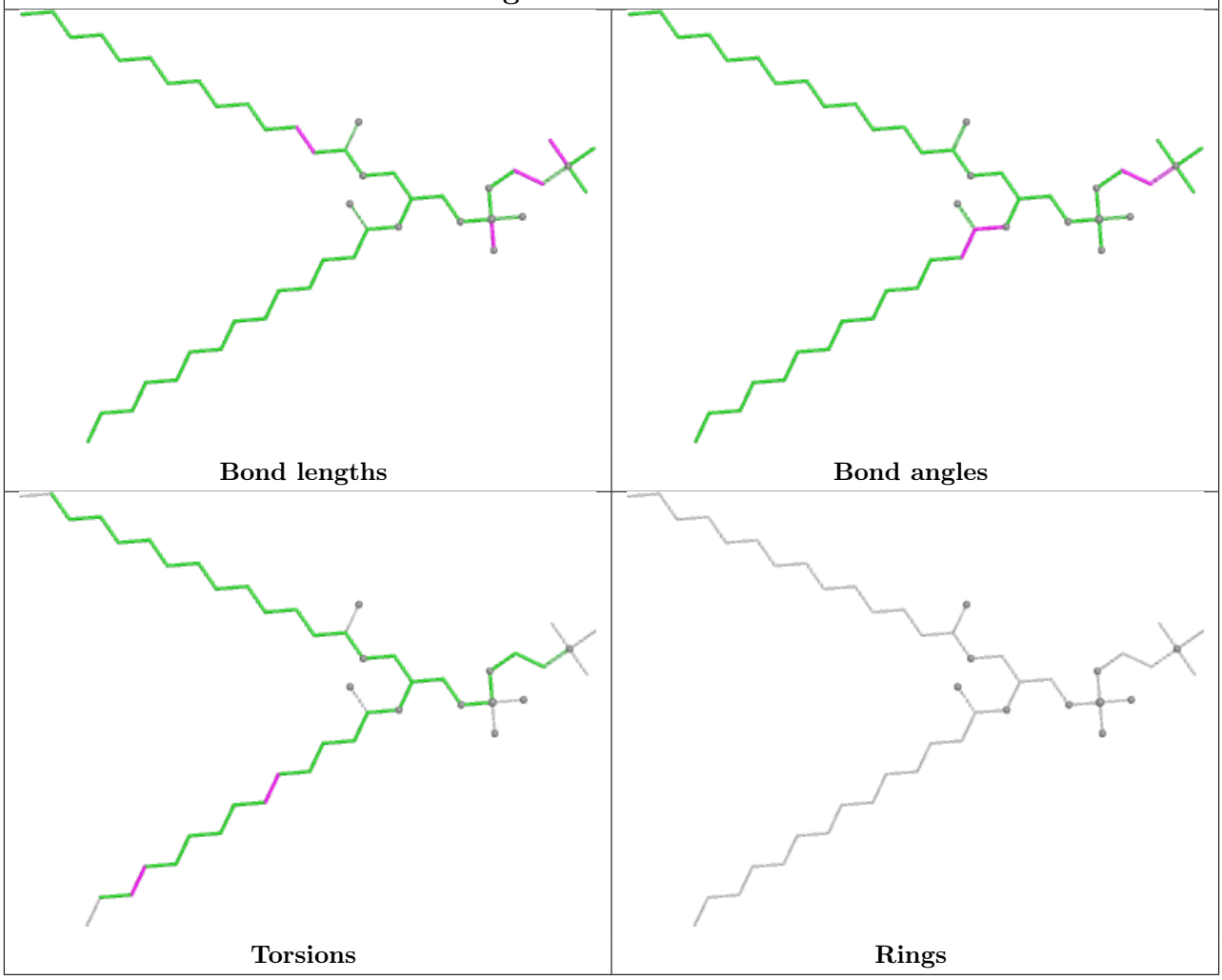


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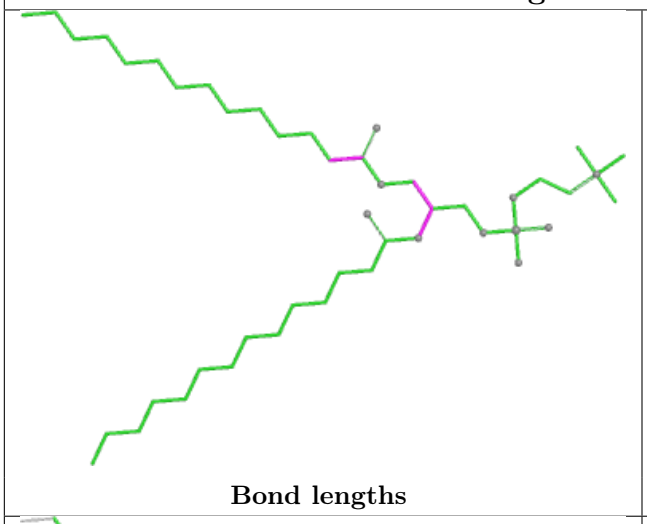


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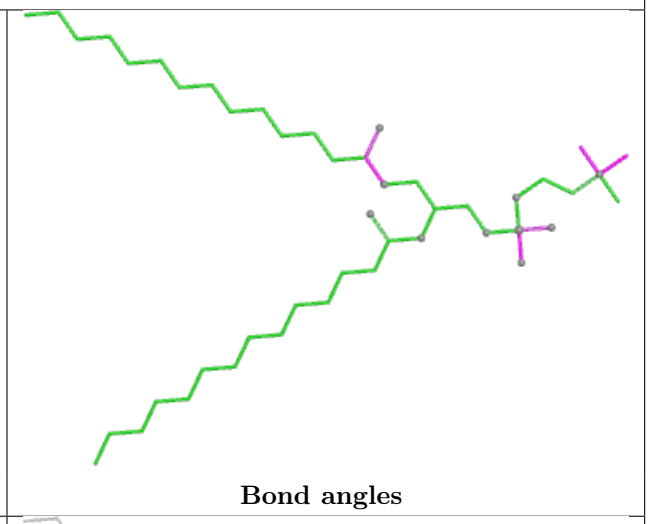
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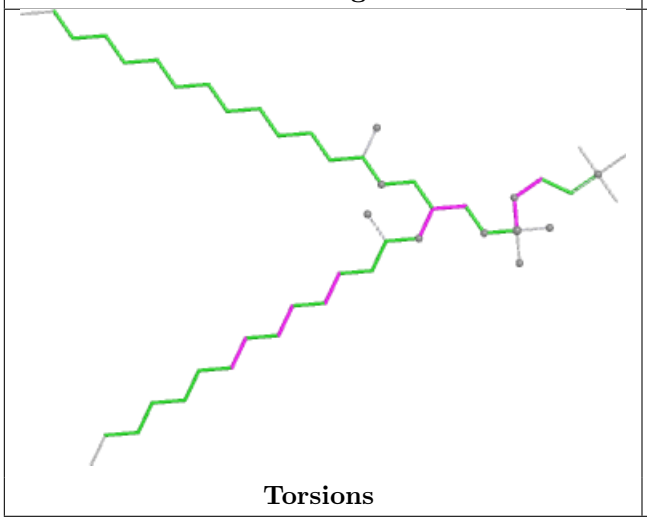
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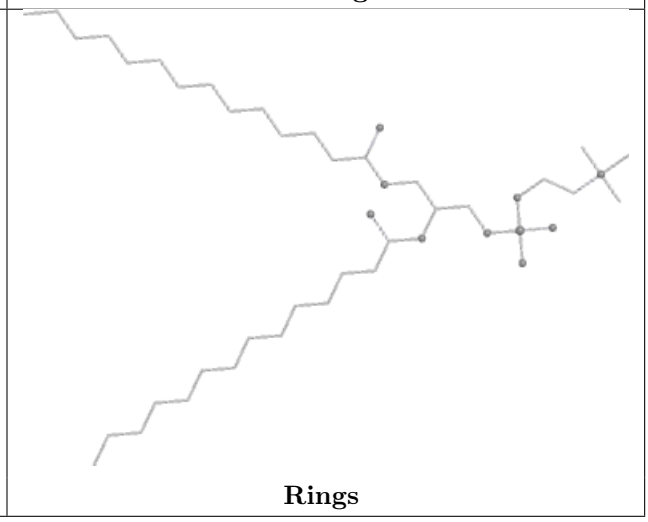
Bond lengths



Bond angles

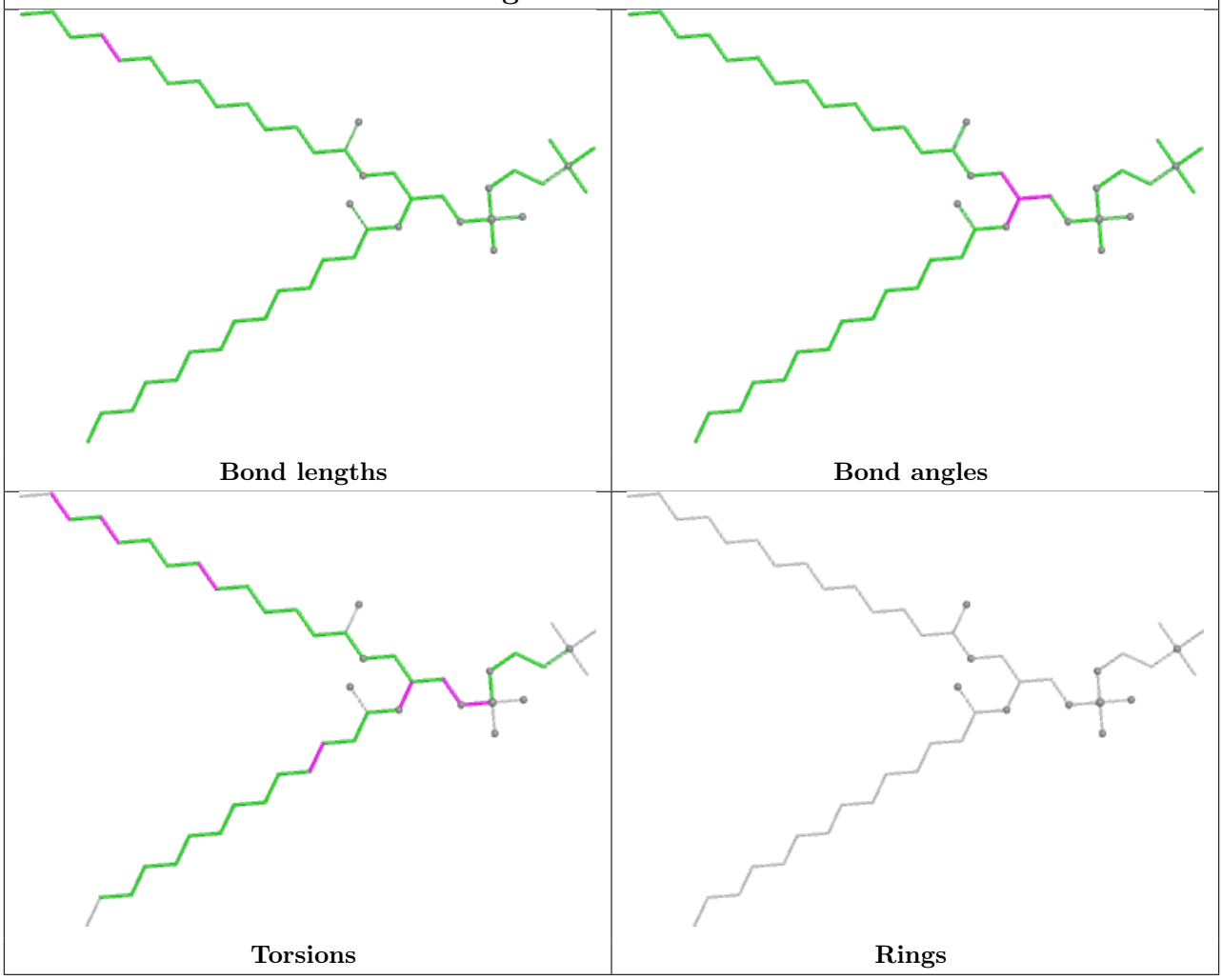


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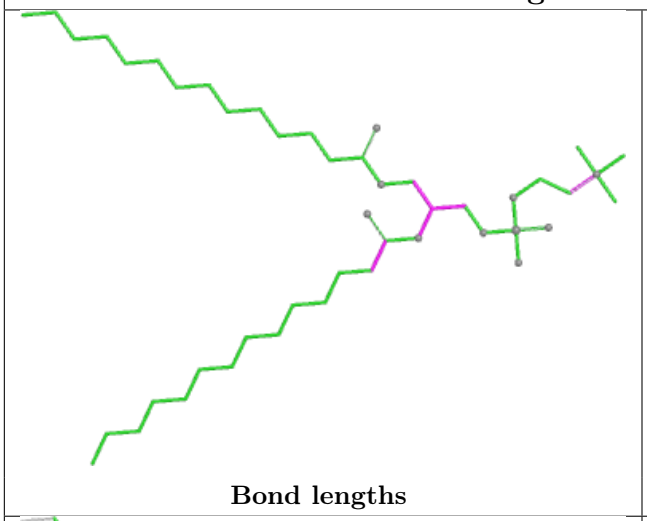


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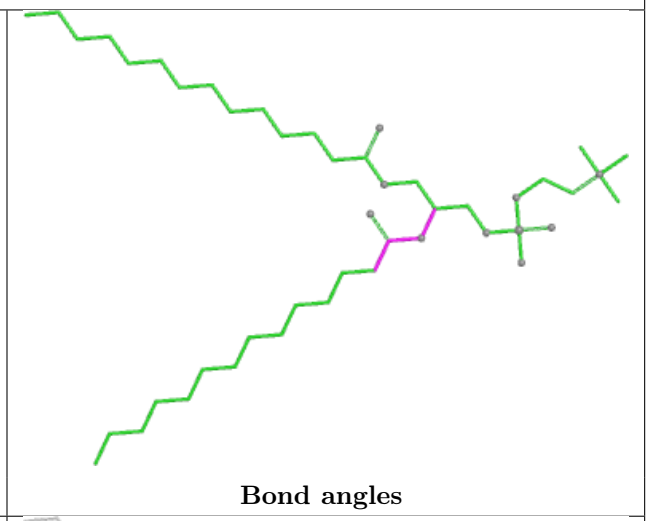
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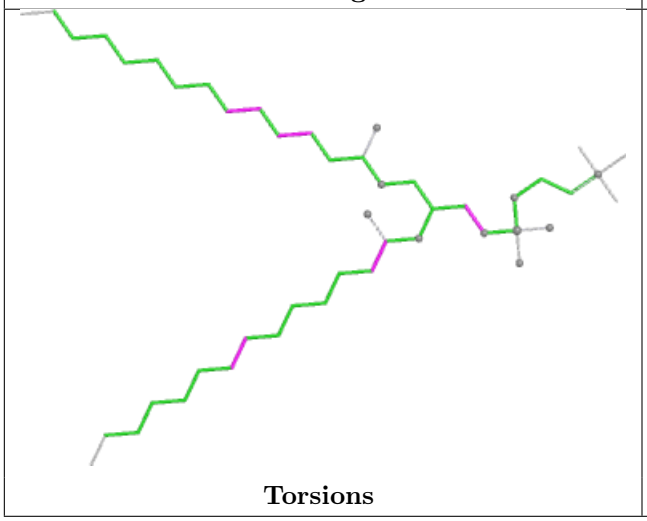
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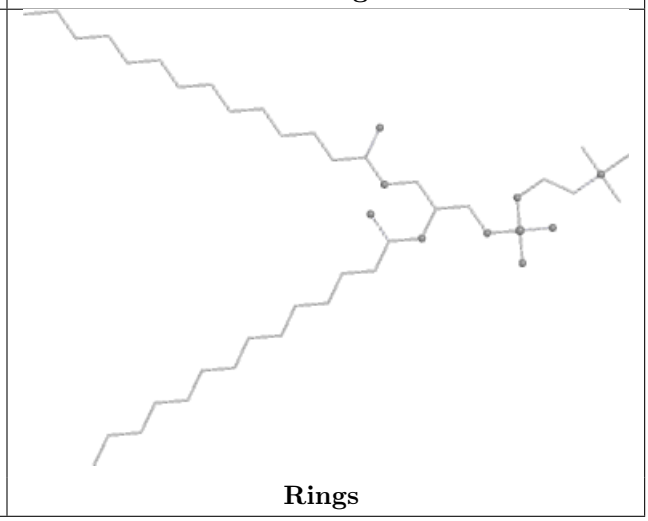
Bond lengths



Bond angles

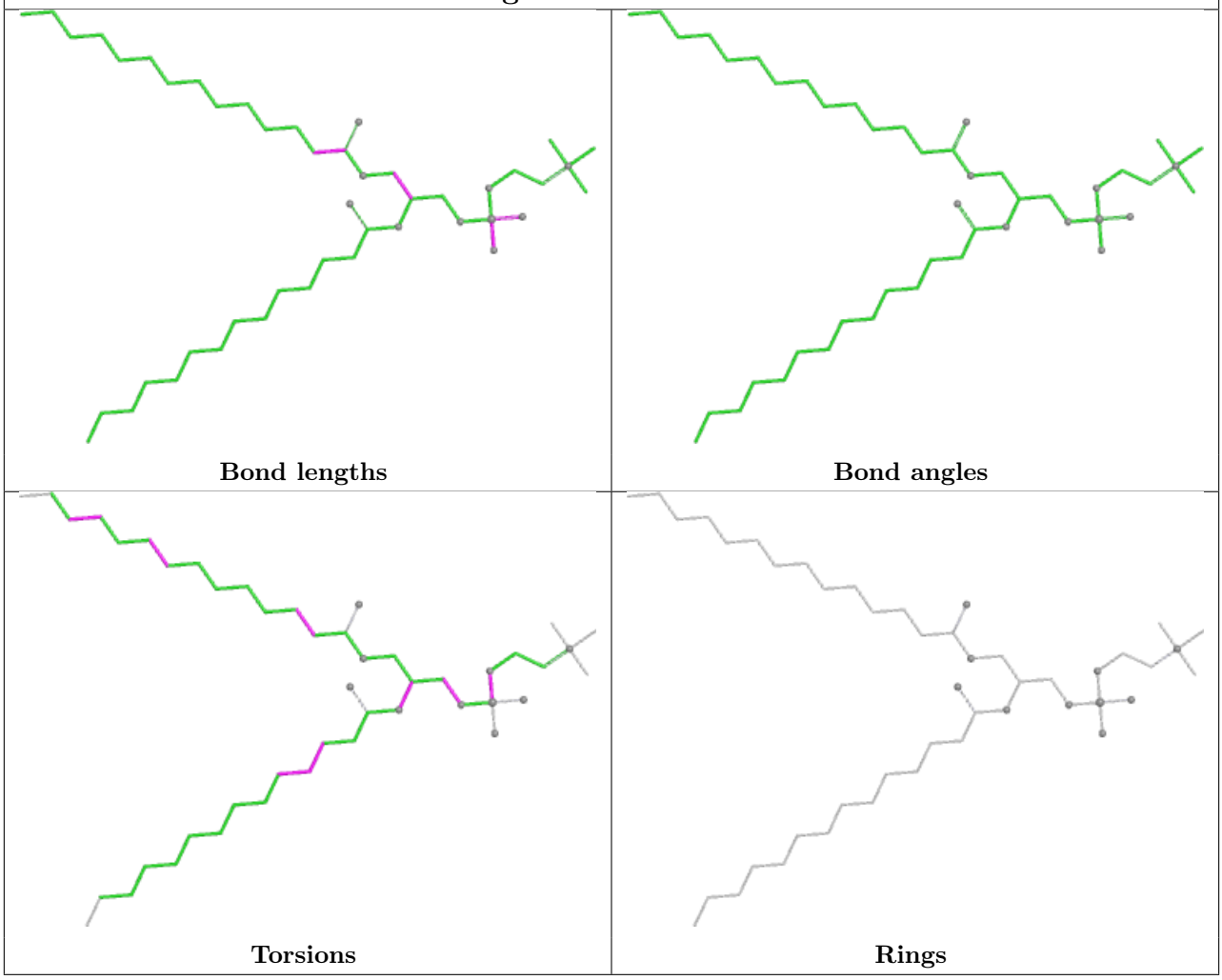


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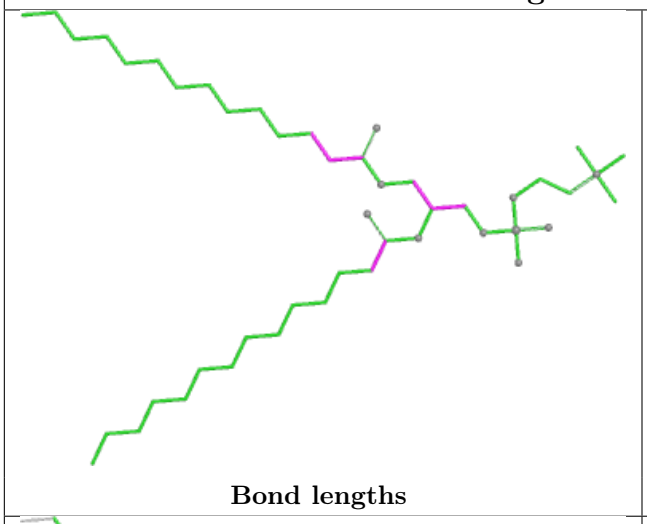


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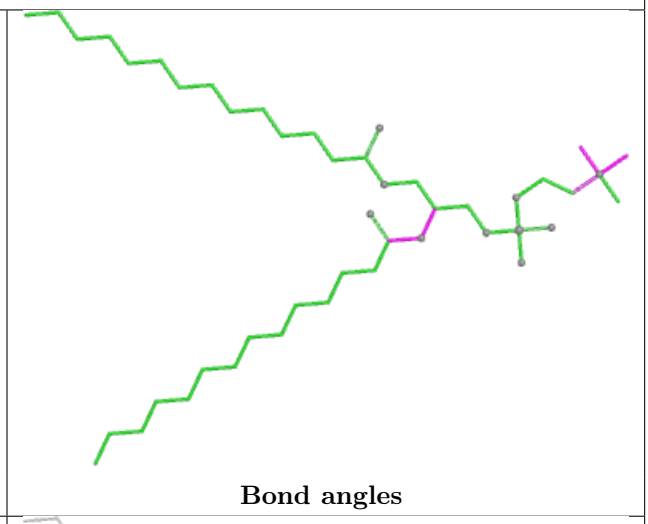
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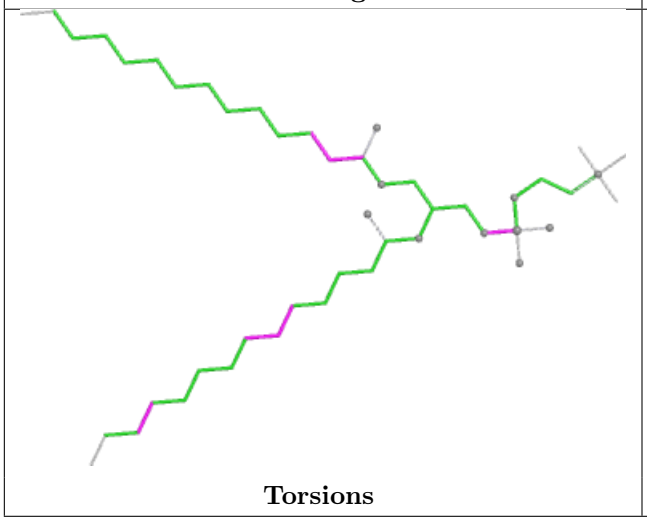
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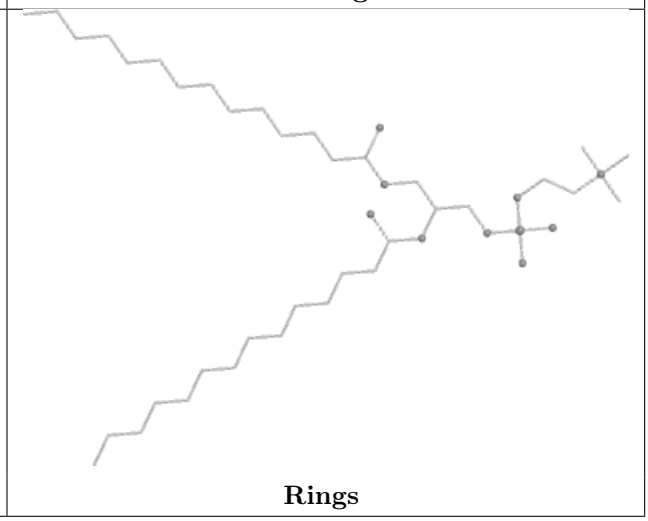
Bond lengths



Bond angles

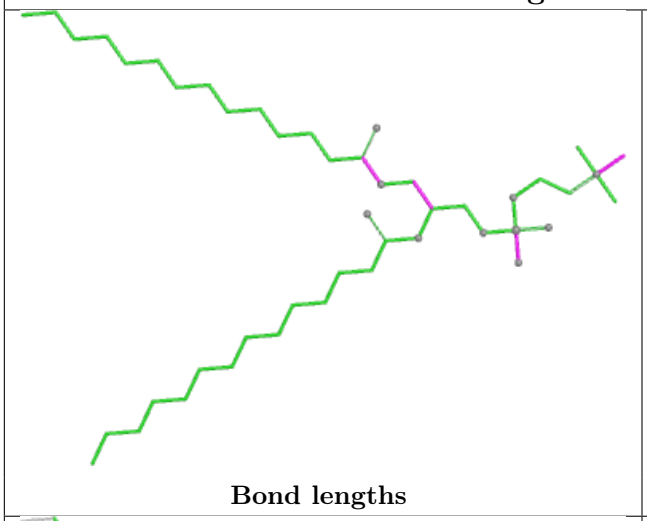


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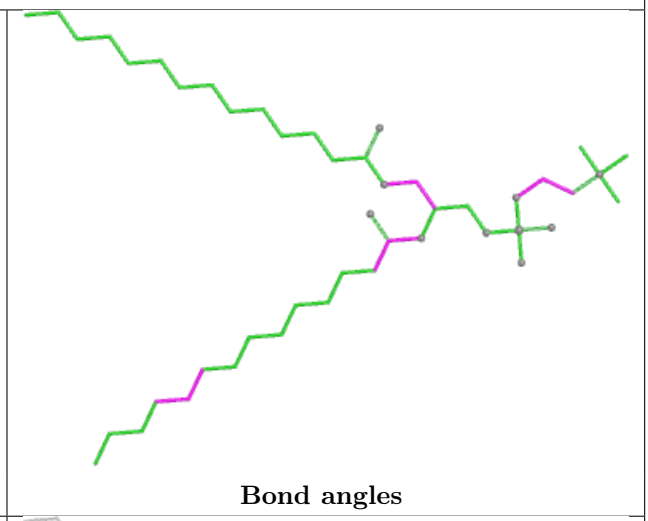


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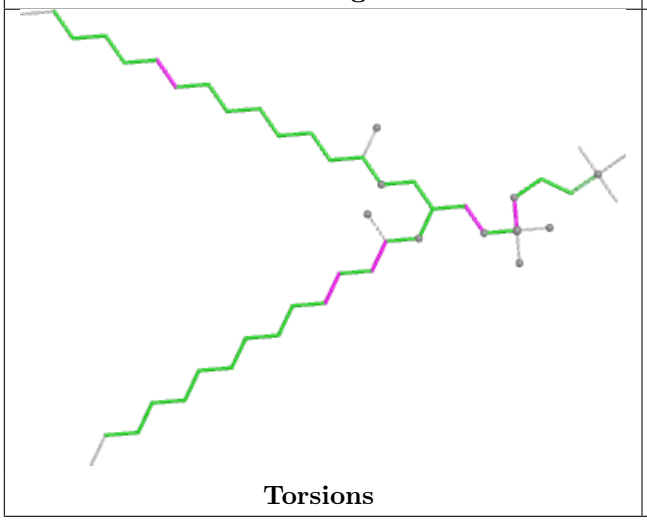
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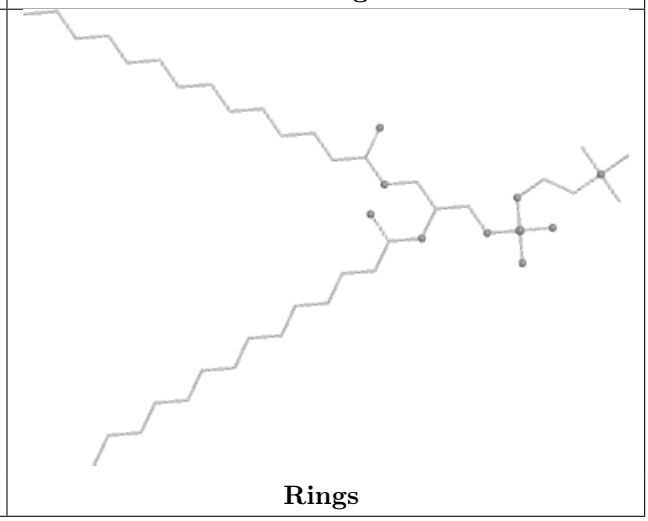
Bond lengths



Bond angles

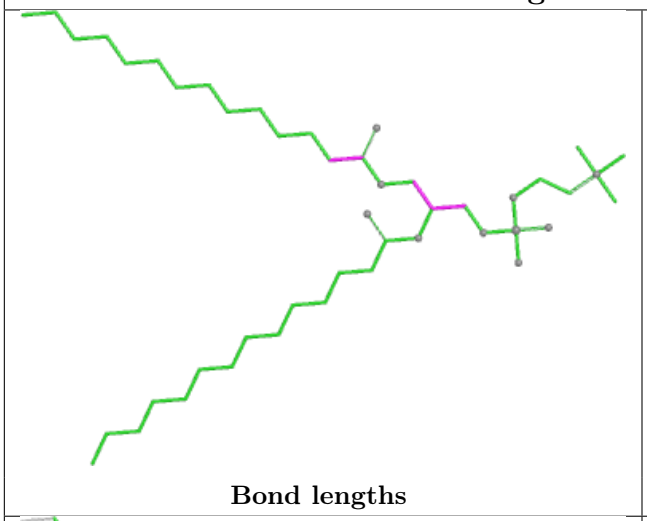


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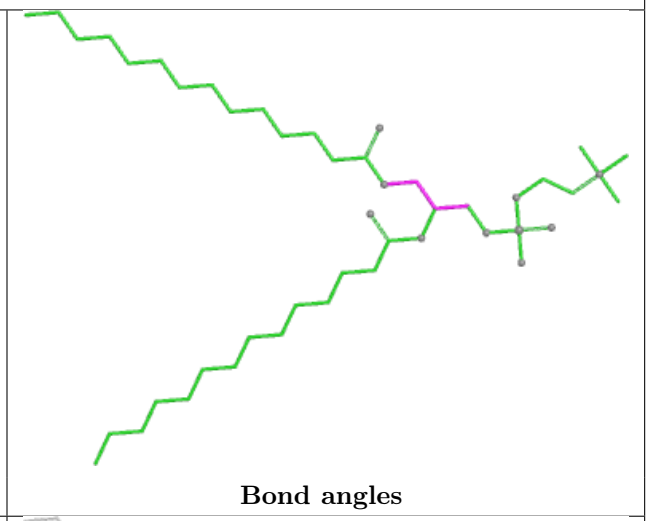


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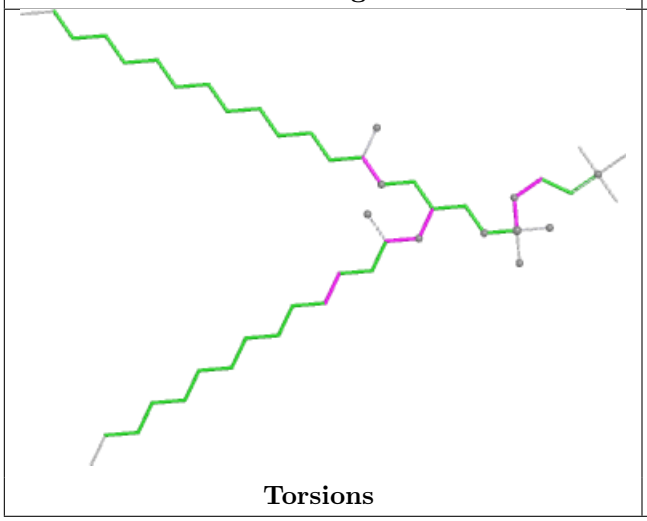
Ligand PX4 C 331



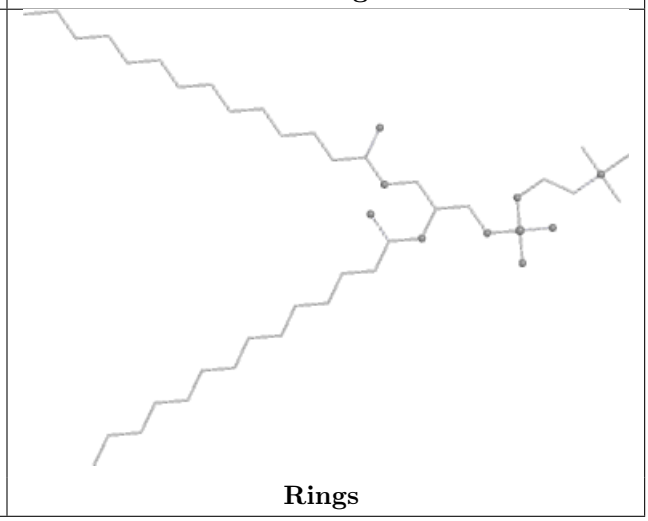
Bond lengths



Bond angles

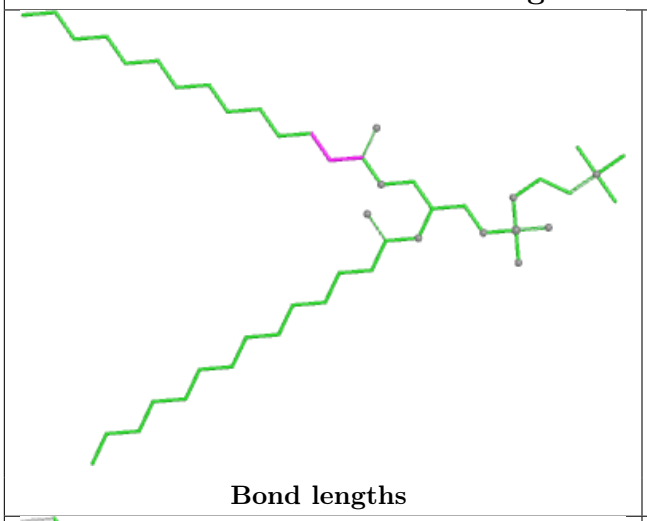


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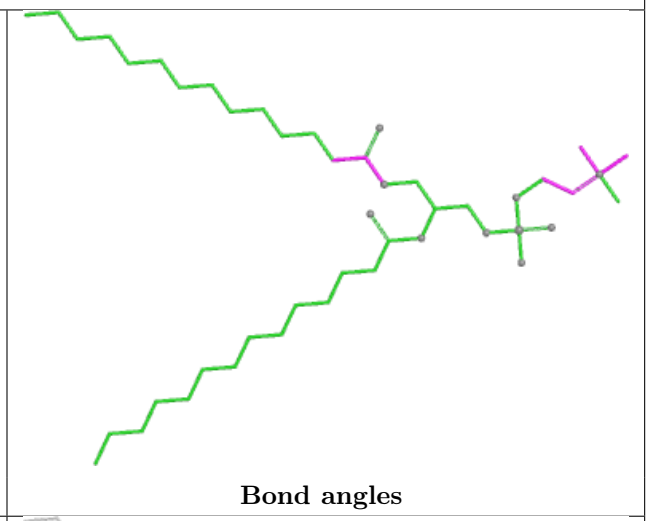


Rings

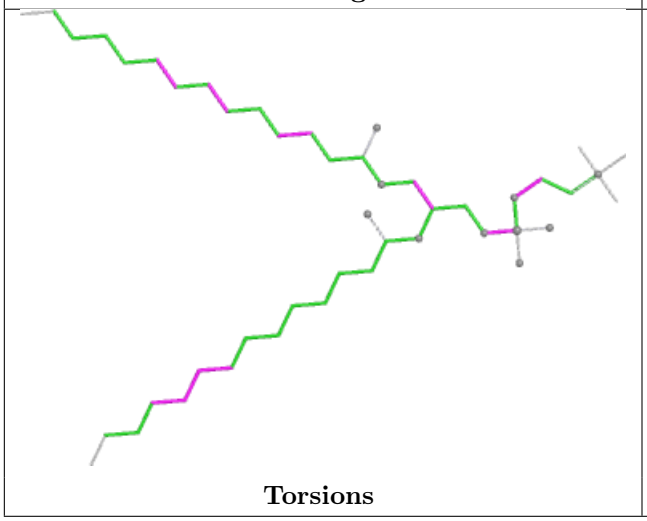
Ligand PX4 A 642



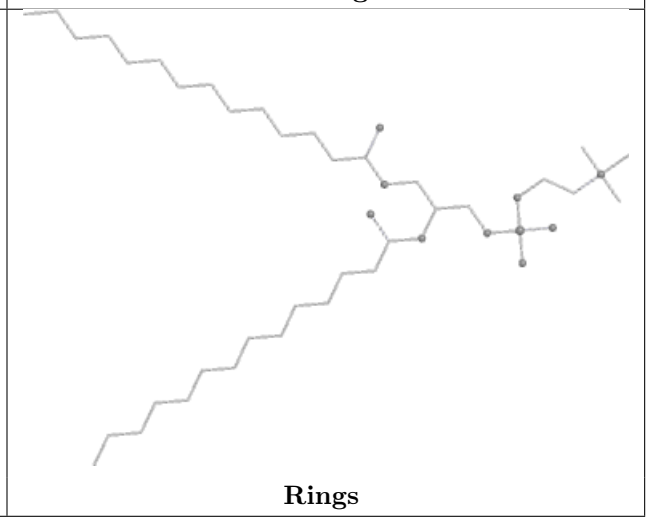
Bond lengths



Bond angles

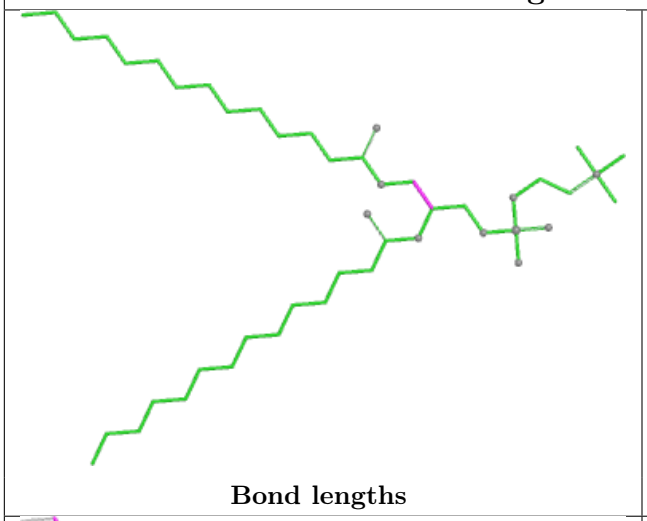


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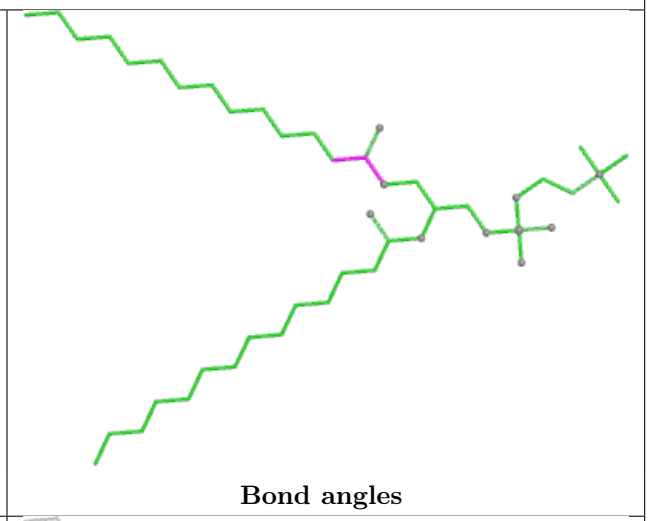


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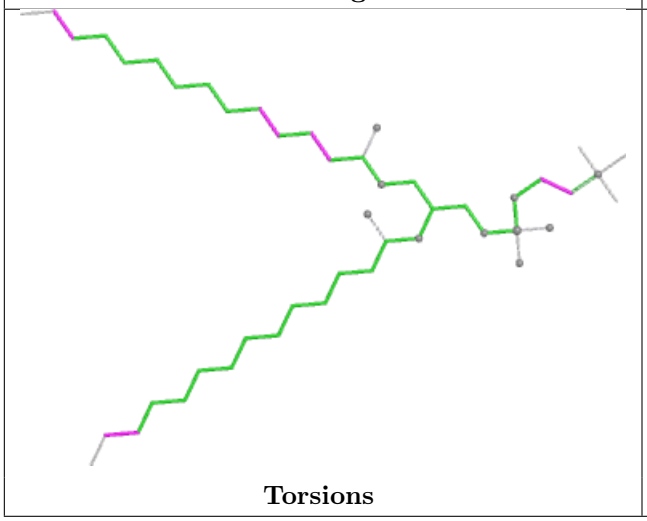
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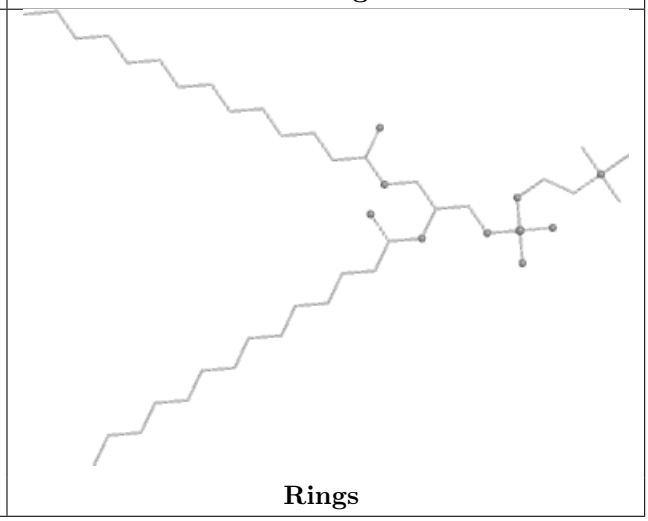
Bond lengths



Bond angles

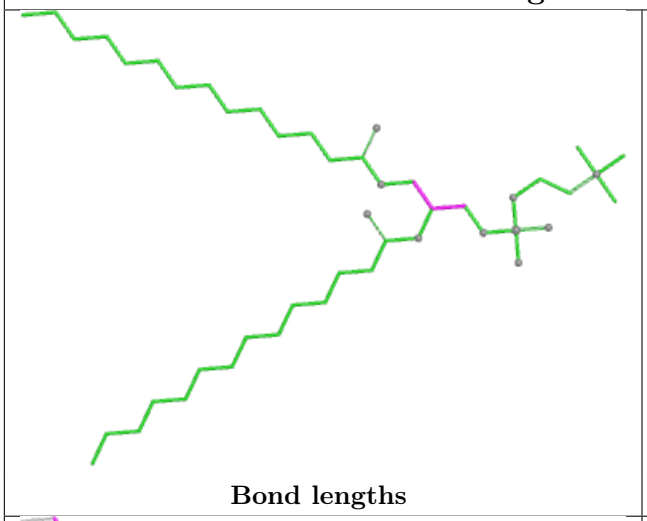


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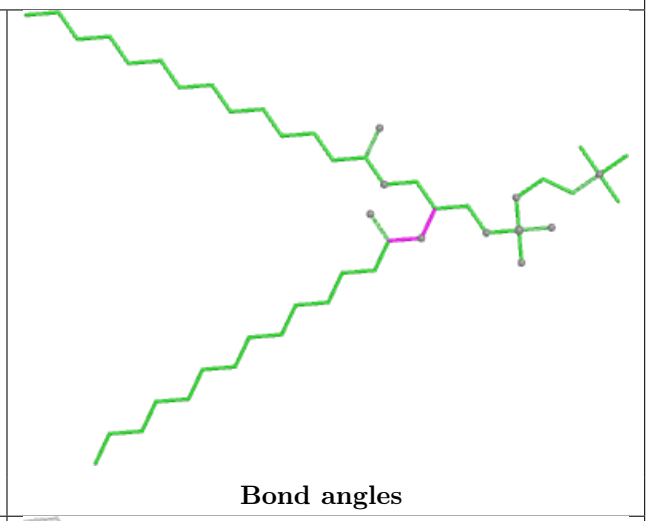


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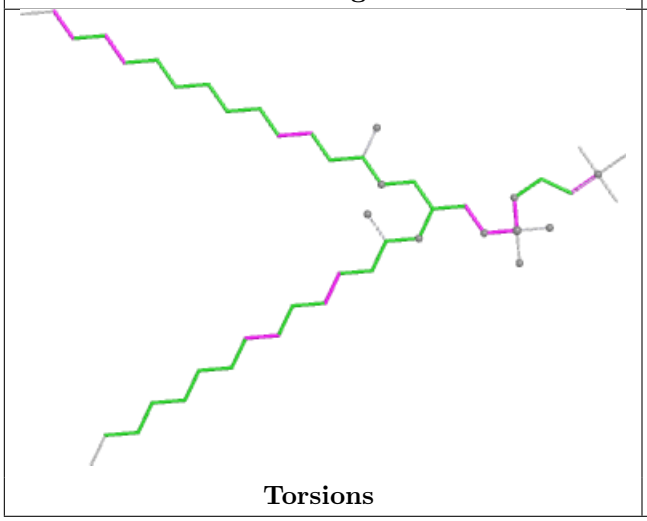
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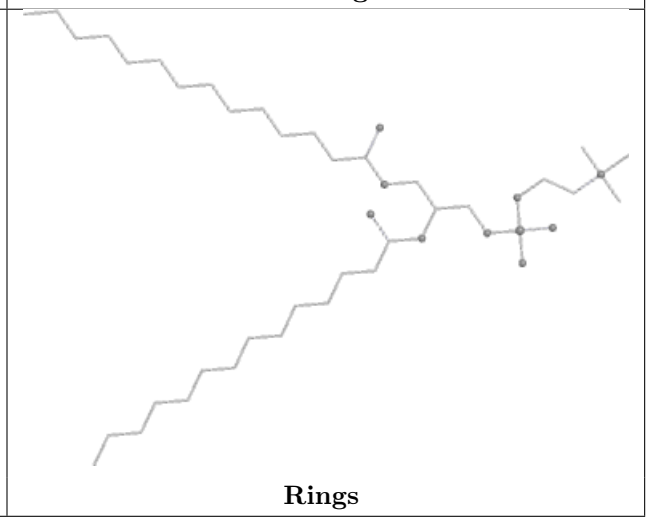
Bond lengths



Bond angles

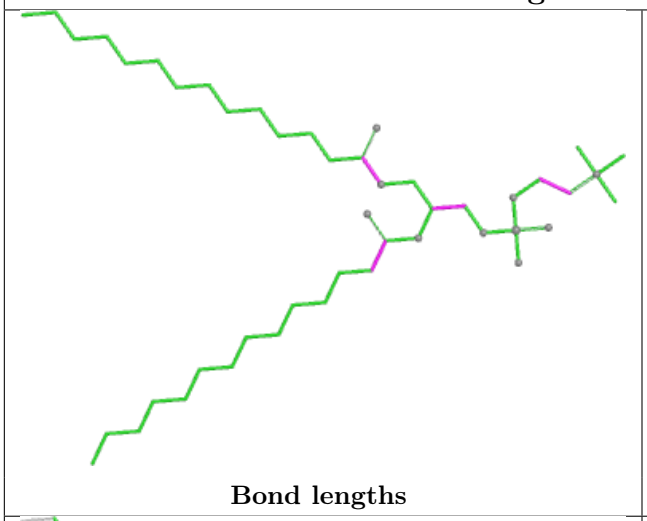


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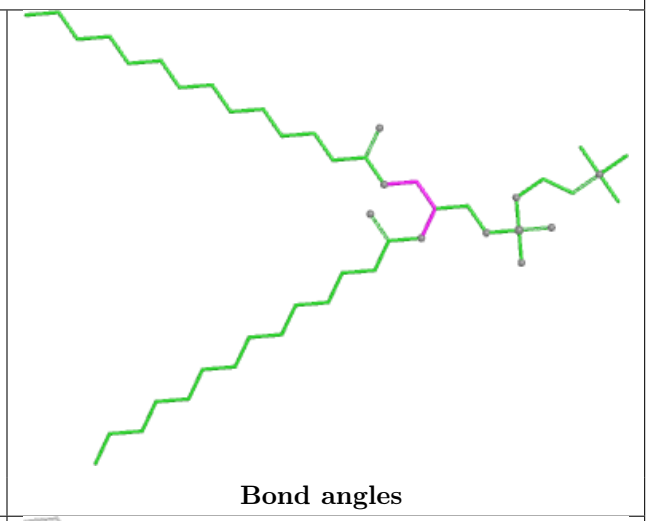


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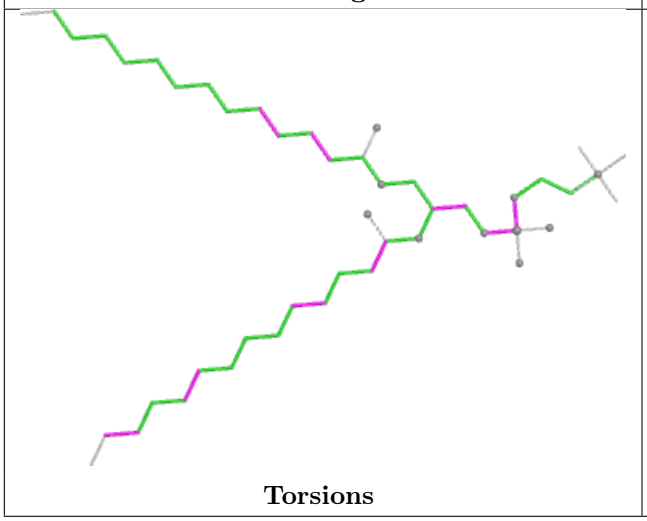
Ligand PX4 C 355



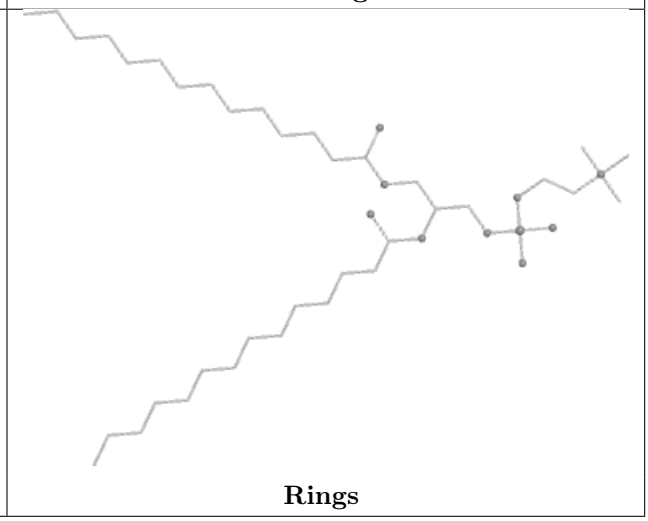
Bond lengths



Bond angles

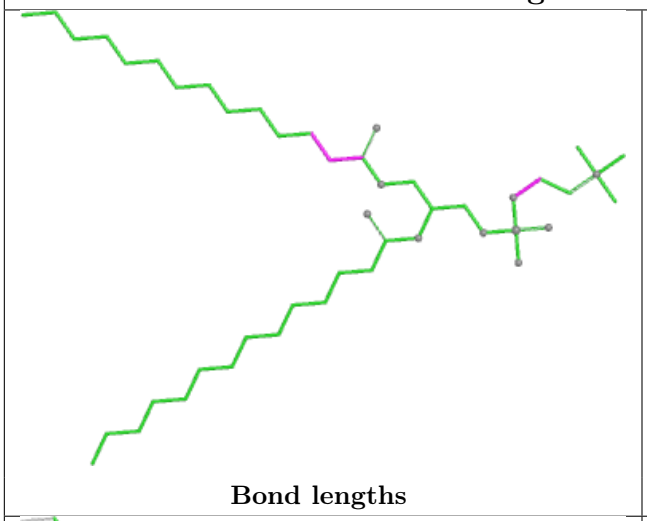


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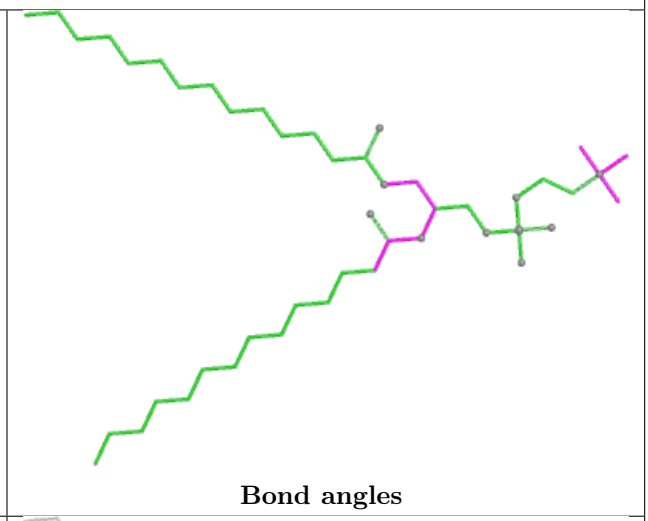


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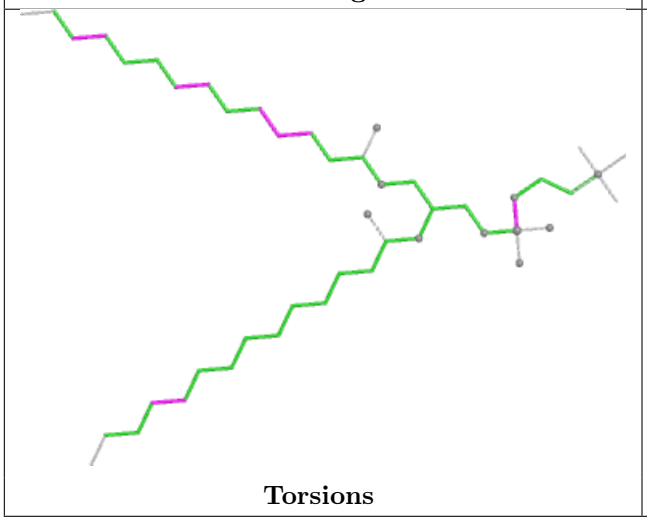
Ligand PX4 A 625



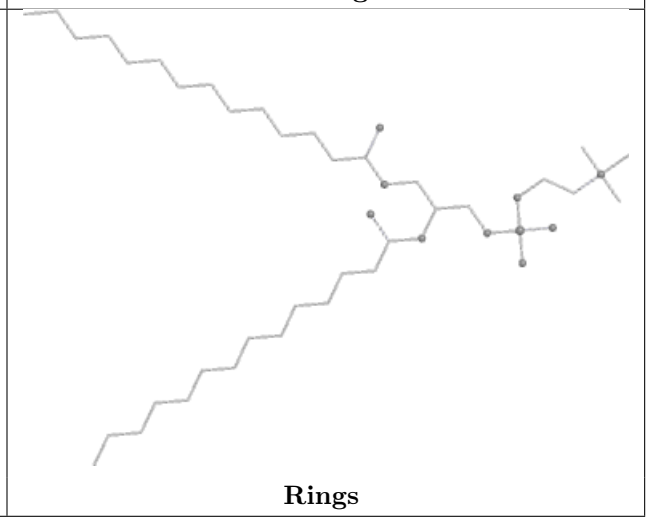
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Bond angles

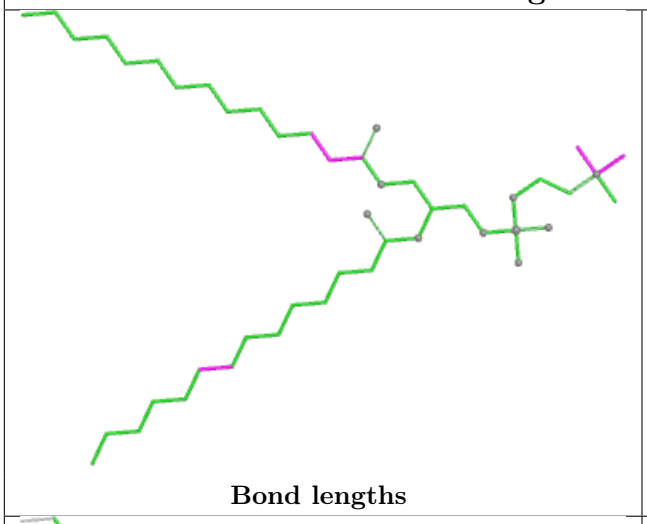


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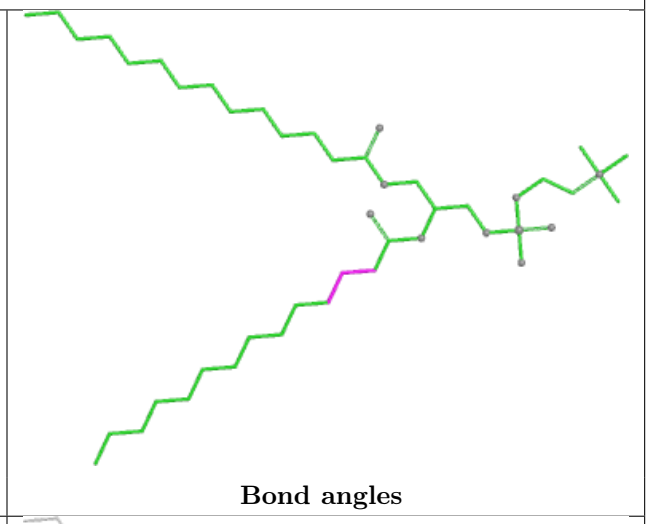


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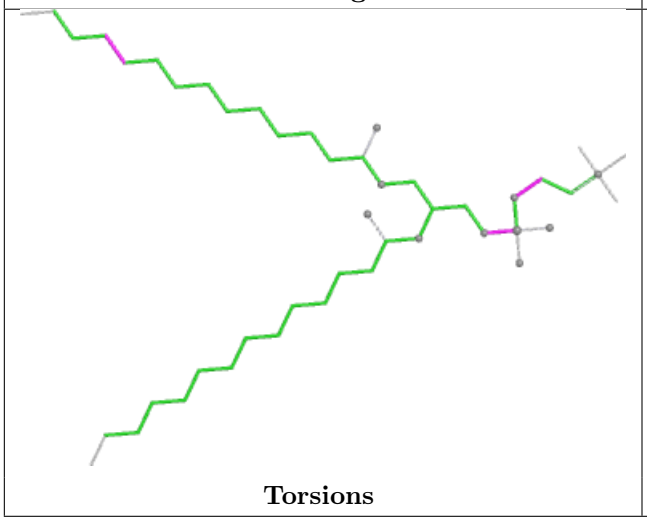
Ligand PX4 B 301



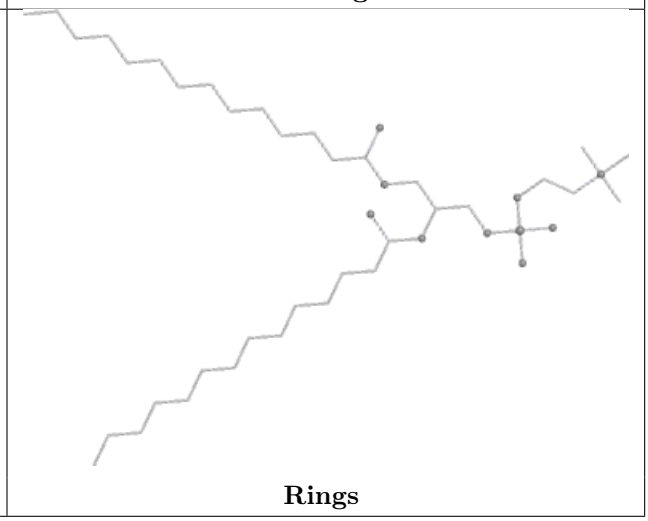
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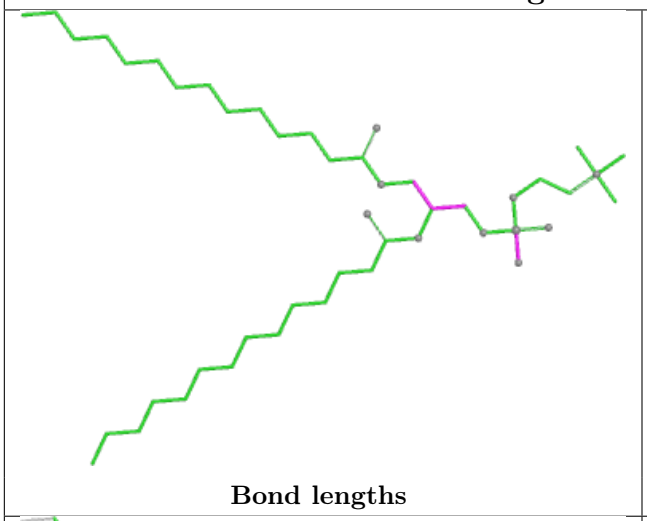


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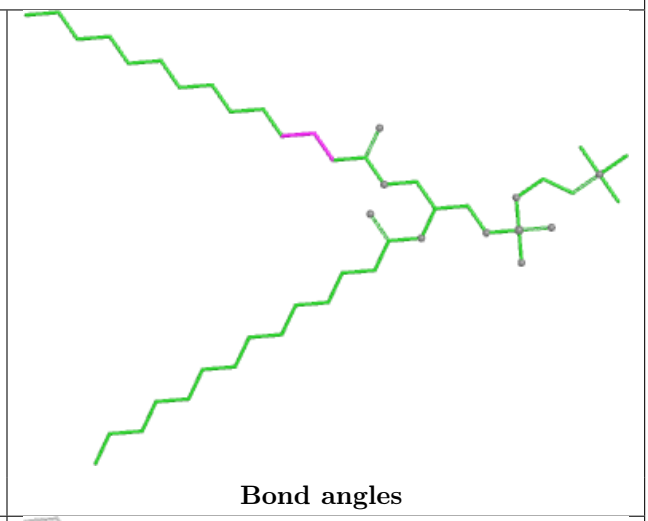


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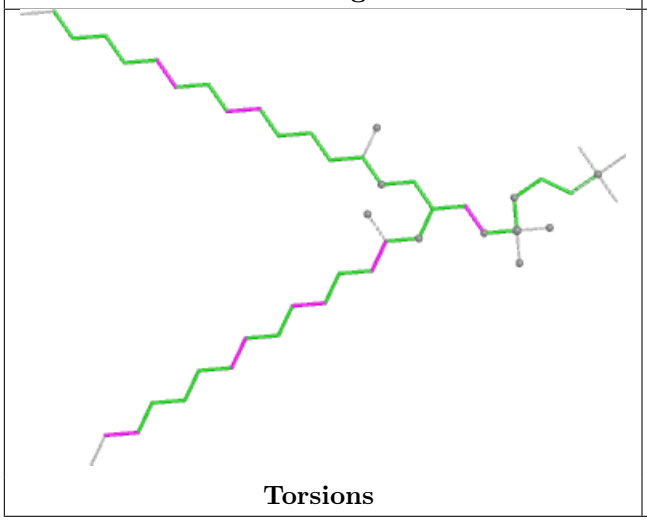
Ligand PX4 A 653



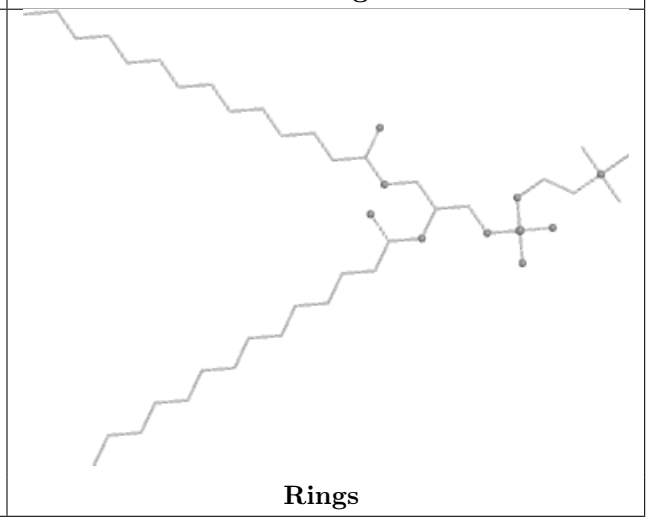
Bond lengths



Bond angles

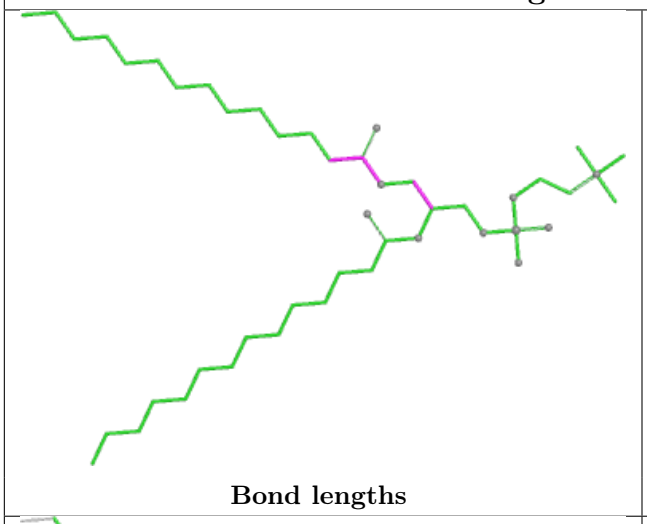


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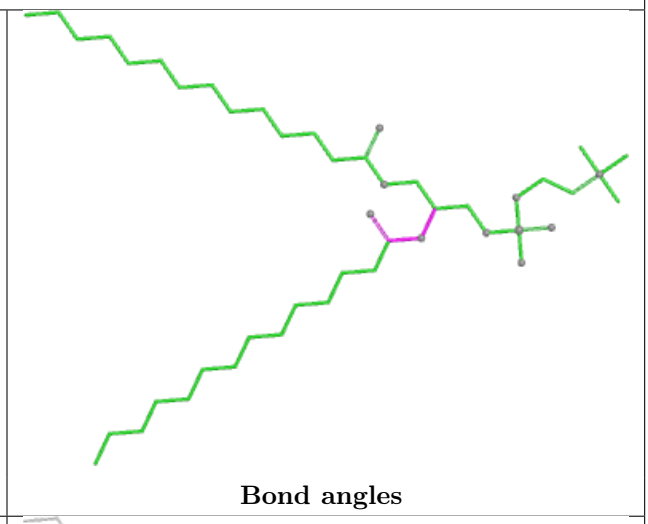


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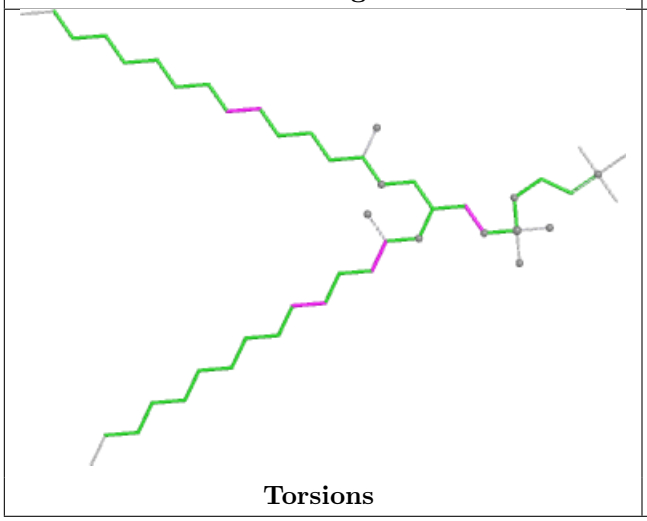
Ligand PX4 B 375



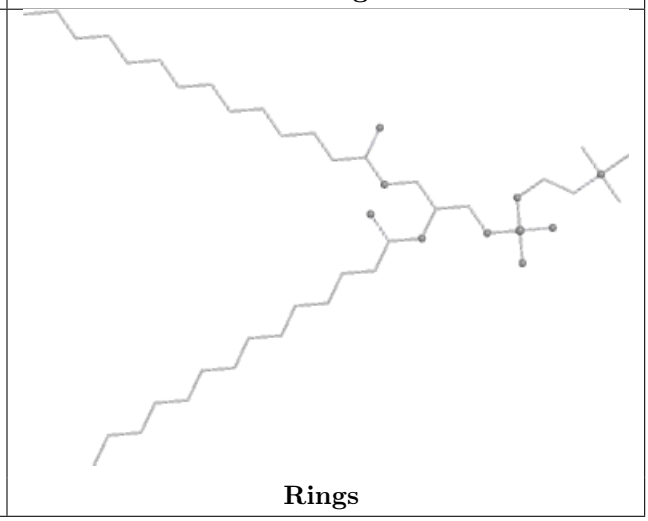
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Bond angles

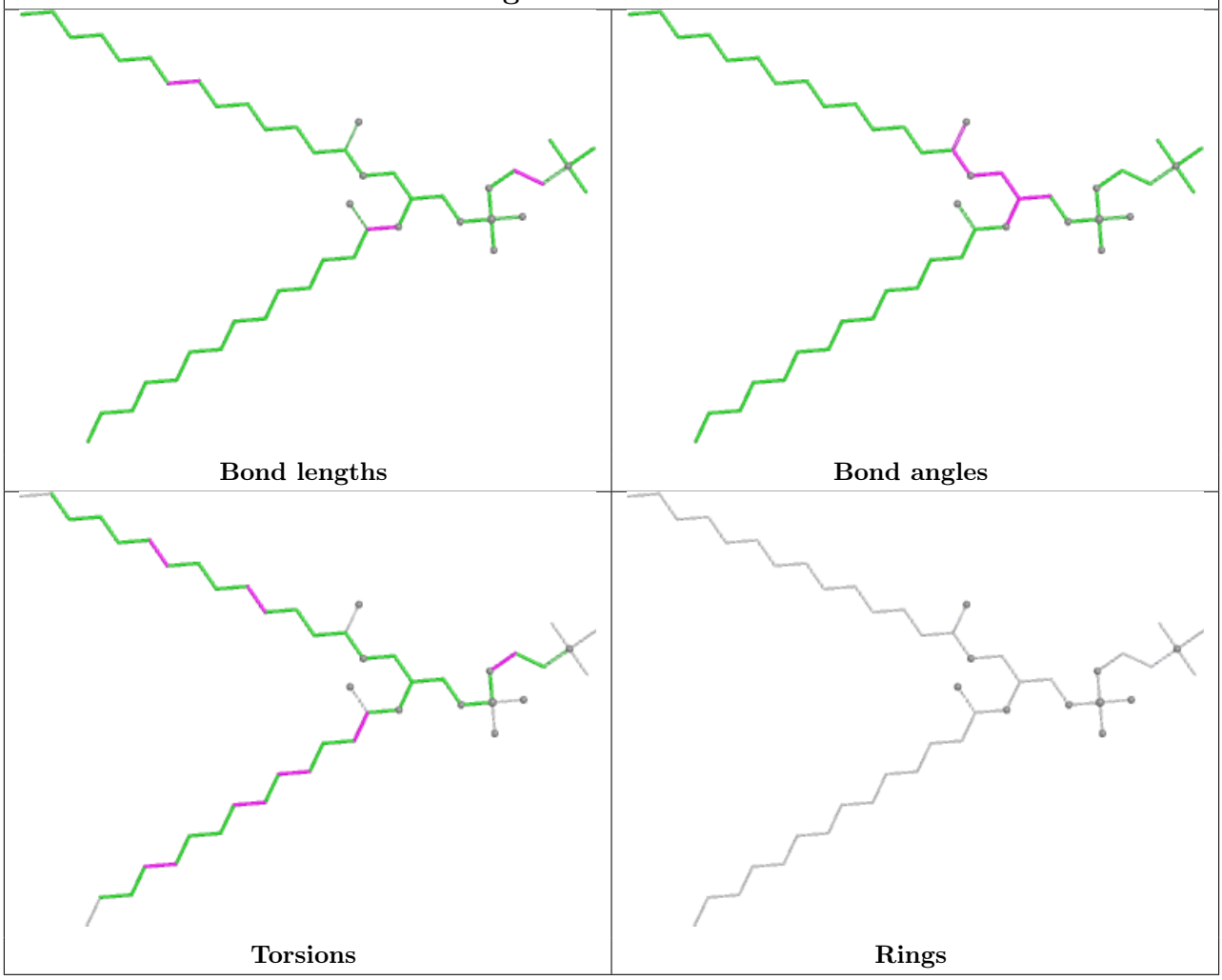


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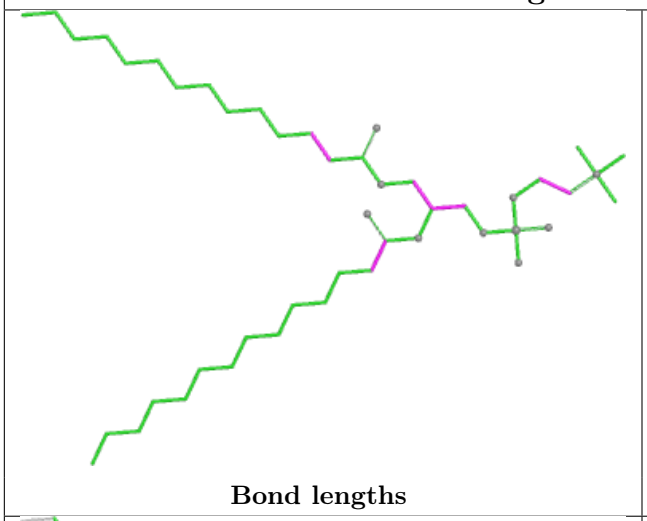


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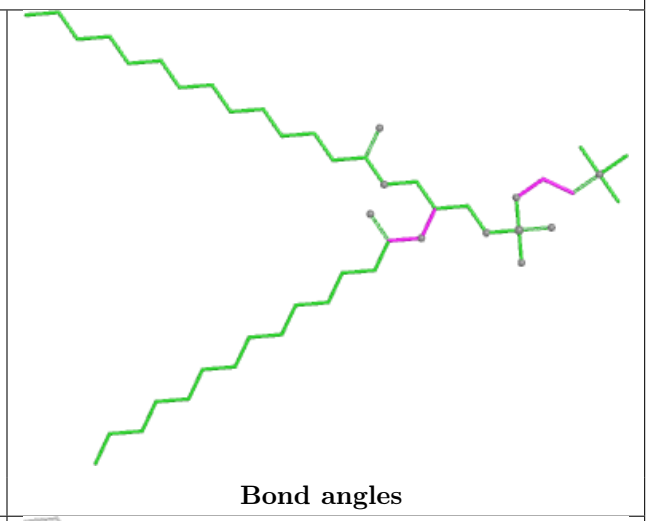
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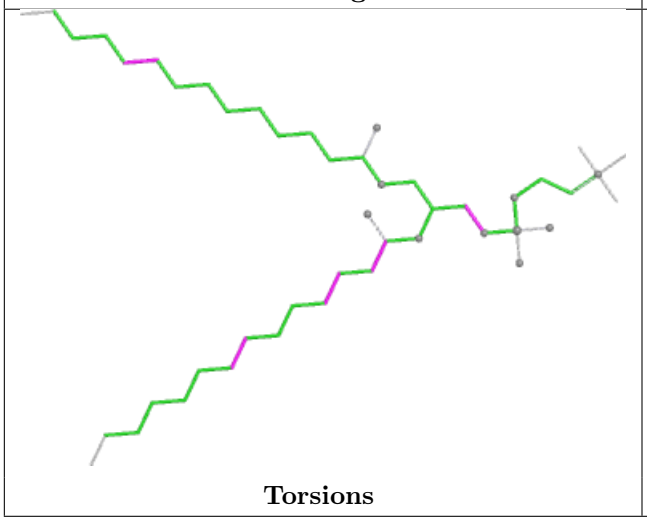
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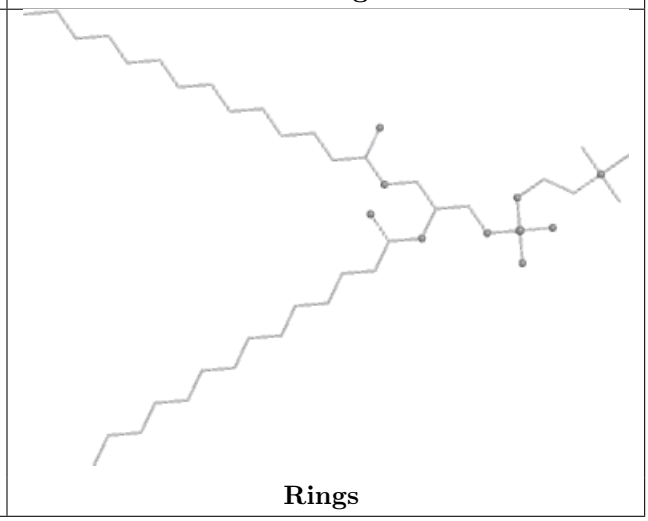
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Bond angles

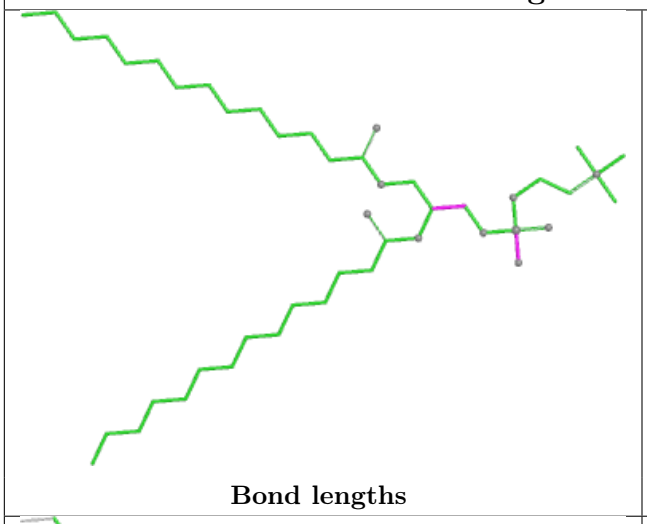


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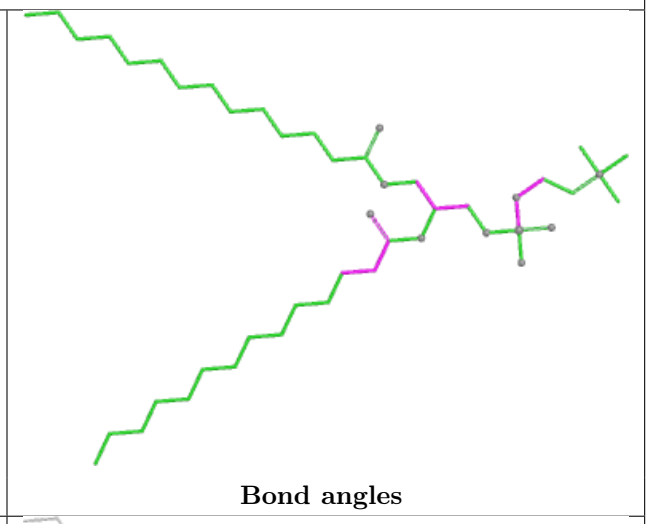


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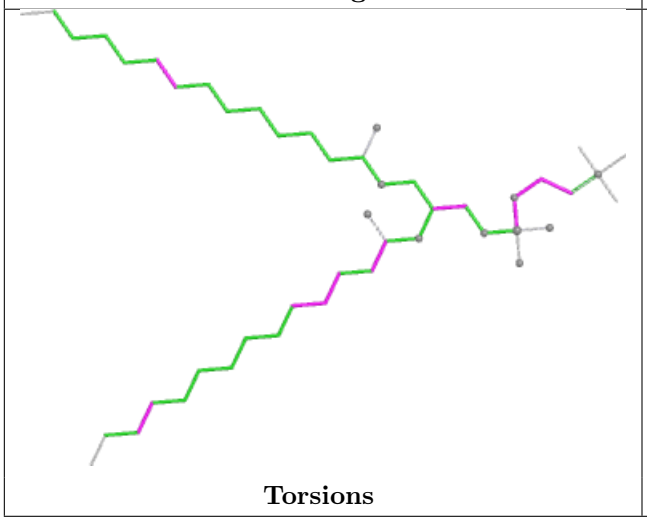
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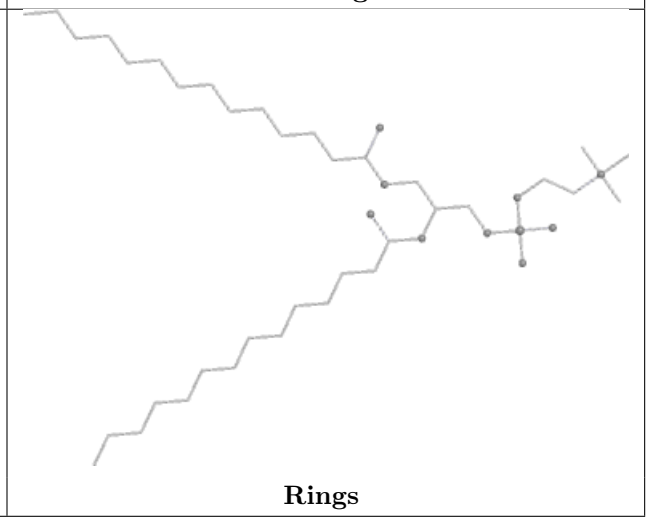
Bond lengths



Bond angles

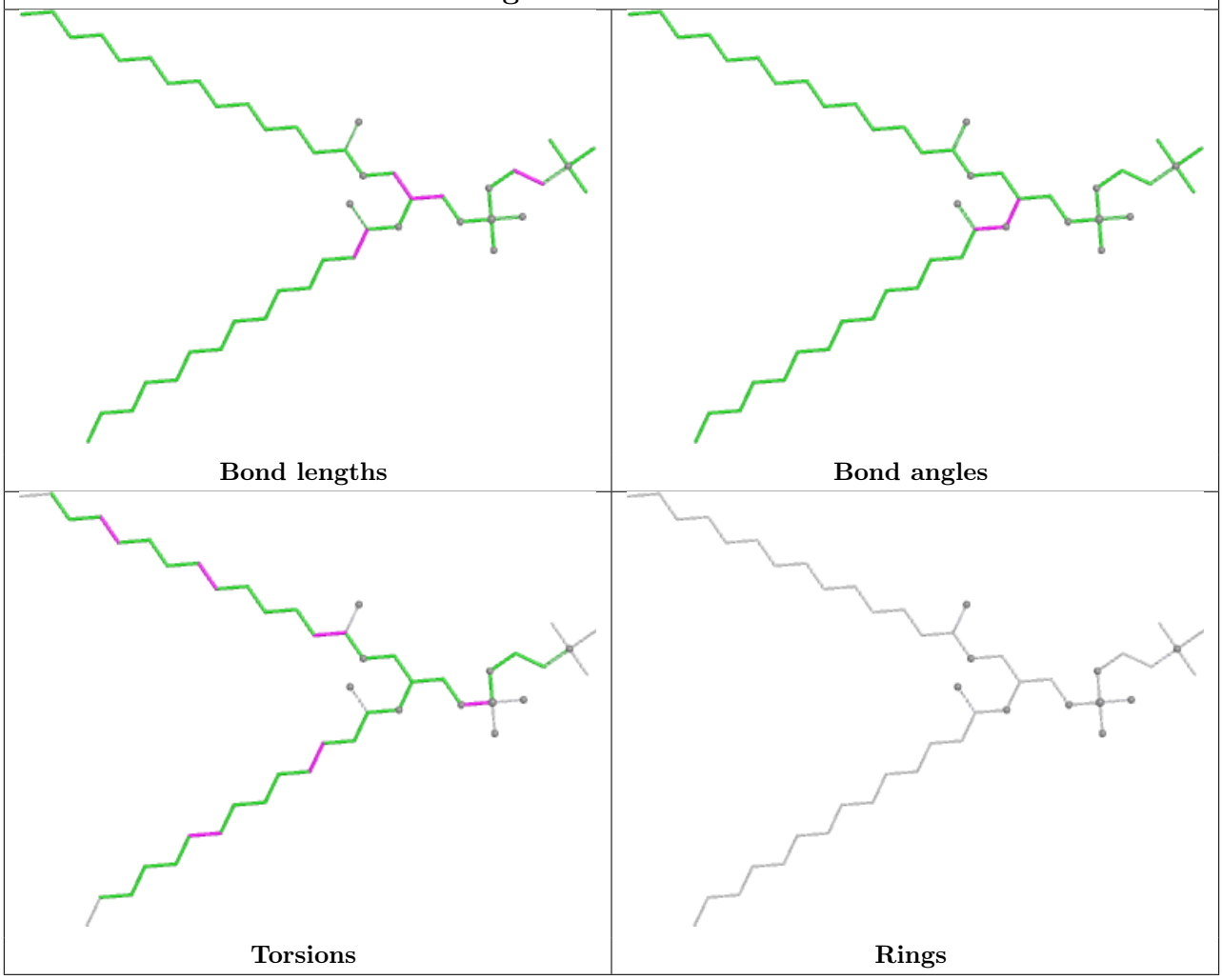


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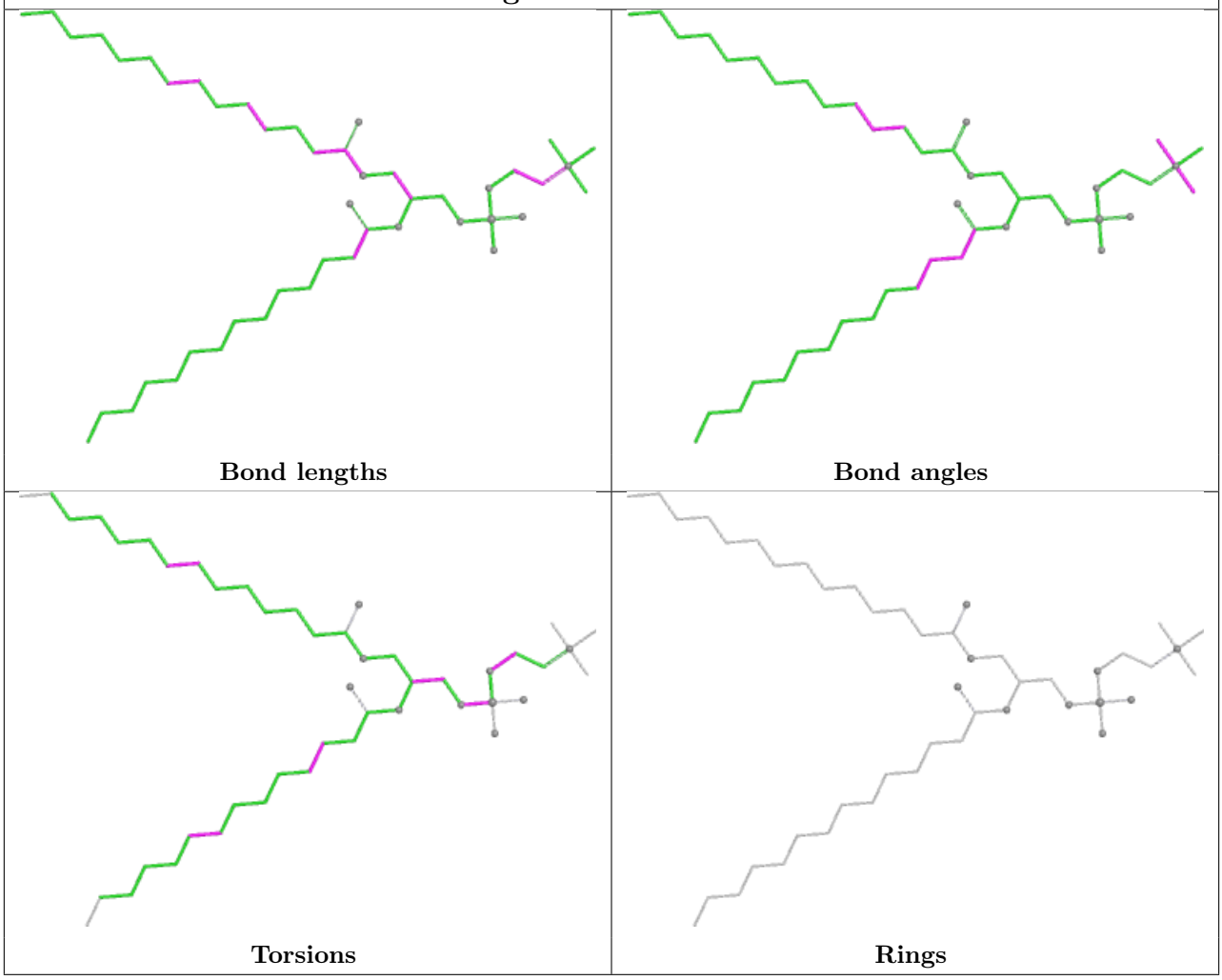


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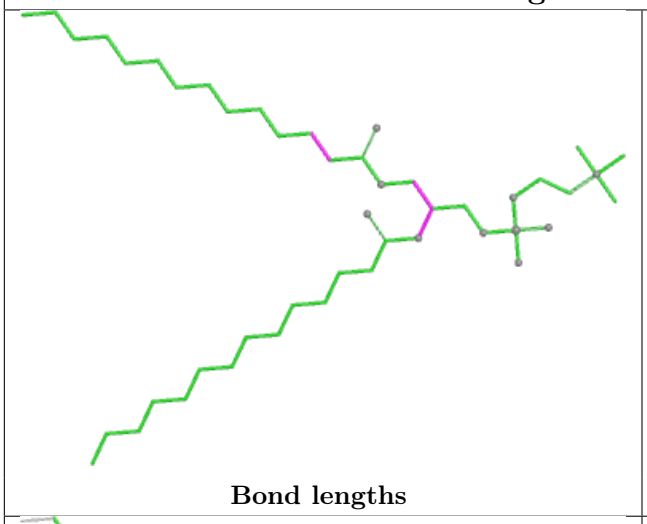
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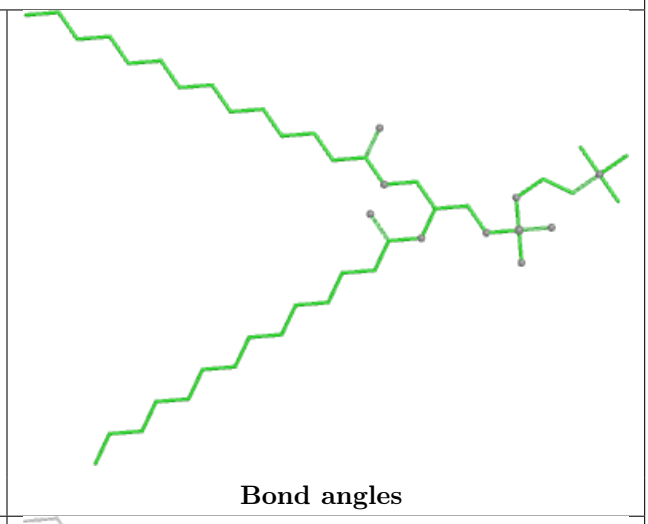
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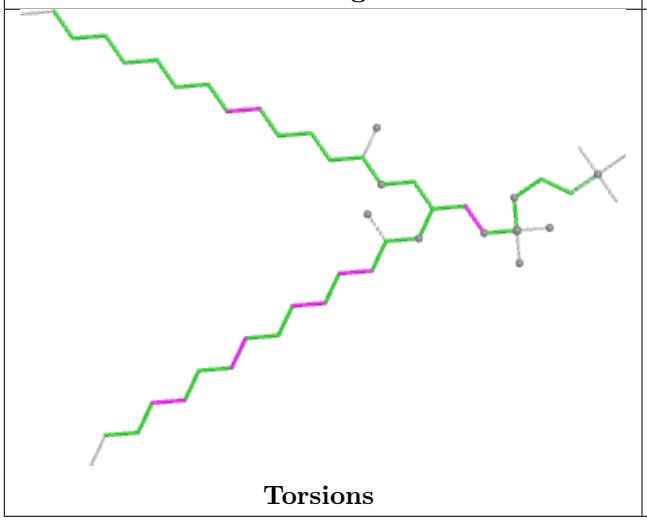
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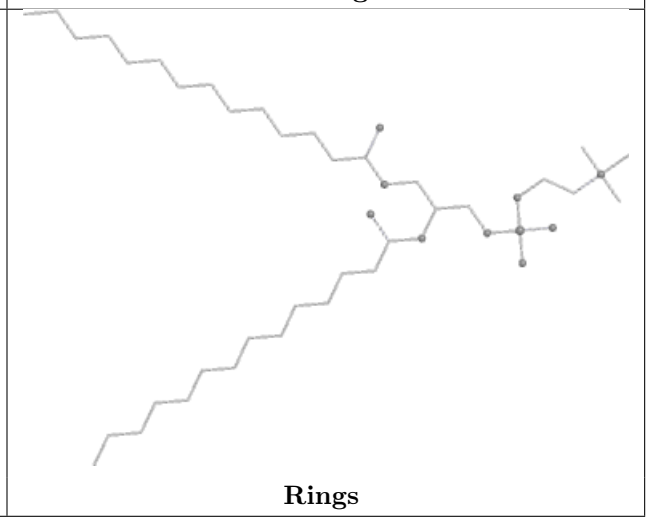
Bond lengths



Bond angles

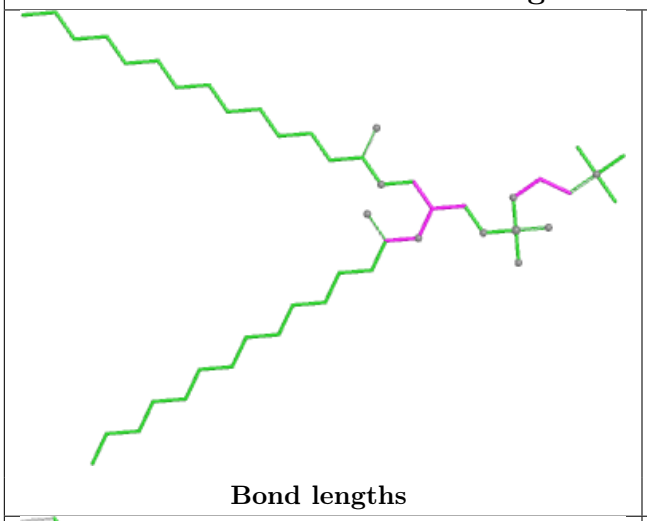


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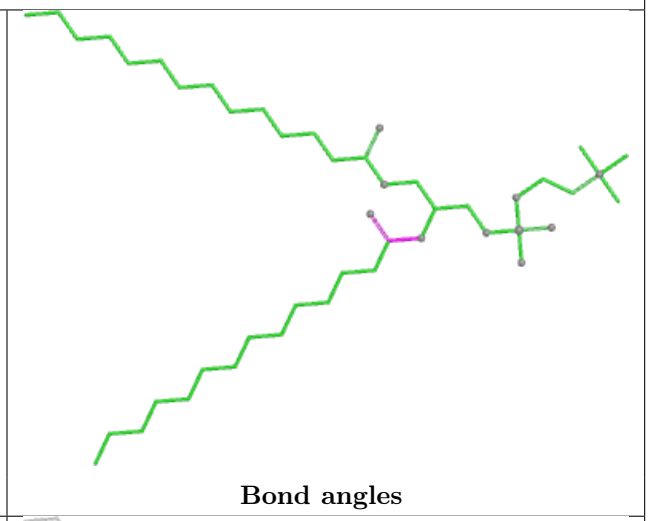


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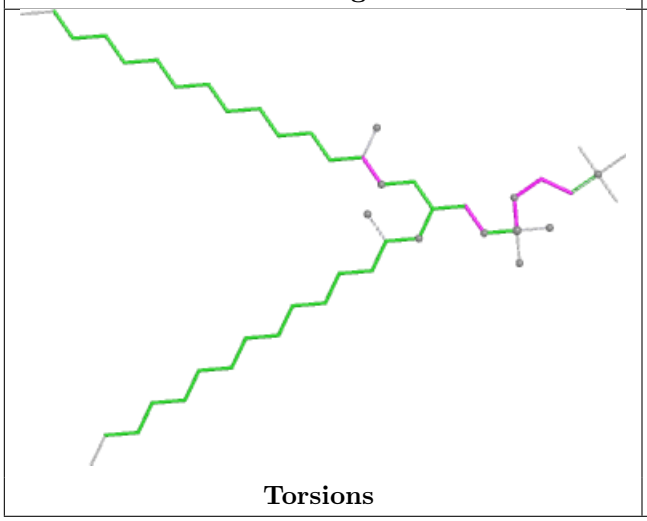
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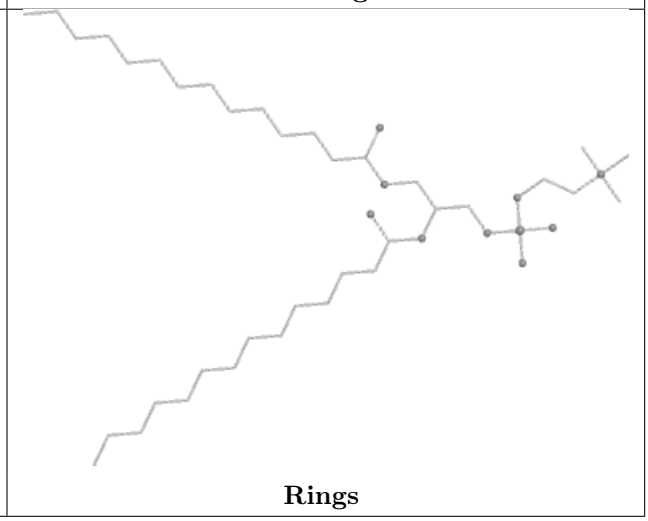
Bond lengths



Bond angles

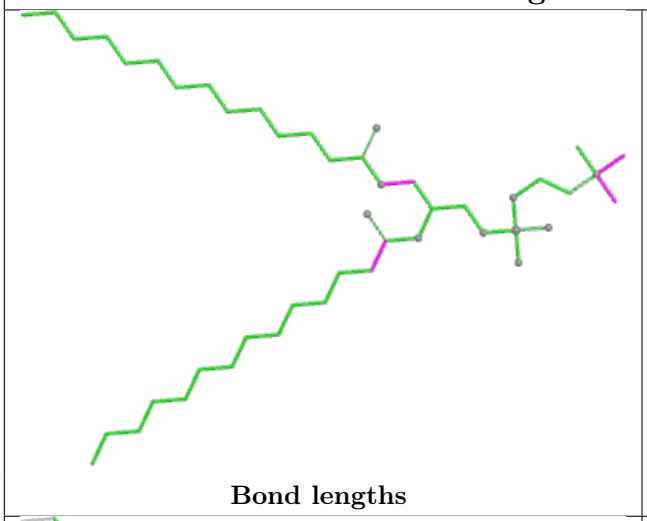


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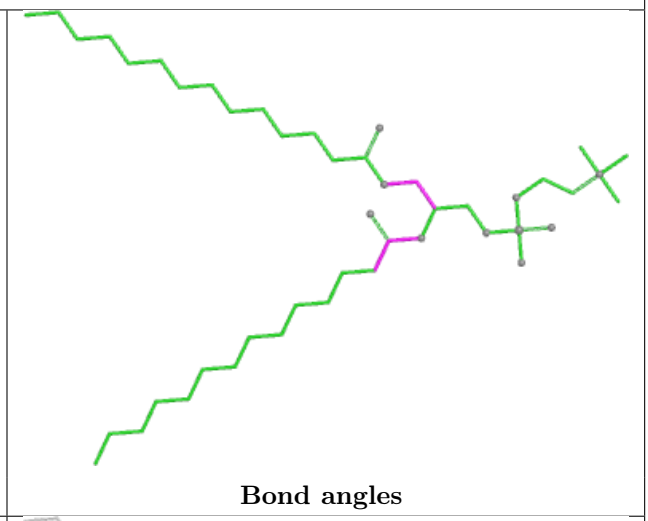


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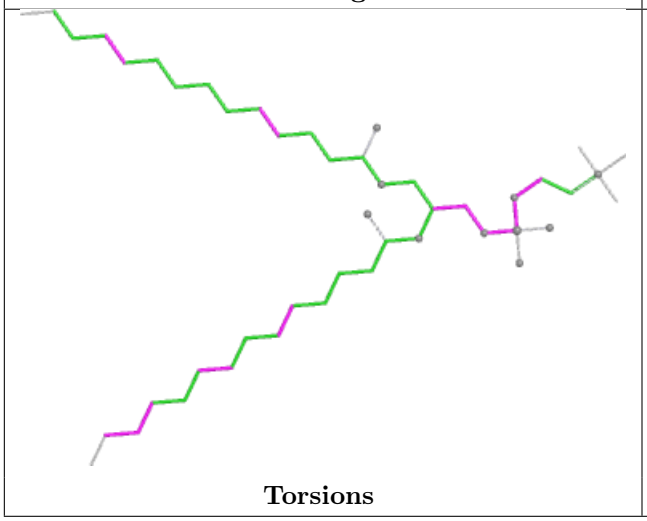
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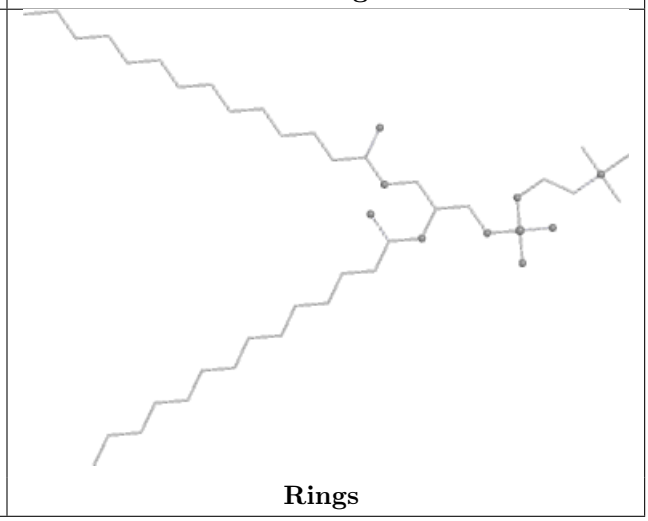
Bond lengths



Bond angles

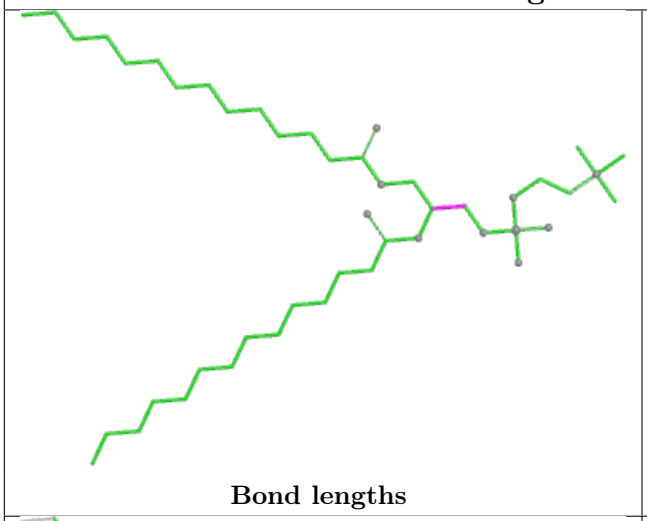


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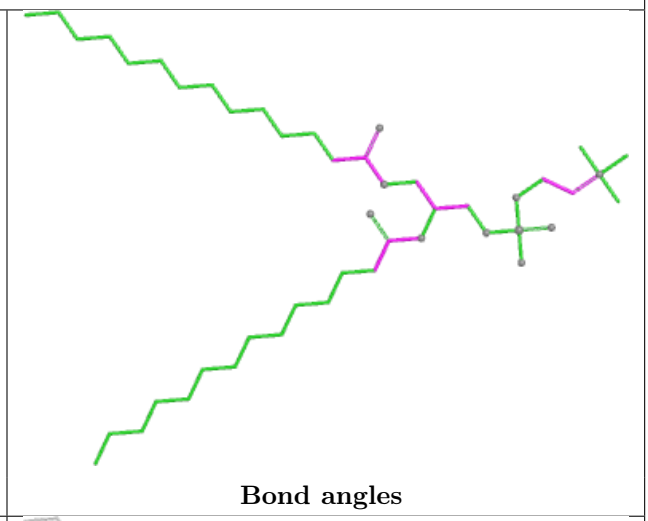


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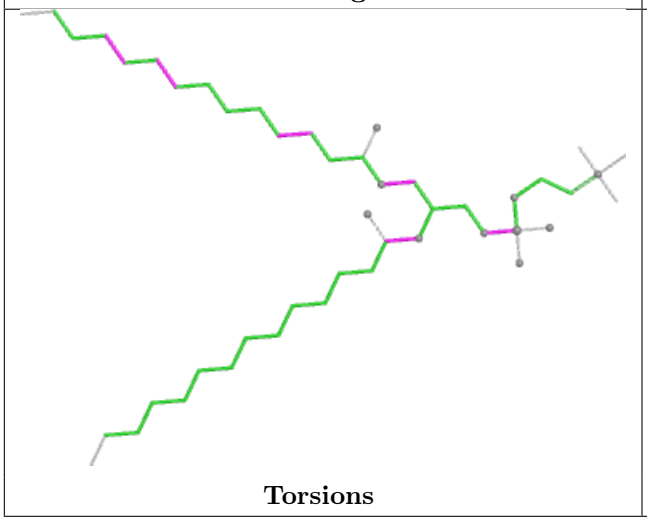
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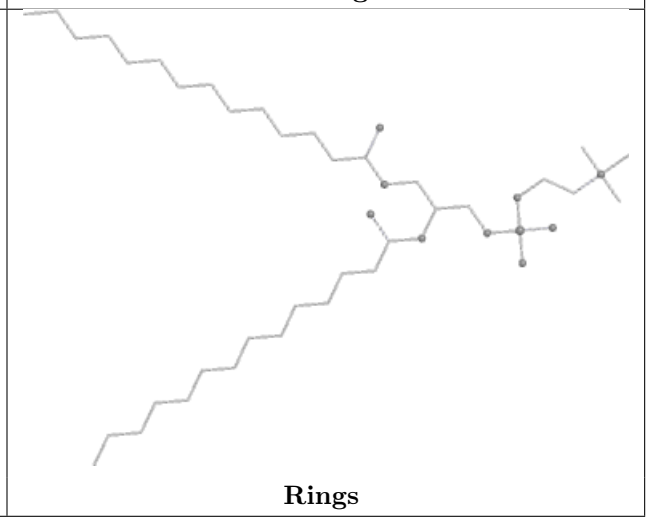
Bond lengths



Bond angles

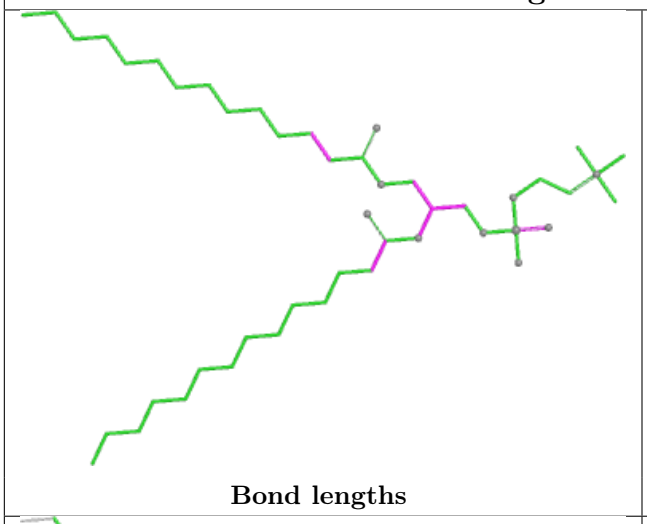


Torsions

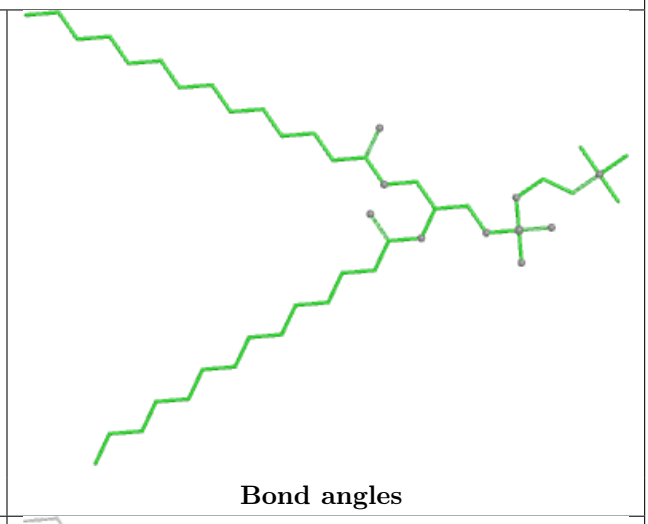


Rings

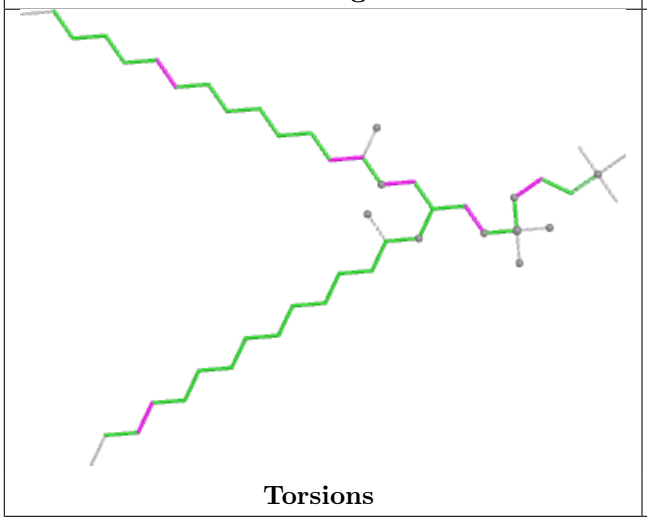
Ligand PX4 B 377



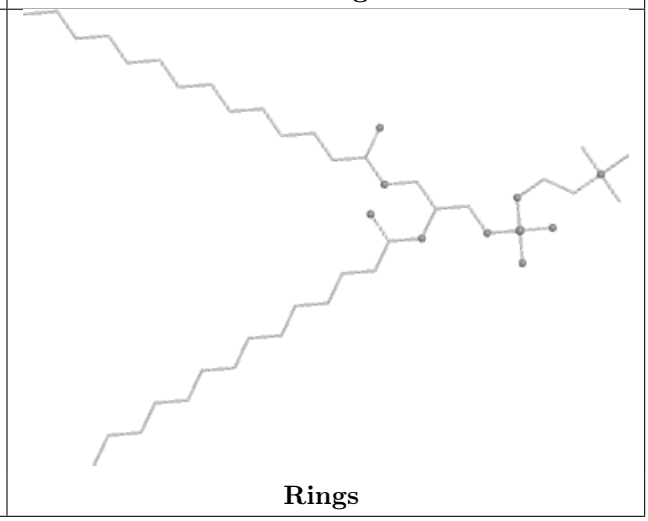
Bond lengths



Bond angles

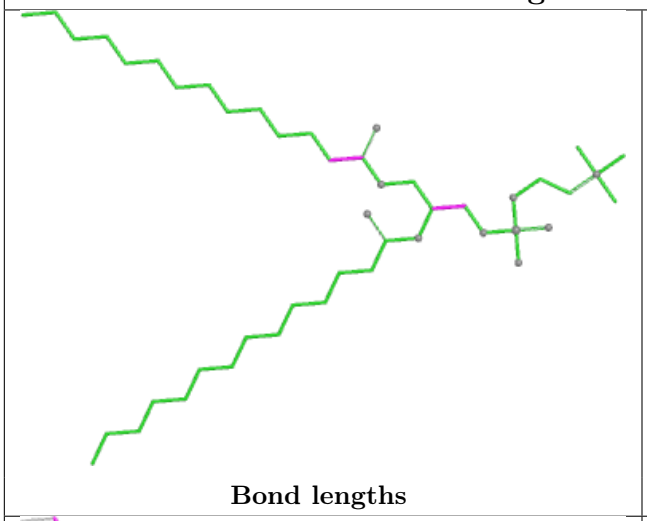


Torsions

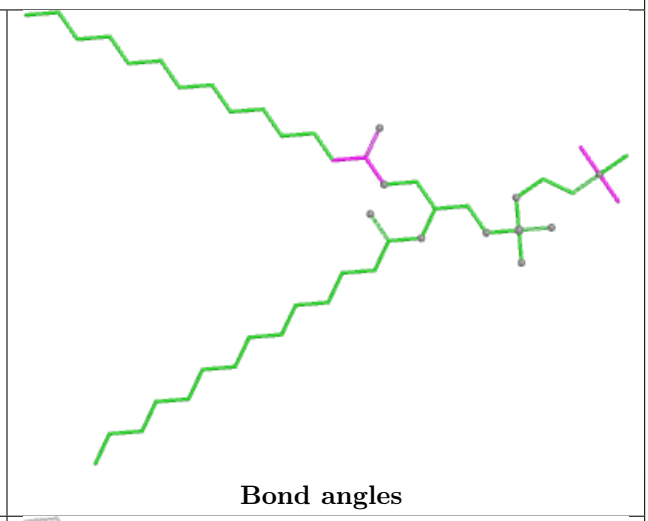


Rings

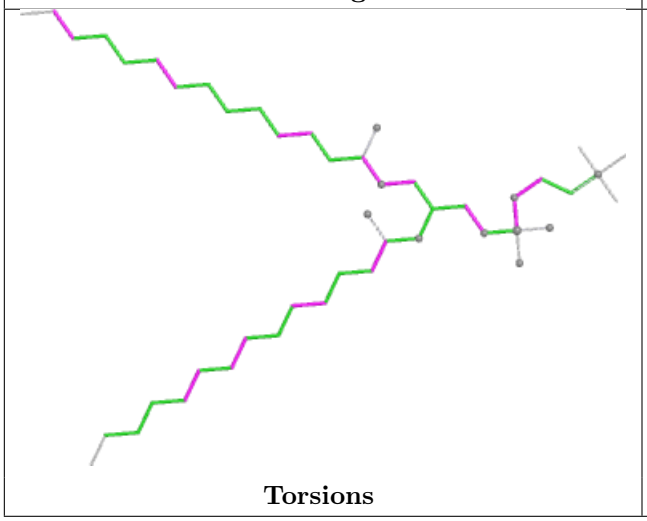
Ligand PX4 C 342



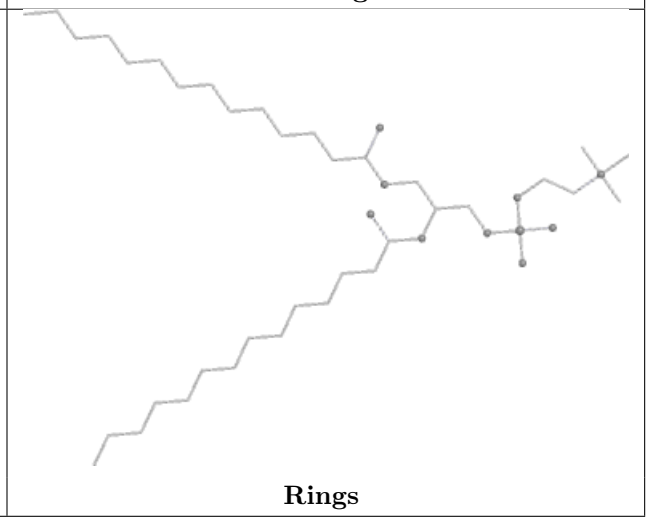
Bond lengths



Bond angles

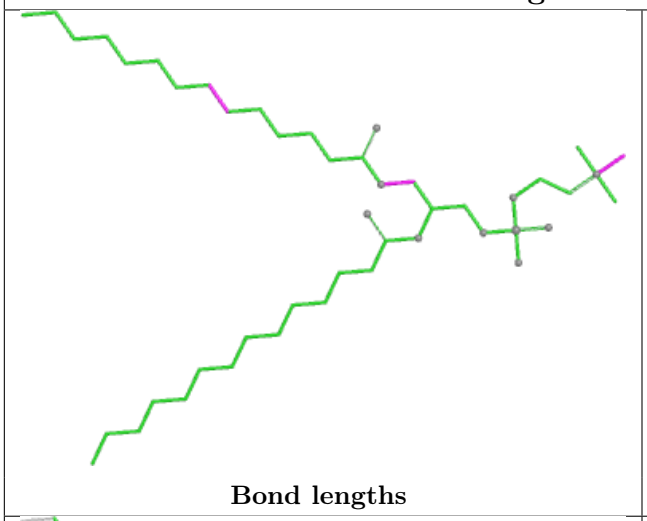


Torsions

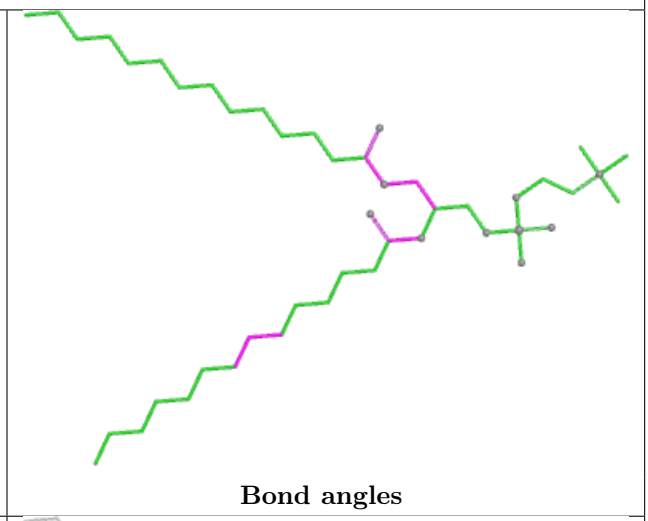


Rings

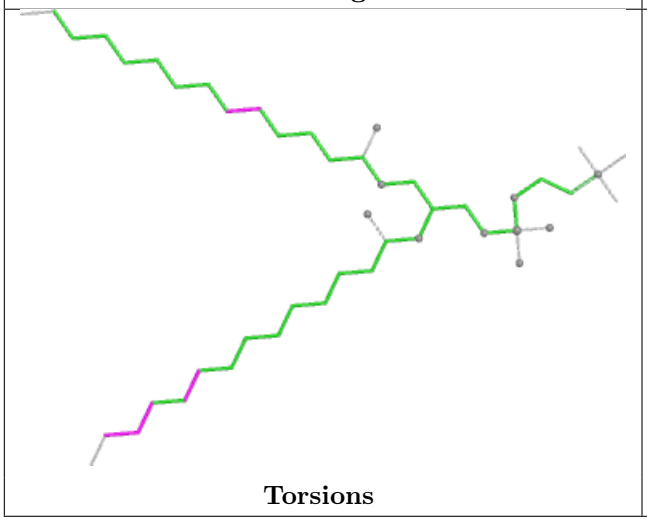
Ligand PX4 C 351



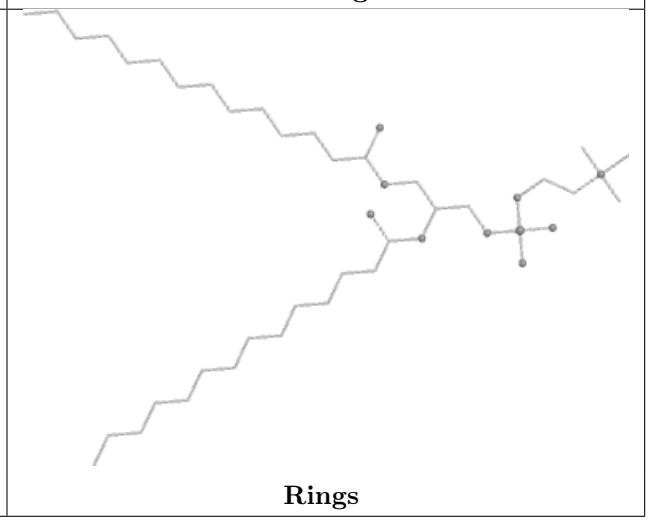
Bond lengths



Bond angles

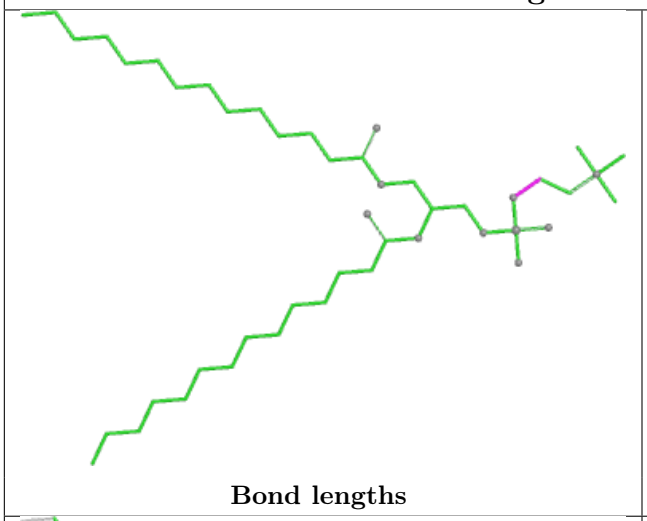


Torsions

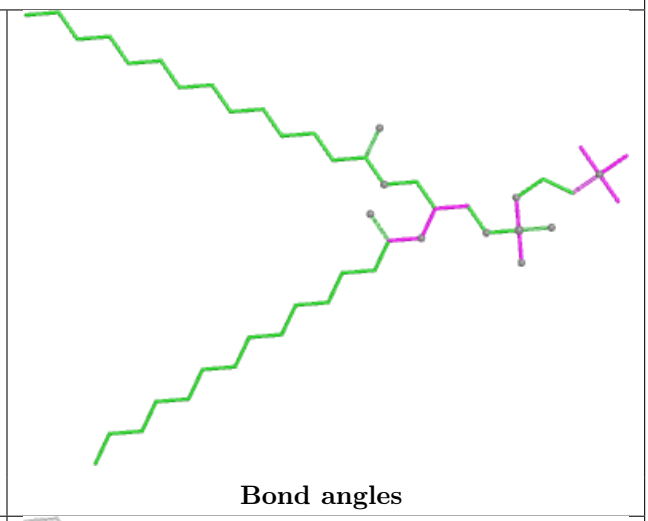


Rings

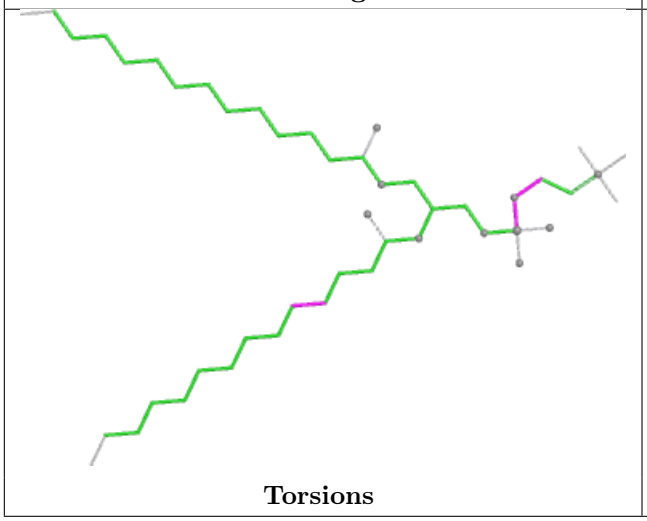
Ligand PX4 C 315



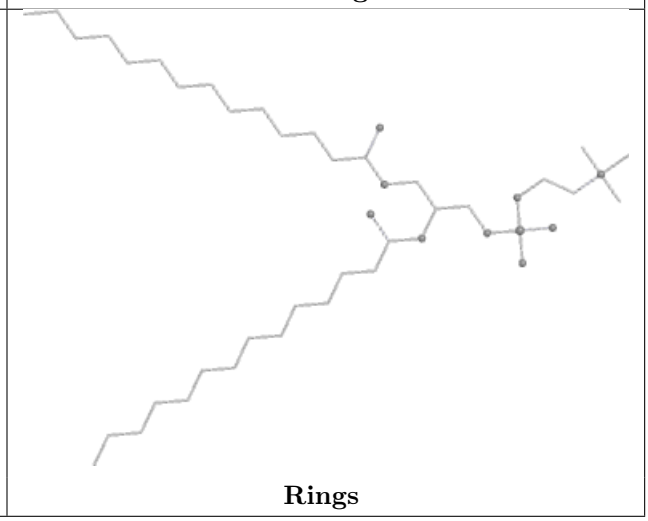
Bond lengths



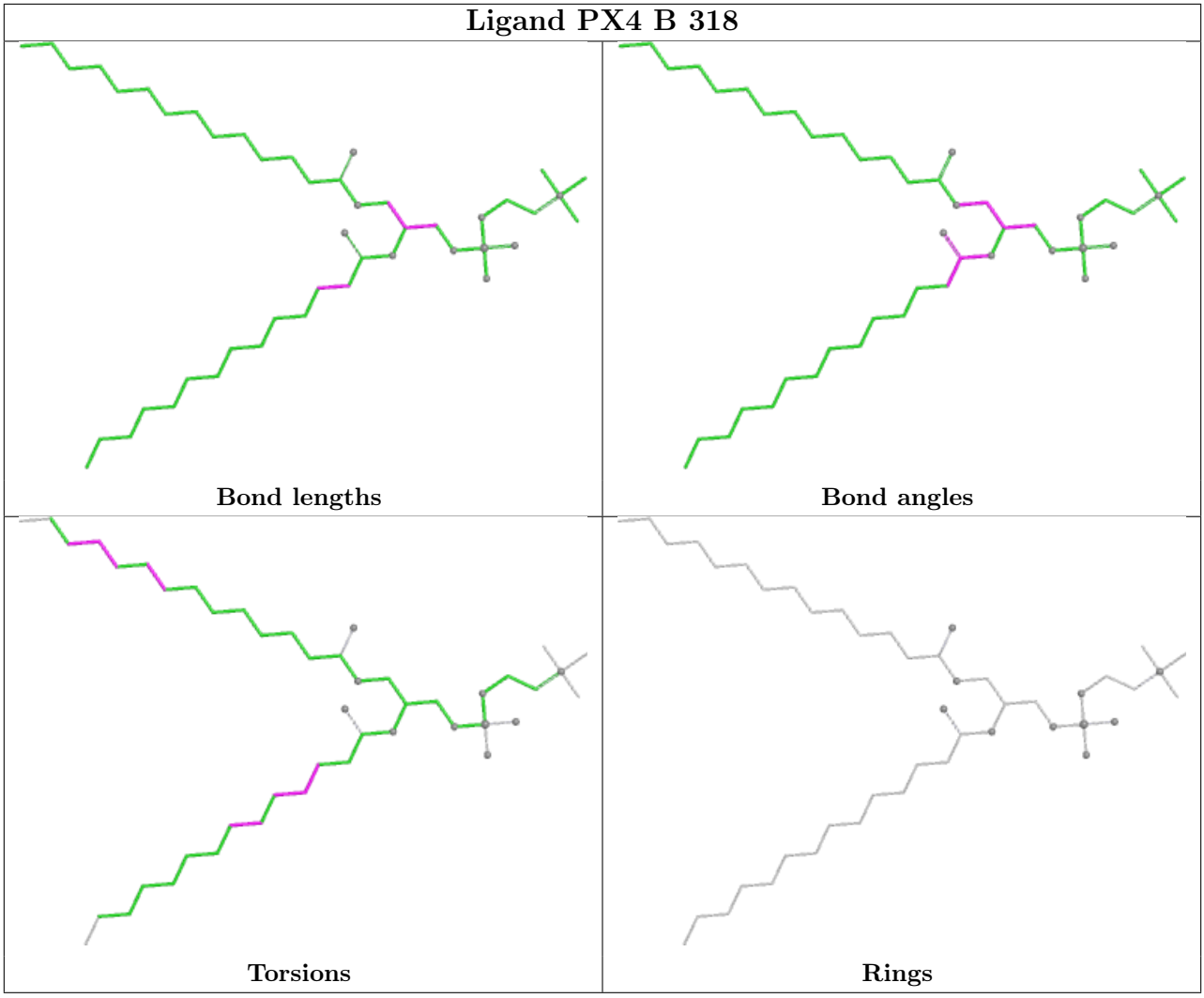
Bond angles



Torsions



Rings



6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

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: *Deposition_nmr_coordinates_6Aug18.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 8785. 0 out of 99 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	184/3048 (6%)	92/1233 (7%)	0/1230 (0%)	92/585 (16%)
Sidechain	140/4970 (3%)	105/3181 (3%)	35/1554 (2%)	0/235 (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	324/8785 (4%)	197/4791 (4%)	35/3148 (1%)	92/846 (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:

