Full wwPDB NMR Structure Validation Report (i)

Jun 3, 2023 – 10:16 PM EDT

PDB ID	:	2MZH
BMRB ID	:	25488
Title	:	NMR Solution Structure of the PRO Form of Human Matrilysin (proMMP-7) in Complex with Zwitterionic Membrane
Authors	:	Prior, S.H.; Van Doren, S.R.
Deposited on	:	2015-02-12

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

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

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

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

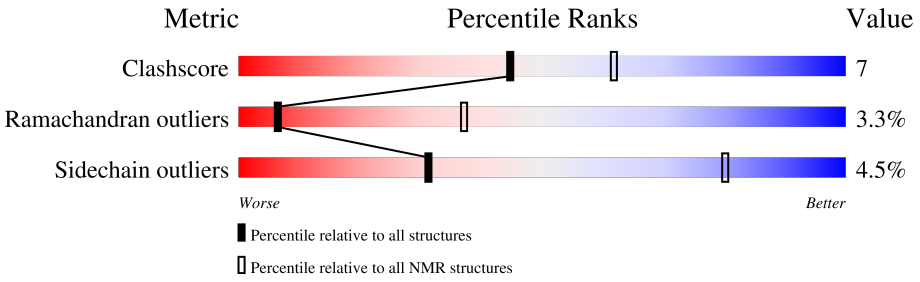
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

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 48%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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

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

Mol	Chain	Length	Quality of chain
1	A	248	74% 17% • 8%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 11 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *fewest violations*.

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:11-A:239 (229)	1.15	11

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 3 clusters and 2 single-model clusters were found.

Cluster number	Models
1	1, 2, 4, 5, 6, 7, 8, 10, 11, 12, 13, 14, 17, 19
2	9, 18
3	3, 15
Single-model clusters	16; 20

3 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9696 atoms, of which 1898 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Matrilysin.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	248	3850	1240	1898	339	364	9	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	195	ALA	GLU	engineered mutation	UNP P09237

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

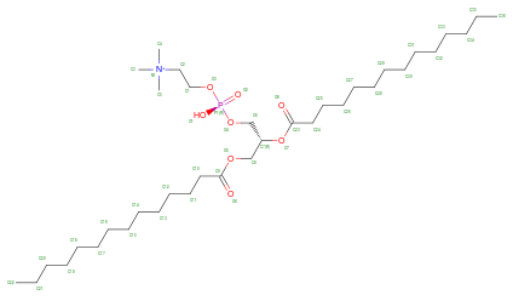
Mol	Chain	Residues	Atoms	
			Total	Ca
2	A	2	2	2

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	
			Total	Zn
3	A	2	2	2

- Molecule 4 is 1,2-DIMYRISTOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PX4) (formula: $C_{36}H_{73}NO_8P$).

PX4



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

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

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

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

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

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

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

4 Residue-property plots (i)

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: Matrilysin

Chain A: 74% 17% • 8%

L0 P1 Q2 E3 A4 G5 G6 M7 S8 E9 L10 Q11 W12 Y18 R21 F22 Y23 L24 Y25 D26 N31 F45 F46 L54 R57 P65 R66 D71 V72 A73 E74 Y75 F78 Y91 R92 Y96 T97 R98 R107 R125 W129 F138 A139 R140

D145 S146 Y147 P148 F149 D150 T155 L156 D169 D175 E176 R177 D180 F188 L189 Y190 Y213 Y216 Y238 G239 K240 R241 S242 N243 S244 R245 K246 K247

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: Matrilysin

Chain A: 69% 19% • 8%

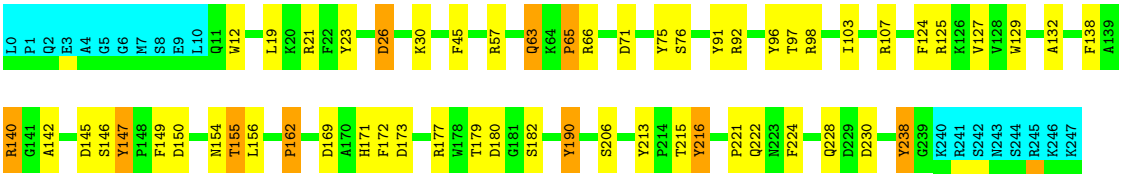
L0 P1 Q2 E3 A4 G5 G6 M7 S8 E9 L10 Q11 W12 Y18 Y23 L24 Y25 D26 K30 N31 F45 F46 L54 R57 V58 I59 P65 R66 D71 V72 A73 E74 Y75 F78 P79 N80 K83 Y91 R92 Y96 T97 R98 D99 D106 R107 P121

R125 V128 W129 D133 F138 A139 R140 D145 S146 Y147 D150 T155 A159 F160 T164 D173 E174 D175 E176 R177 D180 G185 F188 L189 Y190 Y213 Y216 Q222 L226 D230 L237 Y238 G239 K240 R241 S242 N243 S244 R245 K246 K247

4.2.2 Score per residue for model 2

• Molecule 1: Matrilysin

Chain A: 69% 19% • 8%



4.2.3 Score per residue for model 3

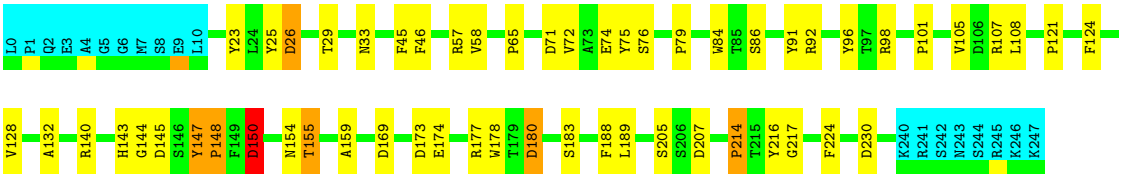
- Molecule 1: Matrilysin

Chain A: 67% 21% • 8%

4.2.4 Score per residue for model 4

- Molecule 1: Matrilysin

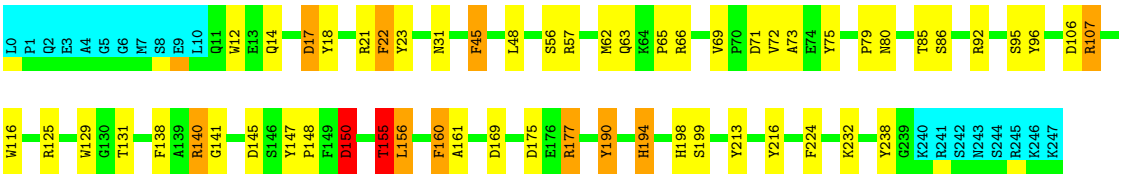
Chain A: 70% 20% • 8%



4.2.5 Score per residue for model 5

- Molecule 1: Matrilysin

Chain A: 69% 18% • • 8%



4.2.6 Score per residue for model 6

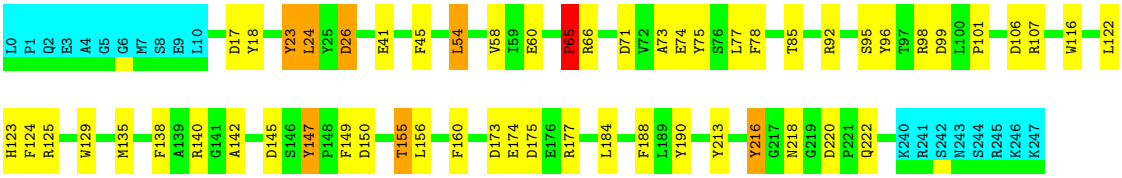
- Molecule 1: Matrilysin

Chain A: 68% 20% • 8%

4.2.7 Score per residue for model 7

- Molecule 1: Matrilysin

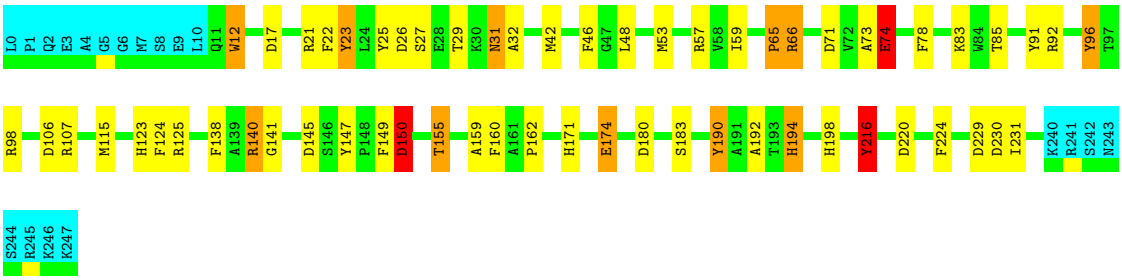
Chain A: 70% 19% • 8%



4.2.8 Score per residue for model 8

- Molecule 1: Matrilysin

Chain A: 68% 19% • • 8%



4.2.9 Score per residue for model 9

- Molecule 1: Matrilysin

Chain A: 62% 27% • • 8%

L0 P1 Q2 E3 A4 G5 G6 M7 S8 E9 L10 Q11 W12 Y18 R21 F22 Y23 L24 Y25 D26 T29 K30 N31 M42 F45 F46 L54 R57 V58 I59 P65 R66 V69 P70 D71 V72 A73 E74 Y75 S76 L77 F78 S81 T85 Y91 R92 I93 V94

S95 Y96 T97 R98 D99 T104 L108 V109 R125 K126 V127 V128 R140 G141 A142 H143 G144 D145 S146 Y147 P148 F149 D150 N154 T155 L156 A161 P162 F172 D173 E174 D175 E176 R177 S183 F188 L189 Y190 H194 H198 D207 V211 M212 Y213 Y216

N223 D229 D230 I231 K232 Q235 Y238 G239 K240 R241 S242 N243 S244 R245 K246 K247

4.2.10 Score per residue for model 10

- Molecule 1: Matrilysin

Chain A: 72% 17% • 8%

L0 P1 Q2 E3 A4 G5 G6 M7 S8 E9 L10 Y18 L19 K20 R21 F22 Y23 L24 Y25 N31 L39 L54 N55 S56 R57 V58 P65 R66 V69 P70 D71 Y75 F78 W84 V89 T90 Y91 R92 Y96 T97 R98 D99 T104 V105 D106 R107 L113

N114 M115 W116 H123 F124 R125 G130 F138 A139 R140 H143 G144 D145 P148 F149 D150 T155 L156 F160 D169 F172 R177 G185 F188 P214 T215 Y216 Y238 G239 K240 R241 S242 N243 S244 R245 K246 K247

4.2.11 Score per residue for model 11 (medoid)

- Molecule 1: Matrilysin

Chain A: 71% 19% • 8%

L0 P1 Q2 E3 A4 G5 G6 M7 S8 E9 L10 Q11 W12 D17 Y18 L19 K20 R21 F22 Y23 N31 A32 L39 K40 E41 F45 F46 L54 N55 S56 R57 V58 P65 R66 P70 D71 E74 Y75 R92 T97 R98 D99 R125 W129 F138 A139 R140

H143 G144 D145 F149 D150 T155 F160 D169 F172 D173 R177 D180 L184 F188 L189 Y190 L200 A210 Y213 P214 T215 Y216 D220 K240 R241 S242 N243 S244 R245 K246 K247

4.2.12 Score per residue for model 12

- Molecule 1: Matrilysin

Chain A: 68% 20% • 8%

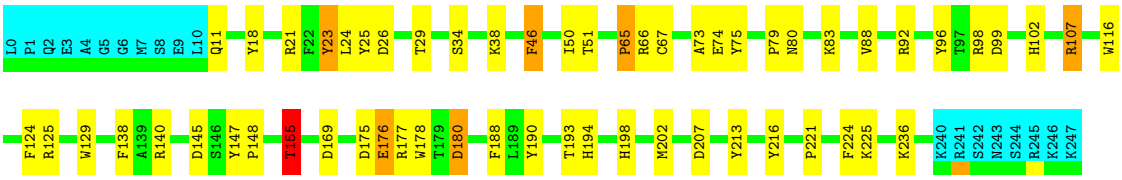
L0 P1 Q2 E3 A4 G5 G6 M7 S8 E9 L10 K20 R21 F22 Y23 L24 Y25 N31 A32 N33 K40 E41 R57 P65 R66 V69 P70 D71 V72 Y75 S76 L77 F78 P79 N80 K83 Y91 R92 Y96 T97 R98 D99 L100 T104 V109 W116

H123 F124 R125 W129 D133 F138 A139 R140 G141 A142 H143 G144 D145 S146 Y147 P148 F149 D150 T155 L156 F160 D169 D175 W178 A195 S205 S206 D207 P208 M212 Y213 Y216 D229 G233 K240 R241 S242 N243 S244 R245 K246 K247

4.2.13 Score per residue for model 13

- Molecule 1: Matrilysin

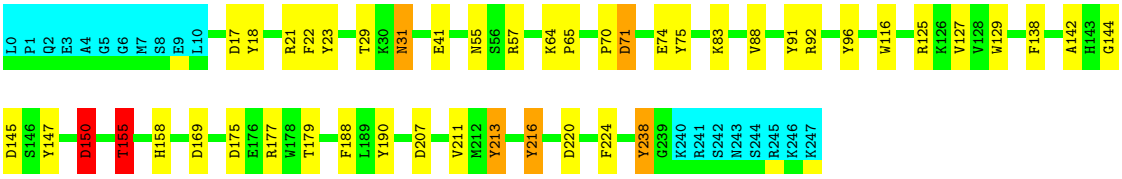
Chain A: 69% 21% • 8%



4.2.14 Score per residue for model 14

- Molecule 1: Matrilysin

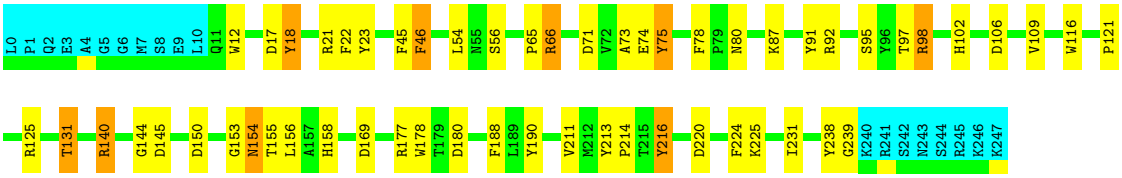
Chain A: 74% 16% •• 8%



4.2.15 Score per residue for model 15

- Molecule 1: Matrilysin

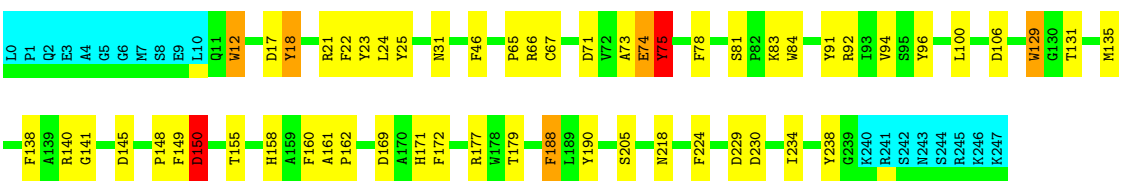
Chain A: 70% 19% • 8%



4.2.16 Score per residue for model 16

- Molecule 1: Matrilysin

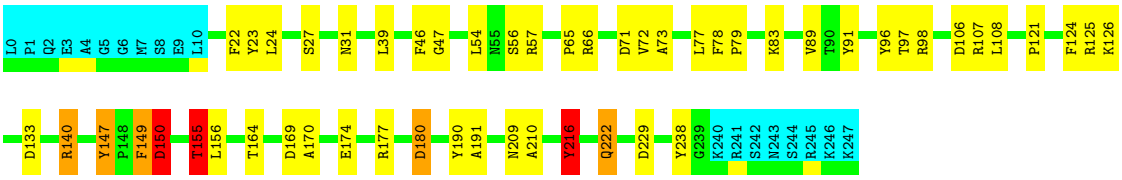
Chain A: 70% 20% •• 8%



4.2.17 Score per residue for model 17

- Molecule 1: Matrilysin

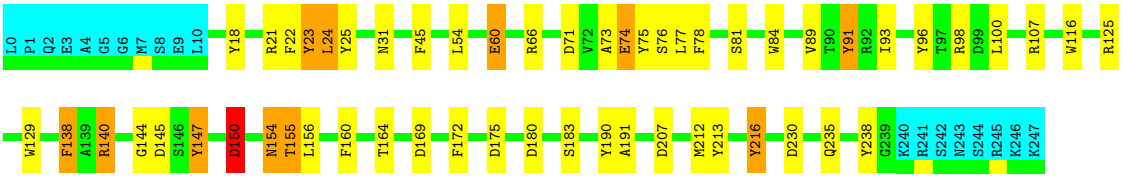
Chain A: 71% 18% • • 8%



4.2.18 Score per residue for model 18

- Molecule 1: Matrilysin

Chain A: 70% 17% • 8%



4.2.19 Score per residue for model 19

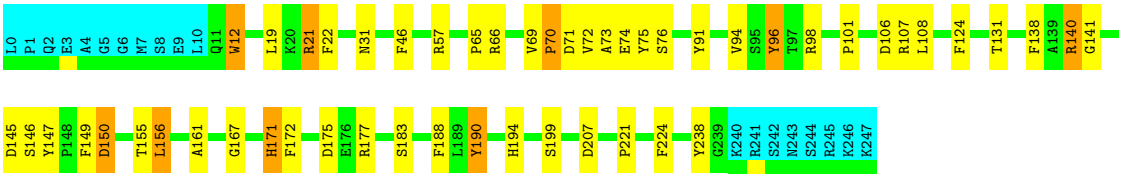
- Molecule 1: Matrilysin

Chain A: 67% 22% • 8%

4.2.20 Score per residue for model 20

- Molecule 1: Matrilysin

Chain A: 71% 17% • 8%


L0
P1
Q2
E3
A4
G5
G6
M7
S8
E9
L10
Q11
W12
L19
K20
R21
F22
N31
F46
R57
P65
R66
V69
P70
D71
V72
A73
E74
Y75
S76
Y91
V94
S95
Y96
I97
R98
P101
D106
R107
L108
F124
T131
F138
A139
R140
G141
D145
S146
Y147
P148
F149
D150
T155
L156
A161
G167
H171
F172
D175
E176
R177
S183
F188
L189
Y190
H194
S199
D207
P221
F224
Y238
G239
K240
R241
S242
N243
S244
R245
K246
K247

5 Refinement protocol and experimental data overview (i)

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

Of the 10000 calculated structures, 20 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	**Classification**	**Version**
HADDOCK	structure solution	2.1
GROMOS	refinement	4.5.7

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	1503
Number of shifts mapped to atoms	1503
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	48%

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: ZN, PX4, CA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.52±0.00	0±0/1858 (0.0± 0.0%)	2.04±0.04	58±6/2520 (2.3± 0.2%)
All	All	0.52	0/37160 (0.0%)	2.04	1156/50400 (2.3%)

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	6.8±2.3
All	All	0	135

There are no bond-length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	140	ARG	NE-CZ-NH2	-20.93	109.84	120.30	5	9
1	A	75	TYR	CB-CG-CD2	-17.54	110.47	121.00	4	5
1	A	177	ARG	NE-CZ-NH2	-17.42	111.59	120.30	13	9
1	A	18	TYR	CB-CG-CD2	-17.28	110.63	121.00	7	9
1	A	98	ARG	NE-CZ-NH2	-16.76	111.92	120.30	18	8
1	A	140	ARG	NE-CZ-NH1	16.44	128.52	120.30	17	14
1	A	238	TYR	CB-CG-CD2	-16.14	111.32	121.00	3	5
1	A	107	ARG	NE-CZ-NH1	15.30	127.95	120.30	17	10
1	A	57	ARG	NE-CZ-NH1	15.19	127.90	120.30	2	8
1	A	125	ARG	NE-CZ-NH2	-15.00	112.80	120.30	12	9
1	A	213	TYR	CB-CG-CD2	-14.55	112.27	121.00	5	6
1	A	21	ARG	NE-CZ-NH1	13.74	127.17	120.30	20	9

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	71	ASP	CB-CG-OD2	13.22	130.19	118.30	2	13
1	A	230	ASP	CB-CG-OD2	12.96	129.97	118.30	18	3
1	A	57	ARG	NE-CZ-NH2	-12.71	113.94	120.30	17	8
1	A	125	ARG	NE-CZ-NH1	12.68	126.64	120.30	19	11
1	A	145	ASP	CB-CG-OD1	12.29	129.36	118.30	5	13
1	A	98	ARG	NE-CZ-NH1	12.08	126.34	120.30	17	10
1	A	91	TYR	CB-CG-CD2	-12.02	113.79	121.00	15	9
1	A	46	PHE	CB-CG-CD1	-12.01	112.39	120.80	17	7
1	A	71	ASP	CB-CG-OD1	12.00	129.10	118.30	10	15
1	A	21	ARG	NE-CZ-NH2	-11.95	114.32	120.30	2	9
1	A	92	ARG	NE-CZ-NH1	11.78	126.19	120.30	14	9
1	A	224	PHE	CB-CG-CD2	-11.73	112.59	120.80	20	4
1	A	66	ARG	NE-CZ-NH2	-11.67	114.47	120.30	3	8
1	A	91	TYR	CB-CG-CD1	-11.66	114.00	121.00	4	8
1	A	107	ARG	NE-CZ-NH2	-11.38	114.61	120.30	17	7
1	A	177	ARG	NE-CZ-NH1	11.36	125.98	120.30	9	10
1	A	22	PHE	CB-CG-CD2	-11.33	112.87	120.80	5	9
1	A	92	ARG	NE-CZ-NH2	-11.16	114.72	120.30	13	9
1	A	23	TYR	CB-CG-CD1	-11.14	114.31	121.00	4	6
1	A	145	ASP	CB-CG-OD2	10.92	128.13	118.30	3	13
1	A	45	PHE	CB-CG-CD1	-10.91	113.16	120.80	15	5
1	A	190	TYR	CB-CG-CD1	-10.71	114.58	121.00	5	6
1	A	91	TYR	CG-CD1-CE1	-10.61	112.81	121.30	6	2
1	A	213	TYR	CB-CG-CD1	-10.42	114.75	121.00	11	7
1	A	96	TYR	CB-CG-CD2	10.29	127.18	121.00	20	6
1	A	91	TYR	CG-CD2-CE2	-10.28	113.07	121.30	4	3
1	A	18	TYR	CB-CG-CD1	-10.21	114.88	121.00	9	4
1	A	150	ASP	CB-CG-OD1	10.19	127.47	118.30	18	4
1	A	138	PHE	CB-CG-CD2	-10.16	113.69	120.80	13	7
1	A	175	ASP	CB-CG-OD1	10.13	127.42	118.30	19	5
1	A	169	ASP	CB-CG-OD1	9.92	127.23	118.30	2	8
1	A	224	PHE	CB-CG-CD1	9.87	127.71	120.80	20	5
1	A	238	TYR	CB-CG-CD1	-9.84	115.09	121.00	5	9
1	A	96	TYR	CB-CG-CD1	-9.72	115.17	121.00	4	9
1	A	23	TYR	CB-CG-CD2	-9.72	115.17	121.00	1	9
1	A	188	PHE	CB-CG-CD2	-9.69	114.02	120.80	10	8
1	A	18	TYR	CG-CD2-CE2	-9.63	113.60	121.30	7	2
1	A	190	TYR	CB-CG-CD2	-9.42	115.35	121.00	16	7
1	A	66	ARG	NE-CZ-NH1	9.36	124.98	120.30	10	5
1	A	216	TYR	CB-CG-CD2	9.33	126.60	121.00	15	6
1	A	46	PHE	CB-CG-CD2	-9.26	114.32	120.80	13	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	155	THR	CA-CB-CG2	9.11	125.16	112.40	17	4
1	A	133	ASP	CB-CG-OD1	9.06	126.45	118.30	17	3
1	A	74	GLU	OE1-CD-OE2	-9.01	112.48	123.30	16	2
1	A	188	PHE	CB-CG-CD1	-8.98	114.52	120.80	15	5
1	A	71	ASP	OD1-CG-OD2	-8.96	106.27	123.30	19	15
1	A	220	ASP	CB-CG-OD2	-8.94	110.25	118.30	6	3
1	A	140	ARG	CD-NE-CZ	8.92	136.09	123.60	1	7
1	A	172	PHE	CB-CG-CD1	-8.86	114.60	120.80	18	4
1	A	29	THR	CA-CB-CG2	8.73	124.62	112.40	3	5
1	A	78	PHE	CB-CG-CD2	-8.71	114.70	120.80	8	4
1	A	216	TYR	CB-CG-CD1	-8.60	115.84	121.00	15	9
1	A	116	TRP	NE1-CE2-CD2	-8.59	98.71	107.30	5	6
1	A	150	ASP	CB-CG-OD2	8.57	126.02	118.30	16	4
1	A	172	PHE	CB-CG-CD2	-8.53	114.83	120.80	2	4
1	A	72	VAL	CA-CB-CG1	8.45	123.58	110.90	19	1
1	A	127	VAL	CA-CB-CG1	8.41	123.51	110.90	2	3
1	A	138	PHE	CB-CG-CD1	-8.40	114.92	120.80	18	6
1	A	106	ASP	CB-CG-OD2	8.39	125.85	118.30	15	6
1	A	94	VAL	CA-CB-CG2	8.39	123.48	110.90	20	2
1	A	145	ASP	OD1-CG-OD2	-8.31	107.51	123.30	5	15
1	A	213	TYR	CG-CD2-CE2	-8.20	114.74	121.30	18	3
1	A	149	PHE	CB-CG-CD1	-8.15	115.10	120.80	16	6
1	A	99	ASP	CB-CG-OD2	-8.12	110.99	118.30	11	7
1	A	159	ALA	CB-CA-C	8.12	122.27	110.10	3	4
1	A	207	ASP	CB-CG-OD2	-8.00	111.10	118.30	13	5
1	A	65	PRO	N-CA-CB	7.96	112.85	103.30	2	3
1	A	206	SER	CB-CA-C	7.94	125.18	110.10	12	1
1	A	169	ASP	CB-CG-OD2	7.91	125.42	118.30	12	6
1	A	210	ALA	CB-CA-C	-7.89	98.26	110.10	11	2
1	A	116	TRP	CE2-CD2-CG	7.86	113.59	107.30	5	4
1	A	91	TYR	CD1-CG-CD2	7.79	126.47	117.90	4	2
1	A	229	ASP	CB-CG-OD1	7.75	125.27	118.30	8	3
1	A	129	TRP	CD1-NE1-CE2	7.75	115.97	109.00	14	4
1	A	25	TYR	CG-CD1-CE1	-7.72	115.12	121.30	4	2
1	A	12	TRP	CB-CG-CD2	7.68	136.58	126.60	2	1
1	A	12	TRP	CD1-NE1-CE2	7.66	115.90	109.00	16	5
1	A	124	PHE	CB-CG-CD1	-7.66	115.44	120.80	4	4
1	A	75	TYR	CB-CG-CD1	7.65	125.59	121.00	4	6
1	A	18	TYR	CA-CB-CG	7.65	127.93	113.40	19	2
1	A	12	TRP	CD1-CG-CD2	-7.62	100.21	106.30	5	1
1	A	129	TRP	NE1-CE2-CD2	-7.60	99.70	107.30	14	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	116	TRP	CZ3-CH2-CZ2	-7.58	112.50	121.60	19	1
1	A	14	GLN	N-CA-CB	-7.55	97.01	110.60	5	1
1	A	79	PRO	N-CA-CB	7.54	112.35	103.30	13	1
1	A	106	ASP	CB-CG-OD1	-7.48	111.57	118.30	20	4
1	A	116	TRP	CH2-CZ2-CE2	7.48	124.88	117.40	19	1
1	A	78	PHE	CB-CG-CD1	7.44	126.01	120.80	3	3
1	A	75	TYR	CG-CD1-CE1	-7.41	115.37	121.30	4	3
1	A	116	TRP	CD1-NE1-CE2	7.41	115.67	109.00	5	6
1	A	98	ARG	NH1-CZ-NH2	7.41	127.55	119.40	4	1
1	A	131	THR	CA-CB-CG2	-7.40	102.05	112.40	15	1
1	A	17	ASP	CB-CG-OD2	7.39	124.95	118.30	14	3
1	A	214	PRO	N-CA-CB	7.34	112.10	103.30	10	1
1	A	66	ARG	CD-NE-CZ	7.29	133.80	123.60	5	5
1	A	149	PHE	CB-CG-CD2	-7.27	115.71	120.80	11	4
1	A	129	TRP	CE2-CD2-CG	7.27	113.11	107.30	1	2
1	A	98	ARG	CD-NE-CZ	7.25	133.75	123.60	2	3
1	A	150	ASP	CB-CA-C	7.24	124.87	110.40	14	7
1	A	18	TYR	CG-CD1-CE1	-7.21	115.53	121.30	15	2
1	A	164	THR	C-N-CA	7.21	137.45	122.30	18	1
1	A	96	TYR	CG-CD1-CE1	-7.20	115.54	121.30	4	6
1	A	140	ARG	NH1-CZ-NH2	7.18	127.30	119.40	5	4
1	A	238	TYR	CG-CD1-CE1	-7.18	115.56	121.30	16	5
1	A	69	VAL	CA-CB-CG2	7.13	121.59	110.90	20	4
1	A	147	TYR	CB-CG-CD2	7.11	125.27	121.00	5	3
1	A	17	ASP	CB-CG-OD1	7.09	124.68	118.30	7	3
1	A	180	ASP	CB-CA-C	7.09	124.58	110.40	4	2
1	A	238	TYR	CG-CD2-CE2	-7.09	115.63	121.30	16	2
1	A	91	TYR	CD1-CE1-CZ	7.08	126.17	119.80	6	3
1	A	108	LEU	CB-CG-CD1	7.08	123.04	111.00	4	4
1	A	116	TRP	NE1-CE2-CZ2	7.06	138.16	130.40	5	2
1	A	107	ARG	NH1-CZ-NH2	7.04	127.14	119.40	1	1
1	A	84	TRP	CD1-NE1-CE2	7.00	115.30	109.00	18	1
1	A	60	GLU	OE1-CD-OE2	-7.00	114.90	123.30	18	1
1	A	45	PHE	CB-CG-CD2	-6.99	115.91	120.80	9	5
1	A	191	ALA	CB-CA-C	-6.99	99.62	110.10	19	1
1	A	22	PHE	CB-CG-CD1	6.98	125.69	120.80	15	4
1	A	116	TRP	CE3-CZ3-CH2	-6.98	113.52	121.20	18	1
1	A	89	VAL	CA-CB-CG1	6.96	121.33	110.90	17	2
1	A	133	ASP	CB-CG-OD2	6.92	124.53	118.30	19	2
1	A	23	TYR	CD1-CE1-CZ	6.92	126.03	119.80	7	4
1	A	65	PRO	CA-N-CD	-6.91	101.83	111.50	7	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	23	TYR	CG-CD2-CE2	-6.90	115.78	121.30	13	1
1	A	18	TYR	CD1-CG-CD2	6.89	125.48	117.90	7	1
1	A	124	PHE	CB-CG-CD2	6.86	125.60	120.80	4	4
1	A	207	ASP	CB-CG-OD1	6.84	124.46	118.30	9	3
1	A	213	TYR	CD1-CG-CD2	6.84	125.43	117.90	12	1
1	A	220	ASP	CB-CG-OD1	-6.84	112.14	118.30	7	2
1	A	102	HIS	CA-CB-CG	6.83	125.22	113.60	6	1
1	A	31	ASN	N-CA-CB	6.80	122.84	110.60	14	2
1	A	73	ALA	C-N-CA	6.80	138.69	121.70	17	8
1	A	199	SER	N-CA-CB	-6.80	100.31	110.50	19	2
1	A	95	SER	CB-CA-C	6.79	123.01	110.10	15	4
1	A	70	PRO	N-CD-CG	6.79	113.38	103.20	19	1
1	A	57	ARG	CD-NE-CZ	6.79	133.10	123.60	9	4
1	A	116	TRP	CB-CG-CD2	6.78	135.41	126.60	19	1
1	A	125	ARG	CD-NE-CZ	6.78	133.09	123.60	13	4
1	A	190	TYR	N-CA-CB	-6.75	98.45	110.60	7	2
1	A	96	TYR	CG-CD2-CE2	-6.75	115.90	121.30	19	4
1	A	154	ASN	C-N-CA	6.72	138.50	121.70	9	3
1	A	150	ASP	OD1-CG-OD2	-6.69	110.58	123.30	20	1
1	A	161	ALA	N-CA-CB	-6.69	100.73	110.10	20	3
1	A	105	VAL	CA-CB-CG2	6.68	120.92	110.90	4	1
1	A	26	ASP	CB-CG-OD2	6.67	124.30	118.30	9	3
1	A	147	TYR	CB-CG-CD1	-6.66	117.00	121.00	5	3
1	A	96	TYR	CD1-CG-CD2	6.65	125.22	117.90	19	3
1	A	12	TRP	NE1-CE2-CD2	-6.64	100.66	107.30	20	5
1	A	183	SER	CB-CA-C	6.63	122.70	110.10	8	5
1	A	84	TRP	NE1-CE2-CD2	-6.60	100.70	107.30	18	1
1	A	171	HIS	CG-ND1-CE1	-6.59	97.14	105.70	16	1
1	A	69	VAL	CB-CA-C	6.57	123.89	111.40	10	1
1	A	25	TYR	CD1-CE1-CZ	6.57	125.71	119.80	4	2
1	A	25	TYR	CB-CG-CD2	-6.57	117.06	121.00	8	4
1	A	231	ILE	CA-CB-CG2	6.56	124.02	110.90	8	2
1	A	178	TRP	N-CA-CB	-6.55	98.80	110.60	4	1
1	A	86	SER	CB-CA-C	6.55	122.54	110.10	19	2
1	A	205	SER	N-CA-CB	-6.55	100.68	110.50	12	1
1	A	109	VAL	CA-CB-CG2	6.54	120.71	110.90	9	3
1	A	234	ILE	CA-CB-CG1	6.53	123.41	111.00	3	1
1	A	211	VAL	CG1-CB-CG2	-6.53	100.46	110.90	14	1
1	A	25	TYR	CB-CG-CD1	6.50	124.90	121.00	18	2
1	A	75	TYR	CD1-CE1-CZ	6.49	125.64	119.80	7	2
1	A	142	ALA	N-CA-CB	-6.49	101.02	110.10	14	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	54	LEU	C-N-CA	6.49	137.92	121.70	19	1
1	A	42	MET	CA-CB-CG	-6.48	102.28	113.30	8	1
1	A	160	PHE	CD1-CE1-CZ	-6.45	112.36	120.10	8	1
1	A	175	ASP	CB-CG-OD2	-6.45	112.50	118.30	9	2
1	A	45	PHE	CG-CD2-CE2	-6.44	113.71	120.80	5	1
1	A	88	VAL	CA-CB-CG2	6.44	120.56	110.90	13	1
1	A	92	ARG	NH1-CZ-NH2	6.41	126.45	119.40	1	1
1	A	85	THR	CA-CB-CG2	6.41	121.37	112.40	9	1
1	A	54	LEU	CB-CG-CD2	6.38	121.85	111.00	7	1
1	A	169	ASP	OD1-CG-OD2	-6.38	111.19	123.30	2	5
1	A	101	PRO	N-CD-CG	6.37	112.75	103.20	7	3
1	A	178	TRP	NE1-CE2-CZ2	6.36	137.40	130.40	3	1
1	A	96	TYR	CZ-CE2-CD2	-6.34	114.10	119.80	10	2
1	A	23	TYR	CG-CD1-CE1	-6.32	116.25	121.30	7	1
1	A	54	LEU	CB-CG-CD1	6.31	121.73	111.00	18	3
1	A	182	SER	C-N-CA	6.29	137.44	121.70	2	1
1	A	92	ARG	CD-NE-CZ	6.28	132.38	123.60	2	5
1	A	45	PHE	CZ-CE2-CD2	6.27	127.63	120.10	5	1
1	A	147	TYR	CG-CD2-CE2	-6.26	116.29	121.30	13	2
1	A	73	ALA	O-C-N	6.26	132.72	122.70	16	1
1	A	139	ALA	CB-CA-C	6.23	119.45	110.10	6	1
1	A	84	TRP	CH2-CZ2-CE2	6.23	123.63	117.40	4	2
1	A	213	TYR	N-CA-CB	-6.22	99.40	110.60	7	2
1	A	73	ALA	N-CA-CB	-6.21	101.41	110.10	1	2
1	A	84	TRP	CD1-CG-CD2	-6.20	101.34	106.30	3	1
1	A	89	VAL	CA-CB-CG2	6.20	120.20	110.90	10	2
1	A	173	ASP	CB-CG-OD1	6.19	123.87	118.30	4	3
1	A	193	THR	CA-CB-CG2	6.19	121.07	112.40	13	1
1	A	173	ASP	CB-CG-OD2	-6.19	112.73	118.30	7	3
1	A	12	TRP	CE2-CD2-CG	6.18	112.25	107.30	8	2
1	A	190	TYR	CA-CB-CG	6.18	125.14	113.40	14	4
1	A	160	PHE	CB-CG-CD1	-6.18	116.48	120.80	12	3
1	A	71	ASP	C-N-CA	6.16	137.10	121.70	1	2
1	A	190	TYR	CZ-CE2-CD2	-6.15	114.27	119.80	3	2
1	A	99	ASP	N-CA-CB	-6.13	99.57	110.60	7	2
1	A	130	GLY	O-C-N	6.12	132.49	122.70	10	1
1	A	144	GLY	C-N-CA	6.12	137.00	121.70	14	2
1	A	72	VAL	O-C-N	-6.09	112.95	122.70	12	2
1	A	96	TYR	CB-CA-C	6.08	122.56	110.40	7	2
1	A	238	TYR	CD1-CG-CD2	6.08	124.58	117.90	16	2
1	A	27	SER	N-CA-CB	-6.08	101.39	110.50	17	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	129	TRP	CA-CB-CG	6.07	125.24	113.70	12	1
1	A	26	ASP	CB-CG-OD1	6.07	123.76	118.30	1	3
1	A	70	PRO	N-CA-CB	6.07	110.58	103.30	14	3
1	A	156	LEU	CB-CA-C	6.06	121.71	110.20	20	1
1	A	200	LEU	CB-CG-CD1	6.02	121.23	111.00	3	1
1	A	74	GLU	CA-CB-CG	6.01	126.62	113.40	8	1
1	A	212	MET	CB-CA-C	6.00	122.41	110.40	18	2
1	A	84	TRP	NE1-CE2-CZ2	6.00	137.00	130.40	4	1
1	A	178	TRP	CB-CG-CD1	-6.00	119.20	127.00	12	1
1	A	32	ALA	N-CA-CB	-5.99	101.72	110.10	11	1
1	A	65	PRO	N-CD-CG	5.97	112.16	103.20	7	3
1	A	20	LYS	N-CA-CB	-5.97	99.86	110.60	12	1
1	A	58	VAL	O-C-N	-5.96	113.16	122.70	7	1
1	A	192	ALA	CB-CA-C	-5.96	101.16	110.10	19	1
1	A	91	TYR	CA-CB-CG	5.95	124.71	113.40	17	2
1	A	121	PRO	N-CA-CB	5.94	110.43	103.30	4	1
1	A	160	PHE	CB-CG-CD2	5.94	124.96	120.80	12	3
1	A	160	PHE	CG-CD1-CE1	5.93	127.33	120.80	8	2
1	A	129	TRP	CB-CG-CD2	5.93	134.31	126.60	1	2
1	A	104	THR	CA-CB-CG2	5.92	120.69	112.40	10	1
1	A	99	ASP	CB-CG-OD1	5.92	123.63	118.30	12	2
1	A	75	TYR	CG-CD2-CE2	-5.92	116.56	121.30	16	3
1	A	75	TYR	N-CA-CB	5.89	121.20	110.60	9	1
1	A	158	HIS	CB-CA-C	5.89	122.17	110.40	14	1
1	A	107	ARG	CD-NE-CZ	5.88	131.83	123.60	4	1
1	A	131	THR	C-N-CA	5.88	136.40	121.70	16	2
1	A	190	TYR	CG-CD2-CE2	-5.88	116.60	121.30	18	2
1	A	202	MET	CG-SD-CE	5.88	109.60	100.20	13	2
1	A	34	SER	N-CA-CB	-5.88	101.69	110.50	13	1
1	A	177	ARG	N-CA-CB	-5.86	100.06	110.60	4	1
1	A	123	HIS	CA-CB-CG	5.85	123.55	113.60	7	3
1	A	173	ASP	N-CA-CB	-5.84	100.08	110.60	9	1
1	A	29	THR	O-C-N	-5.84	113.35	122.70	14	1
1	A	140	ARG	C-N-CA	5.84	134.56	122.30	20	3
1	A	216	TYR	CG-CD2-CE2	-5.82	116.64	121.30	8	2
1	A	129	TRP	CG-CD2-CE3	-5.82	128.66	133.90	13	1
1	A	126	LYS	C-N-CA	5.81	136.24	121.70	17	1
1	A	41	GLU	CA-CB-CG	5.81	126.19	113.40	11	1
1	A	148	PRO	N-CA-CB	5.80	110.26	103.30	3	1
1	A	50	ILE	CA-CB-CG1	5.79	122.00	111.00	13	1
1	A	91	TYR	CZ-CE2-CD2	-5.79	114.59	119.80	20	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	178	TRP	NE1-CE2-CD2	-5.78	101.52	107.30	3	3
1	A	23	TYR	CZ-CE2-CD2	-5.78	114.60	119.80	18	1
1	A	55	ASN	O-C-N	-5.77	113.47	122.70	14	1
1	A	129	TRP	CB-CA-C	5.77	121.93	110.40	7	2
1	A	75	TYR	C-N-CA	5.76	136.10	121.70	19	3
1	A	39	LEU	CB-CG-CD1	5.76	120.79	111.00	10	2
1	A	97	THR	O-C-N	-5.76	113.49	122.70	15	1
1	A	58	VAL	CG1-CB-CG2	-5.75	101.70	110.90	7	2
1	A	70	PRO	C-N-CA	5.75	136.07	121.70	12	1
1	A	146	SER	N-CA-CB	-5.74	101.89	110.50	20	3
1	A	171	HIS	CB-CA-C	5.73	121.86	110.40	16	1
1	A	132	ALA	N-CA-CB	-5.72	102.09	110.10	2	1
1	A	180	ASP	CB-CG-OD2	5.72	123.45	118.30	19	1
1	A	213	TYR	CG-CD1-CE1	-5.71	116.73	121.30	11	1
1	A	161	ALA	CB-CA-C	5.71	118.66	110.10	16	1
1	A	87	LYS	CB-CG-CD	5.70	126.42	111.60	15	1
1	A	170	ALA	CB-CA-C	5.70	118.65	110.10	3	2
1	A	129	TRP	C-N-CA	5.68	134.24	122.30	12	1
1	A	81	SER	CB-CA-C	5.68	120.89	110.10	16	1
1	A	179	THR	CA-CB-OG1	5.68	120.92	109.00	14	1
1	A	229	ASP	CB-CG-OD2	5.67	123.41	118.30	12	2
1	A	159	ALA	O-C-N	5.67	131.76	122.70	3	1
1	A	76	SER	CB-CA-C	5.64	120.83	110.10	12	2
1	A	67	CYS	CA-CB-SG	5.63	124.14	114.00	16	1
1	A	178	TRP	CD1-NE1-CE2	5.63	114.07	109.00	3	2
1	A	178	TRP	CB-CG-CD2	5.62	133.91	126.60	12	1
1	A	12	TRP	CE3-CZ3-CH2	-5.60	115.04	121.20	6	1
1	A	116	TRP	CB-CG-CD1	-5.60	119.72	127.00	19	1
1	A	18	TYR	CD1-CE1-CZ	5.58	124.83	119.80	15	1
1	A	173	ASP	CA-CB-CG	5.58	125.67	113.40	11	1
1	A	58	VAL	CA-CB-CG2	5.57	119.26	110.90	11	2
1	A	75	TYR	CB-CA-C	5.57	121.54	110.40	14	1
1	A	194	HIS	CA-CB-CG	5.56	123.06	113.60	5	2
1	A	22	PHE	CD1-CE1-CZ	5.56	126.78	120.10	17	1
1	A	129	TRP	NE1-CE2-CZ2	5.56	136.51	130.40	3	2
1	A	147	TYR	CB-CA-C	5.55	121.50	110.40	1	2
1	A	100	LEU	CB-CA-C	5.55	120.74	110.20	18	1
1	A	18	TYR	CZ-CE2-CD2	5.54	124.79	119.80	7	2
1	A	162	PRO	N-CD-CG	5.54	111.52	103.20	9	1
1	A	41	GLU	O-C-N	-5.54	113.84	122.70	12	1
1	A	192	ALA	N-CA-CB	5.54	117.85	110.10	8	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	12	TRP	CB-CG-CD1	-5.53	119.81	127.00	2	1
1	A	221	PRO	N-CD-CG	5.53	111.49	103.20	2	1
1	A	108	LEU	CB-CG-CD2	5.52	120.39	111.00	9	2
1	A	222	GLN	CB-CG-CD	5.51	125.94	111.60	17	1
1	A	132	ALA	CB-CA-C	5.51	118.37	110.10	4	1
1	A	129	TRP	CE2-CD2-CE3	-5.51	112.09	118.70	1	2
1	A	27	SER	CB-CA-C	5.51	120.56	110.10	19	1
1	A	150	ASP	N-CA-CB	5.50	120.50	110.60	4	1
1	A	79	PRO	C-N-CA	5.50	135.44	121.70	4	3
1	A	206	SER	N-CA-CB	-5.49	102.27	110.50	2	2
1	A	162	PRO	C-N-CA	5.49	133.82	122.30	8	1
1	A	79	PRO	CA-N-CD	-5.49	103.82	111.50	13	1
1	A	194	HIS	N-CA-CB	-5.48	100.74	110.60	3	1
1	A	42	MET	O-C-N	-5.47	113.94	122.70	9	1
1	A	89	VAL	CG1-CB-CG2	-5.47	102.14	110.90	18	1
1	A	143	HIS	CA-CB-CG	5.47	122.91	113.60	9	4
1	A	174	GLU	OE1-CD-OE2	-5.47	116.73	123.30	8	2
1	A	237	LEU	CB-CG-CD2	5.47	120.30	111.00	6	1
1	A	176	GLU	OE1-CD-OE2	-5.46	116.74	123.30	3	2
1	A	178	TRP	CH2-CZ2-CE2	-5.46	111.94	117.40	15	1
1	A	148	PRO	N-CD-CG	5.46	111.39	103.20	4	2
1	A	142	ALA	CB-CA-C	5.46	118.29	110.10	9	1
1	A	48	LEU	CB-CG-CD2	-5.46	101.73	111.00	5	1
1	A	221	PRO	C-N-CA	5.44	135.30	121.70	13	1
1	A	160	PHE	CZ-CE2-CD2	-5.44	113.57	120.10	18	2
1	A	234	ILE	CA-CB-CG2	5.43	121.77	110.90	16	1
1	A	216	TYR	CG-CD1-CE1	-5.43	116.95	121.30	11	1
1	A	23	TYR	C-N-CA	5.43	135.27	121.70	5	1
1	A	85	THR	C-N-CA	5.43	135.27	121.70	5	1
1	A	156	LEU	CB-CG-CD2	5.43	120.23	111.00	12	1
1	A	30	LYS	C-N-CA	5.42	135.26	121.70	2	2
1	A	150	ASP	C-N-CA	5.41	133.67	122.30	1	1
1	A	12	TRP	NE1-CE2-CZ2	5.40	136.34	130.40	8	2
1	A	51	THR	CA-CB-OG1	5.40	120.34	109.00	13	1
1	A	72	VAL	CA-CB-CG2	5.40	118.99	110.90	5	2
1	A	97	THR	CA-CB-CG2	5.40	119.95	112.40	19	2
1	A	128	VAL	CA-CB-CG2	5.38	118.96	110.90	1	1
1	A	225	LYS	CB-CA-C	5.37	121.14	110.40	13	2
1	A	24	LEU	CB-CA-C	5.37	120.40	110.20	18	1
1	A	220	ASP	N-CA-CB	-5.37	100.94	110.60	3	1
1	A	208	PRO	N-CA-CB	5.37	109.74	103.30	12	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	12	TRP	CH2-CZ2-CE2	5.36	122.76	117.40	1	1
1	A	155	THR	CB-CA-C	5.36	126.08	111.60	5	1
1	A	226	LEU	CB-CA-C	-5.36	100.01	110.20	1	1
1	A	195	ALA	N-CA-CB	5.36	117.60	110.10	12	1
1	A	230	ASP	CB-CG-OD1	-5.36	113.48	118.30	2	2
1	A	158	HIS	CA-CB-CG	5.36	122.71	113.60	6	2
1	A	212	MET	CG-SD-CE	5.35	108.77	100.20	12	1
1	A	200	LEU	CB-CA-C	-5.35	100.03	110.20	11	1
1	A	213	TYR	CD1-CE1-CZ	5.34	124.61	119.80	11	1
1	A	21	ARG	O-C-N	-5.34	114.15	122.70	12	1
1	A	79	PRO	N-CD-CG	5.34	111.21	103.20	13	1
1	A	47	GLY	CA-C-O	-5.33	111.00	120.60	17	1
1	A	40	LYS	O-C-N	-5.33	114.17	122.70	12	1
1	A	124	PHE	CG-CD2-CE2	5.33	126.66	120.80	6	1
1	A	38	LYS	O-C-N	-5.33	114.18	122.70	13	1
1	A	191	ALA	N-CA-CB	-5.32	102.66	110.10	17	2
1	A	26	ASP	CB-CA-C	5.31	121.02	110.40	2	1
1	A	214	PRO	N-CA-C	5.31	125.91	112.10	4	1
1	A	218	ASN	CB-CA-C	5.30	121.01	110.40	16	1
1	A	67	CYS	O-C-N	-5.30	114.19	123.20	13	1
1	A	155	THR	OG1-CB-CG2	-5.30	97.80	110.00	18	1
1	A	235	GLN	O-C-N	-5.30	114.22	122.70	3	1
1	A	55	ASN	N-CA-CB	5.30	120.13	110.60	11	1
1	A	171	HIS	CA-CB-CG	5.29	122.59	113.60	20	1
1	A	228	GLN	N-CA-CB	-5.29	101.09	110.60	2	1
1	A	139	ALA	N-CA-CB	-5.28	102.71	110.10	11	1
1	A	180	ASP	CB-CG-OD1	-5.28	113.55	118.30	13	1
1	A	116	TRP	CD2-CE3-CZ3	5.28	125.66	118.80	18	1
1	A	24	LEU	N-CA-CB	5.27	120.93	110.40	7	1
1	A	22	PHE	C-N-CA	5.27	134.87	121.70	12	1
1	A	205	SER	CB-CA-C	5.25	120.08	110.10	16	1
1	A	125	ARG	CG-CD-NE	5.25	122.82	111.80	12	1
1	A	198	HIS	O-C-N	5.25	131.10	122.70	3	1
1	A	56	SER	N-CA-CB	-5.25	102.63	110.50	15	1
1	A	29	THR	OG1-CB-CG2	-5.24	97.95	110.00	8	1
1	A	46	PHE	CZ-CE2-CD2	-5.23	113.82	120.10	19	1
1	A	86	SER	C-N-CA	5.23	134.78	121.70	4	1
1	A	88	VAL	CA-CB-CG1	5.22	118.74	110.90	14	1
1	A	183	SER	N-CA-CB	5.22	118.33	110.50	20	1
1	A	188	PHE	CZ-CE2-CD2	-5.22	113.84	120.10	1	1
1	A	105	VAL	CA-CB-CG1	5.21	118.72	110.90	19	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	19	LEU	O-C-N	-5.21	114.36	122.70	20	1
1	A	224	PHE	N-CA-CB	-5.21	101.23	110.60	5	1
1	A	103	ILE	CB-CA-C	5.20	122.00	111.60	3	1
1	A	128	VAL	CB-CA-C	5.20	121.28	111.40	9	1
1	A	95	SER	C-N-CA	5.20	134.70	121.70	6	2
1	A	33	ASN	N-CA-CB	-5.20	101.25	110.60	4	1
1	A	102	HIS	C-N-CA	5.19	134.68	121.70	15	1
1	A	45	PHE	CA-CB-CG	5.19	126.35	113.90	18	1
1	A	32	ALA	CB-CA-C	-5.19	102.32	110.10	8	2
1	A	221	PRO	O-C-N	-5.19	114.40	122.70	20	1
1	A	226	LEU	CB-CG-CD2	5.18	119.81	111.00	1	1
1	A	159	ALA	N-CA-CB	5.18	117.35	110.10	6	1
1	A	133	ASP	N-CA-CB	5.18	119.92	110.60	17	1
1	A	156	LEU	CB-CG-CD1	5.17	119.80	111.00	9	1
1	A	59	ILE	CA-CB-CG1	5.16	120.81	111.00	1	1
1	A	160	PHE	O-C-N	-5.16	114.45	122.70	11	1
1	A	135	MET	CG-SD-CE	5.16	108.45	100.20	16	1
1	A	57	ARG	NH1-CZ-NH2	5.16	125.07	119.40	17	1
1	A	19	LEU	CB-CG-CD2	5.15	119.75	111.00	2	1
1	A	23	TYR	CD1-CG-CD2	5.15	123.56	117.90	13	1
1	A	213	TYR	CA-CB-CG	5.14	123.17	113.40	2	1
1	A	62	MET	CG-SD-CE	5.13	108.41	100.20	5	1
1	A	184	LEU	C-N-CA	5.13	133.06	122.30	19	1
1	A	156	LEU	N-CA-CB	5.12	120.65	110.40	18	1
1	A	121	PRO	N-CD-CG	5.11	110.86	103.20	1	1
1	A	115	MET	CA-CB-CG	5.11	121.98	113.30	8	1
1	A	171	HIS	N-CA-CB	-5.11	101.41	110.60	19	1
1	A	83	LYS	O-C-N	-5.11	114.53	122.70	17	1
1	A	74	GLU	CG-CD-OE1	5.10	128.50	118.30	16	1
1	A	64	LYS	CA-C-O	-5.09	109.42	120.10	14	1
1	A	213	TYR	CZ-CE2-CD2	5.08	124.38	119.80	18	1
1	A	162	PRO	N-CA-C	5.08	125.31	112.10	2	1
1	A	154	ASN	CB-CA-C	5.08	120.56	110.40	15	1
1	A	149	PHE	CG-CD2-CE2	-5.07	115.22	120.80	2	1
1	A	153	GLY	C-N-CA	5.07	134.37	121.70	15	1
1	A	41	GLU	OE1-CD-OE2	-5.07	117.22	123.30	14	1
1	A	19	LEU	N-CA-CB	-5.06	100.27	110.40	11	1
1	A	75	TYR	CA-CB-CG	5.06	123.02	113.40	6	1
1	A	77	LEU	CB-CG-CD1	5.06	119.60	111.00	7	1
1	A	19	LEU	CB-CG-CD1	5.06	119.59	111.00	10	1
1	A	156	LEU	N-CA-C	5.05	124.65	111.00	5	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	155	THR	C-N-CA	5.05	134.33	121.70	14	1
1	A	217	GLY	N-CA-C	5.05	125.72	113.10	4	1
1	A	158	HIS	ND1-CE1-NE2	5.04	121.00	109.90	16	1
1	A	215	THR	C-N-CA	5.04	134.30	121.70	11	1
1	A	77	LEU	CB-CA-C	5.03	119.76	110.20	17	1
1	A	51	THR	CA-CB-CG2	-5.02	105.37	112.40	6	1
1	A	78	PHE	CG-CD1-CE1	-5.02	115.28	120.80	8	1
1	A	33	ASN	O-C-N	-5.02	114.67	122.70	12	1
1	A	17	ASP	CB-CA-C	5.02	120.44	110.40	16	1
1	A	84	TRP	CB-CG-CD2	5.01	133.12	126.60	6	1
1	A	199	SER	C-N-CA	5.01	134.24	121.70	20	1
1	A	176	GLU	CG-CD-OE1	-5.00	108.29	118.30	19	1
1	A	94	VAL	CG1-CB-CG2	-5.00	102.89	110.90	9	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	23	TYR	Sidechain,Peptide	9
1	A	147	TYR	Sidechain	6
1	A	140	ARG	Sidechain,Peptide	6
1	A	238	TYR	Sidechain	6
1	A	96	TYR	Sidechain,Mainchain	6
1	A	216	TYR	Sidechain	6
1	A	190	TYR	Sidechain	5
1	A	18	TYR	Sidechain	5
1	A	46	PHE	Sidechain	4
1	A	91	TYR	Sidechain	4
1	A	78	PHE	Sidechain	4
1	A	25	TYR	Sidechain	4
1	A	21	ARG	Sidechain	4
1	A	138	PHE	Sidechain	3
1	A	107	ARG	Sidechain	3
1	A	75	TYR	Sidechain	3
1	A	74	GLU	Peptide	3
1	A	149	PHE	Sidechain	3
1	A	185	GLY	Mainchain	2
1	A	213	TYR	Sidechain	2
1	A	71	ASP	Sidechain	2
1	A	73	ALA	Peptide	2

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	148	PRO	Peptide	2
1	A	188	PHE	Sidechain	2
1	A	160	PHE	Sidechain	2
1	A	102	HIS	Sidechain	2
1	A	194	HIS	Sidechain	2
1	A	92	ARG	Sidechain	1
1	A	97	THR	Mainchain	1
1	A	32	ALA	Mainchain	1
1	A	144	GLY	Peptide	1
1	A	224	PHE	Sidechain	1
1	A	22	PHE	Sidechain	1
1	A	45	PHE	Sidechain	1
1	A	69	VAL	Mainchain	1
1	A	232	LYS	Mainchain	1
1	A	128	VAL	Peptide	1
1	A	157	ALA	Peptide	1
1	A	180	ASP	Mainchain	1
1	A	171	HIS	Sidechain	1
1	A	72	VAL	Peptide	1
1	A	113	LEU	Mainchain	1
1	A	172	PHE	Sidechain	1
1	A	100	LEU	Mainchain	1
1	A	233	GLY	Mainchain	1
1	A	66	ARG	Sidechain	1
1	A	155	THR	Mainchain	1
1	A	131	THR	Mainchain	1
1	A	154	ASN	Peptide	1
1	A	177	ARG	Sidechain	1
1	A	239	GLY	Mainchain	1
1	A	83	LYS	Peptide	1
1	A	79	PRO	Peptide	1
1	A	121	PRO	Peptide	1
1	A	124	PHE	Sidechain	1
1	A	94	VAL	Mainchain	1
1	A	168	GLY	Peptide	1
1	A	181	GLY	Peptide	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	1805	1741	1741	2±2
4	A	5842	0	9144	125±14
All	All	153020	34820	217699	2534

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 7.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:320:PX4:H17	4:A:353:PX4:H16	0.96	1.32	10	1
4:A:373:PX4:H41	4:A:421:PX4:H66	0.96	1.37	1	1
4:A:389:PX4:H50	4:A:398:PX4:H22	0.95	1.37	2	1
4:A:313:PX4:H25	4:A:348:PX4:H64	0.95	1.39	6	1
4:A:313:PX4:H26	4:A:354:PX4:H50	0.94	1.35	5	1
4:A:349:PX4:H19	4:A:363:PX4:H21	0.93	1.41	16	1
4:A:382:PX4:H17	4:A:385:PX4:H49	0.92	1.38	1	1
4:A:361:PX4:H49	4:A:362:PX4:H22	0.91	1.41	4	1
4:A:329:PX4:H60	4:A:336:PX4:H49	0.89	1.42	14	1
4:A:378:PX4:H49	4:A:411:PX4:H54	0.89	1.43	18	1
4:A:369:PX4:H19	4:A:370:PX4:H22	0.86	1.47	14	1
4:A:336:PX4:H40	4:A:399:PX4:H33	0.86	1.45	15	1
4:A:308:PX4:H55	4:A:318:PX4:H27	0.86	1.46	7	1
4:A:381:PX4:H21	4:A:385:PX4:H54	0.85	1.48	16	1
4:A:324:PX4:H20	4:A:340:PX4:H54	0.85	1.48	16	1
4:A:374:PX4:H47	4:A:398:PX4:H19	0.85	1.48	2	1
4:A:325:PX4:H53	4:A:350:PX4:H54	0.85	1.48	14	1
4:A:328:PX4:H21	4:A:335:PX4:H16	0.84	1.45	6	2
4:A:386:PX4:H21	4:A:387:PX4:H17	0.83	1.50	15	2
4:A:336:PX4:H67	4:A:352:PX4:H58	0.83	1.49	14	1
4:A:324:PX4:H64	4:A:339:PX4:H26	0.83	1.48	12	1
4:A:320:PX4:H29	4:A:328:PX4:H37	0.82	1.50	3	1
4:A:355:PX4:H20	4:A:356:PX4:H17	0.81	1.52	11	2
4:A:376:PX4:H58	4:A:430:PX4:H32	0.81	1.52	11	1
4:A:315:PX4:H67	4:A:319:PX4:H16	0.81	1.51	2	1
4:A:377:PX4:H57	4:A:384:PX4:H59	0.80	1.51	3	1
4:A:375:PX4:H66	4:A:421:PX4:H44	0.80	1.52	14	1
4:A:376:PX4:H42	4:A:398:PX4:H59	0.80	1.52	17	1
4:A:373:PX4:H20	4:A:380:PX4:H54	0.80	1.53	15	1
4:A:385:PX4:H51	4:A:387:PX4:H49	0.80	1.53	14	1
4:A:305:PX4:H53	4:A:305:PX4:H31	0.80	1.51	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:328:PX4:H16	4:A:335:PX4:H20	0.80	1.50	14	1
4:A:348:PX4:H37	4:A:349:PX4:H31	0.80	1.50	19	1
4:A:381:PX4:H22	4:A:395:PX4:H53	0.80	1.53	9	1
4:A:387:PX4:H60	4:A:395:PX4:H29	0.80	1.51	17	1
4:A:386:PX4:H48	4:A:395:PX4:H21	0.79	1.54	2	1
4:A:337:PX4:H16	4:A:354:PX4:H16	0.79	1.54	20	1
4:A:324:PX4:H67	4:A:331:PX4:H34	0.79	1.54	17	1
4:A:398:PX4:H66	4:A:403:PX4:H40	0.79	1.52	15	1
4:A:405:PX4:H48	4:A:414:PX4:H22	0.78	1.55	14	1
4:A:371:PX4:H55	4:A:412:PX4:H16	0.78	1.56	17	1
4:A:401:PX4:H42	4:A:410:PX4:H40	0.78	1.54	19	1
4:A:424:PX4:H14	4:A:424:PX4:H6	0.78	1.55	19	1
4:A:371:PX4:H58	4:A:412:PX4:H49	0.78	1.56	15	1
1:A:140:ARG:CZ	4:A:330:PX4:H4	0.78	2.09	20	3
4:A:374:PX4:H19	4:A:383:PX4:H16	0.78	1.56	10	1
4:A:404:PX4:H61	4:A:414:PX4:H29	0.77	1.57	14	1
4:A:348:PX4:H42	4:A:374:PX4:H67	0.77	1.55	16	1
4:A:347:PX4:H22	4:A:354:PX4:H20	0.77	1.57	18	1
4:A:405:PX4:H15	4:A:414:PX4:H18	0.77	1.56	1	2
4:A:402:PX4:H60	4:A:427:PX4:H31	0.77	1.57	14	1
4:A:376:PX4:H66	4:A:425:PX4:H26	0.76	1.57	18	1
4:A:346:PX4:H27	4:A:346:PX4:H52	0.76	1.54	12	1
4:A:375:PX4:H21	4:A:421:PX4:H25	0.76	1.56	19	1
4:A:318:PX4:H68	4:A:322:PX4:H59	0.76	1.57	1	1
4:A:370:PX4:H41	4:A:377:PX4:H41	0.75	1.56	10	1
4:A:305:PX4:H16	4:A:328:PX4:H4	0.75	1.57	11	1
4:A:339:PX4:H48	4:A:355:PX4:H56	0.75	1.56	13	1
4:A:357:PX4:H17	4:A:358:PX4:H22	0.75	1.56	8	1
4:A:312:PX4:H32	4:A:327:PX4:H63	0.75	1.57	7	1
4:A:375:PX4:H6	4:A:375:PX4:H14	0.75	1.58	5	1
4:A:392:PX4:H55	4:A:409:PX4:H67	0.75	1.58	7	1
4:A:387:PX4:H55	4:A:395:PX4:H60	0.74	1.58	12	1
4:A:328:PX4:H58	4:A:335:PX4:H23	0.74	1.59	20	1
4:A:336:PX4:H51	4:A:344:PX4:H53	0.74	1.59	7	1
4:A:329:PX4:H57	4:A:346:PX4:H31	0.74	1.58	8	1
4:A:332:PX4:H16	4:A:340:PX4:H26	0.74	1.58	9	1
4:A:333:PX4:H51	4:A:348:PX4:H53	0.74	1.60	16	1
4:A:339:PX4:H16	4:A:355:PX4:H50	0.74	1.57	19	1
4:A:321:PX4:H16	4:A:330:PX4:H49	0.74	1.59	1	1
4:A:376:PX4:H27	4:A:383:PX4:H25	0.74	1.58	16	1
4:A:325:PX4:H67	4:A:376:PX4:H45	0.73	1.56	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:394:PX4:H52	4:A:402:PX4:H31	0.73	1.58	12	1
4:A:313:PX4:H26	4:A:356:PX4:H28	0.73	1.61	6	1
4:A:348:PX4:H27	4:A:349:PX4:H48	0.73	1.59	7	2
4:A:396:PX4:H24	4:A:396:PX4:H54	0.73	1.59	10	1
4:A:376:PX4:H46	4:A:430:PX4:H17	0.72	1.61	13	4
4:A:383:PX4:H19	4:A:398:PX4:H50	0.72	1.61	13	1
4:A:307:PX4:H70	4:A:309:PX4:H21	0.72	1.61	15	1
4:A:370:PX4:H20	4:A:419:PX4:H51	0.72	1.61	9	2
4:A:328:PX4:H38	4:A:351:PX4:H34	0.72	1.59	2	1
4:A:424:PX4:H49	4:A:430:PX4:H25	0.72	1.61	6	1
4:A:379:PX4:H37	4:A:427:PX4:H37	0.72	1.61	7	1
4:A:330:PX4:H24	4:A:331:PX4:H27	0.72	1.60	14	1
4:A:388:PX4:H41	4:A:402:PX4:H32	0.72	1.61	8	1
4:A:378:PX4:H62	4:A:380:PX4:H34	0.72	1.62	13	1
4:A:404:PX4:H23	4:A:412:PX4:H48	0.72	1.62	18	1
4:A:368:PX4:H1	4:A:368:PX4:H22	0.72	1.61	1	1
4:A:352:PX4:H17	4:A:365:PX4:H22	0.72	1.60	1	1
4:A:329:PX4:H19	4:A:338:PX4:H24	0.72	1.62	12	1
4:A:352:PX4:H27	4:A:416:PX4:H44	0.72	1.59	14	1
4:A:310:PX4:H55	4:A:363:PX4:H51	0.72	1.62	10	1
4:A:362:PX4:H39	4:A:379:PX4:H39	0.71	1.61	13	1
4:A:379:PX4:H21	4:A:427:PX4:H16	0.71	1.60	20	1
4:A:325:PX4:H33	4:A:325:PX4:H65	0.71	1.60	13	1
4:A:334:PX4:H67	4:A:341:PX4:H35	0.71	1.61	17	1
4:A:324:PX4:H42	4:A:324:PX4:H62	0.71	1.61	10	1
4:A:370:PX4:H44	4:A:378:PX4:H40	0.71	1.60	5	1
4:A:368:PX4:H58	4:A:376:PX4:H57	0.71	1.60	3	1
4:A:328:PX4:H49	4:A:335:PX4:H28	0.71	1.63	8	1
4:A:336:PX4:H15	4:A:351:PX4:H58	0.71	1.62	8	1
4:A:378:PX4:H59	4:A:379:PX4:H37	0.71	1.61	16	1
4:A:332:PX4:H38	4:A:340:PX4:H67	0.70	1.62	8	1
4:A:329:PX4:H22	4:A:351:PX4:H53	0.70	1.62	20	1
4:A:348:PX4:H49	4:A:356:PX4:H49	0.70	1.63	8	1
4:A:401:PX4:H16	4:A:427:PX4:H47	0.70	1.63	6	2
4:A:407:PX4:H37	4:A:423:PX4:H41	0.70	1.61	13	1
4:A:308:PX4:H24	4:A:315:PX4:H17	0.70	1.61	7	2
4:A:308:PX4:H65	4:A:314:PX4:H61	0.70	1.62	18	1
4:A:407:PX4:H32	4:A:423:PX4:H29	0.70	1.61	19	1
4:A:312:PX4:H62	4:A:317:PX4:H64	0.70	1.64	19	1
4:A:381:PX4:H60	4:A:387:PX4:H35	0.70	1.63	2	1
4:A:342:PX4:H19	4:A:351:PX4:H22	0.70	1.62	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:406:PX4:H23	4:A:408:PX4:H39	0.70	1.62	5	1
4:A:424:PX4:H30	4:A:424:PX4:H58	0.70	1.62	8	1
4:A:306:PX4:H63	4:A:333:PX4:H59	0.69	1.62	6	1
4:A:380:PX4:H20	4:A:411:PX4:H47	0.69	1.61	13	1
4:A:390:PX4:H48	4:A:399:PX4:H49	0.69	1.64	20	1
4:A:425:PX4:H25	4:A:430:PX4:H21	0.69	1.64	20	1
4:A:392:PX4:H66	4:A:402:PX4:H62	0.69	1.62	6	1
4:A:324:PX4:H72	4:A:355:PX4:H67	0.69	1.64	10	1
4:A:337:PX4:H20	4:A:346:PX4:H26	0.69	1.64	15	1
4:A:353:PX4:H63	4:A:360:PX4:H49	0.69	1.62	9	1
4:A:384:PX4:H16	4:A:400:PX4:H20	0.69	1.65	9	1
4:A:372:PX4:O2	4:A:373:PX4:H18	0.69	1.87	7	1
4:A:380:PX4:H17	4:A:381:PX4:O6	0.69	1.88	7	2
4:A:309:PX4:H67	4:A:399:PX4:H67	0.69	1.64	8	1
4:A:391:PX4:H52	4:A:400:PX4:H57	0.69	1.64	14	1
4:A:316:PX4:H68	4:A:317:PX4:H30	0.69	1.63	20	1
4:A:393:PX4:H39	4:A:400:PX4:H40	0.69	1.64	2	1
4:A:424:PX4:H35	4:A:425:PX4:H67	0.69	1.63	3	1
4:A:334:PX4:H15	4:A:341:PX4:H16	0.69	1.64	6	1
4:A:344:PX4:H57	4:A:346:PX4:H31	0.69	1.64	10	1
4:A:317:PX4:H46	4:A:343:PX4:H17	0.69	1.65	6	1
4:A:328:PX4:H57	4:A:335:PX4:H31	0.68	1.65	17	1
4:A:377:PX4:H22	4:A:378:PX4:H16	0.68	1.64	20	1
4:A:394:PX4:H38	4:A:418:PX4:H27	0.68	1.64	14	1
4:A:305:PX4:H28	4:A:335:PX4:H28	0.68	1.65	4	1
4:A:392:PX4:H59	4:A:418:PX4:H27	0.68	1.65	8	1
4:A:403:PX4:H56	4:A:404:PX4:H62	0.68	1.64	12	1
4:A:373:PX4:H33	4:A:421:PX4:H72	0.68	1.64	14	1
4:A:377:PX4:H16	4:A:378:PX4:H20	0.68	1.66	10	2
4:A:373:PX4:H54	4:A:381:PX4:H52	0.68	1.66	7	1
4:A:376:PX4:H22	4:A:390:PX4:H25	0.68	1.64	7	1
4:A:332:PX4:H22	4:A:340:PX4:H25	0.68	1.65	20	1
4:A:331:PX4:H61	4:A:346:PX4:H60	0.68	1.65	15	1
4:A:388:PX4:H20	4:A:395:PX4:H17	0.68	1.66	7	2
4:A:417:PX4:H46	4:A:426:PX4:H19	0.68	1.66	2	1
4:A:384:PX4:H20	4:A:400:PX4:H16	0.68	1.66	4	5
4:A:419:PX4:H37	4:A:426:PX4:H66	0.68	1.65	4	1
4:A:308:PX4:H64	4:A:372:PX4:H42	0.67	1.64	5	1
4:A:386:PX4:H66	4:A:402:PX4:H33	0.67	1.64	15	1
4:A:378:PX4:H42	4:A:387:PX4:H31	0.67	1.65	17	1
4:A:379:PX4:H28	4:A:427:PX4:H28	0.67	1.65	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:305:PX4:H25	4:A:320:PX4:H33	0.67	1.64	2	1
4:A:337:PX4:H29	4:A:355:PX4:H33	0.67	1.65	10	1
4:A:394:PX4:H23	4:A:412:PX4:H49	0.67	1.65	10	1
4:A:409:PX4:H65	4:A:410:PX4:H65	0.67	1.66	18	1
4:A:386:PX4:H62	4:A:402:PX4:H29	0.67	1.67	16	1
4:A:337:PX4:H46	4:A:346:PX4:H48	0.67	1.66	17	1
4:A:333:PX4:H35	4:A:339:PX4:H67	0.67	1.65	12	1
4:A:345:PX4:H46	4:A:354:PX4:H16	0.67	1.65	19	1
4:A:369:PX4:H47	4:A:370:PX4:H25	0.67	1.66	19	1
4:A:325:PX4:H31	4:A:349:PX4:H59	0.67	1.65	1	1
4:A:307:PX4:H21	4:A:363:PX4:H26	0.67	1.65	7	1
4:A:390:PX4:H17	4:A:397:PX4:H66	0.67	1.65	8	1
4:A:384:PX4:H28	4:A:400:PX4:H52	0.67	1.65	12	1
4:A:384:PX4:H17	4:A:393:PX4:H20	0.67	1.65	14	1
4:A:337:PX4:H61	4:A:355:PX4:H40	0.67	1.67	18	1
4:A:305:PX4:H51	4:A:362:PX4:H48	0.67	1.67	12	1
4:A:417:PX4:H69	4:A:426:PX4:H40	0.67	1.66	12	1
4:A:399:PX4:H19	4:A:408:PX4:H14	0.67	1.65	1	2
4:A:413:PX4:H29	4:A:422:PX4:H24	0.67	1.67	4	1
4:A:355:PX4:H21	4:A:356:PX4:H15	0.67	1.67	7	1
4:A:400:PX4:H49	4:A:425:PX4:H27	0.67	1.66	12	1
4:A:419:PX4:H22	4:A:426:PX4:H50	0.67	1.66	18	1
4:A:309:PX4:H19	4:A:366:PX4:H49	0.67	1.64	5	1
4:A:405:PX4:H19	4:A:420:PX4:H21	0.67	1.64	5	1
4:A:306:PX4:H59	4:A:311:PX4:H55	0.67	1.67	15	1
4:A:339:PX4:H9	4:A:340:PX4:H51	0.66	1.66	14	1
4:A:384:PX4:H28	4:A:400:PX4:H58	0.66	1.65	19	1
4:A:308:PX4:H70	4:A:382:PX4:H39	0.66	1.67	5	1
4:A:376:PX4:H24	4:A:429:PX4:H31	0.66	1.64	10	1
4:A:336:PX4:H45	4:A:399:PX4:H29	0.66	1.66	15	1
4:A:401:PX4:H25	4:A:427:PX4:H48	0.66	1.67	18	1
4:A:337:PX4:H67	4:A:355:PX4:H40	0.66	1.67	2	1
4:A:347:PX4:H72	4:A:351:PX4:H21	0.66	1.67	2	1
4:A:379:PX4:H71	4:A:380:PX4:H45	0.66	1.66	4	1
4:A:388:PX4:H54	4:A:389:PX4:H48	0.66	1.64	7	1
4:A:348:PX4:H60	4:A:355:PX4:H32	0.66	1.66	10	1
4:A:316:PX4:H19	4:A:334:PX4:H66	0.66	1.65	18	1
4:A:327:PX4:H39	4:A:360:PX4:H32	0.66	1.67	18	1
4:A:334:PX4:H26	4:A:341:PX4:H22	0.66	1.68	17	1
4:A:309:PX4:H67	4:A:383:PX4:H66	0.66	1.67	9	1
4:A:305:PX4:H38	4:A:322:PX4:H26	0.66	1.67	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:373:PX4:H20	4:A:380:PX4:H20	0.66	1.68	18	1
4:A:369:PX4:O8	4:A:391:PX4:H5	0.66	1.90	2	1
4:A:330:PX4:H15	4:A:331:PX4:H18	0.66	1.68	20	1
4:A:329:PX4:H27	4:A:347:PX4:H54	0.66	1.67	1	1
4:A:393:PX4:H58	4:A:408:PX4:H41	0.66	1.67	9	1
4:A:338:PX4:H32	4:A:346:PX4:H67	0.66	1.66	14	1
4:A:423:PX4:H17	4:A:424:PX4:H24	0.66	1.65	16	1
4:A:384:PX4:H60	4:A:393:PX4:H29	0.65	1.67	4	1
4:A:318:PX4:H28	4:A:319:PX4:H65	0.65	1.68	20	1
4:A:325:PX4:H63	4:A:341:PX4:H59	0.65	1.68	20	1
4:A:309:PX4:H27	4:A:366:PX4:H23	0.65	1.68	4	1
4:A:354:PX4:H22	4:A:356:PX4:H29	0.65	1.69	4	1
4:A:336:PX4:H62	4:A:366:PX4:H16	0.65	1.67	8	1
4:A:383:PX4:H45	4:A:412:PX4:H63	0.65	1.68	3	1
4:A:392:PX4:H17	4:A:409:PX4:H61	0.65	1.67	15	3
4:A:332:PX4:H20	4:A:340:PX4:H16	0.65	1.67	11	4
4:A:411:PX4:H36	4:A:419:PX4:H54	0.65	1.68	5	1
4:A:308:PX4:H17	4:A:318:PX4:H49	0.65	1.68	16	1
4:A:384:PX4:H68	4:A:386:PX4:H55	0.65	1.68	1	1
4:A:371:PX4:H69	4:A:389:PX4:H45	0.65	1.66	2	1
4:A:417:PX4:H57	4:A:427:PX4:H63	0.65	1.67	3	1
4:A:370:PX4:H17	4:A:419:PX4:H47	0.65	1.65	2	1
4:A:326:PX4:H14	4:A:343:PX4:H15	0.65	1.68	4	1
4:A:313:PX4:H60	4:A:348:PX4:H20	0.65	1.67	13	1
4:A:381:PX4:H46	4:A:385:PX4:H16	0.65	1.67	14	1
4:A:314:PX4:H28	4:A:354:PX4:H56	0.65	1.69	4	1
4:A:401:PX4:H64	4:A:410:PX4:H33	0.65	1.67	18	1
4:A:380:PX4:H29	4:A:381:PX4:H32	0.65	1.69	3	1
4:A:376:PX4:H51	4:A:430:PX4:H48	0.65	1.68	7	1
4:A:322:PX4:H29	4:A:332:PX4:H28	0.65	1.67	5	1
4:A:338:PX4:H66	4:A:400:PX4:H38	0.65	1.68	4	1
4:A:404:PX4:H21	4:A:405:PX4:H40	0.65	1.69	9	1
4:A:328:PX4:H62	4:A:332:PX4:H29	0.65	1.68	14	1
4:A:325:PX4:H39	4:A:382:PX4:H41	0.65	1.69	20	1
4:A:322:PX4:H21	4:A:332:PX4:H49	0.64	1.68	8	1
4:A:322:PX4:H39	4:A:340:PX4:H21	0.64	1.67	8	1
4:A:418:PX4:H67	4:A:420:PX4:H72	0.64	1.67	10	1
4:A:347:PX4:H20	4:A:355:PX4:H47	0.64	1.69	2	1
4:A:359:PX4:H28	4:A:407:PX4:H37	0.64	1.67	2	1
4:A:423:PX4:H55	4:A:426:PX4:H22	0.64	1.70	2	1
4:A:328:PX4:H60	4:A:328:PX4:H39	0.64	1.67	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:333:PX4:H39	4:A:389:PX4:H67	0.64	1.68	3	1
4:A:319:PX4:H43	4:A:407:PX4:H33	0.64	1.68	7	1
4:A:384:PX4:H25	4:A:400:PX4:H16	0.64	1.69	12	1
4:A:401:PX4:H69	4:A:417:PX4:H44	0.64	1.67	13	1
4:A:409:PX4:H21	4:A:416:PX4:H21	0.64	1.67	13	1
4:A:330:PX4:H68	4:A:331:PX4:H42	0.64	1.68	1	1
4:A:372:PX4:H46	4:A:428:PX4:H59	0.64	1.70	5	1
4:A:424:PX4:H34	4:A:424:PX4:H62	0.64	1.69	8	1
4:A:387:PX4:H33	4:A:387:PX4:H53	0.64	1.70	14	1
4:A:336:PX4:H67	4:A:360:PX4:H63	0.64	1.69	16	1
4:A:313:PX4:H46	4:A:348:PX4:H54	0.64	1.69	18	1
4:A:342:PX4:H36	4:A:351:PX4:H49	0.64	1.69	7	1
4:A:306:PX4:H24	4:A:313:PX4:H38	0.64	1.69	7	1
4:A:409:PX4:H19	4:A:410:PX4:H51	0.64	1.70	8	1
4:A:385:PX4:H47	4:A:387:PX4:H16	0.64	1.68	16	1
4:A:347:PX4:H68	4:A:351:PX4:H70	0.64	1.69	16	1
4:A:325:PX4:H44	4:A:382:PX4:H35	0.64	1.69	20	1
4:A:393:PX4:H48	4:A:394:PX4:C25	0.64	2.22	6	1
4:A:316:PX4:H47	4:A:325:PX4:H55	0.64	1.69	16	1
4:A:321:PX4:H16	4:A:330:PX4:H19	0.64	1.68	20	1
4:A:329:PX4:H37	4:A:336:PX4:H32	0.64	1.69	2	1
4:A:422:PX4:H19	4:A:431:PX4:H49	0.64	1.67	4	1
4:A:411:PX4:H18	4:A:427:PX4:H49	0.64	1.70	10	2
4:A:330:PX4:H53	4:A:331:PX4:H21	0.64	1.69	12	1
4:A:390:PX4:H26	4:A:398:PX4:H66	0.64	1.68	13	1
4:A:375:PX4:H28	4:A:413:PX4:H66	0.64	1.70	16	1
4:A:336:PX4:H43	4:A:399:PX4:H23	0.64	1.70	17	1
4:A:413:PX4:H65	4:A:383:PX4:H63	0.63	1.70	1	1
4:A:307:PX4:H64	4:A:396:PX4:H64	0.63	1.70	5	1
4:A:369:PX4:H64	4:A:391:PX4:H29	0.63	1.70	7	1
4:A:409:PX4:H18	4:A:416:PX4:H14	0.63	1.70	15	1
4:A:329:PX4:H28	4:A:338:PX4:H62	0.63	1.70	18	1
4:A:400:PX4:H49	4:A:408:PX4:H11	0.63	1.68	20	1
4:A:380:PX4:H17	4:A:381:PX4:H18	0.63	1.69	2	1
4:A:379:PX4:H38	4:A:427:PX4:H71	0.63	1.70	4	1
4:A:408:PX4:H51	4:A:415:PX4:H59	0.63	1.69	14	1
4:A:318:PX4:H62	4:A:340:PX4:H28	0.63	1.70	15	1
4:A:399:PX4:H37	4:A:408:PX4:H67	0.63	1.70	18	1
4:A:317:PX4:H27	4:A:318:PX4:H17	0.63	1.70	2	1
4:A:321:PX4:H33	4:A:331:PX4:H62	0.63	1.70	7	1
4:A:335:PX4:H21	4:A:342:PX4:H47	0.63	1.68	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:369:PX4:H67	4:A:370:PX4:H39	0.63	1.71	11	1
4:A:407:PX4:H1	4:A:417:PX4:H8	0.63	1.70	16	1
4:A:355:PX4:H59	4:A:356:PX4:H65	0.63	1.70	14	1
4:A:417:PX4:O2	4:A:419:PX4:H10	0.63	1.94	16	1
4:A:372:PX4:H36	4:A:421:PX4:H38	0.63	1.70	7	1
4:A:373:PX4:H65	4:A:380:PX4:H65	0.63	1.71	9	1
4:A:389:PX4:H54	4:A:398:PX4:H26	0.63	1.69	2	1
4:A:333:PX4:H18	4:A:356:PX4:H56	0.63	1.69	14	1
4:A:337:PX4:H19	4:A:344:PX4:H50	0.63	1.70	18	1
4:A:326:PX4:H52	4:A:343:PX4:H47	0.63	1.69	1	1
4:A:371:PX4:H68	4:A:412:PX4:H63	0.63	1.71	5	1
4:A:371:PX4:H68	4:A:388:PX4:H28	0.63	1.69	7	1
4:A:307:PX4:H56	4:A:310:PX4:H53	0.63	1.70	12	1
4:A:317:PX4:O6	4:A:318:PX4:H11	0.63	1.94	17	1
4:A:392:PX4:H25	4:A:393:PX4:H47	0.62	1.69	1	1
4:A:378:PX4:H65	4:A:411:PX4:H59	0.62	1.70	9	1
4:A:391:PX4:H24	4:A:425:PX4:H49	0.62	1.70	18	1
4:A:374:PX4:H51	4:A:385:PX4:H58	0.62	1.71	7	1
4:A:414:PX4:H34	4:A:431:PX4:H25	0.62	1.71	8	1
4:A:421:PX4:H58	4:A:428:PX4:H21	0.62	1.70	13	1
4:A:358:PX4:H70	4:A:408:PX4:H70	0.62	1.70	16	1
1:A:142:ALA:HB2	4:A:321:PX4:H7	0.62	1.70	3	1
4:A:337:PX4:H36	4:A:338:PX4:H44	0.62	1.72	9	1
4:A:308:PX4:H4	4:A:319:PX4:O3	0.62	1.94	11	1
4:A:345:PX4:H62	4:A:354:PX4:H30	0.62	1.72	19	1
4:A:336:PX4:H48	4:A:352:PX4:H13	0.62	1.71	9	1
4:A:374:PX4:H46	4:A:382:PX4:H16	0.62	1.72	13	1
4:A:403:PX4:H49	4:A:403:PX4:H27	0.62	1.72	20	1
4:A:380:PX4:H20	4:A:411:PX4:H49	0.62	1.71	7	1
4:A:371:PX4:H48	4:A:404:PX4:H18	0.62	1.72	16	1
4:A:384:PX4:H39	4:A:400:PX4:H33	0.62	1.70	19	1
4:A:406:PX4:H25	4:A:409:PX4:H34	0.61	1.72	3	1
4:A:423:PX4:H38	4:A:424:PX4:H34	0.61	1.71	3	1
4:A:305:PX4:H60	4:A:362:PX4:H59	0.61	1.69	4	1
4:A:404:PX4:H56	4:A:405:PX4:H49	0.61	1.72	13	2
4:A:350:PX4:H50	4:A:363:PX4:H51	0.61	1.70	15	1
4:A:327:PX4:H31	4:A:353:PX4:H65	0.61	1.69	18	1
4:A:347:PX4:H31	4:A:355:PX4:H26	0.61	1.71	19	1
4:A:396:PX4:H23	4:A:405:PX4:H56	0.61	1.70	19	1
4:A:348:PX4:H35	4:A:363:PX4:H54	0.61	1.70	8	1
4:A:387:PX4:H48	4:A:387:PX4:H32	0.61	1.72	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:333:PX4:H69	4:A:371:PX4:H70	0.61	1.70	19	1
4:A:402:PX4:H52	4:A:392:PX4:H54	0.61	1.73	1	1
4:A:371:PX4:H58	4:A:404:PX4:H28	0.61	1.72	4	1
4:A:394:PX4:H53	4:A:402:PX4:H30	0.61	1.71	6	1
4:A:403:PX4:H48	4:A:412:PX4:H17	0.61	1.72	14	1
4:A:324:PX4:H37	4:A:382:PX4:H37	0.61	1.72	16	1
4:A:375:PX4:H47	4:A:421:PX4:H27	0.61	1.72	16	1
4:A:319:PX4:H22	4:A:327:PX4:H65	0.61	1.72	17	1
4:A:368:PX4:H62	4:A:390:PX4:H34	0.61	1.71	5	1
4:A:369:PX4:H55	4:A:391:PX4:H22	0.61	1.72	11	1
4:A:402:PX4:H65	4:A:392:PX4:H66	0.61	1.73	1	1
4:A:405:PX4:H62	4:A:414:PX4:H29	0.61	1.71	6	1
4:A:401:PX4:H23	4:A:427:PX4:H31	0.61	1.72	7	1
4:A:385:PX4:H26	4:A:387:PX4:H24	0.61	1.71	13	1
4:A:345:PX4:H38	4:A:365:PX4:H33	0.61	1.72	12	1
4:A:359:PX4:H48	4:A:367:PX4:H23	0.61	1.72	2	1
4:A:386:PX4:H39	4:A:387:PX4:H36	0.61	1.71	2	1
4:A:386:PX4:O8	4:A:394:PX4:H13	0.61	1.96	12	1
4:A:325:PX4:H48	4:A:339:PX4:H61	0.61	1.71	17	1
4:A:354:PX4:H23	4:A:356:PX4:H57	0.61	1.72	20	1
4:A:361:PX4:H40	4:A:364:PX4:H37	0.61	1.72	20	1
4:A:371:PX4:H53	4:A:388:PX4:H17	0.61	1.72	6	1
4:A:342:PX4:H39	4:A:357:PX4:H43	0.61	1.73	12	1
4:A:320:PX4:H65	4:A:328:PX4:H57	0.61	1.71	13	1
4:A:308:PX4:H36	4:A:312:PX4:H41	0.61	1.73	18	1
4:A:329:PX4:H14	4:A:351:PX4:H15	0.61	1.73	1	1
4:A:342:PX4:H31	4:A:358:PX4:H39	0.61	1.73	2	1
4:A:423:PX4:H34	4:A:424:PX4:H34	0.61	1.71	19	1
4:A:307:PX4:H61	4:A:311:PX4:H28	0.60	1.72	7	1
4:A:307:PX4:H8	4:A:310:PX4:O3	0.60	1.95	10	1
4:A:338:PX4:H30	4:A:347:PX4:H56	0.60	1.73	17	1
4:A:341:PX4:H47	4:A:341:PX4:H28	0.60	1.73	17	1
4:A:377:PX4:H68	4:A:391:PX4:H58	0.60	1.73	10	1
4:A:373:PX4:H17	4:A:380:PX4:H49	0.60	1.74	12	1
4:A:307:PX4:H43	4:A:405:PX4:H57	0.60	1.73	13	1
4:A:368:PX4:H63	4:A:376:PX4:H43	0.60	1.71	15	1
4:A:347:PX4:H29	4:A:356:PX4:H63	0.60	1.73	16	1
4:A:419:PX4:H20	4:A:426:PX4:H16	0.60	1.73	2	5
4:A:308:PX4:H51	4:A:318:PX4:H25	0.60	1.73	3	1
4:A:419:PX4:H32	4:A:424:PX4:H38	0.60	1.73	9	1
4:A:383:PX4:H38	4:A:389:PX4:H49	0.60	1.71	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:394:PX4:H48	4:A:402:PX4:H27	0.60	1.73	12	1
4:A:377:PX4:H58	4:A:387:PX4:H22	0.60	1.72	16	1
4:A:313:PX4:H17	4:A:348:PX4:H52	0.60	1.74	1	1
4:A:369:PX4:H66	4:A:425:PX4:H69	0.60	1.74	1	1
4:A:385:PX4:H15	4:A:387:PX4:H19	0.60	1.71	6	1
4:A:354:PX4:H63	4:A:356:PX4:H42	0.60	1.71	9	1
4:A:321:PX4:H52	4:A:330:PX4:H28	0.60	1.72	15	1
4:A:308:PX4:H23	4:A:319:PX4:H48	0.60	1.72	16	1
4:A:388:PX4:O2	4:A:389:PX4:H8	0.60	1.96	7	1
4:A:378:PX4:H50	4:A:411:PX4:H15	0.60	1.73	8	1
4:A:341:PX4:H59	4:A:350:PX4:H58	0.60	1.74	7	1
4:A:325:PX4:O6	4:A:349:PX4:H9	0.60	1.97	11	1
4:A:335:PX4:H67	4:A:353:PX4:H38	0.60	1.72	15	1
4:A:318:PX4:H50	4:A:323:PX4:H49	0.60	1.72	6	1
4:A:342:PX4:H32	4:A:351:PX4:H53	0.60	1.71	16	1
4:A:377:PX4:H59	4:A:386:PX4:H20	0.60	1.72	16	1
4:A:336:PX4:H30	4:A:351:PX4:H60	0.60	1.74	18	1
4:A:352:PX4:H41	4:A:358:PX4:H57	0.60	1.74	18	1
4:A:373:PX4:H57	4:A:380:PX4:H55	0.60	1.72	8	1
4:A:324:PX4:H47	4:A:339:PX4:H15	0.60	1.73	9	1
4:A:387:PX4:H18	4:A:387:PX4:H1	0.60	1.72	12	2
4:A:379:PX4:H62	4:A:380:PX4:H37	0.59	1.74	2	1
4:A:309:PX4:H38	4:A:357:PX4:H70	0.59	1.74	4	1
4:A:392:PX4:H19	4:A:393:PX4:H49	0.59	1.74	4	1
4:A:370:PX4:H47	4:A:419:PX4:H17	0.59	1.74	17	2
4:A:309:PX4:H35	4:A:366:PX4:H42	0.59	1.72	18	1
4:A:385:PX4:H15	4:A:387:PX4:H20	0.59	1.72	1	2
4:A:354:PX4:H65	4:A:364:PX4:H39	0.59	1.71	7	1
4:A:384:PX4:H48	4:A:400:PX4:H19	0.59	1.74	7	1
4:A:377:PX4:H58	4:A:378:PX4:H31	0.59	1.71	13	1
4:A:375:PX4:H57	4:A:382:PX4:H50	0.59	1.73	20	1
4:A:323:PX4:H33	4:A:375:PX4:H43	0.59	1.74	1	1
4:A:348:PX4:H63	4:A:356:PX4:H32	0.59	1.74	6	1
4:A:317:PX4:H40	4:A:318:PX4:H53	0.59	1.72	11	1
4:A:378:PX4:H17	4:A:385:PX4:H19	0.59	1.74	13	1
4:A:394:PX4:H33	4:A:418:PX4:H26	0.59	1.74	15	1
4:A:351:PX4:H61	4:A:358:PX4:H66	0.59	1.72	17	1
4:A:348:PX4:H25	4:A:349:PX4:H22	0.59	1.73	3	1
4:A:311:PX4:H71	4:A:404:PX4:H69	0.59	1.73	5	1
4:A:382:PX4:H38	4:A:421:PX4:H30	0.59	1.75	5	1
4:A:418:PX4:H17	4:A:427:PX4:H23	0.59	1.73	16	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:321:PX4:H16	4:A:330:PX4:H21	0.59	1.75	11	1
4:A:375:PX4:H52	4:A:382:PX4:H19	0.59	1.74	14	1
4:A:332:PX4:H43	4:A:375:PX4:H43	0.59	1.74	15	1
4:A:345:PX4:H38	4:A:395:PX4:H42	0.59	1.74	18	1
4:A:405:PX4:H26	4:A:431:PX4:H27	0.59	1.74	18	1
4:A:369:PX4:H62	4:A:391:PX4:H33	0.59	1.74	5	1
4:A:337:PX4:H27	4:A:344:PX4:H51	0.59	1.73	6	1
4:A:397:PX4:H37	4:A:403:PX4:H36	0.59	1.75	14	1
4:A:418:PX4:H52	4:A:427:PX4:H33	0.59	1.73	15	1
4:A:375:PX4:H27	4:A:421:PX4:H41	0.59	1.73	16	1
4:A:413:PX4:H26	4:A:431:PX4:H17	0.59	1.73	16	1
4:A:305:PX4:H41	4:A:321:PX4:H67	0.59	1.75	6	1
4:A:342:PX4:H28	4:A:358:PX4:H35	0.59	1.74	11	1
4:A:314:PX4:H24	4:A:354:PX4:H46	0.59	1.73	19	1
4:A:371:PX4:H26	4:A:418:PX4:H50	0.59	1.73	10	1
4:A:383:PX4:H61	4:A:390:PX4:H31	0.59	1.75	14	1
4:A:313:PX4:H19	4:A:354:PX4:H23	0.59	1.74	19	1
4:A:313:PX4:H34	4:A:364:PX4:H34	0.59	1.73	3	1
4:A:424:PX4:H33	4:A:426:PX4:H55	0.59	1.72	4	1
4:A:325:PX4:H19	4:A:349:PX4:H53	0.59	1.73	9	1
4:A:312:PX4:H19	4:A:327:PX4:H54	0.59	1.75	19	1
4:A:379:PX4:H19	4:A:427:PX4:H20	0.58	1.75	2	1
4:A:413:PX4:H42	4:A:431:PX4:H28	0.58	1.75	4	1
4:A:306:PX4:H47	4:A:364:PX4:H33	0.58	1.74	9	1
4:A:344:PX4:H16	4:A:345:PX4:H17	0.58	1.74	9	1
4:A:420:PX4:H16	4:A:428:PX4:H47	0.58	1.75	16	2
4:A:369:PX4:H3	4:A:370:PX4:H18	0.58	1.74	5	1
4:A:401:PX4:H57	4:A:417:PX4:H48	0.58	1.74	6	1
4:A:378:PX4:H45	4:A:380:PX4:H35	0.58	1.75	10	1
4:A:368:PX4:H61	4:A:376:PX4:H56	0.58	1.73	17	1
4:A:339:PX4:H48	4:A:355:PX4:H60	0.58	1.73	6	1
4:A:320:PX4:H60	4:A:328:PX4:H56	0.58	1.75	7	1
4:A:369:PX4:H52	4:A:391:PX4:H22	0.58	1.75	10	1
4:A:382:PX4:H52	4:A:389:PX4:H54	0.58	1.74	11	1
4:A:333:PX4:H24	4:A:339:PX4:H53	0.58	1.73	14	1
4:A:409:PX4:H18	4:A:416:PX4:O6	0.58	1.98	18	1
4:A:337:PX4:H19	4:A:346:PX4:H28	0.58	1.74	2	1
4:A:384:PX4:H66	4:A:395:PX4:H35	0.58	1.74	2	1
4:A:305:PX4:H17	4:A:362:PX4:O7	0.58	1.99	5	1
4:A:398:PX4:H39	4:A:429:PX4:H41	0.58	1.74	5	1
4:A:389:PX4:H27	4:A:403:PX4:H49	0.58	1.76	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:313:PX4:H36	4:A:364:PX4:H33	0.58	1.76	10	1
4:A:313:PX4:H19	4:A:348:PX4:H65	0.58	1.73	11	1
4:A:343:PX4:H69	4:A:343:PX4:H37	0.58	1.74	15	1
4:A:392:PX4:H23	4:A:399:PX4:H21	0.58	1.73	15	1
4:A:402:PX4:H48	4:A:418:PX4:H26	0.58	1.74	17	1
4:A:344:PX4:H49	4:A:345:PX4:H49	0.58	1.75	18	1
4:A:312:PX4:H59	4:A:317:PX4:H61	0.58	1.74	19	1
4:A:376:PX4:H34	4:A:398:PX4:H72	0.58	1.76	4	1
4:A:369:PX4:H27	4:A:370:PX4:H34	0.58	1.76	11	1
4:A:341:PX4:H34	4:A:408:PX4:H66	0.58	1.76	13	1
4:A:357:PX4:H41	4:A:408:PX4:H58	0.58	1.75	14	1
4:A:401:PX4:H48	4:A:410:PX4:H19	0.58	1.75	15	1
4:A:346:PX4:H38	4:A:346:PX4:H62	0.58	1.76	19	1
4:A:413:PX4:H56	4:A:421:PX4:H17	0.58	1.74	4	1
4:A:419:PX4:H21	4:A:426:PX4:H20	0.58	1.76	7	1
4:A:362:PX4:H28	4:A:365:PX4:H49	0.58	1.76	14	1
4:A:332:PX4:H16	4:A:340:PX4:C10	0.58	2.29	20	1
4:A:374:PX4:H26	4:A:429:PX4:H34	0.58	1.75	3	1
4:A:370:PX4:H31	4:A:377:PX4:H35	0.58	1.76	4	1
4:A:337:PX4:H31	4:A:344:PX4:H55	0.58	1.76	6	1
4:A:327:PX4:H41	4:A:353:PX4:H41	0.58	1.74	8	1
4:A:392:PX4:H16	4:A:393:PX4:H15	0.58	1.75	8	1
4:A:372:PX4:H17	4:A:428:PX4:H22	0.58	1.74	14	1
4:A:373:PX4:H17	4:A:380:PX4:H46	0.58	1.75	17	1
4:A:375:PX4:H27	4:A:429:PX4:H20	0.58	1.76	18	1
4:A:325:PX4:H20	4:A:348:PX4:H24	0.58	1.76	13	2
4:A:386:PX4:H52	4:A:394:PX4:H2	0.58	1.74	5	1
4:A:327:PX4:H24	4:A:353:PX4:H31	0.58	1.75	19	1
4:A:311:PX4:H49	4:A:363:PX4:H31	0.57	1.76	1	1
4:A:368:PX4:H14	4:A:429:PX4:H14	0.57	1.75	6	2
4:A:338:PX4:H54	4:A:351:PX4:H24	0.57	1.74	7	1
4:A:353:PX4:H39	4:A:362:PX4:H68	0.57	1.76	20	1
4:A:423:PX4:H47	4:A:426:PX4:H17	0.57	1.75	3	1
4:A:392:PX4:H56	4:A:409:PX4:H54	0.57	1.76	9	1
4:A:400:PX4:H23	4:A:393:PX4:H27	0.57	1.75	1	1
4:A:401:PX4:H71	4:A:401:PX4:H39	0.57	1.75	2	1
4:A:357:PX4:H40	4:A:358:PX4:H37	0.57	1.75	8	1
4:A:377:PX4:H14	4:A:378:PX4:O1	0.57	1.99	9	1
4:A:334:PX4:H48	4:A:343:PX4:H19	0.57	1.77	10	1
4:A:357:PX4:H17	4:A:358:PX4:H20	0.57	1.75	14	1
4:A:379:PX4:H53	4:A:418:PX4:H55	0.57	1.76	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:312:PX4:H14	4:A:319:PX4:H15	0.57	1.76	19	1
4:A:394:PX4:H66	4:A:400:PX4:H34	0.57	1.75	8	1
4:A:338:PX4:H31	4:A:346:PX4:H29	0.57	1.75	18	1
4:A:374:PX4:H10	4:A:382:PX4:H18	0.57	1.75	20	1
4:A:378:PX4:H59	4:A:411:PX4:H24	0.57	1.76	20	1
4:A:407:PX4:H34	4:A:423:PX4:H28	0.57	1.75	20	1
4:A:330:PX4:H46	4:A:331:PX4:H7	0.57	1.75	1	1
4:A:305:PX4:H24	4:A:320:PX4:H59	0.57	1.77	10	1
4:A:328:PX4:H19	4:A:335:PX4:H16	0.57	1.76	15	2
4:A:391:PX4:H56	4:A:425:PX4:H67	0.57	1.76	14	1
4:A:369:PX4:H59	4:A:391:PX4:H28	0.57	1.77	20	1
4:A:417:PX4:H51	4:A:419:PX4:H49	0.57	1.77	4	1
4:A:326:PX4:H16	4:A:327:PX4:C26	0.57	2.29	9	1
4:A:418:PX4:H64	4:A:428:PX4:H66	0.57	1.77	16	1
4:A:328:PX4:H16	4:A:342:PX4:H57	0.57	1.75	17	1
4:A:378:PX4:H58	4:A:380:PX4:H32	0.57	1.76	8	1
4:A:333:PX4:H34	4:A:339:PX4:H55	0.57	1.76	9	1
4:A:357:PX4:H34	4:A:429:PX4:H39	0.57	1.76	9	1
4:A:338:PX4:H71	4:A:425:PX4:H66	0.57	1.77	14	1
4:A:381:PX4:C11	4:A:385:PX4:H54	0.57	2.26	16	1
4:A:389:PX4:H32	4:A:403:PX4:H29	0.57	1.77	2	1
4:A:331:PX4:H60	4:A:346:PX4:H65	0.57	1.76	7	1
4:A:377:PX4:H42	4:A:419:PX4:H51	0.57	1.77	11	1
4:A:390:PX4:H20	4:A:430:PX4:H55	0.57	1.75	17	1
4:A:317:PX4:H36	4:A:319:PX4:H56	0.57	1.76	1	1
4:A:352:PX4:H4	4:A:365:PX4:H15	0.57	1.76	1	1
4:A:372:PX4:H21	4:A:421:PX4:H48	0.57	1.77	2	1
4:A:397:PX4:H12	4:A:397:PX4:H14	0.57	1.76	8	1
4:A:368:PX4:H35	4:A:429:PX4:H64	0.57	1.77	12	1
4:A:319:PX4:H62	4:A:429:PX4:H71	0.57	1.76	13	1
4:A:331:PX4:H50	4:A:347:PX4:H18	0.57	1.75	15	1
4:A:315:PX4:H67	4:A:319:PX4:H32	0.57	1.75	19	1
4:A:313:PX4:H29	4:A:364:PX4:H40	0.57	1.77	2	1
4:A:388:PX4:H51	4:A:412:PX4:H46	0.57	1.76	6	1
4:A:414:PX4:H53	4:A:422:PX4:H25	0.57	1.75	14	1
4:A:325:PX4:H21	4:A:349:PX4:H46	0.57	1.75	16	1
4:A:392:PX4:H55	4:A:402:PX4:H63	0.57	1.76	17	1
4:A:372:PX4:H55	4:A:373:PX4:H34	0.57	1.76	19	1
4:A:330:PX4:H17	4:A:331:PX4:H20	0.56	1.78	3	1
4:A:342:PX4:H38	4:A:358:PX4:H21	0.56	1.77	17	1
4:A:391:PX4:H3	4:A:425:PX4:H14	0.56	1.77	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:318:PX4:H1	4:A:323:PX4:H18	0.56	1.77	8	2
4:A:418:PX4:H17	4:A:427:PX4:H19	0.56	1.75	8	1
4:A:338:PX4:H28	4:A:346:PX4:H56	0.56	1.76	11	1
4:A:337:PX4:H58	4:A:337:PX4:H25	0.56	1.76	12	1
4:A:320:PX4:H23	4:A:353:PX4:H65	0.56	1.76	3	1
4:A:351:PX4:H42	4:A:391:PX4:H71	0.56	1.76	3	1
4:A:348:PX4:H64	4:A:354:PX4:H33	0.56	1.76	9	1
4:A:308:PX4:H48	4:A:315:PX4:H51	0.56	1.76	11	1
4:A:338:PX4:H24	4:A:346:PX4:H24	0.56	1.77	15	1
4:A:330:PX4:H66	4:A:346:PX4:H64	0.56	1.78	18	1
4:A:309:PX4:H20	4:A:357:PX4:H54	0.56	1.78	20	1
4:A:326:PX4:H16	4:A:327:PX4:H50	0.56	1.77	9	1
4:A:305:PX4:H11	4:A:362:PX4:O6	0.56	2.00	10	1
4:A:311:PX4:H58	4:A:405:PX4:H36	0.56	1.77	13	1
4:A:335:PX4:O2	4:A:342:PX4:H4	0.56	2.00	14	1
4:A:404:PX4:H65	4:A:414:PX4:H33	0.56	1.77	14	1
4:A:412:PX4:H30	4:A:420:PX4:H63	0.56	1.76	14	1
4:A:414:PX4:H59	4:A:422:PX4:H47	0.56	1.78	15	1
4:A:341:PX4:H65	4:A:343:PX4:H45	0.56	1.75	20	1
4:A:377:PX4:H60	4:A:391:PX4:H49	0.56	1.77	5	1
4:A:392:PX4:H44	4:A:399:PX4:H39	0.56	1.77	6	1
4:A:416:PX4:H55	4:A:422:PX4:H52	0.56	1.77	9	1
4:A:334:PX4:H48	4:A:343:PX4:H20	0.56	1.76	12	1
4:A:354:PX4:O6	4:A:355:PX4:H17	0.56	2.00	20	1
4:A:355:PX4:H48	4:A:356:PX4:H50	0.56	1.78	2	1
4:A:338:PX4:H69	4:A:384:PX4:H34	0.56	1.77	4	1
4:A:321:PX4:H3	4:A:328:PX4:H11	0.56	1.77	8	1
4:A:318:PX4:H16	4:A:323:PX4:H14	0.56	1.78	9	1
4:A:332:PX4:H16	4:A:340:PX4:H19	0.56	1.77	20	1
4:A:320:PX4:H23	4:A:320:PX4:H58	0.56	1.77	1	1
4:A:310:PX4:H59	4:A:349:PX4:H21	0.56	1.78	2	1
4:A:413:PX4:H60	4:A:421:PX4:O6	0.56	2.00	4	1
4:A:393:PX4:H48	4:A:394:PX4:H49	0.56	1.78	6	1
4:A:371:PX4:H41	4:A:420:PX4:H35	0.56	1.77	11	1
4:A:411:PX4:H56	4:A:427:PX4:H60	0.56	1.77	2	1
4:A:372:PX4:H16	4:A:373:PX4:H25	0.56	1.76	4	1
4:A:361:PX4:H38	4:A:427:PX4:H38	0.56	1.77	5	1
4:A:377:PX4:H47	4:A:378:PX4:H24	0.56	1.78	12	1
4:A:417:PX4:O4	4:A:419:PX4:H8	0.56	2.00	4	1
4:A:308:PX4:H13	4:A:319:PX4:O2	0.56	2.01	11	1
4:A:404:PX4:H47	4:A:405:PX4:H16	0.56	1.78	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:413:PX4:H25	4:A:431:PX4:H52	0.56	1.78	12	1
4:A:377:PX4:H68	4:A:378:PX4:H35	0.56	1.77	14	1
4:A:376:PX4:H19	4:A:383:PX4:H22	0.56	1.77	17	1
4:A:414:PX4:H20	4:A:422:PX4:H37	0.56	1.78	20	1
4:A:409:PX4:H21	4:A:410:PX4:H46	0.56	1.79	2	1
4:A:391:PX4:C12	4:A:425:PX4:H48	0.56	2.31	4	1
4:A:346:PX4:H39	4:A:358:PX4:H70	0.56	1.77	5	1
4:A:328:PX4:O4	4:A:335:PX4:H16	0.56	2.01	17	1
4:A:426:PX4:H57	4:A:426:PX4:H25	0.56	1.78	19	1
4:A:324:PX4:H70	4:A:374:PX4:H66	0.55	1.78	11	1
4:A:357:PX4:H56	4:A:358:PX4:H65	0.55	1.76	20	1
4:A:308:PX4:H56	4:A:340:PX4:H45	0.55	1.78	1	1
4:A:374:PX4:H17	4:A:398:PX4:O1	0.55	2.02	2	1
4:A:396:PX4:H35	4:A:414:PX4:H38	0.55	1.77	2	1
4:A:373:PX4:H61	4:A:385:PX4:H45	0.55	1.78	3	1
4:A:319:PX4:H25	4:A:367:PX4:H34	0.55	1.78	9	1
4:A:309:PX4:O6	4:A:366:PX4:H17	0.55	2.02	15	2
4:A:413:PX4:H71	4:A:429:PX4:H21	0.55	1.78	13	1
1:A:48:LEU:HD23	1:A:53:MET:SD	0.55	2.41	8	1
4:A:331:PX4:H21	4:A:339:PX4:H23	0.55	1.78	11	1
4:A:423:PX4:H51	4:A:426:PX4:H57	0.55	1.77	11	1
4:A:316:PX4:H28	4:A:325:PX4:H60	0.55	1.76	13	1
4:A:372:PX4:H54	4:A:421:PX4:H56	0.55	1.78	17	1
4:A:315:PX4:H21	4:A:322:PX4:H48	0.55	1.78	4	1
4:A:370:PX4:H48	4:A:419:PX4:H17	0.55	1.78	13	1
4:A:391:PX4:H37	4:A:425:PX4:H34	0.55	1.78	13	1
4:A:386:PX4:H4	4:A:400:PX4:O1	0.55	2.01	17	1
4:A:396:PX4:H18	4:A:398:PX4:H55	0.55	1.77	20	1
4:A:403:PX4:H56	4:A:405:PX4:H56	0.55	1.76	3	1
4:A:399:PX4:H46	4:A:408:PX4:H59	0.55	1.78	8	1
4:A:396:PX4:H67	4:A:405:PX4:H72	0.55	1.79	11	1
4:A:409:PX4:H20	4:A:416:PX4:H16	0.55	1.78	12	3
4:A:387:PX4:H53	4:A:395:PX4:H21	0.55	1.78	16	1
4:A:374:PX4:H47	4:A:398:PX4:C10	0.55	2.28	2	1
4:A:385:PX4:H12	4:A:387:PX4:H16	0.55	1.77	2	1
4:A:357:PX4:H21	4:A:358:PX4:H27	0.55	1.78	4	1
4:A:308:PX4:H57	4:A:318:PX4:H46	0.55	1.78	7	1
4:A:323:PX4:H64	4:A:331:PX4:H45	0.55	1.78	7	1
4:A:348:PX4:H36	4:A:349:PX4:H65	0.55	1.76	10	1
4:A:371:PX4:H34	4:A:418:PX4:H68	0.55	1.78	10	1
4:A:305:PX4:H42	4:A:305:PX4:H61	0.55	1.77	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:360:PX4:H28	4:A:360:PX4:H67	0.55	1.78	14	1
4:A:320:PX4:H72	4:A:362:PX4:H64	0.55	1.78	17	1
4:A:326:PX4:H18	4:A:327:PX4:H49	0.55	1.76	18	1
4:A:371:PX4:H19	4:A:418:PX4:H48	0.55	1.79	19	1
4:A:357:PX4:H55	4:A:358:PX4:H61	0.55	1.78	20	1
4:A:419:PX4:H56	4:A:426:PX4:H32	0.55	1.79	2	1
4:A:429:PX4:H4	4:A:429:PX4:H19	0.55	1.77	2	1
4:A:375:PX4:H28	4:A:429:PX4:H24	0.55	1.77	4	1
4:A:384:PX4:H69	4:A:393:PX4:H39	0.55	1.78	4	1
4:A:329:PX4:H19	4:A:338:PX4:H47	0.55	1.79	8	1
4:A:388:PX4:H61	4:A:388:PX4:H34	0.55	1.79	12	1
4:A:382:PX4:H17	4:A:385:PX4:H58	0.55	1.77	13	1
4:A:318:PX4:H69	4:A:373:PX4:H40	0.55	1.77	14	1
4:A:404:PX4:H49	4:A:405:PX4:H52	0.55	1.77	16	1
4:A:375:PX4:H13	4:A:429:PX4:H16	0.55	1.77	17	1
4:A:378:PX4:C25	4:A:411:PX4:H54	0.55	2.28	18	1
4:A:389:PX4:H50	4:A:395:PX4:H52	0.55	1.79	1	1
4:A:384:PX4:H26	4:A:400:PX4:H23	0.55	1.79	3	1
4:A:327:PX4:H38	4:A:353:PX4:H37	0.55	1.77	8	1
4:A:329:PX4:H30	4:A:351:PX4:H24	0.55	1.79	9	1
4:A:322:PX4:O2	4:A:361:PX4:H4	0.55	2.02	15	1
4:A:369:PX4:H24	4:A:370:PX4:H27	0.55	1.77	16	1
4:A:378:PX4:H8	4:A:385:PX4:O2	0.55	2.02	20	1
4:A:328:PX4:H48	4:A:335:PX4:H22	0.55	1.79	1	1
4:A:392:PX4:H28	4:A:409:PX4:H58	0.55	1.79	8	1
4:A:329:PX4:H67	4:A:338:PX4:H62	0.55	1.78	9	1
4:A:369:PX4:H34	4:A:400:PX4:H27	0.55	1.78	16	1
4:A:346:PX4:H46	4:A:347:PX4:H17	0.55	1.78	13	1
4:A:312:PX4:H23	4:A:327:PX4:H55	0.55	1.77	14	1
4:A:378:PX4:H54	4:A:385:PX4:H28	0.55	1.79	15	1
4:A:348:PX4:H26	4:A:349:PX4:H30	0.55	1.79	17	1
4:A:318:PX4:H48	4:A:323:PX4:H53	0.55	1.79	20	1
4:A:318:PX4:H8	4:A:324:PX4:H23	0.54	1.79	7	1
4:A:384:PX4:H21	4:A:400:PX4:H26	0.54	1.79	8	1
4:A:312:PX4:H19	4:A:359:PX4:H15	0.54	1.78	9	1
4:A:320:PX4:H17	4:A:353:PX4:H49	0.54	1.79	12	1
4:A:324:PX4:H38	4:A:340:PX4:H39	0.54	1.79	15	1
4:A:369:PX4:H60	4:A:391:PX4:H25	0.54	1.79	16	1
4:A:328:PX4:H16	4:A:335:PX4:H18	0.54	1.79	1	1
4:A:372:PX4:H44	4:A:421:PX4:H37	0.54	1.80	5	1
4:A:317:PX4:H21	4:A:318:PX4:H5	0.54	1.78	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:335:PX4:H70	4:A:391:PX4:H66	0.54	1.79	7	1
4:A:374:PX4:H15	4:A:383:PX4:H49	0.54	1.79	16	1
4:A:393:PX4:H27	4:A:400:PX4:H27	0.54	1.80	2	1
4:A:308:PX4:H4	4:A:319:PX4:O2	0.54	2.03	6	1
4:A:377:PX4:H33	4:A:411:PX4:H34	0.54	1.79	8	1
4:A:368:PX4:H62	4:A:429:PX4:H30	0.54	1.77	12	1
4:A:321:PX4:H27	4:A:338:PX4:H49	0.54	1.80	15	1
4:A:332:PX4:H19	4:A:340:PX4:H16	0.54	1.78	18	1
4:A:391:PX4:H17	4:A:400:PX4:H47	0.54	1.80	11	2
4:A:357:PX4:H46	4:A:358:PX4:H48	0.54	1.80	7	1
4:A:396:PX4:H65	4:A:396:PX4:H33	0.54	1.79	14	2
4:A:312:PX4:H19	4:A:327:PX4:H57	0.54	1.78	17	1
4:A:379:PX4:H66	4:A:380:PX4:H42	0.54	1.80	3	1
4:A:320:PX4:H72	4:A:353:PX4:H70	0.54	1.79	7	1
4:A:371:PX4:H25	4:A:418:PX4:H53	0.54	1.78	14	1
4:A:376:PX4:H51	4:A:430:PX4:H57	0.54	1.79	8	1
4:A:383:PX4:H58	4:A:429:PX4:H31	0.54	1.80	12	1
4:A:332:PX4:H39	4:A:340:PX4:H29	0.54	1.80	15	1
4:A:355:PX4:H9	4:A:355:PX4:O2	0.54	2.02	2	1
4:A:377:PX4:H43	4:A:378:PX4:H71	0.54	1.80	7	1
4:A:329:PX4:H51	4:A:338:PX4:H25	0.54	1.80	14	1
4:A:424:PX4:H46	4:A:426:PX4:H54	0.54	1.78	16	1
4:A:324:PX4:H52	4:A:339:PX4:H17	0.54	1.78	18	1
4:A:371:PX4:H47	4:A:404:PX4:H20	0.54	1.80	2	1
4:A:414:PX4:H45	4:A:421:PX4:H49	0.54	1.80	9	1
4:A:320:PX4:C8	4:A:353:PX4:H16	0.54	2.21	10	1
4:A:388:PX4:H62	4:A:412:PX4:H64	0.54	1.80	11	1
4:A:396:PX4:H15	4:A:397:PX4:O1	0.54	2.02	14	1
4:A:350:PX4:H26	4:A:357:PX4:H20	0.54	1.80	15	1
4:A:392:PX4:H30	4:A:393:PX4:H17	0.54	1.80	20	1
4:A:370:PX4:H19	4:A:419:PX4:H47	0.54	1.79	1	1
4:A:316:PX4:O6	4:A:324:PX4:H19	0.54	2.03	4	1
4:A:364:PX4:H55	4:A:412:PX4:H43	0.54	1.78	7	1
4:A:338:PX4:H16	4:A:346:PX4:H47	0.54	1.80	12	1
4:A:357:PX4:H2	4:A:358:PX4:O6	0.54	2.03	12	1
4:A:312:PX4:H39	4:A:319:PX4:H16	0.54	1.79	16	1
4:A:321:PX4:H46	4:A:328:PX4:H48	0.54	1.78	17	1
4:A:324:PX4:H30	4:A:339:PX4:H62	0.54	1.78	18	1
4:A:384:PX4:H66	4:A:386:PX4:H47	0.54	1.79	18	1
4:A:407:PX4:H49	4:A:416:PX4:H13	0.54	1.78	18	1
4:A:401:PX4:H52	4:A:417:PX4:H49	0.54	1.80	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:371:PX4:H46	4:A:412:PX4:H16	0.54	1.80	1	1
4:A:341:PX4:H38	4:A:358:PX4:H35	0.54	1.79	3	1
4:A:328:PX4:H20	4:A:342:PX4:H55	0.54	1.79	5	1
4:A:376:PX4:H16	4:A:383:PX4:H47	0.54	1.79	20	2
4:A:399:PX4:H10	4:A:408:PX4:O4	0.54	2.02	7	1
4:A:316:PX4:H36	4:A:343:PX4:H39	0.54	1.79	9	1
4:A:369:PX4:H47	4:A:370:PX4:H21	0.54	1.80	15	2
4:A:404:PX4:H59	4:A:414:PX4:H19	0.54	1.78	19	1
1:A:84:TRP:CE2	1:A:162:PRO:HB3	0.53	2.38	16	1
4:A:306:PX4:H48	4:A:364:PX4:H27	0.53	1.78	18	1
4:A:390:PX4:H20	4:A:398:PX4:H62	0.53	1.79	19	1
4:A:326:PX4:H56	4:A:343:PX4:H51	0.53	1.79	1	1
1:A:142:ALA:O	4:A:335:PX4:H6	0.53	2.03	2	1
4:A:348:PX4:H41	4:A:397:PX4:H40	0.53	1.77	2	1
4:A:333:PX4:H61	4:A:348:PX4:H54	0.53	1.81	3	1
4:A:309:PX4:O2	4:A:366:PX4:H12	0.53	2.02	5	1
4:A:344:PX4:H59	4:A:344:PX4:H24	0.53	1.79	8	1
4:A:334:PX4:H56	4:A:341:PX4:H21	0.53	1.78	12	1
4:A:306:PX4:O2	4:A:313:PX4:H10	0.53	2.02	14	1
4:A:312:PX4:H48	4:A:326:PX4:H54	0.53	1.79	15	1
4:A:392:PX4:O2	4:A:409:PX4:H9	0.53	2.01	17	1
4:A:390:PX4:O3	4:A:390:PX4:H18	0.53	2.03	18	1
4:A:337:PX4:H50	4:A:355:PX4:H22	0.53	1.81	2	1
4:A:325:PX4:H23	4:A:356:PX4:H65	0.53	1.80	6	1
4:A:331:PX4:H48	4:A:355:PX4:H53	0.53	1.80	9	1
4:A:316:PX4:H70	4:A:390:PX4:H45	0.53	1.80	13	1
4:A:322:PX4:H20	4:A:332:PX4:H17	0.53	1.79	14	1
4:A:409:PX4:H59	4:A:416:PX4:H24	0.53	1.80	16	1
4:A:305:PX4:H62	4:A:362:PX4:H55	0.53	1.78	20	1
4:A:370:PX4:H36	4:A:425:PX4:H67	0.53	1.78	5	1
4:A:325:PX4:H8	4:A:350:PX4:O8	0.53	2.03	6	1
4:A:305:PX4:H53	4:A:305:PX4:H27	0.53	1.80	8	1
4:A:305:PX4:H39	4:A:330:PX4:H27	0.53	1.79	8	1
4:A:381:PX4:H62	4:A:385:PX4:H61	0.53	1.79	11	1
4:A:312:PX4:H69	4:A:383:PX4:H69	0.53	1.80	13	1
4:A:331:PX4:H60	4:A:347:PX4:H51	0.53	1.81	14	1
4:A:319:PX4:H34	4:A:407:PX4:H39	0.53	1.79	15	1
4:A:345:PX4:H67	4:A:354:PX4:H44	0.53	1.80	15	1
4:A:333:PX4:H17	4:A:339:PX4:H64	0.53	1.80	17	1
4:A:404:PX4:H22	4:A:412:PX4:H16	0.53	1.80	18	1
4:A:404:PX4:H14	4:A:412:PX4:O1	0.53	2.04	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:391:PX4:H39	4:A:425:PX4:H68	0.53	1.80	3	1
4:A:324:PX4:H60	4:A:340:PX4:H56	0.53	1.79	5	1
4:A:316:PX4:H19	4:A:324:PX4:H26	0.53	1.81	8	1
4:A:377:PX4:H48	4:A:386:PX4:H7	0.53	1.81	14	1
4:A:402:PX4:H63	4:A:418:PX4:H29	0.53	1.81	14	1
4:A:414:PX4:H51	4:A:431:PX4:H24	0.53	1.80	14	1
4:A:409:PX4:H17	4:A:410:PX4:H48	0.53	1.80	15	1
4:A:329:PX4:H48	4:A:351:PX4:H50	0.53	1.79	3	1
4:A:369:PX4:H32	4:A:378:PX4:H31	0.53	1.81	6	1
4:A:373:PX4:H65	4:A:380:PX4:H63	0.53	1.80	8	1
4:A:377:PX4:H35	4:A:411:PX4:H19	0.53	1.79	9	1
4:A:308:PX4:H23	4:A:359:PX4:H65	0.53	1.79	13	1
4:A:424:PX4:H54	4:A:430:PX4:H41	0.53	1.81	16	1
4:A:361:PX4:H60	4:A:427:PX4:H45	0.53	1.80	17	1
4:A:388:PX4:H54	4:A:395:PX4:H53	0.53	1.80	17	1
4:A:381:PX4:H28	4:A:382:PX4:H25	0.53	1.80	18	1
4:A:411:PX4:H32	4:A:417:PX4:H64	0.53	1.79	20	1
4:A:326:PX4:H32	4:A:353:PX4:H34	0.53	1.79	16	1
4:A:337:PX4:H16	4:A:354:PX4:C7	0.53	2.30	20	1
4:A:388:PX4:H1	4:A:412:PX4:H49	0.53	1.79	20	1
4:A:321:PX4:H49	4:A:330:PX4:H24	0.53	1.78	5	1
4:A:305:PX4:H53	4:A:362:PX4:H17	0.53	1.81	9	1
4:A:413:PX4:H60	4:A:429:PX4:H52	0.53	1.79	9	1
4:A:369:PX4:H49	4:A:370:PX4:H27	0.53	1.81	11	1
4:A:329:PX4:O6	4:A:351:PX4:H17	0.53	2.03	16	1
4:A:359:PX4:H16	4:A:367:PX4:H18	0.53	1.80	19	1
4:A:317:PX4:H29	4:A:323:PX4:H38	0.53	1.81	13	1
4:A:307:PX4:H4	4:A:363:PX4:O6	0.53	2.04	1	1
4:A:396:PX4:H25	4:A:405:PX4:H51	0.53	1.80	6	1
4:A:339:PX4:H21	4:A:355:PX4:H57	0.53	1.81	7	1
4:A:344:PX4:H60	4:A:366:PX4:H60	0.53	1.79	7	1
4:A:335:PX4:H23	4:A:342:PX4:H53	0.53	1.81	9	1
4:A:355:PX4:H24	4:A:356:PX4:H30	0.53	1.80	9	1
4:A:331:PX4:H62	4:A:339:PX4:H31	0.53	1.78	11	1
4:A:380:PX4:H30	4:A:385:PX4:H36	0.53	1.80	12	1
4:A:320:PX4:H49	4:A:362:PX4:H47	0.53	1.80	14	1
4:A:305:PX4:H68	4:A:321:PX4:H62	0.53	1.80	19	1
4:A:377:PX4:H51	4:A:386:PX4:H11	0.53	1.80	20	1
4:A:346:PX4:H52	4:A:347:PX4:H53	0.52	1.82	2	1
4:A:380:PX4:O6	4:A:381:PX4:H9	0.52	2.02	2	1
4:A:349:PX4:H60	4:A:350:PX4:H61	0.52	1.80	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:321:PX4:H59	4:A:328:PX4:H60	0.52	1.79	13	1
4:A:369:PX4:H56	4:A:425:PX4:H55	0.52	1.81	14	1
4:A:385:PX4:H60	4:A:386:PX4:H32	0.52	1.82	15	1
4:A:316:PX4:H38	4:A:375:PX4:H71	0.52	1.80	16	1
4:A:316:PX4:H43	4:A:318:PX4:H26	0.52	1.81	18	1
4:A:305:PX4:H33	4:A:321:PX4:H55	0.52	1.81	1	1
1:A:147:TYR:HB3	1:A:148:PRO:HD2	0.52	1.82	19	2
4:A:376:PX4:H35	4:A:383:PX4:H29	0.52	1.81	11	1
4:A:383:PX4:H28	4:A:389:PX4:H67	0.52	1.81	12	1
4:A:386:PX4:H19	4:A:395:PX4:H34	0.52	1.81	13	1
4:A:398:PX4:H66	4:A:403:PX4:C20	0.52	2.33	15	1
4:A:409:PX4:H30	4:A:417:PX4:H26	0.52	1.81	16	1
4:A:416:PX4:H56	4:A:422:PX4:H60	0.52	1.80	1	1
4:A:409:PX4:H30	4:A:410:PX4:H69	0.52	1.81	9	1
4:A:379:PX4:H58	4:A:380:PX4:H27	0.52	1.81	11	1
4:A:423:PX4:H25	4:A:424:PX4:H22	0.52	1.81	13	1
4:A:385:PX4:H51	4:A:387:PX4:C25	0.52	2.32	14	1
4:A:309:PX4:H20	4:A:366:PX4:H20	0.52	1.80	16	1
4:A:321:PX4:H43	4:A:338:PX4:H49	0.52	1.79	20	1
4:A:319:PX4:H34	4:A:312:PX4:H37	0.52	1.82	1	1
4:A:330:PX4:O2	4:A:339:PX4:H3	0.52	2.05	5	1
4:A:377:PX4:H16	4:A:387:PX4:H5	0.52	1.81	7	1
4:A:329:PX4:H72	4:A:344:PX4:H27	0.52	1.81	11	1
4:A:377:PX4:H65	4:A:384:PX4:H62	0.52	1.80	12	1
4:A:414:PX4:H56	4:A:422:PX4:H29	0.52	1.80	14	1
4:A:305:PX4:H33	4:A:328:PX4:H62	0.52	1.81	15	1
4:A:348:PX4:H19	4:A:349:PX4:H17	0.52	1.80	19	1
4:A:305:PX4:H37	4:A:328:PX4:H65	0.52	1.81	5	1
4:A:391:PX4:O6	4:A:400:PX4:H6	0.52	2.05	6	1
4:A:387:PX4:H56	4:A:395:PX4:H51	0.52	1.82	8	1
4:A:370:PX4:H27	4:A:377:PX4:H30	0.52	1.81	9	1
4:A:336:PX4:H20	4:A:358:PX4:H15	0.52	1.81	18	1
4:A:311:PX4:O8	4:A:364:PX4:H47	0.52	2.05	1	1
4:A:422:PX4:H16	4:A:431:PX4:H20	0.52	1.80	19	5
4:A:316:PX4:H18	4:A:324:PX4:H19	0.52	1.81	2	1
4:A:324:PX4:H50	4:A:339:PX4:H50	0.52	1.80	2	1
4:A:383:PX4:H37	4:A:389:PX4:H17	0.52	1.81	10	2
4:A:352:PX4:H20	4:A:360:PX4:H46	0.52	1.81	6	1
4:A:308:PX4:H21	4:A:315:PX4:H49	0.52	1.82	7	1
4:A:325:PX4:H23	4:A:349:PX4:H56	0.52	1.79	9	1
4:A:307:PX4:O6	4:A:348:PX4:H11	0.52	2.03	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:369:PX4:H6	4:A:419:PX4:O1	0.52	2.05	1	1
4:A:377:PX4:H49	4:A:378:PX4:H24	0.52	1.80	2	1
4:A:374:PX4:H57	4:A:398:PX4:H31	0.52	1.80	4	1
4:A:374:PX4:H50	4:A:382:PX4:H16	0.52	1.80	6	1
4:A:324:PX4:H32	4:A:413:PX4:H43	0.52	1.81	9	1
4:A:370:PX4:H43	4:A:411:PX4:H39	0.52	1.80	9	1
4:A:309:PX4:H33	4:A:366:PX4:H71	0.52	1.81	11	1
4:A:374:PX4:H18	4:A:382:PX4:H56	0.52	1.82	18	1
4:A:306:PX4:H66	4:A:364:PX4:H35	0.52	1.81	10	1
4:A:392:PX4:H47	4:A:409:PX4:H58	0.52	1.79	10	1
4:A:388:PX4:H28	4:A:394:PX4:H51	0.52	1.82	13	1
4:A:406:PX4:H36	4:A:409:PX4:H33	0.52	1.82	15	1
4:A:396:PX4:H30	4:A:414:PX4:H53	0.52	1.82	17	1
4:A:369:PX4:H65	4:A:400:PX4:H52	0.52	1.82	6	1
4:A:333:PX4:H21	4:A:356:PX4:H53	0.52	1.82	7	1
4:A:372:PX4:H15	4:A:428:PX4:H7	0.52	1.80	8	1
4:A:409:PX4:C8	4:A:416:PX4:H14	0.52	2.34	15	1
4:A:404:PX4:O8	4:A:420:PX4:H3	0.52	2.05	18	1
4:A:318:PX4:H17	4:A:323:PX4:H20	0.52	1.80	1	1
4:A:333:PX4:H40	4:A:355:PX4:H57	0.52	1.82	1	1
4:A:345:PX4:O6	4:A:352:PX4:H7	0.52	2.05	1	1
4:A:384:PX4:H56	4:A:395:PX4:H27	0.52	1.82	1	1
4:A:368:PX4:H29	4:A:413:PX4:H56	0.52	1.82	5	1
4:A:336:PX4:H54	4:A:344:PX4:H49	0.52	1.82	6	1
4:A:370:PX4:H26	4:A:370:PX4:H55	0.52	1.82	7	1
4:A:342:PX4:H27	4:A:351:PX4:H16	0.52	1.80	10	1
4:A:392:PX4:H16	4:A:393:PX4:H9	0.52	1.82	10	1
4:A:377:PX4:H59	4:A:384:PX4:H57	0.52	1.81	15	1
4:A:394:PX4:H46	4:A:402:PX4:H24	0.52	1.82	15	1
4:A:320:PX4:H21	4:A:353:PX4:H24	0.52	1.80	16	1
4:A:388:PX4:H49	4:A:389:PX4:H16	0.52	1.81	16	1
4:A:312:PX4:H23	4:A:359:PX4:H19	0.52	1.82	18	1
4:A:322:PX4:H22	4:A:332:PX4:H13	0.51	1.80	2	1
4:A:419:PX4:H36	4:A:424:PX4:H34	0.51	1.83	4	1
4:A:369:PX4:H72	4:A:391:PX4:H57	0.51	1.82	5	1
4:A:377:PX4:H21	4:A:378:PX4:H25	0.51	1.81	11	1
4:A:321:PX4:H31	4:A:335:PX4:H25	0.51	1.81	12	1
4:A:336:PX4:H8	4:A:344:PX4:O1	0.51	2.05	12	1
4:A:399:PX4:H51	4:A:408:PX4:H57	0.51	1.82	15	1
4:A:329:PX4:H19	4:A:338:PX4:H28	0.51	1.82	7	1
4:A:375:PX4:H9	4:A:421:PX4:O6	0.51	2.05	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:381:PX4:H25	4:A:382:PX4:H47	0.51	1.81	9	1
4:A:347:PX4:H8	4:A:355:PX4:O6	0.51	2.05	11	1
4:A:312:PX4:O2	4:A:327:PX4:H13	0.51	2.06	14	1
4:A:338:PX4:H36	4:A:346:PX4:H72	0.51	1.82	14	1
4:A:337:PX4:H51	4:A:346:PX4:H23	0.51	1.81	16	1
4:A:370:PX4:H21	4:A:425:PX4:H51	0.51	1.81	16	1
4:A:384:PX4:H49	4:A:386:PX4:H7	0.51	1.80	2	1
4:A:392:PX4:H62	4:A:418:PX4:H44	0.51	1.81	4	1
4:A:354:PX4:H21	4:A:355:PX4:H22	0.51	1.82	9	1
4:A:331:PX4:H57	4:A:347:PX4:H52	0.51	1.82	15	1
4:A:392:PX4:H54	4:A:409:PX4:H49	0.51	1.81	18	1
4:A:369:PX4:O8	4:A:391:PX4:H11	0.51	2.05	19	1
4:A:399:PX4:H44	4:A:402:PX4:H39	0.51	1.81	4	1
4:A:322:PX4:H24	4:A:332:PX4:H17	0.51	1.82	7	2
4:A:338:PX4:H3	4:A:342:PX4:O2	0.51	2.05	7	1
4:A:317:PX4:H24	4:A:323:PX4:H30	0.51	1.81	9	1
4:A:318:PX4:H1	4:A:323:PX4:O3	0.51	2.05	11	1
4:A:392:PX4:H26	4:A:399:PX4:H29	0.51	1.83	13	1
4:A:334:PX4:H62	4:A:341:PX4:H55	0.51	1.81	17	1
4:A:353:PX4:H66	4:A:362:PX4:H67	0.51	1.82	18	1
4:A:337:PX4:C7	4:A:354:PX4:H16	0.51	2.31	20	1
4:A:379:PX4:H53	4:A:380:PX4:H32	0.51	1.82	3	1
4:A:311:PX4:H16	4:A:364:PX4:H5	0.51	1.82	5	1
4:A:383:PX4:H49	4:A:429:PX4:H11	0.51	1.81	5	1
4:A:320:PX4:H30	4:A:321:PX4:H63	0.51	1.83	9	1
4:A:314:PX4:H44	4:A:345:PX4:H63	0.51	1.82	11	1
4:A:312:PX4:H39	4:A:327:PX4:H70	0.51	1.80	14	1
4:A:352:PX4:H29	4:A:416:PX4:H39	0.51	1.82	14	1
4:A:335:PX4:H54	4:A:342:PX4:H17	0.51	1.82	15	1
4:A:373:PX4:H24	4:A:380:PX4:H58	0.51	1.82	15	1
4:A:404:PX4:H43	4:A:405:PX4:H34	0.51	1.82	15	1
4:A:316:PX4:H51	4:A:317:PX4:H49	0.51	1.81	16	1
4:A:373:PX4:O2	4:A:373:PX4:H6	0.51	2.06	16	1
4:A:409:PX4:H17	4:A:410:PX4:H15	0.51	1.81	16	1
4:A:333:PX4:H36	4:A:339:PX4:H40	0.51	1.82	19	1
4:A:305:PX4:H17	4:A:362:PX4:H13	0.51	1.82	20	1
4:A:329:PX4:H27	4:A:347:PX4:C28	0.51	2.35	1	1
4:A:401:PX4:H47	4:A:410:PX4:H16	0.51	1.81	2	1
4:A:354:PX4:H62	4:A:364:PX4:H39	0.51	1.83	4	1
4:A:321:PX4:O2	4:A:332:PX4:H5	0.51	2.06	8	2
4:A:371:PX4:H9	4:A:420:PX4:O2	0.51	2.06	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:329:PX4:O6	4:A:338:PX4:H17	0.51	2.05	10	1
4:A:358:PX4:H32	4:A:399:PX4:H70	0.51	1.83	14	1
4:A:392:PX4:O2	4:A:409:PX4:H48	0.51	2.05	15	1
4:A:352:PX4:H31	4:A:366:PX4:H63	0.51	1.82	4	1
4:A:307:PX4:H46	4:A:310:PX4:H10	0.51	1.82	12	1
4:A:308:PX4:H39	4:A:322:PX4:H65	0.51	1.81	14	1
4:A:328:PX4:C10	4:A:335:PX4:H16	0.51	2.35	15	1
4:A:397:PX4:H30	4:A:403:PX4:H27	0.51	1.82	17	1
4:A:347:PX4:H26	4:A:355:PX4:H53	0.51	1.83	18	1
4:A:336:PX4:H30	4:A:352:PX4:H35	0.51	1.82	20	1
4:A:312:PX4:H45	4:A:423:PX4:H43	0.51	1.82	10	1
4:A:320:PX4:H59	4:A:328:PX4:H21	0.51	1.81	13	1
4:A:368:PX4:H25	4:A:424:PX4:H19	0.51	1.83	13	1
4:A:333:PX4:H22	4:A:356:PX4:H53	0.51	1.81	1	1
4:A:360:PX4:H28	4:A:426:PX4:H70	0.51	1.83	2	1
4:A:330:PX4:H46	4:A:331:PX4:H9	0.51	1.83	4	1
4:A:392:PX4:H55	4:A:410:PX4:H68	0.51	1.82	6	1
4:A:320:PX4:O8	4:A:362:PX4:H4	0.51	2.06	12	1
4:A:328:PX4:H23	4:A:342:PX4:H59	0.51	1.82	16	1
4:A:348:PX4:H49	4:A:356:PX4:H20	0.51	1.82	18	1
4:A:369:PX4:O1	4:A:377:PX4:H18	0.51	2.06	20	1
4:A:362:PX4:H34	4:A:362:PX4:H63	0.51	1.83	3	1
4:A:341:PX4:H50	4:A:350:PX4:H54	0.51	1.82	5	1
4:A:313:PX4:H33	4:A:354:PX4:H52	0.51	1.83	7	1
4:A:383:PX4:H38	4:A:389:PX4:C25	0.51	2.36	10	1
4:A:350:PX4:H44	4:A:390:PX4:H70	0.51	1.81	11	1
4:A:391:PX4:H27	4:A:400:PX4:H52	0.51	1.83	11	1
4:A:394:PX4:H7	4:A:395:PX4:H18	0.51	1.82	12	1
4:A:335:PX4:H55	4:A:342:PX4:H17	0.51	1.83	14	1
4:A:306:PX4:H61	4:A:313:PX4:H48	0.51	1.82	15	1
4:A:336:PX4:H28	4:A:358:PX4:H63	0.51	1.83	16	1
4:A:406:PX4:H32	4:A:409:PX4:H31	0.51	1.81	17	1
4:A:337:PX4:H70	4:A:402:PX4:H38	0.50	1.83	1	1
4:A:346:PX4:H13	4:A:347:PX4:O4	0.50	2.05	3	1
4:A:374:PX4:H30	4:A:398:PX4:H29	0.50	1.84	5	1
4:A:346:PX4:H32	4:A:346:PX4:H55	0.50	1.82	6	1
4:A:347:PX4:H19	4:A:355:PX4:H51	0.50	1.82	9	1
4:A:396:PX4:H39	4:A:414:PX4:H57	0.50	1.83	12	1
4:A:348:PX4:H58	4:A:356:PX4:H30	0.50	1.83	13	1
4:A:329:PX4:H49	4:A:336:PX4:H5	0.50	1.82	15	1
4:A:420:PX4:H26	4:A:428:PX4:H31	0.50	1.83	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:369:PX4:H40	4:A:391:PX4:H64	0.50	1.82	3	1
4:A:324:PX4:C22	4:A:375:PX4:H39	0.50	2.36	4	1
4:A:398:PX4:H10	4:A:398:PX4:O6	0.50	2.06	6	1
4:A:346:PX4:H20	4:A:347:PX4:H14	0.50	1.81	9	1
4:A:321:PX4:H51	4:A:335:PX4:H23	0.50	1.83	13	1
4:A:408:PX4:H48	4:A:415:PX4:H55	0.50	1.84	14	1
4:A:394:PX4:H61	4:A:394:PX4:H28	0.50	1.82	16	1
4:A:337:PX4:H20	4:A:345:PX4:H55	0.50	1.84	18	1
4:A:349:PX4:H55	4:A:363:PX4:H49	0.50	1.83	20	1
4:A:393:PX4:H50	4:A:402:PX4:H27	0.50	1.82	6	1
4:A:329:PX4:H16	4:A:351:PX4:H47	0.50	1.83	7	2
4:A:407:PX4:H32	4:A:423:PX4:H34	0.50	1.82	7	1
4:A:305:PX4:O6	4:A:362:PX4:H15	0.50	2.06	8	1
4:A:347:PX4:H43	4:A:388:PX4:H66	0.50	1.84	13	1
4:A:327:PX4:H36	4:A:360:PX4:H29	0.50	1.83	18	1
4:A:328:PX4:H44	4:A:342:PX4:H63	0.50	1.81	19	1
4:A:413:PX4:H50	4:A:431:PX4:H51	0.50	1.84	4	1
4:A:377:PX4:H33	4:A:378:PX4:H30	0.50	1.83	6	1
4:A:362:PX4:H71	4:A:411:PX4:H40	0.50	1.83	10	1
4:A:317:PX4:H41	4:A:382:PX4:H43	0.50	1.83	11	1
4:A:409:PX4:H28	4:A:416:PX4:H55	0.50	1.82	15	1
4:A:375:PX4:H15	4:A:421:PX4:H20	0.50	1.82	16	1
4:A:307:PX4:H60	4:A:310:PX4:H20	0.50	1.83	18	1
4:A:386:PX4:H72	4:A:402:PX4:H38	0.50	1.81	19	1
4:A:391:PX4:H28	4:A:425:PX4:H52	0.50	1.84	2	1
4:A:311:PX4:H64	4:A:412:PX4:H34	0.50	1.83	5	1
4:A:313:PX4:H5	4:A:348:PX4:O2	0.50	2.07	8	1
4:A:407:PX4:H18	4:A:422:PX4:H15	0.50	1.84	12	1
4:A:424:PX4:H46	4:A:430:PX4:H19	0.50	1.83	15	1
4:A:397:PX4:H41	4:A:398:PX4:H34	0.50	1.83	16	1
4:A:413:PX4:H17	4:A:421:PX4:H46	0.50	1.83	17	1
4:A:419:PX4:H71	4:A:419:PX4:H45	0.50	1.84	19	1
4:A:312:PX4:H16	4:A:319:PX4:H53	0.50	1.82	20	1
4:A:349:PX4:H66	4:A:382:PX4:H45	0.50	1.84	20	1
4:A:404:PX4:H71	4:A:422:PX4:H45	0.50	1.83	20	1
4:A:424:PX4:O8	4:A:430:PX4:H4	0.50	2.07	3	1
1:A:194:HIS:CD2	1:A:198:HIS:CE1	0.50	3.00	8	4
4:A:331:PX4:O6	4:A:339:PX4:H4	0.50	2.06	6	1
4:A:372:PX4:O2	4:A:428:PX4:H4	0.50	2.07	10	1
4:A:339:PX4:H16	4:A:355:PX4:H55	0.50	1.82	11	1
4:A:308:PX4:H71	4:A:340:PX4:H27	0.50	1.83	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:338:PX4:H31	4:A:346:PX4:H34	0.50	1.84	20	1
4:A:345:PX4:H38	4:A:352:PX4:H72	0.50	1.84	20	1
4:A:307:PX4:H42	4:A:403:PX4:H55	0.50	1.82	1	1
4:A:333:PX4:H29	4:A:355:PX4:H62	0.50	1.84	1	1
4:A:374:PX4:O6	4:A:398:PX4:H14	0.50	2.07	2	1
4:A:321:PX4:H52	4:A:335:PX4:H25	0.50	1.83	5	1
4:A:344:PX4:H34	4:A:345:PX4:H66	0.50	1.82	5	1
4:A:359:PX4:H59	4:A:364:PX4:H50	0.50	1.83	5	1
4:A:399:PX4:H26	4:A:408:PX4:H14	0.50	1.82	7	1
4:A:417:PX4:H64	4:A:427:PX4:H69	0.50	1.83	8	1
4:A:305:PX4:H56	4:A:361:PX4:H62	0.50	1.84	14	1
4:A:349:PX4:H41	4:A:405:PX4:H67	0.50	1.84	14	1
4:A:384:PX4:H67	4:A:393:PX4:H42	0.50	1.84	17	1
4:A:413:PX4:H37	4:A:428:PX4:H31	0.50	1.82	17	1
4:A:318:PX4:H60	4:A:403:PX4:H44	0.50	1.83	18	1
4:A:382:PX4:H26	4:A:385:PX4:H53	0.50	1.83	18	1
4:A:351:PX4:H42	4:A:391:PX4:H44	0.50	1.83	19	1
4:A:387:PX4:H63	4:A:395:PX4:H56	0.50	1.84	11	1
4:A:318:PX4:O2	4:A:324:PX4:H7	0.50	2.07	12	1
4:A:384:PX4:H57	4:A:400:PX4:H27	0.50	1.84	14	1
4:A:307:PX4:H5	4:A:310:PX4:H48	0.50	1.84	15	1
4:A:388:PX4:H35	4:A:393:PX4:H40	0.50	1.82	15	1
4:A:338:PX4:O2	4:A:346:PX4:H3	0.50	2.06	16	1
4:A:318:PX4:H26	4:A:319:PX4:H48	0.50	1.83	17	1
4:A:320:PX4:H51	4:A:327:PX4:H26	0.50	1.84	18	1
4:A:380:PX4:H69	4:A:381:PX4:H38	0.50	1.84	2	1
4:A:406:PX4:H8	4:A:409:PX4:H16	0.50	1.82	2	1
4:A:360:PX4:H60	4:A:360:PX4:H28	0.50	1.84	3	1
4:A:332:PX4:O8	4:A:340:PX4:H13	0.50	2.06	5	1
4:A:373:PX4:H57	4:A:382:PX4:H34	0.50	1.84	6	1
4:A:370:PX4:C9	4:A:419:PX4:H47	0.50	2.37	9	1
4:A:334:PX4:H56	4:A:341:PX4:H16	0.50	1.83	10	1
4:A:326:PX4:H28	4:A:343:PX4:H63	0.50	1.84	12	1
4:A:379:PX4:H52	4:A:381:PX4:H23	0.50	1.84	17	1
4:A:328:PX4:H25	4:A:342:PX4:H50	0.50	1.83	19	1
4:A:334:PX4:H48	4:A:343:PX4:H23	0.50	1.82	20	1
4:A:329:PX4:H25	4:A:342:PX4:H33	0.49	1.84	3	1
4:A:399:PX4:H16	4:A:408:PX4:H46	0.49	1.84	10	2
4:A:373:PX4:H32	4:A:421:PX4:H28	0.49	1.83	5	1
4:A:338:PX4:H24	4:A:347:PX4:H61	0.49	1.84	8	1
4:A:410:PX4:H53	4:A:417:PX4:H42	0.49	1.81	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:348:PX4:H66	4:A:356:PX4:H35	0.49	1.82	12	1
4:A:401:PX4:H60	4:A:417:PX4:H54	0.49	1.83	12	1
4:A:388:PX4:H32	4:A:402:PX4:H32	0.49	1.83	13	1
4:A:316:PX4:H32	4:A:325:PX4:H67	0.49	1.83	17	1
4:A:343:PX4:H50	4:A:353:PX4:H26	0.49	1.84	17	1
4:A:390:PX4:H15	4:A:399:PX4:O1	0.49	2.07	20	1
4:A:378:PX4:H48	4:A:380:PX4:H21	0.49	1.83	1	1
4:A:312:PX4:H50	4:A:317:PX4:H20	0.49	1.82	5	1
4:A:347:PX4:H44	4:A:355:PX4:H35	0.49	1.82	8	1
4:A:371:PX4:H72	4:A:388:PX4:H37	0.49	1.82	11	1
4:A:359:PX4:H69	4:A:364:PX4:H61	0.49	1.84	1	1
4:A:413:PX4:H33	4:A:428:PX4:H33	0.49	1.83	4	1
4:A:320:PX4:H49	4:A:362:PX4:H46	0.49	1.83	13	1
4:A:376:PX4:H42	4:A:390:PX4:H42	0.49	1.84	15	1
4:A:370:PX4:H16	4:A:425:PX4:H46	0.49	1.83	16	1
4:A:347:PX4:H70	4:A:378:PX4:H70	0.49	1.82	18	1
4:A:348:PX4:H28	4:A:349:PX4:H22	0.49	1.84	19	1
4:A:371:PX4:H63	4:A:412:PX4:H20	0.49	1.84	4	1
4:A:349:PX4:H43	4:A:415:PX4:H43	0.49	1.82	7	1
4:A:333:PX4:H21	4:A:356:PX4:H61	0.49	1.84	9	1
4:A:330:PX4:H56	4:A:330:PX4:H30	0.49	1.84	13	2
4:A:388:PX4:H70	4:A:395:PX4:H72	0.49	1.83	15	1
4:A:384:PX4:H22	4:A:400:PX4:H49	0.49	1.83	16	1
4:A:321:PX4:H22	4:A:330:PX4:O5	0.49	2.08	20	1
4:A:347:PX4:H39	4:A:355:PX4:H69	0.49	1.85	20	1
4:A:313:PX4:O6	4:A:356:PX4:H23	0.49	2.07	3	1
4:A:321:PX4:H22	4:A:335:PX4:H23	0.49	1.85	7	1
4:A:348:PX4:H19	4:A:349:PX4:H9	0.49	1.85	7	1
4:A:319:PX4:H56	4:A:359:PX4:H23	0.49	1.84	9	1
4:A:313:PX4:H33	4:A:314:PX4:H22	0.49	1.84	10	1
4:A:381:PX4:H30	4:A:381:PX4:H59	0.49	1.85	11	1
4:A:310:PX4:H27	4:A:311:PX4:H35	0.49	1.84	1	1
4:A:377:PX4:H50	4:A:391:PX4:H46	0.49	1.83	1	1
4:A:364:PX4:H60	4:A:414:PX4:H43	0.49	1.84	6	1
4:A:423:PX4:H48	4:A:426:PX4:H47	0.49	1.85	11	1
4:A:333:PX4:H50	4:A:348:PX4:H48	0.49	1.84	13	1
4:A:311:PX4:O2	4:A:364:PX4:H9	0.49	2.08	15	1
4:A:338:PX4:H59	4:A:351:PX4:H32	0.49	1.83	15	1
4:A:391:PX4:H29	4:A:425:PX4:H63	0.49	1.83	18	1
4:A:387:PX4:H59	4:A:395:PX4:H59	0.49	1.85	19	1
4:A:323:PX4:H47	4:A:339:PX4:H5	0.49	1.84	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:369:PX4:H9	4:A:370:PX4:O2	0.49	2.07	5	1
4:A:346:PX4:H64	4:A:347:PX4:H30	0.49	1.83	7	1
4:A:305:PX4:H8	4:A:365:PX4:O6	0.49	2.06	8	1
4:A:381:PX4:H22	4:A:395:PX4:C27	0.49	2.33	9	1
4:A:371:PX4:H64	4:A:403:PX4:H53	0.49	1.83	11	1
4:A:339:PX4:O1	4:A:355:PX4:H11	0.49	2.08	19	2
4:A:388:PX4:H23	4:A:412:PX4:H61	0.49	1.83	14	1
4:A:376:PX4:H16	4:A:383:PX4:H48	0.49	1.83	19	1
4:A:420:PX4:H7	4:A:420:PX4:H15	0.49	1.85	1	1
4:A:309:PX4:H28	4:A:406:PX4:H41	0.49	1.85	2	1
4:A:384:PX4:O6	4:A:408:PX4:H8	0.49	2.08	2	1
4:A:392:PX4:H50	4:A:409:PX4:H58	0.49	1.84	2	1
4:A:337:PX4:H55	4:A:354:PX4:H19	0.49	1.84	3	2
4:A:404:PX4:H9	4:A:420:PX4:O3	0.49	2.07	4	1
4:A:371:PX4:H52	4:A:404:PX4:H25	0.49	1.85	5	1
4:A:386:PX4:O1	4:A:387:PX4:H9	0.49	2.08	7	1
4:A:399:PX4:H61	4:A:425:PX4:H35	0.49	1.84	7	1
4:A:377:PX4:H46	4:A:386:PX4:H12	0.49	1.85	8	1
4:A:329:PX4:H40	4:A:338:PX4:H60	0.49	1.84	11	1
4:A:337:PX4:H62	4:A:339:PX4:H37	0.49	1.85	17	1
4:A:392:PX4:H36	4:A:393:PX4:H60	0.49	1.85	17	1
4:A:337:PX4:H19	4:A:344:PX4:C26	0.49	2.36	18	1
4:A:425:PX4:H17	4:A:430:PX4:H14	0.49	1.85	3	2
4:A:313:PX4:H26	4:A:354:PX4:C26	0.49	2.25	5	1
4:A:376:PX4:H52	4:A:430:PX4:H17	0.49	1.83	5	1
4:A:309:PX4:H26	4:A:366:PX4:H50	0.49	1.84	7	1
4:A:377:PX4:O8	4:A:387:PX4:H8	0.49	2.08	7	1
4:A:402:PX4:H66	4:A:418:PX4:H42	0.49	1.84	8	1
4:A:316:PX4:H38	4:A:317:PX4:H18	0.49	1.84	9	1
4:A:305:PX4:H36	4:A:361:PX4:H62	0.49	1.85	10	1
4:A:326:PX4:H49	4:A:343:PX4:H17	0.49	1.84	12	1
4:A:314:PX4:H45	4:A:365:PX4:H59	0.49	1.84	15	1
4:A:320:PX4:H32	4:A:321:PX4:H56	0.49	1.83	18	1
4:A:330:PX4:H55	4:A:331:PX4:H51	0.49	1.83	18	1
4:A:332:PX4:H29	4:A:340:PX4:H48	0.49	1.84	20	1
4:A:305:PX4:H16	4:A:328:PX4:H6	0.49	1.85	1	1
4:A:399:PX4:O6	4:A:408:PX4:H9	0.49	2.07	1	1
4:A:362:PX4:H19	4:A:365:PX4:H16	0.49	1.85	6	1
4:A:389:PX4:H3	4:A:403:PX4:H2	0.49	1.85	8	1
4:A:354:PX4:H35	4:A:355:PX4:H69	0.49	1.84	9	1
4:A:390:PX4:H36	4:A:429:PX4:H38	0.49	1.85	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:418:PX4:H17	4:A:427:PX4:H22	0.49	1.85	11	1
4:A:381:PX4:H48	4:A:387:PX4:H31	0.49	1.85	12	1
4:A:336:PX4:H51	4:A:366:PX4:H50	0.49	1.85	13	1
4:A:329:PX4:H54	4:A:336:PX4:H19	0.49	1.84	14	1
4:A:330:PX4:H71	4:A:335:PX4:H42	0.48	1.84	1	1
4:A:318:PX4:H67	4:A:332:PX4:H60	0.48	1.83	3	1
4:A:338:PX4:H18	4:A:338:PX4:H13	0.48	1.85	4	1
4:A:373:PX4:H61	4:A:380:PX4:H59	0.48	1.85	8	1
4:A:369:PX4:H20	4:A:369:PX4:H53	0.48	1.84	11	1
4:A:360:PX4:H20	4:A:367:PX4:H49	0.48	1.85	12	1
4:A:399:PX4:H2	4:A:408:PX4:H6	0.48	1.84	13	1
4:A:388:PX4:H57	4:A:412:PX4:H54	0.48	1.83	15	1
4:A:350:PX4:H61	4:A:363:PX4:H61	0.48	1.84	16	1
4:A:353:PX4:H48	4:A:362:PX4:H50	0.48	1.84	16	1
4:A:401:PX4:O6	4:A:418:PX4:H10	0.48	2.08	16	1
4:A:316:PX4:H49	4:A:341:PX4:H61	0.48	1.85	8	1
4:A:336:PX4:H41	4:A:384:PX4:H37	0.48	1.84	10	1
4:A:369:PX4:H48	4:A:425:PX4:H55	0.48	1.84	10	1
4:A:339:PX4:H53	4:A:355:PX4:H56	0.48	1.84	15	1
4:A:344:PX4:H40	4:A:401:PX4:H39	0.48	1.84	7	1
4:A:396:PX4:H30	4:A:414:PX4:H55	0.48	1.84	7	1
4:A:390:PX4:H22	4:A:430:PX4:H52	0.48	1.86	8	1
4:A:396:PX4:H23	4:A:396:PX4:H57	0.48	1.84	8	1
4:A:305:PX4:O8	4:A:362:PX4:H11	0.48	2.08	9	1
4:A:320:PX4:H38	4:A:328:PX4:H36	0.48	1.84	10	1
4:A:379:PX4:H62	4:A:380:PX4:H38	0.48	1.86	10	1
4:A:370:PX4:O1	4:A:426:PX4:H10	0.48	2.09	12	1
4:A:403:PX4:H48	4:A:412:PX4:H57	0.48	1.85	16	1
4:A:306:PX4:H23	4:A:314:PX4:H49	0.48	1.85	17	1
4:A:400:PX4:H8	4:A:425:PX4:H23	0.48	1.85	1	1
4:A:319:PX4:H26	4:A:327:PX4:H61	0.48	1.85	2	1
4:A:306:PX4:H24	4:A:314:PX4:H19	0.48	1.84	3	1
4:A:359:PX4:H20	4:A:367:PX4:H9	0.48	1.85	3	1
4:A:306:PX4:H4	4:A:354:PX4:O3	0.48	2.07	8	1
4:A:388:PX4:H18	4:A:395:PX4:O7	0.48	2.08	10	1
4:A:396:PX4:O2	4:A:414:PX4:H7	0.48	2.09	10	1
4:A:381:PX4:O8	4:A:382:PX4:H11	0.48	2.08	11	2
4:A:391:PX4:H19	4:A:425:PX4:H23	0.48	1.85	11	1
1:A:93:ILE:HD12	1:A:93:ILE:N	0.48	2.24	18	1
4:A:307:PX4:H12	4:A:307:PX4:H15	0.48	1.84	19	1
4:A:384:PX4:H35	4:A:400:PX4:H30	0.48	1.84	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:320:PX4:H49	4:A:362:PX4:H50	0.48	1.83	20	1
4:A:425:PX4:C13	4:A:430:PX4:H21	0.48	2.36	20	1
4:A:375:PX4:H56	4:A:382:PX4:H26	0.48	1.85	2	1
4:A:326:PX4:C6	4:A:343:PX4:H15	0.48	2.37	4	1
4:A:399:PX4:O6	4:A:408:PX4:H3	0.48	2.07	9	1
4:A:348:PX4:H4	4:A:349:PX4:O1	0.48	2.09	11	1
4:A:322:PX4:H48	4:A:332:PX4:H55	0.48	1.84	14	1
4:A:334:PX4:C9	4:A:334:PX4:H3	0.48	2.39	14	1
4:A:317:PX4:H52	4:A:343:PX4:H25	0.48	1.85	16	1
4:A:374:PX4:H10	4:A:374:PX4:O4	0.48	2.07	18	1
4:A:336:PX4:H19	4:A:351:PX4:H57	0.48	1.85	17	2
4:A:391:PX4:H31	4:A:400:PX4:H49	0.48	1.85	3	1
4:A:314:PX4:H18	4:A:361:PX4:H18	0.48	1.85	8	1
4:A:334:PX4:H40	4:A:425:PX4:H41	0.48	1.85	10	1
4:A:309:PX4:H27	4:A:416:PX4:H43	0.48	1.86	14	1
4:A:383:PX4:H34	4:A:398:PX4:H17	0.48	1.84	17	1
4:A:318:PX4:H60	4:A:340:PX4:H23	0.48	1.85	19	1
4:A:402:PX4:H72	4:A:410:PX4:H35	0.48	1.85	19	1
4:A:305:PX4:H16	4:A:321:PX4:H55	0.48	1.84	20	1
4:A:336:PX4:H46	4:A:344:PX4:H12	0.48	1.85	20	1
4:A:407:PX4:H28	4:A:423:PX4:H30	0.48	1.85	7	1
4:A:324:PX4:H63	4:A:339:PX4:H57	0.48	1.86	9	1
4:A:369:PX4:H63	4:A:391:PX4:H51	0.48	1.86	10	1
4:A:369:PX4:H14	4:A:370:PX4:H21	0.48	1.86	17	1
4:A:333:PX4:H11	4:A:339:PX4:O8	0.48	2.09	18	1
4:A:392:PX4:P1	4:A:409:PX4:H11	0.48	2.48	19	1
1:A:98:ARG:NH2	4:A:331:PX4:O1	0.48	2.46	20	1
4:A:412:PX4:H67	4:A:389:PX4:H41	0.48	1.85	1	1
4:A:379:PX4:H37	4:A:427:PX4:H68	0.48	1.86	2	1
4:A:406:PX4:H10	4:A:416:PX4:O6	0.48	2.08	3	1
4:A:387:PX4:O6	4:A:387:PX4:H7	0.48	2.09	6	1
4:A:320:PX4:H42	4:A:351:PX4:H42	0.48	1.84	7	1
4:A:308:PX4:H19	4:A:315:PX4:H49	0.48	1.86	8	1
4:A:321:PX4:H49	4:A:332:PX4:H19	0.48	1.85	14	1
4:A:331:PX4:H64	4:A:347:PX4:H60	0.48	1.85	15	1
4:A:335:PX4:H64	4:A:341:PX4:H29	0.48	1.84	15	1
4:A:327:PX4:H55	4:A:360:PX4:H24	0.48	1.86	18	1
4:A:355:PX4:H25	4:A:356:PX4:H47	0.48	1.84	19	1
4:A:374:PX4:H27	4:A:383:PX4:H54	0.48	1.84	9	1
4:A:420:PX4:H22	4:A:428:PX4:H22	0.48	1.84	16	1
4:A:306:PX4:H17	4:A:313:PX4:H24	0.48	1.85	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:334:PX4:H59	4:A:341:PX4:H27	0.48	1.86	17	1
4:A:382:PX4:H58	4:A:395:PX4:H60	0.48	1.85	1	1
1:A:22:PHE:CE2	1:A:66:ARG:CZ	0.48	2.96	3	1
4:A:361:PX4:H58	4:A:362:PX4:H32	0.48	1.86	3	1
4:A:370:PX4:H60	4:A:426:PX4:H32	0.48	1.84	5	1
4:A:344:PX4:H30	4:A:345:PX4:H30	0.48	1.86	6	1
4:A:348:PX4:H35	4:A:363:PX4:C28	0.48	2.37	8	1
4:A:394:PX4:H66	4:A:400:PX4:C17	0.48	2.39	8	1
4:A:372:PX4:H45	4:A:429:PX4:H60	0.48	1.86	14	1
4:A:352:PX4:H47	4:A:365:PX4:H25	0.48	1.86	15	1
4:A:329:PX4:H68	4:A:337:PX4:H23	0.48	1.85	16	1
4:A:375:PX4:H5	4:A:421:PX4:O6	0.48	2.09	17	1
4:A:325:PX4:H16	4:A:349:PX4:H51	0.48	1.85	19	1
4:A:326:PX4:H17	4:A:326:PX4:H10	0.47	1.86	1	1
4:A:369:PX4:H57	4:A:391:PX4:H46	0.47	1.86	2	1
4:A:330:PX4:H68	4:A:342:PX4:H72	0.47	1.83	4	1
4:A:371:PX4:H69	4:A:389:PX4:H59	0.47	1.86	6	1
4:A:324:PX4:H71	4:A:331:PX4:H34	0.47	1.86	10	1
4:A:381:PX4:H66	4:A:385:PX4:H64	0.47	1.85	12	1
4:A:413:PX4:H37	4:A:428:PX4:H32	0.47	1.86	12	1
4:A:407:PX4:H29	4:A:423:PX4:H20	0.47	1.86	16	1
4:A:381:PX4:H25	4:A:382:PX4:H48	0.47	1.85	18	1
4:A:384:PX4:H6	4:A:393:PX4:O2	0.47	2.08	20	1
4:A:335:PX4:H20	4:A:342:PX4:H46	0.47	1.85	1	1
4:A:366:PX4:H35	4:A:409:PX4:H40	0.47	1.86	1	1
4:A:312:PX4:H49	4:A:318:PX4:H19	0.47	1.86	3	1
4:A:383:PX4:H30	4:A:389:PX4:H17	0.47	1.85	3	1
4:A:306:PX4:H27	4:A:314:PX4:H47	0.47	1.84	4	1
4:A:308:PX4:H37	4:A:315:PX4:H23	0.47	1.84	6	1
4:A:376:PX4:H64	4:A:430:PX4:H67	0.47	1.86	7	1
4:A:424:PX4:H46	4:A:430:PX4:H23	0.47	1.86	10	1
4:A:425:PX4:H10	4:A:425:PX4:H17	0.47	1.86	12	1
4:A:348:PX4:H19	4:A:349:PX4:C9	0.47	2.39	14	1
4:A:420:PX4:H22	4:A:428:PX4:C11	0.47	2.39	16	1
4:A:327:PX4:H59	4:A:360:PX4:H27	0.47	1.85	18	1
4:A:321:PX4:H40	4:A:347:PX4:H63	0.47	1.86	19	1
4:A:346:PX4:H42	4:A:346:PX4:H66	0.47	1.85	19	1
4:A:360:PX4:H60	4:A:360:PX4:C14	0.47	2.39	3	1
4:A:384:PX4:H56	4:A:393:PX4:H25	0.47	1.86	4	1
4:A:404:PX4:H25	4:A:412:PX4:H19	0.47	1.86	4	1
4:A:331:PX4:H50	4:A:347:PX4:H24	0.47	1.85	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:380:PX4:H52	4:A:385:PX4:H46	0.47	1.87	9	1
4:A:329:PX4:H13	4:A:338:PX4:O6	0.47	2.09	12	1
4:A:330:PX4:H28	4:A:331:PX4:H32	0.47	1.85	14	1
4:A:341:PX4:H51	4:A:350:PX4:H14	0.47	1.87	15	1
4:A:362:PX4:H20	4:A:365:PX4:H16	0.47	1.87	16	1
4:A:348:PX4:H12	4:A:349:PX4:H22	0.47	1.84	18	1
4:A:366:PX4:O6	4:A:366:PX4:H12	0.47	2.08	18	1
4:A:370:PX4:H49	4:A:424:PX4:H59	0.47	1.85	18	1
4:A:389:PX4:O6	4:A:403:PX4:H7	0.47	2.10	3	1
4:A:309:PX4:H68	4:A:357:PX4:H33	0.47	1.86	4	1
4:A:305:PX4:H27	4:A:362:PX4:H54	0.47	1.86	6	1
4:A:363:PX4:H43	4:A:405:PX4:H42	0.47	1.85	6	1
4:A:336:PX4:H43	4:A:400:PX4:H62	0.47	1.84	9	1
4:A:341:PX4:H45	4:A:408:PX4:H65	0.47	1.86	14	1
4:A:406:PX4:O2	4:A:415:PX4:H14	0.47	2.09	16	1
4:A:318:PX4:H47	4:A:323:PX4:H49	0.47	1.85	19	1
4:A:386:PX4:H36	4:A:387:PX4:H57	0.47	1.86	19	1
4:A:370:PX4:H47	4:A:419:PX4:H19	0.47	1.85	20	1
4:A:399:PX4:H31	4:A:409:PX4:H53	0.47	1.87	2	1
4:A:321:PX4:H37	4:A:347:PX4:H58	0.47	1.86	10	1
4:A:413:PX4:O6	4:A:428:PX4:H11	0.47	2.10	10	1
4:A:328:PX4:H25	4:A:335:PX4:H57	0.47	1.85	11	1
4:A:332:PX4:H29	4:A:340:PX4:H26	0.47	1.87	15	1
4:A:329:PX4:H17	4:A:338:PX4:H17	0.47	1.86	16	1
4:A:401:PX4:H30	4:A:410:PX4:H39	0.47	1.86	16	1
4:A:337:PX4:H23	4:A:337:PX4:H57	0.47	1.85	3	2
4:A:403:PX4:H52	4:A:405:PX4:H53	0.47	1.85	3	1
4:A:349:PX4:H21	4:A:363:PX4:H17	0.47	1.86	6	1
4:A:327:PX4:H40	4:A:343:PX4:H63	0.47	1.87	8	1
4:A:369:PX4:H49	4:A:370:PX4:H26	0.47	1.86	8	1
4:A:376:PX4:H21	4:A:383:PX4:H21	0.47	1.85	8	1
4:A:342:PX4:H14	4:A:342:PX4:H13	0.47	1.86	10	1
4:A:374:PX4:C10	4:A:383:PX4:H16	0.47	2.37	10	1
4:A:394:PX4:H64	4:A:400:PX4:H38	0.47	1.87	13	1
4:A:357:PX4:H38	4:A:408:PX4:H62	0.47	1.87	14	1
4:A:305:PX4:H47	4:A:362:PX4:H52	0.47	1.85	19	1
4:A:311:PX4:H56	4:A:315:PX4:H31	0.47	1.85	20	1
4:A:321:PX4:H34	4:A:330:PX4:H57	0.47	1.87	20	1
4:A:344:PX4:O6	4:A:344:PX4:H4	0.47	2.09	20	1
4:A:361:PX4:H36	4:A:364:PX4:H33	0.47	1.87	20	1
4:A:339:PX4:H44	4:A:381:PX4:H66	0.47	1.86	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:405:PX4:H15	4:A:414:PX4:O4	0.47	2.09	11	2
4:A:314:PX4:O2	4:A:354:PX4:H11	0.47	2.09	3	1
4:A:316:PX4:H50	4:A:317:PX4:H50	0.47	1.86	5	1
4:A:419:PX4:H35	4:A:426:PX4:H58	0.47	1.86	5	1
4:A:306:PX4:H60	4:A:313:PX4:H57	0.47	1.85	7	1
4:A:320:PX4:H61	4:A:362:PX4:H58	0.47	1.85	7	1
4:A:380:PX4:H24	4:A:411:PX4:H52	0.47	1.86	7	1
4:A:321:PX4:H31	4:A:335:PX4:H38	0.47	1.86	8	1
4:A:318:PX4:H43	4:A:422:PX4:H67	0.47	1.87	9	1
4:A:328:PX4:H19	4:A:342:PX4:H61	0.47	1.86	10	1
4:A:375:PX4:H9	4:A:429:PX4:O4	0.47	2.08	10	1
4:A:387:PX4:H58	4:A:388:PX4:H68	0.47	1.87	10	1
4:A:361:PX4:H43	4:A:411:PX4:H64	0.47	1.87	11	1
4:A:406:PX4:H38	4:A:417:PX4:H33	0.47	1.86	11	1
4:A:337:PX4:H47	4:A:346:PX4:H23	0.47	1.86	12	1
4:A:375:PX4:H16	4:A:382:PX4:H24	0.47	1.85	13	1
4:A:377:PX4:H54	4:A:378:PX4:H27	0.47	1.86	13	1
4:A:310:PX4:H68	4:A:397:PX4:H44	0.47	1.86	14	1
4:A:392:PX4:H20	4:A:393:PX4:H46	0.47	1.86	14	1
4:A:392:PX4:H68	4:A:394:PX4:H45	0.47	1.86	14	1
4:A:392:PX4:H55	4:A:402:PX4:H51	0.47	1.84	14	1
4:A:320:PX4:H16	4:A:328:PX4:H52	0.47	1.87	15	1
4:A:340:PX4:H69	4:A:387:PX4:H70	0.47	1.86	15	1
4:A:333:PX4:H11	4:A:339:PX4:H48	0.47	1.86	16	1
4:A:392:PX4:H57	4:A:402:PX4:H19	0.47	1.87	16	1
4:A:382:PX4:H35	4:A:421:PX4:H30	0.47	1.87	17	1
4:A:377:PX4:H69	4:A:378:PX4:H35	0.47	1.87	18	1
4:A:406:PX4:H17	4:A:415:PX4:H21	0.47	1.87	18	1
4:A:383:PX4:H19	4:A:398:PX4:H16	0.47	1.86	19	1
4:A:411:PX4:H17	4:A:411:PX4:H10	0.47	1.86	19	1
4:A:411:PX4:H18	4:A:427:PX4:H58	0.47	1.87	19	1
4:A:336:PX4:H52	4:A:352:PX4:H53	0.47	1.85	20	1
4:A:379:PX4:H28	4:A:401:PX4:H24	0.47	1.86	20	1
4:A:322:PX4:H20	4:A:332:PX4:O7	0.47	2.09	1	1
4:A:309:PX4:H24	4:A:366:PX4:H53	0.47	1.87	5	1
4:A:368:PX4:H28	4:A:429:PX4:H51	0.47	1.87	5	1
4:A:403:PX4:H58	4:A:412:PX4:H55	0.47	1.86	9	1
4:A:375:PX4:H15	4:A:375:PX4:H6	0.47	1.87	11	1
4:A:410:PX4:H25	4:A:423:PX4:H71	0.47	1.85	11	1
4:A:322:PX4:H45	4:A:332:PX4:H58	0.47	1.87	12	1
4:A:344:PX4:H23	4:A:345:PX4:H26	0.47	1.86	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:338:PX4:H40	4:A:346:PX4:H35	0.47	1.86	19	1
4:A:321:PX4:H52	4:A:328:PX4:H47	0.47	1.87	20	1
4:A:330:PX4:H32	4:A:332:PX4:H23	0.47	1.87	20	1
4:A:309:PX4:H64	4:A:363:PX4:H59	0.47	1.86	2	1
4:A:337:PX4:H52	4:A:356:PX4:H25	0.47	1.85	3	1
4:A:377:PX4:H53	4:A:395:PX4:H41	0.47	1.87	5	1
4:A:321:PX4:H41	4:A:338:PX4:H60	0.47	1.87	7	1
4:A:378:PX4:H13	4:A:385:PX4:O2	0.47	2.09	8	1
4:A:306:PX4:H7	4:A:313:PX4:O2	0.47	2.10	9	1
4:A:329:PX4:H36	4:A:358:PX4:H44	0.47	1.85	9	1
4:A:419:PX4:H23	4:A:426:PX4:H48	0.47	1.85	9	1
4:A:310:PX4:H50	4:A:363:PX4:H16	0.47	1.86	10	1
4:A:381:PX4:H27	4:A:385:PX4:H37	0.47	1.86	10	1
4:A:385:PX4:H59	4:A:387:PX4:H53	0.47	1.85	12	1
4:A:342:PX4:H20	4:A:351:PX4:O5	0.47	2.09	16	1
4:A:374:PX4:O6	4:A:398:PX4:H6	0.47	2.10	16	1
4:A:429:PX4:H61	4:A:431:PX4:H65	0.47	1.87	16	1
4:A:417:PX4:O8	4:A:419:PX4:H11	0.47	2.08	17	1
4:A:307:PX4:H17	4:A:363:PX4:O6	0.47	2.10	19	1
4:A:312:PX4:H65	4:A:319:PX4:H68	0.47	1.86	20	1
4:A:401:PX4:H16	4:A:427:PX4:H48	0.47	1.86	20	1
4:A:403:PX4:H16	4:A:412:PX4:H8	0.47	1.86	1	1
4:A:318:PX4:H17	4:A:323:PX4:H24	0.47	1.85	3	1
4:A:323:PX4:O2	4:A:324:PX4:H11	0.47	2.10	4	1
4:A:347:PX4:H22	4:A:355:PX4:H48	0.47	1.87	5	1
4:A:357:PX4:H17	4:A:358:PX4:H21	0.47	1.87	5	1
4:A:344:PX4:H56	4:A:366:PX4:H67	0.47	1.87	6	1
4:A:329:PX4:H20	4:A:347:PX4:H55	0.47	1.85	7	1
4:A:331:PX4:H17	4:A:339:PX4:H14	0.47	1.85	7	1
4:A:334:PX4:H22	4:A:353:PX4:H37	0.47	1.86	7	1
4:A:392:PX4:H27	4:A:393:PX4:H61	0.47	1.85	8	1
4:A:369:PX4:H21	4:A:377:PX4:H46	0.47	1.85	12	1
4:A:337:PX4:H45	4:A:388:PX4:H36	0.47	1.86	13	1
4:A:391:PX4:O7	4:A:400:PX4:H17	0.47	2.10	13	1
4:A:348:PX4:H16	4:A:349:PX4:H10	0.47	1.85	17	2
4:A:321:PX4:H25	4:A:335:PX4:H32	0.47	1.87	18	1
4:A:321:PX4:H32	4:A:330:PX4:H64	0.47	1.87	19	1
4:A:322:PX4:H66	4:A:372:PX4:H39	0.46	1.87	1	1
4:A:388:PX4:O6	4:A:394:PX4:H7	0.46	2.10	2	1
4:A:390:PX4:H20	4:A:430:PX4:H51	0.46	1.86	2	1
4:A:334:PX4:H27	4:A:351:PX4:H28	0.46	1.85	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:383:PX4:H57	4:A:429:PX4:H32	0.46	1.86	6	1
4:A:397:PX4:O8	4:A:398:PX4:H56	0.46	2.10	11	1
4:A:359:PX4:H19	4:A:367:PX4:H20	0.46	1.86	13	1
4:A:396:PX4:H48	4:A:422:PX4:H46	0.46	1.86	13	1
4:A:309:PX4:H67	4:A:363:PX4:H62	0.46	1.87	14	1
4:A:424:PX4:H21	4:A:425:PX4:H55	0.46	1.86	15	1
4:A:333:PX4:H34	4:A:339:PX4:H39	0.46	1.87	16	1
4:A:369:PX4:H14	4:A:370:PX4:C11	0.46	2.40	17	1
4:A:377:PX4:H47	4:A:395:PX4:H39	0.46	1.86	19	1
4:A:325:PX4:H23	4:A:333:PX4:H22	0.46	1.86	20	1
4:A:402:PX4:H22	4:A:392:PX4:H53	0.46	1.87	1	1
4:A:325:PX4:H22	4:A:333:PX4:H47	0.46	1.87	6	1
4:A:393:PX4:H51	4:A:402:PX4:H27	0.46	1.87	8	1
4:A:316:PX4:H20	4:A:325:PX4:H57	0.46	1.86	9	1
4:A:369:PX4:H69	4:A:393:PX4:H43	0.46	1.88	9	1
4:A:307:PX4:H16	4:A:311:PX4:H14	0.46	1.87	19	2
4:A:313:PX4:H62	4:A:403:PX4:H35	0.46	1.87	11	1
4:A:361:PX4:H28	4:A:427:PX4:H44	0.46	1.87	17	1
4:A:369:PX4:H55	4:A:400:PX4:H59	0.46	1.86	20	1
4:A:361:PX4:H30	4:A:365:PX4:H61	0.46	1.86	2	1
4:A:386:PX4:H57	4:A:394:PX4:H46	0.46	1.86	3	1
4:A:306:PX4:H17	4:A:313:PX4:H22	0.46	1.87	7	1
4:A:382:PX4:H38	4:A:421:PX4:H32	0.46	1.86	10	1
4:A:392:PX4:H50	4:A:409:PX4:H59	0.46	1.86	11	1
4:A:318:PX4:H69	4:A:373:PX4:H70	0.46	1.87	13	1
4:A:372:PX4:H48	4:A:421:PX4:H53	0.46	1.87	13	1
4:A:430:PX4:H2	4:A:430:PX4:O6	0.46	2.10	15	1
4:A:416:PX4:H53	4:A:417:PX4:H21	0.46	1.86	16	1
4:A:336:PX4:H66	4:A:366:PX4:H14	0.46	1.88	17	1
4:A:309:PX4:H53	4:A:357:PX4:H55	0.46	1.87	18	1
4:A:418:PX4:H19	4:A:427:PX4:H22	0.46	1.87	18	1
4:A:333:PX4:H41	4:A:347:PX4:H33	0.46	1.86	1	1
4:A:406:PX4:H36	4:A:408:PX4:H31	0.46	1.88	2	1
4:A:340:PX4:H69	4:A:382:PX4:H65	0.46	1.87	11	1
4:A:406:PX4:H25	4:A:416:PX4:H22	0.46	1.86	11	1
4:A:358:PX4:H40	4:A:399:PX4:H70	0.46	1.88	12	1
4:A:320:PX4:H16	4:A:362:PX4:H5	0.46	1.87	14	1
4:A:343:PX4:H45	4:A:390:PX4:H44	0.46	1.88	15	1
4:A:413:PX4:H20	4:A:421:PX4:H51	0.46	1.87	15	1
4:A:399:PX4:H25	4:A:408:PX4:H14	0.46	1.88	17	1
4:A:306:PX4:H31	4:A:314:PX4:H47	0.46	1.88	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:305:PX4:H29	4:A:321:PX4:H51	0.46	1.88	1	1
4:A:326:PX4:H41	4:A:424:PX4:H43	0.46	1.87	2	1
4:A:324:PX4:H24	4:A:325:PX4:H50	0.46	1.87	3	1
4:A:373:PX4:H42	4:A:421:PX4:H39	0.46	1.87	4	1
4:A:383:PX4:H45	4:A:388:PX4:H54	0.46	1.88	5	1
4:A:307:PX4:H60	4:A:311:PX4:H32	0.46	1.86	6	1
4:A:321:PX4:H26	4:A:347:PX4:H46	0.46	1.87	10	1
4:A:391:PX4:H53	4:A:400:PX4:H55	0.46	1.88	12	2
4:A:305:PX4:H18	4:A:362:PX4:H3	0.46	1.87	13	1
4:A:308:PX4:H22	4:A:359:PX4:H59	0.46	1.88	13	1
4:A:314:PX4:H31	4:A:354:PX4:H57	0.46	1.86	13	1
4:A:318:PX4:H49	4:A:340:PX4:H5	0.46	1.87	15	1
4:A:316:PX4:H31	4:A:316:PX4:H53	0.46	1.88	18	1
4:A:313:PX4:H38	4:A:306:PX4:H27	0.46	1.87	1	1
4:A:337:PX4:H23	4:A:344:PX4:H51	0.46	1.86	1	1
4:A:389:PX4:H42	4:A:404:PX4:H69	0.46	1.88	4	1
4:A:378:PX4:H8	4:A:380:PX4:O1	0.46	2.11	9	1
4:A:372:PX4:H72	4:A:379:PX4:H70	0.46	1.88	12	1
4:A:393:PX4:H29	4:A:394:PX4:H59	0.46	1.87	13	1
4:A:401:PX4:H14	4:A:410:PX4:O2	0.46	2.10	13	1
4:A:392:PX4:C10	4:A:393:PX4:H46	0.46	2.41	14	1
4:A:315:PX4:H51	4:A:318:PX4:H56	0.46	1.87	15	1
4:A:357:PX4:H54	4:A:358:PX4:H45	0.46	1.86	16	1
4:A:328:PX4:O2	4:A:335:PX4:H14	0.46	2.10	17	1
4:A:334:PX4:H38	4:A:400:PX4:H64	0.46	1.87	1	1
4:A:336:PX4:O6	4:A:358:PX4:H17	0.46	2.11	5	1
4:A:337:PX4:H48	4:A:346:PX4:H56	0.46	1.85	5	1
4:A:401:PX4:H22	4:A:410:PX4:H19	0.46	1.87	6	1
4:A:351:PX4:H70	4:A:357:PX4:H47	0.46	1.86	7	1
4:A:321:PX4:H14	4:A:330:PX4:O5	0.46	2.10	15	1
4:A:336:PX4:H72	4:A:365:PX4:H45	0.46	1.87	15	1
4:A:419:PX4:H10	4:A:426:PX4:O2	0.46	2.11	15	1
4:A:372:PX4:H19	4:A:421:PX4:H16	0.46	1.87	16	1
4:A:369:PX4:H52	4:A:425:PX4:H51	0.46	1.88	17	1
4:A:380:PX4:H2	4:A:385:PX4:O6	0.46	2.09	18	1
4:A:305:PX4:H59	4:A:305:PX4:H33	0.46	1.87	19	1
4:A:323:PX4:H58	4:A:340:PX4:H22	0.46	1.88	19	1
4:A:420:PX4:H26	4:A:428:PX4:H27	0.46	1.87	20	1
4:A:384:PX4:H52	4:A:400:PX4:H20	0.46	1.88	2	1
4:A:348:PX4:H38	4:A:349:PX4:H30	0.46	1.86	4	1
4:A:335:PX4:H58	4:A:353:PX4:H42	0.46	1.87	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:377:PX4:H59	4:A:391:PX4:H50	0.46	1.88	8	1
4:A:338:PX4:H45	4:A:347:PX4:H71	0.46	1.88	9	1
4:A:396:PX4:H11	4:A:403:PX4:O6	0.46	2.10	9	1
4:A:393:PX4:H28	4:A:394:PX4:H56	0.46	1.88	10	1
4:A:316:PX4:H3	4:A:324:PX4:O2	0.46	2.11	11	1
4:A:424:PX4:H53	4:A:430:PX4:H27	0.46	1.88	13	1
4:A:341:PX4:H55	4:A:357:PX4:H24	0.46	1.88	15	1
4:A:352:PX4:H3	4:A:365:PX4:O4	0.46	2.11	15	1
4:A:403:PX4:H34	4:A:403:PX4:H61	0.46	1.85	16	1
4:A:391:PX4:H15	4:A:400:PX4:O7	0.46	2.11	17	1
4:A:393:PX4:H65	4:A:400:PX4:H40	0.46	1.88	17	1
4:A:368:PX4:H54	4:A:430:PX4:H20	0.46	1.87	19	1
4:A:340:PX4:H59	4:A:355:PX4:H67	0.46	1.88	1	1
4:A:384:PX4:H17	4:A:393:PX4:H22	0.46	1.87	1	1
4:A:409:PX4:H71	4:A:410:PX4:H63	0.46	1.87	5	1
4:A:409:PX4:H28	4:A:417:PX4:H23	0.46	1.88	6	1
4:A:311:PX4:H32	4:A:396:PX4:H43	0.46	1.88	7	1
4:A:399:PX4:H26	4:A:408:PX4:C6	0.46	2.40	7	1
4:A:414:PX4:H10	4:A:422:PX4:O8	0.46	2.11	9	1
4:A:333:PX4:H26	4:A:339:PX4:H58	0.46	1.87	15	1
1:A:129:TRP:CD2	4:A:313:PX4:H1	0.46	2.46	16	1
4:A:337:PX4:H51	4:A:347:PX4:H22	0.46	1.88	17	1
4:A:401:PX4:H36	4:A:410:PX4:H36	0.46	1.88	18	1
4:A:371:PX4:H63	4:A:403:PX4:H49	0.46	1.87	2	1
4:A:374:PX4:H49	4:A:382:PX4:O5	0.46	2.11	2	1
4:A:337:PX4:H24	4:A:346:PX4:H35	0.46	1.87	3	1
4:A:322:PX4:H58	4:A:332:PX4:H61	0.46	1.87	5	1
4:A:392:PX4:H34	4:A:399:PX4:H39	0.46	1.87	5	1
4:A:399:PX4:C9	4:A:408:PX4:H3	0.46	2.41	6	1
4:A:329:PX4:H70	4:A:402:PX4:H39	0.46	1.88	7	1
4:A:336:PX4:H18	4:A:358:PX4:H15	0.46	1.86	7	1
4:A:328:PX4:H14	4:A:335:PX4:H21	0.46	1.87	9	1
4:A:323:PX4:H54	4:A:340:PX4:H48	0.46	1.87	11	1
4:A:381:PX4:H23	4:A:385:PX4:H41	0.46	1.88	12	1
4:A:366:PX4:H45	4:A:417:PX4:H34	0.46	1.88	15	1
4:A:417:PX4:O1	4:A:417:PX4:H17	0.46	2.11	15	1
1:A:129:TRP:CG	4:A:313:PX4:H1	0.46	2.46	16	1
4:A:329:PX4:H40	4:A:391:PX4:H67	0.46	1.88	17	1
4:A:399:PX4:H18	4:A:408:PX4:H1	0.46	1.88	17	1
4:A:318:PX4:H43	4:A:431:PX4:H38	0.46	1.87	18	1
4:A:313:PX4:H66	4:A:349:PX4:H39	0.46	1.87	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:344:PX4:H16	4:A:345:PX4:H47	0.45	1.88	1	1
4:A:336:PX4:H27	4:A:341:PX4:H26	0.45	1.87	6	1
4:A:362:PX4:H71	4:A:365:PX4:H65	0.45	1.88	6	1
4:A:313:PX4:H24	4:A:354:PX4:H55	0.45	1.87	11	1
4:A:329:PX4:H33	4:A:384:PX4:H42	0.45	1.88	13	1
4:A:358:PX4:H35	4:A:399:PX4:H68	0.45	1.86	15	1
4:A:310:PX4:H19	4:A:307:PX4:H55	0.45	1.88	1	1
4:A:390:PX4:H52	4:A:399:PX4:H15	0.45	1.87	2	1
4:A:321:PX4:H17	4:A:328:PX4:H49	0.45	1.88	4	1
4:A:321:PX4:H32	4:A:330:PX4:H63	0.45	1.87	5	1
4:A:347:PX4:H20	4:A:355:PX4:H17	0.45	1.87	7	1
4:A:405:PX4:H58	4:A:406:PX4:H59	0.45	1.87	7	1
4:A:392:PX4:H60	4:A:402:PX4:H58	0.45	1.88	8	1
4:A:331:PX4:H66	4:A:380:PX4:H43	0.45	1.87	9	1
4:A:424:PX4:H59	4:A:425:PX4:H39	0.45	1.86	9	1
4:A:306:PX4:H71	4:A:364:PX4:H39	0.45	1.88	10	1
4:A:380:PX4:O6	4:A:381:PX4:H6	0.45	2.12	10	1
4:A:375:PX4:H11	4:A:413:PX4:H54	0.45	1.87	11	1
4:A:407:PX4:H37	4:A:423:PX4:C21	0.45	2.38	13	1
4:A:327:PX4:H20	4:A:353:PX4:H52	0.45	1.88	17	1
4:A:317:PX4:H32	4:A:323:PX4:H33	0.45	1.87	18	1
4:A:390:PX4:H48	4:A:430:PX4:H59	0.45	1.88	19	1
4:A:372:PX4:H9	4:A:372:PX4:H15	0.45	1.88	20	1
4:A:391:PX4:H31	4:A:425:PX4:H56	0.45	1.89	2	1
4:A:401:PX4:H39	4:A:401:PX4:C36	0.45	2.41	2	1
1:A:12:TRP:CE3	1:A:59:ILE:HD11	0.45	2.47	6	3
4:A:407:PX4:H1	4:A:423:PX4:O1	0.45	2.10	7	1
4:A:315:PX4:H68	4:A:318:PX4:H23	0.45	1.88	8	1
4:A:373:PX4:H64	4:A:381:PX4:H34	0.45	1.87	8	1
4:A:394:PX4:H63	4:A:400:PX4:H33	0.45	1.88	8	1
4:A:313:PX4:H55	4:A:333:PX4:H53	0.45	1.89	9	1
4:A:407:PX4:O6	4:A:407:PX4:H7	0.45	2.11	10	1
4:A:319:PX4:H42	4:A:340:PX4:H45	0.45	1.88	14	1
4:A:371:PX4:H17	4:A:404:PX4:O6	0.45	2.11	15	1
4:A:308:PX4:H31	4:A:315:PX4:H26	0.45	1.89	17	1
4:A:357:PX4:H15	4:A:358:PX4:O5	0.45	2.10	17	1
4:A:374:PX4:O1	4:A:375:PX4:H15	0.45	2.11	17	1
4:A:318:PX4:O2	4:A:323:PX4:H14	0.45	2.10	2	1
4:A:358:PX4:H42	4:A:399:PX4:H64	0.45	1.87	2	1
4:A:406:PX4:H23	4:A:416:PX4:H20	0.45	1.87	2	1
4:A:337:PX4:H60	4:A:356:PX4:H32	0.45	1.87	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:389:PX4:H43	4:A:404:PX4:H25	0.45	1.89	8	1
4:A:357:PX4:H55	4:A:358:PX4:H55	0.45	1.87	12	1
4:A:384:PX4:H26	4:A:400:PX4:H21	0.45	1.86	12	1
4:A:369:PX4:H30	4:A:369:PX4:H60	0.45	1.89	13	1
4:A:311:PX4:H3	4:A:364:PX4:O8	0.45	2.12	14	1
4:A:369:PX4:H30	4:A:369:PX4:H64	0.45	1.89	15	1
4:A:374:PX4:H26	4:A:375:PX4:H29	0.45	1.89	15	1
4:A:382:PX4:H17	4:A:385:PX4:H56	0.45	1.88	19	1
4:A:316:PX4:H5	4:A:325:PX4:O6	0.45	2.11	20	1
4:A:334:PX4:H25	4:A:341:PX4:H25	0.45	1.88	20	1
4:A:380:PX4:H5	4:A:411:PX4:O8	0.45	2.11	20	1
4:A:360:PX4:H71	4:A:360:PX4:H20	0.45	1.87	2	1
4:A:335:PX4:H72	4:A:343:PX4:H68	0.45	1.89	4	1
4:A:337:PX4:H17	4:A:346:PX4:H21	0.45	1.89	7	1
4:A:349:PX4:H69	4:A:350:PX4:H66	0.45	1.87	7	1
4:A:375:PX4:H5	4:A:429:PX4:O8	0.45	2.12	7	1
4:A:322:PX4:H70	4:A:372:PX4:H37	0.45	1.88	8	1
4:A:369:PX4:C27	4:A:391:PX4:H22	0.45	2.40	10	1
4:A:370:PX4:H69	4:A:426:PX4:H34	0.45	1.89	12	1
4:A:409:PX4:H21	4:A:410:PX4:H47	0.45	1.88	16	1
4:A:361:PX4:H60	4:A:427:PX4:C22	0.45	2.41	17	1
4:A:384:PX4:H58	4:A:393:PX4:H30	0.45	1.89	17	1
4:A:405:PX4:O2	4:A:414:PX4:H6	0.45	2.11	17	1
4:A:396:PX4:H5	4:A:403:PX4:O6	0.45	2.10	18	1
4:A:378:PX4:H4	4:A:381:PX4:O3	0.45	2.12	1	1
4:A:373:PX4:H54	4:A:381:PX4:H53	0.45	1.88	3	1
4:A:347:PX4:H11	4:A:355:PX4:H17	0.45	1.89	4	1
4:A:316:PX4:H19	4:A:324:PX4:H28	0.45	1.88	5	1
4:A:370:PX4:C10	4:A:419:PX4:H51	0.45	2.38	9	1
4:A:340:PX4:H41	4:A:428:PX4:H41	0.45	1.89	14	1
4:A:403:PX4:H51	4:A:412:PX4:H52	0.45	1.87	15	1
4:A:410:PX4:H54	4:A:410:PX4:H21	0.45	1.87	15	1
4:A:425:PX4:O6	4:A:430:PX4:H16	0.45	2.11	15	1
4:A:382:PX4:H47	4:A:387:PX4:H46	0.45	1.89	19	1
4:A:377:PX4:H23	4:A:411:PX4:H25	0.45	1.88	20	1
4:A:388:PX4:H54	4:A:412:PX4:H54	0.45	1.88	3	1
4:A:369:PX4:H1	4:A:370:PX4:O2	0.45	2.11	4	1
4:A:319:PX4:H70	4:A:375:PX4:H43	0.45	1.88	5	1
4:A:337:PX4:H25	4:A:346:PX4:H35	0.45	1.88	9	1
4:A:357:PX4:C15	4:A:429:PX4:H44	0.45	2.41	9	1
4:A:310:PX4:H67	4:A:363:PX4:H24	0.45	1.88	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:338:PX4:H25	4:A:346:PX4:H21	0.45	1.87	10	1
4:A:376:PX4:H17	4:A:390:PX4:H19	0.45	1.89	10	1
4:A:411:PX4:H34	4:A:426:PX4:H35	0.45	1.88	10	1
4:A:306:PX4:H46	4:A:313:PX4:O8	0.45	2.12	11	1
4:A:329:PX4:H4	4:A:338:PX4:O1	0.45	2.11	16	1
4:A:368:PX4:H4	4:A:429:PX4:O1	0.45	2.11	18	1
4:A:405:PX4:H60	4:A:396:PX4:H27	0.45	1.87	1	1
4:A:336:PX4:H24	4:A:351:PX4:H50	0.45	1.89	5	1
4:A:313:PX4:H26	4:A:348:PX4:H60	0.45	1.88	7	1
4:A:312:PX4:H46	4:A:317:PX4:C6	0.45	2.42	10	1
4:A:340:PX4:H28	4:A:340:PX4:H9	0.45	1.88	10	1
1:A:100:LEU:HB3	1:A:104:THR:HG21	0.45	1.89	12	1
4:A:323:PX4:H15	4:A:339:PX4:H5	0.45	1.89	17	1
4:A:332:PX4:H56	4:A:410:PX4:H44	0.45	1.89	18	1
4:A:333:PX4:H55	4:A:333:PX4:H19	0.45	1.86	18	1
4:A:314:PX4:H32	4:A:345:PX4:H25	0.45	1.88	19	1
4:A:361:PX4:H46	4:A:362:PX4:H23	0.45	1.88	19	1
4:A:360:PX4:H43	4:A:401:PX4:H45	0.45	1.87	3	1
4:A:370:PX4:H53	4:A:424:PX4:H20	0.45	1.89	3	1
4:A:391:PX4:H44	4:A:400:PX4:H62	0.45	1.89	3	1
4:A:367:PX4:H45	4:A:421:PX4:H68	0.45	1.88	4	1
4:A:372:PX4:H16	4:A:373:PX4:C11	0.45	2.42	6	1
4:A:306:PX4:H21	4:A:314:PX4:H15	0.45	1.89	7	1
4:A:305:PX4:H21	4:A:328:PX4:H17	0.45	1.89	13	1
4:A:389:PX4:H3	4:A:403:PX4:O1	0.45	2.12	13	1
4:A:338:PX4:H55	4:A:346:PX4:H64	0.45	1.88	16	1
4:A:374:PX4:H24	4:A:398:PX4:H16	0.45	1.89	16	1
4:A:376:PX4:H19	4:A:383:PX4:C11	0.45	2.41	17	1
4:A:316:PX4:H19	4:A:334:PX4:C34	0.45	2.39	18	1
4:A:328:PX4:H58	4:A:342:PX4:H66	0.45	1.89	5	1
4:A:339:PX4:H33	4:A:347:PX4:H35	0.45	1.88	5	1
4:A:399:PX4:O2	4:A:408:PX4:H12	0.45	2.11	6	1
4:A:322:PX4:H37	4:A:332:PX4:H62	0.45	1.88	7	1
4:A:349:PX4:H16	4:A:363:PX4:H47	0.45	1.88	8	1
4:A:337:PX4:H40	4:A:388:PX4:H44	0.45	1.89	11	1
4:A:376:PX4:H17	4:A:390:PX4:H24	0.45	1.89	11	1
4:A:389:PX4:H24	4:A:403:PX4:H24	0.45	1.87	12	1
4:A:312:PX4:H26	4:A:327:PX4:H60	0.45	1.89	13	1
4:A:305:PX4:H22	4:A:328:PX4:H9	0.45	1.89	17	1
4:A:372:PX4:H5	4:A:380:PX4:O1	0.45	2.11	17	1
4:A:328:PX4:C30	4:A:335:PX4:H23	0.45	2.36	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:336:PX4:H22	4:A:351:PX4:H57	0.44	1.89	1	1
4:A:368:PX4:H22	4:A:368:PX4:C1	0.44	2.39	1	1
4:A:381:PX4:H34	4:A:387:PX4:H38	0.44	1.89	2	1
4:A:392:PX4:H30	4:A:394:PX4:H60	0.44	1.89	4	1
4:A:324:PX4:H51	4:A:339:PX4:H49	0.44	1.89	5	1
4:A:394:PX4:H40	4:A:402:PX4:H18	0.44	1.88	5	1
4:A:368:PX4:H65	4:A:376:PX4:H62	0.44	1.88	7	1
4:A:389:PX4:O1	4:A:398:PX4:H3	0.44	2.13	12	1
4:A:326:PX4:O1	4:A:343:PX4:H15	0.44	2.13	14	1
4:A:392:PX4:H34	4:A:393:PX4:H69	0.44	1.89	15	1
4:A:343:PX4:H30	4:A:350:PX4:H36	0.44	1.88	3	1
4:A:354:PX4:H61	4:A:354:PX4:H35	0.44	1.89	3	1
4:A:352:PX4:H27	4:A:366:PX4:H60	0.44	1.90	4	1
4:A:354:PX4:H26	4:A:356:PX4:H34	0.44	1.89	4	1
4:A:422:PX4:H59	4:A:431:PX4:H32	0.44	1.89	5	1
4:A:392:PX4:H68	4:A:394:PX4:H31	0.44	1.89	7	1
4:A:399:PX4:H23	4:A:408:PX4:H24	0.44	1.88	8	1
4:A:393:PX4:H4	4:A:402:PX4:O2	0.44	2.12	11	1
4:A:326:PX4:H4	4:A:353:PX4:O6	0.44	2.10	16	1
4:A:318:PX4:H64	4:A:332:PX4:H64	0.44	1.89	19	1
4:A:390:PX4:H17	4:A:399:PX4:H48	0.44	1.90	20	1
4:A:341:PX4:H17	4:A:350:PX4:H20	0.44	1.90	1	1
4:A:394:PX4:H34	4:A:412:PX4:H39	0.44	1.89	3	1
1:A:140:ARG:NE	1:A:175:ASP:OD1	0.44	2.46	5	1
4:A:403:PX4:H47	4:A:412:PX4:H17	0.44	1.89	5	1
4:A:376:PX4:H19	4:A:390:PX4:H31	0.44	1.90	8	1
1:A:143:HIS:CE1	1:A:145:ASP:OD2	0.44	2.69	10	1
4:A:319:PX4:H22	4:A:327:PX4:H58	0.44	1.88	11	1
4:A:379:PX4:H57	4:A:381:PX4:H32	0.44	1.89	11	1
4:A:396:PX4:H34	4:A:414:PX4:H60	0.44	1.89	11	1
4:A:329:PX4:O6	4:A:338:PX4:H11	0.44	2.13	12	1
4:A:419:PX4:H30	4:A:424:PX4:H16	0.44	1.89	14	1
4:A:329:PX4:H36	4:A:338:PX4:H67	0.44	1.90	15	1
4:A:336:PX4:H43	4:A:399:PX4:H57	0.44	1.88	15	1
4:A:368:PX4:H28	4:A:431:PX4:H53	0.44	1.88	16	1
4:A:319:PX4:H64	4:A:429:PX4:H72	0.44	1.89	17	1
4:A:316:PX4:H49	4:A:317:PX4:H46	0.44	1.89	20	1
4:A:376:PX4:H55	4:A:430:PX4:H19	0.44	1.88	1	1
4:A:348:PX4:H38	4:A:349:PX4:H33	0.44	1.89	7	1
4:A:331:PX4:H66	4:A:346:PX4:H69	0.44	1.89	10	1
4:A:378:PX4:C22	4:A:380:PX4:H35	0.44	2.41	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:327:PX4:H53	4:A:327:PX4:H5	0.44	1.89	13	1
4:A:379:PX4:O3	4:A:379:PX4:H13	0.44	2.12	14	1
4:A:312:PX4:O6	4:A:327:PX4:H12	0.44	2.12	15	1
4:A:320:PX4:H4	4:A:353:PX4:H46	0.44	1.88	15	1
4:A:377:PX4:H14	4:A:387:PX4:H11	0.44	1.89	15	1
4:A:308:PX4:H5	4:A:359:PX4:H53	0.44	1.89	19	1
4:A:306:PX4:H27	4:A:313:PX4:H22	0.44	1.88	20	1
4:A:338:PX4:H24	4:A:346:PX4:H60	0.44	1.90	20	1
4:A:332:PX4:H59	4:A:340:PX4:H24	0.44	1.88	3	1
4:A:309:PX4:H58	4:A:357:PX4:H16	0.44	1.89	6	1
4:A:380:PX4:O6	4:A:411:PX4:H14	0.44	2.13	7	1
4:A:379:PX4:H17	4:A:380:PX4:H11	0.44	1.88	8	1
4:A:369:PX4:H29	4:A:378:PX4:H29	0.44	1.88	9	1
4:A:337:PX4:H42	4:A:388:PX4:H45	0.44	1.89	14	1
4:A:306:PX4:H58	4:A:348:PX4:H63	0.44	1.88	15	1
4:A:336:PX4:H55	4:A:345:PX4:H26	0.44	1.90	16	1
4:A:405:PX4:O6	4:A:420:PX4:H17	0.44	2.12	20	1
4:A:363:PX4:H26	4:A:364:PX4:H68	0.44	1.88	4	1
4:A:368:PX4:H58	4:A:383:PX4:H63	0.44	1.88	5	1
4:A:334:PX4:H36	4:A:353:PX4:H40	0.44	1.88	6	1
4:A:375:PX4:H24	4:A:429:PX4:H24	0.44	1.89	11	1
4:A:396:PX4:H61	4:A:396:PX4:H29	0.44	1.90	11	1
4:A:387:PX4:H62	4:A:395:PX4:H52	0.44	1.90	13	1
4:A:338:PX4:H5	4:A:351:PX4:O6	0.44	2.13	15	1
4:A:331:PX4:H40	4:A:340:PX4:H68	0.44	1.90	17	1
4:A:307:PX4:H49	4:A:310:PX4:O3	0.44	2.13	18	1
4:A:315:PX4:O8	4:A:340:PX4:H5	0.44	2.13	20	1
4:A:310:PX4:H33	4:A:359:PX4:H31	0.44	1.89	1	1
4:A:315:PX4:H70	4:A:319:PX4:O8	0.44	2.12	1	1
4:A:309:PX4:H52	4:A:357:PX4:H59	0.44	1.89	2	1
4:A:422:PX4:H34	4:A:431:PX4:H44	0.44	1.89	8	1
4:A:320:PX4:H71	4:A:342:PX4:H72	0.44	1.88	10	1
4:A:319:PX4:H71	4:A:431:PX4:H71	0.44	1.89	12	1
4:A:330:PX4:H37	4:A:380:PX4:H44	0.44	1.88	12	1
4:A:359:PX4:H39	4:A:367:PX4:H64	0.44	1.88	13	1
4:A:390:PX4:H26	4:A:430:PX4:H57	0.44	1.90	14	1
4:A:419:PX4:H16	4:A:426:PX4:H19	0.44	1.89	14	1
4:A:308:PX4:H57	4:A:318:PX4:H28	0.44	1.90	15	1
4:A:314:PX4:H8	4:A:364:PX4:O6	0.44	2.13	15	1
4:A:375:PX4:H66	4:A:421:PX4:H71	0.44	1.88	18	1
4:A:411:PX4:H33	4:A:427:PX4:H67	0.44	1.90	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:305:PX4:H21	4:A:321:PX4:H71	0.44	1.88	20	1
4:A:315:PX4:H35	4:A:373:PX4:H43	0.44	1.89	1	1
4:A:399:PX4:H46	4:A:408:PX4:H57	0.44	1.89	3	1
4:A:333:PX4:H25	4:A:355:PX4:H66	0.44	1.89	6	1
4:A:326:PX4:H32	4:A:326:PX4:H64	0.44	1.90	7	1
4:A:366:PX4:H7	4:A:366:PX4:O6	0.44	2.13	7	1
4:A:333:PX4:H3	4:A:339:PX4:H70	0.44	1.89	8	1
4:A:385:PX4:O1	4:A:387:PX4:H14	0.44	2.13	9	1
4:A:348:PX4:H51	4:A:348:PX4:H57	0.44	1.52	12	1
4:A:419:PX4:H27	4:A:426:PX4:H55	0.44	1.88	14	1
4:A:347:PX4:H13	4:A:355:PX4:H18	0.44	1.90	16	1
4:A:388:PX4:H16	4:A:395:PX4:H50	0.44	1.90	17	1
4:A:333:PX4:H32	4:A:339:PX4:H61	0.44	1.90	3	1
4:A:372:PX4:H19	4:A:421:PX4:O8	0.44	2.13	5	1
4:A:417:PX4:H68	4:A:427:PX4:H69	0.44	1.90	6	1
4:A:376:PX4:H55	4:A:430:PX4:H61	0.44	1.88	8	1
4:A:378:PX4:H34	4:A:385:PX4:H30	0.44	1.90	9	1
4:A:315:PX4:H49	4:A:322:PX4:H50	0.44	1.88	10	1
4:A:322:PX4:H42	4:A:323:PX4:H65	0.44	1.89	10	1
4:A:404:PX4:H62	4:A:404:PX4:H57	0.44	1.35	10	1
4:A:324:PX4:H60	4:A:339:PX4:H22	0.44	1.89	12	1
4:A:413:PX4:H64	4:A:429:PX4:H47	0.44	1.89	12	1
4:A:377:PX4:H62	4:A:378:PX4:H35	0.44	1.90	13	1
4:A:337:PX4:H41	4:A:354:PX4:H43	0.44	1.90	14	1
4:A:430:PX4:H42	4:A:430:PX4:H35	0.44	1.37	16	1
4:A:320:PX4:H46	4:A:353:PX4:H52	0.44	1.90	18	1
4:A:384:PX4:H53	4:A:386:PX4:H46	0.44	1.89	18	1
4:A:318:PX4:H8	4:A:324:PX4:H21	0.44	1.89	19	1
4:A:413:PX4:H60	4:A:413:PX4:H67	0.43	1.52	1	1
4:A:346:PX4:H63	4:A:346:PX4:H32	0.43	1.89	2	1
4:A:377:PX4:O8	4:A:387:PX4:H9	0.43	2.13	5	1
4:A:428:PX4:H48	4:A:428:PX4:H54	0.43	1.62	5	1
4:A:336:PX4:H30	4:A:358:PX4:H31	0.43	1.89	6	1
4:A:419:PX4:H25	4:A:426:PX4:H23	0.43	1.90	7	1
4:A:321:PX4:H42	4:A:342:PX4:H63	0.43	1.89	11	1
4:A:379:PX4:H66	4:A:380:PX4:H36	0.43	1.90	11	1
4:A:406:PX4:H32	4:A:408:PX4:H30	0.43	1.88	11	1
4:A:419:PX4:H44	4:A:419:PX4:H38	0.43	1.53	12	1
4:A:334:PX4:H50	4:A:341:PX4:H53	0.43	1.90	15	1
4:A:397:PX4:H59	4:A:398:PX4:H68	0.43	1.90	17	1
4:A:401:PX4:H65	4:A:401:PX4:H38	0.43	1.90	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:329:PX4:H11	4:A:346:PX4:O1	0.43	2.13	20	1
4:A:321:PX4:H36	4:A:333:PX4:H44	0.43	1.90	1	1
4:A:388:PX4:H37	4:A:388:PX4:H31	0.43	1.58	3	1
4:A:368:PX4:H48	4:A:429:PX4:H47	0.43	1.89	4	1
4:A:334:PX4:H20	4:A:342:PX4:H25	0.43	1.89	6	1
4:A:389:PX4:H60	4:A:395:PX4:H55	0.43	1.90	6	1
4:A:347:PX4:H19	4:A:355:PX4:C26	0.43	2.43	9	1
4:A:370:PX4:H22	4:A:419:PX4:H54	0.43	1.90	10	1
4:A:321:PX4:H46	4:A:328:PX4:H51	0.43	1.91	12	1
4:A:365:PX4:H20	4:A:365:PX4:H26	0.43	1.48	12	1
4:A:309:PX4:H7	4:A:366:PX4:O7	0.43	2.12	13	1
4:A:389:PX4:H37	4:A:403:PX4:H63	0.43	1.90	13	1
4:A:323:PX4:H63	4:A:340:PX4:H56	0.43	1.89	14	1
4:A:376:PX4:H54	4:A:430:PX4:H52	0.43	1.89	15	1
4:A:373:PX4:O2	4:A:380:PX4:H14	0.43	2.12	16	1
4:A:349:PX4:H53	4:A:350:PX4:H46	0.43	1.89	1	1
4:A:340:PX4:H2	4:A:340:PX4:O6	0.43	2.14	2	1
4:A:307:PX4:H36	4:A:307:PX4:H41	0.43	1.54	6	1
4:A:314:PX4:H20	4:A:354:PX4:H51	0.43	1.90	7	1
4:A:312:PX4:H31	4:A:319:PX4:H54	0.43	1.89	9	1
4:A:396:PX4:H53	4:A:414:PX4:H50	0.43	1.90	10	1
4:A:374:PX4:H33	4:A:382:PX4:H28	0.43	1.90	11	1
4:A:339:PX4:H21	4:A:355:PX4:H61	0.43	1.90	12	1
1:A:98:ARG:CZ	4:A:355:PX4:H13	0.43	2.44	15	1
4:A:399:PX4:H22	4:A:408:PX4:O7	0.43	2.14	15	1
4:A:379:PX4:H27	4:A:401:PX4:C12	0.43	2.43	16	1
4:A:419:PX4:H28	4:A:426:PX4:H48	0.43	1.88	16	1
4:A:334:PX4:C13	4:A:341:PX4:H22	0.43	2.42	17	1
4:A:351:PX4:H42	4:A:391:PX4:C22	0.43	2.43	19	1
4:A:419:PX4:H29	4:A:426:PX4:H29	0.43	1.89	1	1
4:A:337:PX4:O4	4:A:346:PX4:H16	0.43	2.13	2	1
4:A:354:PX4:O6	4:A:356:PX4:H26	0.43	2.14	2	1
4:A:374:PX4:H62	4:A:374:PX4:H39	0.43	1.90	2	1
4:A:313:PX4:H29	4:A:364:PX4:H29	0.43	1.91	4	1
4:A:305:PX4:H47	4:A:362:PX4:O6	0.43	2.13	6	1
4:A:390:PX4:O6	4:A:390:PX4:H6	0.43	2.13	9	1
4:A:413:PX4:H16	4:A:431:PX4:H15	0.43	1.91	9	1
4:A:386:PX4:H20	4:A:395:PX4:H19	0.43	1.90	10	1
4:A:410:PX4:H54	4:A:410:PX4:H49	0.43	1.60	11	1
4:A:346:PX4:H27	4:A:346:PX4:C27	0.43	2.37	12	1
4:A:374:PX4:H25	4:A:429:PX4:H28	0.43	1.90	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:358:PX4:H39	4:A:399:PX4:H64	0.43	1.90	15	1
4:A:378:PX4:H38	4:A:387:PX4:H40	0.43	1.90	16	1
4:A:402:PX4:H57	4:A:402:PX4:H50	0.43	1.62	20	1
4:A:359:PX4:H21	4:A:367:PX4:H16	0.43	1.91	3	1
4:A:373:PX4:H54	4:A:375:PX4:H55	0.43	1.89	4	1
4:A:350:PX4:H29	4:A:350:PX4:H53	0.43	1.88	5	1
4:A:333:PX4:H20	4:A:356:PX4:H55	0.43	1.90	6	1
4:A:320:PX4:H56	4:A:362:PX4:H54	0.43	1.91	7	1
4:A:308:PX4:H57	4:A:318:PX4:H48	0.43	1.90	10	1
4:A:317:PX4:H33	4:A:318:PX4:H23	0.43	1.91	13	1
4:A:362:PX4:O2	4:A:365:PX4:H11	0.43	2.14	14	1
4:A:381:PX4:H42	4:A:381:PX4:H35	0.43	1.41	14	1
4:A:324:PX4:C10	4:A:340:PX4:H54	0.43	2.34	16	1
4:A:314:PX4:H53	4:A:315:PX4:H72	0.43	1.90	18	1
4:A:331:PX4:H47	4:A:331:PX4:H16	0.43	1.64	18	1
4:A:397:PX4:H47	4:A:415:PX4:H10	0.43	1.91	19	1
4:A:338:PX4:H8	4:A:351:PX4:O6	0.43	2.14	20	1
4:A:338:PX4:H50	4:A:342:PX4:H52	0.43	1.90	20	1
4:A:383:PX4:H35	4:A:397:PX4:H30	0.43	1.88	2	1
4:A:329:PX4:H66	4:A:338:PX4:H43	0.43	1.90	3	1
4:A:338:PX4:C35	4:A:384:PX4:H34	0.43	2.43	4	1
4:A:383:PX4:H4	4:A:398:PX4:O1	0.43	2.12	4	1
4:A:373:PX4:H67	4:A:375:PX4:H66	0.43	1.89	6	1
4:A:341:PX4:H52	4:A:350:PX4:H19	0.43	1.90	7	1
4:A:329:PX4:H65	4:A:346:PX4:H40	0.43	1.89	8	1
4:A:305:PX4:H4	4:A:361:PX4:O8	0.43	2.13	15	1
4:A:369:PX4:H45	4:A:378:PX4:H42	0.43	1.89	15	1
4:A:422:PX4:H19	4:A:431:PX4:H24	0.43	1.91	15	1
4:A:375:PX4:H27	4:A:421:PX4:H37	0.43	1.90	16	1
4:A:322:PX4:H64	4:A:332:PX4:H65	0.43	1.91	17	1
4:A:378:PX4:H15	4:A:380:PX4:H3	0.43	1.90	18	1
4:A:321:PX4:H14	4:A:330:PX4:O8	0.43	2.13	19	1
4:A:334:PX4:H52	4:A:334:PX4:H39	0.43	1.90	19	1
4:A:364:PX4:H38	4:A:420:PX4:H63	0.43	1.89	19	1
4:A:306:PX4:C10	4:A:314:PX4:H17	0.43	2.43	20	1
4:A:381:PX4:H55	4:A:387:PX4:H54	0.43	1.89	20	1
1:A:74:GLU:HG3	1:A:75:TYR:H	0.43	1.74	1	2
4:A:359:PX4:H35	4:A:359:PX4:H30	0.43	1.65	2	1
4:A:419:PX4:H61	4:A:425:PX4:H59	0.43	1.90	2	1
4:A:364:PX4:H35	4:A:405:PX4:H41	0.43	1.90	3	1
4:A:386:PX4:H7	4:A:400:PX4:O6	0.43	2.14	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:424:PX4:H24	4:A:425:PX4:H55	0.43	1.90	3	1
4:A:407:PX4:H16	4:A:422:PX4:H3	0.43	1.91	4	1
4:A:316:PX4:H17	4:A:317:PX4:H22	0.43	1.89	6	1
4:A:346:PX4:H42	4:A:355:PX4:H31	0.43	1.89	6	1
4:A:320:PX4:H66	4:A:362:PX4:H62	0.43	1.91	7	1
4:A:413:PX4:H26	4:A:421:PX4:H50	0.43	1.89	7	1
1:A:12:TRP:CZ2	1:A:54:LEU:HD22	0.43	2.49	9	1
1:A:73:ALA:HB1	1:A:78:PHE:CZ	0.43	2.49	9	1
4:A:312:PX4:H72	4:A:317:PX4:H68	0.43	1.89	10	1
4:A:369:PX4:H58	4:A:391:PX4:H48	0.43	1.90	10	1
4:A:305:PX4:O8	4:A:328:PX4:H9	0.43	2.13	11	1
4:A:414:PX4:H58	4:A:422:PX4:H58	0.43	1.89	11	1
4:A:369:PX4:H20	4:A:377:PX4:H22	0.43	1.90	12	1
4:A:384:PX4:C13	4:A:391:PX4:H57	0.43	2.43	13	1
4:A:321:PX4:H19	4:A:330:PX4:H69	0.43	1.88	14	1
4:A:349:PX4:H50	4:A:350:PX4:H51	0.43	1.90	14	1
4:A:334:PX4:H49	4:A:341:PX4:H16	0.43	1.89	16	1
4:A:344:PX4:H9	4:A:345:PX4:O6	0.43	2.13	16	1
4:A:379:PX4:H47	4:A:380:PX4:H5	0.43	1.89	17	1
4:A:311:PX4:H16	4:A:363:PX4:H27	0.43	1.90	19	1
4:A:305:PX4:H47	4:A:321:PX4:H65	0.43	1.90	20	1
4:A:403:PX4:H21	4:A:403:PX4:H28	0.43	1.55	20	1
4:A:423:PX4:H40	4:A:423:PX4:H34	0.43	1.65	1	1
4:A:328:PX4:H19	4:A:335:PX4:H48	0.43	1.91	2	1
4:A:391:PX4:H6	4:A:391:PX4:H20	0.43	1.89	2	1
4:A:384:PX4:O8	4:A:386:PX4:H3	0.43	2.14	3	2
4:A:332:PX4:H45	4:A:381:PX4:H40	0.43	1.90	6	1
4:A:376:PX4:H53	4:A:383:PX4:H55	0.43	1.90	7	1
4:A:384:PX4:H58	4:A:394:PX4:H53	0.43	1.91	9	1
4:A:332:PX4:H31	4:A:340:PX4:H57	0.43	1.90	10	1
4:A:394:PX4:O2	4:A:394:PX4:H7	0.43	2.13	11	1
4:A:423:PX4:H35	4:A:424:PX4:H64	0.43	1.89	13	1
4:A:398:PX4:H65	4:A:398:PX4:H58	0.43	1.44	14	1
4:A:352:PX4:C1	4:A:365:PX4:H17	0.43	2.44	15	1
4:A:379:PX4:H64	4:A:381:PX4:H35	0.43	1.90	17	1
4:A:334:PX4:H39	4:A:334:PX4:H59	0.43	1.89	19	1
4:A:329:PX4:H21	4:A:351:PX4:H17	0.43	1.90	20	1
4:A:383:PX4:H30	4:A:397:PX4:H27	0.43	1.91	4	1
4:A:399:PX4:H56	4:A:399:PX4:H63	0.43	1.53	4	1
4:A:422:PX4:H25	4:A:431:PX4:H37	0.43	1.90	4	1
4:A:407:PX4:H20	4:A:423:PX4:O6	0.43	2.13	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:372:PX4:H16	4:A:373:PX4:H22	0.43	1.89	6	2
4:A:393:PX4:H48	4:A:394:PX4:H48	0.43	1.91	6	1
4:A:305:PX4:H57	4:A:305:PX4:H51	0.43	1.73	9	1
4:A:316:PX4:H68	4:A:316:PX4:H63	0.43	1.61	10	1
4:A:431:PX4:H56	4:A:431:PX4:H62	0.43	1.53	10	1
4:A:318:PX4:H54	4:A:318:PX4:H60	0.43	1.67	13	1
4:A:312:PX4:H30	4:A:319:PX4:H49	0.43	1.90	18	1
4:A:375:PX4:H1	4:A:421:PX4:O3	0.43	2.13	18	1
4:A:415:PX4:H57	4:A:415:PX4:H62	0.43	1.53	18	1
4:A:413:PX4:H28	4:A:413:PX4:H22	0.43	1.68	3	1
4:A:336:PX4:H71	4:A:344:PX4:H42	0.43	1.91	4	1
4:A:377:PX4:H64	4:A:386:PX4:H32	0.43	1.91	12	1
4:A:402:PX4:H31	4:A:402:PX4:H38	0.43	1.44	14	1
4:A:328:PX4:H65	4:A:342:PX4:H71	0.43	1.91	17	1
4:A:337:PX4:H25	4:A:356:PX4:H21	0.43	1.91	17	1
4:A:396:PX4:H17	4:A:414:PX4:H16	0.43	1.91	19	1
4:A:421:PX4:H22	4:A:421:PX4:H27	0.42	1.61	2	1
4:A:329:PX4:H53	4:A:336:PX4:H47	0.42	1.91	3	1
4:A:309:PX4:H16	4:A:357:PX4:H51	0.42	1.91	5	1
4:A:372:PX4:H22	4:A:421:PX4:H50	0.42	1.91	5	1
4:A:378:PX4:H60	4:A:380:PX4:H28	0.42	1.91	5	1
4:A:313:PX4:H30	4:A:348:PX4:H68	0.42	1.91	6	1
4:A:357:PX4:H47	4:A:358:PX4:H16	0.42	1.90	8	1
4:A:369:PX4:H29	4:A:370:PX4:H40	0.42	1.89	8	1
4:A:414:PX4:H29	4:A:431:PX4:H19	0.42	1.91	9	1
4:A:382:PX4:H43	4:A:398:PX4:H43	0.42	1.92	13	1
4:A:424:PX4:H27	4:A:429:PX4:H59	0.42	1.91	19	1
4:A:399:PX4:H36	4:A:408:PX4:H36	0.42	1.91	1	1
4:A:418:PX4:H7	4:A:427:PX4:O2	0.42	2.14	1	1
4:A:325:PX4:H28	4:A:325:PX4:H63	0.42	1.90	3	1
4:A:333:PX4:H42	4:A:395:PX4:H62	0.42	1.91	3	1
4:A:417:PX4:H6	4:A:423:PX4:O8	0.42	2.14	4	1
4:A:371:PX4:H36	4:A:427:PX4:H44	0.42	1.92	7	1
4:A:373:PX4:H66	4:A:382:PX4:H38	0.42	1.91	8	1
4:A:384:PX4:H57	4:A:386:PX4:H55	0.42	1.91	9	1
1:A:96:TYR:OH	4:A:333:PX4:H2	0.42	2.14	10	1
4:A:388:PX4:H23	4:A:394:PX4:H17	0.42	1.92	10	1
4:A:341:PX4:H23	4:A:358:PX4:H37	0.42	1.92	11	1
4:A:346:PX4:H34	4:A:346:PX4:H27	0.42	1.56	11	1
4:A:402:PX4:H67	4:A:427:PX4:H37	0.42	1.91	11	1
4:A:336:PX4:H68	4:A:366:PX4:H67	0.42	1.90	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:371:PX4:H52	4:A:412:PX4:H21	0.42	1.92	13	1
4:A:387:PX4:H30	4:A:395:PX4:H35	0.42	1.91	13	1
4:A:328:PX4:H35	4:A:328:PX4:H30	0.42	1.49	14	1
4:A:383:PX4:H31	4:A:398:PX4:H26	0.42	1.91	14	1
4:A:392:PX4:H51	4:A:402:PX4:H15	0.42	1.91	16	1
4:A:306:PX4:H50	4:A:364:PX4:H23	0.42	1.91	17	1
4:A:323:PX4:H70	4:A:428:PX4:H68	0.42	1.90	18	1
4:A:307:PX4:H12	4:A:310:PX4:O4	0.42	2.13	20	1
4:A:377:PX4:C11	4:A:378:PX4:H16	0.42	2.40	20	1
4:A:365:PX4:H70	4:A:379:PX4:H45	0.42	1.92	1	1
4:A:420:PX4:H21	4:A:420:PX4:H27	0.42	1.56	1	1
4:A:320:PX4:C15	4:A:328:PX4:H37	0.42	2.36	3	1
4:A:336:PX4:H39	4:A:358:PX4:H65	0.42	1.90	3	1
4:A:325:PX4:H42	4:A:325:PX4:H65	0.42	1.91	5	1
4:A:352:PX4:O2	4:A:365:PX4:H10	0.42	2.14	5	1
4:A:388:PX4:H25	4:A:394:PX4:O6	0.42	2.15	5	1
4:A:386:PX4:O1	4:A:387:PX4:H7	0.42	2.14	8	1
4:A:369:PX4:H56	4:A:369:PX4:H31	0.42	1.90	9	1
4:A:337:PX4:H63	4:A:346:PX4:H39	0.42	1.91	10	1
4:A:317:PX4:H18	4:A:318:PX4:H8	0.42	1.91	11	1
4:A:314:PX4:H37	4:A:365:PX4:H58	0.42	1.90	12	1
4:A:404:PX4:H57	4:A:412:PX4:H23	0.42	1.90	12	1
4:A:408:PX4:H30	4:A:408:PX4:H36	0.42	1.62	13	1
4:A:352:PX4:H24	4:A:366:PX4:H20	0.42	1.91	14	1
4:A:408:PX4:H18	4:A:415:PX4:H27	0.42	1.91	14	1
4:A:318:PX4:H58	4:A:318:PX4:H65	0.42	1.66	16	1
4:A:388:PX4:H55	4:A:389:PX4:H53	0.42	1.91	16	1
4:A:419:PX4:H27	4:A:424:PX4:H56	0.42	1.90	16	1
4:A:429:PX4:H25	4:A:429:PX4:H31	0.42	1.61	16	1
4:A:403:PX4:H63	4:A:403:PX4:C21	0.42	2.44	17	1
4:A:411:PX4:O2	4:A:381:PX4:H11	0.42	2.15	1	1
4:A:397:PX4:O5	4:A:398:PX4:H52	0.42	2.14	2	1
4:A:318:PX4:H71	4:A:322:PX4:H55	0.42	1.90	3	1
4:A:399:PX4:O6	4:A:408:PX4:H7	0.42	2.14	3	1
4:A:310:PX4:H58	4:A:363:PX4:H32	0.42	1.92	4	1
4:A:384:PX4:H56	4:A:395:PX4:H34	0.42	1.90	6	1
4:A:322:PX4:H16	4:A:332:PX4:H47	0.42	1.92	7	1
4:A:374:PX4:O3	4:A:429:PX4:H5	0.42	2.14	7	1
4:A:386:PX4:H31	4:A:387:PX4:H31	0.42	1.89	7	1
4:A:404:PX4:H33	4:A:420:PX4:H55	0.42	1.90	8	1
4:A:384:PX4:H29	4:A:400:PX4:H30	0.42	1.91	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:411:PX4:H54	4:A:411:PX4:H61	0.42	1.76	10	1
4:A:419:PX4:H41	4:A:419:PX4:H36	0.42	1.61	14	1
4:A:421:PX4:H66	4:A:421:PX4:H34	0.42	1.90	14	1
4:A:404:PX4:H23	4:A:418:PX4:H20	0.42	1.91	15	1
4:A:391:PX4:H8	4:A:400:PX4:O2	0.42	2.14	16	1
4:A:333:PX4:H25	4:A:356:PX4:H53	0.42	1.90	17	1
4:A:389:PX4:O7	4:A:398:PX4:H15	0.42	2.15	17	1
4:A:307:PX4:H54	4:A:310:PX4:H18	0.42	1.89	20	1
1:A:63:GLN:HE21	1:A:63:GLN:HA	0.42	1.75	2	1
1:A:234:ILE:HG23	1:A:237:LEU:HD12	0.42	1.90	3	1
4:A:376:PX4:C19	4:A:397:PX4:H67	0.42	2.44	4	1
4:A:376:PX4:H60	4:A:430:PX4:H22	0.42	1.90	4	1
4:A:418:PX4:H38	4:A:418:PX4:H31	0.42	1.60	5	1
4:A:400:PX4:H54	4:A:425:PX4:H35	0.42	1.91	6	1
4:A:403:PX4:O4	4:A:412:PX4:H8	0.42	2.14	6	1
4:A:369:PX4:O8	4:A:391:PX4:H8	0.42	2.14	8	1
4:A:382:PX4:H48	4:A:382:PX4:H55	0.42	1.58	13	1
4:A:322:PX4:H52	4:A:332:PX4:H47	0.42	1.91	15	1
4:A:346:PX4:H58	4:A:346:PX4:H64	0.42	1.62	15	1
4:A:364:PX4:H30	4:A:364:PX4:H23	0.42	1.64	15	1
4:A:316:PX4:H23	4:A:339:PX4:H55	0.42	1.92	16	1
4:A:406:PX4:H12	4:A:415:PX4:O6	0.42	2.15	16	1
4:A:378:PX4:H62	4:A:411:PX4:H54	0.42	1.91	17	1
4:A:315:PX4:H66	4:A:318:PX4:H23	0.42	1.90	2	1
4:A:373:PX4:H37	4:A:421:PX4:H36	0.42	1.90	2	1
4:A:320:PX4:H19	4:A:353:PX4:H61	0.42	1.90	3	1
4:A:333:PX4:H18	4:A:333:PX4:H9	0.42	1.91	3	1
4:A:420:PX4:H53	4:A:420:PX4:H36	0.42	1.92	3	1
4:A:318:PX4:H22	4:A:319:PX4:H58	0.42	1.90	5	1
4:A:399:PX4:H20	4:A:408:PX4:H14	0.42	1.89	6	1
4:A:342:PX4:H37	4:A:342:PX4:H32	0.42	1.63	8	1
4:A:426:PX4:H67	4:A:426:PX4:H35	0.42	1.90	8	1
4:A:383:PX4:H69	4:A:429:PX4:H31	0.42	1.92	9	1
4:A:397:PX4:H21	4:A:398:PX4:H48	0.42	1.91	9	1
4:A:379:PX4:H65	4:A:385:PX4:H41	0.42	1.91	10	1
4:A:306:PX4:H21	4:A:364:PX4:H21	0.42	1.92	12	1
4:A:305:PX4:O6	4:A:362:PX4:H4	0.42	2.14	13	1
4:A:379:PX4:H25	4:A:427:PX4:H48	0.42	1.91	15	1
4:A:313:PX4:H62	4:A:313:PX4:H69	0.42	1.64	16	1
4:A:321:PX4:C24	4:A:328:PX4:H48	0.42	2.45	17	1
4:A:379:PX4:H60	4:A:381:PX4:H31	0.42	1.90	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:370:PX4:O1	4:A:426:PX4:H5	0.42	2.15	18	1
4:A:307:PX4:H16	4:A:311:PX4:O1	0.42	2.15	19	1
4:A:399:PX4:H7	4:A:408:PX4:O4	0.42	2.15	20	1
4:A:318:PX4:C8	4:A:323:PX4:H20	0.42	2.45	1	1
4:A:403:PX4:H51	4:A:404:PX4:H55	0.42	1.91	1	1
4:A:428:PX4:H28	4:A:428:PX4:H21	0.42	1.61	1	1
4:A:318:PX4:H20	4:A:319:PX4:H11	0.42	1.91	3	1
4:A:386:PX4:H25	4:A:387:PX4:H54	0.42	1.91	3	1
4:A:326:PX4:H29	4:A:360:PX4:H70	0.42	1.91	4	1
4:A:331:PX4:H27	4:A:331:PX4:H34	0.42	1.60	4	1
4:A:414:PX4:H65	4:A:422:PX4:H56	0.42	1.92	5	1
4:A:311:PX4:H22	4:A:359:PX4:H50	0.42	1.92	7	1
4:A:392:PX4:H55	4:A:409:PX4:C34	0.42	2.39	7	1
4:A:384:PX4:O6	4:A:408:PX4:H11	0.42	2.15	9	2
4:A:330:PX4:H49	4:A:331:PX4:H16	0.42	1.92	10	1
4:A:374:PX4:H58	4:A:382:PX4:H58	0.42	1.92	11	1
4:A:389:PX4:H23	4:A:403:PX4:H21	0.42	1.91	11	1
4:A:374:PX4:H45	4:A:375:PX4:H24	0.42	1.91	13	1
4:A:405:PX4:H52	4:A:405:PX4:H59	0.42	1.66	13	1
4:A:416:PX4:H39	4:A:416:PX4:H34	0.42	1.53	13	1
4:A:321:PX4:H64	4:A:321:PX4:H59	0.42	1.61	15	1
4:A:413:PX4:H55	4:A:413:PX4:H48	0.42	1.59	18	1
4:A:387:PX4:H32	4:A:395:PX4:H35	0.42	1.92	3	1
4:A:371:PX4:H17	4:A:404:PX4:H22	0.42	1.91	5	1
4:A:371:PX4:H16	4:A:388:PX4:H6	0.42	1.91	6	1
4:A:388:PX4:H14	4:A:395:PX4:O1	0.42	2.15	8	1
4:A:379:PX4:H24	4:A:411:PX4:H18	0.42	1.92	9	1
4:A:315:PX4:H62	4:A:315:PX4:H69	0.42	1.40	11	1
4:A:335:PX4:H19	4:A:342:PX4:H58	0.42	1.90	11	1
4:A:365:PX4:H41	4:A:379:PX4:H40	0.42	1.89	11	1
4:A:374:PX4:H45	4:A:374:PX4:H37	0.42	1.60	12	2
4:A:381:PX4:H61	4:A:381:PX4:H55	0.42	1.45	12	1
4:A:336:PX4:O3	4:A:336:PX4:H16	0.42	2.15	13	1
4:A:305:PX4:H25	4:A:328:PX4:H55	0.42	1.91	15	1
4:A:332:PX4:C10	4:A:340:PX4:H16	0.42	2.45	18	2
4:A:321:PX4:H16	4:A:330:PX4:H20	0.42	1.91	17	1
4:A:370:PX4:H51	4:A:419:PX4:H17	0.42	1.90	17	1
4:A:421:PX4:H45	4:A:421:PX4:H37	0.42	1.62	17	1
4:A:431:PX4:H33	4:A:431:PX4:H28	0.42	1.49	17	1
4:A:372:PX4:H45	4:A:372:PX4:H37	0.42	1.74	18	1
4:A:363:PX4:H68	4:A:374:PX4:H59	0.42	1.91	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:355:PX4:H67	4:A:355:PX4:H60	0.42	1.54	1	1
4:A:373:PX4:H49	4:A:421:PX4:H20	0.42	1.91	2	1
4:A:305:PX4:O6	4:A:362:PX4:H13	0.42	2.15	4	1
4:A:330:PX4:H58	4:A:347:PX4:H47	0.42	1.90	4	1
4:A:342:PX4:H13	4:A:342:PX4:O8	0.42	2.15	5	1
4:A:400:PX4:H67	4:A:400:PX4:H60	0.42	1.57	6	1
4:A:321:PX4:H48	4:A:335:PX4:H31	0.42	1.90	8	1
1:A:59:ILE:HD12	1:A:59:ILE:H	0.42	1.73	9	1
4:A:376:PX4:C12	4:A:429:PX4:H31	0.42	2.41	10	1
4:A:405:PX4:H13	4:A:414:PX4:O6	0.42	2.15	11	1
4:A:309:PX4:H42	4:A:352:PX4:H69	0.42	1.92	14	1
4:A:329:PX4:H58	4:A:329:PX4:H65	0.42	1.58	14	1
4:A:341:PX4:H54	4:A:350:PX4:H16	0.42	1.92	15	1
4:A:351:PX4:H24	4:A:351:PX4:H29	0.42	1.41	15	1
4:A:386:PX4:H26	4:A:386:PX4:H31	0.42	1.49	15	1
4:A:329:PX4:H66	4:A:337:PX4:H67	0.42	1.90	16	1
4:A:334:PX4:H54	4:A:334:PX4:H61	0.42	1.20	16	1
4:A:341:PX4:H61	4:A:341:PX4:H38	0.42	1.92	16	1
4:A:338:PX4:H16	4:A:347:PX4:C26	0.42	2.45	17	1
4:A:391:PX4:H51	4:A:400:PX4:H22	0.42	1.92	17	1
4:A:328:PX4:H14	4:A:335:PX4:O2	0.42	2.15	19	1
4:A:343:PX4:H43	4:A:425:PX4:H36	0.42	1.92	19	1
4:A:349:PX4:H40	4:A:349:PX4:H33	0.42	1.61	19	1
4:A:325:PX4:H68	4:A:341:PX4:H68	0.42	1.92	20	1
4:A:409:PX4:H25	4:A:409:PX4:H61	0.42	1.89	20	1
4:A:330:PX4:H60	4:A:331:PX4:H29	0.42	1.92	1	1
4:A:374:PX4:H68	4:A:398:PX4:H44	0.42	1.91	3	1
4:A:404:PX4:H8	4:A:405:PX4:O6	0.42	2.15	3	1
4:A:312:PX4:H66	4:A:312:PX4:H61	0.42	1.60	5	1
1:A:143:HIS:NE2	1:A:171:HIS:CE1	0.42	2.87	6	1
4:A:312:PX4:H9	4:A:312:PX4:O1	0.42	2.15	6	1
4:A:344:PX4:H26	4:A:345:PX4:H26	0.42	1.90	6	1
4:A:390:PX4:H22	4:A:398:PX4:H69	0.42	1.91	10	1
4:A:359:PX4:H29	4:A:359:PX4:H36	0.42	1.36	11	1
4:A:412:PX4:H25	4:A:412:PX4:H20	0.42	1.49	11	1
4:A:360:PX4:H36	4:A:360:PX4:H29	0.42	1.66	13	1
4:A:328:PX4:H53	4:A:335:PX4:H28	0.42	1.91	14	1
4:A:368:PX4:H17	4:A:429:PX4:H47	0.42	1.92	14	1
4:A:372:PX4:H61	4:A:372:PX4:H54	0.42	1.47	14	1
4:A:375:PX4:H17	4:A:421:PX4:H22	0.42	1.91	14	1
4:A:308:PX4:H48	4:A:315:PX4:H53	0.42	1.92	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:386:PX4:H48	4:A:395:PX4:H22	0.42	1.91	15	1
4:A:325:PX4:H29	4:A:348:PX4:H23	0.42	1.90	16	1
4:A:337:PX4:H47	4:A:346:PX4:H19	0.42	1.90	16	1
4:A:320:PX4:H14	4:A:353:PX4:O8	0.42	2.14	18	1
4:A:373:PX4:H51	4:A:381:PX4:H20	0.42	1.90	19	1
4:A:332:PX4:H54	4:A:332:PX4:H61	0.42	1.65	20	1
4:A:360:PX4:H14	4:A:360:PX4:H9	0.42	1.91	20	1
4:A:344:PX4:H39	4:A:344:PX4:H34	0.41	1.59	1	1
4:A:403:PX4:H72	4:A:397:PX4:H32	0.41	1.91	1	1
4:A:370:PX4:H57	4:A:430:PX4:H33	0.41	1.92	2	1
4:A:329:PX4:H53	4:A:336:PX4:C24	0.41	2.45	3	1
4:A:370:PX4:H38	4:A:370:PX4:H31	0.41	1.69	3	1
4:A:354:PX4:H41	4:A:354:PX4:H36	0.41	1.59	4	1
4:A:328:PX4:H36	4:A:338:PX4:H57	0.41	1.92	5	1
4:A:333:PX4:H30	4:A:333:PX4:H35	0.41	1.65	7	1
4:A:338:PX4:H4	4:A:351:PX4:O2	0.41	2.15	7	1
4:A:363:PX4:H69	4:A:415:PX4:H50	0.41	1.90	8	1
4:A:338:PX4:H44	4:A:400:PX4:H42	0.41	1.92	11	1
4:A:368:PX4:H29	4:A:431:PX4:H55	0.41	1.92	12	1
4:A:431:PX4:H53	4:A:431:PX4:H46	0.41	1.68	12	1
4:A:338:PX4:H3	4:A:342:PX4:O3	0.41	2.15	13	1
4:A:363:PX4:H68	4:A:363:PX4:H62	0.41	1.37	13	1
4:A:307:PX4:H52	4:A:310:PX4:H52	0.41	1.91	15	1
4:A:376:PX4:H31	4:A:383:PX4:C15	0.41	2.46	16	1
4:A:387:PX4:H17	4:A:395:PX4:H20	0.41	1.90	16	1
4:A:305:PX4:H60	4:A:305:PX4:H55	0.41	1.64	17	1
4:A:331:PX4:H15	4:A:339:PX4:O1	0.41	2.15	17	1
4:A:396:PX4:H17	4:A:414:PX4:C7	0.41	2.45	19	1
4:A:337:PX4:H62	4:A:347:PX4:H36	0.41	1.92	20	1
4:A:351:PX4:H35	4:A:391:PX4:H43	0.41	1.92	20	1
4:A:337:PX4:H17	4:A:346:PX4:H24	0.41	1.91	1	1
4:A:326:PX4:H51	4:A:343:PX4:H17	0.41	1.91	2	1
4:A:419:PX4:H65	4:A:426:PX4:H39	0.41	1.92	3	1
4:A:379:PX4:H51	4:A:380:PX4:H24	0.41	1.92	4	1
4:A:335:PX4:H48	4:A:342:PX4:H49	0.41	1.92	7	1
4:A:410:PX4:H62	4:A:410:PX4:H30	0.41	1.92	8	1
4:A:381:PX4:H56	4:A:395:PX4:H56	0.41	1.92	9	1
4:A:425:PX4:H25	4:A:425:PX4:H32	0.41	1.62	10	1
4:A:397:PX4:H28	4:A:397:PX4:H21	0.41	1.51	11	1
4:A:305:PX4:O1	4:A:362:PX4:H13	0.41	2.15	13	1
4:A:388:PX4:H22	4:A:394:PX4:H17	0.41	1.91	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:364:PX4:H38	4:A:412:PX4:H42	0.41	1.91	14	1
4:A:331:PX4:H44	4:A:335:PX4:H45	0.41	1.92	15	1
4:A:406:PX4:H23	4:A:416:PX4:H22	0.41	1.92	15	1
4:A:407:PX4:H14	4:A:416:PX4:H51	0.41	1.91	16	1
4:A:417:PX4:C26	4:A:419:PX4:H24	0.41	2.45	18	1
4:A:389:PX4:O6	4:A:403:PX4:H1	0.41	2.15	19	1
4:A:379:PX4:H53	4:A:420:PX4:H43	0.41	1.91	1	1
4:A:383:PX4:H54	4:A:429:PX4:H24	0.41	1.91	1	1
4:A:360:PX4:H66	4:A:360:PX4:H14	0.41	1.92	2	1
4:A:317:PX4:H22	4:A:324:PX4:H26	0.41	1.91	4	1
4:A:326:PX4:H14	4:A:343:PX4:C6	0.41	2.44	4	1
4:A:341:PX4:O6	4:A:351:PX4:H9	0.41	2.15	4	1
4:A:343:PX4:H39	4:A:343:PX4:H69	0.41	1.91	4	1
4:A:310:PX4:H19	4:A:310:PX4:H26	0.41	1.57	5	1
4:A:317:PX4:H11	4:A:343:PX4:H18	0.41	1.91	5	1
4:A:381:PX4:H64	4:A:381:PX4:H72	0.41	1.44	6	1
4:A:335:PX4:H37	4:A:391:PX4:H69	0.41	1.91	10	1
4:A:311:PX4:H72	4:A:412:PX4:H38	0.41	1.91	11	1
4:A:329:PX4:H34	4:A:351:PX4:H50	0.41	1.90	12	1
4:A:355:PX4:H35	4:A:356:PX4:H55	0.41	1.92	13	1
4:A:414:PX4:H52	4:A:431:PX4:H22	0.41	1.92	13	1
4:A:384:PX4:H51	4:A:386:PX4:H47	0.41	1.92	14	1
4:A:396:PX4:H68	4:A:396:PX4:H63	0.41	1.48	15	1
4:A:314:PX4:H54	4:A:361:PX4:H19	0.41	1.92	16	1
4:A:417:PX4:H3	4:A:423:PX4:H49	0.41	1.90	16	1
4:A:366:PX4:H62	4:A:366:PX4:H69	0.41	1.39	17	1
4:A:338:PX4:H6	4:A:342:PX4:O4	0.41	2.14	19	1
4:A:308:PX4:H34	4:A:308:PX4:H39	0.41	1.62	20	1
4:A:322:PX4:H36	4:A:332:PX4:H53	0.41	1.91	20	1
4:A:352:PX4:H50	4:A:352:PX4:H57	0.41	1.70	20	1
4:A:378:PX4:H46	4:A:411:PX4:O1	0.41	2.15	20	1
4:A:340:PX4:H52	4:A:340:PX4:H59	0.41	1.55	3	1
4:A:381:PX4:H2	4:A:381:PX4:H18	0.41	1.92	3	1
4:A:346:PX4:H69	4:A:346:PX4:H62	0.41	1.59	4	1
4:A:312:PX4:H3	4:A:319:PX4:O1	0.41	2.15	6	1
4:A:368:PX4:H19	4:A:429:PX4:H50	0.41	1.93	7	1
4:A:387:PX4:H25	4:A:395:PX4:H40	0.41	1.93	7	1
4:A:378:PX4:H3	4:A:385:PX4:O4	0.41	2.14	8	1
4:A:370:PX4:H37	4:A:370:PX4:H45	0.41	1.46	11	1
4:A:372:PX4:H55	4:A:372:PX4:H48	0.41	1.55	11	1
4:A:418:PX4:H47	4:A:427:PX4:H19	0.41	1.91	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:360:PX4:H48	4:A:360:PX4:H55	0.41	1.69	14	1
4:A:381:PX4:H21	4:A:385:PX4:H25	0.41	1.92	15	1
4:A:306:PX4:H19	4:A:314:PX4:H17	0.41	1.93	20	2
4:A:308:PX4:H19	4:A:319:PX4:H15	0.41	1.92	16	1
4:A:315:PX4:H14	4:A:315:PX4:H12	0.41	1.92	16	1
4:A:340:PX4:H70	4:A:380:PX4:H69	0.41	1.92	16	1
4:A:349:PX4:H48	4:A:350:PX4:H54	0.41	1.91	16	1
4:A:346:PX4:H52	4:A:346:PX4:H47	0.41	1.65	17	1
4:A:350:PX4:H39	4:A:350:PX4:H33	0.41	1.70	17	1
4:A:348:PX4:H60	4:A:356:PX4:H61	0.41	1.90	18	1
4:A:386:PX4:H66	4:A:394:PX4:H62	0.41	1.92	18	1
4:A:403:PX4:H3	4:A:412:PX4:O1	0.41	2.16	18	1
4:A:411:PX4:H36	4:A:426:PX4:H42	0.41	1.92	18	1
4:A:346:PX4:H47	4:A:347:PX4:H18	0.41	1.92	19	1
4:A:350:PX4:H48	4:A:350:PX4:H26	0.41	1.93	19	1
4:A:401:PX4:H15	4:A:410:PX4:C8	0.41	2.45	19	1
4:A:322:PX4:H40	4:A:332:PX4:H56	0.41	1.92	20	1
4:A:329:PX4:H23	4:A:329:PX4:H30	0.41	1.67	20	1
1:A:83:LYS:CD	1:A:237:LEU:HD22	0.41	2.46	1	1
4:A:361:PX4:H57	4:A:361:PX4:H50	0.41	1.66	2	1
4:A:371:PX4:H22	4:A:404:PX4:H25	0.41	1.91	2	1
4:A:384:PX4:H48	4:A:400:PX4:O6	0.41	2.16	2	1
4:A:396:PX4:H29	4:A:396:PX4:H36	0.41	1.61	2	1
4:A:318:PX4:H58	4:A:340:PX4:H23	0.41	1.92	3	1
4:A:333:PX4:H44	4:A:389:PX4:H63	0.41	1.91	3	1
4:A:358:PX4:H26	4:A:358:PX4:H19	0.41	1.57	4	1
4:A:361:PX4:H45	4:A:427:PX4:H70	0.41	1.91	4	1
4:A:397:PX4:H52	4:A:397:PX4:H59	0.41	1.66	5	1
4:A:337:PX4:H71	4:A:346:PX4:H41	0.41	1.90	6	1
4:A:424:PX4:H24	4:A:430:PX4:H33	0.41	1.92	6	1
4:A:307:PX4:H21	4:A:363:PX4:C13	0.41	2.39	7	1
4:A:312:PX4:C9	4:A:319:PX4:H17	0.41	2.46	7	1
4:A:332:PX4:H33	4:A:340:PX4:H63	0.41	1.92	8	1
4:A:404:PX4:H20	4:A:404:PX4:H26	0.41	1.65	8	1
1:A:194:HIS:CD2	1:A:198:HIS:NE2	0.41	2.89	9	1
4:A:400:PX4:H15	4:A:400:PX4:H13	0.41	1.91	10	1
4:A:371:PX4:H16	4:A:418:PX4:H20	0.41	1.90	11	1
4:A:306:PX4:H70	4:A:389:PX4:H41	0.41	1.91	12	1
4:A:375:PX4:H52	4:A:382:PX4:H50	0.41	1.92	16	1
4:A:312:PX4:H33	4:A:367:PX4:H37	0.41	1.92	18	1
4:A:414:PX4:H22	4:A:431:PX4:H28	0.41	1.92	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:315:PX4:H72	4:A:319:PX4:H27	0.41	1.93	19	1
4:A:350:PX4:H71	4:A:350:PX4:H65	0.41	1.57	19	1
4:A:372:PX4:H14	4:A:373:PX4:H2	0.41	1.92	20	1
4:A:388:PX4:H1	4:A:412:PX4:C25	0.41	2.46	20	1
4:A:352:PX4:H17	4:A:365:PX4:C11	0.41	2.41	1	1
4:A:381:PX4:H17	4:A:385:PX4:H21	0.41	1.92	1	1
4:A:346:PX4:H36	4:A:346:PX4:H67	0.41	1.93	2	1
4:A:373:PX4:H55	4:A:380:PX4:H62	0.41	1.92	2	1
4:A:392:PX4:H21	4:A:409:PX4:H57	0.41	1.92	5	1
4:A:311:PX4:H51	4:A:311:PX4:H56	0.41	1.50	6	1
4:A:322:PX4:H31	4:A:322:PX4:H26	0.41	1.56	6	1
4:A:406:PX4:H11	4:A:416:PX4:O6	0.41	2.15	6	1
4:A:339:PX4:H11	4:A:340:PX4:H48	0.41	1.92	7	1
4:A:347:PX4:H45	4:A:412:PX4:H70	0.41	1.92	7	1
4:A:401:PX4:H18	4:A:427:PX4:O7	0.41	2.16	8	1
4:A:323:PX4:H55	4:A:340:PX4:H52	0.41	1.91	10	1
4:A:360:PX4:H53	4:A:367:PX4:H50	0.41	1.92	10	1
4:A:390:PX4:H31	4:A:429:PX4:H34	0.41	1.93	10	1
4:A:314:PX4:H36	4:A:345:PX4:H29	0.41	1.91	11	1
4:A:322:PX4:H34	4:A:332:PX4:H17	0.41	1.91	11	1
4:A:362:PX4:H72	4:A:426:PX4:H44	0.41	1.93	12	1
4:A:347:PX4:H38	4:A:355:PX4:H37	0.41	1.93	13	1
4:A:309:PX4:H55	4:A:309:PX4:H60	0.41	1.57	15	1
4:A:332:PX4:H25	4:A:340:PX4:H22	0.41	1.90	15	1
4:A:312:PX4:H51	4:A:319:PX4:H46	0.41	1.92	19	1
4:A:313:PX4:H58	4:A:313:PX4:H65	0.41	1.50	19	1
4:A:418:PX4:H51	4:A:418:PX4:H56	0.41	1.47	19	1
4:A:365:PX4:H36	4:A:365:PX4:H41	0.41	1.50	20	1
4:A:310:PX4:H68	4:A:363:PX4:H25	0.41	1.92	6	1
4:A:327:PX4:H35	4:A:334:PX4:H39	0.41	1.91	6	1
4:A:331:PX4:H63	4:A:347:PX4:H22	0.41	1.93	6	1
4:A:384:PX4:H4	4:A:393:PX4:O5	0.41	2.15	8	1
4:A:316:PX4:H10	4:A:333:PX4:H15	0.41	1.93	9	1
4:A:318:PX4:H39	4:A:319:PX4:H65	0.41	1.91	9	1
1:A:98:ARG:NH1	4:A:330:PX4:O1	0.41	2.53	10	1
4:A:342:PX4:H62	4:A:342:PX4:H69	0.41	1.69	10	1
4:A:386:PX4:H38	4:A:386:PX4:H32	0.41	1.59	10	1
4:A:307:PX4:H24	4:A:311:PX4:H47	0.41	1.92	11	1
4:A:321:PX4:H23	4:A:321:PX4:H30	0.41	1.68	11	1
4:A:329:PX4:H63	4:A:344:PX4:H52	0.41	1.92	13	1
4:A:336:PX4:H62	4:A:336:PX4:H57	0.41	1.72	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:336:PX4:H62	4:A:366:PX4:H49	0.41	1.93	13	1
4:A:376:PX4:H7	4:A:376:PX4:O1	0.41	2.15	14	1
1:A:116:TRP:CH2	1:A:211:VAL:HG11	0.41	2.50	15	1
4:A:329:PX4:H65	4:A:337:PX4:H36	0.41	1.92	15	1
4:A:384:PX4:O6	4:A:394:PX4:H68	0.41	2.14	15	1
4:A:386:PX4:H36	4:A:386:PX4:H29	0.41	1.63	16	1
4:A:398:PX4:H25	4:A:398:PX4:H20	0.41	1.57	16	1
4:A:336:PX4:O6	4:A:358:PX4:H15	0.41	2.16	17	1
4:A:344:PX4:H51	4:A:346:PX4:H24	0.41	1.93	17	1
4:A:346:PX4:H59	4:A:347:PX4:H57	0.41	1.92	17	1
4:A:395:PX4:H32	4:A:395:PX4:H25	0.41	1.45	17	1
4:A:430:PX4:O6	4:A:430:PX4:H12	0.41	2.15	18	1
4:A:308:PX4:H68	4:A:322:PX4:H70	0.41	1.93	20	1
4:A:387:PX4:H27	4:A:387:PX4:H33	0.41	1.70	1	1
4:A:340:PX4:H32	4:A:421:PX4:H43	0.41	1.92	2	1
4:A:374:PX4:H18	4:A:398:PX4:H19	0.41	1.92	4	1
4:A:347:PX4:H69	4:A:351:PX4:H31	0.41	1.92	5	1
4:A:351:PX4:H33	4:A:391:PX4:H68	0.41	1.92	5	1
4:A:351:PX4:H37	4:A:391:PX4:H65	0.41	1.92	5	1
4:A:308:PX4:H10	4:A:359:PX4:O8	0.41	2.15	6	1
4:A:326:PX4:H11	4:A:353:PX4:O6	0.41	2.15	6	1
4:A:339:PX4:C7	4:A:355:PX4:H58	0.41	2.46	6	1
4:A:330:PX4:H33	4:A:332:PX4:H35	0.41	1.91	10	1
4:A:331:PX4:H43	4:A:387:PX4:H63	0.41	1.92	10	1
4:A:324:PX4:H44	4:A:398:PX4:H37	0.41	1.93	11	1
4:A:347:PX4:H30	4:A:356:PX4:H59	0.41	1.92	11	1
4:A:318:PX4:H63	4:A:318:PX4:H68	0.41	1.62	13	1
4:A:334:PX4:H23	4:A:335:PX4:H66	0.41	1.91	13	1
4:A:338:PX4:H41	4:A:338:PX4:H36	0.41	1.55	13	1
4:A:368:PX4:H67	4:A:424:PX4:H62	0.41	1.92	13	1
4:A:376:PX4:H45	4:A:376:PX4:H37	0.41	1.43	13	1
4:A:360:PX4:H50	4:A:360:PX4:H57	0.41	1.70	15	1
4:A:377:PX4:H68	4:A:377:PX4:H63	0.41	1.75	15	1
4:A:403:PX4:H55	4:A:404:PX4:H51	0.41	1.93	15	1
4:A:328:PX4:H27	4:A:342:PX4:H55	0.41	1.92	17	1
4:A:333:PX4:H44	4:A:374:PX4:H68	0.41	1.93	17	1
4:A:317:PX4:H17	4:A:318:PX4:H4	0.41	1.93	18	1
4:A:324:PX4:H49	4:A:339:PX4:H15	0.41	1.93	18	1
4:A:409:PX4:H68	4:A:410:PX4:H69	0.41	1.92	18	1
4:A:360:PX4:H50	4:A:360:PX4:H32	0.41	1.93	19	1
4:A:378:PX4:H26	4:A:387:PX4:H29	0.41	1.93	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:313:PX4:H52	4:A:333:PX4:H55	0.41	1.93	2	1
4:A:378:PX4:H3	4:A:385:PX4:H17	0.41	1.92	3	1
4:A:423:PX4:H55	4:A:426:PX4:H26	0.41	1.92	3	1
4:A:312:PX4:H44	4:A:318:PX4:H36	0.41	1.93	4	1
4:A:383:PX4:H35	4:A:389:PX4:H17	0.41	1.92	4	1
4:A:325:PX4:O2	4:A:349:PX4:H4	0.41	2.15	5	1
4:A:391:PX4:H31	4:A:391:PX4:H26	0.41	1.50	5	1
4:A:409:PX4:H9	4:A:409:PX4:O4	0.41	2.16	5	1
4:A:415:PX4:H29	4:A:415:PX4:H24	0.41	1.59	5	1
4:A:330:PX4:H15	4:A:331:PX4:O4	0.41	2.16	6	1
4:A:389:PX4:H37	4:A:389:PX4:H32	0.41	1.36	6	1
4:A:326:PX4:H64	4:A:326:PX4:H71	0.41	1.67	7	1
4:A:338:PX4:H29	4:A:338:PX4:H36	0.41	1.29	7	1
4:A:349:PX4:H69	4:A:375:PX4:H33	0.41	1.93	9	1
4:A:373:PX4:H58	4:A:381:PX4:H54	0.41	1.92	10	1
4:A:388:PX4:H49	4:A:388:PX4:H54	0.41	1.51	10	1
4:A:391:PX4:H33	4:A:391:PX4:H40	0.41	1.65	10	1
4:A:399:PX4:H20	4:A:399:PX4:H25	0.41	1.61	10	1
4:A:423:PX4:H58	4:A:423:PX4:H64	0.41	1.67	10	1
4:A:375:PX4:H68	4:A:421:PX4:H27	0.41	1.91	12	1
4:A:339:PX4:H51	4:A:355:PX4:H64	0.41	1.92	13	1
4:A:384:PX4:H2	4:A:393:PX4:O4	0.41	2.15	14	1
4:A:345:PX4:H40	4:A:345:PX4:H34	0.41	1.67	15	1
4:A:366:PX4:H41	4:A:366:PX4:H36	0.41	1.69	15	1
4:A:307:PX4:H33	4:A:363:PX4:H41	0.41	1.92	16	1
4:A:338:PX4:H71	4:A:338:PX4:H65	0.41	1.49	16	1
4:A:369:PX4:H20	4:A:369:PX4:H26	0.41	1.51	16	1
4:A:374:PX4:H26	4:A:374:PX4:H31	0.41	1.60	16	1
4:A:376:PX4:H55	4:A:429:PX4:H45	0.41	1.92	16	1
4:A:411:PX4:H34	4:A:426:PX4:H31	0.41	1.93	16	1
4:A:321:PX4:H26	4:A:330:PX4:H54	0.41	1.93	17	1
4:A:344:PX4:H49	4:A:344:PX4:H54	0.41	1.48	17	1
4:A:357:PX4:H28	4:A:357:PX4:H22	0.41	1.61	17	1
4:A:379:PX4:H59	4:A:428:PX4:H64	0.41	1.93	17	1
4:A:388:PX4:H17	4:A:388:PX4:H13	0.41	1.93	17	1
4:A:402:PX4:H18	4:A:418:PX4:H27	0.41	1.92	17	1
4:A:312:PX4:H60	4:A:312:PX4:H54	0.41	1.64	18	1
4:A:381:PX4:H69	4:A:381:PX4:H62	0.41	1.60	18	1
1:A:72:VAL:HG13	1:A:74:GLU:HB3	0.41	1.91	19	1
4:A:326:PX4:H22	4:A:326:PX4:H52	0.41	1.93	19	1
4:A:349:PX4:H14	4:A:363:PX4:C6	0.41	2.46	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:390:PX4:H29	4:A:390:PX4:H36	0.41	1.61	19	1
4:A:406:PX4:H25	4:A:409:PX4:H32	0.41	1.92	19	1
4:A:374:PX4:H17	4:A:398:PX4:H8	0.41	1.91	20	1
4:A:372:PX4:H25	4:A:421:PX4:H26	0.41	1.90	2	1
4:A:358:PX4:H60	4:A:358:PX4:H55	0.41	1.60	7	1
4:A:383:PX4:H26	4:A:398:PX4:H53	0.41	1.93	7	1
4:A:307:PX4:H25	4:A:313:PX4:H52	0.41	1.92	8	1
4:A:309:PX4:H34	4:A:309:PX4:H40	0.41	1.69	8	1
4:A:326:PX4:H41	4:A:360:PX4:H27	0.41	1.92	8	1
4:A:350:PX4:H55	4:A:350:PX4:H61	0.41	1.66	8	1
4:A:393:PX4:H34	4:A:400:PX4:H42	0.41	1.92	8	1
4:A:405:PX4:H31	4:A:405:PX4:H26	0.41	1.32	9	1
4:A:315:PX4:H54	4:A:319:PX4:H45	0.41	1.91	10	1
4:A:341:PX4:H31	4:A:341:PX4:H38	0.41	1.65	11	1
4:A:341:PX4:H67	4:A:341:PX4:H60	0.41	1.60	11	1
4:A:349:PX4:H55	4:A:349:PX4:H60	0.41	1.79	12	1
4:A:346:PX4:H59	4:A:347:PX4:H56	0.41	1.92	13	1
4:A:382:PX4:O8	4:A:398:PX4:H5	0.41	2.16	13	1
4:A:391:PX4:H58	4:A:400:PX4:H62	0.41	1.93	13	1
4:A:352:PX4:H29	4:A:352:PX4:H35	0.41	1.69	14	1
4:A:348:PX4:H37	4:A:348:PX4:H32	0.41	1.63	15	1
4:A:392:PX4:H37	4:A:392:PX4:H31	0.41	1.61	15	1
4:A:414:PX4:H63	4:A:422:PX4:H53	0.41	1.93	15	1
4:A:305:PX4:C29	4:A:320:PX4:H54	0.41	2.46	16	1
4:A:384:PX4:H60	4:A:395:PX4:H35	0.41	1.92	17	1
4:A:394:PX4:H8	4:A:395:PX4:O2	0.41	2.16	17	1
4:A:429:PX4:H64	4:A:429:PX4:H59	0.41	1.63	18	1
4:A:305:PX4:H13	4:A:362:PX4:O1	0.41	2.16	19	1
4:A:375:PX4:H16	4:A:382:PX4:H3	0.41	1.92	20	1
4:A:375:PX4:H5	4:A:413:PX4:H58	0.40	1.92	1	1
4:A:379:PX4:H33	4:A:427:PX4:H32	0.40	1.93	1	1
4:A:385:PX4:H28	4:A:387:PX4:H30	0.40	1.93	1	1
4:A:318:PX4:H41	4:A:319:PX4:H38	0.40	1.93	2	1
4:A:353:PX4:H41	4:A:353:PX4:H36	0.40	1.67	2	1
4:A:419:PX4:H30	4:A:424:PX4:H33	0.40	1.93	2	1
4:A:377:PX4:H27	4:A:411:PX4:H31	0.40	1.92	3	1
4:A:397:PX4:H32	4:A:397:PX4:H37	0.40	1.70	3	1
4:A:307:PX4:H23	4:A:307:PX4:H30	0.40	1.72	4	1
4:A:354:PX4:H25	4:A:354:PX4:C28	0.40	2.46	4	1
4:A:362:PX4:H39	4:A:362:PX4:H70	0.40	1.93	6	1
4:A:329:PX4:O5	4:A:338:PX4:H24	0.40	2.16	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:399:PX4:C10	4:A:408:PX4:H14	0.40	2.46	7	1
4:A:336:PX4:H25	4:A:351:PX4:H57	0.40	1.91	9	1
4:A:413:PX4:H25	4:A:431:PX4:H50	0.40	1.92	9	1
4:A:312:PX4:H35	4:A:312:PX4:H30	0.40	1.53	10	1
4:A:370:PX4:H66	4:A:425:PX4:H66	0.40	1.93	10	1
4:A:377:PX4:C35	4:A:391:PX4:H58	0.40	2.44	10	1
4:A:321:PX4:H30	4:A:321:PX4:H35	0.40	1.64	11	1
4:A:361:PX4:H59	4:A:365:PX4:C16	0.40	2.45	11	1
4:A:336:PX4:H27	4:A:336:PX4:H34	0.40	1.57	13	1
4:A:313:PX4:H36	4:A:314:PX4:H27	0.40	1.92	14	1
4:A:368:PX4:H44	4:A:429:PX4:H67	0.40	1.92	14	1
4:A:387:PX4:H38	4:A:387:PX4:H31	0.40	1.55	14	1
4:A:370:PX4:H47	4:A:419:PX4:O6	0.40	2.16	15	1
4:A:415:PX4:H28	4:A:415:PX4:H21	0.40	1.50	16	1
4:A:312:PX4:O1	4:A:327:PX4:H13	0.40	2.15	17	1
4:A:329:PX4:H47	4:A:338:PX4:H24	0.40	1.92	17	1
4:A:326:PX4:O6	4:A:327:PX4:H14	0.40	2.16	18	1
4:A:430:PX4:H54	4:A:430:PX4:H49	0.40	1.55	19	1
4:A:307:PX4:H17	4:A:363:PX4:H22	0.40	1.92	1	1
4:A:329:PX4:H63	4:A:338:PX4:H38	0.40	1.92	1	1
4:A:372:PX4:H34	4:A:373:PX4:H41	0.40	1.94	4	1
4:A:352:PX4:H43	4:A:409:PX4:H43	0.40	1.93	5	1
4:A:368:PX4:H48	4:A:429:PX4:H49	0.40	1.92	5	1
4:A:384:PX4:H26	4:A:391:PX4:H56	0.40	1.91	6	1
4:A:429:PX4:H59	4:A:429:PX4:H52	0.40	1.60	7	1
4:A:357:PX4:H68	4:A:357:PX4:H63	0.40	1.48	9	1
4:A:310:PX4:C28	4:A:363:PX4:H51	0.40	2.40	10	1
4:A:309:PX4:H56	4:A:309:PX4:H62	0.40	1.71	11	1
4:A:316:PX4:H49	4:A:316:PX4:H54	0.40	1.64	15	1
4:A:389:PX4:H47	4:A:398:PX4:H17	0.40	1.91	15	1
4:A:348:PX4:H54	4:A:356:PX4:H48	0.40	1.94	16	1
4:A:352:PX4:H12	4:A:352:PX4:H2	0.40	1.62	17	1
4:A:331:PX4:H41	4:A:339:PX4:H45	0.40	1.91	18	1
4:A:406:PX4:C13	4:A:409:PX4:H32	0.40	2.45	19	1
4:A:415:PX4:H30	4:A:415:PX4:H35	0.40	1.73	19	1
4:A:306:PX4:H72	4:A:348:PX4:H35	0.40	1.93	20	1
4:A:379:PX4:H48	4:A:379:PX4:H55	0.40	1.74	20	1
4:A:334:PX4:H57	4:A:334:PX4:H50	0.40	1.73	1	1
4:A:420:PX4:H30	4:A:420:PX4:H35	0.40	1.61	3	1
4:A:330:PX4:O2	4:A:339:PX4:H9	0.40	2.16	4	1
4:A:378:PX4:O7	4:A:381:PX4:H11	0.40	2.16	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:384:PX4:H57	4:A:384:PX4:H51	0.40	1.77	5	1
4:A:328:PX4:O5	4:A:335:PX4:H14	0.40	2.16	6	1
4:A:312:PX4:O2	4:A:327:PX4:H3	0.40	2.16	7	1
4:A:318:PX4:H41	4:A:421:PX4:H69	0.40	1.92	7	1
4:A:354:PX4:H21	4:A:354:PX4:H28	0.40	1.20	7	1
4:A:370:PX4:H23	4:A:377:PX4:H26	0.40	1.93	8	1
4:A:391:PX4:H45	4:A:391:PX4:H37	0.40	1.71	8	1
4:A:306:PX4:H54	4:A:349:PX4:H29	0.40	1.94	9	1
4:A:414:PX4:H27	4:A:414:PX4:H33	0.40	1.54	9	1
4:A:328:PX4:H34	4:A:328:PX4:H39	0.40	1.57	10	1
4:A:332:PX4:H23	4:A:332:PX4:H30	0.40	1.69	10	1
4:A:349:PX4:H14	4:A:363:PX4:O1	0.40	2.17	10	1
4:A:395:PX4:H59	4:A:412:PX4:H58	0.40	1.92	10	1
4:A:312:PX4:H52	4:A:317:PX4:H22	0.40	1.93	11	1
4:A:386:PX4:H38	4:A:387:PX4:H35	0.40	1.92	11	1
4:A:315:PX4:H64	4:A:315:PX4:H72	0.40	1.56	13	1
4:A:393:PX4:H5	4:A:402:PX4:O1	0.40	2.17	14	1
4:A:423:PX4:H59	4:A:426:PX4:H54	0.40	1.93	14	1
1:A:213:TYR:CG	1:A:214:PRO:HD2	0.40	2.51	15	1
4:A:305:PX4:H19	4:A:328:PX4:H52	0.40	1.93	16	1
4:A:326:PX4:H40	4:A:353:PX4:H42	0.40	1.93	16	1
4:A:320:PX4:H37	4:A:328:PX4:H33	0.40	1.92	19	1
4:A:368:PX4:H72	4:A:430:PX4:H27	0.40	1.92	19	1
4:A:393:PX4:O6	4:A:408:PX4:H5	0.40	2.16	19	1
4:A:394:PX4:H34	4:A:394:PX4:H27	0.40	1.44	19	1
4:A:402:PX4:H64	4:A:410:PX4:H63	0.40	1.93	19	1
4:A:408:PX4:H63	4:A:408:PX4:H68	0.40	1.74	19	1
4:A:330:PX4:H15	4:A:331:PX4:C8	0.40	2.44	20	1
4:A:391:PX4:H35	4:A:391:PX4:H30	0.40	1.70	20	1
4:A:318:PX4:H17	4:A:323:PX4:H23	0.40	1.92	1	1
4:A:423:PX4:H55	4:A:426:PX4:C11	0.40	2.44	2	1
4:A:316:PX4:H9	4:A:316:PX4:H14	0.40	1.92	3	1
1:A:129:TRP:CE2	4:A:313:PX4:H3	0.40	2.51	5	1
4:A:310:PX4:H38	4:A:310:PX4:H31	0.40	1.73	5	1
4:A:406:PX4:H34	4:A:406:PX4:H27	0.40	1.53	5	1
4:A:318:PX4:H44	4:A:375:PX4:H42	0.40	1.92	6	1
4:A:341:PX4:O6	4:A:357:PX4:H5	0.40	2.16	6	1
4:A:346:PX4:H52	4:A:347:PX4:H49	0.40	1.92	6	1
4:A:353:PX4:H15	4:A:353:PX4:O8	0.40	2.15	6	1
4:A:420:PX4:H33	4:A:420:PX4:H28	0.40	1.75	8	1
4:A:418:PX4:H2	4:A:427:PX4:O1	0.40	2.16	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:321:PX4:H54	4:A:335:PX4:H23	0.40	1.92	10	1
4:A:374:PX4:H34	4:A:375:PX4:H21	0.40	1.93	10	1
4:A:330:PX4:C27	4:A:331:PX4:H21	0.40	2.42	12	1
4:A:384:PX4:H58	4:A:395:PX4:H27	0.40	1.93	13	1
4:A:305:PX4:H56	4:A:362:PX4:H56	0.40	1.93	16	1
4:A:323:PX4:H59	4:A:340:PX4:H56	0.40	1.93	17	1
4:A:342:PX4:H16	4:A:351:PX4:H22	0.40	1.92	17	1
4:A:383:PX4:H65	4:A:429:PX4:H36	0.40	1.94	17	1
4:A:318:PX4:H22	4:A:318:PX4:H28	0.40	1.65	19	1
4:A:325:PX4:H56	4:A:349:PX4:H58	0.40	1.93	19	1
4:A:419:PX4:O4	4:A:426:PX4:H10	0.40	2.16	19	1
4:A:318:PX4:H2	4:A:323:PX4:H1	0.40	1.94	1	1
4:A:431:PX4:H72	4:A:431:PX4:H64	0.40	1.74	2	1
4:A:397:PX4:H56	4:A:397:PX4:H50	0.40	1.67	3	1
4:A:343:PX4:H54	4:A:353:PX4:H27	0.40	1.93	4	1
4:A:365:PX4:H45	4:A:379:PX4:H43	0.40	1.92	4	1
4:A:370:PX4:H30	4:A:377:PX4:H35	0.40	1.93	4	1
4:A:378:PX4:H69	4:A:380:PX4:H38	0.40	1.94	4	1
4:A:313:PX4:H34	4:A:364:PX4:H30	0.40	1.94	6	1
4:A:390:PX4:H26	4:A:397:PX4:H59	0.40	1.94	6	1
4:A:408:PX4:H28	4:A:416:PX4:H36	0.40	1.94	6	1
4:A:316:PX4:H59	4:A:317:PX4:H52	0.40	1.93	8	1
4:A:316:PX4:H20	4:A:325:PX4:H50	0.40	1.92	9	1
4:A:331:PX4:H46	4:A:331:PX4:H16	0.40	1.64	9	1
4:A:345:PX4:H53	4:A:354:PX4:H53	0.40	1.94	9	1
4:A:416:PX4:H58	4:A:417:PX4:H21	0.40	1.94	11	1
4:A:374:PX4:H71	4:A:398:PX4:H35	0.40	1.93	12	1
4:A:354:PX4:H50	4:A:354:PX4:H21	0.40	1.94	13	1
4:A:373:PX4:H48	4:A:375:PX4:H52	0.40	1.94	13	1
4:A:341:PX4:H31	4:A:341:PX4:H26	0.40	1.62	15	1
4:A:314:PX4:H47	4:A:364:PX4:H20	0.40	1.93	16	1
4:A:316:PX4:H47	4:A:325:PX4:C28	0.40	2.45	16	1
4:A:344:PX4:H47	4:A:344:PX4:H52	0.40	1.30	16	1
4:A:398:PX4:H67	4:A:398:PX4:H60	0.40	1.69	16	1
4:A:413:PX4:O1	4:A:428:PX4:H11	0.40	2.17	16	1
4:A:343:PX4:H54	4:A:353:PX4:H30	0.40	1.94	17	1
4:A:366:PX4:H58	4:A:366:PX4:H53	0.40	1.66	17	1
4:A:315:PX4:H39	4:A:388:PX4:H57	0.40	1.93	18	1
4:A:405:PX4:H19	4:A:414:PX4:H24	0.40	1.93	18	1
4:A:420:PX4:H63	4:A:420:PX4:H68	0.40	1.43	18	1
4:A:341:PX4:H34	4:A:341:PX4:H27	0.40	1.64	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:385:PX4:H46	4:A:385:PX4:H53	0.40	1.32	19	1
4:A:332:PX4:H34	4:A:340:PX4:H53	0.40	1.93	20	1
4:A:368:PX4:H38	4:A:368:PX4:H44	0.40	1.58	20	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	229/248 (92%)	202±3 (88±1%)	20±3 (9±1%)	8±2 (3±1%)	6 37
All	All	4580/4960 (92%)	4036 (88%)	391 (9%)	153 (3%)	6 37

All 32 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	155	THR	20
1	A	65	PRO	17
1	A	31	ASN	15
1	A	150	ASP	13
1	A	74	GLU	11
1	A	147	TYR	11
1	A	24	LEU	9
1	A	80	ASN	6
1	A	76	SER	5
1	A	141	GLY	5
1	A	75	TYR	5
1	A	121	PRO	3
1	A	162	PRO	3
1	A	144	GLY	3
1	A	148	PRO	3
1	A	56	SER	3
1	A	154	ASN	2
1	A	70	PRO	2
1	A	166	LEU	2

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Mol	Chain	Res	Type	Models (Total)
1	A	72	VAL	2
1	A	81	SER	2
1	A	103	ILE	1
1	A	215	THR	1
1	A	214	PRO	1
1	A	73	ALA	1
1	A	142	ALA	1
1	A	211	VAL	1
1	A	232	LYS	1
1	A	11	GLN	1
1	A	164	THR	1
1	A	216	TYR	1
1	A	167	GLY	1

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	190/206 (92%)	182±3 (96±2%)	8±3 (4±2%)	31 80
All	All	3800/4120 (92%)	3630 (96%)	170 (4%)	31 80

All 60 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	155	THR	13
1	A	150	ASP	13
1	A	216	TYR	11
1	A	156	LEU	11
1	A	180	ASP	9
1	A	26	ASP	7
1	A	177	ARG	6
1	A	175	ASP	6
1	A	66	ARG	5
1	A	174	GLU	5
1	A	54	LEU	5
1	A	138	PHE	5

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Mol	Chain	Res	Type	Models (Total)
1	A	222	GLN	4
1	A	171	HIS	4
1	A	83	LYS	4
1	A	12	TRP	4
1	A	184	LEU	3
1	A	77	LEU	3
1	A	128	VAL	2
1	A	63	GLN	2
1	A	179	THR	2
1	A	220	ASP	2
1	A	230	ASP	2
1	A	60	GLU	2
1	A	65	PRO	2
1	A	85	THR	2
1	A	235	GLN	2
1	A	131	THR	2
1	A	106	ASP	1
1	A	164	THR	1
1	A	224	PHE	1
1	A	72	VAL	1
1	A	189	LEU	1
1	A	205	SER	1
1	A	17	ASP	1
1	A	81	SER	1
1	A	92	ARG	1
1	A	225	LYS	1
1	A	41	GLU	1
1	A	122	LEU	1
1	A	135	MET	1
1	A	218	ASN	1
1	A	123	HIS	1
1	A	104	THR	1
1	A	223	ASN	1
1	A	114	ASN	1
1	A	11	GLN	1
1	A	39	LEU	1
1	A	148	PRO	1
1	A	176	GLU	1
1	A	71	ASP	1
1	A	213	TYR	1
1	A	231	ILE	1
1	A	75	TYR	1

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Mol	Chain	Res	Type	Models (Total)
1	A	100	LEU	1
1	A	97	THR	1
1	A	209	ASN	1
1	A	207	ASP	1
1	A	48	LEU	1
1	A	228	GLN	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

Of 131 ligands modelled in this entry, 4 are monoatomic - leaving 127 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
4	PX4	A	372	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	312	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	373	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	355	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	339	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	395	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	378	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	426	-	45,45,45	0.63±0.00	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
4	PX4	A	306	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	370	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	345	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	376	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	404	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	369	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	415	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	366	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	386	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	341	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	371	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	335	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	350	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	361	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	344	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	327	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	349	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	381	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	411	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	347	-	45,45,45	0.63±0.01	0±0 (0±0%)
4	PX4	A	389	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	363	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	362	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	393	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	318	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	308	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	410	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	307	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	417	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	360	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	374	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	398	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	400	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	390	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	305	-	45,45,45	0.63±0.01	0±0 (0±0%)
4	PX4	A	407	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	323	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	354	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	321	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	365	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	399	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	409	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	422	-	45,45,45	0.63±0.00	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
4	PX4	A	403	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	412	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	423	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	382	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	314	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	385	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	329	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	342	-	45,45,45	0.63±0.01	0±0 (0±0%)
4	PX4	A	421	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	375	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	353	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	315	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	317	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	333	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	387	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	405	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	368	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	367	-	45,45,45	0.63±0.01	0±0 (0±0%)
4	PX4	A	346	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	425	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	392	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	328	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	419	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	356	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	391	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	340	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	309	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	401	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	413	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	420	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	406	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	377	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	331	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	359	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	384	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	320	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	428	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	394	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	332	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	431	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	357	-	45,45,45	0.63±0.01	0±0 (0±0%)
4	PX4	A	322	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	343	-	45,45,45	0.63±0.00	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
4	PX4	A	430	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	326	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	313	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	414	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	310	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	380	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	337	-	45,45,45	0.63±0.01	0±0 (0±0%)
4	PX4	A	348	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	311	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	379	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	324	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	402	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	416	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	336	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	383	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	334	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	429	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	330	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	351	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	418	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	352	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	424	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	364	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	358	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	338	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	427	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	408	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	396	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	316	-	45,45,45	0.63±0.01	0±0 (0±0%)
4	PX4	A	388	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	397	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	319	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	325	-	45,45,45	0.63±0.00	0±0 (0±0%)

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

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
4	PX4	A	372	-	51,53,53	1.55±0.16	10±2 (19±4%)
4	PX4	A	312	-	51,53,53	1.55±0.17	10±3 (19±5%)
4	PX4	A	373	-	51,53,53	1.55±0.18	10±3 (19±5%)
4	PX4	A	355	-	51,53,53	1.54±0.12	10±2 (19±3%)
4	PX4	A	339	-	51,53,53	1.46±0.14	8±2 (16±4%)
4	PX4	A	395	-	51,53,53	1.54±0.12	9±2 (18±3%)
4	PX4	A	378	-	51,53,53	1.49±0.14	10±2 (18±4%)
4	PX4	A	426	-	51,53,53	1.45±0.17	8±2 (16±4%)
4	PX4	A	306	-	51,53,53	1.53±0.16	9±2 (18±4%)
4	PX4	A	370	-	51,53,53	1.53±0.14	10±2 (19±3%)
4	PX4	A	345	-	51,53,53	1.49±0.10	9±3 (17±4%)
4	PX4	A	376	-	51,53,53	1.54±0.19	9±3 (18±6%)
4	PX4	A	404	-	51,53,53	1.43±0.12	9±2 (16±4%)
4	PX4	A	369	-	51,53,53	1.52±0.19	9±2 (16±4%)
4	PX4	A	415	-	51,53,53	1.53±0.12	10±2 (19±3%)
4	PX4	A	366	-	51,53,53	1.45±0.13	8±2 (16±4%)
4	PX4	A	386	-	51,53,53	1.52±0.14	9±3 (18±5%)
4	PX4	A	341	-	51,53,53	1.47±0.09	8±2 (16±3%)
4	PX4	A	371	-	51,53,53	1.46±0.12	9±2 (17±4%)
4	PX4	A	335	-	51,53,53	1.50±0.11	10±2 (18±4%)
4	PX4	A	350	-	51,53,53	1.43±0.18	8±2 (15±4%)
4	PX4	A	361	-	51,53,53	1.51±0.11	9±2 (17±3%)
4	PX4	A	344	-	51,53,53	1.48±0.08	9±2 (16±3%)
4	PX4	A	327	-	51,53,53	1.45±0.15	8±3 (16±5%)
4	PX4	A	349	-	51,53,53	1.54±0.13	9±2 (18±4%)
4	PX4	A	381	-	51,53,53	1.51±0.15	9±3 (17±5%)
4	PX4	A	411	-	51,53,53	1.55±0.12	9±2 (18±4%)
4	PX4	A	347	-	51,53,53	1.45±0.11	8±3 (15±5%)
4	PX4	A	389	-	51,53,53	1.47±0.14	8±2 (15±4%)
4	PX4	A	363	-	51,53,53	1.54±0.13	10±2 (19±4%)
4	PX4	A	362	-	51,53,53	1.44±0.14	8±2 (15±4%)
4	PX4	A	393	-	51,53,53	1.49±0.12	9±2 (16±4%)
4	PX4	A	318	-	51,53,53	1.53±0.13	9±3 (18±5%)
4	PX4	A	308	-	51,53,53	1.44±0.11	9±2 (17±3%)
4	PX4	A	410	-	51,53,53	1.51±0.17	9±3 (17±5%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
4	PX4	A	307	-	51,53,53	1.50±0.17	9±3 (18±6%)
4	PX4	A	417	-	51,53,53	1.45±0.15	9±3 (16±5%)
4	PX4	A	360	-	51,53,53	1.48±0.13	9±2 (17±4%)
4	PX4	A	374	-	51,53,53	1.53±0.10	9±2 (17±3%)
4	PX4	A	398	-	51,53,53	1.47±0.15	9±3 (17±6%)
4	PX4	A	400	-	51,53,53	1.45±0.17	9±3 (17±5%)
4	PX4	A	390	-	51,53,53	1.53±0.17	8±2 (16±4%)
4	PX4	A	305	-	51,53,53	1.48±0.15	8±2 (15±4%)
4	PX4	A	407	-	51,53,53	1.51±0.16	9±2 (16±4%)
4	PX4	A	323	-	51,53,53	1.44±0.12	8±2 (14±4%)
4	PX4	A	354	-	51,53,53	1.50±0.17	10±3 (18±6%)
4	PX4	A	321	-	51,53,53	1.51±0.18	10±2 (19±4%)
4	PX4	A	365	-	51,53,53	1.45±0.16	8±2 (15±4%)
4	PX4	A	399	-	51,53,53	1.44±0.17	8±3 (16±5%)
4	PX4	A	409	-	51,53,53	1.49±0.13	9±3 (17±5%)
4	PX4	A	422	-	51,53,53	1.49±0.14	8±2 (16±4%)
4	PX4	A	403	-	51,53,53	1.52±0.13	9±2 (16±4%)
4	PX4	A	412	-	51,53,53	1.51±0.17	9±3 (18±5%)
4	PX4	A	423	-	51,53,53	1.52±0.17	9±3 (17±5%)
4	PX4	A	382	-	51,53,53	1.49±0.12	9±2 (16±3%)
4	PX4	A	314	-	51,53,53	1.52±0.11	9±2 (18±3%)
4	PX4	A	385	-	51,53,53	1.53±0.17	10±3 (19±5%)
4	PX4	A	329	-	51,53,53	1.46±0.13	9±2 (17±4%)
4	PX4	A	342	-	51,53,53	1.48±0.12	8±2 (15±4%)
4	PX4	A	421	-	51,53,53	1.53±0.15	10±2 (18±4%)
4	PX4	A	375	-	51,53,53	1.45±0.17	9±3 (17±6%)
4	PX4	A	353	-	51,53,53	1.55±0.16	10±2 (19±4%)
4	PX4	A	315	-	51,53,53	1.50±0.15	9±3 (17±5%)
4	PX4	A	317	-	51,53,53	1.47±0.16	9±2 (16±3%)
4	PX4	A	333	-	51,53,53	1.49±0.12	8±2 (16±3%)
4	PX4	A	387	-	51,53,53	1.42±0.11	8±2 (15±4%)
4	PX4	A	405	-	51,53,53	1.50±0.15	9±2 (17±4%)
4	PX4	A	368	-	51,53,53	1.52±0.13	9±3 (18±4%)
4	PX4	A	367	-	51,53,53	1.51±0.18	9±3 (17±5%)
4	PX4	A	346	-	51,53,53	1.48±0.15	8±2 (16±4%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
4	PX4	A	425	-	51,53,53	1.50±0.14	9±3 (17±5%)
4	PX4	A	392	-	51,53,53	1.53±0.14	9±2 (16±4%)
4	PX4	A	328	-	51,53,53	1.47±0.14	9±2 (17±4%)
4	PX4	A	419	-	51,53,53	1.51±0.15	10±2 (19±4%)
4	PX4	A	356	-	51,53,53	1.49±0.13	9±3 (17±5%)
4	PX4	A	391	-	51,53,53	1.50±0.14	9±2 (16±3%)
4	PX4	A	340	-	51,53,53	1.44±0.13	7±2 (14±4%)
4	PX4	A	309	-	51,53,53	1.46±0.11	8±2 (16±4%)
4	PX4	A	401	-	51,53,53	1.51±0.17	10±3 (19±5%)
4	PX4	A	413	-	51,53,53	1.46±0.14	9±2 (17±4%)
4	PX4	A	420	-	51,53,53	1.51±0.14	9±3 (17±5%)
4	PX4	A	406	-	51,53,53	1.52±0.14	9±2 (16±3%)
4	PX4	A	377	-	51,53,53	1.49±0.14	9±2 (17±3%)
4	PX4	A	331	-	51,53,53	1.50±0.18	9±3 (17±5%)
4	PX4	A	359	-	51,53,53	1.48±0.13	9±3 (17±5%)
4	PX4	A	384	-	51,53,53	1.55±0.18	9±2 (18±4%)
4	PX4	A	320	-	51,53,53	1.47±0.15	9±2 (17±3%)
4	PX4	A	428	-	51,53,53	1.52±0.16	10±3 (19±5%)
4	PX4	A	394	-	51,53,53	1.43±0.14	8±2 (15±3%)
4	PX4	A	332	-	51,53,53	1.51±0.15	10±3 (18±6%)
4	PX4	A	431	-	51,53,53	1.53±0.13	10±3 (19±4%)
4	PX4	A	357	-	51,53,53	1.48±0.14	9±3 (16±5%)
4	PX4	A	322	-	51,53,53	1.47±0.13	9±2 (16±3%)
4	PX4	A	343	-	51,53,53	1.49±0.13	9±2 (18±4%)
4	PX4	A	430	-	51,53,53	1.48±0.17	9±2 (16±4%)
4	PX4	A	326	-	51,53,53	1.55±0.13	10±3 (19±6%)
4	PX4	A	313	-	51,53,53	1.50±0.14	9±2 (17±4%)
4	PX4	A	414	-	51,53,53	1.54±0.13	9±3 (17±4%)
4	PX4	A	310	-	51,53,53	1.50±0.10	9±2 (17±4%)
4	PX4	A	380	-	51,53,53	1.50±0.15	9±3 (18±4%)
4	PX4	A	337	-	51,53,53	1.55±0.17	9±3 (17±5%)
4	PX4	A	348	-	51,53,53	1.51±0.13	9±2 (17±4%)
4	PX4	A	311	-	51,53,53	1.56±0.13	10±2 (19±4%)
4	PX4	A	379	-	51,53,53	1.47±0.21	8±3 (16±5%)
4	PX4	A	324	-	51,53,53	1.50±0.14	8±2 (15±4%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
4	PX4	A	402	-	51,53,53	1.49±0.13	9±3 (18±5%)
4	PX4	A	416	-	51,53,53	1.43±0.10	8±1 (16±2%)
4	PX4	A	336	-	51,53,53	1.48±0.17	9±2 (16±4%)
4	PX4	A	383	-	51,53,53	1.48±0.14	9±2 (17±4%)
4	PX4	A	334	-	51,53,53	1.48±0.11	9±2 (17±4%)
4	PX4	A	429	-	51,53,53	1.45±0.18	8±3 (16±5%)
4	PX4	A	330	-	51,53,53	1.49±0.17	9±3 (18±5%)
4	PX4	A	351	-	51,53,53	1.52±0.15	9±2 (17±4%)
4	PX4	A	418	-	51,53,53	1.52±0.08	9±2 (18±3%)
4	PX4	A	352	-	51,53,53	1.49±0.19	9±3 (16±5%)
4	PX4	A	424	-	51,53,53	1.43±0.14	8±2 (15±4%)
4	PX4	A	364	-	51,53,53	1.45±0.12	9±2 (17±3%)
4	PX4	A	358	-	51,53,53	1.48±0.11	9±2 (17±4%)
4	PX4	A	338	-	51,53,53	1.46±0.08	8±1 (15±2%)
4	PX4	A	427	-	51,53,53	1.47±0.13	9±2 (17±4%)
4	PX4	A	408	-	51,53,53	1.49±0.12	8±2 (16±3%)
4	PX4	A	396	-	51,53,53	1.46±0.12	8±2 (15±4%)
4	PX4	A	316	-	51,53,53	1.53±0.10	9±2 (18±3%)
4	PX4	A	388	-	51,53,53	1.53±0.17	9±2 (17±4%)
4	PX4	A	397	-	51,53,53	1.48±0.07	9±2 (17±3%)
4	PX4	A	319	-	51,53,53	1.55±0.15	10±2 (18±4%)
4	PX4	A	325	-	51,53,53	1.49±0.16	9±2 (17±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
4	PX4	A	417	-	-	0±0,49,49,49	-
4	PX4	A	374	-	-	0±0,49,49,49	-
4	PX4	A	407	-	-	0±0,49,49,49	-
4	PX4	A	375	-	-	0±0,49,49,49	-
4	PX4	A	333	-	-	0±0,49,49,49	-
4	PX4	A	405	-	-	0±0,49,49,49	-
4	PX4	A	342	-	-	0±0,49,49,49	-
4	PX4	A	315	-	-	0±0,49,49,49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PX4	A	419	-	-	0±0,49,49,49	-
4	PX4	A	380	-	-	0±0,49,49,49	-
4	PX4	A	341	-	-	0±0,49,49,49	-
4	PX4	A	399	-	-	0±0,49,49,49	-
4	PX4	A	365	-	-	0±0,49,49,49	-
4	PX4	A	391	-	-	0±0,49,49,49	-
4	PX4	A	367	-	-	0±0,49,49,49	-
4	PX4	A	386	-	-	0±0,49,49,49	-
4	PX4	A	429	-	-	0±0,49,49,49	-
4	PX4	A	369	-	-	0±0,49,49,49	-
4	PX4	A	350	-	-	0±0,49,49,49	-
4	PX4	A	353	-	-	0±0,49,49,49	-
4	PX4	A	408	-	-	0±0,49,49,49	-
4	PX4	A	338	-	-	0±0,49,49,49	-
4	PX4	A	352	-	-	0±0,49,49,49	-
4	PX4	A	390	-	-	0±0,49,49,49	-
4	PX4	A	314	-	-	0±0,49,49,49	-
4	PX4	A	371	-	-	0±0,49,49,49	-
4	PX4	A	324	-	-	0±0,49,49,49	-
4	PX4	A	398	-	-	0±0,49,49,49	-
4	PX4	A	349	-	-	0±0,49,49,49	-
4	PX4	A	337	-	-	0±0,49,49,49	-
4	PX4	A	351	-	-	0±0,49,49,49	-
4	PX4	A	348	-	-	0±0,49,49,49	-
4	PX4	A	431	-	-	0±0,49,49,49	-
4	PX4	A	335	-	-	0±0,49,49,49	-
4	PX4	A	354	-	-	0±0,49,49,49	-
4	PX4	A	388	-	-	0±0,49,49,49	-
4	PX4	A	370	-	-	0±0,49,49,49	-
4	PX4	A	361	-	-	0±0,49,49,49	-
4	PX4	A	420	-	-	0±0,49,49,49	-
4	PX4	A	340	-	-	0±0,49,49,49	-
4	PX4	A	334	-	-	0±0,49,49,49	-
4	PX4	A	403	-	-	0±0,49,49,49	-
4	PX4	A	372	-	-	0±0,49,49,49	-
4	PX4	A	309	-	-	0±0,49,49,49	-
4	PX4	A	397	-	-	0±0,49,49,49	-
4	PX4	A	355	-	-	0±0,49,49,49	-
4	PX4	A	326	-	-	0±0,49,49,49	-
4	PX4	A	383	-	-	0±0,49,49,49	-
4	PX4	A	406	-	-	0±0,49,49,49	-
4	PX4	A	331	-	-	0±0,49,49,49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PX4	A	421	-	-	0±0,49,49,49	-
4	PX4	A	409	-	-	0±0,49,49,49	-
4	PX4	A	362	-	-	0±0,49,49,49	-
4	PX4	A	373	-	-	0±0,49,49,49	-
4	PX4	A	412	-	-	0±0,49,49,49	-
4	PX4	A	430	-	-	0±0,49,49,49	-
4	PX4	A	411	-	-	0±0,49,49,49	-
4	PX4	A	316	-	-	0±0,49,49,49	-
4	PX4	A	423	-	-	0±0,49,49,49	-
4	PX4	A	416	-	-	0±0,49,49,49	-
4	PX4	A	339	-	-	0±0,49,49,49	-
4	PX4	A	330	-	-	0±0,49,49,49	-
4	PX4	A	318	-	-	0±0,49,49,49	-
4	PX4	A	384	-	-	0±0,49,49,49	-
4	PX4	A	336	-	-	0±0,49,49,49	-
4	PX4	A	402	-	-	0±0,49,49,49	-
4	PX4	A	401	-	-	0±0,49,49,49	-
4	PX4	A	321	-	-	0±0,49,49,49	-
4	PX4	A	327	-	-	0±0,49,49,49	-
4	PX4	A	422	-	-	0±0,49,49,49	-
4	PX4	A	404	-	-	0±0,49,49,49	-
4	PX4	A	394	-	-	0±0,49,49,49	-
4	PX4	A	413	-	-	0±0,49,49,49	-
4	PX4	A	357	-	-	0±0,49,49,49	-
4	PX4	A	376	-	-	0±0,49,49,49	-
4	PX4	A	323	-	-	0±0,49,49,49	-
4	PX4	A	415	-	-	0±0,49,49,49	-
4	PX4	A	345	-	-	0±0,49,49,49	-
4	PX4	A	306	-	-	0±0,49,49,49	-
4	PX4	A	385	-	-	0±0,49,49,49	-
4	PX4	A	359	-	-	0±0,49,49,49	-
4	PX4	A	389	-	-	0±0,49,49,49	-
4	PX4	A	400	-	-	0±0,49,49,49	-
4	PX4	A	368	-	-	0±0,49,49,49	-
4	PX4	A	313	-	-	0±0,49,49,49	-
4	PX4	A	343	-	-	0±0,49,49,49	-
4	PX4	A	358	-	-	0±0,49,49,49	-
4	PX4	A	325	-	-	0±0,49,49,49	-
4	PX4	A	328	-	-	0±0,49,49,49	-
4	PX4	A	396	-	-	0±0,49,49,49	-
4	PX4	A	307	-	-	0±0,49,49,49	-
4	PX4	A	378	-	-	0±0,49,49,49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PX4	A	414	-	-	1±0,49,49,49	-
4	PX4	A	312	-	-	0±0,49,49,49	-
4	PX4	A	305	-	-	0±0,49,49,49	-
4	PX4	A	427	-	-	0±0,49,49,49	-
4	PX4	A	308	-	-	0±0,49,49,49	-
4	PX4	A	379	-	-	0±0,49,49,49	-
4	PX4	A	418	-	-	0±0,49,49,49	-
4	PX4	A	319	-	-	0±0,49,49,49	-
4	PX4	A	363	-	-	0±0,49,49,49	-
4	PX4	A	364	-	-	0±0,49,49,49	-
4	PX4	A	382	-	-	0±0,49,49,49	-
4	PX4	A	424	-	-	0±0,49,49,49	-
4	PX4	A	428	-	-	0±0,49,49,49	-
4	PX4	A	387	-	-	0±0,49,49,49	-
4	PX4	A	344	-	-	0±0,49,49,49	-
4	PX4	A	360	-	-	0±0,49,49,49	-
4	PX4	A	425	-	-	0±0,49,49,49	-
4	PX4	A	395	-	-	0±0,49,49,49	-
4	PX4	A	310	-	-	0±0,49,49,49	-
4	PX4	A	381	-	-	0±0,49,49,49	-
4	PX4	A	347	-	-	0±0,49,49,49	-
4	PX4	A	377	-	-	0±0,49,49,49	-
4	PX4	A	322	-	-	0±0,49,49,49	-
4	PX4	A	356	-	-	0±0,49,49,49	-
4	PX4	A	392	-	-	0±0,49,49,49	-
4	PX4	A	410	-	-	0±0,49,49,49	-
4	PX4	A	329	-	-	0±0,49,49,49	-
4	PX4	A	317	-	-	0±0,49,49,49	-
4	PX4	A	426	-	-	0±0,49,49,49	-
4	PX4	A	346	-	-	0±0,49,49,49	-
4	PX4	A	311	-	-	0±0,49,49,49	-
4	PX4	A	332	-	-	0±0,49,49,49	-
4	PX4	A	366	-	-	0±0,49,49,49	-
4	PX4	A	320	-	-	0±0,49,49,49	-
4	PX4	A	393	-	-	0±0,49,49,49	-

There are no bond-length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	343	PX4	C8-C7-C6	7.96	92.97	111.79	16	8
4	A	392	PX4	C7-O7-C23	7.71	136.78	117.79	11	7
4	A	384	PX4	C5-N1-C4	7.66	89.28	108.97	6	5
4	A	369	PX4	C8-C7-C6	7.48	94.09	111.79	12	15
4	A	356	PX4	C8-C7-C6	7.31	94.49	111.79	5	11
4	A	398	PX4	C8-C7-C6	7.11	94.98	111.79	15	13
4	A	426	PX4	O7-C23-O8	7.08	106.60	123.70	12	5
4	A	307	PX4	C8-C7-C6	6.98	95.28	111.79	8	13
4	A	349	PX4	O5-C8-C7	6.96	128.70	108.43	8	13
4	A	384	PX4	C8-C7-C6	6.94	95.37	111.79	7	14
4	A	319	PX4	O5-C8-C7	6.93	128.62	108.43	19	9
4	A	331	PX4	C8-C7-C6	6.93	95.40	111.79	19	16
4	A	337	PX4	O7-C23-C24	6.93	126.43	111.50	16	15
4	A	311	PX4	C7-O7-C23	6.90	134.79	117.79	15	12
4	A	407	PX4	O7-C23-C24	6.87	126.31	111.50	10	9
4	A	403	PX4	C8-C7-C6	6.84	95.61	111.79	14	11
4	A	391	PX4	O5-C8-C7	6.83	128.31	108.43	14	8
4	A	331	PX4	C7-O7-C23	6.80	134.53	117.79	16	2
4	A	373	PX4	O7-C23-C24	6.73	126.00	111.50	13	10
4	A	406	PX4	O7-C23-C24	6.72	125.98	111.50	9	9
4	A	419	PX4	P1-O3-C1	6.57	89.26	121.59	13	11
4	A	321	PX4	C8-C7-C6	6.54	96.31	111.79	11	9
4	A	337	PX4	O5-C8-C7	6.52	127.42	108.43	18	15
4	A	386	PX4	O5-C8-C7	6.49	127.33	108.43	7	12
4	A	377	PX4	C8-C7-C6	6.48	96.46	111.79	8	14
4	A	420	PX4	C8-C7-C6	6.47	96.49	111.79	9	16
4	A	309	PX4	C4-N1-C3	6.43	92.43	108.97	12	4
4	A	370	PX4	O7-C23-C24	6.40	125.28	111.50	4	9
4	A	326	PX4	O5-C8-C7	6.39	127.04	108.43	9	15
4	A	363	PX4	O7-C23-C24	6.32	125.13	111.50	10	11
4	A	390	PX4	C4-N1-C3	6.29	92.79	108.97	8	3
4	A	390	PX4	C8-C7-C6	6.29	96.92	111.79	1	15
4	A	318	PX4	O5-C8-C7	6.26	126.65	108.43	1	15
4	A	306	PX4	C8-C7-C6	6.21	97.09	111.79	7	14
4	A	408	PX4	P1-O3-C1	6.21	91.04	121.59	11	15
4	A	414	PX4	O7-C23-C24	6.20	124.87	111.50	8	12
4	A	324	PX4	C8-C7-C6	6.20	97.13	111.79	8	15
4	A	341	PX4	C8-C7-C6	6.19	97.15	111.79	7	13
4	A	352	PX4	O7-C23-C24	6.17	124.81	111.50	18	12
4	A	357	PX4	C8-C7-C6	6.15	97.24	111.79	3	13
4	A	424	PX4	C8-C7-C6	6.14	97.27	111.79	14	10
4	A	418	PX4	C8-C7-C6	6.14	97.27	111.79	19	12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	332	PX4	O7-C23-C24	6.12	124.68	111.50	15	14
4	A	403	PX4	O5-C8-C7	6.11	126.21	108.43	12	12
4	A	337	PX4	C8-C7-C6	6.09	97.39	111.79	5	14
4	A	392	PX4	O7-C23-C24	6.09	124.62	111.50	6	9
4	A	417	PX4	C8-C7-C6	6.09	97.39	111.79	9	10
4	A	428	PX4	C8-C7-C6	6.07	97.42	111.79	5	14
4	A	393	PX4	O3-P1-O2	6.05	85.42	109.07	16	4
4	A	351	PX4	O5-C8-C7	6.04	126.01	108.43	7	9
4	A	372	PX4	C8-C7-C6	6.03	97.52	111.79	17	15
4	A	376	PX4	O3-P1-O2	6.02	85.56	109.07	7	8
4	A	384	PX4	C7-O7-C23	6.01	132.59	117.79	15	11
4	A	355	PX4	O7-C23-C24	6.01	124.45	111.50	16	11
4	A	352	PX4	C8-C7-C6	6.00	97.60	111.79	16	12
4	A	330	PX4	O7-C23-C24	5.99	124.41	111.50	9	8
4	A	312	PX4	O5-C8-C7	5.98	125.85	108.43	12	14
4	A	392	PX4	C8-C7-C6	5.98	97.65	111.79	17	13
4	A	393	PX4	C8-C7-C6	5.98	97.66	111.79	11	16
4	A	369	PX4	O7-C23-C24	5.97	124.37	111.50	16	14
4	A	385	PX4	C8-C7-C6	5.97	97.68	111.79	20	12
4	A	430	PX4	O7-C23-C24	5.95	124.33	111.50	3	10
4	A	311	PX4	O5-C8-C7	5.93	125.70	108.43	16	11
4	A	418	PX4	O5-C8-C7	5.93	125.69	108.43	8	13
4	A	321	PX4	O7-C23-C24	5.91	124.25	111.50	10	11
4	A	316	PX4	C8-C7-C6	5.90	97.82	111.79	4	15
4	A	305	PX4	O7-C23-C24	5.90	124.22	111.50	3	8
4	A	325	PX4	O7-C23-O8	5.89	109.48	123.70	4	7
4	A	390	PX4	O7-C23-C24	5.87	124.16	111.50	4	10
4	A	412	PX4	O5-C8-C7	5.86	125.50	108.43	14	10
4	A	350	PX4	C8-C7-C6	5.83	98.00	111.79	15	8
4	A	430	PX4	O5-C8-C7	5.83	125.40	108.43	3	12
4	A	366	PX4	O5-C8-C7	5.82	125.37	108.43	5	10
4	A	313	PX4	O3-P1-O2	5.80	86.41	109.07	11	5
4	A	379	PX4	C8-C7-C6	5.79	98.09	111.79	19	9
4	A	407	PX4	C8-C7-C6	5.77	98.14	111.79	3	15
4	A	319	PX4	C8-C7-C6	5.77	98.15	111.79	1	15
4	A	305	PX4	O7-C23-O8	5.76	109.78	123.70	12	7
4	A	328	PX4	C8-C7-C6	5.76	98.17	111.79	11	17
4	A	356	PX4	O5-C8-C7	5.76	125.19	108.43	11	11
4	A	310	PX4	C8-C7-C6	5.75	98.18	111.79	7	14
4	A	341	PX4	O5-C8-C7	5.75	125.16	108.43	15	13
4	A	369	PX4	O5-C8-C7	5.74	125.15	108.43	9	9

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	320	PX4	O7-C23-C24	5.74	123.86	111.50	4	12
4	A	370	PX4	C7-O7-C23	5.73	131.89	117.79	9	8
4	A	410	PX4	O5-C8-C7	5.73	125.10	108.43	18	8
4	A	424	PX4	O7-C23-C24	5.72	123.83	111.50	9	8
4	A	310	PX4	O7-C23-C24	5.71	123.81	111.50	1	9
4	A	415	PX4	O7-C23-O8	5.71	109.89	123.70	10	7
4	A	400	PX4	O5-C8-C7	5.71	125.06	108.43	9	14
4	A	430	PX4	C8-C7-C6	5.71	98.28	111.79	18	16
4	A	391	PX4	C7-O7-C23	5.71	131.85	117.79	1	9
4	A	396	PX4	C8-C7-C6	5.70	98.30	111.79	2	12
4	A	410	PX4	C8-C7-C6	5.70	98.31	111.79	5	15
4	A	372	PX4	O7-C23-O8	5.69	109.94	123.70	15	7
4	A	407	PX4	O7-C23-O8	5.69	109.95	123.70	10	4
4	A	313	PX4	O7-C23-C24	5.68	123.75	111.50	5	12
4	A	325	PX4	O7-C23-C24	5.66	123.69	111.50	8	9
4	A	317	PX4	O5-C8-C7	5.65	124.88	108.43	19	11
4	A	401	PX4	O7-C23-C24	5.65	123.68	111.50	9	4
4	A	407	PX4	O5-C8-C7	5.65	124.89	108.43	1	16
4	A	343	PX4	O5-C9-O6	5.64	109.37	123.59	4	7
4	A	423	PX4	O7-C23-C24	5.63	123.64	111.50	5	10
4	A	397	PX4	C7-O7-C23	5.63	131.65	117.79	20	8
4	A	388	PX4	O5-C8-C7	5.62	124.80	108.43	9	9
4	A	353	PX4	O7-C23-C24	5.61	123.59	111.50	17	11
4	A	354	PX4	O7-C23-O8	5.61	110.15	123.70	3	10
4	A	406	PX4	O5-C8-C7	5.60	124.74	108.43	7	12
4	A	307	PX4	O7-C23-C24	5.59	123.56	111.50	16	4
4	A	372	PX4	O7-C23-C24	5.59	123.55	111.50	13	9
4	A	399	PX4	P1-O3-C1	5.59	94.09	121.59	15	10
4	A	388	PX4	C5-N1-C4	5.58	94.63	108.97	11	3
4	A	379	PX4	O7-C23-C24	5.58	123.52	111.50	4	9
4	A	417	PX4	O5-C8-C7	5.58	124.67	108.43	13	11
4	A	367	PX4	O7-C23-C24	5.58	123.52	111.50	17	14
4	A	318	PX4	O7-C23-C24	5.57	123.50	111.50	16	9
4	A	388	PX4	C8-C7-C6	5.57	98.62	111.79	9	15
4	A	397	PX4	O5-C8-C7	5.57	124.64	108.43	5	8
4	A	337	PX4	C26-C25-C24	5.56	93.19	113.19	13	3
4	A	429	PX4	C5-N1-C3	5.56	94.67	108.97	7	4
4	A	355	PX4	C8-C7-C6	5.56	98.63	111.79	10	10
4	A	313	PX4	O5-C8-C7	5.55	124.58	108.43	19	15
4	A	395	PX4	C5-N1-C4	5.54	94.74	108.97	3	2
4	A	306	PX4	O7-C23-C24	5.53	123.41	111.50	16	12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	305	PX4	P1-O3-C1	5.52	94.40	121.59	12	12
4	A	410	PX4	O7-C23-C24	5.52	123.40	111.50	6	12
4	A	386	PX4	O7-C23-C24	5.52	123.39	111.50	4	7
4	A	342	PX4	C8-C7-C6	5.52	98.74	111.79	8	11
4	A	431	PX4	C8-C7-C6	5.52	98.74	111.79	1	15
4	A	382	PX4	O5-C9-O6	5.51	109.68	123.59	15	4
4	A	312	PX4	O7-C23-O8	5.50	110.41	123.70	1	9
4	A	325	PX4	O5-C8-C7	5.50	124.44	108.43	11	13
4	A	403	PX4	O7-C23-C24	5.50	123.36	111.50	13	10
4	A	382	PX4	C8-C7-C6	5.50	98.78	111.79	8	11
4	A	362	PX4	C8-C7-C6	5.49	98.81	111.79	4	8
4	A	319	PX4	C5-N1-C3	5.48	123.07	108.97	8	9
4	A	319	PX4	C7-O7-C23	5.48	131.28	117.79	20	9
4	A	346	PX4	O3-P1-O2	5.47	87.68	109.07	1	5
4	A	400	PX4	O7-C23-C24	5.47	123.30	111.50	19	10
4	A	414	PX4	C8-C7-C6	5.47	98.86	111.79	11	11
4	A	376	PX4	O7-C23-C24	5.46	123.27	111.50	3	11
4	A	405	PX4	C4-N1-C3	5.46	94.94	108.97	8	5
4	A	373	PX4	C8-C7-C6	5.45	98.90	111.79	16	11
4	A	331	PX4	O7-C23-C24	5.44	123.23	111.50	18	11
4	A	427	PX4	C8-C7-C6	5.44	98.92	111.79	14	11
4	A	348	PX4	O5-C8-C7	5.42	124.20	108.43	8	13
4	A	314	PX4	C8-C7-C6	5.42	98.98	111.79	13	9
4	A	346	PX4	O5-C8-C7	5.42	124.20	108.43	15	12
4	A	351	PX4	C8-C7-C6	5.41	98.99	111.79	12	16
4	A	404	PX4	O7-C23-O8	5.41	110.63	123.70	17	8
4	A	419	PX4	O7-C23-C24	5.40	123.14	111.50	14	10
4	A	322	PX4	O5-C8-C7	5.39	124.11	108.43	14	11
4	A	415	PX4	C8-C7-C6	5.37	99.08	111.79	20	12
4	A	340	PX4	C7-O7-C23	5.37	131.01	117.79	12	5
4	A	347	PX4	O7-C23-C24	5.37	123.08	111.50	17	10
4	A	326	PX4	C4-N1-C3	5.36	95.19	108.97	6	4
4	A	347	PX4	C7-O7-C23	5.36	130.98	117.79	4	5
4	A	310	PX4	O5-C8-C7	5.36	124.02	108.43	12	11
4	A	386	PX4	C7-O7-C23	5.35	130.97	117.79	14	7
4	A	416	PX4	O7-C23-C24	5.34	123.01	111.50	7	12
4	A	410	PX4	O7-C23-O8	5.33	110.81	123.70	17	7
4	A	314	PX4	C7-O7-C23	5.33	130.91	117.79	18	8
4	A	355	PX4	O7-C23-O8	5.33	110.83	123.70	16	6
4	A	395	PX4	O7-C23-C24	5.32	122.97	111.50	11	10
4	A	396	PX4	O5-C8-C7	5.32	123.92	108.43	16	11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	307	PX4	O5-C8-C7	5.32	123.92	108.43	10	11
4	A	380	PX4	O5-C8-C7	5.32	123.92	108.43	1	11
4	A	345	PX4	C8-C7-C6	5.32	99.22	111.79	20	11
4	A	389	PX4	O7-C23-C24	5.31	122.95	111.50	14	9
4	A	316	PX4	P1-O3-C1	5.31	95.46	121.59	9	15
4	A	404	PX4	C8-C7-C6	5.31	99.24	111.79	17	9
4	A	431	PX4	O5-C8-C7	5.31	123.88	108.43	17	14
4	A	335	PX4	C8-C7-C6	5.30	99.25	111.79	7	14
4	A	344	PX4	O7-C23-C24	5.29	122.90	111.50	12	5
4	A	358	PX4	C7-O7-C23	5.28	130.79	117.79	7	5
4	A	405	PX4	O7-C23-C24	5.28	122.87	111.50	5	11
4	A	348	PX4	C8-C7-C6	5.27	99.32	111.79	18	14
4	A	396	PX4	O7-C23-C24	5.26	122.85	111.50	12	10
4	A	413	PX4	O7-C23-C24	5.26	122.84	111.50	8	10
4	A	421	PX4	O5-C8-C7	5.26	123.75	108.43	18	14
4	A	387	PX4	O5-C8-C7	5.24	123.69	108.43	15	8
4	A	389	PX4	O5-C8-C7	5.24	123.69	108.43	12	9
4	A	412	PX4	C7-O7-C23	5.24	104.89	117.79	20	8
4	A	340	PX4	C8-C7-C6	5.24	99.40	111.79	18	12
4	A	364	PX4	C8-C7-C6	5.23	99.41	111.79	9	15
4	A	323	PX4	C5-N1-C3	5.23	95.53	108.97	7	5
4	A	389	PX4	C8-C7-C6	5.23	99.43	111.79	6	12
4	A	335	PX4	O7-C23-C24	5.22	122.76	111.50	8	9
4	A	354	PX4	C8-C7-C6	5.22	99.44	111.79	16	10
4	A	414	PX4	C7-O7-C23	5.22	130.65	117.79	17	13
4	A	374	PX4	O3-P1-O2	5.22	88.68	109.07	7	3
4	A	366	PX4	C8-C7-C6	5.22	99.45	111.79	12	14
4	A	393	PX4	O5-C8-C7	5.22	123.61	108.43	13	8
4	A	421	PX4	C8-C7-C6	5.21	99.46	111.79	12	16
4	A	422	PX4	C7-O7-C23	5.21	130.62	117.79	18	7
4	A	336	PX4	O7-C23-C24	5.21	122.73	111.50	13	10
4	A	345	PX4	O7-C23-C24	5.21	122.72	111.50	18	10
4	A	361	PX4	O7-C23-C24	5.21	122.72	111.50	13	13
4	A	422	PX4	O7-C23-C24	5.21	122.72	111.50	5	10
4	A	372	PX4	O5-C8-C7	5.20	123.58	108.43	2	12
4	A	364	PX4	P1-O3-C1	5.20	95.98	121.59	17	15
4	A	402	PX4	O5-C8-C7	5.20	123.58	108.43	1	13
4	A	411	PX4	O5-C8-C7	5.20	123.57	108.43	14	12
4	A	349	PX4	C8-C7-C6	5.20	99.49	111.79	16	12
4	A	398	PX4	C4-N1-C3	5.20	95.60	108.97	13	8
4	A	339	PX4	O7-C23-C24	5.20	122.70	111.50	19	8

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	382	PX4	O5-C8-C7	5.19	123.54	108.43	20	14
4	A	315	PX4	O7-C23-C24	5.19	122.68	111.50	3	9
4	A	319	PX4	O3-P1-O2	5.19	88.80	109.07	7	5
4	A	332	PX4	C8-C7-C6	5.19	99.52	111.79	2	16
4	A	346	PX4	C7-O7-C23	5.18	105.04	117.79	5	5
4	A	422	PX4	C8-C7-C6	5.17	99.55	111.79	6	11
4	A	369	PX4	O7-C23-O8	5.17	111.21	123.70	16	10
4	A	374	PX4	P1-O3-C1	5.17	96.14	121.59	10	14
4	A	391	PX4	C8-C7-C6	5.17	99.57	111.79	16	14
4	A	310	PX4	O7-C23-O8	5.17	111.22	123.70	1	4
4	A	312	PX4	O7-C23-C24	5.16	122.62	111.50	10	15
4	A	325	PX4	C8-C7-C6	5.16	99.59	111.79	20	13
4	A	380	PX4	C8-C7-C6	5.15	99.61	111.79	11	16
4	A	333	PX4	C5-N1-C3	5.14	95.75	108.97	17	4
4	A	357	PX4	C5-N1-C4	5.14	95.76	108.97	6	3
4	A	383	PX4	O5-C8-C7	5.14	123.38	108.43	17	8
4	A	332	PX4	O5-C8-C7	5.13	123.38	108.43	7	14
4	A	314	PX4	O7-C23-O8	5.13	111.31	123.70	18	8
4	A	326	PX4	P1-O3-C1	5.13	96.34	121.59	12	14
4	A	356	PX4	C7-O7-C23	5.13	130.41	117.79	20	5
4	A	392	PX4	O5-C8-C7	5.13	123.36	108.43	1	13
4	A	383	PX4	C5-N1-C3	5.12	95.80	108.97	15	6
4	A	379	PX4	O5-C8-C7	5.12	123.34	108.43	15	14
4	A	322	PX4	C7-O7-C23	5.11	130.37	117.79	5	7
4	A	374	PX4	C8-C7-C6	5.11	99.70	111.79	9	16
4	A	373	PX4	C26-C25-C24	5.11	94.83	113.19	3	3
4	A	427	PX4	P1-O3-C1	5.11	96.45	121.59	1	17
4	A	421	PX4	O5-C9-O6	5.10	110.71	123.59	14	5
4	A	412	PX4	O7-C23-C24	5.10	122.49	111.50	13	12
4	A	321	PX4	O5-C8-C7	5.09	123.26	108.43	18	7
4	A	367	PX4	P1-O4-C6	5.09	91.82	121.68	19	10
4	A	429	PX4	C8-C7-C6	5.09	99.75	111.79	11	16
4	A	390	PX4	P1-O3-C1	5.08	96.57	121.59	1	13
4	A	425	PX4	O7-C23-C24	5.08	122.45	111.50	8	17
4	A	427	PX4	O5-C8-C7	5.08	123.23	108.43	12	12
4	A	341	PX4	C7-O7-C23	5.08	130.30	117.79	1	5
4	A	376	PX4	O5-C8-C7	5.08	123.21	108.43	1	11
4	A	344	PX4	C8-C7-C6	5.07	99.79	111.79	11	12
4	A	396	PX4	O7-C7-C8	5.07	126.76	108.40	13	7
4	A	426	PX4	O7-C23-C24	5.07	122.42	111.50	12	9
4	A	383	PX4	O7-C23-O8	5.06	111.48	123.70	16	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	395	PX4	O5-C8-C7	5.06	123.15	108.43	16	13
4	A	333	PX4	O5-C8-C7	5.05	123.12	108.43	9	8
4	A	353	PX4	O5-C8-C7	5.04	123.11	108.43	2	15
4	A	327	PX4	C8-C7-C6	5.04	99.86	111.79	1	11
4	A	340	PX4	O7-C7-C8	5.04	126.64	108.40	9	7
4	A	384	PX4	P1-O3-C1	5.04	96.78	121.59	16	14
4	A	423	PX4	C5-N1-C4	5.04	96.02	108.97	6	8
4	A	350	PX4	O7-C23-C24	5.03	122.34	111.50	1	10
4	A	420	PX4	C5-N1-C4	5.03	121.90	108.97	19	6
4	A	325	PX4	C5-N1-C4	5.02	96.06	108.97	11	8
4	A	405	PX4	C8-C7-C6	5.02	99.92	111.79	10	11
4	A	363	PX4	C8-C7-C6	5.02	99.92	111.79	11	11
4	A	343	PX4	C7-O7-C23	5.01	130.14	117.79	11	7
4	A	352	PX4	O5-C8-C7	5.01	123.03	108.43	13	16
4	A	370	PX4	C8-C7-C6	5.01	99.94	111.79	14	9
4	A	423	PX4	O5-C8-C7	5.01	123.02	108.43	12	13
4	A	334	PX4	O7-C23-C24	5.01	122.29	111.50	17	9
4	A	338	PX4	O5-C8-C7	5.00	123.00	108.43	5	13
4	A	381	PX4	C8-C7-C6	5.00	99.95	111.79	4	13
4	A	394	PX4	C8-C7-C6	5.00	99.96	111.79	9	10
4	A	314	PX4	C8-O5-C9	5.00	98.61	117.12	12	2
4	A	324	PX4	P1-O3-C1	4.99	97.01	121.59	1	15
4	A	339	PX4	C8-C7-C6	4.99	99.98	111.79	11	12
4	A	350	PX4	C4-N1-C3	4.99	121.81	108.97	1	5
4	A	374	PX4	O5-C8-C7	4.99	122.96	108.43	14	12
4	A	430	PX4	C7-O7-C23	4.98	130.06	117.79	3	5
4	A	350	PX4	O5-C8-C7	4.98	122.94	108.43	18	9
4	A	378	PX4	O7-C23-C24	4.97	122.22	111.50	4	14
4	A	367	PX4	C7-O7-C23	4.97	130.02	117.79	17	13
4	A	375	PX4	P1-O3-C1	4.97	97.13	121.59	3	17
4	A	398	PX4	C7-O7-C23	4.97	130.02	117.79	11	4
4	A	425	PX4	C8-C7-C6	4.96	100.05	111.79	2	11
4	A	342	PX4	P1-O4-C6	4.96	92.61	121.68	15	10
4	A	348	PX4	O7-C23-C24	4.96	122.19	111.50	15	13
4	A	400	PX4	C7-O7-C23	4.96	130.00	117.79	11	7
4	A	324	PX4	O7-C23-C24	4.96	122.18	111.50	16	10
4	A	336	PX4	C8-C7-C6	4.96	100.07	111.79	7	15
4	A	358	PX4	C8-C7-C6	4.95	100.08	111.79	20	13
4	A	357	PX4	O7-C23-C24	4.94	122.15	111.50	17	11
4	A	399	PX4	O7-C23-C24	4.94	122.15	111.50	6	11
4	A	402	PX4	C7-O7-C23	4.94	129.96	117.79	12	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	340	PX4	O7-C23-C24	4.94	122.15	111.50	5	6
4	A	317	PX4	C8-C7-C6	4.93	100.12	111.79	5	15
4	A	411	PX4	O7-C23-C24	4.93	122.13	111.50	10	10
4	A	342	PX4	O5-C8-C7	4.92	122.76	108.43	6	11
4	A	352	PX4	C7-O7-C23	4.92	105.67	117.79	8	4
4	A	408	PX4	O5-C8-C7	4.92	122.76	108.43	5	12
4	A	322	PX4	C8-C7-C6	4.92	100.15	111.79	4	11
4	A	395	PX4	P1-O3-C1	4.92	97.36	121.59	6	16
4	A	417	PX4	O7-C7-C8	4.92	126.22	108.40	14	9
4	A	403	PX4	P1-O3-C1	4.92	97.39	121.59	11	19
4	A	405	PX4	O5-C8-C7	4.92	122.74	108.43	14	15
4	A	370	PX4	O3-P1-O2	4.91	89.89	109.07	5	12
4	A	377	PX4	O7-C23-C24	4.90	122.07	111.50	9	10
4	A	425	PX4	O7-C7-C8	4.91	126.16	108.40	2	8
4	A	335	PX4	O5-C8-C7	4.90	122.69	108.43	13	12
4	A	361	PX4	O5-C8-C7	4.90	122.69	108.43	11	12
4	A	316	PX4	C5-N1-C4	4.90	96.39	108.97	11	6
4	A	360	PX4	C8-C7-C6	4.90	100.21	111.79	2	14
4	A	389	PX4	O1-P1-O3	4.90	85.01	107.75	13	2
4	A	352	PX4	O7-C7-C8	4.89	126.12	108.40	18	5
4	A	385	PX4	O3-P1-O2	4.89	89.96	109.07	6	3
4	A	389	PX4	P1-O3-C1	4.89	97.50	121.59	6	16
4	A	402	PX4	P1-O3-C1	4.89	97.53	121.59	6	17
4	A	375	PX4	C5-N1-C4	4.89	96.41	108.97	9	6
4	A	410	PX4	C7-O7-C23	4.88	129.81	117.79	12	7
4	A	355	PX4	O7-C7-C8	4.88	126.06	108.40	6	12
4	A	383	PX4	O7-C23-C24	4.88	122.01	111.50	18	9
4	A	341	PX4	O7-C23-C24	4.87	122.00	111.50	8	9
4	A	323	PX4	C8-C7-C6	4.87	100.28	111.79	9	13
4	A	378	PX4	O5-C8-C7	4.87	122.60	108.43	4	14
4	A	317	PX4	O7-C23-C24	4.86	121.98	111.50	12	11
4	A	354	PX4	O7-C23-C24	4.86	121.98	111.50	19	13
4	A	421	PX4	C5-N1-C4	4.86	96.49	108.97	9	6
4	A	395	PX4	O7-C7-C6	4.85	125.97	108.40	15	7
4	A	385	PX4	O5-C8-C7	4.85	122.56	108.43	5	12
4	A	315	PX4	P1-O3-C1	4.85	97.71	121.59	5	14
4	A	415	PX4	C7-O7-C23	4.85	129.73	117.79	6	16
4	A	324	PX4	O7-C7-C8	4.85	125.95	108.40	7	7
4	A	406	PX4	O7-C23-O8	4.85	111.99	123.70	8	9
4	A	381	PX4	C4-N1-C3	4.84	96.52	108.97	10	4
4	A	320	PX4	O7-C23-O8	4.84	112.01	123.70	10	9

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	327	PX4	C7-O7-C23	4.84	129.70	117.79	15	3
4	A	363	PX4	O7-C23-O8	4.84	112.01	123.70	18	9
4	A	355	PX4	C5-N1-C3	4.84	96.54	108.97	5	13
4	A	426	PX4	C8-C7-C6	4.84	100.35	111.79	20	11
4	A	351	PX4	P1-O3-C1	4.83	97.80	121.59	3	16
4	A	414	PX4	C5-N1-C4	4.83	96.55	108.97	12	7
4	A	342	PX4	C5-N1-C4	4.83	96.56	108.97	13	9
4	A	388	PX4	O7-C7-C8	4.83	125.88	108.40	9	10
4	A	370	PX4	C4-N1-C3	4.82	96.57	108.97	13	7
4	A	418	PX4	C5-N1-C3	4.82	96.57	108.97	15	8
4	A	337	PX4	O7-C23-O8	4.82	112.05	123.70	16	7
4	A	355	PX4	P1-O3-C1	4.82	97.85	121.59	10	16
4	A	416	PX4	O5-C8-C7	4.82	122.47	108.43	6	9
4	A	330	PX4	O3-P1-O2	4.82	90.25	109.07	7	8
4	A	420	PX4	P1-O3-C1	4.81	97.90	121.59	9	14
4	A	338	PX4	C8-C7-C6	4.81	100.42	111.79	2	12
4	A	411	PX4	P1-O3-C1	4.81	97.93	121.59	9	16
4	A	314	PX4	P1-O3-C1	4.80	97.94	121.59	10	19
4	A	365	PX4	O7-C23-C24	4.80	121.86	111.50	2	9
4	A	419	PX4	C8-C7-C6	4.80	100.44	111.79	10	10
4	A	425	PX4	C5-N1-C4	4.79	121.29	108.97	4	3
4	A	329	PX4	O7-C23-C24	4.79	121.82	111.50	5	7
4	A	431	PX4	O7-C23-C24	4.78	121.80	111.50	13	11
4	A	313	PX4	C8-C7-C6	4.78	100.49	111.79	12	12
4	A	326	PX4	C8-C7-C6	4.78	100.49	111.79	10	15
4	A	401	PX4	C8-C7-C6	4.78	100.49	111.79	17	13
4	A	320	PX4	O3-P1-O2	4.77	90.42	109.07	19	6
4	A	376	PX4	C7-O7-C23	4.77	129.54	117.79	10	7
4	A	379	PX4	C4-N1-C3	4.77	96.72	108.97	11	5
4	A	385	PX4	O5-C9-C10	4.77	126.87	111.91	13	5
4	A	429	PX4	O5-C8-C7	4.76	122.30	108.43	3	13
4	A	307	PX4	C7-O7-C23	4.76	106.07	117.79	15	5
4	A	359	PX4	C8-C7-C6	4.76	100.53	111.79	19	10
4	A	384	PX4	O5-C8-C7	4.76	122.29	108.43	12	15
4	A	350	PX4	P1-O3-C1	4.75	98.18	121.59	10	14
4	A	347	PX4	C8-C7-C6	4.75	100.55	111.79	19	11
4	A	364	PX4	O7-C23-C24	4.75	121.75	111.50	17	8
4	A	332	PX4	C5-N1-C4	4.75	121.18	108.97	17	5
4	A	312	PX4	C8-C7-C6	4.74	100.57	111.79	20	10
4	A	413	PX4	C4-N1-C3	4.74	96.78	108.97	12	7
4	A	430	PX4	O7-C7-C8	4.74	125.55	108.40	8	8

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	330	PX4	P1-O3-C1	4.73	98.29	121.59	20	15
4	A	381	PX4	C5-N1-C4	4.73	96.80	108.97	20	6
4	A	387	PX4	C8-C7-C6	4.73	100.59	111.79	11	12
4	A	416	PX4	O7-C23-O8	4.73	112.27	123.70	10	5
4	A	310	PX4	P1-O3-C1	4.73	98.31	121.59	3	17
4	A	362	PX4	O1-P1-O3	4.73	85.80	107.75	3	1
4	A	368	PX4	C8-C7-C6	4.73	100.61	111.79	4	15
4	A	398	PX4	O7-C23-C24	4.72	121.68	111.50	13	10
4	A	313	PX4	C5-N1-C4	4.72	96.84	108.97	8	3
4	A	352	PX4	C5-N1-C3	4.72	96.84	108.97	15	5
4	A	327	PX4	O7-C23-C24	4.72	121.67	111.50	13	9
4	A	354	PX4	C5-N1-C3	4.72	96.85	108.97	5	8
4	A	374	PX4	O7-C23-C24	4.71	121.66	111.50	10	11
4	A	390	PX4	O5-C8-C7	4.71	122.14	108.43	5	8
4	A	360	PX4	O7-C23-C24	4.71	121.65	111.50	8	13
4	A	364	PX4	C7-O7-C23	4.71	129.38	117.79	13	3
4	A	404	PX4	O5-C8-C7	4.70	122.12	108.43	11	12
4	A	373	PX4	O7-C7-C8	4.70	125.42	108.40	19	11
4	A	414	PX4	P1-O3-C1	4.70	98.45	121.59	16	17
4	A	353	PX4	C7-O7-C23	4.70	129.35	117.79	15	6
4	A	382	PX4	O7-C23-C24	4.70	121.62	111.50	19	8
4	A	363	PX4	C4-N1-C3	4.69	96.91	108.97	12	10
4	A	334	PX4	C8-C7-C6	4.69	100.69	111.79	5	8
4	A	376	PX4	P1-O3-C1	4.69	98.51	121.59	18	18
4	A	326	PX4	C5-N1-C3	4.69	96.92	108.97	1	4
4	A	327	PX4	P1-O3-C1	4.68	98.53	121.59	18	15
4	A	423	PX4	O3-P1-O2	4.68	90.77	109.07	8	2
4	A	365	PX4	C8-C7-C6	4.68	100.72	111.79	17	12
4	A	413	PX4	C5-N1-C3	4.67	96.96	108.97	11	6
4	A	327	PX4	O7-C7-C8	4.67	125.30	108.40	12	10
4	A	336	PX4	P1-O3-C1	4.66	98.62	121.59	4	13
4	A	359	PX4	O5-C8-C7	4.66	122.01	108.43	7	13
4	A	367	PX4	O7-C7-C8	4.67	125.29	108.40	12	11
4	A	370	PX4	O5-C9-O6	4.67	111.82	123.59	1	7
4	A	386	PX4	C8-C7-C6	4.66	100.76	111.79	2	15
4	A	318	PX4	C8-C7-C6	4.66	100.77	111.79	19	15
4	A	386	PX4	P1-O3-C1	4.66	98.64	121.59	14	16
4	A	314	PX4	O5-C8-C7	4.66	121.99	108.43	4	14
4	A	407	PX4	P1-O3-C1	4.66	98.66	121.59	13	14
4	A	418	PX4	O7-C23-C24	4.66	121.54	111.50	17	14
4	A	416	PX4	C8-C7-C6	4.65	100.79	111.79	11	8

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	325	PX4	O7-C7-C6	4.64	125.22	108.40	9	10
4	A	425	PX4	C7-O7-C23	4.65	129.23	117.79	16	6
4	A	348	PX4	C7-O7-C23	4.64	129.22	117.79	2	8
4	A	357	PX4	O5-C8-C7	4.64	121.94	108.43	20	13
4	A	309	PX4	O5-C8-C7	4.64	121.93	108.43	13	11
4	A	427	PX4	O7-C23-C24	4.64	121.49	111.50	17	10
4	A	306	PX4	O7-C7-C8	4.63	125.18	108.40	18	6
4	A	324	PX4	O7-C7-C6	4.63	125.18	108.40	17	9
4	A	428	PX4	P1-O3-C1	4.63	98.79	121.59	2	17
4	A	321	PX4	C7-O7-C23	4.63	129.19	117.79	3	11
4	A	411	PX4	C4-N1-C3	4.63	97.07	108.97	9	6
4	A	308	PX4	C5-N1-C4	4.63	97.08	108.97	19	6
4	A	316	PX4	O5-C8-C7	4.62	121.89	108.43	4	7
4	A	381	PX4	O7-C7-C8	4.62	125.15	108.40	3	7
4	A	343	PX4	O7-C23-O8	4.62	112.53	123.70	9	8
4	A	375	PX4	C7-O7-C23	4.62	129.17	117.79	16	3
4	A	377	PX4	O5-C8-C7	4.62	121.88	108.43	2	12
4	A	425	PX4	C4-N1-C3	4.62	97.10	108.97	20	7
4	A	353	PX4	P1-O3-C1	4.62	98.86	121.59	15	17
4	A	354	PX4	O7-C7-C8	4.62	125.12	108.40	11	4
4	A	353	PX4	C11-C10-C9	4.62	96.83	113.62	2	2
4	A	401	PX4	P1-O3-C1	4.62	98.87	121.59	8	16
4	A	368	PX4	C4-N1-C3	4.61	97.11	108.97	15	4
4	A	407	PX4	O7-C7-C8	4.61	125.11	108.40	16	11
4	A	426	PX4	P1-O3-C1	4.61	98.87	121.59	16	17
4	A	397	PX4	P1-O3-C1	4.61	98.88	121.59	14	13
4	A	359	PX4	C7-O7-C23	4.61	129.14	117.79	4	8
4	A	362	PX4	O7-C23-C24	4.61	121.44	111.50	9	9
4	A	322	PX4	O1-P1-O3	4.61	86.35	107.75	3	2
4	A	353	PX4	C8-C7-C6	4.61	100.89	111.79	20	13
4	A	402	PX4	O7-C23-C24	4.61	121.43	111.50	18	10
4	A	311	PX4	O7-C23-C24	4.60	121.42	111.50	6	12
4	A	312	PX4	C7-O7-C23	4.60	129.13	117.79	11	6
4	A	329	PX4	O3-P1-O2	4.60	91.07	109.07	9	7
4	A	326	PX4	O7-C23-C24	4.60	121.41	111.50	7	13
4	A	372	PX4	P1-O3-C1	4.60	98.96	121.59	18	17
4	A	320	PX4	O5-C8-C7	4.59	121.80	108.43	19	11
4	A	347	PX4	O5-C8-C7	4.59	121.80	108.43	2	11
4	A	380	PX4	C1-C2-N1	4.59	131.11	115.78	2	4
4	A	334	PX4	O5-C8-C7	4.59	121.78	108.43	16	11
4	A	381	PX4	O4-P1-O2	4.58	126.98	109.07	20	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	365	PX4	O7-C7-C6	4.58	124.99	108.40	2	5
4	A	388	PX4	O7-C23-C24	4.58	121.37	111.50	6	12
4	A	317	PX4	C5-N1-C3	4.58	97.21	108.97	17	6
4	A	312	PX4	C11-C10-C9	4.58	96.98	113.62	19	4
4	A	393	PX4	C4-N1-C3	4.58	97.21	108.97	3	7
4	A	353	PX4	C1-C2-N1	4.58	131.06	115.78	15	7
4	A	409	PX4	C8-C7-C6	4.57	100.97	111.79	7	13
4	A	352	PX4	O3-P1-O2	4.57	91.22	109.07	16	4
4	A	406	PX4	O5-C9-O6	4.57	112.06	123.59	20	7
4	A	330	PX4	O5-C8-C7	4.56	121.72	108.43	10	15
4	A	318	PX4	C5-N1-C4	4.56	97.24	108.97	8	6
4	A	354	PX4	O5-C8-C7	4.56	121.70	108.43	3	11
4	A	322	PX4	O7-C23-O8	4.55	112.70	123.70	10	5
4	A	358	PX4	O5-C8-C7	4.55	121.69	108.43	1	11
4	A	415	PX4	C5-N1-C3	4.55	120.68	108.97	19	5
4	A	341	PX4	O7-C23-O8	4.55	112.70	123.70	14	4
4	A	382	PX4	C7-O7-C23	4.54	128.98	117.79	18	7
4	A	395	PX4	C5-N1-C3	4.55	97.29	108.97	2	9
4	A	360	PX4	O7-C23-O8	4.54	112.72	123.70	10	7
4	A	362	PX4	P1-O3-C1	4.54	99.23	121.59	13	12
4	A	369	PX4	O3-P1-O2	4.54	91.32	109.07	8	5
4	A	326	PX4	P1-O4-C6	4.54	95.06	121.68	8	11
4	A	416	PX4	P1-O3-C1	4.54	99.26	121.59	15	14
4	A	339	PX4	P1-O4-C6	4.53	95.10	121.68	15	11
4	A	331	PX4	O7-C23-O8	4.53	112.75	123.70	18	8
4	A	360	PX4	O7-C7-C8	4.53	124.81	108.40	10	10
4	A	350	PX4	O7-C23-O8	4.53	112.75	123.70	1	6
4	A	401	PX4	O3-P1-O2	4.53	91.38	109.07	17	9
4	A	340	PX4	C5-N1-C3	4.52	97.34	108.97	5	5
4	A	371	PX4	C8-C7-C6	4.52	101.09	111.79	20	13
4	A	409	PX4	O7-C23-C24	4.53	121.25	111.50	20	11
4	A	398	PX4	O7-C23-O8	4.53	112.77	123.70	4	6
4	A	320	PX4	C5-N1-C3	4.52	120.58	108.97	9	5
4	A	338	PX4	O7-C23-C24	4.51	121.23	111.50	3	10
4	A	324	PX4	O7-C23-O8	4.51	112.81	123.70	2	4
4	A	361	PX4	C7-O7-C23	4.51	128.89	117.79	18	7
4	A	408	PX4	C7-O7-C23	4.51	128.89	117.79	8	7
4	A	421	PX4	C7-O7-C23	4.51	128.89	117.79	14	3
4	A	343	PX4	O5-C8-C7	4.50	121.54	108.43	12	11
4	A	417	PX4	O7-C23-C24	4.50	121.20	111.50	20	10
4	A	382	PX4	C5-N1-C3	4.50	97.40	108.97	14	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	429	PX4	O5-C9-O6	4.49	112.25	123.59	19	6
4	A	305	PX4	P1-O4-C6	4.49	95.34	121.68	3	15
4	A	351	PX4	C5-N1-C3	4.49	120.52	108.97	20	4
4	A	333	PX4	C8-C7-C6	4.49	101.17	111.79	12	8
4	A	358	PX4	C4-N1-C3	4.49	97.43	108.97	6	5
4	A	368	PX4	C11-C10-C9	4.49	97.29	113.62	15	1
4	A	352	PX4	C1-C2-N1	4.49	130.76	115.78	9	8
4	A	395	PX4	C8-C7-C6	4.48	101.19	111.79	11	10
4	A	415	PX4	O7-C23-C24	4.48	121.16	111.50	10	8
4	A	363	PX4	O5-C8-C7	4.48	121.47	108.43	3	12
4	A	385	PX4	O7-C23-C24	4.48	121.15	111.50	13	12
4	A	368	PX4	O5-C8-C7	4.48	121.46	108.43	2	10
4	A	342	PX4	O7-C23-C24	4.47	121.14	111.50	14	11
4	A	380	PX4	O7-C23-C24	4.47	121.14	111.50	15	9
4	A	359	PX4	P1-O3-C1	4.47	99.57	121.59	20	10
4	A	420	PX4	O5-C8-C7	4.47	121.45	108.43	2	9
4	A	372	PX4	O7-C7-C8	4.47	124.59	108.40	17	7
4	A	379	PX4	O1-P1-O3	4.47	86.98	107.75	18	2
4	A	429	PX4	O3-P1-O2	4.47	91.60	109.07	5	2
4	A	377	PX4	C5-N1-C4	4.47	97.48	108.97	3	6
4	A	381	PX4	O7-C23-C24	4.47	121.13	111.50	18	9
4	A	373	PX4	P1-O3-C1	4.46	99.62	121.59	8	17
4	A	380	PX4	P1-O3-C1	4.46	99.62	121.59	17	15
4	A	366	PX4	P1-O3-C1	4.46	99.63	121.59	6	15
4	A	308	PX4	C8-C7-C6	4.46	101.24	111.79	20	12
4	A	314	PX4	O7-C23-C24	4.46	121.11	111.50	7	10
4	A	417	PX4	O5-C9-O6	4.46	112.35	123.59	12	8
4	A	305	PX4	C8-C7-C6	4.45	101.25	111.79	18	12
4	A	308	PX4	O7-C7-C8	4.45	124.52	108.40	4	8
4	A	315	PX4	C7-O7-C23	4.45	128.76	117.79	20	10
4	A	374	PX4	C7-O7-C23	4.45	128.76	117.79	1	8
4	A	337	PX4	O3-P1-O2	4.45	91.68	109.07	15	3
4	A	409	PX4	O5-C8-C7	4.45	121.38	108.43	11	9
4	A	404	PX4	O7-C23-C24	4.45	121.08	111.50	5	6
4	A	345	PX4	O7-C7-C8	4.44	124.49	108.40	17	10
4	A	315	PX4	C11-C10-C9	4.44	97.47	113.62	1	5
4	A	338	PX4	C7-O7-C23	4.44	128.73	117.79	3	4
4	A	341	PX4	C5-N1-C4	4.44	120.39	108.97	6	3
4	A	355	PX4	C5-N1-C4	4.44	97.56	108.97	13	3
4	A	367	PX4	C8-C7-C6	4.44	101.29	111.79	16	12
4	A	333	PX4	C7-O7-C23	4.44	128.72	117.79	2	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	335	PX4	C7-O7-C23	4.44	106.87	117.79	5	6
4	A	406	PX4	P1-O3-C1	4.44	99.75	121.59	4	17
4	A	417	PX4	O7-C23-O8	4.43	112.98	123.70	12	7
4	A	419	PX4	O7-C7-C8	4.43	124.46	108.40	6	7
4	A	419	PX4	O3-P1-O2	4.43	91.74	109.07	6	6
4	A	387	PX4	O7-C23-C24	4.43	121.05	111.50	16	13
4	A	319	PX4	C5-N1-C4	4.43	97.59	108.97	16	5
4	A	323	PX4	O5-C8-C7	4.42	121.31	108.43	5	10
4	A	399	PX4	O5-C9-C10	4.42	125.79	111.91	12	2
4	A	429	PX4	P1-O3-C1	4.42	99.81	121.59	12	15
4	A	345	PX4	O5-C8-C7	4.42	121.30	108.43	10	8
4	A	400	PX4	O7-C23-O8	4.42	113.02	123.70	9	4
4	A	339	PX4	C1-C2-N1	4.42	130.53	115.78	4	7
4	A	344	PX4	P1-O3-C1	4.41	99.86	121.59	20	17
4	A	380	PX4	C7-O7-C23	4.41	128.65	117.79	5	8
4	A	384	PX4	O7-C23-C24	4.41	121.01	111.50	20	9
4	A	421	PX4	O7-C23-C24	4.41	121.01	111.50	14	9
4	A	326	PX4	O7-C7-C6	4.40	124.35	108.40	1	6
4	A	375	PX4	C8-C7-C6	4.40	101.38	111.79	18	10
4	A	330	PX4	O7-C23-O8	4.40	113.07	123.70	9	7
4	A	389	PX4	O3-P1-O2	4.40	91.89	109.07	8	5
4	A	349	PX4	O5-C9-O6	4.39	112.51	123.59	11	5
4	A	349	PX4	O7-C23-C24	4.39	120.97	111.50	14	11
4	A	320	PX4	O7-C7-C8	4.39	124.28	108.40	10	12
4	A	334	PX4	O7-C23-O8	4.39	113.10	123.70	2	7
4	A	305	PX4	O5-C9-C10	4.38	125.66	111.91	19	4
4	A	316	PX4	C7-O7-C23	4.38	128.58	117.79	6	4
4	A	351	PX4	C4-N1-C3	4.38	97.71	108.97	20	3
4	A	367	PX4	O7-C7-C6	4.38	124.25	108.40	16	13
4	A	385	PX4	O1-P1-O3	4.38	87.41	107.75	6	5
4	A	322	PX4	O7-C7-C8	4.37	124.23	108.40	5	6
4	A	327	PX4	C5-N1-C4	4.37	120.22	108.97	19	6
4	A	408	PX4	O7-C23-O8	4.37	113.13	123.70	9	8
4	A	340	PX4	O5-C9-O6	4.37	112.56	123.59	10	6
4	A	397	PX4	C5-N1-C4	4.37	97.73	108.97	2	7
4	A	321	PX4	P1-O3-C1	4.37	100.08	121.59	18	15
4	A	351	PX4	O7-C23-C24	4.37	120.92	111.50	20	10
4	A	373	PX4	C4-N1-C3	4.37	97.74	108.97	18	5
4	A	385	PX4	P1-O3-C1	4.37	100.10	121.59	1	13
4	A	394	PX4	O5-C9-O6	4.37	112.58	123.59	12	8
4	A	413	PX4	O3-P1-O2	4.37	92.01	109.07	5	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	312	PX4	O7-C7-C8	4.36	124.20	108.40	11	9
4	A	349	PX4	C5-N1-C3	4.36	97.76	108.97	10	8
4	A	423	PX4	C8-C7-C6	4.36	101.47	111.79	5	10
4	A	396	PX4	O5-C9-O6	4.36	112.59	123.59	18	3
4	A	322	PX4	P1-O3-C1	4.36	100.13	121.59	13	16
4	A	406	PX4	C8-C7-C6	4.36	101.48	111.79	9	13
4	A	362	PX4	C7-O7-C23	4.36	128.52	117.79	17	7
4	A	392	PX4	O3-P1-O2	4.36	92.04	109.07	10	5
4	A	379	PX4	O7-C23-O8	4.36	113.18	123.70	4	2
4	A	431	PX4	P1-O3-C1	4.36	100.15	121.59	20	18
4	A	330	PX4	C7-O7-C23	4.35	128.50	117.79	5	8
4	A	332	PX4	P1-O3-C1	4.35	100.18	121.59	12	15
4	A	333	PX4	O7-C23-C24	4.35	120.88	111.50	1	11
4	A	352	PX4	P1-O3-C1	4.35	100.17	121.59	8	14
4	A	333	PX4	O7-C7-C6	4.34	124.11	108.40	15	8
4	A	339	PX4	C7-O7-C23	4.34	128.46	117.79	11	6
4	A	414	PX4	O7-C23-O8	4.33	113.23	123.70	5	7
4	A	306	PX4	O5-C8-C7	4.33	121.04	108.43	8	10
4	A	356	PX4	P1-O3-C1	4.33	100.26	121.59	15	17
4	A	313	PX4	P1-O4-C6	4.33	96.29	121.68	2	12
4	A	315	PX4	C8-C7-C6	4.33	101.55	111.79	20	9
4	A	394	PX4	O5-C8-C7	4.32	121.02	108.43	3	12
4	A	332	PX4	C7-O7-C23	4.32	128.43	117.79	19	5
4	A	364	PX4	O5-C8-C7	4.32	121.01	108.43	15	13
4	A	402	PX4	C5-N1-C3	4.32	97.86	108.97	8	2
4	A	374	PX4	O7-C7-C8	4.32	124.05	108.40	14	8
4	A	424	PX4	P1-O3-C1	4.32	100.31	121.59	6	16
4	A	342	PX4	C4-N1-C3	4.32	97.87	108.97	9	7
4	A	377	PX4	O7-C7-C8	4.32	124.04	108.40	13	8
4	A	365	PX4	P1-O3-C1	4.32	100.34	121.59	4	18
4	A	311	PX4	P1-O4-C6	4.31	96.39	121.68	3	12
4	A	368	PX4	P1-O4-C6	4.31	96.40	121.68	10	10
4	A	417	PX4	C5-N1-C3	4.31	97.89	108.97	5	1
4	A	309	PX4	C8-C7-C6	4.31	101.59	111.79	6	12
4	A	315	PX4	O5-C8-C7	4.31	120.98	108.43	7	8
4	A	370	PX4	C5-N1-C4	4.31	97.89	108.97	18	2
4	A	335	PX4	P1-O3-C1	4.31	100.37	121.59	7	16
4	A	378	PX4	C8-C7-C6	4.31	101.59	111.79	14	15
4	A	324	PX4	C1-C2-N1	4.31	130.16	115.78	12	5
4	A	353	PX4	C17-C16-C15	4.31	92.56	114.42	13	1
4	A	374	PX4	C5-N1-C4	4.30	97.91	108.97	16	7

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	381	PX4	P1-O3-C1	4.30	100.41	121.59	20	13
4	A	319	PX4	O7-C7-C8	4.30	123.98	108.40	1	8
4	A	336	PX4	O3-P1-O2	4.30	92.26	109.07	7	6
4	A	391	PX4	O7-C23-C24	4.30	120.77	111.50	13	9
4	A	394	PX4	O7-C23-C24	4.30	120.77	111.50	15	9
4	A	411	PX4	C12-C11-C10	4.30	97.74	113.19	4	3
4	A	318	PX4	C7-O7-C23	4.29	128.37	117.79	18	5
4	A	375	PX4	O5-C8-C7	4.29	120.93	108.43	15	10
4	A	430	PX4	C5-N1-C3	4.29	97.94	108.97	4	6
4	A	323	PX4	O7-C23-O8	4.29	113.34	123.70	9	8
4	A	376	PX4	C8-C7-C6	4.29	101.65	111.79	19	11
4	A	308	PX4	O7-C23-C24	4.29	120.74	111.50	11	9
4	A	373	PX4	C7-O7-C23	4.29	128.34	117.79	18	7
4	A	412	PX4	C8-C7-C6	4.29	101.65	111.79	10	12
4	A	312	PX4	C5-N1-C4	4.29	97.95	108.97	10	7
4	A	333	PX4	P1-O3-C1	4.28	100.51	121.59	7	12
4	A	338	PX4	P1-O3-C1	4.28	100.51	121.59	7	17
4	A	311	PX4	O3-P1-O2	4.28	92.35	109.07	16	4
4	A	393	PX4	P1-O3-C1	4.28	100.52	121.59	2	17
4	A	403	PX4	C5-N1-C2	4.28	127.42	109.92	17	5
4	A	399	PX4	C5-N1-C3	4.27	97.99	108.97	2	7
4	A	423	PX4	P1-O3-C1	4.27	100.55	121.59	9	18
4	A	413	PX4	C8-C7-C6	4.27	101.69	111.79	13	12
4	A	318	PX4	P1-O4-C6	4.27	96.67	121.68	14	10
4	A	324	PX4	O5-C8-C7	4.27	120.85	108.43	5	10
4	A	354	PX4	O4-P1-O2	4.27	125.74	109.07	8	5
4	A	425	PX4	P1-O3-C1	4.27	100.59	121.59	2	17
4	A	326	PX4	O7-C23-O8	4.26	113.40	123.70	12	8
4	A	347	PX4	C12-C11-C10	4.26	97.87	113.19	11	5
4	A	384	PX4	C1-C2-N1	4.26	130.01	115.78	7	7
4	A	308	PX4	O5-C8-C7	4.26	120.83	108.43	13	14
4	A	382	PX4	P1-O3-C1	4.26	100.62	121.59	14	15
4	A	367	PX4	O5-C8-C7	4.25	120.82	108.43	6	11
4	A	376	PX4	C4-N1-C3	4.25	98.04	108.97	8	6
4	A	386	PX4	C4-N1-C3	4.25	119.91	108.97	18	4
4	A	428	PX4	C4-N1-C3	4.25	98.04	108.97	18	8
4	A	318	PX4	C8-O5-C9	4.25	101.38	117.12	12	3
4	A	322	PX4	C1-C2-N1	4.25	129.97	115.78	11	8
4	A	330	PX4	O7-C7-C6	4.25	123.79	108.40	5	5
4	A	361	PX4	P1-O4-C6	4.25	96.77	121.68	16	16
4	A	312	PX4	P1-O4-C6	4.25	96.78	121.68	10	12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	341	PX4	P1-O3-C1	4.25	100.68	121.59	1	14
4	A	368	PX4	P1-O3-C1	4.25	100.69	121.59	3	16
4	A	426	PX4	O5-C8-C7	4.25	120.80	108.43	16	11
4	A	377	PX4	P1-O3-C1	4.25	100.69	121.59	2	18
4	A	327	PX4	O5-C8-C7	4.24	120.78	108.43	7	10
4	A	334	PX4	C12-C11-C10	4.24	97.93	113.19	8	4
4	A	321	PX4	O7-C7-C6	4.24	123.76	108.40	2	8
4	A	368	PX4	C1-C2-N1	4.24	129.94	115.78	7	4
4	A	400	PX4	C8-C7-C6	4.24	101.76	111.79	20	12
4	A	428	PX4	O3-P1-O2	4.24	92.50	109.07	19	6
4	A	369	PX4	C7-O7-C23	4.24	128.23	117.79	6	4
4	A	351	PX4	C1-C2-N1	4.23	129.91	115.78	12	6
4	A	370	PX4	O7-C23-O8	4.23	113.47	123.70	4	6
4	A	390	PX4	O5-C9-C10	4.23	125.19	111.91	10	5
4	A	412	PX4	O7-C7-C8	4.23	123.72	108.40	10	10
4	A	315	PX4	O4-P1-O2	4.23	125.59	109.07	20	4
4	A	375	PX4	O7-C23-C24	4.23	120.61	111.50	1	13
4	A	388	PX4	P1-O3-C1	4.23	100.78	121.59	18	15
4	A	413	PX4	O5-C8-C7	4.23	120.73	108.43	13	11
4	A	426	PX4	C5-N1-C3	4.23	98.11	108.97	3	2
4	A	356	PX4	O7-C7-C8	4.22	123.69	108.40	6	7
4	A	382	PX4	P1-O4-C6	4.22	96.91	121.68	17	12
4	A	382	PX4	C4-N1-C3	4.22	98.11	108.97	20	6
4	A	410	PX4	P1-O3-C1	4.22	100.79	121.59	4	14
4	A	420	PX4	O7-C23-C24	4.22	120.60	111.50	4	10
4	A	426	PX4	P1-O4-C6	4.22	96.92	121.68	17	12
4	A	358	PX4	O7-C7-C8	4.22	123.69	108.40	19	7
4	A	420	PX4	C7-O7-C23	4.22	128.18	117.79	16	4
4	A	316	PX4	O7-C23-C24	4.22	120.59	111.50	19	14
4	A	320	PX4	C12-C11-C10	4.22	98.02	113.19	3	4
4	A	369	PX4	P1-O4-C6	4.22	96.94	121.68	8	13
4	A	395	PX4	C7-O7-C23	4.22	128.18	117.79	16	5
4	A	398	PX4	O5-C8-C7	4.22	120.71	108.43	19	11
4	A	430	PX4	C4-N1-C3	4.22	98.13	108.97	6	4
4	A	328	PX4	O7-C7-C8	4.22	123.67	108.40	7	6
4	A	409	PX4	C5-N1-C3	4.22	98.13	108.97	5	4
4	A	346	PX4	C8-C7-C6	4.21	101.82	111.79	18	10
4	A	378	PX4	C5-N1-C4	4.21	119.80	108.97	14	5
4	A	422	PX4	P1-O3-C1	4.21	100.85	121.59	15	16
4	A	405	PX4	O4-P1-O2	4.21	125.51	109.07	1	3
4	A	420	PX4	C11-C10-C9	4.21	98.32	113.62	12	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	319	PX4	O7-C23-C24	4.20	120.56	111.50	15	8
4	A	373	PX4	O5-C8-C7	4.20	120.65	108.43	2	12
4	A	391	PX4	C5-N1-C4	4.20	98.18	108.97	18	3
4	A	406	PX4	C26-C25-C24	4.19	98.11	113.19	6	4
4	A	344	PX4	O7-C7-C6	4.19	123.58	108.40	14	7
4	A	351	PX4	C12-C11-C10	4.19	98.12	113.19	18	4
4	A	359	PX4	O7-C23-O8	4.19	113.57	123.70	15	9
4	A	381	PX4	O7-C7-C6	4.19	123.57	108.40	8	6
4	A	383	PX4	P1-O3-C1	4.19	100.96	121.59	11	13
4	A	424	PX4	O5-C8-C7	4.19	120.63	108.43	12	12
4	A	403	PX4	O7-C23-O8	4.19	113.58	123.70	8	6
4	A	366	PX4	C7-O7-C23	4.18	128.09	117.79	8	6
4	A	393	PX4	C11-C10-C9	4.18	98.41	113.62	2	1
4	A	342	PX4	C5-N1-C3	4.18	119.72	108.97	13	4
4	A	407	PX4	C7-O7-C23	4.18	128.09	117.79	12	5
4	A	383	PX4	C7-O7-C23	4.18	128.09	117.79	7	5
4	A	358	PX4	O5-C9-C10	4.18	125.02	111.91	20	4
4	A	393	PX4	O7-C23-C24	4.18	120.51	111.50	18	10
4	A	405	PX4	P1-O3-C1	4.18	101.02	121.59	6	16
4	A	306	PX4	C12-C11-C10	4.18	98.18	113.19	13	5
4	A	358	PX4	C26-C25-C24	4.17	98.18	113.19	9	1
4	A	414	PX4	O7-C7-C8	4.17	123.52	108.40	16	10
4	A	419	PX4	C4-N1-C3	4.18	98.24	108.97	6	6
4	A	395	PX4	P1-O4-C6	4.17	97.21	121.68	10	11
4	A	382	PX4	O3-P1-O2	4.17	92.77	109.07	18	3
4	A	334	PX4	P1-O3-C1	4.17	101.07	121.59	4	12
4	A	337	PX4	P1-O3-C1	4.17	101.07	121.59	15	16
4	A	402	PX4	C8-C7-C6	4.17	101.93	111.79	20	11
4	A	359	PX4	O7-C23-C24	4.17	120.48	111.50	3	12
4	A	389	PX4	O7-C7-C6	4.17	123.48	108.40	15	7
4	A	339	PX4	O4-P1-O2	4.16	92.80	109.07	11	3
4	A	348	PX4	P1-O3-C1	4.16	101.09	121.59	15	14
4	A	317	PX4	P1-O4-C6	4.16	97.28	121.68	13	9
4	A	334	PX4	O1-P1-O3	4.16	88.43	107.75	14	3
4	A	313	PX4	O7-C7-C8	4.16	123.45	108.40	18	6
4	A	359	PX4	O5-C9-O6	4.16	113.11	123.59	13	2
4	A	420	PX4	O7-C7-C8	4.16	123.45	108.40	4	8
4	A	356	PX4	O7-C7-C6	4.15	123.44	108.40	13	5
4	A	323	PX4	O7-C7-C6	4.15	123.42	108.40	12	4
4	A	358	PX4	P1-O3-C1	4.15	101.17	121.59	7	16
4	A	339	PX4	O5-C8-C7	4.15	120.50	108.43	9	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	393	PX4	O7-C7-C6	4.14	123.41	108.40	8	7
4	A	317	PX4	P1-O3-C1	4.14	101.19	121.59	9	16
4	A	409	PX4	C7-O7-C23	4.14	127.99	117.79	3	6
4	A	318	PX4	P1-O3-C1	4.14	101.20	121.59	2	15
4	A	361	PX4	C8-C7-C6	4.14	101.99	111.79	5	13
4	A	366	PX4	O5-C9-C10	4.14	124.90	111.91	18	7
4	A	421	PX4	P1-O3-C1	4.14	101.20	121.59	6	12
4	A	307	PX4	P1-O3-C1	4.14	101.23	121.59	5	17
4	A	388	PX4	O7-C7-C6	4.14	123.37	108.40	6	7
4	A	430	PX4	P1-O3-C1	4.13	101.24	121.59	1	14
4	A	329	PX4	O5-C8-C7	4.13	120.46	108.43	17	12
4	A	388	PX4	O3-P1-O2	4.13	92.92	109.07	2	5
4	A	339	PX4	O7-C23-O8	4.13	113.72	123.70	20	3
4	A	327	PX4	O5-C9-O6	4.13	113.18	123.59	2	2
4	A	355	PX4	O5-C8-C7	4.13	120.44	108.43	2	14
4	A	386	PX4	C5-N1-C3	4.13	98.36	108.97	11	6
4	A	408	PX4	C5-N1-C4	4.12	98.37	108.97	16	7
4	A	331	PX4	O5-C8-C7	4.12	120.43	108.43	19	9
4	A	347	PX4	O7-C7-C6	4.12	123.32	108.40	14	8
4	A	380	PX4	C5-N1-C4	4.12	98.38	108.97	9	2
4	A	429	PX4	O7-C23-C24	4.12	120.38	111.50	9	8
4	A	429	PX4	C1-C2-N1	4.12	129.54	115.78	18	4
4	A	330	PX4	O5-C9-O6	4.12	113.20	123.59	9	6
4	A	343	PX4	C5-N1-C4	4.12	98.38	108.97	15	5
4	A	370	PX4	O5-C8-C7	4.12	120.42	108.43	8	9
4	A	330	PX4	C4-N1-C3	4.12	98.39	108.97	16	7
4	A	411	PX4	C7-O7-C23	4.12	127.93	117.79	2	6
4	A	312	PX4	C5-N1-C3	4.12	119.56	108.97	8	4
4	A	330	PX4	C8-C7-C6	4.11	102.06	111.79	11	12
4	A	413	PX4	O7-C23-O8	4.11	113.77	123.70	5	6
4	A	306	PX4	C7-O7-C23	4.11	127.91	117.79	3	7
4	A	378	PX4	P1-O3-C1	4.11	101.35	121.59	3	18
4	A	325	PX4	P1-O3-C1	4.11	101.36	121.59	4	17
4	A	360	PX4	O5-C9-C10	4.11	124.80	111.91	16	4
4	A	414	PX4	C5-N1-C3	4.11	98.41	108.97	6	4
4	A	405	PX4	O5-C9-C10	4.11	124.79	111.91	19	8
4	A	317	PX4	C7-O7-C23	4.10	107.69	117.79	7	5
4	A	399	PX4	C8-C7-C6	4.10	102.09	111.79	10	16
4	A	383	PX4	O5-C9-C10	4.10	124.78	111.91	17	5
4	A	406	PX4	C7-O7-C23	4.10	127.89	117.79	8	4
4	A	310	PX4	P1-O4-C6	4.10	97.65	121.68	2	12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	329	PX4	C5-N1-C4	4.10	119.51	108.97	9	3
4	A	342	PX4	P1-O3-C1	4.10	101.42	121.59	3	15
4	A	390	PX4	P1-O4-C6	4.10	97.66	121.68	17	14
4	A	407	PX4	C5-N1-C4	4.09	119.50	108.97	9	4
4	A	410	PX4	C5-N1-C3	4.09	98.45	108.97	18	6
4	A	363	PX4	C7-O7-C23	4.09	127.87	117.79	6	6
4	A	423	PX4	C5-N1-C3	4.09	98.45	108.97	13	7
4	A	312	PX4	P1-O3-C1	4.09	101.45	121.59	15	18
4	A	345	PX4	C1-C2-N1	4.09	129.44	115.78	4	3
4	A	362	PX4	C4-N1-C3	4.09	98.45	108.97	17	5
4	A	362	PX4	O5-C8-C7	4.09	120.34	108.43	10	7
4	A	404	PX4	P1-O3-C1	4.09	101.45	121.59	16	16
4	A	382	PX4	O1-P1-O2	4.09	132.46	112.24	9	8
4	A	418	PX4	C7-O7-C23	4.09	127.86	117.79	16	6
4	A	333	PX4	O4-P1-O2	4.09	93.10	109.07	19	4
4	A	305	PX4	O3-P1-O2	4.09	93.11	109.07	17	5
4	A	414	PX4	C1-C2-N1	4.09	129.42	115.78	20	6
4	A	371	PX4	C26-C25-C24	4.08	98.51	113.19	3	4
4	A	372	PX4	C4-N1-C3	4.08	98.48	108.97	7	7
4	A	381	PX4	C7-O7-C23	4.08	127.84	117.79	7	8
4	A	408	PX4	C8-C7-C6	4.08	102.14	111.79	19	15
4	A	320	PX4	C11-C10-C9	4.08	98.79	113.62	3	3
4	A	305	PX4	O7-C7-C6	4.08	123.17	108.40	2	8
4	A	414	PX4	O5-C8-C7	4.08	120.30	108.43	11	13
4	A	428	PX4	O5-C8-C7	4.08	120.30	108.43	6	11
4	A	320	PX4	C4-N1-C3	4.08	98.50	108.97	12	5
4	A	402	PX4	O7-C7-C6	4.08	123.16	108.40	19	5
4	A	430	PX4	O3-P1-O2	4.07	124.98	109.07	17	4
4	A	327	PX4	C5-N1-C3	4.07	119.44	108.97	13	3
4	A	309	PX4	O5-C9-O6	4.07	113.33	123.59	19	5
4	A	338	PX4	C26-C25-C24	4.07	98.56	113.19	12	4
4	A	371	PX4	O5-C8-C7	4.07	120.28	108.43	4	12
4	A	363	PX4	P1-O4-C6	4.07	97.83	121.68	14	13
4	A	311	PX4	P1-O3-C1	4.07	101.57	121.59	17	15
4	A	357	PX4	O7-C23-O8	4.07	113.88	123.70	5	5
4	A	352	PX4	O7-C7-C6	4.07	123.12	108.40	16	8
4	A	420	PX4	O4-P1-O2	4.07	124.95	109.07	16	2
4	A	383	PX4	C8-C7-C6	4.06	102.18	111.79	6	11
4	A	411	PX4	P1-O4-C6	4.06	97.85	121.68	11	12
4	A	311	PX4	C5-N1-C3	4.06	98.53	108.97	5	8
4	A	419	PX4	O7-C23-O8	4.06	113.88	123.70	5	9

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	369	PX4	P1-O3-C1	4.06	101.60	121.59	5	15
4	A	378	PX4	O7-C23-O8	4.06	113.89	123.70	19	7
4	A	308	PX4	P1-O4-C6	4.06	97.90	121.68	13	11
4	A	312	PX4	O5-C9-C10	4.05	124.63	111.91	4	7
4	A	329	PX4	P1-O4-C6	4.06	97.90	121.68	2	11
4	A	327	PX4	O7-C23-O8	4.05	113.91	123.70	20	6
4	A	334	PX4	O5-C9-O6	4.05	113.37	123.59	6	8
4	A	392	PX4	O1-P1-O2	4.05	132.27	112.24	9	10
4	A	411	PX4	C8-C7-C6	4.05	102.21	111.79	19	10
4	A	371	PX4	P1-O3-C1	4.05	101.67	121.59	4	18
4	A	346	PX4	P1-O4-C6	4.04	97.97	121.68	9	12
4	A	314	PX4	C5-N1-C3	4.04	98.59	108.97	4	3
4	A	423	PX4	C7-O7-C23	4.04	127.74	117.79	1	6
4	A	312	PX4	C12-C11-C10	4.04	98.67	113.19	1	3
4	A	393	PX4	O1-P1-O3	4.04	88.98	107.75	2	3
4	A	377	PX4	C1-C2-N1	4.04	129.26	115.78	3	8
4	A	385	PX4	C7-O7-C23	4.04	127.73	117.79	11	8
4	A	340	PX4	O5-C8-C7	4.04	120.18	108.43	1	5
4	A	418	PX4	C1-C2-N1	4.04	129.26	115.78	13	6
4	A	331	PX4	O3-P1-O2	4.03	93.31	109.07	13	7
4	A	338	PX4	O7-C7-C6	4.03	123.01	108.40	7	5
4	A	377	PX4	O3-P1-O2	4.03	93.31	109.07	6	4
4	A	425	PX4	O1-P1-O2	4.03	132.18	112.24	15	8
4	A	397	PX4	C8-C7-C6	4.03	102.25	111.79	15	14
4	A	311	PX4	C8-C7-C6	4.03	102.26	111.79	19	10
4	A	347	PX4	P1-O3-C1	4.03	101.76	121.59	18	15
4	A	379	PX4	P1-O3-C1	4.02	101.78	121.59	17	15
4	A	417	PX4	P1-O3-C1	4.03	101.77	121.59	7	13
4	A	309	PX4	O7-C23-C24	4.02	120.17	111.50	19	8
4	A	370	PX4	P1-O3-C1	4.02	101.80	121.59	15	11
4	A	401	PX4	O5-C8-C7	4.02	120.14	108.43	10	9
4	A	411	PX4	O7-C7-C8	4.02	122.96	108.40	19	8
4	A	312	PX4	C25-C24-C23	4.02	99.00	113.62	17	3
4	A	354	PX4	P1-O4-C6	4.02	98.12	121.68	3	12
4	A	351	PX4	P1-O4-C6	4.01	98.14	121.68	11	10
4	A	410	PX4	O7-C7-C8	4.01	122.94	108.40	3	9
4	A	389	PX4	O7-C23-O8	4.01	114.00	123.70	15	6
4	A	420	PX4	C4-N1-C3	4.01	98.66	108.97	14	6
4	A	402	PX4	C33-C32-C31	4.01	94.06	114.42	17	3
4	A	424	PX4	P1-O4-C6	4.01	98.16	121.68	20	12
4	A	313	PX4	O4-P1-O2	4.01	124.72	109.07	17	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	332	PX4	O1-P1-O2	4.01	132.06	112.24	17	7
4	A	418	PX4	P1-O4-C6	4.01	98.18	121.68	1	15
4	A	429	PX4	P1-O4-C6	4.01	98.17	121.68	7	10
4	A	410	PX4	O5-C9-O6	4.01	113.48	123.59	6	7
4	A	428	PX4	O7-C23-O8	4.01	114.02	123.70	3	7
4	A	328	PX4	C5-N1-C3	4.00	98.68	108.97	12	2
4	A	344	PX4	O5-C8-C7	4.00	120.09	108.43	2	14
4	A	352	PX4	P1-O4-C6	4.01	98.19	121.68	12	11
4	A	309	PX4	C5-N1-C4	4.00	98.68	108.97	8	4
4	A	333	PX4	O7-C7-C8	4.00	122.89	108.40	14	10
4	A	396	PX4	O7-C23-O8	4.00	114.04	123.70	1	6
4	A	415	PX4	O5-C9-O6	4.00	113.51	123.59	6	5
4	A	315	PX4	C4-N1-C3	3.99	98.71	108.97	10	4
4	A	412	PX4	O5-C9-O6	3.99	113.52	123.59	3	3
4	A	397	PX4	C5-N1-C3	3.99	98.71	108.97	14	6
4	A	315	PX4	P1-O4-C6	3.99	98.29	121.68	8	15
4	A	365	PX4	C5-N1-C4	3.99	98.72	108.97	20	6
4	A	336	PX4	O5-C8-C7	3.99	120.04	108.43	6	14
4	A	323	PX4	O3-P1-O2	3.99	93.49	109.07	8	6
4	A	368	PX4	O7-C7-C6	3.99	122.84	108.40	15	11
4	A	408	PX4	O1-P1-O2	3.99	131.95	112.24	4	7
4	A	422	PX4	C5-N1-C3	3.99	98.72	108.97	10	3
4	A	305	PX4	O5-C9-O6	3.98	113.54	123.59	8	5
4	A	323	PX4	O7-C23-C24	3.98	120.08	111.50	16	4
4	A	361	PX4	P1-O3-C1	3.98	101.99	121.59	17	17
4	A	368	PX4	O7-C23-C24	3.98	120.08	111.50	5	13
4	A	387	PX4	P1-O3-C1	3.98	102.00	121.59	15	14
4	A	428	PX4	O5-C9-O6	3.98	113.55	123.59	17	5
4	A	396	PX4	P1-O3-C1	3.98	102.01	121.59	19	14
4	A	409	PX4	P1-O3-C1	3.98	102.02	121.59	20	15
4	A	324	PX4	C7-O7-C23	3.97	127.57	117.79	17	9
4	A	350	PX4	O7-C7-C8	3.97	122.79	108.40	4	7
4	A	402	PX4	C4-N1-C3	3.97	98.76	108.97	3	6
4	A	426	PX4	C7-O7-C23	3.97	127.57	117.79	12	5
4	A	322	PX4	O7-C23-C24	3.97	120.06	111.50	19	12
4	A	310	PX4	O3-P1-O2	3.97	93.56	109.07	16	3
4	A	314	PX4	C25-C24-C23	3.97	99.18	113.62	4	2
4	A	320	PX4	C8-C7-C6	3.97	102.40	111.79	17	8
4	A	321	PX4	C12-C11-C10	3.97	98.92	113.19	8	3
4	A	368	PX4	O7-C23-O8	3.97	114.11	123.70	17	6
4	A	351	PX4	C7-O7-C23	3.97	127.56	117.79	8	9

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	398	PX4	P1-O3-C1	3.97	102.06	121.59	8	17
4	A	399	PX4	C11-C10-C9	3.97	99.20	113.62	10	2
4	A	376	PX4	P1-O4-C6	3.97	98.42	121.68	17	11
4	A	407	PX4	O1-P1-O3	3.97	126.17	107.75	2	2
4	A	315	PX4	O7-C23-O8	3.96	114.13	123.70	9	5
4	A	349	PX4	O7-C7-C8	3.96	122.75	108.40	4	6
4	A	431	PX4	P1-O4-C6	3.96	98.45	121.68	7	14
4	A	360	PX4	O7-C7-C6	3.96	122.73	108.40	7	9
4	A	423	PX4	C1-C2-N1	3.96	129.00	115.78	5	6
4	A	307	PX4	O3-P1-O2	3.96	93.61	109.07	15	6
4	A	365	PX4	C7-O7-C23	3.95	108.06	117.79	7	4
4	A	407	PX4	O1-P1-O2	3.95	131.77	112.24	14	8
4	A	327	PX4	C1-C2-N1	3.95	128.97	115.78	13	4
4	A	376	PX4	O4-P1-O2	3.95	124.50	109.07	14	2
4	A	388	PX4	C4-N1-C3	3.95	98.82	108.97	4	7
4	A	367	PX4	C26-C25-C24	3.95	99.00	113.19	17	1
4	A	412	PX4	P1-O3-C1	3.94	102.17	121.59	7	16
4	A	425	PX4	O5-C8-C7	3.95	119.92	108.43	8	10
4	A	306	PX4	C5-N1-C4	3.94	98.85	108.97	13	5
4	A	355	PX4	C4-N1-C3	3.94	98.84	108.97	4	3
4	A	408	PX4	O7-C7-C8	3.94	122.67	108.40	16	9
4	A	386	PX4	O7-C7-C8	3.94	122.66	108.40	1	7
4	A	311	PX4	C1-C2-N1	3.93	128.92	115.78	7	8
4	A	318	PX4	C4-N1-C3	3.93	98.86	108.97	19	6
4	A	338	PX4	O4-P1-O2	3.93	124.43	109.07	15	3
4	A	332	PX4	O5-C9-O6	3.93	113.67	123.59	5	4
4	A	390	PX4	O7-C23-O8	3.93	114.21	123.70	3	4
4	A	397	PX4	O7-C7-C8	3.93	122.63	108.40	11	10
4	A	306	PX4	O5-C9-C10	3.93	124.23	111.91	5	5
4	A	424	PX4	C5-N1-C4	3.93	98.88	108.97	10	6
4	A	395	PX4	C34-C33-C32	3.92	94.50	114.42	2	5
4	A	397	PX4	O7-C23-O8	3.92	114.22	123.70	4	4
4	A	398	PX4	O3-P1-O2	3.92	93.74	109.07	1	3
4	A	305	PX4	O5-C8-C7	3.92	119.85	108.43	20	7
4	A	329	PX4	P1-O3-C1	3.92	102.29	121.59	16	17
4	A	383	PX4	P1-O4-C6	3.92	98.69	121.68	15	17
4	A	354	PX4	P1-O3-C1	3.92	102.30	121.59	9	17
4	A	360	PX4	O3-P1-O2	3.92	93.77	109.07	16	7
4	A	365	PX4	P1-O4-C6	3.92	98.72	121.68	1	12
4	A	367	PX4	C1-C2-N1	3.92	128.86	115.78	20	3
4	A	377	PX4	O5-C9-O6	3.92	113.71	123.59	18	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	387	PX4	C5-N1-C4	3.92	98.90	108.97	17	1
4	A	418	PX4	O1-P1-O2	3.92	131.60	112.24	4	15
4	A	316	PX4	O7-C7-C6	3.92	122.58	108.40	2	8
4	A	373	PX4	C5-N1-C4	3.92	98.91	108.97	13	8
4	A	389	PX4	C4-N1-C3	3.91	119.04	108.97	19	7
4	A	390	PX4	C26-C25-C24	3.91	99.12	113.19	1	7
4	A	391	PX4	O1-P1-O2	3.91	131.59	112.24	17	6
4	A	385	PX4	O7-C23-O8	3.91	114.24	123.70	13	7
4	A	306	PX4	C5-N1-C3	3.91	98.92	108.97	1	7
4	A	338	PX4	C5-N1-C4	3.91	119.03	108.97	1	1
4	A	371	PX4	P1-O4-C6	3.91	98.74	121.68	3	14
4	A	346	PX4	O1-P1-O2	3.91	131.57	112.24	20	17
4	A	430	PX4	O5-C9-O6	3.91	113.72	123.59	10	6
4	A	393	PX4	O1-P1-O2	3.91	131.56	112.24	14	14
4	A	415	PX4	O7-C7-C8	3.91	122.55	108.40	3	10
4	A	361	PX4	O7-C7-C6	3.91	122.55	108.40	11	9
4	A	400	PX4	O5-C9-C10	3.90	124.16	111.91	19	6
4	A	396	PX4	O5-C9-C10	3.91	124.16	111.91	1	6
4	A	349	PX4	P1-O3-C1	3.90	102.37	121.59	18	14
4	A	338	PX4	O7-C7-C8	3.90	122.52	108.40	9	8
4	A	355	PX4	P1-O4-C6	3.90	98.82	121.68	20	13
4	A	308	PX4	O7-C7-C6	3.90	122.51	108.40	9	5
4	A	399	PX4	C7-O7-C23	3.90	127.39	117.79	12	7
4	A	411	PX4	C31-C30-C29	3.90	94.64	114.42	3	2
4	A	347	PX4	C1-C2-N1	3.89	128.78	115.78	7	4
4	A	381	PX4	C25-C24-C23	3.90	99.45	113.62	7	1
4	A	408	PX4	O4-P1-O2	3.89	124.28	109.07	8	1
4	A	361	PX4	O7-C7-C8	3.89	122.50	108.40	3	9
4	A	394	PX4	C4-N1-C3	3.89	98.97	108.97	12	2
4	A	345	PX4	C5-N1-C4	3.89	98.98	108.97	2	4
4	A	395	PX4	O7-C23-O8	3.89	114.30	123.70	19	8
4	A	381	PX4	P1-O4-C6	3.89	98.88	121.68	14	11
4	A	427	PX4	C7-O7-C23	3.89	108.22	117.79	14	8
4	A	329	PX4	O7-C7-C8	3.88	122.47	108.40	4	8
4	A	411	PX4	C5-N1-C4	3.89	98.98	108.97	18	5
4	A	330	PX4	O7-C7-C8	3.88	122.45	108.40	4	8
4	A	325	PX4	C1-C2-N1	3.88	128.73	115.78	9	4
4	A	332	PX4	C8-O5-C9	3.88	102.76	117.12	13	3
4	A	346	PX4	O7-C7-C6	3.88	122.44	108.40	16	4
4	A	356	PX4	C4-N1-C3	3.88	99.00	108.97	20	5
4	A	305	PX4	O4-P1-O2	3.87	124.21	109.07	3	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	405	PX4	O7-C7-C8	3.88	122.43	108.40	1	7
4	A	334	PX4	C4-N1-C3	3.87	99.02	108.97	13	3
4	A	326	PX4	O7-C7-C8	3.87	122.42	108.40	5	12
4	A	359	PX4	C26-C25-C24	3.87	99.28	113.19	5	4
4	A	384	PX4	O1-P1-O2	3.87	131.37	112.24	3	6
4	A	361	PX4	C4-N1-C3	3.87	99.03	108.97	2	6
4	A	346	PX4	P1-O3-C1	3.87	102.55	121.59	20	16
4	A	401	PX4	C1-C2-N1	3.87	128.69	115.78	12	6
4	A	353	PX4	O3-P1-O2	3.86	93.97	109.07	18	3
4	A	305	PX4	C5-N1-C3	3.86	99.04	108.97	8	3
4	A	319	PX4	O5-C9-C10	3.86	124.03	111.91	20	5
4	A	413	PX4	P1-O3-C1	3.86	102.57	121.59	1	14
4	A	340	PX4	P1-O3-C1	3.86	102.58	121.59	8	13
4	A	392	PX4	P1-O4-C6	3.86	99.04	121.68	20	12
4	A	394	PX4	P1-O4-C6	3.86	99.05	121.68	10	14
4	A	375	PX4	O7-C7-C8	3.86	122.37	108.40	16	7
4	A	381	PX4	O3-P1-O2	3.86	93.99	109.07	10	4
4	A	325	PX4	O5-C9-O6	3.86	113.86	123.59	11	1
4	A	391	PX4	P1-O3-C1	3.86	102.60	121.59	16	13
4	A	344	PX4	P1-O4-C6	3.86	99.07	121.68	19	15
4	A	416	PX4	O4-P1-O2	3.86	124.13	109.07	12	5
4	A	350	PX4	O5-C9-C10	3.85	124.00	111.91	20	5
4	A	306	PX4	P1-O3-C1	3.85	102.62	121.59	14	15
4	A	307	PX4	O5-C9-C10	3.85	124.00	111.91	18	4
4	A	414	PX4	C12-C11-C10	3.85	99.34	113.19	12	2
4	A	308	PX4	O4-P1-O2	3.85	94.02	109.07	14	5
4	A	373	PX4	O7-C23-O8	3.85	114.39	123.70	8	6
4	A	362	PX4	P1-O4-C6	3.85	99.12	121.68	9	10
4	A	366	PX4	C11-C10-C9	3.85	99.63	113.62	3	3
4	A	328	PX4	O7-C23-O8	3.85	114.41	123.70	11	8
4	A	342	PX4	C7-O7-C23	3.85	127.26	117.79	14	5
4	A	313	PX4	C4-N1-C3	3.84	99.09	108.97	19	4
4	A	329	PX4	C7-O7-C23	3.84	127.25	117.79	2	6
4	A	389	PX4	P1-O4-C6	3.85	99.13	121.68	2	13
4	A	329	PX4	O1-P1-O2	3.84	131.24	112.24	8	18
4	A	339	PX4	P1-O3-C1	3.84	102.67	121.59	4	13
4	A	383	PX4	O3-P1-O2	3.84	94.05	109.07	11	5
4	A	360	PX4	O5-C8-C7	3.84	119.61	108.43	14	13
4	A	431	PX4	C7-O7-C23	3.84	127.25	117.79	9	13
4	A	338	PX4	O5-C9-O6	3.84	113.91	123.59	17	5
4	A	343	PX4	O7-C23-C24	3.84	119.77	111.50	16	9

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	376	PX4	O7-C23-O8	3.84	114.43	123.70	2	7
4	A	420	PX4	O7-C7-C6	3.84	122.30	108.40	9	12
4	A	321	PX4	O3-P1-O2	3.84	94.08	109.07	9	6
4	A	343	PX4	P1-O4-C6	3.84	99.19	121.68	2	11
4	A	334	PX4	C7-O7-C23	3.83	127.23	117.79	4	4
4	A	306	PX4	O3-P1-O2	3.83	94.09	109.07	5	3
4	A	332	PX4	O7-C23-O8	3.83	114.44	123.70	5	9
4	A	345	PX4	C7-O7-C23	3.83	127.22	117.79	4	6
4	A	392	PX4	O7-C7-C6	3.83	122.27	108.40	5	7
4	A	387	PX4	C1-C2-N1	3.83	128.57	115.78	6	4
4	A	430	PX4	O7-C7-C6	3.83	122.27	108.40	18	11
4	A	344	PX4	C7-O7-C23	3.83	127.21	117.79	5	3
4	A	346	PX4	C26-C25-C24	3.83	99.43	113.19	7	6
4	A	391	PX4	O7-C23-O8	3.83	114.45	123.70	19	5
4	A	310	PX4	C26-C25-C24	3.83	99.44	113.19	9	3
4	A	354	PX4	C11-C10-C9	3.82	99.71	113.62	12	4
4	A	404	PX4	C5-N1-C3	3.82	99.14	108.97	9	5
4	A	368	PX4	C12-C11-C10	3.82	99.45	113.19	1	2
4	A	394	PX4	C7-O7-C23	3.82	127.20	117.79	12	5
4	A	351	PX4	O3-P1-O2	3.82	94.13	109.07	8	5
4	A	360	PX4	P1-O3-C1	3.82	102.78	121.59	3	17
4	A	346	PX4	O7-C23-C24	3.82	119.73	111.50	8	9
4	A	328	PX4	O5-C8-C7	3.82	119.55	108.43	12	8
4	A	354	PX4	O7-C7-C6	3.82	122.22	108.40	16	6
4	A	374	PX4	O5-C9-O6	3.82	113.95	123.59	12	7
4	A	397	PX4	O7-C23-C24	3.82	119.72	111.50	4	11
4	A	397	PX4	C20-C19-C18	3.82	95.05	114.42	9	3
4	A	420	PX4	C1-C2-N1	3.82	128.52	115.78	13	4
4	A	325	PX4	C3-N1-C2	3.81	125.52	109.92	16	2
4	A	342	PX4	O1-P1-O2	3.81	131.10	112.24	10	8
4	A	369	PX4	O4-P1-O2	3.81	123.97	109.07	7	2
4	A	341	PX4	C4-N1-C3	3.81	99.17	108.97	16	6
4	A	361	PX4	O5-C9-O6	3.81	113.97	123.59	10	4
4	A	387	PX4	O5-C9-O6	3.81	113.97	123.59	18	6
4	A	419	PX4	O5-C8-C7	3.81	119.53	108.43	16	10
4	A	379	PX4	C7-O7-C23	3.81	127.17	117.79	4	5
4	A	400	PX4	P1-O3-C1	3.81	102.85	121.59	18	14
4	A	424	PX4	O7-C7-C8	3.81	122.19	108.40	14	10
4	A	412	PX4	C4-N1-C3	3.81	99.19	108.97	10	3
4	A	406	PX4	C12-C11-C10	3.80	99.52	113.19	19	2
4	A	340	PX4	C4-N1-C3	3.80	99.20	108.97	7	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	366	PX4	O7-C23-C24	3.80	119.69	111.50	1	4
4	A	407	PX4	C26-C25-C24	3.80	99.52	113.19	4	4
4	A	399	PX4	P1-O4-C6	3.80	99.40	121.68	20	16
4	A	333	PX4	O1-P1-O3	3.80	90.10	107.75	7	5
4	A	355	PX4	C7-O7-C23	3.80	127.14	117.79	9	6
4	A	386	PX4	O7-C23-O8	3.80	114.52	123.70	13	5
4	A	340	PX4	O7-C23-O8	3.80	114.53	123.70	5	3
4	A	407	PX4	O7-C7-C6	3.79	122.14	108.40	7	6
4	A	321	PX4	O7-C23-O8	3.79	114.54	123.70	5	6
4	A	314	PX4	P1-O4-C6	3.79	99.47	121.68	17	17
4	A	312	PX4	O3-P1-O2	3.79	94.26	109.07	9	3
4	A	343	PX4	O5-C9-C10	3.79	123.80	111.91	7	2
4	A	360	PX4	O1-P1-O3	3.79	90.15	107.75	16	3
4	A	410	PX4	C26-C25-C24	3.79	126.81	113.19	14	4
4	A	389	PX4	C5-N1-C3	3.79	99.24	108.97	5	4
4	A	418	PX4	O7-C7-C8	3.79	122.11	108.40	9	6
4	A	422	PX4	O5-C9-C10	3.79	123.79	111.91	18	4
4	A	345	PX4	P1-O3-C1	3.78	102.96	121.59	11	16
4	A	364	PX4	C5-N1-C4	3.78	99.25	108.97	12	3
4	A	353	PX4	C26-C25-C24	3.78	99.60	113.19	18	4
4	A	354	PX4	O3-P1-O2	3.78	94.29	109.07	10	7
4	A	357	PX4	P1-O4-C6	3.78	99.50	121.68	19	12
4	A	380	PX4	C5-N1-C3	3.78	118.70	108.97	9	8
4	A	386	PX4	P1-O4-C6	3.78	99.49	121.68	13	15
4	A	399	PX4	O1-P1-O4	3.78	125.31	107.75	6	4
4	A	347	PX4	C4-N1-C3	3.78	99.25	108.97	2	5
4	A	331	PX4	O7-C7-C6	3.78	122.08	108.40	2	11
4	A	402	PX4	C1-C2-N1	3.78	128.40	115.78	19	4
4	A	355	PX4	O7-C7-C6	3.78	122.08	108.40	20	9
4	A	316	PX4	C30-C29-C28	3.78	95.25	114.42	12	3
4	A	339	PX4	O7-C7-C6	3.78	122.07	108.40	3	7
4	A	311	PX4	O5-C9-O6	3.77	114.07	123.59	9	6
4	A	421	PX4	O7-C23-O8	3.77	114.58	123.70	3	6
4	A	340	PX4	O5-C9-C10	3.77	123.75	111.91	9	4
4	A	416	PX4	C7-O7-C23	3.77	127.08	117.79	18	4
4	A	314	PX4	O4-P1-O2	3.77	123.80	109.07	14	4
4	A	328	PX4	P1-O3-C1	3.77	103.03	121.59	6	14
4	A	335	PX4	O5-C9-O6	3.77	114.08	123.59	14	6
4	A	361	PX4	C5-N1-C3	3.77	99.29	108.97	16	3
4	A	346	PX4	O7-C7-C8	3.77	122.04	108.40	20	8
4	A	363	PX4	P1-O3-C1	3.77	103.05	121.59	9	17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	364	PX4	O5-C9-C10	3.77	123.73	111.91	15	8
4	A	330	PX4	P1-O4-C6	3.76	99.61	121.68	1	10
4	A	370	PX4	O5-C9-C10	3.76	123.72	111.91	1	6
4	A	393	PX4	C5-N1-C3	3.76	99.30	108.97	17	5
4	A	370	PX4	C1-C2-N1	3.76	128.34	115.78	16	4
4	A	422	PX4	O5-C8-C7	3.76	119.38	108.43	16	12
4	A	321	PX4	P1-O4-C6	3.76	99.63	121.68	17	14
4	A	333	PX4	O7-C23-O8	3.76	114.62	123.70	18	7
4	A	363	PX4	O1-P1-O2	3.76	130.83	112.24	1	14
4	A	424	PX4	C7-O7-C23	3.76	127.05	117.79	4	5
4	A	376	PX4	C33-C32-C31	3.76	95.34	114.42	13	1
4	A	407	PX4	C11-C10-C9	3.76	99.95	113.62	7	2
4	A	392	PX4	P1-O3-C1	3.76	103.09	121.59	10	15
4	A	328	PX4	O1-P1-O2	3.76	130.81	112.24	6	8
4	A	396	PX4	C4-N1-C3	3.76	118.63	108.97	2	5
4	A	377	PX4	C5-N1-C3	3.75	99.32	108.97	1	6
4	A	331	PX4	O7-C7-C8	3.75	121.98	108.40	17	9
4	A	393	PX4	O7-C7-C8	3.75	121.98	108.40	19	9
4	A	359	PX4	O3-P1-O2	3.75	94.42	109.07	4	5
4	A	404	PX4	C7-O7-C23	3.75	127.02	117.79	7	6
4	A	337	PX4	C5-N1-C4	3.75	99.34	108.97	5	2
4	A	344	PX4	C5-N1-C4	3.75	99.34	108.97	19	7
4	A	349	PX4	C1-C2-N1	3.75	128.29	115.78	13	7
4	A	350	PX4	O7-C7-C6	3.75	121.97	108.40	9	4
4	A	380	PX4	O1-P1-O2	3.75	130.77	112.24	14	10
4	A	382	PX4	O7-C23-O8	3.75	114.64	123.70	4	9
4	A	390	PX4	C5-N1-C3	3.75	99.34	108.97	5	3
4	A	310	PX4	C7-O7-C23	3.75	127.01	117.79	9	6
4	A	338	PX4	O5-C9-C10	3.75	123.66	111.91	6	4
4	A	410	PX4	C12-C11-C10	3.75	99.72	113.19	13	4
4	A	313	PX4	O5-C9-O6	3.74	114.14	123.59	20	6
4	A	307	PX4	O1-P1-O4	3.74	125.14	107.75	15	5
4	A	316	PX4	O3-P1-O2	3.74	94.44	109.07	18	5
4	A	384	PX4	O5-C9-C10	3.74	123.65	111.91	15	7
4	A	409	PX4	C4-N1-C3	3.74	99.35	108.97	19	4
4	A	310	PX4	O7-C7-C8	3.74	121.94	108.40	8	11
4	A	421	PX4	O6-C9-C10	3.74	109.14	123.73	11	2
4	A	311	PX4	O7-C7-C6	3.74	121.93	108.40	1	5
4	A	336	PX4	C7-O7-C23	3.74	126.99	117.79	5	3
4	A	327	PX4	O3-P1-O2	3.74	94.47	109.07	3	8
4	A	394	PX4	P1-O3-C1	3.74	103.19	121.59	10	14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	422	PX4	P1-O4-C6	3.74	99.77	121.68	11	13
4	A	418	PX4	C4-N1-C3	3.73	118.57	108.97	20	5
4	A	406	PX4	O5-C9-C10	3.73	123.62	111.91	12	7
4	A	391	PX4	O7-C7-C8	3.73	121.91	108.40	7	6
4	A	422	PX4	O5-C9-O6	3.73	114.17	123.59	18	8
4	A	399	PX4	O3-P1-O2	3.73	94.49	109.07	16	3
4	A	309	PX4	O7-C7-C8	3.73	121.91	108.40	19	9
4	A	376	PX4	O7-C7-C8	3.73	121.91	108.40	6	13
4	A	328	PX4	O5-C9-O6	3.73	114.19	123.59	7	3
4	A	382	PX4	O4-P1-O2	3.73	123.63	109.07	18	3
4	A	403	PX4	C5-N1-C3	3.73	99.39	108.97	8	3
4	A	380	PX4	O7-C7-C8	3.72	121.89	108.40	8	7
4	A	308	PX4	P1-O3-C1	3.72	103.27	121.59	18	15
4	A	373	PX4	C1-C2-N1	3.72	128.21	115.78	13	4
4	A	384	PX4	O7-C23-O8	3.72	114.71	123.70	10	4
4	A	317	PX4	O6-C9-C10	3.72	109.22	123.73	17	2
4	A	358	PX4	O7-C7-C6	3.72	121.87	108.40	20	9
4	A	373	PX4	P1-O4-C6	3.72	99.87	121.68	9	15
4	A	409	PX4	O1-P1-O2	3.72	130.63	112.24	8	10
4	A	341	PX4	O3-P1-O2	3.72	94.54	109.07	13	4
4	A	336	PX4	P1-O4-C6	3.72	99.89	121.68	5	10
4	A	355	PX4	C1-C2-N1	3.72	128.19	115.78	17	7
4	A	367	PX4	O4-P1-O2	3.71	123.58	109.07	10	2
4	A	336	PX4	O5-C9-C10	3.71	123.56	111.91	8	6
4	A	342	PX4	O4-P1-O2	3.71	123.56	109.07	2	3
4	A	375	PX4	C1-C2-N1	3.71	128.16	115.78	19	4
4	A	423	PX4	O5-C9-O6	3.71	114.23	123.59	8	5
4	A	420	PX4	O3-P1-O2	3.71	94.58	109.07	16	7
4	A	346	PX4	C5-N1-C3	3.71	118.50	108.97	1	4
4	A	366	PX4	C26-C25-C24	3.71	99.87	113.19	9	2
4	A	367	PX4	O3-P1-O2	3.71	94.59	109.07	6	3
4	A	347	PX4	P1-O4-C6	3.70	99.96	121.68	12	16
4	A	389	PX4	C7-O7-C23	3.71	126.91	117.79	10	2
4	A	309	PX4	P1-O3-C1	3.70	103.36	121.59	11	13
4	A	346	PX4	O7-C23-O8	3.70	114.75	123.70	13	6
4	A	419	PX4	C12-C11-C10	3.70	99.88	113.19	1	5
4	A	307	PX4	O1-P1-O2	3.70	130.54	112.24	10	12
4	A	330	PX4	C1-C2-N1	3.70	128.13	115.78	13	8
4	A	406	PX4	O7-C7-C8	3.70	121.80	108.40	18	4
4	A	413	PX4	O1-P1-O4	3.70	124.94	107.75	6	6
4	A	309	PX4	O7-C7-C6	3.70	121.79	108.40	11	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	335	PX4	C5-N1-C4	3.70	99.46	108.97	4	4
4	A	366	PX4	O5-C9-O6	3.70	114.25	123.59	19	2
4	A	397	PX4	C4-N1-C3	3.70	99.46	108.97	19	4
4	A	344	PX4	C4-N1-C3	3.70	99.47	108.97	3	4
4	A	348	PX4	O5-C9-O6	3.70	114.26	123.59	4	4
4	A	371	PX4	O7-C23-C24	3.70	119.47	111.50	14	9
4	A	411	PX4	O5-C9-O6	3.69	114.27	123.59	15	7
4	A	393	PX4	P1-O4-C6	3.70	100.01	121.68	9	11
4	A	431	PX4	O1-P1-O2	3.70	130.51	112.24	6	10
4	A	314	PX4	O3-P1-O2	3.69	94.64	109.07	16	6
4	A	357	PX4	C4-N1-C2	3.69	94.80	109.92	14	3
4	A	408	PX4	O5-C9-O6	3.69	114.27	123.59	9	9
4	A	350	PX4	C14-C13-C12	3.69	95.68	114.42	11	1
4	A	364	PX4	O5-C9-O6	3.69	114.27	123.59	1	5
4	A	311	PX4	O7-C23-O8	3.69	114.78	123.70	18	9
4	A	378	PX4	C7-O7-C23	3.69	108.70	117.79	7	6
4	A	407	PX4	P1-O4-C6	3.69	100.03	121.68	11	14
4	A	313	PX4	O7-C7-C6	3.69	121.76	108.40	19	9
4	A	428	PX4	C12-C11-C10	3.69	99.92	113.19	1	6
4	A	324	PX4	O5-C9-C10	3.69	123.48	111.91	7	4
4	A	336	PX4	O4-P1-O2	3.69	123.47	109.07	20	5
4	A	353	PX4	O5-C9-C10	3.68	123.47	111.91	9	7
4	A	319	PX4	P1-O3-C1	3.68	103.46	121.59	1	15
4	A	359	PX4	O1-P1-O3	3.68	90.64	107.75	9	3
4	A	401	PX4	O7-C7-C8	3.68	121.74	108.40	2	11
4	A	343	PX4	O4-P1-O2	3.68	123.46	109.07	20	3
4	A	366	PX4	P1-O4-C6	3.68	100.08	121.68	7	11
4	A	360	PX4	O1-P1-O2	3.68	130.43	112.24	16	8
4	A	306	PX4	O7-C23-O8	3.68	114.82	123.70	16	6
4	A	316	PX4	C1-C2-N1	3.68	128.06	115.78	14	6
4	A	427	PX4	O7-C7-C8	3.68	121.72	108.40	8	9
4	A	400	PX4	C5-N1-C3	3.68	99.52	108.97	8	5
4	A	405	PX4	P1-O4-C6	3.68	100.13	121.68	16	14
4	A	387	PX4	C7-O7-C23	3.67	126.84	117.79	7	4
4	A	423	PX4	O1-P1-O2	3.67	130.40	112.24	3	6
4	A	334	PX4	C8-O5-C9	3.67	103.52	117.12	9	2
4	A	412	PX4	P1-O4-C6	3.67	100.14	121.68	20	12
4	A	431	PX4	C4-N1-C3	3.67	99.53	108.97	6	7
4	A	356	PX4	C5-N1-C4	3.67	99.54	108.97	3	5
4	A	319	PX4	P1-O4-C6	3.67	100.16	121.68	8	16
4	A	416	PX4	O1-P1-O2	3.67	130.38	112.24	7	11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	328	PX4	P1-O4-C6	3.67	100.17	121.68	5	13
4	A	329	PX4	O7-C23-O8	3.67	114.84	123.70	1	5
4	A	372	PX4	C5-N1-C3	3.67	99.55	108.97	20	6
4	A	344	PX4	O5-C9-C10	3.66	123.41	111.91	15	5
4	A	425	PX4	O7-C23-O8	3.66	114.84	123.70	20	7
4	A	362	PX4	O3-P1-O2	3.66	94.75	109.07	15	6
4	A	318	PX4	O5-C9-C10	3.66	123.40	111.91	6	6
4	A	379	PX4	O7-C7-C6	3.66	121.66	108.40	4	6
4	A	322	PX4	O1-P1-O2	3.66	130.34	112.24	7	13
4	A	403	PX4	O7-C7-C8	3.66	121.66	108.40	18	10
4	A	416	PX4	O3-P1-O2	3.66	94.76	109.07	7	11
4	A	331	PX4	P1-O3-C1	3.66	103.57	121.59	17	16
4	A	428	PX4	C1-C2-N1	3.66	128.00	115.78	19	7
4	A	352	PX4	C26-C25-C24	3.66	100.04	113.19	9	4
4	A	427	PX4	C3-N1-C2	3.66	124.88	109.92	20	2
4	A	319	PX4	C1-C2-N1	3.66	127.98	115.78	12	7
4	A	320	PX4	P1-O3-C1	3.66	103.59	121.59	14	13
4	A	367	PX4	C32-C31-C30	3.66	95.87	114.42	15	5
4	A	426	PX4	C1-C2-N1	3.66	127.98	115.78	20	7
4	A	359	PX4	O5-C9-C10	3.65	123.37	111.91	14	6
4	A	363	PX4	C18-C17-C16	3.65	95.88	114.42	7	2
4	A	415	PX4	C4-N1-C3	3.65	99.58	108.97	17	5
4	A	390	PX4	C1-C2-N1	3.65	127.97	115.78	9	7
4	A	411	PX4	O5-C9-C10	3.65	123.36	111.91	1	4
4	A	339	PX4	O7-C7-C8	3.65	121.61	108.40	14	6
4	A	316	PX4	O7-C7-C8	3.65	121.61	108.40	17	9
4	A	341	PX4	O5-C9-C10	3.65	123.35	111.91	18	5
4	A	367	PX4	P1-O3-C1	3.65	103.64	121.59	7	15
4	A	399	PX4	O5-C8-C7	3.65	119.05	108.43	8	10
4	A	377	PX4	O7-C23-O8	3.65	114.89	123.70	13	9
4	A	383	PX4	O1-P1-O2	3.65	130.26	112.24	20	8
4	A	428	PX4	C7-O7-C23	3.65	126.77	117.79	8	5
4	A	411	PX4	C1-C2-N1	3.65	127.95	115.78	7	7
4	A	408	PX4	O7-C7-C6	3.64	121.60	108.40	19	11
4	A	398	PX4	O5-C9-C10	3.65	123.35	111.91	11	5
4	A	371	PX4	O3-P1-O2	3.64	94.83	109.07	8	4
4	A	356	PX4	O7-C23-C24	3.64	119.35	111.50	8	10
4	A	323	PX4	C27-C26-C25	3.64	95.95	114.42	11	1
4	A	361	PX4	O1-P1-O2	3.64	130.23	112.24	6	5
4	A	390	PX4	C5-N1-C4	3.64	99.62	108.97	10	6
4	A	395	PX4	O3-P1-O2	3.64	94.85	109.07	16	8

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	326	PX4	C25-C24-C23	3.64	100.39	113.62	19	4
4	A	317	PX4	O7-C7-C8	3.64	121.57	108.40	16	7
4	A	326	PX4	O1-P1-O3	3.64	90.85	107.75	4	1
4	A	348	PX4	O7-C23-O8	3.64	114.91	123.70	18	6
4	A	385	PX4	O7-C7-C6	3.64	121.57	108.40	7	5
4	A	376	PX4	O1-P1-O3	3.64	90.86	107.75	14	2
4	A	385	PX4	C1-C2-N1	3.64	127.92	115.78	18	5
4	A	419	PX4	O7-C7-C6	3.64	121.57	108.40	12	7
4	A	381	PX4	O5-C8-C7	3.63	119.01	108.43	20	13
4	A	382	PX4	O7-C7-C8	3.63	121.56	108.40	2	9
4	A	317	PX4	O7-C7-C6	3.63	121.55	108.40	5	7
4	A	365	PX4	O5-C8-C7	3.63	119.00	108.43	19	11
4	A	427	PX4	O1-P1-O2	3.63	130.19	112.24	14	9
4	A	309	PX4	O1-P1-O2	3.63	130.18	112.24	3	10
4	A	341	PX4	C5-N1-C3	3.63	99.64	108.97	1	4
4	A	401	PX4	C26-C25-C24	3.63	100.15	113.19	8	5
4	A	372	PX4	P1-O4-C6	3.63	100.40	121.68	8	13
4	A	337	PX4	O1-P1-O2	3.63	130.17	112.24	9	10
4	A	356	PX4	O5-C9-C10	3.63	123.28	111.91	14	5
4	A	366	PX4	O7-C7-C6	3.63	121.53	108.40	1	7
4	A	409	PX4	O5-C9-O6	3.63	114.44	123.59	5	3
4	A	375	PX4	C5-N1-C3	3.62	99.66	108.97	18	5
4	A	339	PX4	C12-C11-C10	3.62	100.18	113.19	1	4
4	A	394	PX4	O7-C7-C8	3.62	121.51	108.40	3	2
4	A	347	PX4	O7-C7-C8	3.62	121.50	108.40	18	4
4	A	400	PX4	C1-C2-N1	3.62	127.86	115.78	20	7
4	A	371	PX4	O5-C9-O6	3.62	114.46	123.59	11	6
4	A	423	PX4	O7-C7-C6	3.62	121.50	108.40	13	7
4	A	360	PX4	O5-C9-O6	3.62	114.47	123.59	16	8
4	A	403	PX4	C11-C10-C9	3.61	100.48	113.62	3	2
4	A	396	PX4	C5-N1-C3	3.61	99.68	108.97	2	4
4	A	315	PX4	O5-C9-C10	3.61	123.25	111.91	7	5
4	A	322	PX4	C5-N1-C3	3.61	99.69	108.97	16	3
4	A	344	PX4	O1-P1-O2	3.61	130.08	112.24	2	7
4	A	362	PX4	O1-P1-O2	3.61	130.09	112.24	15	10
4	A	372	PX4	O7-C7-C6	3.61	121.47	108.40	7	11
4	A	364	PX4	O7-C7-C8	3.61	121.47	108.40	4	9
4	A	317	PX4	C11-C10-C9	3.61	100.50	113.62	14	3
4	A	364	PX4	C4-N1-C2	3.61	124.68	109.92	16	4
4	A	400	PX4	O5-C9-O6	3.61	114.49	123.59	19	7
4	A	415	PX4	P1-O3-C1	3.61	103.83	121.59	12	16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	377	PX4	P1-O4-C6	3.61	100.54	121.68	12	17
4	A	323	PX4	O5-C9-C10	3.60	123.22	111.91	7	4
4	A	378	PX4	C12-C11-C10	3.60	100.23	113.19	11	3
4	A	394	PX4	C1-C2-N1	3.60	127.81	115.78	12	2
4	A	428	PX4	C5-N1-C4	3.60	118.24	108.97	7	4
4	A	318	PX4	O1-P1-O2	3.60	130.04	112.24	8	9
4	A	372	PX4	C17-C16-C15	3.60	96.14	114.42	13	2
4	A	380	PX4	O5-C9-O6	3.60	114.50	123.59	14	4
4	A	318	PX4	O5-C9-O6	3.60	114.51	123.59	5	8
4	A	321	PX4	O4-P1-O2	3.60	123.13	109.07	11	4
4	A	365	PX4	C4-N1-C2	3.60	95.19	109.92	5	1
4	A	421	PX4	C5-N1-C3	3.60	99.72	108.97	12	4
4	A	422	PX4	O1-P1-O4	3.60	124.46	107.75	2	3
4	A	428	PX4	O4-P1-O2	3.60	123.13	109.07	13	5
4	A	335	PX4	C5-N1-C3	3.60	118.22	108.97	13	2
4	A	305	PX4	C25-C24-C23	3.60	100.54	113.62	16	4
4	A	350	PX4	P1-O4-C6	3.60	100.60	121.68	6	10
4	A	361	PX4	O7-C23-O8	3.60	115.01	123.70	6	7
4	A	372	PX4	C27-C26-C25	3.60	96.17	114.42	11	2
4	A	326	PX4	C16-C15-C14	3.59	96.19	114.42	11	3
4	A	424	PX4	O7-C7-C6	3.59	121.41	108.40	17	6
4	A	427	PX4	O5-C9-O6	3.59	114.53	123.59	14	2
4	A	337	PX4	O5-C9-O6	3.59	114.54	123.59	17	7
4	A	410	PX4	P1-O4-C6	3.59	100.64	121.68	9	12
4	A	309	PX4	P1-O4-C6	3.59	100.65	121.68	1	11
4	A	313	PX4	O1-P1-O3	3.59	91.09	107.75	6	3
4	A	388	PX4	O5-C9-O6	3.59	114.54	123.59	18	3
4	A	394	PX4	O1-P1-O2	3.59	129.97	112.24	1	9
4	A	374	PX4	P1-O4-C6	3.58	100.66	121.68	6	11
4	A	425	PX4	P1-O4-C6	3.58	100.66	121.68	14	16
4	A	426	PX4	O1-P1-O3	3.59	91.09	107.75	7	1
4	A	305	PX4	O1-P1-O2	3.58	129.95	112.24	16	10
4	A	315	PX4	C1-C2-N1	3.58	127.74	115.78	3	4
4	A	307	PX4	O7-C7-C8	3.58	121.36	108.40	8	9
4	A	338	PX4	C4-N1-C3	3.58	99.77	108.97	19	3
4	A	348	PX4	O7-C7-C8	3.58	121.37	108.40	3	3
4	A	357	PX4	P1-O3-C1	3.58	103.96	121.59	14	13
4	A	400	PX4	P1-O4-C6	3.58	100.68	121.68	12	16
4	A	396	PX4	O7-C7-C6	3.58	121.37	108.40	6	8
4	A	334	PX4	C5-N1-C3	3.58	99.77	108.97	18	11
4	A	334	PX4	O7-C7-C8	3.58	121.36	108.40	10	7

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	428	PX4	O1-P1-O2	3.58	129.93	112.24	1	11
4	A	402	PX4	C25-C24-C23	3.58	100.61	113.62	4	3
4	A	332	PX4	O7-C7-C8	3.58	121.35	108.40	20	5
4	A	353	PX4	O7-C7-C6	3.58	121.35	108.40	3	9
4	A	310	PX4	O1-P1-O2	3.57	129.91	112.24	4	14
4	A	324	PX4	C4-N1-C3	3.57	99.78	108.97	16	4
4	A	382	PX4	C14-C13-C12	3.58	96.28	114.42	17	2
4	A	396	PX4	P1-O4-C6	3.58	100.72	121.68	4	8
4	A	336	PX4	C4-N1-C3	3.57	99.79	108.97	19	2
4	A	370	PX4	P1-O4-C6	3.57	100.73	121.68	19	16
4	A	378	PX4	C5-N1-C3	3.57	99.79	108.97	16	7
4	A	388	PX4	P1-O4-C6	3.57	100.73	121.68	9	13
4	A	390	PX4	C7-O7-C23	3.57	126.58	117.79	4	4
4	A	423	PX4	O7-C7-C8	3.57	121.33	108.40	17	7
4	A	374	PX4	O7-C23-O8	3.57	115.07	123.70	16	4
4	A	388	PX4	O7-C23-O8	3.57	115.07	123.70	12	5
4	A	323	PX4	O7-C7-C8	3.57	121.31	108.40	1	4
4	A	387	PX4	O1-P1-O2	3.57	129.88	112.24	14	8
4	A	315	PX4	C32-C31-C30	3.56	96.33	114.42	6	2
4	A	332	PX4	C12-C11-C10	3.56	100.38	113.19	13	1
4	A	361	PX4	O5-C9-C10	3.57	123.10	111.91	1	7
4	A	348	PX4	C4-N1-C3	3.56	118.14	108.97	13	6
4	A	341	PX4	O7-C7-C6	3.56	121.30	108.40	17	8
4	A	391	PX4	O1-P1-O3	3.56	91.20	107.75	2	8
4	A	426	PX4	O5-C9-O6	3.56	114.60	123.59	12	6
4	A	307	PX4	O7-C7-C6	3.56	121.29	108.40	19	6
4	A	415	PX4	C5-N1-C4	3.56	99.83	108.97	11	3
4	A	322	PX4	O6-C9-C10	3.55	109.87	123.73	5	2
4	A	362	PX4	C26-C25-C24	3.55	125.97	113.19	1	3
4	A	317	PX4	C8-O5-C9	3.55	103.97	117.12	15	2
4	A	344	PX4	O4-P1-O2	3.55	95.18	109.07	5	1
4	A	409	PX4	P1-O4-C6	3.55	100.84	121.68	12	14
4	A	331	PX4	C28-C27-C26	3.55	96.39	114.42	6	1
4	A	391	PX4	P1-O4-C6	3.55	100.85	121.68	7	12
4	A	408	PX4	P1-O4-C6	3.55	100.86	121.68	9	14
4	A	321	PX4	C18-C17-C16	3.55	96.42	114.42	7	4
4	A	353	PX4	O7-C7-C8	3.55	121.24	108.40	4	7
4	A	380	PX4	O3-P1-O2	3.55	95.21	109.07	8	2
4	A	408	PX4	C1-C2-N1	3.55	127.62	115.78	2	8
4	A	322	PX4	P1-O4-C6	3.54	100.89	121.68	15	13
4	A	430	PX4	P1-O4-C6	3.55	100.89	121.68	14	9

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	351	PX4	O7-C7-C8	3.54	121.23	108.40	6	4
4	A	402	PX4	O7-C7-C8	3.54	121.23	108.40	4	5
4	A	401	PX4	C5-N1-C3	3.54	99.87	108.97	11	4
4	A	419	PX4	C1-C2-N1	3.54	127.61	115.78	13	8
4	A	309	PX4	C14-C13-C12	3.54	96.45	114.42	9	2
4	A	390	PX4	O7-C7-C6	3.54	121.22	108.40	2	7
4	A	307	PX4	P1-O4-C6	3.54	100.94	121.68	9	14
4	A	342	PX4	O5-C9-O6	3.54	114.66	123.59	18	5
4	A	410	PX4	O7-C7-C6	3.54	121.22	108.40	1	8
4	A	328	PX4	O7-C7-C6	3.54	121.21	108.40	3	5
4	A	398	PX4	O7-C7-C6	3.53	121.20	108.40	8	6
4	A	422	PX4	O7-C7-C8	3.53	121.20	108.40	15	10
4	A	429	PX4	C7-O7-C23	3.54	109.09	117.79	1	5
4	A	334	PX4	O1-P1-O2	3.53	129.71	112.24	8	9
4	A	370	PX4	O7-C7-C8	3.53	121.19	108.40	5	9
4	A	401	PX4	O6-C9-C10	3.53	109.96	123.73	13	3
4	A	403	PX4	C25-C24-C23	3.53	100.78	113.62	7	2
4	A	326	PX4	C1-C2-N1	3.53	127.57	115.78	11	4
4	A	334	PX4	P1-O4-C6	3.53	100.98	121.68	15	12
4	A	335	PX4	O7-C7-C8	3.53	121.18	108.40	12	11
4	A	348	PX4	C1-C2-N1	3.53	127.57	115.78	12	2
4	A	372	PX4	O5-C9-O6	3.53	114.68	123.59	18	8
4	A	315	PX4	C5-N1-C4	3.53	99.90	108.97	17	5
4	A	393	PX4	C5-N1-C4	3.53	99.90	108.97	1	2
4	A	333	PX4	O5-C9-C10	3.53	122.97	111.91	6	2
4	A	398	PX4	P1-O4-C6	3.53	101.01	121.68	20	7
4	A	429	PX4	C5-N1-C4	3.53	99.91	108.97	16	4
4	A	384	PX4	C4-N1-C3	3.52	99.91	108.97	4	4
4	A	409	PX4	O3-P1-O2	3.52	95.30	109.07	7	4
4	A	417	PX4	C1-C2-N1	3.52	127.55	115.78	5	9
4	A	341	PX4	O1-P1-O2	3.52	129.66	112.24	10	12
4	A	349	PX4	P1-O4-C6	3.52	101.03	121.68	14	15
4	A	381	PX4	O1-P1-O2	3.52	129.66	112.24	11	11
4	A	422	PX4	O7-C23-O8	3.52	115.19	123.70	18	5
4	A	425	PX4	C16-C15-C14	3.52	96.54	114.42	18	2
4	A	354	PX4	C7-O7-C23	3.52	126.46	117.79	18	6
4	A	415	PX4	O5-C8-C7	3.52	118.69	108.43	18	10
4	A	325	PX4	P1-O4-C6	3.52	101.05	121.68	5	16
4	A	332	PX4	C3-N1-C2	3.52	124.32	109.92	8	2
4	A	412	PX4	C1-C2-N1	3.52	127.53	115.78	2	9
4	A	341	PX4	O5-C9-O6	3.52	114.71	123.59	20	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	312	PX4	C26-C25-C24	3.52	100.55	113.19	14	3
4	A	366	PX4	O1-P1-O3	3.52	91.41	107.75	2	3
4	A	403	PX4	C5-N1-C4	3.52	99.93	108.97	6	3
4	A	431	PX4	C5-N1-C3	3.52	99.93	108.97	11	4
4	A	306	PX4	C1-C2-N1	3.52	127.52	115.78	12	6
4	A	320	PX4	O1-P1-O2	3.51	129.62	112.24	15	12
4	A	380	PX4	P1-O4-C6	3.52	101.07	121.68	18	13
4	A	386	PX4	O1-P1-O2	3.52	129.62	112.24	9	7
4	A	321	PX4	C26-C25-C24	3.51	100.56	113.19	18	5
4	A	348	PX4	O7-C7-C6	3.51	121.12	108.40	1	11
4	A	351	PX4	C5-N1-C4	3.51	99.94	108.97	16	4
4	A	414	PX4	P1-O4-C6	3.51	101.07	121.68	11	14
4	A	398	PX4	O1-P1-O2	3.51	129.61	112.24	9	7
4	A	342	PX4	O3-P1-O2	3.51	95.35	109.07	17	5
4	A	384	PX4	C26-C25-C24	3.51	100.57	113.19	4	6
4	A	340	PX4	O3-P1-O2	3.51	95.36	109.07	4	3
4	A	350	PX4	C5-N1-C3	3.51	99.95	108.97	15	4
4	A	370	PX4	C25-C24-C23	3.51	100.86	113.62	9	5
4	A	374	PX4	O1-P1-O2	3.51	129.59	112.24	11	10
4	A	386	PX4	C12-C11-C10	3.51	100.58	113.19	16	5
4	A	413	PX4	C1-C2-N1	3.51	127.49	115.78	15	4
4	A	305	PX4	C12-C11-C10	3.51	100.58	113.19	13	3
4	A	366	PX4	C1-C2-N1	3.51	127.48	115.78	6	6
4	A	390	PX4	O7-C7-C8	3.51	121.09	108.40	19	6
4	A	349	PX4	O7-C23-O8	3.50	115.23	123.70	10	5
4	A	402	PX4	C32-C31-C30	3.50	96.64	114.42	9	2
4	A	383	PX4	O1-P1-O3	3.50	91.47	107.75	15	3
4	A	313	PX4	P1-O3-C1	3.50	104.34	121.59	6	12
4	A	370	PX4	C17-C16-C15	3.50	96.65	114.42	2	2
4	A	405	PX4	C5-N1-C4	3.50	99.97	108.97	12	5
4	A	391	PX4	C5-N1-C3	3.50	99.97	108.97	20	3
4	A	327	PX4	O1-P1-O2	3.50	129.54	112.24	11	15
4	A	308	PX4	C7-O7-C23	3.50	109.18	117.79	8	3
4	A	399	PX4	C5-N1-C4	3.50	99.98	108.97	3	3
4	A	431	PX4	O7-C23-O8	3.50	115.25	123.70	13	4
4	A	317	PX4	C26-C25-C24	3.50	100.62	113.19	5	4
4	A	322	PX4	O7-C7-C6	3.50	121.06	108.40	4	5
4	A	347	PX4	O5-C9-O6	3.50	114.77	123.59	7	5
4	A	366	PX4	O7-C7-C8	3.50	121.06	108.40	10	8
4	A	419	PX4	P1-O4-C6	3.49	101.19	121.68	8	15
4	A	420	PX4	P1-O4-C6	3.50	101.18	121.68	14	15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	428	PX4	O7-C7-C6	3.50	121.06	108.40	11	6
4	A	335	PX4	O7-C7-C6	3.49	121.05	108.40	18	4
4	A	357	PX4	O7-C7-C6	3.49	121.05	108.40	2	9
4	A	430	PX4	C4-N1-C2	3.49	95.63	109.92	10	1
4	A	431	PX4	C1-C2-N1	3.49	127.44	115.78	8	3
4	A	371	PX4	C1-C2-N1	3.49	127.43	115.78	20	7
4	A	408	PX4	O5-C9-C10	3.49	122.86	111.91	3	7
4	A	345	PX4	O7-C7-C6	3.49	121.03	108.40	10	6
4	A	364	PX4	O7-C23-O8	3.49	115.27	123.70	13	5
4	A	410	PX4	O3-P1-O2	3.49	95.44	109.07	5	5
4	A	343	PX4	O1-P1-O2	3.49	129.47	112.24	11	11
4	A	385	PX4	P1-O4-C6	3.49	101.23	121.68	6	13
4	A	427	PX4	O5-C9-C10	3.49	122.85	111.91	6	1
4	A	391	PX4	O7-C7-C6	3.49	121.02	108.40	4	8
4	A	373	PX4	O5-C9-O6	3.48	114.80	123.59	13	9
4	A	374	PX4	C5-N1-C3	3.48	100.02	108.97	4	6
4	A	420	PX4	O1-P1-O2	3.48	129.47	112.24	12	8
4	A	424	PX4	C16-C15-C14	3.48	96.74	114.42	15	4
4	A	319	PX4	O1-P1-O2	3.48	129.45	112.24	20	10
4	A	329	PX4	C8-C7-C6	3.48	103.55	111.79	19	8
4	A	324	PX4	O3-P1-O2	3.48	95.47	109.07	7	1
4	A	345	PX4	P1-O4-C6	3.48	101.27	121.68	18	15
4	A	326	PX4	O5-C9-O6	3.48	114.81	123.59	16	4
4	A	384	PX4	O7-C7-C8	3.48	121.00	108.40	18	6
4	A	389	PX4	C28-C27-C26	3.48	96.76	114.42	17	1
4	A	412	PX4	O1-P1-O2	3.48	129.45	112.24	13	10
4	A	400	PX4	C25-C24-C23	3.48	100.97	113.62	15	3
4	A	384	PX4	O8-C23-C24	3.48	110.16	123.73	3	1
4	A	426	PX4	O7-C7-C8	3.48	121.00	108.40	5	8
4	A	427	PX4	P1-O4-C6	3.48	101.28	121.68	3	16
4	A	370	PX4	C3-N1-C2	3.48	95.69	109.92	14	2
4	A	390	PX4	O5-C9-O6	3.48	114.81	123.59	10	6
4	A	411	PX4	O4-P1-O2	3.48	95.48	109.07	2	4
4	A	419	PX4	C17-C16-C15	3.48	96.78	114.42	9	3
4	A	418	PX4	P1-O3-C1	3.47	104.49	121.59	15	13
4	A	427	PX4	C4-N1-C3	3.48	100.04	108.97	19	5
4	A	331	PX4	C5-N1-C3	3.47	100.05	108.97	19	5
4	A	334	PX4	O4-P1-O2	3.47	95.49	109.07	5	3
4	A	385	PX4	O7-C7-C8	3.47	120.98	108.40	2	14
4	A	384	PX4	O7-C7-C6	3.47	120.97	108.40	4	8
4	A	410	PX4	O5-C9-C10	3.47	122.80	111.91	14	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	307	PX4	C1-C2-N1	3.47	127.37	115.78	7	10
4	A	384	PX4	O1-P1-O3	3.47	123.86	107.75	19	1
4	A	332	PX4	O1-P1-O4	3.47	123.85	107.75	13	3
4	A	353	PX4	P1-O4-C6	3.47	101.34	121.68	17	12
4	A	359	PX4	C11-C10-C9	3.47	101.01	113.62	6	2
4	A	377	PX4	O7-C7-C6	3.47	120.96	108.40	4	7
4	A	409	PX4	C25-C24-C23	3.47	126.23	113.62	1	4
4	A	357	PX4	C1-C2-N1	3.47	127.36	115.78	3	6
4	A	377	PX4	O1-P1-O2	3.47	129.38	112.24	10	9
4	A	389	PX4	O7-C7-C8	3.46	120.94	108.40	11	5
4	A	352	PX4	O7-C23-O8	3.46	115.34	123.70	2	8
4	A	358	PX4	P1-O4-C6	3.46	101.38	121.68	8	13
4	A	400	PX4	C4-N1-C3	3.46	100.07	108.97	12	4
4	A	401	PX4	C5-N1-C4	3.46	100.07	108.97	8	6
4	A	397	PX4	O5-C9-C10	3.46	122.77	111.91	9	5
4	A	326	PX4	C12-C11-C10	3.46	100.75	113.19	15	1
4	A	330	PX4	O5-C9-C10	3.46	122.77	111.91	20	7
4	A	369	PX4	O5-C9-O6	3.46	114.86	123.59	11	3
4	A	315	PX4	O1-P1-O2	3.46	129.33	112.24	13	12
4	A	357	PX4	O1-P1-O2	3.46	129.32	112.24	4	12
4	A	415	PX4	O5-C9-C10	3.45	122.75	111.91	7	6
4	A	362	PX4	O7-C23-O8	3.45	115.36	123.70	20	9
4	A	364	PX4	P1-O4-C6	3.45	101.44	121.68	17	10
4	A	397	PX4	C26-C25-C24	3.45	100.78	113.19	10	2
4	A	391	PX4	C1-C2-N1	3.45	127.30	115.78	8	7
4	A	418	PX4	O5-C9-O6	3.45	114.88	123.59	10	4
4	A	372	PX4	C7-O7-C23	3.45	109.30	117.79	9	10
4	A	415	PX4	P1-O4-C6	3.45	101.45	121.68	1	14
4	A	314	PX4	C11-C10-C9	3.45	101.08	113.62	6	2
4	A	337	PX4	O5-C9-C10	3.45	122.73	111.91	4	4
4	A	336	PX4	C25-C24-C23	3.45	101.09	113.62	18	2
4	A	321	PX4	O5-C9-O6	3.44	114.90	123.59	18	6
4	A	347	PX4	C5-N1-C2	3.45	124.02	109.92	9	2
4	A	391	PX4	O1-P1-O4	3.45	123.75	107.75	18	6
4	A	341	PX4	P1-O4-C6	3.44	101.48	121.68	5	14
4	A	350	PX4	O1-P1-O2	3.44	129.27	112.24	11	9
4	A	389	PX4	C12-C11-C10	3.44	100.81	113.19	1	4
4	A	364	PX4	O3-P1-O2	3.44	95.62	109.07	14	5
4	A	358	PX4	C5-N1-C4	3.44	100.13	108.97	20	3
4	A	413	PX4	O1-P1-O2	3.44	129.26	112.24	3	8
4	A	383	PX4	O7-C7-C8	3.44	120.86	108.40	6	8

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	358	PX4	O7-C23-C24	3.44	118.91	111.50	4	7
4	A	307	PX4	O5-C9-O6	3.44	114.92	123.59	5	1
4	A	329	PX4	C5-N1-C3	3.44	100.14	108.97	9	1
4	A	366	PX4	O4-P1-O2	3.44	122.50	109.07	2	3
4	A	366	PX4	C5-N1-C4	3.44	100.14	108.97	16	5
4	A	423	PX4	O5-C9-C10	3.44	122.70	111.91	1	5
4	A	308	PX4	C1-C2-N1	3.44	127.25	115.78	17	3
4	A	331	PX4	O4-P1-O2	3.44	122.49	109.07	13	5
4	A	382	PX4	C18-C17-C16	3.44	96.98	114.42	1	1
4	A	391	PX4	C4-N1-C3	3.44	100.14	108.97	13	3
4	A	336	PX4	C18-C17-C16	3.44	96.98	114.42	20	3
4	A	429	PX4	O7-C23-O8	3.44	115.40	123.70	2	4
4	A	308	PX4	O1-P1-O2	3.43	129.22	112.24	17	12
4	A	345	PX4	C25-C24-C23	3.43	101.13	113.62	2	1
4	A	340	PX4	P1-O4-C6	3.43	101.55	121.68	7	11
4	A	378	PX4	P1-O4-C6	3.43	101.56	121.68	14	16
4	A	418	PX4	O5-C9-C10	3.43	122.68	111.91	6	9
4	A	351	PX4	O7-C7-C6	3.43	120.82	108.40	19	8
4	A	348	PX4	P1-O4-C6	3.43	101.57	121.68	5	7
4	A	320	PX4	C16-C15-C14	3.43	97.02	114.42	2	2
4	A	319	PX4	C12-C11-C10	3.43	100.88	113.19	7	3
4	A	343	PX4	C4-N1-C3	3.43	100.16	108.97	1	5
4	A	350	PX4	C12-C11-C10	3.43	100.88	113.19	8	4
4	A	355	PX4	O5-C9-O6	3.43	114.94	123.59	13	4
4	A	403	PX4	O3-P1-O2	3.43	95.68	109.07	18	4
4	A	381	PX4	C26-C25-C24	3.43	100.87	113.19	13	4
4	A	313	PX4	C7-O7-C23	3.42	126.22	117.79	18	8
4	A	384	PX4	C25-C24-C23	3.43	101.16	113.62	6	3
4	A	391	PX4	O3-P1-O2	3.43	95.68	109.07	17	5
4	A	429	PX4	O7-C7-C8	3.42	120.80	108.40	4	4
4	A	355	PX4	O1-P1-O2	3.42	129.16	112.24	4	8
4	A	365	PX4	C5-N1-C3	3.42	117.77	108.97	5	7
4	A	343	PX4	P1-O3-C1	3.42	104.75	121.59	10	14
4	A	421	PX4	O5-C9-C10	3.42	122.64	111.91	16	7
4	A	319	PX4	O4-P1-O2	3.42	95.71	109.07	16	4
4	A	334	PX4	O7-C7-C6	3.42	120.78	108.40	16	10
4	A	406	PX4	O1-P1-O2	3.42	129.13	112.24	13	12
4	A	411	PX4	C13-C12-C11	3.42	97.08	114.42	6	4
4	A	392	PX4	O4-P1-O2	3.42	95.72	109.07	6	4
4	A	392	PX4	C5-N1-C3	3.42	100.19	108.97	15	3
4	A	315	PX4	O3-P1-O2	3.41	95.73	109.07	20	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	336	PX4	O7-C23-O8	3.41	115.45	123.70	11	3
4	A	383	PX4	C13-C12-C11	3.41	97.09	114.42	10	2
4	A	379	PX4	C5-N1-C3	3.41	100.20	108.97	16	4
4	A	415	PX4	O7-C7-C6	3.41	120.76	108.40	9	6
4	A	429	PX4	O1-P1-O2	3.41	129.11	112.24	15	15
4	A	332	PX4	O5-C9-C10	3.41	122.61	111.91	16	9
4	A	373	PX4	C5-N1-C3	3.41	100.20	108.97	8	7
4	A	379	PX4	O3-P1-O2	3.41	95.74	109.07	18	4
4	A	388	PX4	O4-P1-O2	3.41	95.74	109.07	16	1
4	A	378	PX4	C4-N1-C3	3.41	100.21	108.97	7	4
4	A	413	PX4	C7-O7-C23	3.41	126.18	117.79	5	5
4	A	385	PX4	O5-C9-O6	3.41	114.99	123.59	20	6
4	A	421	PX4	O7-C7-C8	3.41	120.74	108.40	19	6
4	A	316	PX4	O7-C23-O8	3.41	115.47	123.70	9	9
4	A	346	PX4	C25-C24-C23	3.41	101.23	113.62	12	3
4	A	401	PX4	P1-O4-C6	3.41	101.71	121.68	16	12
4	A	430	PX4	C5-N1-C4	3.41	100.22	108.97	18	5
4	A	360	PX4	P1-O4-C6	3.40	101.72	121.68	9	13
4	A	375	PX4	C30-C29-C28	3.40	97.14	114.42	5	2
4	A	413	PX4	C3-N1-C2	3.40	123.84	109.92	16	2
4	A	428	PX4	O7-C7-C8	3.40	120.72	108.40	7	10
4	A	311	PX4	C8-O5-C9	3.40	104.52	117.12	4	6
4	A	327	PX4	C4-N1-C3	3.40	100.23	108.97	16	2
4	A	403	PX4	O5-C9-O6	3.40	115.01	123.59	5	1
4	A	387	PX4	C12-C11-C10	3.40	100.96	113.19	8	1
4	A	318	PX4	C1-C2-N1	3.40	127.13	115.78	13	6
4	A	358	PX4	O3-P1-O2	3.40	95.78	109.07	1	4
4	A	357	PX4	O7-C7-C8	3.40	120.71	108.40	18	6
4	A	349	PX4	O7-C7-C6	3.40	120.70	108.40	11	5
4	A	398	PX4	C1-C2-N1	3.40	127.12	115.78	19	6
4	A	417	PX4	O7-C7-C6	3.40	120.70	108.40	14	6
4	A	316	PX4	P1-O4-C6	3.39	101.78	121.68	2	12
4	A	318	PX4	C5-N1-C3	3.39	100.25	108.97	9	5
4	A	322	PX4	O3-P1-O2	3.39	95.81	109.07	4	3
4	A	347	PX4	O5-C9-C10	3.39	122.56	111.91	8	2
4	A	387	PX4	C18-C17-C16	3.39	97.20	114.42	14	1
4	A	324	PX4	C5-N1-C2	3.39	123.80	109.92	13	6
4	A	328	PX4	C29-C28-C27	3.39	97.20	114.42	10	1
4	A	345	PX4	O7-C23-O8	3.39	115.51	123.70	2	9
4	A	404	PX4	O5-C9-O6	3.39	115.03	123.59	6	5
4	A	380	PX4	O8-C23-C24	3.39	110.50	123.73	15	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	351	PX4	O7-C23-O8	3.39	115.51	123.70	17	6
4	A	368	PX4	O5-C9-O6	3.39	115.04	123.59	3	9
4	A	373	PX4	O4-P1-O2	3.39	122.31	109.07	1	3
4	A	421	PX4	C1-C2-N1	3.39	127.09	115.78	10	6
4	A	306	PX4	C34-C33-C32	3.39	97.23	114.42	1	2
4	A	353	PX4	C5-N1-C3	3.39	100.27	108.97	2	3
4	A	345	PX4	C12-C11-C10	3.38	101.02	113.19	3	4
4	A	345	PX4	C5-N1-C3	3.39	100.27	108.97	9	4
4	A	349	PX4	C4-N1-C3	3.39	100.27	108.97	20	2
4	A	405	PX4	C27-C26-C25	3.39	97.24	114.42	15	5
4	A	333	PX4	O1-P1-O4	3.38	123.46	107.75	13	2
4	A	402	PX4	C4-N1-C2	3.38	123.76	109.92	3	3
4	A	381	PX4	C5-N1-C3	3.38	100.27	108.97	4	4
4	A	369	PX4	C27-C26-C25	3.38	97.25	114.42	3	1
4	A	384	PX4	C28-C27-C26	3.38	97.28	114.42	5	4
4	A	396	PX4	C1-C2-N1	3.38	127.06	115.78	10	8
4	A	428	PX4	P1-O4-C6	3.38	101.87	121.68	9	8
4	A	333	PX4	C16-C15-C14	3.37	97.29	114.42	19	3
4	A	338	PX4	O3-P1-O2	3.38	95.88	109.07	16	3
4	A	386	PX4	C26-C25-C24	3.38	101.05	113.19	19	4
4	A	361	PX4	C5-N1-C4	3.38	100.30	108.97	17	3
4	A	394	PX4	O7-C7-C6	3.38	120.62	108.40	13	5
4	A	365	PX4	O7-C7-C8	3.37	120.62	108.40	1	11
4	A	376	PX4	C26-C25-C24	3.37	101.06	113.19	4	6
4	A	309	PX4	C12-C11-C10	3.37	101.07	113.19	7	4
4	A	341	PX4	O7-C7-C8	3.37	120.61	108.40	17	4
4	A	317	PX4	C5-N1-C4	3.37	117.64	108.97	19	2
4	A	401	PX4	O7-C23-O8	3.37	115.56	123.70	9	4
4	A	371	PX4	C5-N1-C4	3.37	100.31	108.97	13	3
4	A	378	PX4	O7-C7-C8	3.37	120.60	108.40	11	9
4	A	325	PX4	C5-N1-C3	3.37	117.63	108.97	8	4
4	A	332	PX4	C5-N1-C3	3.37	100.31	108.97	4	5
4	A	349	PX4	O3-P1-O2	3.37	95.91	109.07	11	3
4	A	367	PX4	C5-N1-C4	3.37	100.31	108.97	15	5
4	A	316	PX4	O1-P1-O2	3.37	128.88	112.24	20	10
4	A	336	PX4	O7-C7-C8	3.36	120.58	108.40	15	8
4	A	379	PX4	O5-C9-O6	3.36	115.10	123.59	3	5
4	A	430	PX4	O1-P1-O4	3.36	92.12	107.75	17	1
4	A	346	PX4	O5-C9-O6	3.36	115.10	123.59	13	5
4	A	319	PX4	O1-P1-O4	3.36	123.36	107.75	3	4
4	A	377	PX4	C12-C11-C10	3.36	101.10	113.19	11	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	359	PX4	C1-C2-N1	3.36	127.00	115.78	12	4
4	A	398	PX4	O5-C9-O6	3.36	115.11	123.59	8	9
4	A	320	PX4	C26-C25-C24	3.36	101.12	113.19	16	4
4	A	392	PX4	O7-C23-O8	3.36	115.59	123.70	11	2
4	A	416	PX4	P1-O4-C6	3.36	101.99	121.68	11	14
4	A	308	PX4	O7-C23-O8	3.36	115.59	123.70	7	7
4	A	310	PX4	O4-P1-O2	3.36	122.18	109.07	18	3
4	A	371	PX4	O7-C23-O8	3.35	115.59	123.70	19	4
4	A	373	PX4	O1-P1-O2	3.36	128.83	112.24	9	12
4	A	349	PX4	C25-C24-C23	3.35	101.42	113.62	2	4
4	A	403	PX4	C7-O7-C23	3.35	109.53	117.79	19	6
4	A	375	PX4	O1-P1-O2	3.35	128.83	112.24	17	11
4	A	368	PX4	O1-P1-O2	3.35	128.82	112.24	1	10
4	A	377	PX4	C26-C25-C24	3.35	101.14	113.19	7	3
4	A	416	PX4	O7-C7-C6	3.35	120.54	108.40	5	8
4	A	425	PX4	C5-N1-C3	3.35	100.35	108.97	3	4
4	A	333	PX4	C4-N1-C3	3.35	100.36	108.97	19	5
4	A	357	PX4	C5-N1-C3	3.35	100.36	108.97	7	3
4	A	404	PX4	P1-O4-C6	3.35	102.03	121.68	8	13
4	A	413	PX4	P1-O4-C6	3.35	102.03	121.68	11	13
4	A	355	PX4	C25-C24-C23	3.35	101.44	113.62	16	1
4	A	411	PX4	O7-C7-C6	3.35	120.53	108.40	14	10
4	A	393	PX4	O7-C23-O8	3.35	115.61	123.70	2	5
4	A	368	PX4	C26-C25-C24	3.35	101.16	113.19	7	5
4	A	330	PX4	C5-N1-C3	3.34	117.57	108.97	2	3
4	A	342	PX4	O7-C23-O8	3.34	115.62	123.70	16	4
4	A	309	PX4	C11-C10-C9	3.34	101.47	113.62	9	7
4	A	366	PX4	O1-P1-O2	3.34	128.76	112.24	14	8
4	A	328	PX4	C14-C13-C12	3.34	97.47	114.42	19	3
4	A	337	PX4	C5-N1-C3	3.34	100.39	108.97	10	2
4	A	376	PX4	O5-C9-O6	3.34	115.16	123.59	9	6
4	A	345	PX4	O4-P1-O2	3.34	122.10	109.07	6	3
4	A	399	PX4	C1-C2-N1	3.34	126.92	115.78	20	7
4	A	410	PX4	O1-P1-O3	3.34	92.24	107.75	14	4
4	A	405	PX4	C5-N1-C3	3.34	100.39	108.97	2	4
4	A	407	PX4	C4-N1-C3	3.34	100.40	108.97	11	3
4	A	352	PX4	C4-N1-C3	3.33	100.40	108.97	14	3
4	A	403	PX4	P1-O4-C6	3.33	102.13	121.68	17	13
4	A	389	PX4	O5-C9-C10	3.33	122.37	111.91	7	6
4	A	315	PX4	O5-C9-O6	3.33	132.00	123.59	19	3
4	A	353	PX4	O1-P1-O2	3.33	128.71	112.24	9	9

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	412	PX4	O7-C7-C6	3.33	120.47	108.40	12	5
4	A	394	PX4	C14-C13-C12	3.33	97.51	114.42	20	1
4	A	371	PX4	C4-N1-C3	3.33	117.54	108.97	14	6
4	A	376	PX4	O1-P1-O4	3.33	123.22	107.75	7	5
4	A	378	PX4	O7-C7-C6	3.33	120.46	108.40	14	5
4	A	417	PX4	P1-O4-C6	3.33	102.14	121.68	19	11
4	A	347	PX4	C5-N1-C3	3.33	100.42	108.97	16	3
4	A	384	PX4	P1-O4-C6	3.33	102.16	121.68	6	14
4	A	424	PX4	O7-C23-O8	3.33	115.66	123.70	10	5
4	A	424	PX4	C1-C2-N1	3.33	126.90	115.78	18	3
4	A	308	PX4	C12-C11-C10	3.33	101.23	113.19	8	4
4	A	360	PX4	C5-N1-C4	3.33	100.42	108.97	6	1
4	A	426	PX4	C12-C11-C10	3.33	101.23	113.19	14	7
4	A	426	PX4	C5-N1-C4	3.33	100.42	108.97	6	7
4	A	338	PX4	O1-P1-O2	3.33	128.68	112.24	6	12
4	A	417	PX4	C12-C11-C10	3.33	101.23	113.19	5	5
4	A	351	PX4	O5-C9-O6	3.32	115.20	123.59	8	8
4	A	319	PX4	C4-N1-C3	3.32	100.43	108.97	6	4
4	A	336	PX4	O1-P1-O2	3.32	128.66	112.24	4	10
4	A	337	PX4	O7-C7-C8	3.32	120.43	108.40	5	7
4	A	405	PX4	C11-C10-C9	3.32	101.54	113.62	12	3
4	A	418	PX4	C30-C29-C28	3.32	97.56	114.42	7	5
4	A	421	PX4	P1-O4-C6	3.32	102.20	121.68	7	15
4	A	400	PX4	O7-C7-C8	3.32	120.42	108.40	12	6
4	A	371	PX4	O1-P1-O2	3.32	128.65	112.24	9	10
4	A	373	PX4	O3-P1-O2	3.32	96.10	109.07	13	5
4	A	320	PX4	O7-C7-C6	3.32	120.41	108.40	1	9
4	A	328	PX4	C1-C2-N1	3.32	126.86	115.78	8	6
4	A	383	PX4	O4-P1-O2	3.32	96.11	109.07	1	2
4	A	418	PX4	C11-C10-C9	3.32	101.56	113.62	6	1
4	A	309	PX4	C25-C24-C23	3.32	101.56	113.62	11	3
4	A	353	PX4	O5-C9-O6	3.32	115.22	123.59	12	8
4	A	357	PX4	C4-N1-C3	3.32	100.45	108.97	5	4
4	A	311	PX4	O6-C9-C10	3.31	110.81	123.73	20	3
4	A	349	PX4	C5-N1-C4	3.31	117.49	108.97	4	5
4	A	363	PX4	O4-P1-O2	3.31	122.01	109.07	15	5
4	A	389	PX4	O1-P1-O4	3.31	123.11	107.75	17	3
4	A	392	PX4	O5-C9-O6	3.31	115.24	123.59	9	3
4	A	431	PX4	C11-C10-C9	3.31	101.58	113.62	7	3
4	A	384	PX4	O5-C9-O6	3.31	115.24	123.59	19	3
4	A	397	PX4	O1-P1-O2	3.31	128.60	112.24	1	15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	422	PX4	O3-P1-O2	3.31	96.14	109.07	5	5
4	A	401	PX4	O1-P1-O3	3.31	92.39	107.75	9	3
4	A	376	PX4	C1-C2-N1	3.31	126.82	115.78	20	7
4	A	317	PX4	C4-N1-C2	3.31	123.44	109.92	14	2
4	A	409	PX4	O7-C7-C6	3.31	120.37	108.40	8	9
4	A	363	PX4	O3-P1-O2	3.30	96.16	109.07	15	4
4	A	407	PX4	C1-C2-N1	3.30	126.81	115.78	20	2
4	A	416	PX4	O7-C7-C8	3.30	120.36	108.40	13	5
4	A	386	PX4	C32-C31-C30	3.30	97.66	114.42	11	3
4	A	428	PX4	O7-C23-C24	3.30	118.62	111.50	14	6
4	A	335	PX4	O3-P1-O2	3.30	96.17	109.07	18	5
4	A	351	PX4	O5-C9-C10	3.30	122.26	111.91	20	6
4	A	368	PX4	O7-C7-C8	3.30	120.35	108.40	12	6
4	A	359	PX4	O1-P1-O2	3.30	128.54	112.24	13	11
4	A	366	PX4	O3-P1-O2	3.30	96.18	109.07	2	1
4	A	359	PX4	O7-C7-C8	3.30	120.33	108.40	11	8
4	A	387	PX4	O7-C7-C6	3.30	120.33	108.40	14	9
4	A	389	PX4	O4-P1-O2	3.30	121.94	109.07	2	6
4	A	411	PX4	O7-C23-O8	3.30	115.74	123.70	8	7
4	A	431	PX4	O7-C7-C6	3.30	120.33	108.40	9	3
4	A	365	PX4	O7-C23-O8	3.29	115.74	123.70	15	4
4	A	366	PX4	C4-N1-C3	3.29	100.51	108.97	2	4
4	A	380	PX4	O7-C7-C6	3.29	120.33	108.40	10	8
4	A	397	PX4	P1-O4-C6	3.29	102.37	121.68	1	13
4	A	317	PX4	O3-P1-O2	3.29	96.21	109.07	20	3
4	A	335	PX4	P1-O4-C6	3.29	102.38	121.68	20	17
4	A	427	PX4	C29-C28-C27	3.29	97.71	114.42	4	3
4	A	402	PX4	O3-P1-O2	3.29	96.21	109.07	15	5
4	A	316	PX4	C8-O5-C9	3.29	104.94	117.12	20	6
4	A	399	PX4	C12-C11-C10	3.29	101.37	113.19	10	5
4	A	375	PX4	O5-C9-O6	3.29	115.29	123.59	1	6
4	A	380	PX4	C11-C10-C9	3.29	101.67	113.62	2	3
4	A	384	PX4	C31-C30-C29	3.29	97.74	114.42	5	2
4	A	388	PX4	C1-C2-N1	3.29	126.76	115.78	3	4
4	A	412	PX4	O5-C9-C10	3.29	122.23	111.91	13	5
4	A	308	PX4	O3-P1-O2	3.29	96.23	109.07	18	4
4	A	319	PX4	O7-C7-C6	3.29	120.30	108.40	13	12
4	A	336	PX4	C1-C2-N1	3.29	126.75	115.78	6	4
4	A	405	PX4	C7-O7-C23	3.29	125.88	117.79	12	2
4	A	398	PX4	C5-N1-C2	3.29	123.36	109.92	5	3
4	A	337	PX4	O7-C7-C6	3.28	120.29	108.40	1	8

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	358	PX4	C1-C2-N1	3.28	126.74	115.78	10	4
4	A	420	PX4	O7-C23-O8	3.28	115.77	123.70	8	6
4	A	343	PX4	O7-C7-C6	3.28	120.28	108.40	11	3
4	A	354	PX4	O1-P1-O2	3.28	128.46	112.24	16	10
4	A	367	PX4	O1-P1-O2	3.28	128.46	112.24	6	6
4	A	369	PX4	O1-P1-O4	3.28	122.98	107.75	16	3
4	A	315	PX4	O7-C7-C8	3.28	120.27	108.40	8	7
4	A	337	PX4	O1-P1-O4	3.28	122.97	107.75	15	1
4	A	399	PX4	O1-P1-O3	3.28	92.52	107.75	12	2
4	A	372	PX4	O1-P1-O2	3.28	128.45	112.24	18	9
4	A	389	PX4	O3-C1-C2	3.28	126.40	109.16	3	1
4	A	312	PX4	C18-C17-C16	3.27	97.81	114.42	15	2
4	A	343	PX4	C29-C28-C27	3.27	97.81	114.42	3	1
4	A	356	PX4	P1-O4-C6	3.27	102.50	121.68	8	10
4	A	364	PX4	O7-C7-C6	3.27	120.25	108.40	3	7
4	A	371	PX4	C5-N1-C3	3.27	100.56	108.97	12	3
4	A	425	PX4	O7-C7-C6	3.27	120.24	108.40	5	7
4	A	427	PX4	O7-C7-C6	3.27	120.24	108.40	15	7
4	A	338	PX4	C5-N1-C3	3.27	100.57	108.97	7	5
4	A	402	PX4	P1-O4-C6	3.27	102.53	121.68	11	11
4	A	388	PX4	O5-C9-C10	3.26	122.15	111.91	8	2
4	A	410	PX4	O1-P1-O2	3.27	128.38	112.24	20	9
4	A	393	PX4	C1-C2-N1	3.27	126.69	115.78	19	5
4	A	322	PX4	C19-C18-C17	3.27	97.85	114.42	20	3
4	A	309	PX4	C8-O5-C9	3.26	105.03	117.12	18	2
4	A	431	PX4	O7-C7-C8	3.26	120.22	108.40	17	4
4	A	406	PX4	C3-N1-C2	3.26	96.56	109.92	19	2
4	A	387	PX4	C4-N1-C3	3.26	117.36	108.97	17	4
4	A	338	PX4	P1-O4-C6	3.26	102.56	121.68	11	15
4	A	306	PX4	O4-P1-O2	3.26	121.81	109.07	9	4
4	A	365	PX4	C12-C11-C10	3.26	101.47	113.19	12	2
4	A	380	PX4	C4-N1-C3	3.26	100.59	108.97	10	6
4	A	385	PX4	O4-P1-O2	3.26	96.33	109.07	19	3
4	A	385	PX4	C4-N1-C3	3.26	117.36	108.97	3	8
4	A	422	PX4	O1-P1-O3	3.26	92.61	107.75	3	1
4	A	426	PX4	C25-C24-C23	3.26	101.77	113.62	2	2
4	A	424	PX4	O5-C9-C10	3.26	122.13	111.91	3	4
4	A	352	PX4	C32-C31-C30	3.26	97.89	114.42	4	3
4	A	366	PX4	O8-C23-C24	3.26	111.02	123.73	17	1
4	A	329	PX4	C1-C2-N1	3.26	126.65	115.78	12	4
4	A	334	PX4	C20-C19-C18	3.26	97.90	114.42	20	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	343	PX4	O1-P1-O3	3.26	92.63	107.75	4	3
4	A	346	PX4	C16-C15-C14	3.26	97.90	114.42	19	1
4	A	356	PX4	C12-C11-C10	3.26	101.48	113.19	1	1
4	A	375	PX4	C4-N1-C3	3.26	100.60	108.97	19	4
4	A	430	PX4	O1-P1-O2	3.25	128.33	112.24	20	11
4	A	307	PX4	C11-C10-C9	3.25	101.79	113.62	1	1
4	A	314	PX4	O7-C7-C6	3.25	120.18	108.40	19	6
4	A	333	PX4	P1-O4-C6	3.25	102.61	121.68	17	12
4	A	368	PX4	O1-P1-O3	3.25	92.64	107.75	1	1
4	A	402	PX4	O1-P1-O2	3.25	128.32	112.24	20	10
4	A	317	PX4	O7-C23-O8	3.25	115.85	123.70	1	6
4	A	356	PX4	O3-P1-O2	3.25	96.37	109.07	3	6
4	A	364	PX4	C12-C11-C10	3.25	101.51	113.19	4	6
4	A	365	PX4	O4-P1-O2	3.25	121.77	109.07	13	2
4	A	416	PX4	C5-N1-C4	3.25	100.62	108.97	17	4
4	A	419	PX4	O1-P1-O2	3.25	128.31	112.24	4	13
4	A	340	PX4	C15-C14-C13	3.25	97.93	114.42	5	3
4	A	411	PX4	C5-N1-C3	3.25	100.62	108.97	14	7
4	A	401	PX4	C27-C26-C25	3.25	97.94	114.42	14	3
4	A	403	PX4	O7-C7-C6	3.25	120.16	108.40	12	10
4	A	307	PX4	O7-C23-O8	3.25	115.86	123.70	1	7
4	A	320	PX4	O5-C9-O6	3.25	115.40	123.59	17	6
4	A	333	PX4	C1-C2-N1	3.24	126.61	115.78	9	6
4	A	414	PX4	O5-C9-O6	3.24	115.41	123.59	19	7
4	A	398	PX4	C5-N1-C4	3.24	100.63	108.97	5	5
4	A	379	PX4	O7-C7-C8	3.24	120.14	108.40	16	8
4	A	343	PX4	O3-P1-O2	3.24	96.40	109.07	7	7
4	A	351	PX4	O1-P1-O4	3.24	122.80	107.75	4	2
4	A	403	PX4	C4-N1-C3	3.24	100.65	108.97	17	3
4	A	386	PX4	O7-C7-C6	3.24	120.13	108.40	9	11
4	A	310	PX4	O7-C7-C6	3.24	120.12	108.40	18	6
4	A	324	PX4	O1-P1-O2	3.24	128.25	112.24	11	13
4	A	410	PX4	C25-C24-C23	3.24	101.84	113.62	13	2
4	A	347	PX4	C5-N1-C4	3.24	117.30	108.97	17	6
4	A	375	PX4	O5-C9-C10	3.24	122.07	111.91	1	6
4	A	328	PX4	O7-C23-C24	3.24	118.47	111.50	3	7
4	A	353	PX4	O7-C23-O8	3.23	115.88	123.70	1	4
4	A	371	PX4	C12-C11-C10	3.24	101.56	113.19	4	2
4	A	389	PX4	O1-P1-O2	3.24	128.24	112.24	8	10
4	A	418	PX4	C5-N1-C4	3.24	100.65	108.97	5	2
4	A	327	PX4	C26-C25-C24	3.23	124.81	113.19	16	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	328	PX4	O5-C9-C10	3.23	122.05	111.91	17	6
4	A	345	PX4	O3-P1-O2	3.23	96.44	109.07	12	3
4	A	348	PX4	C5-N1-C4	3.23	117.28	108.97	18	7
4	A	381	PX4	C12-C11-C10	3.23	101.58	113.19	5	4
4	A	407	PX4	O3-P1-O2	3.23	96.44	109.07	16	3
4	A	331	PX4	P1-O4-C6	3.23	102.75	121.68	20	12
4	A	344	PX4	O7-C7-C8	3.23	120.09	108.40	19	8
4	A	348	PX4	C5-N1-C3	3.23	100.67	108.97	17	7
4	A	386	PX4	O1-P1-O3	3.23	92.75	107.75	2	1
4	A	418	PX4	O7-C23-O8	3.23	115.90	123.70	5	5
4	A	305	PX4	C5-N1-C4	3.23	117.27	108.97	17	5
4	A	356	PX4	C1-C2-N1	3.23	126.55	115.78	17	4
4	A	310	PX4	C12-C11-C10	3.23	101.60	113.19	15	4
4	A	311	PX4	O7-C7-C8	3.23	120.08	108.40	15	11
4	A	339	PX4	O5-C9-C10	3.23	122.03	111.91	3	6
4	A	413	PX4	C34-C33-C32	3.23	98.05	114.42	1	4
4	A	349	PX4	O5-C9-C10	3.22	122.02	111.91	11	4
4	A	351	PX4	O4-P1-O2	3.22	121.66	109.07	19	5
4	A	397	PX4	C3-N1-C2	3.22	96.72	109.92	18	1
4	A	370	PX4	C5-N1-C3	3.22	100.69	108.97	7	4
4	A	320	PX4	P1-O4-C6	3.22	102.79	121.68	17	11
4	A	393	PX4	C7-O7-C23	3.22	125.72	117.79	11	5
4	A	423	PX4	P1-O4-C6	3.22	102.78	121.68	19	13
4	A	349	PX4	C7-O7-C23	3.22	125.72	117.79	17	9
4	A	429	PX4	O7-C7-C6	3.22	120.07	108.40	6	3
4	A	329	PX4	O5-C9-C10	3.22	122.01	111.91	15	4
4	A	400	PX4	C31-C30-C29	3.22	98.08	114.42	1	3
4	A	371	PX4	O3-C1-C2	3.22	126.09	109.16	12	2
4	A	373	PX4	O7-C7-C6	3.22	120.05	108.40	18	2
4	A	414	PX4	O3-P1-O2	3.22	96.49	109.07	12	2
4	A	332	PX4	P1-O4-C6	3.22	102.81	121.68	6	9
4	A	342	PX4	C12-C11-C10	3.22	101.63	113.19	15	2
4	A	347	PX4	C30-C29-C28	3.22	98.10	114.42	10	1
4	A	402	PX4	C19-C18-C17	3.22	98.10	114.42	4	2
4	A	417	PX4	C30-C29-C28	3.22	98.10	114.42	20	4
4	A	400	PX4	C33-C32-C31	3.21	98.11	114.42	6	1
4	A	380	PX4	C30-C29-C28	3.21	98.11	114.42	2	1
4	A	322	PX4	O5-C9-C10	3.21	121.99	111.91	13	3
4	A	406	PX4	P1-O4-C6	3.21	102.83	121.68	18	9
4	A	406	PX4	C29-C28-C27	3.21	98.12	114.42	11	2
4	A	394	PX4	C13-C12-C11	3.21	98.13	114.42	17	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	340	PX4	C25-C24-C23	3.21	125.28	113.62	16	4
4	A	319	PX4	O5-C9-O6	3.21	115.50	123.59	7	4
4	A	360	PX4	C12-C11-C10	3.21	101.67	113.19	12	3
4	A	327	PX4	O1-P1-O3	3.20	92.86	107.75	19	2
4	A	384	PX4	C27-C26-C25	3.20	98.18	114.42	20	1
4	A	431	PX4	C12-C11-C10	3.20	101.68	113.19	4	2
4	A	305	PX4	C1-C2-N1	3.20	126.46	115.78	4	6
4	A	324	PX4	C26-C25-C24	3.20	101.69	113.19	14	5
4	A	365	PX4	C4-N1-C3	3.20	100.75	108.97	12	7
4	A	393	PX4	C14-C13-C12	3.20	98.18	114.42	10	1
4	A	340	PX4	C19-C18-C17	3.20	98.19	114.42	13	1
4	A	378	PX4	O5-C9-O6	3.20	115.52	123.59	14	8
4	A	419	PX4	C7-O7-C23	3.20	125.66	117.79	12	6
4	A	420	PX4	C29-C28-C27	3.20	98.19	114.42	4	2
4	A	345	PX4	O5-C9-O6	3.20	115.53	123.59	19	5
4	A	426	PX4	O5-C9-C10	3.20	121.94	111.91	12	4
4	A	380	PX4	O1-P1-O4	3.20	122.58	107.75	8	2
4	A	394	PX4	C31-C30-C29	3.20	98.20	114.42	8	3
4	A	333	PX4	C18-C17-C16	3.19	98.21	114.42	7	2
4	A	334	PX4	C5-N1-C4	3.19	100.76	108.97	13	7
4	A	369	PX4	C4-N1-C3	3.19	100.76	108.97	15	4
4	A	422	PX4	C19-C18-C17	3.19	98.21	114.42	16	1
4	A	399	PX4	O1-P1-O2	3.19	128.02	112.24	20	10
4	A	326	PX4	C17-C16-C15	3.19	98.22	114.42	5	1
4	A	312	PX4	O1-P1-O2	3.19	128.01	112.24	9	9
4	A	345	PX4	C4-N1-C3	3.19	100.77	108.97	12	7
4	A	431	PX4	O5-C9-C10	3.19	121.92	111.91	16	4
4	A	335	PX4	O4-P1-O2	3.19	121.53	109.07	6	1
4	A	371	PX4	C7-O7-C23	3.19	125.64	117.79	18	3
4	A	376	PX4	O7-C7-C6	3.19	119.95	108.40	7	9
4	A	386	PX4	C11-C10-C9	3.19	102.02	113.62	9	3
4	A	323	PX4	P1-O3-C1	3.19	105.89	121.59	5	14
4	A	416	PX4	C19-C18-C17	3.19	98.24	114.42	13	4
4	A	326	PX4	C29-C28-C27	3.19	98.24	114.42	18	3
4	A	351	PX4	C15-C14-C13	3.19	98.24	114.42	6	3
4	A	397	PX4	O7-C7-C6	3.19	119.94	108.40	15	7
4	A	335	PX4	C1-C2-N1	3.19	126.42	115.78	20	7
4	A	328	PX4	C3-N1-C2	3.18	96.89	109.92	15	2
4	A	381	PX4	O1-P1-O3	3.18	92.96	107.75	17	4
4	A	326	PX4	O4-P1-O2	3.18	121.50	109.07	19	2
4	A	403	PX4	C12-C11-C10	3.18	101.75	113.19	9	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	406	PX4	C5-N1-C4	3.18	100.79	108.97	6	3
4	A	386	PX4	O5-C9-C10	3.18	121.89	111.91	1	7
4	A	380	PX4	C29-C28-C27	3.18	98.28	114.42	11	1
4	A	410	PX4	C5-N1-C4	3.18	100.79	108.97	20	3
4	A	327	PX4	C25-C24-C23	3.18	102.05	113.62	19	2
4	A	362	PX4	O5-C9-C10	3.18	121.89	111.91	13	9
4	A	325	PX4	O1-P1-O2	3.18	127.96	112.24	5	10
4	A	326	PX4	O5-C9-C10	3.18	121.88	111.91	3	5
4	A	400	PX4	O1-P1-O4	3.18	122.51	107.75	3	2
4	A	380	PX4	C26-C25-C24	3.18	101.76	113.19	3	3
4	A	424	PX4	C11-C10-C9	3.18	102.06	113.62	8	2
4	A	314	PX4	C26-C25-C24	3.18	101.78	113.19	12	2
4	A	361	PX4	O1-P1-O4	3.18	122.50	107.75	4	2
4	A	390	PX4	O1-P1-O2	3.18	127.94	112.24	2	8
4	A	371	PX4	C3-N1-C2	3.18	122.91	109.92	9	3
4	A	313	PX4	O1-P1-O4	3.17	122.48	107.75	7	3
4	A	348	PX4	O1-P1-O2	3.17	127.93	112.24	11	7
4	A	369	PX4	O5-C9-C10	3.17	121.87	111.91	7	3
4	A	353	PX4	O4-P1-O2	3.17	121.46	109.07	11	4
4	A	369	PX4	O7-C7-C8	3.17	119.89	108.40	15	10
4	A	378	PX4	O3-P1-O2	3.17	96.67	109.07	10	6
4	A	390	PX4	C4-N1-C2	3.17	122.90	109.92	10	2
4	A	306	PX4	P1-O4-C6	3.17	103.09	121.68	13	12
4	A	314	PX4	O1-P1-O4	3.17	122.47	107.75	8	3
4	A	323	PX4	C26-C25-C24	3.17	101.80	113.19	15	2
4	A	344	PX4	O5-C9-O6	3.17	115.59	123.59	15	5
4	A	377	PX4	C25-C24-C23	3.17	102.10	113.62	5	2
4	A	406	PX4	O7-C7-C6	3.17	119.88	108.40	12	6
4	A	397	PX4	C1-C2-N1	3.17	126.36	115.78	10	4
4	A	423	PX4	O7-C23-O8	3.17	116.04	123.70	1	7
4	A	376	PX4	O1-P1-O2	3.17	127.89	112.24	14	12
4	A	384	PX4	C12-C11-C10	3.17	101.81	113.19	5	4
4	A	313	PX4	O7-C23-O8	3.17	116.05	123.70	3	5
4	A	359	PX4	C3-N1-C2	3.17	122.87	109.92	11	2
4	A	367	PX4	C4-N1-C3	3.17	100.83	108.97	16	8
4	A	430	PX4	C1-C2-N1	3.17	126.35	115.78	13	5
4	A	430	PX4	C25-C24-C23	3.17	102.10	113.62	13	3
4	A	336	PX4	C8-O5-C9	3.16	128.84	117.12	12	1
4	A	321	PX4	O7-C7-C8	3.16	119.86	108.40	19	8
4	A	310	PX4	C1-C2-N1	3.16	126.34	115.78	15	4
4	A	331	PX4	C1-C2-N1	3.16	126.34	115.78	1	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	350	PX4	C27-C26-C25	3.16	98.37	114.42	15	3
4	A	326	PX4	O1-P1-O2	3.16	127.86	112.24	13	13
4	A	333	PX4	O1-P1-O2	3.16	127.86	112.24	20	15
4	A	400	PX4	O7-C7-C6	3.16	119.84	108.40	12	10
4	A	326	PX4	C4-N1-C2	3.16	96.99	109.92	20	2
4	A	374	PX4	C1-C2-N1	3.16	126.33	115.78	16	10
4	A	367	PX4	O1-P1-O4	3.16	122.41	107.75	18	2
4	A	404	PX4	C4-N1-C3	3.16	100.86	108.97	16	2
4	A	318	PX4	O7-C7-C8	3.16	119.83	108.40	10	9
4	A	426	PX4	O4-P1-O2	3.16	121.40	109.07	4	3
4	A	342	PX4	O7-C7-C6	3.15	119.82	108.40	1	7
4	A	359	PX4	P1-O4-C6	3.15	103.19	121.68	6	9
4	A	363	PX4	O5-C9-C10	3.15	121.81	111.91	15	4
4	A	347	PX4	O1-P1-O2	3.15	127.83	112.24	2	11
4	A	405	PX4	O7-C23-O8	3.15	116.08	123.70	16	5
4	A	413	PX4	O5-C9-O6	3.15	115.63	123.59	8	4
4	A	305	PX4	O7-C7-C8	3.15	119.81	108.40	6	4
4	A	340	PX4	C5-N1-C4	3.15	100.87	108.97	9	3
4	A	387	PX4	P1-O4-C6	3.15	103.21	121.68	5	11
4	A	394	PX4	O7-C23-O8	3.15	116.09	123.70	10	6
4	A	344	PX4	O3-C1-C2	3.15	125.72	109.16	9	2
4	A	394	PX4	C16-C15-C14	3.15	98.43	114.42	19	1
4	A	421	PX4	O3-P1-O2	3.15	96.76	109.07	19	4
4	A	423	PX4	C11-C10-C9	3.15	125.07	113.62	17	2
4	A	425	PX4	O5-C9-O6	3.15	115.64	123.59	15	4
4	A	385	PX4	O1-P1-O4	3.15	93.12	107.75	10	1
4	A	305	PX4	C30-C29-C28	3.15	98.46	114.42	3	3
4	A	340	PX4	C1-C2-N1	3.15	126.28	115.78	10	8
4	A	345	PX4	C8-O5-C9	3.15	105.47	117.12	4	4
4	A	375	PX4	P1-O4-C6	3.15	103.23	121.68	1	12
4	A	401	PX4	C8-O5-C9	3.15	105.47	117.12	2	2
4	A	421	PX4	C12-C11-C10	3.15	124.50	113.19	12	4
4	A	412	PX4	C15-C14-C13	3.15	98.46	114.42	19	2
4	A	430	PX4	O7-C23-O8	3.15	116.10	123.70	3	3
4	A	320	PX4	O1-P1-O3	3.14	93.15	107.75	19	3
4	A	375	PX4	C17-C16-C15	3.14	98.47	114.42	19	2
4	A	403	PX4	C1-C2-N1	3.14	126.26	115.78	8	1
4	A	395	PX4	O1-P1-O2	3.14	127.77	112.24	14	14
4	A	384	PX4	C3-N1-C2	3.14	122.76	109.92	6	1
4	A	408	PX4	O7-C23-C24	3.14	118.27	111.50	2	8
4	A	314	PX4	C1-C2-N1	3.14	126.25	115.78	20	9

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	343	PX4	C11-C10-C9	3.14	102.21	113.62	2	2
4	A	360	PX4	O1-P1-O4	3.14	122.32	107.75	16	3
4	A	415	PX4	O3-P1-O2	3.14	96.81	109.07	6	8
4	A	345	PX4	C11-C10-C9	3.14	102.22	113.62	7	4
4	A	360	PX4	C5-N1-C3	3.14	100.91	108.97	14	3
4	A	369	PX4	C1-C2-N1	3.13	126.25	115.78	1	5
4	A	401	PX4	O7-C7-C6	3.14	119.75	108.40	7	6
4	A	329	PX4	O1-P1-O3	3.13	93.19	107.75	14	8
4	A	357	PX4	C7-O7-C23	3.13	125.51	117.79	7	3
4	A	419	PX4	C5-N1-C4	3.13	100.92	108.97	3	4
4	A	318	PX4	O7-C23-O8	3.13	116.13	123.70	3	5
4	A	383	PX4	C4-N1-C3	3.13	100.92	108.97	7	4
4	A	417	PX4	C7-O7-C23	3.13	125.50	117.79	1	5
4	A	403	PX4	O6-C9-C10	3.13	111.52	123.73	7	3
4	A	309	PX4	O7-C23-O8	3.13	116.14	123.70	8	2
4	A	342	PX4	O7-C7-C8	3.13	119.73	108.40	8	4
4	A	343	PX4	C26-C25-C24	3.13	101.94	113.19	19	5
4	A	320	PX4	C5-N1-C4	3.13	117.02	108.97	11	5
4	A	362	PX4	C5-N1-C3	3.13	100.93	108.97	7	4
4	A	369	PX4	C16-C15-C14	3.13	98.54	114.42	9	3
4	A	405	PX4	O3-P1-O2	3.13	96.84	109.07	19	5
4	A	393	PX4	O5-C9-O6	3.13	115.70	123.59	9	8
4	A	419	PX4	C25-C24-C23	3.13	102.24	113.62	16	4
4	A	317	PX4	O5-C9-C10	3.13	121.72	111.91	9	7
4	A	310	PX4	O1-P1-O4	3.13	122.27	107.75	10	2
4	A	372	PX4	C29-C28-C27	3.13	98.55	114.42	13	2
4	A	335	PX4	C26-C25-C24	3.13	101.95	113.19	13	4
4	A	343	PX4	O3-C1-C2	3.12	125.60	109.16	10	4
4	A	380	PX4	C15-C14-C13	3.13	98.56	114.42	13	3
4	A	409	PX4	O7-C23-O8	3.12	116.15	123.70	17	9
4	A	321	PX4	O1-P1-O2	3.12	127.68	112.24	5	13
4	A	401	PX4	C28-C27-C26	3.12	98.57	114.42	15	2
4	A	386	PX4	C14-C13-C12	3.12	98.57	114.42	6	2
4	A	395	PX4	C1-C2-N1	3.12	126.21	115.78	6	5
4	A	397	PX4	O4-P1-O2	3.12	96.86	109.07	16	2
4	A	317	PX4	O1-P1-O3	3.12	93.25	107.75	13	3
4	A	336	PX4	C30-C29-C28	3.12	98.58	114.42	17	1
4	A	424	PX4	C4-N1-C3	3.12	100.95	108.97	6	7
4	A	318	PX4	O7-C7-C6	3.12	119.70	108.40	18	8
4	A	311	PX4	O1-P1-O2	3.12	127.66	112.24	16	6
4	A	352	PX4	C30-C29-C28	3.12	98.59	114.42	19	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	359	PX4	C14-C13-C12	3.12	98.59	114.42	11	2
4	A	310	PX4	O5-C9-O6	3.12	115.73	123.59	13	4
4	A	323	PX4	O1-P1-O2	3.12	127.65	112.24	19	10
4	A	334	PX4	C11-C10-C9	3.12	102.29	113.62	8	3
4	A	346	PX4	C12-C11-C10	3.12	101.99	113.19	7	2
4	A	379	PX4	O1-P1-O2	3.12	127.65	112.24	3	12
4	A	386	PX4	C5-N1-C4	3.12	100.96	108.97	19	2
4	A	391	PX4	O4-P1-O2	3.12	121.25	109.07	15	7
4	A	355	PX4	O5-C9-C10	3.12	121.69	111.91	13	4
4	A	425	PX4	O3-P1-O2	3.12	96.89	109.07	15	4
4	A	336	PX4	C5-N1-C4	3.11	100.97	108.97	18	5
4	A	351	PX4	C14-C13-C12	3.12	98.61	114.42	11	1
4	A	401	PX4	C17-C16-C15	3.11	98.62	114.42	3	3
4	A	327	PX4	P1-O4-C6	3.11	103.43	121.68	7	9
4	A	342	PX4	O1-P1-O4	3.11	122.20	107.75	9	1
4	A	427	PX4	O7-C23-O8	3.11	116.18	123.70	5	7
4	A	328	PX4	C5-N1-C4	3.11	100.98	108.97	18	6
4	A	329	PX4	C26-C25-C24	3.11	102.01	113.19	20	1
4	A	332	PX4	O7-C7-C6	3.11	119.67	108.40	1	6
4	A	337	PX4	C7-O7-C23	3.11	110.13	117.79	11	5
4	A	346	PX4	C13-C12-C11	3.11	98.63	114.42	11	2
4	A	362	PX4	C18-C17-C16	3.11	98.63	114.42	12	1
4	A	396	PX4	C26-C25-C24	3.11	102.00	113.19	14	2
4	A	330	PX4	C25-C24-C23	3.11	102.31	113.62	18	3
4	A	376	PX4	C31-C30-C29	3.11	98.63	114.42	11	3
4	A	381	PX4	C17-C16-C15	3.11	98.63	114.42	3	3
4	A	348	PX4	C5-N1-C2	3.11	122.64	109.92	17	2
4	A	311	PX4	C5-N1-C4	3.11	100.98	108.97	14	3
4	A	392	PX4	C4-N1-C3	3.11	100.98	108.97	11	8
4	A	402	PX4	O7-C23-O8	3.11	116.19	123.70	7	5
4	A	423	PX4	O1-P1-O4	3.11	122.18	107.75	10	4
4	A	345	PX4	O5-C9-C10	3.11	121.65	111.91	13	3
4	A	368	PX4	C5-N1-C3	3.11	100.99	108.97	8	6
4	A	310	PX4	C5-N1-C4	3.10	116.96	108.97	13	6
4	A	372	PX4	O5-C9-C10	3.11	121.65	111.91	13	7
4	A	402	PX4	C11-C10-C9	3.10	102.33	113.62	13	3
4	A	404	PX4	C25-C24-C23	3.10	102.33	113.62	1	3
4	A	429	PX4	O5-C9-C10	3.10	121.65	111.91	1	6
4	A	309	PX4	O3-P1-O2	3.10	96.94	109.07	12	6
4	A	324	PX4	C8-O5-C9	3.10	105.63	117.12	4	3
4	A	343	PX4	C12-C11-C10	3.10	102.03	113.19	3	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	323	PX4	P1-O4-C6	3.10	103.50	121.68	5	9
4	A	309	PX4	C7-O7-C23	3.10	125.42	117.79	10	4
4	A	334	PX4	C1-C2-N1	3.10	126.12	115.78	17	4
4	A	402	PX4	C31-C30-C29	3.10	98.70	114.42	13	2
4	A	365	PX4	O5-C9-O6	3.10	115.78	123.59	11	1
4	A	322	PX4	C11-C10-C9	3.09	102.37	113.62	2	4
4	A	349	PX4	C5-N1-C2	3.09	122.57	109.92	1	3
4	A	363	PX4	C15-C14-C13	3.09	98.72	114.42	12	2
4	A	368	PX4	O4-P1-O2	3.10	121.16	109.07	8	4
4	A	401	PX4	O5-C9-C10	3.09	121.62	111.91	19	7
4	A	428	PX4	C26-C25-C24	3.09	124.31	113.19	18	6
4	A	341	PX4	C12-C11-C10	3.09	102.08	113.19	20	2
4	A	388	PX4	O1-P1-O2	3.09	127.52	112.24	8	14
4	A	414	PX4	C11-C10-C9	3.09	102.38	113.62	13	2
4	A	400	PX4	C34-C33-C32	3.09	98.74	114.42	8	2
4	A	428	PX4	O5-C9-C10	3.09	121.60	111.91	9	2
4	A	322	PX4	C29-C28-C27	3.09	98.75	114.42	8	3
4	A	338	PX4	C3-N1-C2	3.09	97.28	109.92	13	2
4	A	342	PX4	O8-C23-C24	3.09	111.69	123.73	2	2
4	A	366	PX4	O7-C23-O8	3.09	116.24	123.70	1	5
4	A	375	PX4	O7-C23-O8	3.09	116.24	123.70	5	5
4	A	404	PX4	O7-C7-C8	3.09	119.58	108.40	19	5
4	A	377	PX4	C7-O7-C23	3.09	125.39	117.79	17	8
4	A	422	PX4	O3-C1-C2	3.09	125.40	109.16	8	1
4	A	335	PX4	C25-C24-C23	3.08	124.84	113.62	2	3
4	A	385	PX4	O1-P1-O2	3.08	127.49	112.24	6	8
4	A	409	PX4	C1-C2-N1	3.08	126.08	115.78	11	6
4	A	393	PX4	C33-C32-C31	3.09	98.76	114.42	19	1
4	A	321	PX4	C5-N1-C4	3.08	116.90	108.97	19	5
4	A	424	PX4	O5-C9-O6	3.08	115.81	123.59	3	3
4	A	325	PX4	O3-P1-O2	3.08	97.03	109.07	19	4
4	A	415	PX4	O1-P1-O2	3.08	127.47	112.24	2	8
4	A	415	PX4	C1-C2-N1	3.08	126.07	115.78	11	4
4	A	340	PX4	C8-O5-C9	3.08	105.72	117.12	13	1
4	A	411	PX4	C8-O5-C9	3.08	105.72	117.12	17	3
4	A	352	PX4	O1-P1-O2	3.08	127.46	112.24	11	9
4	A	321	PX4	C8-O5-C9	3.08	105.73	117.12	6	2
4	A	332	PX4	C25-C24-C23	3.08	124.81	113.62	15	1
4	A	378	PX4	C1-C2-N1	3.08	126.05	115.78	14	2
4	A	388	PX4	C4-N1-C2	3.08	97.32	109.92	10	5
4	A	396	PX4	O1-P1-O2	3.08	127.46	112.24	12	9

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	353	PX4	C12-C11-C10	3.08	102.13	113.19	17	4
4	A	312	PX4	C1-C2-N1	3.07	126.04	115.78	19	9
4	A	347	PX4	C31-C30-C29	3.07	98.82	114.42	15	1
4	A	362	PX4	C5-N1-C4	3.07	101.07	108.97	15	4
4	A	371	PX4	O7-C7-C8	3.08	119.54	108.40	6	10
4	A	371	PX4	O1-P1-O4	3.07	122.02	107.75	16	3
4	A	374	PX4	O7-C7-C6	3.07	119.53	108.40	17	7
4	A	393	PX4	O1-P1-O4	3.07	122.03	107.75	20	1
4	A	336	PX4	O7-C7-C6	3.07	119.53	108.40	9	3
4	A	376	PX4	C12-C11-C10	3.07	102.15	113.19	15	2
4	A	404	PX4	C28-C27-C26	3.07	98.83	114.42	11	2
4	A	323	PX4	C7-O7-C23	3.07	125.35	117.79	7	3
4	A	356	PX4	O5-C9-O6	3.07	115.84	123.59	17	4
4	A	362	PX4	O8-C23-C24	3.07	111.75	123.73	7	2
4	A	406	PX4	O3-P1-O2	3.07	97.07	109.07	1	4
4	A	400	PX4	O1-P1-O2	3.07	127.42	112.24	7	7
4	A	379	PX4	C1-C2-N1	3.07	126.03	115.78	18	3
4	A	360	PX4	C30-C29-C28	3.07	98.85	114.42	3	2
4	A	429	PX4	C18-C17-C16	3.07	98.84	114.42	20	1
4	A	318	PX4	C25-C24-C23	3.07	102.47	113.62	14	2
4	A	364	PX4	C4-N1-C3	3.07	101.09	108.97	4	3
4	A	335	PX4	O1-P1-O3	3.07	93.51	107.75	10	4
4	A	402	PX4	C30-C29-C28	3.07	98.86	114.42	4	1
4	A	422	PX4	C5-N1-C4	3.07	116.86	108.97	5	4
4	A	336	PX4	C4-N1-C2	3.06	122.46	109.92	9	2
4	A	399	PX4	O5-C9-O6	3.06	131.33	123.59	6	4
4	A	369	PX4	O7-C7-C6	3.07	119.50	108.40	20	2
4	A	310	PX4	O5-C9-C10	3.06	121.51	111.91	17	4
4	A	323	PX4	C19-C18-C17	3.06	98.88	114.42	10	1
4	A	364	PX4	O1-P1-O3	3.06	93.52	107.75	1	2
4	A	406	PX4	C11-C10-C9	3.06	102.49	113.62	3	2
4	A	310	PX4	C27-C26-C25	3.06	98.90	114.42	20	3
4	A	380	PX4	O7-C23-O8	3.06	116.31	123.70	10	7
4	A	328	PX4	O1-P1-O4	3.06	121.94	107.75	19	4
4	A	339	PX4	O3-P1-O2	3.06	97.13	109.07	4	2
4	A	399	PX4	O7-C7-C6	3.06	119.47	108.40	9	7
4	A	392	PX4	C12-C11-C10	3.06	102.20	113.19	14	3
4	A	327	PX4	O5-C9-C10	3.05	121.49	111.91	5	6
4	A	360	PX4	O4-P1-O2	3.05	121.00	109.07	13	3
4	A	374	PX4	C12-C11-C10	3.05	102.22	113.19	1	5
4	A	416	PX4	C5-N1-C2	3.05	97.43	109.92	15	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	421	PX4	C31-C30-C29	3.05	98.93	114.42	12	2
4	A	335	PX4	C4-N1-C2	3.05	97.43	109.92	13	2
4	A	336	PX4	O5-C9-O6	3.05	115.89	123.59	20	7
4	A	416	PX4	C34-C33-C32	3.05	98.94	114.42	2	1
4	A	359	PX4	O7-C7-C6	3.05	119.44	108.40	3	6
4	A	404	PX4	O3-P1-O2	3.05	97.16	109.07	15	3
4	A	395	PX4	C13-C12-C11	3.05	98.95	114.42	20	2
4	A	424	PX4	O1-P1-O4	3.05	121.90	107.75	2	2
4	A	372	PX4	C34-C33-C32	3.05	98.96	114.42	12	4
4	A	408	PX4	O6-C9-C10	3.05	111.85	123.73	3	2
4	A	306	PX4	C11-C10-C9	3.04	124.69	113.62	7	2
4	A	331	PX4	O1-P1-O4	3.04	121.89	107.75	12	4
4	A	410	PX4	C13-C12-C11	3.05	98.97	114.42	18	1
4	A	336	PX4	C33-C32-C31	3.04	98.97	114.42	6	2
4	A	362	PX4	O7-C7-C8	3.04	119.42	108.40	19	5
4	A	329	PX4	O5-C9-O6	3.04	115.92	123.59	14	5
4	A	350	PX4	C7-O7-C23	3.04	125.28	117.79	6	5
4	A	331	PX4	C5-N1-C4	3.04	101.15	108.97	4	5
4	A	335	PX4	C11-C10-C9	3.04	102.56	113.62	3	4
4	A	359	PX4	C5-N1-C4	3.04	101.15	108.97	18	4
4	A	426	PX4	O1-P1-O2	3.04	127.28	112.24	2	11
4	A	427	PX4	C17-C16-C15	3.04	98.98	114.42	1	3
4	A	335	PX4	O1-P1-O2	3.04	127.27	112.24	10	10
4	A	410	PX4	C14-C13-C12	3.04	98.99	114.42	18	3
4	A	328	PX4	C27-C26-C25	3.04	99.00	114.42	18	2
4	A	344	PX4	C18-C17-C16	3.04	99.00	114.42	4	1
4	A	309	PX4	C5-N1-C3	3.04	101.17	108.97	14	2
4	A	342	PX4	O5-C9-C10	3.04	121.44	111.91	2	5
4	A	363	PX4	C1-C2-N1	3.04	125.92	115.78	10	5
4	A	312	PX4	C30-C29-C28	3.03	99.02	114.42	13	4
4	A	325	PX4	C27-C26-C25	3.03	99.02	114.42	10	5
4	A	352	PX4	C11-C10-C9	3.03	102.59	113.62	9	1
4	A	315	PX4	C31-C30-C29	3.03	99.03	114.42	8	3
4	A	333	PX4	C8-O5-C9	3.03	105.89	117.12	2	2
4	A	340	PX4	O1-P1-O2	3.03	127.23	112.24	3	9
4	A	326	PX4	C7-O7-C23	3.03	110.33	117.79	15	7
4	A	422	PX4	C12-C11-C10	3.03	102.29	113.19	19	5
4	A	388	PX4	C11-C10-C9	3.03	102.60	113.62	16	3
4	A	422	PX4	O7-C7-C6	3.03	119.38	108.40	13	5
4	A	383	PX4	O5-C9-O6	3.03	115.95	123.59	11	6
4	A	413	PX4	C12-C11-C10	3.03	102.30	113.19	11	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	421	PX4	C4-N1-C2	3.03	97.52	109.92	18	4
4	A	350	PX4	C28-C27-C26	3.03	99.06	114.42	1	1
4	A	359	PX4	C5-N1-C3	3.03	101.19	108.97	6	7
4	A	372	PX4	C3-N1-C2	3.03	122.30	109.92	8	4
4	A	342	PX4	C31-C30-C29	3.03	99.06	114.42	11	1
4	A	383	PX4	C5-N1-C4	3.03	101.20	108.97	11	6
4	A	417	PX4	C5-N1-C4	3.03	101.19	108.97	12	5
4	A	423	PX4	C31-C30-C29	3.02	99.07	114.42	12	1
4	A	405	PX4	C26-C25-C24	3.02	102.33	113.19	14	5
4	A	308	PX4	C33-C32-C31	3.02	99.09	114.42	4	2
4	A	322	PX4	O1-P1-O4	3.02	121.78	107.75	3	1
4	A	324	PX4	O5-C9-O6	3.02	115.97	123.59	7	4
4	A	411	PX4	O1-P1-O2	3.02	127.18	112.24	5	11
4	A	394	PX4	C5-N1-C4	3.02	116.74	108.97	18	8
4	A	428	PX4	C5-N1-C3	3.02	116.74	108.97	12	8
4	A	430	PX4	C26-C25-C24	3.02	124.05	113.19	1	1
4	A	348	PX4	O5-C9-C10	3.02	121.39	111.91	4	5
4	A	382	PX4	C5-N1-C4	3.02	101.21	108.97	5	6
4	A	305	PX4	O1-P1-O4	3.02	121.76	107.75	17	3
4	A	306	PX4	C15-C14-C13	3.02	99.11	114.42	17	4
4	A	339	PX4	C4-N1-C3	3.02	101.22	108.97	19	5
4	A	370	PX4	O1-P1-O2	3.02	127.15	112.24	5	12
4	A	408	PX4	C4-N1-C3	3.02	116.73	108.97	15	2
4	A	419	PX4	C5-N1-C3	3.02	101.22	108.97	7	5
4	A	350	PX4	C1-C2-N1	3.01	125.84	115.78	16	6
4	A	373	PX4	O5-C9-C10	3.01	121.37	111.91	3	6
4	A	386	PX4	O5-C9-O6	3.01	115.99	123.59	10	4
4	A	431	PX4	C14-C13-C12	3.01	99.13	114.42	8	2
4	A	326	PX4	C28-C27-C26	3.01	99.14	114.42	8	3
4	A	365	PX4	C11-C10-C9	3.01	102.67	113.62	13	2
4	A	371	PX4	O8-C23-C24	3.01	111.98	123.73	12	1
4	A	379	PX4	O4-P1-O2	3.01	120.83	109.07	5	2
4	A	385	PX4	C18-C17-C16	3.01	99.14	114.42	1	1
4	A	416	PX4	C5-N1-C3	3.01	116.71	108.97	18	3
4	A	337	PX4	C12-C11-C10	3.01	102.38	113.19	6	1
4	A	351	PX4	C25-C24-C23	3.01	102.68	113.62	10	1
4	A	401	PX4	O1-P1-O4	3.01	121.71	107.75	10	3
4	A	371	PX4	C33-C32-C31	3.01	99.16	114.42	1	3
4	A	416	PX4	C1-C2-N1	3.01	125.82	115.78	7	7
4	A	336	PX4	C5-N1-C3	3.01	101.24	108.97	2	2
4	A	323	PX4	C11-C10-C9	3.00	102.70	113.62	5	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	349	PX4	O1-P1-O2	3.00	127.09	112.24	11	11
4	A	365	PX4	O1-P1-O2	3.00	127.09	112.24	9	5
4	A	328	PX4	O3-P1-O2	3.00	97.33	109.07	10	4
4	A	337	PX4	P1-O4-C6	3.00	104.07	121.68	11	11
4	A	394	PX4	C5-N1-C3	3.00	116.70	108.97	13	6
4	A	366	PX4	C14-C13-C12	3.00	99.19	114.42	8	1
4	A	368	PX4	O3-P1-O2	3.00	97.34	109.07	19	6
4	A	331	PX4	C26-C25-C24	3.00	102.41	113.19	18	2
4	A	337	PX4	C27-C26-C25	3.00	99.20	114.42	18	4
4	A	405	PX4	O5-C9-O6	3.00	116.03	123.59	17	2
4	A	393	PX4	O4-P1-O2	3.00	97.36	109.07	7	2
4	A	423	PX4	C8-O5-C9	3.00	106.02	117.12	5	2
4	A	429	PX4	C4-N1-C3	3.00	101.27	108.97	15	2
4	A	334	PX4	C33-C32-C31	3.00	99.22	114.42	11	3
4	A	356	PX4	C26-C25-C24	3.00	123.96	113.19	6	2
4	A	395	PX4	C16-C15-C14	3.00	99.22	114.42	17	3
4	A	422	PX4	C30-C29-C28	3.00	99.22	114.42	19	1
4	A	370	PX4	O1-P1-O4	2.99	121.65	107.75	20	5
4	A	370	PX4	C18-C17-C16	2.99	99.23	114.42	14	4
4	A	404	PX4	C18-C17-C16	2.99	99.22	114.42	12	1
4	A	306	PX4	O1-P1-O4	2.99	121.64	107.75	7	2
4	A	328	PX4	C11-C10-C9	2.99	102.74	113.62	16	4
4	A	339	PX4	C5-N1-C3	2.99	116.67	108.97	4	4
4	A	371	PX4	O1-P1-O3	2.99	93.85	107.75	16	1
4	A	381	PX4	O7-C23-O8	2.99	116.47	123.70	9	6
4	A	313	PX4	O1-P1-O2	2.99	127.02	112.24	7	10
4	A	316	PX4	C16-C15-C14	2.99	99.25	114.42	7	2
4	A	358	PX4	O1-P1-O2	2.99	127.02	112.24	10	11
4	A	379	PX4	C11-C10-C9	2.99	102.75	113.62	4	2
4	A	412	PX4	C5-N1-C4	2.99	116.66	108.97	12	4
4	A	316	PX4	O4-P1-O2	2.99	120.73	109.07	3	4
4	A	329	PX4	C4-N1-C3	2.99	101.30	108.97	3	4
4	A	347	PX4	C8-O5-C9	2.99	106.06	117.12	3	2
4	A	369	PX4	O1-P1-O2	2.98	127.00	112.24	1	10
4	A	372	PX4	C5-N1-C4	2.99	116.65	108.97	15	7
4	A	430	PX4	C28-C27-C26	2.99	99.26	114.42	19	1
4	A	337	PX4	C5-N1-C2	2.98	122.13	109.92	6	2
4	A	385	PX4	C27-C26-C25	2.99	99.27	114.42	19	2
4	A	320	PX4	C7-O7-C23	2.98	110.44	117.79	6	3
4	A	312	PX4	C4-N1-C3	2.98	101.31	108.97	13	3
4	A	320	PX4	O5-C9-C10	2.98	121.27	111.91	9	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	391	PX4	O5-C9-C10	2.98	121.27	111.91	13	4
4	A	422	PX4	C1-C2-N1	2.98	125.74	115.78	2	7
4	A	313	PX4	C26-C25-C24	2.98	102.48	113.19	20	3
4	A	316	PX4	C33-C32-C31	2.98	99.29	114.42	5	3
4	A	332	PX4	C34-C33-C32	2.98	99.29	114.42	12	3
4	A	341	PX4	C26-C25-C24	2.98	102.47	113.19	5	1
4	A	402	PX4	O4-P1-O2	2.98	97.41	109.07	7	4
4	A	322	PX4	C13-C12-C11	2.98	99.30	114.42	2	2
4	A	351	PX4	O1-P1-O2	2.98	126.98	112.24	8	11
4	A	405	PX4	C20-C19-C18	2.98	99.29	114.42	18	1
4	A	329	PX4	O4-P1-O2	2.98	120.71	109.07	19	5
4	A	307	PX4	C19-C18-C17	2.98	99.30	114.42	15	1
4	A	357	PX4	O5-C9-O6	2.98	116.07	123.59	19	4
4	A	381	PX4	O3-C1-C2	2.98	124.83	109.16	17	3
4	A	384	PX4	O1-P1-O4	2.98	121.57	107.75	20	3
4	A	412	PX4	O4-P1-O2	2.98	120.70	109.07	20	3
4	A	416	PX4	C12-C11-C10	2.98	102.49	113.19	15	4
4	A	310	PX4	C5-N1-C2	2.97	97.74	109.92	20	1
4	A	322	PX4	C20-C19-C18	2.97	99.32	114.42	20	3
4	A	339	PX4	O1-P1-O2	2.98	126.95	112.24	12	13
4	A	339	PX4	C11-C10-C9	2.97	102.80	113.62	18	1
4	A	345	PX4	C26-C25-C24	2.97	102.50	113.19	7	4
4	A	417	PX4	O4-P1-O2	2.98	120.69	109.07	17	1
4	A	369	PX4	C12-C11-C10	2.97	102.50	113.19	16	3
4	A	407	PX4	O5-C9-O6	2.97	116.09	123.59	7	3
4	A	329	PX4	O7-C7-C6	2.97	119.16	108.40	2	8
4	A	401	PX4	C11-C10-C9	2.97	102.81	113.62	19	2
4	A	373	PX4	C16-C15-C14	2.97	99.34	114.42	13	2
4	A	410	PX4	C4-N1-C3	2.97	101.33	108.97	5	4
4	A	420	PX4	C26-C25-C24	2.97	102.50	113.19	6	4
4	A	421	PX4	C28-C27-C26	2.97	99.33	114.42	20	3
4	A	307	PX4	C5-N1-C3	2.97	101.33	108.97	5	3
4	A	321	PX4	C5-N1-C3	2.97	101.34	108.97	12	4
4	A	365	PX4	C5-N1-C2	2.97	122.07	109.92	20	1
4	A	331	PX4	O1-P1-O2	2.97	126.92	112.24	19	5
4	A	363	PX4	O7-C7-C6	2.97	119.15	108.40	20	10
4	A	384	PX4	C30-C29-C28	2.97	99.35	114.42	6	4
4	A	361	PX4	C11-C10-C9	2.97	102.83	113.62	15	4
4	A	409	PX4	O7-C7-C8	2.97	119.15	108.40	17	8
4	A	392	PX4	C27-C26-C25	2.97	99.36	114.42	10	3
4	A	308	PX4	C14-C13-C12	2.97	99.37	114.42	17	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	341	PX4	C15-C14-C13	2.97	99.37	114.42	4	3
4	A	374	PX4	C34-C33-C32	2.96	99.37	114.42	12	1
4	A	379	PX4	C19-C18-C17	2.97	99.37	114.42	19	1
4	A	414	PX4	O5-C9-C10	2.97	121.22	111.91	17	4
4	A	407	PX4	C17-C16-C15	2.96	99.37	114.42	9	1
4	A	417	PX4	C27-C26-C25	2.97	99.37	114.42	7	5
4	A	427	PX4	C25-C24-C23	2.97	124.41	113.62	6	1
4	A	346	PX4	C5-N1-C4	2.96	101.36	108.97	7	5
4	A	362	PX4	O5-C9-O6	2.96	116.11	123.59	5	7
4	A	354	PX4	C14-C13-C12	2.96	99.39	114.42	14	3
4	A	326	PX4	C8-O5-C9	2.96	106.16	117.12	17	3
4	A	346	PX4	C20-C19-C18	2.96	99.40	114.42	12	1
4	A	377	PX4	O1-P1-O3	2.96	93.99	107.75	5	2
4	A	379	PX4	C29-C28-C27	2.96	99.40	114.42	4	1
4	A	317	PX4	C14-C13-C12	2.96	99.40	114.42	1	1
4	A	317	PX4	O1-P1-O2	2.96	126.87	112.24	19	10
4	A	347	PX4	C26-C25-C24	2.96	102.56	113.19	4	2
4	A	425	PX4	C29-C28-C27	2.96	99.40	114.42	19	3
4	A	371	PX4	C30-C29-C28	2.96	99.42	114.42	2	4
4	A	404	PX4	O7-C7-C6	2.96	119.11	108.40	17	6
4	A	379	PX4	O5-C9-C10	2.96	121.19	111.91	8	6
4	A	383	PX4	C26-C25-C24	2.96	102.56	113.19	15	4
4	A	314	PX4	O5-C9-O6	2.96	116.13	123.59	7	8
4	A	379	PX4	P1-O4-C6	2.96	104.35	121.68	19	12
4	A	330	PX4	O1-P1-O2	2.95	126.84	112.24	7	8
4	A	343	PX4	O7-C7-C8	2.95	119.10	108.40	20	10
4	A	402	PX4	C12-C11-C10	2.95	102.57	113.19	2	3
4	A	387	PX4	C25-C24-C23	2.95	102.87	113.62	11	3
4	A	306	PX4	O1-P1-O2	2.95	126.83	112.24	15	12
4	A	379	PX4	C17-C16-C15	2.95	99.43	114.42	16	4
4	A	407	PX4	C30-C29-C28	2.95	99.44	114.42	11	2
4	A	421	PX4	C34-C33-C32	2.95	99.43	114.42	3	1
4	A	381	PX4	O5-C9-O6	2.95	116.14	123.59	14	3
4	A	313	PX4	C12-C11-C10	2.95	102.59	113.19	18	4
4	A	377	PX4	O5-C9-C10	2.95	121.17	111.91	1	3
4	A	313	PX4	C5-N1-C3	2.95	101.39	108.97	11	6
4	A	348	PX4	C3-N1-C2	2.95	121.98	109.92	4	2
4	A	361	PX4	C4-N1-C2	2.95	121.98	109.92	1	3
4	A	412	PX4	O1-P1-O3	2.95	94.06	107.75	2	3
4	A	314	PX4	C30-C29-C28	2.95	99.47	114.42	17	4
4	A	321	PX4	C1-C2-N1	2.95	125.61	115.78	19	7

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	351	PX4	C26-C25-C24	2.95	102.60	113.19	10	3
4	A	406	PX4	O4-P1-O2	2.95	120.58	109.07	8	3
4	A	378	PX4	C16-C15-C14	2.94	99.48	114.42	8	2
4	A	431	PX4	C30-C29-C28	2.94	99.48	114.42	11	1
4	A	405	PX4	C12-C11-C10	2.94	102.61	113.19	3	2
4	A	388	PX4	C8-O5-C9	2.94	106.22	117.12	12	3
4	A	428	PX4	C15-C14-C13	2.94	99.48	114.42	9	2
4	A	416	PX4	C26-C25-C24	2.94	102.61	113.19	12	5
4	A	346	PX4	C14-C13-C12	2.94	99.49	114.42	15	2
4	A	307	PX4	C4-N1-C3	2.94	101.42	108.97	15	4
4	A	308	PX4	O5-C9-O6	2.94	116.17	123.59	13	4
4	A	399	PX4	O7-C7-C8	2.94	119.05	108.40	2	4
4	A	411	PX4	C26-C25-C24	2.94	102.62	113.19	9	2
4	A	395	PX4	O5-C9-O6	2.94	116.17	123.59	18	4
4	A	361	PX4	C33-C32-C31	2.94	99.51	114.42	5	1
4	A	363	PX4	C5-N1-C3	2.94	116.53	108.97	9	3
4	A	371	PX4	C11-C10-C9	2.94	102.94	113.62	8	1
4	A	426	PX4	O3-P1-O2	2.94	97.59	109.07	2	1
4	A	382	PX4	C3-N1-C2	2.94	121.93	109.92	14	1
4	A	396	PX4	C7-O7-C23	2.94	125.02	117.79	12	3
4	A	325	PX4	O4-P1-O2	2.93	120.53	109.07	8	3
4	A	406	PX4	C33-C32-C31	2.93	99.53	114.42	20	2
4	A	395	PX4	O7-C7-C8	2.94	119.03	108.40	10	5
4	A	416	PX4	C25-C24-C23	2.93	102.95	113.62	1	1
4	A	416	PX4	O1-P1-O3	2.93	94.12	107.75	3	2
4	A	373	PX4	C30-C29-C28	2.93	99.53	114.42	3	3
4	A	419	PX4	O3-C1-C2	2.93	124.59	109.16	11	3
4	A	315	PX4	O1-P1-O3	2.93	94.13	107.75	16	3
4	A	316	PX4	O5-C9-O6	2.93	130.99	123.59	8	8
4	A	322	PX4	C5-N1-C4	2.93	101.44	108.97	10	4
4	A	341	PX4	O6-C9-C10	2.93	112.30	123.73	18	1
4	A	324	PX4	O6-C9-C10	2.93	112.30	123.73	11	1
4	A	410	PX4	C27-C26-C25	2.93	99.55	114.42	15	1
4	A	346	PX4	C4-N1-C2	2.93	121.90	109.92	12	2
4	A	330	PX4	C26-C25-C24	2.93	102.66	113.19	13	2
4	A	337	PX4	C4-N1-C3	2.93	101.45	108.97	11	4
4	A	374	PX4	C26-C25-C24	2.93	102.67	113.19	19	2
4	A	393	PX4	O5-C9-C10	2.93	121.10	111.91	9	2
4	A	425	PX4	C11-C10-C9	2.93	102.98	113.62	1	2
4	A	430	PX4	C11-C10-C9	2.93	102.98	113.62	15	3
4	A	335	PX4	C32-C31-C30	2.92	99.58	114.42	11	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	362	PX4	O4-P1-O2	2.92	120.49	109.07	3	2
4	A	395	PX4	O5-C9-C10	2.93	121.09	111.91	11	7
4	A	421	PX4	C14-C13-C12	2.93	99.57	114.42	4	2
4	A	356	PX4	C31-C30-C29	2.92	99.59	114.42	6	3
4	A	401	PX4	O1-P1-O2	2.92	126.69	112.24	7	11
4	A	374	PX4	O1-P1-O4	2.92	121.32	107.75	7	2
4	A	411	PX4	O1-P1-O3	2.92	94.17	107.75	6	2
4	A	397	PX4	C5-N1-C2	2.92	121.87	109.92	7	2
4	A	319	PX4	O3-C1-C2	2.92	124.52	109.16	16	3
4	A	377	PX4	C28-C27-C26	2.92	99.60	114.42	6	1
4	A	419	PX4	C29-C28-C27	2.92	99.60	114.42	10	2
4	A	345	PX4	C15-C14-C13	2.92	99.62	114.42	1	3
4	A	358	PX4	O7-C23-O8	2.92	116.65	123.70	18	5
4	A	343	PX4	C20-C19-C18	2.92	99.62	114.42	7	3
4	A	373	PX4	O1-P1-O4	2.92	121.29	107.75	20	3
4	A	412	PX4	C14-C13-C12	2.92	99.62	114.42	4	4
4	A	415	PX4	O6-C9-C10	2.92	112.36	123.73	7	3
4	A	418	PX4	C32-C31-C30	2.92	99.63	114.42	11	1
4	A	332	PX4	C1-C2-N1	2.91	125.51	115.78	20	3
4	A	353	PX4	O6-C9-C10	2.91	112.36	123.73	6	1
4	A	413	PX4	C5-N1-C4	2.91	116.47	108.97	4	6
4	A	414	PX4	O7-C7-C6	2.91	118.95	108.40	5	9
4	A	307	PX4	C3-N1-C2	2.91	98.00	109.92	18	1
4	A	323	PX4	C4-N1-C3	2.91	101.49	108.97	14	1
4	A	330	PX4	C29-C28-C27	2.91	99.64	114.42	6	1
4	A	328	PX4	C12-C11-C10	2.91	102.73	113.19	4	3
4	A	357	PX4	C29-C28-C27	2.91	99.65	114.42	8	1
4	A	361	PX4	C28-C27-C26	2.91	99.65	114.42	9	1
4	A	369	PX4	C5-N1-C4	2.91	101.49	108.97	19	5
4	A	388	PX4	O8-C23-C24	2.91	112.38	123.73	6	2
4	A	382	PX4	C30-C29-C28	2.91	99.67	114.42	6	2
4	A	420	PX4	C17-C16-C15	2.91	99.66	114.42	11	2
4	A	427	PX4	O3-C1-C2	2.91	124.45	109.16	17	2
4	A	350	PX4	C8-O5-C9	2.91	106.36	117.12	13	1
4	A	400	PX4	C16-C15-C14	2.91	99.67	114.42	19	2
4	A	396	PX4	O4-P1-O2	2.91	120.42	109.07	15	1
4	A	347	PX4	O7-C23-O8	2.90	116.68	123.70	17	4
4	A	361	PX4	O4-P1-O2	2.90	97.72	109.07	20	2
4	A	374	PX4	O5-C9-C10	2.90	121.02	111.91	13	5
4	A	348	PX4	C26-C25-C24	2.90	102.75	113.19	12	3
4	A	367	PX4	C33-C32-C31	2.90	99.68	114.42	11	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	386	PX4	C8-O5-C9	2.90	106.37	117.12	2	5
4	A	394	PX4	C20-C19-C18	2.90	99.68	114.42	17	1
4	A	337	PX4	C25-C24-C23	2.90	103.07	113.62	17	3
4	A	359	PX4	O4-P1-O2	2.90	120.41	109.07	9	4
4	A	415	PX4	C28-C27-C26	2.90	99.69	114.42	2	2
4	A	357	PX4	O3-P1-O2	2.90	97.74	109.07	19	5
4	A	325	PX4	C15-C14-C13	2.90	99.71	114.42	7	2
4	A	338	PX4	C11-C10-C9	2.90	103.08	113.62	19	3
4	A	390	PX4	C20-C19-C18	2.90	99.71	114.42	2	2
4	A	320	PX4	C8-O5-C9	2.90	127.85	117.12	13	1
4	A	365	PX4	C8-O5-C9	2.90	127.85	117.12	15	2
4	A	418	PX4	C31-C30-C29	2.90	99.71	114.42	18	1
4	A	425	PX4	C19-C18-C17	2.90	99.71	114.42	14	1
4	A	323	PX4	C20-C19-C18	2.90	99.73	114.42	13	4
4	A	332	PX4	C4-N1-C3	2.90	101.53	108.97	3	2
4	A	336	PX4	O6-C9-C10	2.90	112.43	123.73	2	2
4	A	344	PX4	C20-C19-C18	2.90	99.72	114.42	1	2
4	A	355	PX4	C34-C33-C32	2.90	99.72	114.42	5	4
4	A	366	PX4	C5-N1-C2	2.90	121.77	109.92	7	4
4	A	407	PX4	C34-C33-C32	2.90	99.72	114.42	18	2
4	A	348	PX4	C16-C15-C14	2.89	99.73	114.42	3	2
4	A	353	PX4	O1-P1-O3	2.89	94.30	107.75	6	3
4	A	358	PX4	C12-C11-C10	2.89	102.79	113.19	12	2
4	A	396	PX4	C5-N1-C4	2.89	101.53	108.97	7	2
4	A	334	PX4	O5-C9-C10	2.89	120.98	111.91	6	7
4	A	337	PX4	C1-C2-N1	2.89	125.43	115.78	3	4
4	A	341	PX4	C30-C29-C28	2.89	99.75	114.42	6	2
4	A	346	PX4	O4-P1-O2	2.89	120.36	109.07	12	4
4	A	387	PX4	C20-C19-C18	2.89	99.74	114.42	5	1
4	A	371	PX4	O4-P1-O2	2.89	120.36	109.07	4	3
4	A	324	PX4	C5-N1-C4	2.89	101.55	108.97	8	2
4	A	431	PX4	O1-P1-O3	2.89	94.33	107.75	20	3
4	A	404	PX4	O1-P1-O2	2.89	126.52	112.24	15	12
4	A	392	PX4	C5-N1-C4	2.89	116.40	108.97	2	5
4	A	308	PX4	C30-C29-C28	2.89	99.77	114.42	1	2
4	A	306	PX4	C14-C13-C12	2.88	99.78	114.42	17	1
4	A	314	PX4	C18-C17-C16	2.89	99.77	114.42	14	2
4	A	417	PX4	O5-C9-C10	2.89	120.97	111.91	1	4
4	A	350	PX4	C25-C24-C23	2.88	124.11	113.62	2	2
4	A	377	PX4	C4-N1-C3	2.88	101.56	108.97	10	2
4	A	353	PX4	C5-N1-C4	2.88	101.56	108.97	19	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	354	PX4	C5-N1-C4	2.88	116.39	108.97	11	4
4	A	372	PX4	C1-C2-N1	2.88	125.40	115.78	12	5
4	A	386	PX4	C1-C2-N1	2.88	125.40	115.78	18	3
4	A	420	PX4	O5-C9-O6	2.88	116.31	123.59	7	3
4	A	336	PX4	C5-N1-C2	2.88	98.13	109.92	9	1
4	A	416	PX4	O5-C9-C10	2.88	120.95	111.91	13	3
4	A	386	PX4	C4-N1-C2	2.88	121.69	109.92	14	2
4	A	413	PX4	C22-C21-C20	2.88	91.57	113.42	12	1
4	A	374	PX4	C4-N1-C3	2.88	101.58	108.97	20	3
4	A	316	PX4	C5-N1-C3	2.87	116.36	108.97	4	5
4	A	405	PX4	O1-P1-O2	2.88	126.45	112.24	4	9
4	A	374	PX4	C31-C30-C29	2.87	99.83	114.42	20	3
4	A	378	PX4	C26-C25-C24	2.87	102.86	113.19	2	1
4	A	397	PX4	C13-C12-C11	2.88	99.83	114.42	13	3
4	A	392	PX4	O8-C23-C24	2.87	112.52	123.73	6	2
4	A	393	PX4	C28-C27-C26	2.87	99.83	114.42	6	1
4	A	328	PX4	C4-N1-C3	2.87	101.59	108.97	4	6
4	A	413	PX4	O7-C7-C6	2.87	118.81	108.40	20	9
4	A	317	PX4	C4-N1-C3	2.87	101.59	108.97	3	3
4	A	312	PX4	O5-C9-O6	2.87	116.34	123.59	6	9
4	A	361	PX4	O3-P1-O2	2.87	97.85	109.07	6	3
4	A	383	PX4	C32-C31-C30	2.87	99.84	114.42	18	1
4	A	307	PX4	C5-N1-C4	2.87	101.59	108.97	15	3
4	A	317	PX4	O4-P1-O2	2.87	120.28	109.07	16	1
4	A	415	PX4	O1-P1-O4	2.87	121.08	107.75	5	4
4	A	308	PX4	C4-N1-C2	2.87	98.18	109.92	18	1
4	A	339	PX4	C26-C25-C24	2.87	102.88	113.19	6	3
4	A	343	PX4	C1-C2-N1	2.87	125.36	115.78	19	4
4	A	359	PX4	C20-C19-C18	2.87	99.86	114.42	1	3
4	A	374	PX4	C16-C15-C14	2.87	99.86	114.42	19	3
4	A	396	PX4	C18-C17-C16	2.87	99.86	114.42	16	4
4	A	322	PX4	O3-C1-C2	2.87	124.24	109.16	7	2
4	A	402	PX4	C15-C14-C13	2.87	99.87	114.42	14	1
4	A	387	PX4	O3-C1-C2	2.87	124.24	109.16	15	2
4	A	396	PX4	C13-C12-C11	2.87	99.87	114.42	9	2
4	A	391	PX4	C12-C11-C10	2.87	102.89	113.19	17	3
4	A	392	PX4	C1-C2-N1	2.87	125.35	115.78	10	5
4	A	428	PX4	C11-C10-C9	2.87	103.19	113.62	13	2
4	A	331	PX4	O1-P1-O3	2.87	94.43	107.75	17	4
4	A	350	PX4	C11-C10-C9	2.87	103.20	113.62	17	2
4	A	412	PX4	O7-C23-O8	2.87	116.78	123.70	10	9

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	363	PX4	C4-N1-C2	2.86	98.20	109.92	9	3
4	A	409	PX4	C19-C18-C17	2.86	99.88	114.42	18	2
4	A	403	PX4	C27-C26-C25	2.86	99.89	114.42	17	4
4	A	375	PX4	O3-P1-O2	2.86	97.88	109.07	6	5
4	A	378	PX4	O1-P1-O2	2.86	126.40	112.24	1	9
4	A	419	PX4	C26-C25-C24	2.86	102.89	113.19	18	2
4	A	399	PX4	C19-C18-C17	2.86	99.89	114.42	9	1
4	A	405	PX4	O7-C7-C6	2.86	118.77	108.40	16	6
4	A	406	PX4	C16-C15-C14	2.86	99.89	114.42	5	4
4	A	395	PX4	C12-C11-C10	2.86	102.90	113.19	19	2
4	A	309	PX4	C28-C27-C26	2.86	99.90	114.42	13	3
4	A	360	PX4	C8-O5-C9	2.86	106.53	117.12	9	4
4	A	363	PX4	C28-C27-C26	2.86	99.91	114.42	17	3
4	A	367	PX4	C27-C26-C25	2.86	99.90	114.42	15	1
4	A	387	PX4	C26-C25-C24	2.86	102.91	113.19	12	2
4	A	389	PX4	C8-O5-C9	2.86	106.53	117.12	17	2
4	A	390	PX4	C18-C17-C16	2.86	99.90	114.42	16	2
4	A	311	PX4	C31-C30-C29	2.86	99.91	114.42	9	2
4	A	326	PX4	C3-N1-C2	2.86	98.21	109.92	10	2
4	A	401	PX4	O5-C9-O6	2.86	116.38	123.59	15	4
4	A	402	PX4	O5-C9-C10	2.86	120.87	111.91	11	5
4	A	324	PX4	O8-C23-C24	2.86	112.59	123.73	9	2
4	A	361	PX4	C1-C2-N1	2.86	125.31	115.78	20	4
4	A	364	PX4	C3-N1-C2	2.85	98.23	109.92	16	2
4	A	407	PX4	O5-C9-C10	2.85	120.87	111.91	18	5
4	A	392	PX4	C15-C14-C13	2.86	99.93	114.42	16	2
4	A	414	PX4	C26-C25-C24	2.85	102.93	113.19	17	7
4	A	427	PX4	C5-N1-C4	2.85	101.64	108.97	13	4
4	A	315	PX4	C19-C18-C17	2.85	99.95	114.42	17	4
4	A	337	PX4	C11-C10-C9	2.85	103.25	113.62	9	2
4	A	340	PX4	C26-C25-C24	2.85	102.94	113.19	16	5
4	A	359	PX4	O8-C23-C24	2.85	112.61	123.73	7	2
4	A	397	PX4	O1-P1-O4	2.85	121.00	107.75	2	3
4	A	419	PX4	C5-N1-C2	2.85	121.59	109.92	9	2
4	A	341	PX4	O4-P1-O2	2.85	97.93	109.07	4	2
4	A	412	PX4	O3-P1-O2	2.85	97.93	109.07	7	3
4	A	323	PX4	O5-C9-O6	2.85	116.40	123.59	7	5
4	A	328	PX4	C26-C25-C24	2.85	102.95	113.19	17	4
4	A	353	PX4	C28-C27-C26	2.85	99.96	114.42	3	4
4	A	417	PX4	C4-N1-C2	2.85	121.57	109.92	12	3
4	A	423	PX4	C19-C18-C17	2.85	99.96	114.42	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	424	PX4	C20-C19-C18	2.85	99.96	114.42	4	3
4	A	321	PX4	O1-P1-O3	2.85	120.97	107.75	14	2
4	A	365	PX4	C1-C2-N1	2.85	125.29	115.78	12	6
4	A	308	PX4	C32-C31-C30	2.84	128.87	114.42	12	3
4	A	365	PX4	C25-C24-C23	2.85	103.27	113.62	12	3
4	A	427	PX4	O4-P1-O2	2.85	120.19	109.07	12	3
4	A	341	PX4	C17-C16-C15	2.84	99.98	114.42	4	1
4	A	364	PX4	C33-C32-C31	2.84	99.98	114.42	1	1
4	A	408	PX4	C30-C29-C28	2.84	99.98	114.42	4	1
4	A	424	PX4	O4-P1-O2	2.84	120.18	109.07	3	4
4	A	323	PX4	C13-C12-C11	2.84	99.99	114.42	6	3
4	A	358	PX4	C17-C16-C15	2.84	99.99	114.42	8	3
4	A	374	PX4	C18-C17-C16	2.84	100.00	114.42	2	2
4	A	409	PX4	O6-C9-C10	2.84	112.64	123.73	8	2
4	A	393	PX4	C25-C24-C23	2.84	103.28	113.62	16	2
4	A	415	PX4	C13-C12-C11	2.84	99.99	114.42	6	3
4	A	430	PX4	C3-N1-C2	2.84	121.55	109.92	6	3
4	A	331	PX4	C18-C17-C16	2.84	100.00	114.42	20	3
4	A	348	PX4	C8-O5-C9	2.84	106.60	117.12	20	2
4	A	388	PX4	C16-C15-C14	2.84	100.00	114.42	11	2
4	A	398	PX4	C25-C24-C23	2.84	103.29	113.62	12	3
4	A	319	PX4	O7-C23-O8	2.84	116.84	123.70	8	5
4	A	383	PX4	C1-C2-N1	2.84	125.26	115.78	3	5
4	A	408	PX4	C26-C25-C24	2.84	102.98	113.19	18	3
4	A	365	PX4	O5-C9-C10	2.84	120.82	111.91	14	4
4	A	410	PX4	C1-C2-N1	2.84	125.26	115.78	18	8
4	A	307	PX4	C31-C30-C29	2.84	100.02	114.42	14	2
4	A	388	PX4	C13-C12-C11	2.84	100.02	114.42	20	4
4	A	411	PX4	C34-C33-C32	2.84	100.02	114.42	16	2
4	A	322	PX4	C4-N1-C3	2.84	101.68	108.97	18	4
4	A	334	PX4	C5-N1-C2	2.84	121.52	109.92	18	1
4	A	402	PX4	O6-C9-C10	2.84	112.67	123.73	4	3
4	A	406	PX4	C4-N1-C3	2.84	101.68	108.97	3	4
4	A	398	PX4	C34-C33-C32	2.84	100.02	114.42	7	2
4	A	398	PX4	O4-P1-O2	2.84	97.98	109.07	8	1
4	A	366	PX4	C27-C26-C25	2.84	100.03	114.42	4	2
4	A	380	PX4	C19-C18-C17	2.83	100.04	114.42	15	4
4	A	431	PX4	C25-C24-C23	2.84	103.31	113.62	19	2
4	A	395	PX4	O1-P1-O4	2.83	120.91	107.75	4	4
4	A	323	PX4	C25-C24-C23	2.83	103.33	113.62	19	3
4	A	333	PX4	C3-N1-C2	2.83	121.50	109.92	2	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	368	PX4	C30-C29-C28	2.83	100.05	114.42	5	2
4	A	370	PX4	C34-C33-C32	2.83	100.06	114.42	16	1
4	A	402	PX4	C34-C33-C32	2.83	100.06	114.42	12	2
4	A	381	PX4	C15-C14-C13	2.83	100.06	114.42	10	2
4	A	382	PX4	C16-C15-C14	2.83	100.05	114.42	20	2
4	A	312	PX4	O7-C7-C6	2.83	118.64	108.40	15	5
4	A	340	PX4	O4-P1-O2	2.83	120.12	109.07	19	4
4	A	384	PX4	C11-C10-C9	2.83	103.33	113.62	2	5
4	A	323	PX4	O1-P1-O3	2.83	94.61	107.75	10	2
4	A	377	PX4	C16-C15-C14	2.83	100.07	114.42	18	1
4	A	354	PX4	O5-C9-O6	2.83	116.46	123.59	5	4
4	A	381	PX4	C14-C13-C12	2.83	100.08	114.42	6	2
4	A	408	PX4	C5-N1-C3	2.83	101.71	108.97	3	1
4	A	323	PX4	O3-C1-C2	2.82	124.02	109.16	8	2
4	A	339	PX4	C8-O5-C9	2.82	106.66	117.12	8	4
4	A	392	PX4	C26-C25-C24	2.82	103.04	113.19	13	2
4	A	393	PX4	O8-C23-C24	2.82	112.71	123.73	20	2
4	A	394	PX4	O3-P1-O2	2.83	98.03	109.07	4	2
4	A	363	PX4	C3-N1-C2	2.82	121.47	109.92	17	4
4	A	399	PX4	C30-C29-C28	2.82	100.09	114.42	17	2
4	A	390	PX4	C33-C32-C31	2.82	100.09	114.42	18	3
4	A	431	PX4	C32-C31-C30	2.82	100.09	114.42	12	5
4	A	305	PX4	C8-O5-C9	2.82	106.67	117.12	9	2
4	A	309	PX4	O4-P1-O2	2.82	120.09	109.07	18	2
4	A	321	PX4	C4-N1-C3	2.82	101.72	108.97	11	4
4	A	383	PX4	O1-P1-O4	2.82	120.86	107.75	15	2
4	A	370	PX4	O3-C1-C2	2.82	124.00	109.16	3	3
4	A	424	PX4	O1-P1-O2	2.82	126.19	112.24	6	8
4	A	306	PX4	O7-C7-C6	2.82	118.61	108.40	2	7
4	A	307	PX4	C8-O5-C9	2.82	106.68	117.12	9	3
4	A	342	PX4	C1-C2-N1	2.82	125.19	115.78	6	4
4	A	414	PX4	C4-N1-C3	2.82	101.73	108.97	7	2
4	A	428	PX4	O1-P1-O3	2.82	94.65	107.75	5	2
4	A	311	PX4	O4-P1-O2	2.82	120.08	109.07	8	3
4	A	336	PX4	O1-P1-O3	2.82	94.66	107.75	19	1
4	A	348	PX4	O3-P1-O2	2.82	98.06	109.07	2	4
4	A	349	PX4	C29-C28-C27	2.82	100.12	114.42	2	2
4	A	357	PX4	C26-C25-C24	2.82	103.06	113.19	8	4
4	A	406	PX4	C1-C2-N1	2.82	125.19	115.78	10	6
4	A	414	PX4	C33-C32-C31	2.82	100.12	114.42	12	3
4	A	419	PX4	O5-C9-C10	2.82	120.75	111.91	18	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	311	PX4	C17-C16-C15	2.82	100.13	114.42	7	2
4	A	316	PX4	C4-N1-C3	2.82	116.21	108.97	9	3
4	A	344	PX4	C4-N1-C2	2.82	98.40	109.92	5	1
4	A	356	PX4	C5-N1-C3	2.82	101.73	108.97	4	5
4	A	317	PX4	C18-C17-C16	2.81	100.15	114.42	19	1
4	A	311	PX4	C11-C10-C9	2.81	103.39	113.62	12	1
4	A	353	PX4	C30-C29-C28	2.81	100.14	114.42	7	3
4	A	394	PX4	C26-C25-C24	2.81	103.08	113.19	15	4
4	A	408	PX4	C25-C24-C23	2.81	103.39	113.62	4	4
4	A	307	PX4	C25-C24-C23	2.81	103.40	113.62	15	3
4	A	314	PX4	C29-C28-C27	2.81	100.16	114.42	18	1
4	A	381	PX4	O5-C9-C10	2.81	120.73	111.91	9	4
4	A	315	PX4	C17-C16-C15	2.81	100.16	114.42	4	2
4	A	321	PX4	C32-C31-C30	2.81	100.16	114.42	18	3
4	A	340	PX4	C18-C17-C16	2.81	100.16	114.42	1	1
4	A	317	PX4	C1-C2-N1	2.81	125.15	115.78	3	7
4	A	314	PX4	C19-C18-C17	2.81	100.17	114.42	3	2
4	A	325	PX4	C25-C24-C23	2.81	123.83	113.62	14	4
4	A	339	PX4	C5-N1-C4	2.81	116.19	108.97	20	7
4	A	362	PX4	C3-N1-C2	2.81	121.41	109.92	14	3
4	A	402	PX4	O3-C1-C2	2.81	123.93	109.16	15	3
4	A	406	PX4	C15-C14-C13	2.81	100.17	114.42	1	3
4	A	430	PX4	O5-C9-C10	2.81	120.72	111.91	15	3
4	A	306	PX4	C26-C25-C24	2.81	103.11	113.19	6	3
4	A	317	PX4	C17-C16-C15	2.81	100.18	114.42	13	1
4	A	391	PX4	O3-C1-C2	2.81	123.92	109.16	6	1
4	A	307	PX4	C20-C19-C18	2.80	100.19	114.42	6	1
4	A	358	PX4	O1-P1-O3	2.80	94.72	107.75	4	3
4	A	373	PX4	O1-P1-O3	2.81	94.71	107.75	1	5
4	A	418	PX4	C12-C11-C10	2.81	103.11	113.19	1	6
4	A	423	PX4	C17-C16-C15	2.81	100.18	114.42	15	3
4	A	425	PX4	O4-P1-O2	2.81	120.03	109.07	9	3
4	A	321	PX4	C17-C16-C15	2.80	100.19	114.42	20	1
4	A	324	PX4	C4-N1-C2	2.80	121.38	109.92	4	2
4	A	308	PX4	C31-C30-C29	2.80	100.21	114.42	2	1
4	A	330	PX4	C31-C30-C29	2.80	100.21	114.42	14	3
4	A	335	PX4	O5-C9-C10	2.80	120.70	111.91	19	6
4	A	338	PX4	C1-C2-N1	2.80	125.13	115.78	1	2
4	A	370	PX4	C4-N1-C2	2.80	121.38	109.92	1	3
4	A	377	PX4	C13-C12-C11	2.80	100.20	114.42	15	1
4	A	341	PX4	C1-C2-N1	2.80	125.13	115.78	17	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	358	PX4	C29-C28-C27	2.80	100.21	114.42	20	2
4	A	409	PX4	O4-P1-O2	2.80	120.01	109.07	6	1
4	A	341	PX4	C18-C17-C16	2.80	100.22	114.42	18	2
4	A	359	PX4	C32-C31-C30	2.80	100.21	114.42	8	3
4	A	412	PX4	C25-C24-C23	2.80	103.44	113.62	6	1
4	A	383	PX4	O8-C23-C24	2.80	112.81	123.73	3	2
4	A	417	PX4	O1-P1-O2	2.80	126.08	112.24	14	10
4	A	411	PX4	C5-N1-C2	2.80	121.37	109.92	18	1
4	A	413	PX4	C8-O5-C9	2.80	106.76	117.12	19	1
4	A	420	PX4	C25-C24-C23	2.80	103.44	113.62	19	1
4	A	318	PX4	O4-P1-O2	2.80	120.00	109.07	1	2
4	A	307	PX4	C27-C26-C25	2.80	100.23	114.42	17	2
4	A	368	PX4	O5-C9-C10	2.80	120.69	111.91	9	9
4	A	307	PX4	C26-C25-C24	2.80	103.14	113.19	6	4
4	A	308	PX4	C25-C24-C23	2.80	103.45	113.62	12	3
4	A	368	PX4	C34-C33-C32	2.80	100.23	114.42	4	4
4	A	318	PX4	C18-C17-C16	2.79	100.24	114.42	3	3
4	A	345	PX4	O1-P1-O2	2.79	126.05	112.24	2	7
4	A	375	PX4	O1-P1-O3	2.79	94.78	107.75	6	2
4	A	388	PX4	C7-O7-C23	2.79	124.67	117.79	10	8
4	A	419	PX4	O5-C9-O6	2.79	116.54	123.59	12	4
4	A	310	PX4	C16-C15-C14	2.79	100.25	114.42	11	4
4	A	315	PX4	C33-C32-C31	2.79	100.26	114.42	18	2
4	A	317	PX4	O1-P1-O4	2.79	94.79	107.75	5	4
4	A	324	PX4	P1-O4-C6	2.79	105.33	121.68	14	7
4	A	363	PX4	O7-C7-C8	2.79	118.50	108.40	15	5
4	A	402	PX4	C14-C13-C12	2.79	100.26	114.42	2	1
4	A	397	PX4	C19-C18-C17	2.79	100.26	114.42	11	3
4	A	395	PX4	O4-P1-O2	2.79	119.97	109.07	16	3
4	A	332	PX4	C26-C25-C24	2.79	103.17	113.19	19	5
4	A	333	PX4	O3-P1-O2	2.79	98.18	109.07	16	4
4	A	419	PX4	C28-C27-C26	2.79	100.27	114.42	17	5
4	A	329	PX4	C29-C28-C27	2.78	100.29	114.42	17	2
4	A	353	PX4	C4-N1-C3	2.79	101.81	108.97	12	5
4	A	387	PX4	O4-P1-O2	2.79	119.95	109.07	19	3
4	A	429	PX4	C8-O5-C9	2.78	106.81	117.12	20	3
4	A	316	PX4	C28-C27-C26	2.78	100.31	114.42	2	4
4	A	333	PX4	C15-C14-C13	2.78	100.30	114.42	17	2
4	A	367	PX4	C12-C11-C10	2.78	103.19	113.19	9	2
4	A	372	PX4	O4-P1-O2	2.78	98.20	109.07	1	3
4	A	403	PX4	O5-C9-C10	2.78	120.64	111.91	3	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	395	PX4	C28-C27-C26	2.78	100.31	114.42	18	2
4	A	430	PX4	C30-C29-C28	2.78	100.31	114.42	11	1
4	A	325	PX4	C4-N1-C3	2.78	116.12	108.97	10	4
4	A	357	PX4	O8-C23-C24	2.78	112.89	123.73	19	2
4	A	308	PX4	C13-C12-C11	2.78	100.33	114.42	1	1
4	A	319	PX4	C33-C32-C31	2.78	100.32	114.42	1	1
4	A	366	PX4	O3-C1-C2	2.78	123.77	109.16	15	2
4	A	422	PX4	C16-C15-C14	2.78	100.32	114.42	11	1
4	A	305	PX4	C18-C17-C16	2.78	100.33	114.42	17	2
4	A	334	PX4	C31-C30-C29	2.78	100.33	114.42	16	1
4	A	405	PX4	C28-C27-C26	2.78	100.33	114.42	4	2
4	A	339	PX4	C14-C13-C12	2.78	100.33	114.42	6	1
4	A	413	PX4	O7-C7-C8	2.78	118.45	108.40	20	4
4	A	325	PX4	C12-C11-C10	2.77	103.22	113.19	13	2
4	A	338	PX4	C29-C28-C27	2.77	100.34	114.42	14	3
4	A	346	PX4	O5-C9-C10	2.77	120.62	111.91	18	2
4	A	328	PX4	C7-O7-C23	2.77	110.96	117.79	8	5
4	A	352	PX4	C5-N1-C2	2.77	121.26	109.92	19	2
4	A	387	PX4	O5-C9-C10	2.77	120.61	111.91	7	4
4	A	392	PX4	C33-C32-C31	2.77	100.35	114.42	3	1
4	A	314	PX4	C5-N1-C4	2.77	101.85	108.97	15	5
4	A	330	PX4	C15-C14-C13	2.77	100.36	114.42	1	3
4	A	362	PX4	C1-C2-N1	2.77	125.03	115.78	15	3
4	A	400	PX4	C5-N1-C2	2.77	121.25	109.92	9	1
4	A	385	PX4	C5-N1-C3	2.77	101.85	108.97	2	5
4	A	326	PX4	C5-N1-C4	2.77	116.09	108.97	16	6
4	A	330	PX4	O1-P1-O3	2.77	94.88	107.75	19	2
4	A	331	PX4	C12-C11-C10	2.77	103.23	113.19	11	2
4	A	341	PX4	O1-P1-O4	2.77	120.60	107.75	13	3
4	A	349	PX4	C8-O5-C9	2.77	106.87	117.12	3	2
4	A	358	PX4	C27-C26-C25	2.77	100.37	114.42	18	3
4	A	428	PX4	C17-C16-C15	2.77	100.36	114.42	18	3
4	A	431	PX4	C4-N1-C2	2.77	121.25	109.92	12	1
4	A	314	PX4	C12-C11-C10	2.77	103.24	113.19	13	3
4	A	382	PX4	O7-C7-C6	2.77	118.42	108.40	17	8
4	A	335	PX4	C17-C16-C15	2.77	100.38	114.42	17	1
4	A	375	PX4	C16-C15-C14	2.77	100.38	114.42	10	3
4	A	410	PX4	C11-C10-C9	2.77	103.56	113.62	14	2
4	A	392	PX4	C8-O5-C9	2.77	106.88	117.12	15	2
4	A	358	PX4	C19-C18-C17	2.76	100.39	114.42	13	5
4	A	362	PX4	O7-C7-C6	2.76	118.41	108.40	3	7

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	369	PX4	C18-C17-C16	2.76	100.40	114.42	6	2
4	A	371	PX4	C20-C19-C18	2.76	100.39	114.42	8	1
4	A	389	PX4	C26-C25-C24	2.76	123.12	113.19	16	2
4	A	392	PX4	O5-C9-C10	2.76	120.58	111.91	19	5
4	A	417	PX4	O3-C1-C2	2.76	123.70	109.16	4	2
4	A	325	PX4	C31-C30-C29	2.76	100.40	114.42	18	1
4	A	376	PX4	C25-C24-C23	2.76	103.58	113.62	11	2
4	A	388	PX4	C12-C11-C10	2.76	103.26	113.19	10	1
4	A	392	PX4	O7-C7-C8	2.76	118.40	108.40	1	5
4	A	412	PX4	C30-C29-C28	2.76	100.40	114.42	15	2
4	A	314	PX4	C4-N1-C3	2.76	101.88	108.97	13	2
4	A	404	PX4	C12-C11-C10	2.76	103.27	113.19	19	3
4	A	386	PX4	C25-C24-C23	2.76	103.58	113.62	16	3
4	A	307	PX4	O4-P1-O2	2.76	119.85	109.07	11	3
4	A	335	PX4	O1-P1-O4	2.76	120.56	107.75	18	3
4	A	345	PX4	C33-C32-C31	2.76	100.42	114.42	7	3
4	A	368	PX4	C18-C17-C16	2.76	100.42	114.42	14	3
4	A	369	PX4	C25-C24-C23	2.76	103.59	113.62	9	5
4	A	418	PX4	C13-C12-C11	2.76	100.42	114.42	14	2
4	A	424	PX4	O3-P1-O2	2.76	98.28	109.07	11	5
4	A	360	PX4	C7-O7-C23	2.76	124.58	117.79	13	6
4	A	365	PX4	C19-C18-C17	2.76	100.42	114.42	10	3
4	A	325	PX4	C34-C33-C32	2.76	100.43	114.42	7	1
4	A	328	PX4	C15-C14-C13	2.76	100.43	114.42	6	2
4	A	391	PX4	C14-C13-C12	2.76	100.42	114.42	16	1
4	A	419	PX4	C33-C32-C31	2.76	100.43	114.42	2	2
4	A	421	PX4	O1-P1-O3	2.76	94.94	107.75	15	1
4	A	317	PX4	C12-C11-C10	2.76	103.28	113.19	20	4
4	A	395	PX4	C20-C19-C18	2.76	100.43	114.42	9	2
4	A	308	PX4	C11-C10-C9	2.75	103.60	113.62	20	5
4	A	334	PX4	O3-P1-O2	2.76	98.30	109.07	13	4
4	A	415	PX4	C8-O5-C9	2.76	106.92	117.12	18	4
4	A	424	PX4	C15-C14-C13	2.76	100.44	114.42	11	1
4	A	326	PX4	C19-C18-C17	2.75	100.45	114.42	18	1
4	A	330	PX4	C5-N1-C4	2.75	101.89	108.97	5	6
4	A	342	PX4	C30-C29-C28	2.75	100.45	114.42	9	1
4	A	347	PX4	C28-C27-C26	2.75	100.44	114.42	3	1
4	A	348	PX4	O4-P1-O2	2.75	98.30	109.07	16	2
4	A	348	PX4	O8-C23-C24	2.75	112.99	123.73	20	2
4	A	332	PX4	C18-C17-C16	2.75	100.45	114.42	14	3
4	A	353	PX4	C5-N1-C2	2.75	121.18	109.92	1	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	369	PX4	C8-O5-C9	2.75	106.93	117.12	10	2
4	A	397	PX4	C28-C27-C26	2.75	100.45	114.42	8	1
4	A	418	PX4	O1-P1-O4	2.75	120.53	107.75	10	1
4	A	423	PX4	C15-C14-C13	2.75	100.45	114.42	19	2
4	A	308	PX4	C15-C14-C13	2.75	100.46	114.42	7	2
4	A	333	PX4	O3-C1-C2	2.75	123.63	109.16	2	2
4	A	335	PX4	C19-C18-C17	2.75	100.46	114.42	16	1
4	A	371	PX4	O7-C7-C6	2.75	118.36	108.40	10	8
4	A	421	PX4	O1-P1-O2	2.75	125.84	112.24	13	10
4	A	355	PX4	C31-C30-C29	2.75	100.47	114.42	11	3
4	A	371	PX4	O5-C9-C10	2.75	120.54	111.91	12	2
4	A	306	PX4	C4-N1-C3	2.75	116.04	108.97	9	5
4	A	318	PX4	C27-C26-C25	2.75	100.48	114.42	4	2
4	A	316	PX4	O1-P1-O4	2.75	120.50	107.75	2	2
4	A	357	PX4	C27-C26-C25	2.75	100.48	114.42	15	1
4	A	358	PX4	C5-N1-C3	2.75	101.91	108.97	15	4
4	A	390	PX4	O1-P1-O3	2.75	120.51	107.75	17	2
4	A	327	PX4	C12-C11-C10	2.75	103.32	113.19	15	3
4	A	393	PX4	C12-C11-C10	2.74	103.32	113.19	19	3
4	A	422	PX4	C4-N1-C3	2.75	101.92	108.97	7	5
4	A	344	PX4	C1-C2-N1	2.74	124.94	115.78	17	5
4	A	404	PX4	O1-P1-O4	2.74	120.49	107.75	16	3
4	A	392	PX4	C3-N1-C2	2.74	121.14	109.92	5	2
4	A	364	PX4	C18-C17-C16	2.74	100.52	114.42	16	2
4	A	402	PX4	C27-C26-C25	2.74	100.52	114.42	1	2
4	A	347	PX4	C14-C13-C12	2.74	100.53	114.42	4	1
4	A	348	PX4	O1-P1-O4	2.74	95.03	107.75	12	2
4	A	403	PX4	C19-C18-C17	2.74	100.53	114.42	16	3
4	A	375	PX4	O7-C7-C6	2.74	118.31	108.40	17	8
4	A	430	PX4	C15-C14-C13	2.74	100.53	114.42	18	1
4	A	412	PX4	O1-P1-O4	2.74	120.46	107.75	17	4
4	A	327	PX4	C8-O5-C9	2.74	106.99	117.12	5	1
4	A	319	PX4	C30-C29-C28	2.73	100.55	114.42	8	1
4	A	331	PX4	O5-C9-C10	2.73	120.49	111.91	1	2
4	A	350	PX4	C31-C30-C29	2.73	100.54	114.42	7	4
4	A	356	PX4	C18-C17-C16	2.73	100.55	114.42	8	1
4	A	367	PX4	O1-P1-O3	2.73	95.05	107.75	17	1
4	A	405	PX4	C3-N1-C2	2.73	121.10	109.92	15	2
4	A	398	PX4	C30-C29-C28	2.73	100.54	114.42	6	2
4	A	417	PX4	C11-C10-C9	2.74	103.67	113.62	17	4
4	A	420	PX4	O1-P1-O3	2.73	95.05	107.75	3	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	367	PX4	C25-C24-C23	2.73	103.69	113.62	17	1
4	A	380	PX4	O5-C9-C10	2.73	120.48	111.91	15	6
4	A	381	PX4	C33-C32-C31	2.73	100.57	114.42	18	1
4	A	407	PX4	C20-C19-C18	2.73	100.56	114.42	16	3
4	A	421	PX4	O7-C7-C6	2.73	118.29	108.40	16	7
4	A	336	PX4	O1-P1-O4	2.73	120.42	107.75	7	2
4	A	394	PX4	C11-C10-C9	2.73	103.69	113.62	4	4
4	A	413	PX4	O1-P1-O3	2.73	95.08	107.75	6	3
4	A	311	PX4	C29-C28-C27	2.73	100.59	114.42	2	3
4	A	348	PX4	C11-C10-C9	2.72	103.71	113.62	12	4
4	A	375	PX4	C33-C32-C31	2.73	100.59	114.42	14	3
4	A	404	PX4	C26-C25-C24	2.73	103.39	113.19	5	3
4	A	322	PX4	O4-P1-O2	2.72	119.71	109.07	4	3
4	A	354	PX4	C4-N1-C3	2.72	101.97	108.97	2	4
4	A	369	PX4	O1-P1-O3	2.72	95.10	107.75	4	2
4	A	378	PX4	C3-N1-C2	2.72	121.05	109.92	19	4
4	A	428	PX4	O1-P1-O4	2.72	120.39	107.75	19	4
4	A	327	PX4	C27-C26-C25	2.72	100.61	114.42	15	3
4	A	334	PX4	O1-P1-O4	2.72	120.38	107.75	11	1
4	A	340	PX4	C27-C26-C25	2.72	100.61	114.42	19	2
4	A	400	PX4	C14-C13-C12	2.72	100.61	114.42	16	2
4	A	382	PX4	C1-C2-N1	2.72	124.86	115.78	10	5
4	A	319	PX4	C8-O5-C9	2.72	107.05	117.12	6	4
4	A	364	PX4	C5-N1-C3	2.72	101.98	108.97	14	5
4	A	411	PX4	O3-C1-C2	2.72	123.47	109.16	9	1
4	A	342	PX4	C19-C18-C17	2.72	100.63	114.42	9	1
4	A	372	PX4	C4-N1-C2	2.72	121.04	109.92	10	4
4	A	406	PX4	C5-N1-C2	2.72	121.04	109.92	16	1
4	A	343	PX4	C28-C27-C26	2.72	100.63	114.42	18	4
4	A	372	PX4	C18-C17-C16	2.72	100.63	114.42	10	3
4	A	407	PX4	C5-N1-C2	2.72	121.04	109.92	16	1
4	A	386	PX4	C20-C19-C18	2.72	100.63	114.42	14	1
4	A	412	PX4	C16-C15-C14	2.72	100.63	114.42	15	1
4	A	330	PX4	C27-C26-C25	2.72	100.64	114.42	9	2
4	A	356	PX4	C29-C28-C27	2.72	100.64	114.42	19	4
4	A	401	PX4	C13-C12-C11	2.72	100.64	114.42	12	2
4	A	383	PX4	C25-C24-C23	2.72	103.75	113.62	20	2
4	A	408	PX4	O1-P1-O3	2.72	120.36	107.75	17	1
4	A	393	PX4	C19-C18-C17	2.72	100.63	114.42	15	2
4	A	387	PX4	C13-C12-C11	2.72	100.64	114.42	14	1
4	A	422	PX4	O1-P1-O2	2.72	125.67	112.24	3	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	323	PX4	C17-C16-C15	2.71	100.65	114.42	13	2
4	A	352	PX4	C20-C19-C18	2.71	100.65	114.42	5	1
4	A	352	PX4	C13-C12-C11	2.71	100.66	114.42	2	2
4	A	363	PX4	C26-C25-C24	2.71	103.44	113.19	12	2
4	A	372	PX4	C33-C32-C31	2.71	100.66	114.42	12	2
4	A	411	PX4	C19-C18-C17	2.71	100.66	114.42	5	1
4	A	366	PX4	C19-C18-C17	2.71	100.66	114.42	17	3
4	A	403	PX4	C14-C13-C12	2.71	100.66	114.42	14	3
4	A	412	PX4	C13-C12-C11	2.71	100.66	114.42	11	2
4	A	394	PX4	C28-C27-C26	2.71	100.67	114.42	12	3
4	A	428	PX4	O8-C23-C24	2.71	113.16	123.73	1	2
4	A	315	PX4	C5-N1-C3	2.71	102.01	108.97	10	6
4	A	360	PX4	C11-C10-C9	2.71	103.77	113.62	8	1
4	A	373	PX4	C12-C11-C10	2.71	103.45	113.19	7	4
4	A	383	PX4	C16-C15-C14	2.71	100.68	114.42	12	1
4	A	424	PX4	C5-N1-C3	2.71	102.01	108.97	2	1
4	A	399	PX4	O4-P1-O2	2.71	119.64	109.07	15	5
4	A	380	PX4	C27-C26-C25	2.71	100.69	114.42	20	3
4	A	354	PX4	C31-C30-C29	2.70	100.70	114.42	8	1
4	A	399	PX4	C26-C25-C24	2.70	103.47	113.19	20	2
4	A	417	PX4	C26-C25-C24	2.70	103.47	113.19	18	5
4	A	422	PX4	C25-C24-C23	2.70	103.79	113.62	8	1
4	A	425	PX4	C13-C12-C11	2.70	100.69	114.42	19	1
4	A	428	PX4	C19-C18-C17	2.71	100.69	114.42	5	1
4	A	336	PX4	C12-C11-C10	2.70	122.90	113.19	15	3
4	A	344	PX4	O7-C23-O8	2.70	117.17	123.70	4	6
4	A	407	PX4	C25-C24-C23	2.70	103.79	113.62	19	1
4	A	390	PX4	C5-N1-C2	2.70	120.98	109.92	12	2
4	A	405	PX4	C14-C13-C12	2.70	100.71	114.42	11	2
4	A	397	PX4	C16-C15-C14	2.70	100.71	114.42	1	2
4	A	336	PX4	C26-C25-C24	2.70	103.48	113.19	5	3
4	A	384	PX4	C34-C33-C32	2.70	100.72	114.42	9	2
4	A	311	PX4	C12-C11-C10	2.70	103.50	113.19	6	3
4	A	312	PX4	O4-P1-O2	2.70	119.60	109.07	12	3
4	A	360	PX4	O3-C1-C2	2.70	123.34	109.16	11	5
4	A	383	PX4	O3-C1-C2	2.70	123.34	109.16	17	1
4	A	387	PX4	C31-C30-C29	2.70	100.73	114.42	10	1
4	A	421	PX4	O4-P1-O2	2.70	119.60	109.07	19	5
4	A	427	PX4	C12-C11-C10	2.70	122.88	113.19	12	3
4	A	311	PX4	C20-C19-C18	2.69	100.75	114.42	20	3
4	A	353	PX4	C33-C32-C31	2.69	100.74	114.42	8	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	425	PX4	C1-C2-N1	2.70	124.78	115.78	4	5
4	A	343	PX4	O1-P1-O4	2.69	120.25	107.75	5	2
4	A	427	PX4	C27-C26-C25	2.69	100.75	114.42	15	2
4	A	387	PX4	O7-C7-C8	2.69	118.15	108.40	9	5
4	A	421	PX4	C33-C32-C31	2.69	100.76	114.42	2	2
4	A	425	PX4	C12-C11-C10	2.69	103.51	113.19	16	4
4	A	431	PX4	O4-P1-O2	2.69	119.59	109.07	9	3
4	A	324	PX4	C30-C29-C28	2.69	100.76	114.42	15	1
4	A	333	PX4	C34-C33-C32	2.69	100.76	114.42	2	1
4	A	344	PX4	O3-P1-O2	2.69	98.55	109.07	8	3
4	A	347	PX4	C25-C24-C23	2.69	123.40	113.62	7	3
4	A	342	PX4	C4-N1-C2	2.69	120.92	109.92	15	2
4	A	380	PX4	C16-C15-C14	2.69	100.77	114.42	17	2
4	A	318	PX4	C11-C10-C9	2.69	103.85	113.62	2	1
4	A	328	PX4	O6-C9-C10	2.69	113.25	123.73	20	1
4	A	361	PX4	C26-C25-C24	2.69	122.85	113.19	9	3
4	A	367	PX4	O5-C9-O6	2.69	116.81	123.59	8	4
4	A	426	PX4	O7-C7-C6	2.69	118.14	108.40	17	4
4	A	332	PX4	C11-C10-C9	2.69	103.85	113.62	9	4
4	A	315	PX4	C13-C12-C11	2.69	100.79	114.42	9	1
4	A	333	PX4	C5-N1-C2	2.68	120.90	109.92	17	2
4	A	349	PX4	C12-C11-C10	2.68	103.54	113.19	10	3
4	A	350	PX4	C5-N1-C4	2.69	102.07	108.97	7	3
4	A	401	PX4	O4-P1-O2	2.69	119.56	109.07	17	3
4	A	382	PX4	O5-C9-C10	2.69	120.34	111.91	1	6
4	A	362	PX4	C30-C29-C28	2.68	100.80	114.42	1	1
4	A	406	PX4	C4-N1-C2	2.68	98.93	109.92	2	2
4	A	307	PX4	C32-C31-C30	2.68	100.81	114.42	17	2
4	A	318	PX4	C26-C25-C24	2.68	103.55	113.19	16	4
4	A	346	PX4	C3-N1-C2	2.68	120.89	109.92	14	1
4	A	325	PX4	C8-O5-C9	2.68	107.19	117.12	8	4
4	A	332	PX4	C30-C29-C28	2.68	100.81	114.42	12	3
4	A	359	PX4	C25-C24-C23	2.68	103.86	113.62	8	3
4	A	368	PX4	C7-O7-C23	2.68	111.19	117.79	2	5
4	A	364	PX4	C14-C13-C12	2.68	100.81	114.42	2	2
4	A	354	PX4	C3-N1-C2	2.68	98.95	109.92	18	2
4	A	359	PX4	C4-N1-C2	2.68	120.88	109.92	15	2
4	A	321	PX4	O3-C1-C2	2.68	123.25	109.16	8	4
4	A	366	PX4	C17-C16-C15	2.68	100.83	114.42	19	1
4	A	396	PX4	C17-C16-C15	2.68	100.82	114.42	1	2
4	A	375	PX4	C34-C33-C32	2.68	100.83	114.42	16	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	415	PX4	C5-N1-C2	2.68	120.88	109.92	11	2
4	A	309	PX4	O1-P1-O3	2.68	95.32	107.75	20	2
4	A	306	PX4	C8-O5-C9	2.68	107.21	117.12	15	3
4	A	352	PX4	C15-C14-C13	2.68	100.84	114.42	12	2
4	A	356	PX4	O4-P1-O2	2.68	119.53	109.07	19	6
4	A	382	PX4	C11-C10-C9	2.68	123.35	113.62	13	3
4	A	414	PX4	C34-C33-C32	2.68	100.83	114.42	7	1
4	A	327	PX4	O7-C7-C6	2.67	118.09	108.40	7	4
4	A	431	PX4	O5-C9-O6	2.68	116.84	123.59	16	2
4	A	409	PX4	C14-C13-C12	2.67	100.85	114.42	9	2
4	A	392	PX4	C30-C29-C28	2.67	100.85	114.42	16	1
4	A	431	PX4	C34-C33-C32	2.67	100.85	114.42	18	4
4	A	394	PX4	C15-C14-C13	2.67	100.86	114.42	10	2
4	A	378	PX4	C8-O5-C9	2.67	107.23	117.12	17	2
4	A	348	PX4	C27-C26-C25	2.67	100.87	114.42	19	1
4	A	354	PX4	C13-C12-C11	2.67	100.87	114.42	7	1
4	A	385	PX4	C12-C11-C10	2.67	103.59	113.19	4	2
4	A	425	PX4	C15-C14-C13	2.67	100.87	114.42	1	1
4	A	425	PX4	C34-C33-C32	2.67	100.86	114.42	19	1
4	A	332	PX4	C19-C18-C17	2.67	100.88	114.42	14	5
4	A	376	PX4	O3-C1-C2	2.67	123.19	109.16	4	3
4	A	404	PX4	C13-C12-C11	2.67	100.88	114.42	6	3
4	A	409	PX4	C5-N1-C4	2.67	102.11	108.97	19	6
4	A	402	PX4	O5-C9-O6	2.67	116.86	123.59	8	4
4	A	379	PX4	C5-N1-C4	2.67	102.12	108.97	13	3
4	A	382	PX4	C8-O5-C9	2.67	107.25	117.12	16	2
4	A	392	PX4	C14-C13-C12	2.67	100.88	114.42	9	2
4	A	327	PX4	C11-C10-C9	2.67	123.31	113.62	8	3
4	A	337	PX4	C19-C18-C17	2.67	100.89	114.42	15	2
4	A	339	PX4	C30-C29-C28	2.66	100.90	114.42	5	1
4	A	351	PX4	O1-P1-O3	2.67	95.37	107.75	4	4
4	A	311	PX4	C4-N1-C3	2.66	102.12	108.97	17	4
4	A	352	PX4	O1-P1-O3	2.66	95.37	107.75	9	3
4	A	401	PX4	C30-C29-C28	2.66	100.90	114.42	13	4
4	A	377	PX4	C18-C17-C16	2.66	100.90	114.42	18	1
4	A	391	PX4	O8-C23-C24	2.66	113.34	123.73	8	1
4	A	321	PX4	O5-C9-C10	2.66	120.27	111.91	1	4
4	A	333	PX4	C31-C30-C29	2.66	100.91	114.42	3	1
4	A	374	PX4	C25-C24-C23	2.66	103.94	113.62	11	2
4	A	375	PX4	C25-C24-C23	2.66	103.94	113.62	15	1
4	A	404	PX4	C5-N1-C4	2.66	102.13	108.97	13	7

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	396	PX4	C25-C24-C23	2.66	103.94	113.62	20	2
4	A	353	PX4	C34-C33-C32	2.66	100.91	114.42	17	3
4	A	355	PX4	C20-C19-C18	2.66	100.91	114.42	20	1
4	A	340	PX4	C13-C12-C11	2.66	100.92	114.42	3	2
4	A	366	PX4	O6-C9-C10	2.66	113.35	123.73	20	3
4	A	399	PX4	C13-C12-C11	2.66	100.92	114.42	11	3
4	A	321	PX4	O1-P1-O4	2.66	120.10	107.75	16	2
4	A	404	PX4	C3-N1-C2	2.66	120.80	109.92	11	2
4	A	407	PX4	C12-C11-C10	2.66	103.63	113.19	13	3
4	A	383	PX4	C5-N1-C2	2.66	120.80	109.92	18	2
4	A	392	PX4	C25-C24-C23	2.66	103.95	113.62	7	1
4	A	415	PX4	C27-C26-C25	2.66	100.92	114.42	5	2
4	A	316	PX4	C34-C33-C32	2.66	100.93	114.42	6	3
4	A	352	PX4	O4-P1-O2	2.66	119.46	109.07	16	4
4	A	415	PX4	C25-C24-C23	2.66	103.95	113.62	18	4
4	A	425	PX4	O5-C9-C10	2.66	120.25	111.91	10	3
4	A	309	PX4	C3-N1-C2	2.66	120.78	109.92	3	2
4	A	326	PX4	C32-C31-C30	2.66	100.94	114.42	4	1
4	A	359	PX4	C29-C28-C27	2.66	100.94	114.42	1	2
4	A	365	PX4	C33-C32-C31	2.66	100.93	114.42	17	3
4	A	430	PX4	C33-C32-C31	2.66	100.93	114.42	18	4
4	A	431	PX4	C26-C25-C24	2.66	103.63	113.19	12	1
4	A	310	PX4	C4-N1-C3	2.66	102.15	108.97	16	5
4	A	350	PX4	O3-P1-O2	2.66	98.69	109.07	11	3
4	A	325	PX4	C13-C12-C11	2.66	100.94	114.42	7	1
4	A	331	PX4	C16-C15-C14	2.66	100.94	114.42	2	2
4	A	425	PX4	C26-C25-C24	2.66	103.64	113.19	11	4
4	A	322	PX4	O5-C9-O6	2.65	116.89	123.59	2	2
4	A	400	PX4	C27-C26-C25	2.65	100.96	114.42	17	3
4	A	387	PX4	O3-P1-O2	2.65	98.70	109.07	16	2
4	A	388	PX4	C26-C25-C24	2.65	103.66	113.19	13	2
4	A	395	PX4	C4-N1-C3	2.65	102.16	108.97	10	2
4	A	317	PX4	O3-C1-C2	2.65	123.10	109.16	14	1
4	A	323	PX4	O1-P1-O4	2.65	120.05	107.75	17	2
4	A	353	PX4	C4-N1-C2	2.65	99.07	109.92	18	4
4	A	356	PX4	C8-O5-C9	2.65	126.94	117.12	19	5
4	A	324	PX4	C13-C12-C11	2.65	100.98	114.42	16	2
4	A	328	PX4	O8-C23-C24	2.65	113.39	123.73	15	1
4	A	311	PX4	C16-C15-C14	2.65	100.98	114.42	5	2
4	A	327	PX4	O6-C9-C10	2.65	113.40	123.73	10	1
4	A	363	PX4	C12-C11-C10	2.65	103.67	113.19	1	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	394	PX4	C29-C28-C27	2.65	100.97	114.42	20	2
4	A	364	PX4	C29-C28-C27	2.65	100.98	114.42	10	1
4	A	400	PX4	C8-O5-C9	2.65	107.32	117.12	18	1
4	A	372	PX4	C31-C30-C29	2.65	100.98	114.42	16	1
4	A	390	PX4	C11-C10-C9	2.65	103.99	113.62	18	3
4	A	420	PX4	C5-N1-C3	2.65	115.78	108.97	16	4
4	A	306	PX4	O5-C9-O6	2.65	116.91	123.59	14	6
4	A	334	PX4	C32-C31-C30	2.65	100.99	114.42	15	2
4	A	379	PX4	O8-C23-C24	2.65	113.41	123.73	14	1
4	A	407	PX4	C5-N1-C3	2.65	102.17	108.97	7	7
4	A	422	PX4	C31-C30-C29	2.65	100.99	114.42	3	1
4	A	329	PX4	C25-C24-C23	2.64	104.00	113.62	4	5
4	A	343	PX4	C4-N1-C2	2.64	99.10	109.92	15	2
4	A	347	PX4	C19-C18-C17	2.64	101.00	114.42	10	3
4	A	404	PX4	O5-C9-C10	2.64	120.20	111.91	16	6
4	A	410	PX4	O4-P1-O2	2.64	119.40	109.07	5	2
4	A	357	PX4	O5-C9-C10	2.64	120.20	111.91	10	2
4	A	365	PX4	C14-C13-C12	2.64	101.01	114.42	1	4
4	A	406	PX4	O1-P1-O3	2.64	95.47	107.75	17	3
4	A	419	PX4	C31-C30-C29	2.64	101.01	114.42	20	1
4	A	308	PX4	O1-P1-O3	2.64	95.48	107.75	13	2
4	A	387	PX4	O1-P1-O3	2.64	95.48	107.75	14	2
4	A	395	PX4	O1-P1-O3	2.64	95.48	107.75	5	3
4	A	322	PX4	C28-C27-C26	2.64	101.03	114.42	18	2
4	A	323	PX4	C14-C13-C12	2.64	101.03	114.42	20	1
4	A	423	PX4	C18-C17-C16	2.64	101.02	114.42	18	4
4	A	326	PX4	O1-P1-O4	2.64	95.49	107.75	2	3
4	A	358	PX4	O5-C9-O6	2.64	116.93	123.59	5	5
4	A	358	PX4	C8-O5-C9	2.64	126.89	117.12	15	2
4	A	370	PX4	O7-C7-C6	2.64	117.96	108.40	11	6
4	A	316	PX4	C11-C10-C9	2.64	104.03	113.62	15	1
4	A	338	PX4	O7-C23-O8	2.64	117.33	123.70	13	2
4	A	429	PX4	O1-P1-O4	2.64	120.00	107.75	5	1
4	A	351	PX4	C5-N1-C2	2.64	120.71	109.92	8	1
4	A	305	PX4	C3-N1-C2	2.64	99.13	109.92	15	2
4	A	308	PX4	O5-C9-C10	2.63	120.18	111.91	2	5
4	A	315	PX4	O7-C7-C6	2.64	117.94	108.40	20	3
4	A	322	PX4	O8-C23-C24	2.63	113.45	123.73	19	1
4	A	333	PX4	C5-N1-C4	2.64	102.20	108.97	10	1
4	A	344	PX4	C5-N1-C3	2.64	102.20	108.97	9	3
4	A	310	PX4	C20-C19-C18	2.63	101.05	114.42	6	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	353	PX4	C13-C12-C11	2.64	101.05	114.42	8	1
4	A	354	PX4	C32-C31-C30	2.63	101.05	114.42	1	4
4	A	357	PX4	C19-C18-C17	2.64	101.05	114.42	15	4
4	A	388	PX4	C15-C14-C13	2.64	101.04	114.42	3	1
4	A	330	PX4	O4-P1-O2	2.63	119.36	109.07	6	3
4	A	306	PX4	C30-C29-C28	2.63	101.06	114.42	5	2
4	A	307	PX4	C4-N1-C2	2.63	120.69	109.92	3	2
4	A	361	PX4	C18-C17-C16	2.63	101.06	114.42	20	3
4	A	370	PX4	C30-C29-C28	2.63	101.06	114.42	19	2
4	A	341	PX4	C14-C13-C12	2.63	101.07	114.42	5	3
4	A	364	PX4	C30-C29-C28	2.63	101.07	114.42	12	1
4	A	330	PX4	C20-C19-C18	2.63	101.08	114.42	9	1
4	A	370	PX4	O1-P1-O3	2.63	95.54	107.75	11	3
4	A	406	PX4	O1-P1-O4	2.63	119.95	107.75	7	1
4	A	421	PX4	C32-C31-C30	2.63	101.08	114.42	9	1
4	A	424	PX4	C8-O5-C9	2.63	107.38	117.12	10	1
4	A	330	PX4	C12-C11-C10	2.63	103.74	113.19	20	1
4	A	355	PX4	C28-C27-C26	2.63	101.08	114.42	12	4
4	A	359	PX4	C4-N1-C3	2.63	102.22	108.97	11	2
4	A	423	PX4	C16-C15-C14	2.63	101.08	114.42	13	3
4	A	309	PX4	C29-C28-C27	2.63	101.10	114.42	7	4
4	A	317	PX4	O5-C9-O6	2.63	116.96	123.59	1	3
4	A	356	PX4	C3-N1-C2	2.63	120.66	109.92	4	1
4	A	386	PX4	O3-P1-O2	2.63	98.80	109.07	13	4
4	A	412	PX4	C5-N1-C3	2.63	102.22	108.97	13	4
4	A	391	PX4	C15-C14-C13	2.62	101.11	114.42	5	3
4	A	413	PX4	O5-C9-C10	2.62	120.14	111.91	4	4
4	A	414	PX4	C13-C12-C11	2.62	101.10	114.42	8	2
4	A	417	PX4	C19-C18-C17	2.62	101.10	114.42	5	2
4	A	429	PX4	C15-C14-C13	2.62	101.10	114.42	2	2
4	A	323	PX4	O4-P1-O2	2.62	119.32	109.07	10	4
4	A	310	PX4	C28-C27-C26	2.62	101.11	114.42	15	1
4	A	363	PX4	O6-C9-C10	2.62	113.50	123.73	4	3
4	A	366	PX4	C5-N1-C3	2.62	102.23	108.97	1	3
4	A	409	PX4	C31-C30-C29	2.62	101.11	114.42	12	1
4	A	370	PX4	C14-C13-C12	2.62	101.11	114.42	3	1
4	A	416	PX4	C16-C15-C14	2.62	101.11	114.42	16	3
4	A	422	PX4	C26-C25-C24	2.62	103.76	113.19	19	2
4	A	309	PX4	C26-C25-C24	2.62	103.77	113.19	2	1
4	A	360	PX4	C1-C2-N1	2.62	124.53	115.78	2	5
4	A	363	PX4	C27-C26-C25	2.62	101.12	114.42	10	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	406	PX4	C27-C26-C25	2.62	101.11	114.42	18	2
4	A	305	PX4	C4-N1-C3	2.62	102.24	108.97	7	2
4	A	329	PX4	C32-C31-C30	2.62	101.13	114.42	7	2
4	A	385	PX4	O6-C9-C10	2.62	113.51	123.73	13	2
4	A	316	PX4	O1-P1-O3	2.62	95.58	107.75	12	2
4	A	385	PX4	C19-C18-C17	2.62	101.13	114.42	3	2
4	A	397	PX4	C11-C10-C9	2.62	104.09	113.62	19	1
4	A	337	PX4	C33-C32-C31	2.62	101.14	114.42	2	3
4	A	339	PX4	C17-C16-C15	2.62	101.14	114.42	20	2
4	A	395	PX4	O3-C1-C2	2.62	122.93	109.16	5	4
4	A	420	PX4	O1-P1-O4	2.62	119.91	107.75	1	3
4	A	354	PX4	O1-P1-O3	2.62	95.59	107.75	12	1
4	A	374	PX4	C15-C14-C13	2.62	101.14	114.42	6	2
4	A	407	PX4	O4-P1-O2	2.62	119.29	109.07	20	3
4	A	355	PX4	C26-C25-C24	2.62	103.79	113.19	7	4
4	A	397	PX4	O5-C9-O6	2.62	116.99	123.59	19	4
4	A	305	PX4	C13-C12-C11	2.62	101.15	114.42	12	1
4	A	356	PX4	O1-P1-O2	2.62	125.17	112.24	19	8
4	A	357	PX4	C8-O5-C9	2.61	107.44	117.12	19	3
4	A	363	PX4	O5-C9-O6	2.61	116.99	123.59	11	2
4	A	364	PX4	O1-P1-O4	2.62	119.89	107.75	13	5
4	A	378	PX4	O5-C9-C10	2.62	120.12	111.91	9	2
4	A	424	PX4	C12-C11-C10	2.62	103.79	113.19	19	1
4	A	411	PX4	C25-C24-C23	2.62	104.11	113.62	18	2
4	A	414	PX4	O1-P1-O2	2.61	125.16	112.24	17	6
4	A	420	PX4	C19-C18-C17	2.61	101.15	114.42	14	2
4	A	314	PX4	C32-C31-C30	2.61	101.17	114.42	13	1
4	A	339	PX4	C20-C19-C18	2.61	101.16	114.42	9	2
4	A	345	PX4	C18-C17-C16	2.61	101.17	114.42	13	1
4	A	378	PX4	O1-P1-O4	2.61	119.88	107.75	11	3
4	A	426	PX4	C27-C26-C25	2.61	101.16	114.42	5	3
4	A	313	PX4	C27-C26-C25	2.61	101.17	114.42	15	1
4	A	347	PX4	O3-P1-O2	2.61	98.87	109.07	15	2
4	A	351	PX4	C13-C12-C11	2.61	101.17	114.42	13	2
4	A	307	PX4	C15-C14-C13	2.61	101.18	114.42	12	4
4	A	314	PX4	O1-P1-O2	2.61	125.14	112.24	19	8
4	A	359	PX4	C30-C29-C28	2.61	101.18	114.42	5	3
4	A	405	PX4	C8-O5-C9	2.61	107.46	117.12	4	2
4	A	418	PX4	C4-N1-C2	2.61	120.60	109.92	5	1
4	A	421	PX4	C26-C25-C24	2.61	103.81	113.19	14	2
4	A	429	PX4	C33-C32-C31	2.61	101.18	114.42	7	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	307	PX4	C30-C29-C28	2.61	101.19	114.42	4	2
4	A	324	PX4	O1-P1-O3	2.61	95.64	107.75	17	3
4	A	344	PX4	C15-C14-C13	2.61	101.19	114.42	7	2
4	A	388	PX4	O1-P1-O3	2.61	95.64	107.75	5	3
4	A	413	PX4	C26-C25-C24	2.61	103.82	113.19	5	1
4	A	361	PX4	O1-P1-O3	2.61	119.85	107.75	7	1
4	A	399	PX4	C32-C31-C30	2.61	101.19	114.42	9	2
4	A	397	PX4	O3-P1-O2	2.61	98.88	109.07	20	3
4	A	311	PX4	C19-C18-C17	2.60	101.20	114.42	15	3
4	A	385	PX4	C3-N1-C2	2.60	99.26	109.92	4	2
4	A	410	PX4	C33-C32-C31	2.60	101.20	114.42	2	1
4	A	391	PX4	O5-C9-O6	2.60	117.02	123.59	14	5
4	A	431	PX4	C28-C27-C26	2.60	101.20	114.42	18	1
4	A	387	PX4	O7-C23-O8	2.60	117.41	123.70	16	6
4	A	372	PX4	C12-C11-C10	2.60	103.84	113.19	4	3
4	A	403	PX4	O1-P1-O2	2.60	125.11	112.24	17	7
4	A	417	PX4	C34-C33-C32	2.60	101.21	114.42	20	1
4	A	407	PX4	O8-C23-C24	2.60	113.58	123.73	16	1
4	A	340	PX4	C30-C29-C28	2.60	101.22	114.42	11	2
4	A	385	PX4	C26-C25-C24	2.60	103.84	113.19	3	3
4	A	394	PX4	O1-P1-O3	2.60	95.66	107.75	17	1
4	A	395	PX4	C3-N1-C2	2.60	120.56	109.92	2	2
4	A	398	PX4	O7-C7-C8	2.60	117.82	108.40	14	7
4	A	416	PX4	C4-N1-C3	2.60	102.29	108.97	5	3
4	A	313	PX4	C31-C30-C29	2.60	101.23	114.42	7	2
4	A	343	PX4	C5-N1-C3	2.60	115.66	108.97	8	3
4	A	356	PX4	C16-C15-C14	2.60	101.23	114.42	1	3
4	A	385	PX4	C34-C33-C32	2.60	101.23	114.42	1	3
4	A	314	PX4	O7-C7-C8	2.60	117.80	108.40	14	4
4	A	323	PX4	C29-C28-C27	2.60	101.24	114.42	10	1
4	A	405	PX4	C16-C15-C14	2.60	101.24	114.42	1	2
4	A	405	PX4	O1-P1-O4	2.60	119.81	107.75	19	3
4	A	407	PX4	O1-P1-O4	2.60	119.81	107.75	16	2
4	A	319	PX4	C5-N1-C2	2.60	120.54	109.92	15	2
4	A	329	PX4	C20-C19-C18	2.60	101.24	114.42	10	2
4	A	331	PX4	C4-N1-C3	2.60	115.65	108.97	11	3
4	A	335	PX4	C4-N1-C3	2.60	102.30	108.97	19	4
4	A	399	PX4	C16-C15-C14	2.60	101.24	114.42	9	1
4	A	399	PX4	C4-N1-C2	2.60	99.30	109.92	19	1
4	A	404	PX4	C30-C29-C28	2.60	101.25	114.42	3	4
4	A	404	PX4	C8-O5-C9	2.60	107.51	117.12	19	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	426	PX4	C32-C31-C30	2.60	101.25	114.42	5	2
4	A	306	PX4	C32-C31-C30	2.59	101.25	114.42	7	2
4	A	379	PX4	C12-C11-C10	2.59	103.86	113.19	19	3
4	A	321	PX4	C30-C29-C28	2.59	101.26	114.42	1	4
4	A	323	PX4	C5-N1-C4	2.59	102.31	108.97	9	3
4	A	329	PX4	C12-C11-C10	2.59	103.87	113.19	16	5
4	A	333	PX4	C19-C18-C17	2.59	101.26	114.42	2	3
4	A	344	PX4	C8-O5-C9	2.59	107.52	117.12	2	5
4	A	355	PX4	O1-P1-O3	2.59	95.70	107.75	10	5
4	A	402	PX4	C20-C19-C18	2.59	101.27	114.42	12	1
4	A	383	PX4	C11-C10-C9	2.59	104.19	113.62	8	1
4	A	429	PX4	C12-C11-C10	2.59	103.87	113.19	5	4
4	A	330	PX4	C14-C13-C12	2.59	101.27	114.42	3	3
4	A	334	PX4	C13-C12-C11	2.59	101.28	114.42	9	2
4	A	340	PX4	C20-C19-C18	2.59	101.28	114.42	5	1
4	A	376	PX4	C5-N1-C3	2.59	102.31	108.97	20	5
4	A	344	PX4	C25-C24-C23	2.59	104.21	113.62	19	1
4	A	348	PX4	C19-C18-C17	2.59	101.28	114.42	15	1
4	A	381	PX4	C30-C29-C28	2.59	101.28	114.42	15	3
4	A	360	PX4	C3-N1-C2	2.59	99.33	109.92	3	1
4	A	360	PX4	C20-C19-C18	2.59	101.29	114.42	15	3
4	A	400	PX4	C26-C25-C24	2.59	122.49	113.19	2	3
4	A	391	PX4	C27-C26-C25	2.59	101.29	114.42	8	2
4	A	398	PX4	C33-C32-C31	2.59	101.29	114.42	5	3
4	A	428	PX4	C8-O5-C9	2.59	107.54	117.12	18	1
4	A	312	PX4	C33-C32-C31	2.59	101.30	114.42	14	2
4	A	352	PX4	C12-C11-C10	2.58	122.48	113.19	18	4
4	A	354	PX4	C16-C15-C14	2.58	101.30	114.42	12	4
4	A	338	PX4	C15-C14-C13	2.58	101.31	114.42	12	2
4	A	358	PX4	C31-C30-C29	2.58	101.31	114.42	17	4
4	A	418	PX4	O3-P1-O2	2.58	119.16	109.07	8	3
4	A	423	PX4	C28-C27-C26	2.58	101.31	114.42	12	3
4	A	423	PX4	C5-N1-C2	2.58	120.49	109.92	15	1
4	A	370	PX4	C31-C30-C29	2.58	101.31	114.42	19	3
4	A	383	PX4	C27-C26-C25	2.58	101.31	114.42	13	2
4	A	391	PX4	C26-C25-C24	2.58	103.91	113.19	17	2
4	A	429	PX4	C3-N1-C2	2.58	120.49	109.92	3	1
4	A	323	PX4	C33-C32-C31	2.58	101.31	114.42	4	1
4	A	361	PX4	O3-C1-C2	2.58	122.74	109.16	19	1
4	A	329	PX4	C3-N1-C2	2.58	120.48	109.92	13	1
4	A	380	PX4	O4-P1-O2	2.58	119.15	109.07	11	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	413	PX4	C33-C32-C31	2.58	101.32	114.42	6	1
4	A	427	PX4	C8-O5-C9	2.58	107.56	117.12	10	3
4	A	315	PX4	C8-O5-C9	2.58	107.57	117.12	10	6
4	A	330	PX4	C11-C10-C9	2.58	104.24	113.62	10	2
4	A	343	PX4	C17-C16-C15	2.58	101.34	114.42	12	3
4	A	344	PX4	C3-N1-C2	2.58	120.47	109.92	1	1
4	A	346	PX4	C27-C26-C25	2.58	101.33	114.42	18	2
4	A	361	PX4	C8-O5-C9	2.58	107.57	117.12	3	2
4	A	371	PX4	C32-C31-C30	2.58	101.33	114.42	6	3
4	A	431	PX4	O3-P1-O2	2.58	98.98	109.07	16	4
4	A	401	PX4	C5-N1-C2	2.58	120.47	109.92	13	1
4	A	385	PX4	C25-C24-C23	2.58	104.24	113.62	15	2
4	A	421	PX4	C3-N1-C2	2.58	120.47	109.92	12	2
4	A	408	PX4	C12-C11-C10	2.58	103.92	113.19	19	2
4	A	339	PX4	C34-C33-C32	2.58	101.35	114.42	1	1
4	A	387	PX4	C30-C29-C28	2.58	101.34	114.42	13	1
4	A	394	PX4	C30-C29-C28	2.58	101.34	114.42	1	1
4	A	305	PX4	C26-C25-C24	2.58	103.93	113.19	20	3
4	A	361	PX4	C27-C26-C25	2.58	101.35	114.42	11	1
4	A	429	PX4	C29-C28-C27	2.58	101.34	114.42	17	2
4	A	349	PX4	C17-C16-C15	2.57	101.36	114.42	20	5
4	A	353	PX4	C16-C15-C14	2.57	101.36	114.42	7	2
4	A	359	PX4	C31-C30-C29	2.57	101.36	114.42	17	1
4	A	401	PX4	C29-C28-C27	2.58	101.35	114.42	16	3
4	A	383	PX4	C30-C29-C28	2.58	101.35	114.42	9	3
4	A	389	PX4	C11-C10-C9	2.57	104.26	113.62	14	3
4	A	413	PX4	C30-C29-C28	2.57	101.36	114.42	6	1
4	A	398	PX4	C18-C17-C16	2.58	101.35	114.42	8	3
4	A	419	PX4	C4-N1-C2	2.58	99.38	109.92	4	4
4	A	327	PX4	O1-P1-O4	2.57	119.69	107.75	20	2
4	A	331	PX4	C27-C26-C25	2.57	101.37	114.42	18	1
4	A	338	PX4	C30-C29-C28	2.57	101.37	114.42	4	2
4	A	348	PX4	C17-C16-C15	2.57	101.37	114.42	6	3
4	A	392	PX4	C17-C16-C15	2.57	101.36	114.42	4	1
4	A	351	PX4	C16-C15-C14	2.57	101.37	114.42	17	2
4	A	363	PX4	C17-C16-C15	2.57	101.37	114.42	16	3
4	A	367	PX4	C18-C17-C16	2.57	101.37	114.42	2	1
4	A	403	PX4	C20-C19-C18	2.57	101.37	114.42	3	1
4	A	415	PX4	C34-C33-C32	2.57	101.37	114.42	9	2
4	A	427	PX4	C5-N1-C3	2.57	102.36	108.97	6	2
4	A	343	PX4	C25-C24-C23	2.57	104.28	113.62	11	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	367	PX4	C16-C15-C14	2.57	101.38	114.42	16	2
4	A	374	PX4	C29-C28-C27	2.57	101.38	114.42	3	2
4	A	387	PX4	C5-N1-C3	2.57	102.36	108.97	8	3
4	A	396	PX4	O3-P1-O2	2.57	99.03	109.07	12	3
4	A	419	PX4	O1-P1-O4	2.57	119.68	107.75	3	4
4	A	325	PX4	C7-O7-C23	2.57	124.12	117.79	2	1
4	A	420	PX4	C8-O5-C9	2.57	107.61	117.12	17	1
4	A	377	PX4	C8-O5-C9	2.57	107.61	117.12	7	3
4	A	389	PX4	C20-C19-C18	2.57	101.39	114.42	5	1
4	A	428	PX4	C4-N1-C2	2.57	120.42	109.92	20	3
4	A	431	PX4	C5-N1-C2	2.57	99.41	109.92	7	1
4	A	318	PX4	C14-C13-C12	2.57	101.39	114.42	8	1
4	A	387	PX4	C32-C31-C30	2.57	101.39	114.42	3	3
4	A	333	PX4	C14-C13-C12	2.57	101.40	114.42	20	1
4	A	389	PX4	C16-C15-C14	2.57	101.40	114.42	17	2
4	A	395	PX4	C8-O5-C9	2.57	107.62	117.12	13	3
4	A	425	PX4	C20-C19-C18	2.57	101.40	114.42	15	1
4	A	309	PX4	C19-C18-C17	2.56	101.41	114.42	4	4
4	A	319	PX4	C3-N1-C2	2.56	120.41	109.92	19	3
4	A	331	PX4	C20-C19-C18	2.56	101.41	114.42	12	2
4	A	362	PX4	O6-C9-C10	2.56	113.73	123.73	3	1
4	A	370	PX4	C11-C10-C9	2.56	104.29	113.62	16	4
4	A	399	PX4	C5-N1-C2	2.56	120.40	109.92	19	3
4	A	331	PX4	C30-C29-C28	2.56	101.42	114.42	15	1
4	A	344	PX4	C26-C25-C24	2.56	103.98	113.19	18	4
4	A	350	PX4	O5-C9-O6	2.56	117.13	123.59	6	4
4	A	381	PX4	C20-C19-C18	2.56	101.42	114.42	3	3
4	A	383	PX4	C31-C30-C29	2.56	101.42	114.42	3	3
4	A	388	PX4	C32-C31-C30	2.56	101.42	114.42	4	1
4	A	389	PX4	C4-N1-C2	2.56	120.39	109.92	12	1
4	A	413	PX4	C5-N1-C2	2.56	120.40	109.92	18	4
4	A	426	PX4	C28-C27-C26	2.56	101.42	114.42	5	1
4	A	342	PX4	C11-C10-C9	2.56	104.31	113.62	5	1
4	A	403	PX4	C29-C28-C27	2.56	101.42	114.42	20	2
4	A	390	PX4	O4-P1-O2	2.56	99.07	109.07	16	1
4	A	416	PX4	C17-C16-C15	2.56	101.43	114.42	3	2
4	A	345	PX4	C3-N1-C2	2.56	99.44	109.92	5	2
4	A	309	PX4	O5-C9-C10	2.56	119.94	111.91	19	3
4	A	314	PX4	O5-C9-C10	2.56	119.94	111.91	9	4
4	A	348	PX4	C32-C31-C30	2.56	101.43	114.42	5	1
4	A	402	PX4	C13-C12-C11	2.56	101.43	114.42	18	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	326	PX4	C13-C12-C11	2.56	101.45	114.42	17	2
4	A	334	PX4	C34-C33-C32	2.56	101.44	114.42	6	3
4	A	367	PX4	C30-C29-C28	2.56	101.45	114.42	17	1
4	A	411	PX4	C29-C28-C27	2.56	101.44	114.42	4	2
4	A	412	PX4	C18-C17-C16	2.56	101.44	114.42	18	5
4	A	412	PX4	C12-C11-C10	2.56	122.38	113.19	2	4
4	A	409	PX4	C34-C33-C32	2.56	101.45	114.42	8	3
4	A	396	PX4	O1-P1-O3	2.56	95.87	107.75	16	2
4	A	415	PX4	C14-C13-C12	2.56	101.45	114.42	14	1
4	A	331	PX4	C15-C14-C13	2.55	101.46	114.42	15	1
4	A	336	PX4	C3-N1-C2	2.55	120.37	109.92	13	2
4	A	394	PX4	O5-C9-C10	2.55	119.92	111.91	4	5
4	A	397	PX4	O8-C23-C24	2.55	113.77	123.73	1	2
4	A	318	PX4	C12-C11-C10	2.55	104.02	113.19	10	3
4	A	316	PX4	O5-C9-C10	2.55	119.92	111.91	7	4
4	A	348	PX4	C30-C29-C28	2.55	101.47	114.42	5	1
4	A	331	PX4	C3-N1-C2	2.55	120.35	109.92	8	2
4	A	371	PX4	C25-C24-C23	2.55	104.34	113.62	18	1
4	A	378	PX4	C15-C14-C13	2.55	101.48	114.42	13	1
4	A	416	PX4	C20-C19-C18	2.55	101.47	114.42	14	1
4	A	384	PX4	C14-C13-C12	2.55	127.37	114.42	11	2
4	A	429	PX4	C13-C12-C11	2.55	101.48	114.42	12	3
4	A	320	PX4	C28-C27-C26	2.55	101.48	114.42	15	2
4	A	420	PX4	C27-C26-C25	2.55	101.48	114.42	14	1
4	A	431	PX4	C5-N1-C4	2.55	102.42	108.97	12	8
4	A	321	PX4	C31-C30-C29	2.55	101.49	114.42	6	2
4	A	330	PX4	C4-N1-C2	2.55	120.34	109.92	5	1
4	A	334	PX4	C17-C16-C15	2.55	101.49	114.42	15	1
4	A	322	PX4	C33-C32-C31	2.55	101.50	114.42	18	1
4	A	335	PX4	C28-C27-C26	2.55	101.49	114.42	1	2
4	A	362	PX4	O1-P1-O4	2.55	119.58	107.75	14	3
4	A	381	PX4	C4-N1-C2	2.55	120.34	109.92	5	2
4	A	370	PX4	C16-C15-C14	2.55	101.50	114.42	5	1
4	A	376	PX4	C28-C27-C26	2.55	101.49	114.42	4	2
4	A	376	PX4	O8-C23-C24	2.55	113.79	123.73	3	2
4	A	390	PX4	O3-C1-C2	2.55	122.56	109.16	13	4
4	A	412	PX4	C3-N1-C2	2.55	99.49	109.92	18	1
4	A	313	PX4	C3-N1-C2	2.55	99.50	109.92	10	2
4	A	355	PX4	C33-C32-C31	2.55	101.50	114.42	1	1
4	A	375	PX4	C26-C25-C24	2.54	104.04	113.19	12	4
4	A	388	PX4	C25-C24-C23	2.55	104.36	113.62	18	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	428	PX4	C18-C17-C16	2.55	101.50	114.42	15	1
4	A	308	PX4	C20-C19-C18	2.54	101.51	114.42	19	2
4	A	343	PX4	C32-C31-C30	2.54	101.51	114.42	14	2
4	A	361	PX4	C25-C24-C23	2.54	104.37	113.62	13	2
4	A	392	PX4	C20-C19-C18	2.54	101.51	114.42	10	1
4	A	409	PX4	C15-C14-C13	2.54	101.51	114.42	4	4
4	A	392	PX4	C34-C33-C32	2.54	127.34	114.42	13	2
4	A	308	PX4	C18-C17-C16	2.54	101.52	114.42	16	3
4	A	349	PX4	C16-C15-C14	2.54	101.52	114.42	13	3
4	A	318	PX4	C34-C33-C32	2.54	101.53	114.42	13	2
4	A	350	PX4	C29-C28-C27	2.54	101.53	114.42	19	3
4	A	350	PX4	C4-N1-C2	2.54	120.31	109.92	6	2
4	A	415	PX4	O4-P1-O2	2.54	119.00	109.07	8	4
4	A	429	PX4	C25-C24-C23	2.54	104.38	113.62	19	1
4	A	307	PX4	C12-C11-C10	2.54	104.07	113.19	10	2
4	A	317	PX4	C3-N1-C2	2.54	99.53	109.92	19	2
4	A	335	PX4	C20-C19-C18	2.54	101.54	114.42	9	1
4	A	319	PX4	O6-C9-C10	2.54	113.83	123.73	3	1
4	A	356	PX4	O7-C23-O8	2.54	117.57	123.70	4	5
4	A	374	PX4	C3-N1-C2	2.54	99.53	109.92	17	2
4	A	390	PX4	C12-C11-C10	2.54	104.06	113.19	2	2
4	A	395	PX4	O8-C23-C24	2.54	113.83	123.73	11	4
4	A	359	PX4	C19-C18-C17	2.54	101.54	114.42	1	3
4	A	416	PX4	O5-C9-O6	2.54	117.19	123.59	6	3
4	A	307	PX4	C16-C15-C14	2.53	101.56	114.42	6	2
4	A	317	PX4	C16-C15-C14	2.53	101.56	114.42	17	1
4	A	341	PX4	C19-C18-C17	2.54	101.55	114.42	3	3
4	A	351	PX4	C11-C10-C9	2.54	104.40	113.62	20	1
4	A	426	PX4	C18-C17-C16	2.54	101.56	114.42	12	1
4	A	431	PX4	O1-P1-O4	2.54	119.52	107.75	20	4
4	A	320	PX4	O8-C23-C24	2.53	113.85	123.73	4	3
4	A	331	PX4	C17-C16-C15	2.53	101.56	114.42	12	1
4	A	420	PX4	C34-C33-C32	2.53	101.56	114.42	18	2
4	A	355	PX4	O3-P1-O2	2.53	99.17	109.07	3	3
4	A	386	PX4	O4-P1-O2	2.53	118.96	109.07	13	2
4	A	397	PX4	C14-C13-C12	2.53	101.58	114.42	19	1
4	A	418	PX4	C18-C17-C16	2.53	101.57	114.42	5	2
4	A	428	PX4	C13-C12-C11	2.53	101.57	114.42	1	1
4	A	305	PX4	C29-C28-C27	2.53	101.58	114.42	4	1
4	A	312	PX4	C4-N1-C2	2.53	120.27	109.92	3	1
4	A	385	PX4	O3-C1-C2	2.53	122.47	109.16	4	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	385	PX4	C13-C12-C11	2.53	101.58	114.42	14	1
4	A	327	PX4	C4-N1-C2	2.53	99.57	109.92	5	3
4	A	332	PX4	O3-P1-O2	2.53	99.19	109.07	13	4
4	A	418	PX4	O7-C7-C6	2.53	117.55	108.40	20	8
4	A	426	PX4	C15-C14-C13	2.53	101.59	114.42	10	4
4	A	313	PX4	C4-N1-C2	2.52	120.24	109.92	15	5
4	A	308	PX4	C5-N1-C3	2.52	115.47	108.97	17	3
4	A	335	PX4	O7-C23-O8	2.53	117.60	123.70	4	6
4	A	345	PX4	C17-C16-C15	2.53	101.60	114.42	17	4
4	A	324	PX4	C29-C28-C27	2.52	101.61	114.42	19	1
4	A	326	PX4	O3-P1-O2	2.52	99.20	109.07	16	4
4	A	369	PX4	C34-C33-C32	2.52	101.61	114.42	7	1
4	A	378	PX4	C32-C31-C30	2.52	101.61	114.42	16	3
4	A	320	PX4	C34-C33-C32	2.52	101.62	114.42	3	2
4	A	335	PX4	C12-C11-C10	2.52	104.12	113.19	3	4
4	A	368	PX4	C27-C26-C25	2.52	101.62	114.42	19	2
4	A	313	PX4	C1-C2-N1	2.52	124.19	115.78	12	4
4	A	327	PX4	C33-C32-C31	2.52	101.63	114.42	19	1
4	A	340	PX4	C3-N1-C2	2.52	120.23	109.92	20	1
4	A	342	PX4	C17-C16-C15	2.52	101.63	114.42	7	1
4	A	349	PX4	C19-C18-C17	2.52	101.63	114.42	16	2
4	A	367	PX4	C14-C13-C12	2.52	101.63	114.42	6	3
4	A	404	PX4	C17-C16-C15	2.52	101.63	114.42	4	1
4	A	407	PX4	C14-C13-C12	2.52	101.63	114.42	3	3
4	A	396	PX4	C3-N1-C2	2.52	120.23	109.92	9	2
4	A	420	PX4	C28-C27-C26	2.52	101.63	114.42	3	1
4	A	336	PX4	C27-C26-C25	2.52	101.64	114.42	7	2
4	A	351	PX4	O3-C1-C2	2.52	122.40	109.16	14	1
4	A	353	PX4	C31-C30-C29	2.52	101.64	114.42	20	2
4	A	401	PX4	C12-C11-C10	2.52	122.24	113.19	6	2
4	A	426	PX4	C33-C32-C31	2.52	101.64	114.42	18	1
4	A	339	PX4	O8-C23-C24	2.52	113.92	123.73	1	2
4	A	356	PX4	C32-C31-C30	2.52	101.65	114.42	18	5
4	A	363	PX4	C19-C18-C17	2.52	101.66	114.42	11	3
4	A	364	PX4	C5-N1-C2	2.52	99.62	109.92	14	2
4	A	409	PX4	C20-C19-C18	2.52	101.65	114.42	10	2
4	A	410	PX4	O1-P1-O4	2.52	119.43	107.75	14	2
4	A	408	PX4	C31-C30-C29	2.51	101.66	114.42	11	1
4	A	412	PX4	C34-C33-C32	2.51	101.66	114.42	19	1
4	A	424	PX4	O3-C1-C2	2.51	122.38	109.16	7	2
4	A	335	PX4	C31-C30-C29	2.51	101.67	114.42	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	373	PX4	C18-C17-C16	2.51	101.67	114.42	6	1
4	A	313	PX4	C14-C13-C12	2.51	101.68	114.42	19	4
4	A	329	PX4	O1-P1-O4	2.51	119.40	107.75	18	2
4	A	384	PX4	C15-C14-C13	2.51	101.68	114.42	19	4
4	A	412	PX4	C29-C28-C27	2.51	101.68	114.42	19	2
4	A	352	PX4	C33-C32-C31	2.51	101.69	114.42	10	2
4	A	399	PX4	C3-N1-C2	2.51	120.18	109.92	9	2
4	A	403	PX4	C8-O5-C9	2.51	107.83	117.12	9	2
4	A	391	PX4	C34-C33-C32	2.51	101.69	114.42	6	1
4	A	323	PX4	C12-C11-C10	2.51	104.18	113.19	6	1
4	A	398	PX4	C14-C13-C12	2.51	101.69	114.42	13	3
4	A	329	PX4	C30-C29-C28	2.51	101.70	114.42	2	3
4	A	385	PX4	C15-C14-C13	2.51	101.70	114.42	6	2
4	A	308	PX4	O3-C1-C2	2.50	122.33	109.16	13	2
4	A	323	PX4	C15-C14-C13	2.50	101.71	114.42	10	1
4	A	381	PX4	C5-N1-C2	2.51	120.17	109.92	10	2
4	A	310	PX4	C8-O5-C9	2.50	107.85	117.12	6	2
4	A	329	PX4	C34-C33-C32	2.50	101.71	114.42	3	3
4	A	366	PX4	C25-C24-C23	2.50	104.51	113.62	8	3
4	A	403	PX4	C26-C25-C24	2.50	122.19	113.19	1	1
4	A	396	PX4	C32-C31-C30	2.50	101.71	114.42	5	2
4	A	431	PX4	C16-C15-C14	2.50	101.71	114.42	17	3
4	A	341	PX4	C3-N1-C2	2.50	99.67	109.92	9	2
4	A	384	PX4	O3-P1-O2	2.50	99.28	109.07	20	3
4	A	401	PX4	C3-N1-C2	2.50	120.16	109.92	17	1
4	A	417	PX4	C4-N1-C3	2.50	102.54	108.97	12	3
4	A	327	PX4	O4-P1-O2	2.50	99.30	109.07	5	2
4	A	330	PX4	C17-C16-C15	2.50	101.73	114.42	3	2
4	A	335	PX4	C33-C32-C31	2.50	101.73	114.42	5	3
4	A	312	PX4	O8-C23-C24	2.50	113.98	123.73	4	2
4	A	346	PX4	C28-C27-C26	2.50	101.74	114.42	13	1
4	A	369	PX4	C5-N1-C3	2.50	115.40	108.97	8	4
4	A	409	PX4	O5-C9-C10	2.50	119.75	111.91	14	4
4	A	401	PX4	C15-C14-C13	2.50	101.74	114.42	15	2
4	A	387	PX4	C4-N1-C2	2.50	99.69	109.92	4	1
4	A	410	PX4	C34-C33-C32	2.50	101.74	114.42	15	3
4	A	425	PX4	C5-N1-C2	2.50	99.69	109.92	16	2
4	A	359	PX4	C18-C17-C16	2.50	101.74	114.42	11	1
4	A	397	PX4	C8-O5-C9	2.50	107.87	117.12	18	1
4	A	315	PX4	C29-C28-C27	2.50	101.75	114.42	7	2
4	A	339	PX4	C33-C32-C31	2.49	101.76	114.42	4	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	356	PX4	C5-N1-C2	2.50	120.13	109.92	15	2
4	A	410	PX4	C32-C31-C30	2.50	101.75	114.42	14	1
4	A	398	PX4	C5-N1-C3	2.50	102.56	108.97	2	6
4	A	344	PX4	C19-C18-C17	2.49	101.76	114.42	1	2
4	A	350	PX4	C34-C33-C32	2.49	101.77	114.42	4	2
4	A	362	PX4	C33-C32-C31	2.49	101.76	114.42	8	1
4	A	382	PX4	C20-C19-C18	2.49	101.76	114.42	10	1
4	A	408	PX4	C16-C15-C14	2.49	101.77	114.42	7	1
4	A	371	PX4	C16-C15-C14	2.49	101.77	114.42	7	1
4	A	388	PX4	C27-C26-C25	2.49	101.77	114.42	13	2
4	A	398	PX4	C12-C11-C10	2.49	104.23	113.19	11	1
4	A	427	PX4	C30-C29-C28	2.49	101.77	114.42	5	1
4	A	429	PX4	C26-C25-C24	2.49	104.23	113.19	1	1
4	A	312	PX4	C17-C16-C15	2.49	101.78	114.42	8	2
4	A	344	PX4	C12-C11-C10	2.49	104.23	113.19	6	4
4	A	327	PX4	O8-C23-C24	2.49	114.02	123.73	7	3
4	A	325	PX4	C26-C25-C24	2.49	104.24	113.19	16	4
4	A	327	PX4	C20-C19-C18	2.49	101.78	114.42	14	2
4	A	337	PX4	C29-C28-C27	2.49	101.78	114.42	12	1
4	A	348	PX4	C15-C14-C13	2.49	101.78	114.42	1	2
4	A	358	PX4	C14-C13-C12	2.49	101.78	114.42	12	1
4	A	370	PX4	C28-C27-C26	2.49	101.78	114.42	1	1
4	A	410	PX4	O6-C9-C10	2.49	114.02	123.73	1	2
4	A	398	PX4	C11-C10-C9	2.49	104.56	113.62	10	4
4	A	426	PX4	C5-N1-C2	2.49	120.11	109.92	16	1
4	A	311	PX4	C33-C32-C31	2.49	101.79	114.42	12	4
4	A	318	PX4	C13-C12-C11	2.49	101.79	114.42	6	2
4	A	315	PX4	C16-C15-C14	2.49	101.79	114.42	10	3
4	A	389	PX4	C1-C2-N1	2.49	124.09	115.78	5	5
4	A	393	PX4	C27-C26-C25	2.49	101.79	114.42	17	3
4	A	397	PX4	C34-C33-C32	2.49	101.79	114.42	4	1
4	A	400	PX4	C5-N1-C4	2.49	115.37	108.97	15	4
4	A	401	PX4	C31-C30-C29	2.49	101.80	114.42	17	1
4	A	331	PX4	C11-C10-C9	2.49	104.58	113.62	20	3
4	A	341	PX4	O3-C1-C2	2.49	122.23	109.16	2	2
4	A	363	PX4	C16-C15-C14	2.49	101.81	114.42	8	2
4	A	381	PX4	C28-C27-C26	2.49	101.80	114.42	19	1
4	A	413	PX4	C13-C12-C11	2.49	101.80	114.42	2	2
4	A	396	PX4	O3-C1-C2	2.49	122.23	109.16	4	2
4	A	424	PX4	C3-N1-C2	2.49	120.09	109.92	13	1
4	A	426	PX4	C3-N1-C2	2.49	99.75	109.92	18	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	325	PX4	C33-C32-C31	2.48	101.82	114.42	9	2
4	A	355	PX4	C16-C15-C14	2.48	101.82	114.42	18	2
4	A	366	PX4	C29-C28-C27	2.48	101.81	114.42	15	2
4	A	401	PX4	C4-N1-C2	2.48	120.08	109.92	14	2
4	A	404	PX4	C1-C2-N1	2.48	124.07	115.78	14	4
4	A	357	PX4	C32-C31-C30	2.48	101.82	114.42	15	1
4	A	419	PX4	C27-C26-C25	2.48	101.82	114.42	12	2
4	A	347	PX4	O1-P1-O3	2.48	96.22	107.75	1	2
4	A	384	PX4	C20-C19-C18	2.48	101.84	114.42	13	1
4	A	385	PX4	C5-N1-C4	2.48	102.60	108.97	17	5
4	A	425	PX4	C25-C24-C23	2.48	104.60	113.62	1	2
4	A	305	PX4	O6-C9-C10	2.48	114.06	123.73	6	2
4	A	318	PX4	O1-P1-O3	2.48	119.26	107.75	11	3
4	A	346	PX4	C1-C2-N1	2.48	124.06	115.78	20	4
4	A	355	PX4	C14-C13-C12	2.48	101.84	114.42	6	1
4	A	415	PX4	C19-C18-C17	2.48	101.84	114.42	20	2
4	A	325	PX4	O5-C9-C10	2.48	119.68	111.91	3	2
4	A	327	PX4	C5-N1-C2	2.48	120.05	109.92	5	1
4	A	332	PX4	C4-N1-C2	2.48	120.06	109.92	6	3
4	A	341	PX4	C33-C32-C31	2.48	101.85	114.42	16	1
4	A	350	PX4	C19-C18-C17	2.48	101.85	114.42	18	1
4	A	354	PX4	C12-C11-C10	2.48	104.28	113.19	9	2
4	A	354	PX4	C18-C17-C16	2.48	101.85	114.42	16	3
4	A	361	PX4	C12-C11-C10	2.48	104.28	113.19	10	3
4	A	334	PX4	C18-C17-C16	2.48	101.86	114.42	1	1
4	A	361	PX4	C17-C16-C15	2.48	101.85	114.42	16	2
4	A	419	PX4	C13-C12-C11	2.48	101.85	114.42	17	5
4	A	366	PX4	C34-C33-C32	2.48	101.86	114.42	6	1
4	A	373	PX4	C25-C24-C23	2.48	104.62	113.62	17	3
4	A	383	PX4	C14-C13-C12	2.47	101.86	114.42	4	2
4	A	408	PX4	C29-C28-C27	2.48	101.86	114.42	8	2
4	A	389	PX4	C33-C32-C31	2.48	101.86	114.42	20	2
4	A	392	PX4	O1-P1-O3	2.48	96.25	107.75	5	2
4	A	394	PX4	C3-N1-C2	2.48	120.05	109.92	9	2
4	A	395	PX4	C15-C14-C13	2.48	101.86	114.42	17	1
4	A	360	PX4	C28-C27-C26	2.47	101.87	114.42	7	3
4	A	350	PX4	C26-C25-C24	2.47	104.30	113.19	10	1
4	A	379	PX4	C26-C25-C24	2.47	104.30	113.19	16	3
4	A	381	PX4	O1-P1-O4	2.47	119.23	107.75	17	2
4	A	321	PX4	C34-C33-C32	2.47	101.88	114.42	16	3
4	A	344	PX4	C30-C29-C28	2.47	101.88	114.42	2	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	364	PX4	C8-O5-C9	2.47	107.97	117.12	8	1
4	A	364	PX4	O1-P1-O2	2.47	124.46	112.24	10	4
4	A	373	PX4	C31-C30-C29	2.47	101.88	114.42	14	3
4	A	431	PX4	C29-C28-C27	2.47	101.88	114.42	4	1
4	A	339	PX4	O5-C9-O6	2.47	117.36	123.59	18	7
4	A	368	PX4	C3-N1-C2	2.47	120.02	109.92	13	1
4	A	371	PX4	C17-C16-C15	2.47	101.89	114.42	1	1
4	A	398	PX4	C15-C14-C13	2.47	101.89	114.42	20	1
4	A	357	PX4	C14-C13-C12	2.47	101.89	114.42	5	3
4	A	417	PX4	O3-P1-O2	2.47	99.42	109.07	17	2
4	A	397	PX4	C25-C24-C23	2.47	104.65	113.62	2	3
4	A	420	PX4	C12-C11-C10	2.47	104.32	113.19	20	2
4	A	426	PX4	C11-C10-C9	2.47	104.64	113.62	10	2
4	A	311	PX4	C13-C12-C11	2.47	101.90	114.42	9	2
4	A	426	PX4	C20-C19-C18	2.47	101.90	114.42	2	1
4	A	328	PX4	C17-C16-C15	2.47	101.91	114.42	14	3
4	A	379	PX4	C13-C12-C11	2.47	101.91	114.42	20	1
4	A	322	PX4	C26-C25-C24	2.46	104.33	113.19	19	3
4	A	354	PX4	C1-C2-N1	2.46	124.01	115.78	10	4
4	A	306	PX4	C16-C15-C14	2.46	101.92	114.42	17	1
4	A	308	PX4	C4-N1-C3	2.46	115.31	108.97	18	4
4	A	312	PX4	C20-C19-C18	2.46	101.92	114.42	1	1
4	A	332	PX4	C17-C16-C15	2.46	101.92	114.42	4	1
4	A	339	PX4	C5-N1-C2	2.46	119.99	109.92	6	1
4	A	341	PX4	C11-C10-C9	2.46	104.66	113.62	16	3
4	A	355	PX4	C32-C31-C30	2.46	101.91	114.42	16	4
4	A	411	PX4	C14-C13-C12	2.47	101.91	114.42	15	1
4	A	396	PX4	O6-C9-C10	2.46	114.12	123.73	1	1
4	A	419	PX4	C14-C13-C12	2.47	101.91	114.42	17	2
4	A	379	PX4	O1-P1-O4	2.46	119.19	107.75	18	4
4	A	319	PX4	C17-C16-C15	2.46	101.93	114.42	16	1
4	A	356	PX4	C14-C13-C12	2.46	101.93	114.42	1	2
4	A	391	PX4	C18-C17-C16	2.46	101.92	114.42	10	1
4	A	339	PX4	C25-C24-C23	2.46	104.67	113.62	8	2
4	A	401	PX4	C25-C24-C23	2.46	104.67	113.62	15	3
4	A	372	PX4	C5-N1-C2	2.46	119.99	109.92	3	1
4	A	312	PX4	C27-C26-C25	2.46	101.94	114.42	19	1
4	A	350	PX4	C30-C29-C28	2.46	101.94	114.42	9	2
4	A	380	PX4	C5-N1-C2	2.46	119.98	109.92	3	1
4	A	346	PX4	C5-N1-C2	2.46	99.86	109.92	1	2
4	A	348	PX4	C29-C28-C27	2.46	101.94	114.42	15	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	387	PX4	C19-C18-C17	2.46	101.94	114.42	3	4
4	A	423	PX4	C26-C25-C24	2.46	104.35	113.19	10	3
4	A	319	PX4	C13-C12-C11	2.46	101.94	114.42	5	4
4	A	378	PX4	C30-C29-C28	2.46	101.95	114.42	18	1
4	A	393	PX4	C13-C12-C11	2.46	101.94	114.42	17	1
4	A	319	PX4	C11-C10-C9	2.46	104.69	113.62	2	1
4	A	348	PX4	C33-C32-C31	2.46	101.95	114.42	19	3
4	A	375	PX4	C27-C26-C25	2.46	101.95	114.42	19	4
4	A	414	PX4	O4-P1-O2	2.46	118.67	109.07	14	2
4	A	386	PX4	O1-P1-O4	2.46	96.34	107.75	16	1
4	A	310	PX4	O3-C1-C2	2.45	122.06	109.16	1	2
4	A	312	PX4	C15-C14-C13	2.45	101.97	114.42	19	2
4	A	344	PX4	O1-P1-O4	2.45	119.14	107.75	16	2
4	A	418	PX4	C16-C15-C14	2.45	101.97	114.42	2	3
4	A	365	PX4	C13-C12-C11	2.45	101.97	114.42	4	2
4	A	403	PX4	O1-P1-O4	2.45	119.14	107.75	18	5
4	A	421	PX4	C11-C10-C9	2.45	104.70	113.62	1	2
4	A	332	PX4	O3-C1-C2	2.45	122.05	109.16	4	1
4	A	364	PX4	O3-C1-C2	2.45	122.05	109.16	1	2
4	A	313	PX4	O5-C9-C10	2.45	119.59	111.91	6	3
4	A	358	PX4	C34-C33-C32	2.45	101.99	114.42	13	4
4	A	360	PX4	C13-C12-C11	2.45	101.99	114.42	7	2
4	A	376	PX4	O5-C9-C10	2.45	119.60	111.91	14	2
4	A	414	PX4	C32-C31-C30	2.45	101.98	114.42	9	2
4	A	331	PX4	C8-O5-C9	2.45	108.05	117.12	13	3
4	A	364	PX4	O6-C9-C10	2.45	114.18	123.73	13	1
4	A	354	PX4	C34-C33-C32	2.45	102.00	114.42	12	2
4	A	358	PX4	O4-P1-O2	2.45	118.63	109.07	9	3
4	A	381	PX4	C8-O5-C9	2.45	108.05	117.12	16	3
4	A	409	PX4	C29-C28-C27	2.45	102.00	114.42	19	1
4	A	396	PX4	C15-C14-C13	2.45	102.00	114.42	10	4
4	A	425	PX4	O1-P1-O3	2.45	96.38	107.75	15	2
4	A	430	PX4	C27-C26-C25	2.45	102.00	114.42	8	1
4	A	313	PX4	O3-C1-C2	2.45	122.02	109.16	14	1
4	A	312	PX4	C34-C33-C32	2.45	102.01	114.42	1	2
4	A	315	PX4	C14-C13-C12	2.45	102.01	114.42	20	2
4	A	342	PX4	C25-C24-C23	2.45	104.72	113.62	5	3
4	A	322	PX4	C30-C29-C28	2.44	102.01	114.42	20	2
4	A	406	PX4	C18-C17-C16	2.45	102.01	114.42	15	1
4	A	396	PX4	C34-C33-C32	2.44	102.02	114.42	19	4
4	A	424	PX4	C31-C30-C29	2.44	102.01	114.42	5	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	317	PX4	C13-C12-C11	2.44	102.03	114.42	5	1
4	A	346	PX4	C11-C10-C9	2.44	104.73	113.62	13	1
4	A	320	PX4	C1-C2-N1	2.44	123.93	115.78	1	5
4	A	358	PX4	O3-C1-C2	2.44	122.01	109.16	18	2
4	A	366	PX4	C13-C12-C11	2.44	102.02	114.42	13	1
4	A	345	PX4	C14-C13-C12	2.44	102.03	114.42	9	3
4	A	348	PX4	C20-C19-C18	2.44	102.03	114.42	9	1
4	A	412	PX4	C28-C27-C26	2.44	102.03	114.42	14	1
4	A	400	PX4	C17-C16-C15	2.44	102.04	114.42	8	3
4	A	306	PX4	O3-C1-C2	2.44	121.99	109.16	10	2
4	A	363	PX4	C34-C33-C32	2.44	102.05	114.42	13	1
4	A	423	PX4	O1-P1-O3	2.44	96.42	107.75	4	2
4	A	337	PX4	O4-P1-O2	2.44	118.59	109.07	7	1
4	A	353	PX4	C14-C13-C12	2.44	102.06	114.42	2	1
4	A	361	PX4	C31-C30-C29	2.44	102.05	114.42	14	3
4	A	371	PX4	C5-N1-C2	2.44	119.89	109.92	12	1
4	A	332	PX4	O1-P1-O3	2.44	96.43	107.75	3	1
4	A	311	PX4	C26-C25-C24	2.43	104.44	113.19	10	3
4	A	316	PX4	C12-C11-C10	2.44	121.94	113.19	13	1
4	A	343	PX4	C8-O5-C9	2.44	108.10	117.12	9	2
4	A	414	PX4	O3-C1-C2	2.44	121.97	109.16	9	1
4	A	327	PX4	C16-C15-C14	2.43	102.08	114.42	17	4
4	A	360	PX4	C14-C13-C12	2.43	102.07	114.42	11	1
4	A	383	PX4	O7-C7-C6	2.43	117.21	108.40	11	7
4	A	423	PX4	C30-C29-C28	2.43	102.07	114.42	17	1
4	A	421	PX4	C4-N1-C3	2.43	102.72	108.97	2	1
4	A	370	PX4	C12-C11-C10	2.43	104.45	113.19	17	1
4	A	428	PX4	C32-C31-C30	2.43	102.08	114.42	6	2
4	A	431	PX4	C3-N1-C2	2.43	119.87	109.92	9	1
4	A	320	PX4	C4-N1-C2	2.43	119.86	109.92	7	2
4	A	320	PX4	O4-P1-O2	2.43	118.56	109.07	19	2
4	A	337	PX4	C4-N1-C2	2.43	99.97	109.92	6	3
4	A	337	PX4	C13-C12-C11	2.43	102.09	114.42	5	2
4	A	358	PX4	C5-N1-C2	2.43	119.86	109.92	5	2
4	A	338	PX4	C33-C32-C31	2.43	102.09	114.42	17	2
4	A	348	PX4	C31-C30-C29	2.43	102.09	114.42	11	4
4	A	323	PX4	C1-C2-N1	2.43	123.89	115.78	5	3
4	A	351	PX4	O8-C23-C24	2.43	133.21	123.73	13	1
4	A	354	PX4	C29-C28-C27	2.43	102.09	114.42	1	4
4	A	307	PX4	O1-P1-O3	2.43	96.47	107.75	12	2
4	A	357	PX4	C18-C17-C16	2.43	102.10	114.42	3	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	373	PX4	C27-C26-C25	2.43	102.09	114.42	20	3
4	A	378	PX4	O1-P1-O3	2.43	96.47	107.75	19	2
4	A	419	PX4	C36-C35-C34	2.43	95.00	113.42	9	1
4	A	359	PX4	C34-C33-C32	2.43	102.11	114.42	10	2
4	A	370	PX4	C32-C31-C30	2.43	102.11	114.42	13	3
4	A	388	PX4	C5-N1-C3	2.43	102.74	108.97	18	3
4	A	393	PX4	C18-C17-C16	2.42	102.12	114.42	5	1
4	A	415	PX4	C12-C11-C10	2.42	104.47	113.19	2	4
4	A	332	PX4	O6-C9-C10	2.42	114.28	123.73	9	3
4	A	424	PX4	C17-C16-C15	2.42	102.12	114.42	16	2
4	A	319	PX4	C4-N1-C2	2.42	119.83	109.92	14	1
4	A	309	PX4	C20-C19-C18	2.42	102.14	114.42	2	2
4	A	324	PX4	C28-C27-C26	2.42	102.13	114.42	10	1
4	A	334	PX4	O3-C1-C2	2.42	121.89	109.16	12	3
4	A	336	PX4	C29-C28-C27	2.42	102.13	114.42	8	1
4	A	399	PX4	C25-C24-C23	2.42	122.43	113.62	6	1
4	A	378	PX4	C14-C13-C12	2.42	102.13	114.42	15	1
4	A	381	PX4	O8-C23-C24	2.42	114.28	123.73	1	2
4	A	353	PX4	O1-P1-O4	2.42	118.99	107.75	8	3
4	A	386	PX4	C3-N1-C2	2.42	119.82	109.92	12	1
4	A	396	PX4	C28-C27-C26	2.42	102.13	114.42	11	2
4	A	354	PX4	C8-O5-C9	2.42	108.16	117.12	12	4
4	A	395	PX4	C14-C13-C12	2.42	102.14	114.42	11	1
4	A	353	PX4	C29-C28-C27	2.42	102.15	114.42	10	3
4	A	361	PX4	C13-C12-C11	2.42	102.15	114.42	20	1
4	A	400	PX4	C29-C28-C27	2.42	102.15	114.42	20	2
4	A	404	PX4	C11-C10-C9	2.42	104.82	113.62	7	3
4	A	424	PX4	C5-N1-C2	2.42	119.81	109.92	3	2
4	A	369	PX4	C17-C16-C15	2.42	102.16	114.42	5	2
4	A	369	PX4	C11-C10-C9	2.42	104.83	113.62	17	2
4	A	390	PX4	C29-C28-C27	2.42	102.16	114.42	1	2
4	A	397	PX4	C17-C16-C15	2.42	102.15	114.42	16	1
4	A	420	PX4	C16-C15-C14	2.42	102.15	114.42	14	4
4	A	431	PX4	C33-C32-C31	2.42	102.15	114.42	2	1
4	A	324	PX4	C32-C31-C30	2.42	102.16	114.42	4	1
4	A	399	PX4	C27-C26-C25	2.42	102.16	114.42	19	2
4	A	422	PX4	C29-C28-C27	2.42	102.16	114.42	10	2
4	A	431	PX4	C8-O5-C9	2.42	108.17	117.12	10	5
4	A	413	PX4	O3-C1-C2	2.42	121.86	109.16	9	1
4	A	318	PX4	O1-P1-O4	2.41	118.96	107.75	9	2
4	A	331	PX4	C4-N1-C2	2.41	100.04	109.92	8	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	373	PX4	C14-C13-C12	2.41	102.17	114.42	7	2
4	A	426	PX4	C16-C15-C14	2.41	102.17	114.42	15	3
4	A	307	PX4	C17-C16-C15	2.41	102.18	114.42	20	2
4	A	336	PX4	C13-C12-C11	2.41	126.67	114.42	17	4
4	A	375	PX4	O4-P1-O2	2.41	118.49	109.07	9	3
4	A	306	PX4	O1-P1-O3	2.41	96.55	107.75	5	3
4	A	328	PX4	O3-C1-C2	2.41	121.84	109.16	16	4
4	A	400	PX4	C20-C19-C18	2.41	102.19	114.42	14	1
4	A	312	PX4	C31-C30-C29	2.41	102.19	114.42	17	2
4	A	332	PX4	C5-N1-C2	2.41	119.78	109.92	12	2
4	A	337	PX4	C34-C33-C32	2.41	102.19	114.42	5	3
4	A	343	PX4	C15-C14-C13	2.41	102.19	114.42	5	1
4	A	343	PX4	C3-N1-C2	2.41	119.78	109.92	15	1
4	A	373	PX4	C15-C14-C13	2.41	102.19	114.42	7	2
4	A	391	PX4	C32-C31-C30	2.41	102.19	114.42	19	3
4	A	398	PX4	C28-C27-C26	2.41	102.19	114.42	11	3
4	A	418	PX4	O6-C9-C10	2.41	114.33	123.73	14	1
4	A	427	PX4	O3-P1-O2	2.41	99.65	109.07	17	4
4	A	401	PX4	C4-N1-C3	2.41	102.78	108.97	17	3
4	A	409	PX4	C28-C27-C26	2.41	102.20	114.42	20	2
4	A	428	PX4	C25-C24-C23	2.41	104.86	113.62	13	4
4	A	311	PX4	O5-C9-C10	2.41	119.46	111.91	5	2
4	A	316	PX4	C13-C12-C11	2.41	102.20	114.42	20	1
4	A	380	PX4	C4-N1-C2	2.41	119.76	109.92	6	2
4	A	390	PX4	C13-C12-C11	2.41	102.20	114.42	12	3
4	A	311	PX4	O1-P1-O4	2.41	118.92	107.75	15	5
4	A	402	PX4	O8-C23-C24	2.41	114.35	123.73	1	2
4	A	414	PX4	C3-N1-C2	2.41	100.07	109.92	1	1
4	A	429	PX4	O1-P1-O3	2.41	96.57	107.75	5	1
4	A	323	PX4	C31-C30-C29	2.40	102.22	114.42	12	1
4	A	351	PX4	C27-C26-C25	2.40	102.22	114.42	16	1
4	A	358	PX4	C3-N1-C2	2.40	119.75	109.92	6	1
4	A	363	PX4	O1-P1-O4	2.40	118.91	107.75	13	1
4	A	363	PX4	C13-C12-C11	2.40	102.22	114.42	16	1
4	A	345	PX4	O3-C1-C2	2.40	121.80	109.16	2	3
4	A	371	PX4	C8-O5-C9	2.40	108.22	117.12	16	3
4	A	402	PX4	O1-P1-O4	2.40	96.58	107.75	2	5
4	A	373	PX4	C8-O5-C9	2.40	108.22	117.12	20	1
4	A	425	PX4	C28-C27-C26	2.40	102.22	114.42	15	2
4	A	417	PX4	O6-C9-C10	2.40	114.36	123.73	1	1
4	A	427	PX4	C4-N1-C2	2.40	100.08	109.92	20	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	313	PX4	C16-C15-C14	2.40	102.24	114.42	13	1
4	A	330	PX4	O1-P1-O4	2.40	118.90	107.75	18	6
4	A	324	PX4	C5-N1-C3	2.40	102.80	108.97	14	3
4	A	349	PX4	C20-C19-C18	2.40	102.24	114.42	4	2
4	A	380	PX4	C13-C12-C11	2.40	102.23	114.42	12	2
4	A	368	PX4	C8-O5-C9	2.40	108.23	117.12	20	3
4	A	376	PX4	C17-C16-C15	2.40	102.24	114.42	3	1
4	A	380	PX4	C25-C24-C23	2.40	104.89	113.62	8	2
4	A	380	PX4	O3-C1-C2	2.40	121.78	109.16	11	3
4	A	394	PX4	C18-C17-C16	2.40	102.23	114.42	8	1
4	A	340	PX4	C34-C33-C32	2.40	102.24	114.42	20	1
4	A	387	PX4	C28-C27-C26	2.40	102.24	114.42	16	4
4	A	415	PX4	C31-C30-C29	2.40	102.24	114.42	14	2
4	A	428	PX4	O6-C9-C10	2.40	114.37	123.73	14	1
4	A	310	PX4	C5-N1-C3	2.40	102.81	108.97	11	1
4	A	306	PX4	C18-C17-C16	2.40	102.26	114.42	12	2
4	A	314	PX4	O1-P1-O3	2.40	96.61	107.75	2	4
4	A	380	PX4	C12-C11-C10	2.40	104.58	113.19	13	4
4	A	386	PX4	C33-C32-C31	2.40	102.26	114.42	11	2
4	A	394	PX4	C27-C26-C25	2.40	102.25	114.42	6	2
4	A	311	PX4	C28-C27-C26	2.40	102.26	114.42	10	5
4	A	325	PX4	O3-C1-C2	2.40	121.76	109.16	4	1
4	A	335	PX4	C29-C28-C27	2.40	102.26	114.42	9	3
4	A	409	PX4	C26-C25-C24	2.40	104.58	113.19	19	1
4	A	397	PX4	C27-C26-C25	2.40	102.26	114.42	11	2
4	A	421	PX4	C16-C15-C14	2.40	102.26	114.42	7	4
4	A	398	PX4	O1-P1-O3	2.40	118.87	107.75	4	2
4	A	424	PX4	C13-C12-C11	2.40	102.26	114.42	16	1
4	A	427	PX4	C1-C2-N1	2.40	123.78	115.78	8	4
4	A	325	PX4	C17-C16-C15	2.39	102.27	114.42	15	1
4	A	329	PX4	C31-C30-C29	2.39	102.27	114.42	20	2
4	A	332	PX4	O4-P1-O2	2.39	118.42	109.07	8	2
4	A	410	PX4	C31-C30-C29	2.40	102.27	114.42	9	2
4	A	358	PX4	C25-C24-C23	2.39	104.92	113.62	3	1
4	A	382	PX4	C32-C31-C30	2.39	102.28	114.42	15	2
4	A	386	PX4	C15-C14-C13	2.39	102.28	114.42	15	3
4	A	414	PX4	C17-C16-C15	2.39	102.28	114.42	15	2
4	A	415	PX4	O1-P1-O3	2.39	96.62	107.75	1	3
4	A	326	PX4	C15-C14-C13	2.39	102.28	114.42	12	2
4	A	421	PX4	C25-C24-C23	2.39	104.92	113.62	4	2
4	A	305	PX4	C4-N1-C2	2.39	119.70	109.92	8	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	309	PX4	C1-C2-N1	2.39	123.76	115.78	11	4
4	A	310	PX4	O1-P1-O3	2.39	96.64	107.75	12	2
4	A	347	PX4	O8-C23-C24	2.39	114.40	123.73	6	2
4	A	347	PX4	O3-C1-C2	2.39	121.74	109.16	9	2
4	A	355	PX4	C17-C16-C15	2.39	102.29	114.42	3	1
4	A	356	PX4	C28-C27-C26	2.39	102.29	114.42	13	1
4	A	367	PX4	C34-C33-C32	2.39	102.28	114.42	1	5
4	A	396	PX4	C16-C15-C14	2.39	102.29	114.42	11	2
4	A	420	PX4	C14-C13-C12	2.39	102.28	114.42	10	3
4	A	364	PX4	C11-C10-C9	2.39	104.93	113.62	4	4
4	A	369	PX4	C13-C12-C11	2.39	102.29	114.42	3	1
4	A	409	PX4	O1-P1-O3	2.39	96.64	107.75	6	2
4	A	418	PX4	C33-C32-C31	2.39	102.29	114.42	3	1
4	A	431	PX4	O3-C1-C2	2.39	121.73	109.16	9	1
4	A	314	PX4	C31-C30-C29	2.39	102.30	114.42	18	3
4	A	327	PX4	C32-C31-C30	2.39	102.30	114.42	19	1
4	A	342	PX4	C13-C12-C11	2.39	102.30	114.42	7	3
4	A	356	PX4	O3-C1-C2	2.39	121.72	109.16	18	2
4	A	370	PX4	C29-C28-C27	2.39	102.30	114.42	9	1
4	A	318	PX4	C4-N1-C2	2.39	119.68	109.92	3	2
4	A	356	PX4	C15-C14-C13	2.39	102.30	114.42	9	2
4	A	405	PX4	C15-C14-C13	2.39	102.31	114.42	1	1
4	A	409	PX4	O1-P1-O4	2.39	118.84	107.75	6	3
4	A	305	PX4	C7-O7-C23	2.39	123.67	117.79	8	2
4	A	347	PX4	C17-C16-C15	2.39	102.31	114.42	11	1
4	A	346	PX4	O1-P1-O3	2.38	96.67	107.75	10	1
4	A	354	PX4	C20-C19-C18	2.38	102.32	114.42	19	2
4	A	359	PX4	O6-C9-C10	2.38	114.43	123.73	9	3
4	A	362	PX4	C34-C33-C32	2.38	102.32	114.42	18	2
4	A	363	PX4	C25-C24-C23	2.39	104.95	113.62	6	1
4	A	375	PX4	C29-C28-C27	2.39	102.31	114.42	14	1
4	A	404	PX4	C20-C19-C18	2.39	102.31	114.42	13	2
4	A	391	PX4	C30-C29-C28	2.39	102.31	114.42	19	2
4	A	417	PX4	O8-C23-C24	2.39	114.42	123.73	17	1
4	A	366	PX4	C33-C32-C31	2.38	102.32	114.42	9	2
4	A	367	PX4	C31-C30-C29	2.38	102.33	114.42	8	2
4	A	372	PX4	C32-C31-C30	2.38	102.32	114.42	14	2
4	A	408	PX4	C32-C31-C30	2.38	102.32	114.42	6	1
4	A	352	PX4	O5-C9-O6	2.38	117.58	123.59	8	2
4	A	361	PX4	C14-C13-C12	2.38	102.33	114.42	5	3
4	A	423	PX4	C4-N1-C3	2.38	115.10	108.97	9	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	325	PX4	O1-P1-O4	2.38	118.80	107.75	9	4
4	A	338	PX4	C20-C19-C18	2.38	102.34	114.42	5	1
4	A	341	PX4	C27-C26-C25	2.38	102.34	114.42	6	2
4	A	342	PX4	C20-C19-C18	2.38	102.34	114.42	4	2
4	A	362	PX4	C25-C24-C23	2.38	104.97	113.62	18	5
4	A	390	PX4	C31-C30-C29	2.38	102.35	114.42	9	2
4	A	411	PX4	C33-C32-C31	2.38	102.34	114.42	6	2
4	A	375	PX4	C13-C12-C11	2.38	102.35	114.42	7	1
4	A	417	PX4	C14-C13-C12	2.38	102.35	114.42	20	2
4	A	418	PX4	C25-C24-C23	2.38	104.97	113.62	3	2
4	A	320	PX4	O1-P1-O4	2.38	118.79	107.75	5	6
4	A	346	PX4	O1-P1-O4	2.38	118.79	107.75	2	2
4	A	419	PX4	C34-C33-C32	2.38	102.35	114.42	16	1
4	A	420	PX4	O3-C1-C2	2.38	121.67	109.16	1	2
4	A	422	PX4	C28-C27-C26	2.38	102.35	114.42	6	1
4	A	402	PX4	C26-C25-C24	2.38	104.65	113.19	1	3
4	A	375	PX4	C5-N1-C2	2.38	119.64	109.92	14	1
4	A	413	PX4	C4-N1-C2	2.38	119.64	109.92	8	2
4	A	414	PX4	C19-C18-C17	2.38	102.36	114.42	12	2
4	A	400	PX4	O3-P1-O2	2.37	99.79	109.07	6	2
4	A	403	PX4	C4-N1-C2	2.37	119.63	109.92	15	2
4	A	378	PX4	O8-C23-C24	2.38	114.46	123.73	6	1
4	A	398	PX4	C20-C19-C18	2.38	102.36	114.42	10	4
4	A	423	PX4	C14-C13-C12	2.38	102.36	114.42	18	2
4	A	307	PX4	C5-N1-C2	2.38	100.20	109.92	3	2
4	A	357	PX4	C5-N1-C2	2.38	119.64	109.92	3	1
4	A	364	PX4	C28-C27-C26	2.37	102.37	114.42	5	1
4	A	406	PX4	C13-C12-C11	2.38	102.37	114.42	10	1
4	A	385	PX4	C20-C19-C18	2.37	102.38	114.42	2	1
4	A	413	PX4	C31-C30-C29	2.37	102.38	114.42	12	2
4	A	397	PX4	C18-C17-C16	2.37	102.37	114.42	3	2
4	A	429	PX4	C16-C15-C14	2.37	102.37	114.42	15	1
4	A	430	PX4	C20-C19-C18	2.37	102.37	114.42	16	2
4	A	336	PX4	O3-C1-C2	2.37	121.64	109.16	15	3
4	A	350	PX4	O8-C23-C24	2.37	114.48	123.73	15	2
4	A	363	PX4	O1-P1-O3	2.37	96.73	107.75	8	1
4	A	325	PX4	C5-N1-C2	2.37	100.21	109.92	16	1
4	A	372	PX4	O1-P1-O3	2.37	96.73	107.75	2	3
4	A	319	PX4	C14-C13-C12	2.37	102.39	114.42	9	2
4	A	370	PX4	O4-P1-O2	2.37	118.33	109.07	3	5
4	A	383	PX4	C17-C16-C15	2.37	102.39	114.42	18	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	388	PX4	O3-C1-C2	2.37	121.63	109.16	17	2
4	A	423	PX4	C12-C11-C10	2.37	104.67	113.19	9	1
4	A	407	PX4	C3-N1-C2	2.37	100.23	109.92	6	3
4	A	385	PX4	C33-C32-C31	2.37	102.40	114.42	9	2
4	A	425	PX4	C18-C17-C16	2.37	102.40	114.42	15	1
4	A	426	PX4	C14-C13-C12	2.37	102.40	114.42	18	3
4	A	356	PX4	O1-P1-O4	2.37	118.74	107.75	1	5
4	A	363	PX4	C5-N1-C4	2.37	102.89	108.97	10	3
4	A	431	PX4	C20-C19-C18	2.37	102.40	114.42	15	3
4	A	408	PX4	C28-C27-C26	2.37	102.41	114.42	14	2
4	A	311	PX4	C14-C13-C12	2.37	102.42	114.42	19	3
4	A	332	PX4	C27-C26-C25	2.36	102.42	114.42	7	2
4	A	334	PX4	C29-C28-C27	2.37	102.42	114.42	19	4
4	A	366	PX4	C18-C17-C16	2.37	102.42	114.42	2	2
4	A	333	PX4	C17-C16-C15	2.36	102.42	114.42	11	1
4	A	334	PX4	C3-N1-C2	2.36	119.59	109.92	13	1
4	A	337	PX4	C20-C19-C18	2.36	102.42	114.42	19	3
4	A	349	PX4	O4-P1-O2	2.36	99.83	109.07	1	2
4	A	368	PX4	C5-N1-C2	2.36	100.24	109.92	13	3
4	A	388	PX4	O6-C9-C10	2.36	114.51	123.73	8	1
4	A	425	PX4	C30-C29-C28	2.36	102.42	114.42	18	1
4	A	349	PX4	O1-P1-O3	2.36	118.72	107.75	10	3
4	A	373	PX4	O8-C23-C24	2.36	114.52	123.73	13	2
4	A	382	PX4	C12-C11-C10	2.36	104.70	113.19	12	4
4	A	375	PX4	C20-C19-C18	2.36	102.44	114.42	17	1
4	A	382	PX4	C27-C26-C25	2.36	102.43	114.42	15	2
4	A	383	PX4	C3-N1-C2	2.36	119.58	109.92	16	3
4	A	354	PX4	O5-C9-C10	2.36	119.31	111.91	18	3
4	A	379	PX4	C14-C13-C12	2.36	102.44	114.42	15	1
4	A	412	PX4	C19-C18-C17	2.36	102.44	114.42	1	1
4	A	416	PX4	C15-C14-C13	2.36	102.44	114.42	20	1
4	A	306	PX4	C27-C26-C25	2.36	102.45	114.42	17	1
4	A	331	PX4	O3-C1-C2	2.36	121.57	109.16	15	3
4	A	336	PX4	O8-C23-C24	2.36	114.53	123.73	4	2
4	A	427	PX4	C34-C33-C32	2.36	102.45	114.42	18	1
4	A	308	PX4	C17-C16-C15	2.36	102.46	114.42	15	1
4	A	324	PX4	O4-P1-O2	2.36	99.86	109.07	14	1
4	A	327	PX4	C3-N1-C2	2.36	119.56	109.92	14	2
4	A	348	PX4	C12-C11-C10	2.36	104.72	113.19	8	1
4	A	399	PX4	C34-C33-C32	2.36	102.46	114.42	11	2
4	A	310	PX4	C25-C24-C23	2.35	122.18	113.62	7	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	374	PX4	O4-P1-O2	2.36	118.27	109.07	20	2
4	A	310	PX4	C4-N1-C2	2.35	119.55	109.92	16	4
4	A	322	PX4	C25-C24-C23	2.35	105.06	113.62	7	1
4	A	344	PX4	C28-C27-C26	2.35	102.47	114.42	14	2
4	A	390	PX4	C30-C29-C28	2.35	102.47	114.42	6	3
4	A	316	PX4	C19-C18-C17	2.35	102.48	114.42	8	3
4	A	328	PX4	C18-C17-C16	2.35	102.48	114.42	14	2
4	A	351	PX4	C19-C18-C17	2.35	102.48	114.42	18	1
4	A	352	PX4	C5-N1-C4	2.35	115.02	108.97	17	5
4	A	357	PX4	C12-C11-C10	2.35	104.73	113.19	20	4
4	A	358	PX4	O1-P1-O4	2.35	118.67	107.75	15	1
4	A	377	PX4	C17-C16-C15	2.35	102.48	114.42	1	1
4	A	411	PX4	C28-C27-C26	2.35	102.48	114.42	4	3
4	A	425	PX4	C3-N1-C2	2.35	100.28	109.92	9	2
4	A	312	PX4	C14-C13-C12	2.35	102.50	114.42	13	2
4	A	312	PX4	O6-C9-C10	2.35	114.56	123.73	12	3
4	A	315	PX4	O8-C23-C24	2.35	114.56	123.73	16	2
4	A	340	PX4	C5-N1-C2	2.35	119.53	109.92	13	1
4	A	341	PX4	C8-O5-C9	2.35	108.41	117.12	7	3
4	A	346	PX4	O8-C23-C24	2.35	114.56	123.73	14	1
4	A	404	PX4	C32-C31-C30	2.35	102.48	114.42	6	1
4	A	418	PX4	O1-P1-O3	2.35	96.82	107.75	12	1
4	A	325	PX4	O7-C7-C8	2.35	116.91	108.40	8	5
4	A	368	PX4	C31-C30-C29	2.35	102.50	114.42	3	1
4	A	422	PX4	C15-C14-C13	2.35	102.50	114.42	19	2
4	A	430	PX4	C32-C31-C30	2.35	102.49	114.42	12	2
4	A	314	PX4	C28-C27-C26	2.35	102.50	114.42	2	1
4	A	315	PX4	C5-N1-C2	2.35	119.53	109.92	16	1
4	A	329	PX4	C11-C10-C9	2.35	105.08	113.62	10	1
4	A	402	PX4	C8-O5-C9	2.35	108.42	117.12	4	4
4	A	430	PX4	O3-C1-C2	2.35	121.52	109.16	13	3
4	A	326	PX4	O6-C9-C10	2.35	132.89	123.73	16	2
4	A	326	PX4	C11-C10-C9	2.35	105.08	113.62	14	1
4	A	345	PX4	C29-C28-C27	2.35	102.50	114.42	9	2
4	A	349	PX4	C31-C30-C29	2.35	102.50	114.42	7	1
4	A	415	PX4	C17-C16-C15	2.35	102.50	114.42	17	1
4	A	388	PX4	C5-N1-C2	2.35	119.52	109.92	3	2
4	A	370	PX4	C13-C12-C11	2.35	102.51	114.42	2	1
4	A	372	PX4	O3-P1-O2	2.34	99.91	109.07	17	2
4	A	381	PX4	C34-C33-C32	2.35	102.52	114.42	7	1
4	A	384	PX4	C29-C28-C27	2.35	102.51	114.42	14	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	423	PX4	O3-C1-C2	2.35	121.50	109.16	12	1
4	A	328	PX4	C25-C24-C23	2.35	105.09	113.62	18	1
4	A	352	PX4	C34-C33-C32	2.34	102.52	114.42	9	1
4	A	344	PX4	C11-C10-C9	2.34	105.10	113.62	8	2
4	A	344	PX4	C16-C15-C14	2.34	102.53	114.42	9	1
4	A	363	PX4	C30-C29-C28	2.34	102.53	114.42	9	1
4	A	373	PX4	O6-C9-C10	2.34	114.59	123.73	19	1
4	A	390	PX4	C32-C31-C30	2.34	102.53	114.42	14	1
4	A	394	PX4	C32-C31-C30	2.34	102.53	114.42	8	2
4	A	431	PX4	C17-C16-C15	2.34	102.53	114.42	6	2
4	A	310	PX4	C19-C18-C17	2.34	102.53	114.42	10	3
4	A	313	PX4	C25-C24-C23	2.34	105.11	113.62	2	2
4	A	310	PX4	C33-C32-C31	2.34	102.54	114.42	19	1
4	A	331	PX4	O5-C9-O6	2.34	117.68	123.59	19	3
4	A	337	PX4	C3-N1-C2	2.34	119.50	109.92	2	2
4	A	342	PX4	C8-O5-C9	2.34	108.45	117.12	3	1
4	A	365	PX4	O1-P1-O4	2.34	118.62	107.75	5	2
4	A	381	PX4	C31-C30-C29	2.34	102.54	114.42	12	2
4	A	386	PX4	O8-C23-C24	2.34	114.59	123.73	14	1
4	A	409	PX4	C5-N1-C2	2.34	119.50	109.92	19	3
4	A	423	PX4	C33-C32-C31	2.34	102.53	114.42	19	2
4	A	325	PX4	O1-P1-O3	2.34	96.88	107.75	19	3
4	A	341	PX4	C20-C19-C18	2.34	102.54	114.42	13	1
4	A	344	PX4	C31-C30-C29	2.34	102.55	114.42	19	3
4	A	350	PX4	O3-C1-C2	2.34	121.46	109.16	11	1
4	A	405	PX4	O6-C9-C10	2.34	114.61	123.73	19	2
4	A	408	PX4	C5-N1-C2	2.34	119.49	109.92	18	1
4	A	386	PX4	C17-C16-C15	2.34	102.55	114.42	16	2
4	A	392	PX4	C19-C18-C17	2.34	102.55	114.42	6	2
4	A	355	PX4	O1-P1-O4	2.34	118.61	107.75	12	2
4	A	318	PX4	O3-C1-C2	2.34	121.45	109.16	2	2
4	A	329	PX4	O8-C23-C24	2.34	114.61	123.73	5	1
4	A	375	PX4	C28-C27-C26	2.34	102.56	114.42	15	4
4	A	405	PX4	C25-C24-C23	2.34	105.12	113.62	15	3
4	A	391	PX4	C8-O5-C9	2.34	108.47	117.12	6	4
4	A	402	PX4	O1-P1-O3	2.34	96.89	107.75	17	3
4	A	428	PX4	C3-N1-C2	2.34	100.35	109.92	4	4
4	A	310	PX4	C17-C16-C15	2.34	102.57	114.42	16	1
4	A	312	PX4	C13-C12-C11	2.33	102.58	114.42	8	1
4	A	337	PX4	O1-P1-O3	2.34	96.90	107.75	2	4
4	A	339	PX4	C4-N1-C2	2.33	119.47	109.92	9	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	410	PX4	C20-C19-C18	2.33	102.57	114.42	12	3
4	A	401	PX4	O3-C1-C2	2.33	121.43	109.16	9	4
4	A	420	PX4	C18-C17-C16	2.33	102.58	114.42	3	3
4	A	421	PX4	C29-C28-C27	2.33	102.58	114.42	4	1
4	A	309	PX4	O3-C1-C2	2.33	121.42	109.16	17	2
4	A	313	PX4	C30-C29-C28	2.33	102.58	114.42	9	2
4	A	331	PX4	O6-C9-C10	2.33	114.63	123.73	5	1
4	A	340	PX4	O7-C7-C6	2.33	116.85	108.40	5	4
4	A	360	PX4	C4-N1-C2	2.33	100.37	109.92	7	1
4	A	402	PX4	C5-N1-C4	2.33	102.98	108.97	14	2
4	A	378	PX4	C31-C30-C29	2.33	102.59	114.42	16	2
4	A	377	PX4	C11-C10-C9	2.33	105.15	113.62	12	1
4	A	405	PX4	C29-C28-C27	2.33	102.59	114.42	2	2
4	A	406	PX4	C30-C29-C28	2.33	102.59	114.42	14	1
4	A	388	PX4	C14-C13-C12	2.33	102.59	114.42	10	1
4	A	421	PX4	C8-O5-C9	2.33	108.49	117.12	20	2
4	A	423	PX4	C4-N1-C2	2.33	119.46	109.92	12	3
4	A	316	PX4	C4-N1-C2	2.33	119.45	109.92	18	2
4	A	323	PX4	C28-C27-C26	2.33	102.60	114.42	19	1
4	A	328	PX4	C32-C31-C30	2.33	102.60	114.42	5	1
4	A	349	PX4	C14-C13-C12	2.33	102.60	114.42	6	1
4	A	354	PX4	C25-C24-C23	2.33	105.15	113.62	17	3
4	A	335	PX4	C8-O5-C9	2.33	108.50	117.12	3	2
4	A	336	PX4	C31-C30-C29	2.33	102.60	114.42	18	2
4	A	399	PX4	O7-C23-O8	2.33	118.07	123.70	18	3
4	A	394	PX4	O1-P1-O4	2.33	118.57	107.75	10	1
4	A	416	PX4	C29-C28-C27	2.33	102.59	114.42	13	1
4	A	371	PX4	C13-C12-C11	2.33	102.61	114.42	20	1
4	A	379	PX4	C18-C17-C16	2.33	102.62	114.42	16	2
4	A	398	PX4	C17-C16-C15	2.33	102.61	114.42	1	1
4	A	415	PX4	C32-C31-C30	2.33	102.61	114.42	5	1
4	A	313	PX4	O6-C9-C10	2.32	114.67	123.73	19	1
4	A	326	PX4	C27-C26-C25	2.32	102.63	114.42	20	2
4	A	326	PX4	C30-C29-C28	2.32	102.63	114.42	15	1
4	A	333	PX4	C28-C27-C26	2.32	102.63	114.42	16	2
4	A	354	PX4	O6-C9-C10	2.32	114.66	123.73	2	1
4	A	368	PX4	O8-C23-C24	2.32	114.66	123.73	7	2
4	A	384	PX4	C13-C12-C11	2.32	102.63	114.42	5	1
4	A	411	PX4	C30-C29-C28	2.32	102.63	114.42	20	2
4	A	417	PX4	C8-O5-C9	2.32	108.52	117.12	1	2
4	A	312	PX4	C8-O5-C9	2.32	108.53	117.12	6	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	391	PX4	C3-N1-C2	2.32	119.42	109.92	10	1
4	A	427	PX4	O1-P1-O3	2.32	96.96	107.75	6	3
4	A	357	PX4	C25-C24-C23	2.32	105.18	113.62	18	2
4	A	364	PX4	C26-C25-C24	2.32	104.85	113.19	2	5
4	A	400	PX4	O4-P1-O2	2.32	118.13	109.07	6	1
4	A	417	PX4	C13-C12-C11	2.32	102.64	114.42	3	1
4	A	418	PX4	C26-C25-C24	2.32	104.85	113.19	13	1
4	A	429	PX4	C20-C19-C18	2.32	102.65	114.42	6	2
4	A	429	PX4	C32-C31-C30	2.32	102.64	114.42	7	3
4	A	334	PX4	C14-C13-C12	2.32	102.66	114.42	11	1
4	A	338	PX4	O1-P1-O4	2.32	118.51	107.75	2	1
4	A	400	PX4	C4-N1-C2	2.32	119.41	109.92	12	1
4	A	393	PX4	C26-C25-C24	2.32	104.85	113.19	11	4
4	A	428	PX4	C5-N1-C2	2.32	119.41	109.92	2	2
4	A	389	PX4	C5-N1-C2	2.32	119.40	109.92	5	3
4	A	421	PX4	O3-C1-C2	2.32	121.35	109.16	12	2
4	A	332	PX4	C28-C27-C26	2.32	102.67	114.42	20	3
4	A	355	PX4	C18-C17-C16	2.32	102.67	114.42	20	1
4	A	366	PX4	C8-O5-C9	2.32	108.54	117.12	11	1
4	A	396	PX4	C31-C30-C29	2.32	102.66	114.42	8	1
4	A	416	PX4	C13-C12-C11	2.32	102.67	114.42	6	1
4	A	368	PX4	O3-C1-C2	2.32	121.34	109.16	17	1
4	A	402	PX4	C16-C15-C14	2.31	102.67	114.42	4	1
4	A	385	PX4	C11-C10-C9	2.31	105.20	113.62	1	5
4	A	427	PX4	C16-C15-C14	2.32	102.67	114.42	8	3
4	A	308	PX4	C34-C33-C32	2.31	102.68	114.42	12	2
4	A	329	PX4	C15-C14-C13	2.31	102.68	114.42	10	1
4	A	346	PX4	C15-C14-C13	2.31	102.68	114.42	18	3
4	A	349	PX4	O8-C23-C24	2.31	114.70	123.73	5	1
4	A	371	PX4	C14-C13-C12	2.31	102.68	114.42	19	1
4	A	376	PX4	O6-C9-C10	2.31	114.70	123.73	18	1
4	A	409	PX4	C30-C29-C28	2.31	102.68	114.42	12	1
4	A	328	PX4	C20-C19-C18	2.31	102.69	114.42	9	1
4	A	359	PX4	C12-C11-C10	2.31	104.88	113.19	11	2
4	A	427	PX4	C5-N1-C2	2.31	119.38	109.92	2	3
4	A	418	PX4	C29-C28-C27	2.31	102.69	114.42	5	3
4	A	384	PX4	O6-C9-C10	2.31	114.72	123.73	15	2
4	A	421	PX4	C27-C26-C25	2.31	102.70	114.42	14	5
4	A	430	PX4	O6-C9-C10	2.31	114.72	123.73	12	1
4	A	372	PX4	C15-C14-C13	2.31	102.71	114.42	18	1
4	A	330	PX4	C8-O5-C9	2.31	108.58	117.12	14	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	349	PX4	C27-C26-C25	2.31	102.71	114.42	12	2
4	A	377	PX4	O1-P1-O4	2.31	118.46	107.75	11	2
4	A	379	PX4	O3-C1-C2	2.31	121.30	109.16	11	2
4	A	364	PX4	O4-P1-O2	2.31	118.08	109.07	1	1
4	A	378	PX4	C13-C12-C11	2.31	102.72	114.42	19	3
4	A	414	PX4	C31-C30-C29	2.31	102.71	114.42	4	3
4	A	321	PX4	O8-C23-C24	2.30	114.74	123.73	18	1
4	A	385	PX4	C31-C30-C29	2.30	102.73	114.42	15	1
4	A	387	PX4	O1-P1-O4	2.30	118.45	107.75	18	2
4	A	414	PX4	C4-N1-C2	2.31	119.35	109.92	16	1
4	A	333	PX4	C11-C10-C9	2.30	105.24	113.62	16	1
4	A	336	PX4	C11-C10-C9	2.30	105.24	113.62	17	1
4	A	421	PX4	C18-C17-C16	2.30	102.73	114.42	16	2
4	A	430	PX4	O4-P1-O2	2.30	118.07	109.07	6	3
4	A	374	PX4	C5-N1-C2	2.30	100.49	109.92	2	2
4	A	415	PX4	C4-N1-C2	2.30	100.49	109.92	20	1
4	A	331	PX4	C31-C30-C29	2.30	102.74	114.42	14	2
4	A	420	PX4	C5-N1-C2	2.30	100.50	109.92	16	1
4	A	374	PX4	C8-O5-C9	2.30	108.60	117.12	1	1
4	A	379	PX4	C25-C24-C23	2.30	105.25	113.62	18	5
4	A	324	PX4	C3-N1-C2	2.30	100.51	109.92	4	2
4	A	338	PX4	C14-C13-C12	2.30	102.75	114.42	4	4
4	A	422	PX4	C32-C31-C30	2.30	102.75	114.42	8	1
4	A	312	PX4	O1-P1-O3	2.30	97.07	107.75	7	1
4	A	349	PX4	O1-P1-O4	2.30	118.42	107.75	3	2
4	A	356	PX4	C4-N1-C2	2.30	119.32	109.92	3	2
4	A	400	PX4	O6-C9-C10	2.30	114.77	123.73	9	2
4	A	371	PX4	C18-C17-C16	2.30	102.76	114.42	9	1
4	A	376	PX4	C5-N1-C2	2.30	119.32	109.92	9	1
4	A	429	PX4	C11-C10-C9	2.30	105.26	113.62	10	1
4	A	314	PX4	O3-C1-C2	2.30	121.24	109.16	19	1
4	A	377	PX4	C34-C33-C32	2.30	102.76	114.42	10	2
4	A	381	PX4	C16-C15-C14	2.30	102.76	114.42	19	2
4	A	335	PX4	C16-C15-C14	2.30	102.77	114.42	3	1
4	A	349	PX4	C13-C12-C11	2.30	102.77	114.42	12	2
4	A	365	PX4	C3-N1-C2	2.30	119.31	109.92	15	2
4	A	385	PX4	C17-C16-C15	2.30	102.77	114.42	5	1
4	A	368	PX4	C25-C24-C23	2.29	105.28	113.62	3	1
4	A	382	PX4	C31-C30-C29	2.29	102.78	114.42	1	2
4	A	386	PX4	C29-C28-C27	2.30	102.77	114.42	12	1
4	A	307	PX4	O3-C1-C2	2.29	121.22	109.16	6	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	318	PX4	O6-C9-C10	2.29	114.79	123.73	13	1
4	A	325	PX4	C28-C27-C26	2.29	102.78	114.42	15	3
4	A	337	PX4	O3-C1-C2	2.29	121.22	109.16	2	2
4	A	368	PX4	C28-C27-C26	2.29	102.78	114.42	18	4
4	A	371	PX4	C34-C33-C32	2.29	102.78	114.42	3	1
4	A	397	PX4	C31-C30-C29	2.29	102.78	114.42	6	1
4	A	323	PX4	C8-O5-C9	2.29	125.60	117.12	15	1
4	A	328	PX4	C5-N1-C2	2.29	100.54	109.92	2	1
4	A	332	PX4	C32-C31-C30	2.29	102.79	114.42	19	3
4	A	343	PX4	C18-C17-C16	2.29	126.06	114.42	8	1
4	A	401	PX4	C32-C31-C30	2.29	102.79	114.42	10	2
4	A	404	PX4	C19-C18-C17	2.29	102.79	114.42	1	2
4	A	397	PX4	O6-C9-C10	2.29	114.79	123.73	9	1
4	A	349	PX4	C11-C10-C9	2.29	105.29	113.62	2	1
4	A	398	PX4	C13-C12-C11	2.29	102.79	114.42	16	2
4	A	423	PX4	C25-C24-C23	2.29	105.28	113.62	18	1
4	A	342	PX4	C33-C32-C31	2.29	102.80	114.42	3	2
4	A	344	PX4	C13-C12-C11	2.29	102.80	114.42	16	1
4	A	345	PX4	O6-C9-C10	2.29	114.80	123.73	17	1
4	A	346	PX4	C4-N1-C3	2.29	114.86	108.97	8	2
4	A	361	PX4	C30-C29-C28	2.29	102.80	114.42	11	3
4	A	389	PX4	C27-C26-C25	2.29	102.80	114.42	2	2
4	A	424	PX4	C27-C26-C25	2.29	102.80	114.42	6	1
4	A	429	PX4	C5-N1-C2	2.29	119.29	109.92	16	2
4	A	315	PX4	C26-C25-C24	2.29	121.42	113.19	9	4
4	A	321	PX4	C19-C18-C17	2.29	102.81	114.42	9	2
4	A	334	PX4	C19-C18-C17	2.29	102.81	114.42	1	1
4	A	317	PX4	C33-C32-C31	2.29	102.81	114.42	13	3
4	A	323	PX4	C4-N1-C2	2.29	100.56	109.92	15	3
4	A	349	PX4	C34-C33-C32	2.29	102.81	114.42	8	2
4	A	379	PX4	C31-C30-C29	2.29	102.81	114.42	18	2
4	A	400	PX4	C13-C12-C11	2.29	102.82	114.42	18	1
4	A	316	PX4	C32-C31-C30	2.28	102.83	114.42	9	1
4	A	349	PX4	C15-C14-C13	2.29	102.82	114.42	8	3
4	A	373	PX4	C20-C19-C18	2.29	102.82	114.42	8	2
4	A	403	PX4	C13-C12-C11	2.29	102.82	114.42	15	1
4	A	337	PX4	C28-C27-C26	2.28	102.83	114.42	6	1
4	A	386	PX4	C28-C27-C26	2.28	102.83	114.42	15	1
4	A	357	PX4	C15-C14-C13	2.28	102.84	114.42	18	1
4	A	367	PX4	C17-C16-C15	2.28	102.84	114.42	13	2
4	A	386	PX4	C34-C33-C32	2.28	102.83	114.42	17	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	423	PX4	C13-C12-C11	2.28	102.83	114.42	10	1
4	A	350	PX4	C18-C17-C16	2.28	102.84	114.42	12	3
4	A	356	PX4	C13-C12-C11	2.28	102.85	114.42	10	1
4	A	384	PX4	O4-P1-O2	2.28	100.15	109.07	5	2
4	A	375	PX4	C14-C13-C12	2.28	102.85	114.42	19	2
4	A	426	PX4	C26-C25-C24	2.28	104.99	113.19	10	3
4	A	340	PX4	C12-C11-C10	2.28	105.00	113.19	2	2
4	A	345	PX4	O1-P1-O3	2.28	97.16	107.75	6	1
4	A	405	PX4	O3-C1-C2	2.28	121.15	109.16	11	2
4	A	400	PX4	O1-P1-O3	2.28	97.17	107.75	14	3
4	A	370	PX4	C20-C19-C18	2.28	102.86	114.42	15	1
4	A	401	PX4	C33-C32-C31	2.28	102.86	114.42	1	3
4	A	378	PX4	C20-C19-C18	2.28	102.87	114.42	7	1
4	A	406	PX4	C32-C31-C30	2.28	102.87	114.42	4	2
4	A	381	PX4	C1-C2-N1	2.28	123.38	115.78	7	2
4	A	421	PX4	C13-C12-C11	2.28	102.86	114.42	14	2
4	A	431	PX4	C19-C18-C17	2.28	102.86	114.42	2	3
4	A	412	PX4	C20-C19-C18	2.28	102.87	114.42	20	2
4	A	334	PX4	C25-C24-C23	2.27	105.35	113.62	2	2
4	A	368	PX4	C33-C32-C31	2.27	102.88	114.42	4	1
4	A	372	PX4	C20-C19-C18	2.27	102.89	114.42	13	1
4	A	403	PX4	C21-C20-C19	2.27	94.19	115.30	6	1
4	A	318	PX4	C3-N1-C2	2.27	119.21	109.92	12	2
4	A	318	PX4	C20-C19-C18	2.27	102.89	114.42	15	1
4	A	309	PX4	C13-C12-C11	2.27	102.90	114.42	7	2
4	A	309	PX4	C30-C29-C28	2.27	102.89	114.42	19	1
4	A	321	PX4	C20-C19-C18	2.27	102.89	114.42	2	2
4	A	379	PX4	C5-N1-C2	2.27	119.21	109.92	13	2
4	A	385	PX4	C32-C31-C30	2.27	102.89	114.42	20	3
4	A	391	PX4	C20-C19-C18	2.27	102.89	114.42	10	1
4	A	395	PX4	C30-C29-C28	2.27	102.89	114.42	2	1
4	A	338	PX4	C13-C12-C11	2.27	102.89	114.42	11	3
4	A	420	PX4	C33-C32-C31	2.27	102.89	114.42	18	3
4	A	357	PX4	C11-C10-C9	2.27	105.36	113.62	7	2
4	A	399	PX4	C8-O5-C9	2.27	125.53	117.12	11	1
4	A	404	PX4	C31-C30-C29	2.27	102.90	114.42	10	1
4	A	318	PX4	C5-N1-C2	2.27	119.20	109.92	17	2
4	A	335	PX4	O3-C1-C2	2.27	121.09	109.16	8	3
4	A	354	PX4	O8-C23-C24	2.27	114.88	123.73	13	2
4	A	330	PX4	C5-N1-C2	2.27	119.19	109.92	17	2
4	A	339	PX4	C19-C18-C17	2.27	102.92	114.42	5	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	362	PX4	C13-C12-C11	2.27	102.91	114.42	6	1
4	A	373	PX4	C19-C18-C17	2.27	102.91	114.42	15	4
4	A	409	PX4	C11-C10-C9	2.27	105.37	113.62	17	2
4	A	392	PX4	O1-P1-O4	2.27	118.28	107.75	19	1
4	A	395	PX4	C32-C31-C30	2.27	102.91	114.42	1	1
4	A	374	PX4	C20-C19-C18	2.27	102.92	114.42	5	5
4	A	415	PX4	C11-C10-C9	2.27	121.87	113.62	7	1
4	A	349	PX4	O3-C1-C2	2.27	121.08	109.16	10	1
4	A	429	PX4	C31-C30-C29	2.27	102.92	114.42	19	2
4	A	403	PX4	O4-P1-O2	2.26	117.91	109.07	19	3
4	A	392	PX4	C11-C10-C9	2.26	105.38	113.62	15	2
4	A	423	PX4	O8-C23-C24	2.26	114.90	123.73	1	1
4	A	306	PX4	C3-N1-C2	2.26	119.18	109.92	18	2
4	A	358	PX4	C11-C10-C9	2.26	121.85	113.62	7	1
4	A	347	PX4	C27-C26-C25	2.26	102.94	114.42	19	3
4	A	364	PX4	C1-C2-N1	2.26	123.33	115.78	13	1
4	A	358	PX4	C13-C12-C11	2.26	102.94	114.42	14	1
4	A	375	PX4	C3-N1-C2	2.26	100.66	109.92	14	2
4	A	405	PX4	C1-C2-N1	2.26	123.33	115.78	19	2
4	A	385	PX4	C4-N1-C2	2.26	119.17	109.92	6	1
4	A	398	PX4	C4-N1-C2	2.26	119.17	109.92	12	1
4	A	316	PX4	C31-C30-C29	2.26	102.95	114.42	8	3
4	A	351	PX4	C17-C16-C15	2.26	102.95	114.42	2	2
4	A	353	PX4	C32-C31-C30	2.26	102.95	114.42	17	2
4	A	389	PX4	O6-C9-C10	2.26	114.91	123.73	7	1
4	A	352	PX4	C19-C18-C17	2.26	102.96	114.42	5	2
4	A	357	PX4	C28-C27-C26	2.26	102.95	114.42	19	4
4	A	389	PX4	O5-C9-O6	2.26	117.89	123.59	1	3
4	A	415	PX4	C15-C14-C13	2.26	102.96	114.42	6	3
4	A	334	PX4	C30-C29-C28	2.26	102.96	114.42	10	3
4	A	370	PX4	C15-C14-C13	2.26	102.96	114.42	19	2
4	A	411	PX4	C18-C17-C16	2.26	102.97	114.42	16	1
4	A	306	PX4	C20-C19-C18	2.25	102.98	114.42	18	2
4	A	316	PX4	C27-C26-C25	2.25	102.98	114.42	1	2
4	A	341	PX4	C32-C31-C30	2.25	102.98	114.42	8	1
4	A	343	PX4	C13-C12-C11	2.25	102.98	114.42	14	1
4	A	349	PX4	C28-C27-C26	2.25	102.98	114.42	1	1
4	A	404	PX4	C29-C28-C27	2.25	102.98	114.42	1	2
4	A	405	PX4	C32-C31-C30	2.25	102.98	114.42	12	2
4	A	406	PX4	C19-C18-C17	2.25	102.98	114.42	1	2
4	A	383	PX4	C8-O5-C9	2.25	108.77	117.12	6	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	419	PX4	C20-C19-C18	2.25	102.98	114.42	4	2
4	A	421	PX4	O8-C23-C24	2.26	114.93	123.73	13	1
4	A	411	PX4	C27-C26-C25	2.25	102.98	114.42	8	1
4	A	412	PX4	C26-C25-C24	2.25	121.29	113.19	15	2
4	A	417	PX4	C33-C32-C31	2.25	102.99	114.42	8	3
4	A	308	PX4	C3-N1-C2	2.25	119.13	109.92	19	1
4	A	316	PX4	C3-N1-C2	2.25	119.13	109.92	11	1
4	A	322	PX4	C32-C31-C30	2.25	103.00	114.42	10	1
4	A	367	PX4	O5-C9-C10	2.25	118.97	111.91	6	5
4	A	429	PX4	C34-C33-C32	2.25	103.00	114.42	2	1
4	A	319	PX4	C31-C30-C29	2.25	103.01	114.42	5	1
4	A	340	PX4	C29-C28-C27	2.25	103.01	114.42	3	2
4	A	343	PX4	C34-C33-C32	2.25	103.01	114.42	19	3
4	A	355	PX4	C19-C18-C17	2.25	103.00	114.42	19	3
4	A	400	PX4	C12-C11-C10	2.25	105.10	113.19	20	1
4	A	371	PX4	C29-C28-C27	2.25	103.00	114.42	19	1
4	A	403	PX4	C17-C16-C15	2.25	103.01	114.42	11	1
4	A	387	PX4	C34-C33-C32	2.25	103.01	114.42	2	1
4	A	419	PX4	C15-C14-C13	2.25	103.00	114.42	6	2
4	A	316	PX4	C26-C25-C24	2.25	105.11	113.19	10	2
4	A	355	PX4	O6-C9-C10	2.25	114.96	123.73	7	1
4	A	364	PX4	C17-C16-C15	2.25	103.01	114.42	14	2
4	A	420	PX4	C15-C14-C13	2.25	103.01	114.42	13	2
4	A	421	PX4	C19-C18-C17	2.25	103.00	114.42	20	2
4	A	412	PX4	O3-C1-C2	2.25	120.98	109.16	8	1
4	A	403	PX4	C31-C30-C29	2.25	103.02	114.42	14	2
4	A	416	PX4	C18-C17-C16	2.25	103.02	114.42	7	1
4	A	334	PX4	C4-N1-C2	2.25	119.10	109.92	19	1
4	A	313	PX4	C28-C27-C26	2.24	103.04	114.42	5	2
4	A	345	PX4	C20-C19-C18	2.24	103.03	114.42	14	5
4	A	383	PX4	C15-C14-C13	2.24	103.03	114.42	9	3
4	A	414	PX4	C16-C15-C14	2.24	103.03	114.42	16	1
4	A	427	PX4	C32-C31-C30	2.25	103.03	114.42	5	1
4	A	364	PX4	O8-C23-C24	2.24	114.98	123.73	17	1
4	A	321	PX4	C33-C32-C31	2.24	103.04	114.42	9	2
4	A	343	PX4	O6-C9-C10	2.24	132.48	123.73	4	3
4	A	345	PX4	C32-C31-C30	2.24	103.04	114.42	3	2
4	A	339	PX4	C13-C12-C11	2.24	103.05	114.42	6	3
4	A	351	PX4	C31-C30-C29	2.24	103.04	114.42	16	2
4	A	357	PX4	C17-C16-C15	2.24	103.04	114.42	17	1
4	A	401	PX4	C7-O7-C23	2.24	123.31	117.79	19	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	379	PX4	C34-C33-C32	2.24	103.04	114.42	1	2
4	A	409	PX4	C33-C32-C31	2.24	103.04	114.42	16	1
4	A	392	PX4	C4-N1-C2	2.24	119.09	109.92	13	1
4	A	424	PX4	C25-C24-C23	2.24	105.46	113.62	2	1
4	A	332	PX4	O8-C23-C24	2.24	114.99	123.73	14	1
4	A	337	PX4	C8-O5-C9	2.24	108.82	117.12	3	1
4	A	369	PX4	O6-C9-C10	2.24	114.99	123.73	7	1
4	A	372	PX4	C8-O5-C9	2.24	108.82	117.12	3	1
4	A	419	PX4	O4-P1-O2	2.24	117.83	109.07	11	1
4	A	399	PX4	C20-C19-C18	2.24	103.05	114.42	6	2
4	A	425	PX4	O3-C1-C2	2.24	120.95	109.16	17	1
4	A	340	PX4	C11-C10-C9	2.24	105.48	113.62	18	1
4	A	342	PX4	C18-C17-C16	2.24	103.06	114.42	4	2
4	A	355	PX4	C15-C14-C13	2.24	103.06	114.42	7	1
4	A	380	PX4	C28-C27-C26	2.24	103.06	114.42	9	1
4	A	410	PX4	C19-C18-C17	2.24	103.06	114.42	16	1
4	A	396	PX4	C12-C11-C10	2.24	105.14	113.19	11	2
4	A	317	PX4	C32-C31-C30	2.24	103.07	114.42	12	1
4	A	308	PX4	O6-C9-C10	2.24	115.00	123.73	1	1
4	A	308	PX4	C19-C18-C17	2.24	103.07	114.42	15	1
4	A	365	PX4	C34-C33-C32	2.24	103.06	114.42	15	1
4	A	418	PX4	C28-C27-C26	2.24	103.06	114.42	19	2
4	A	330	PX4	C13-C12-C11	2.24	103.08	114.42	7	1
4	A	333	PX4	C25-C24-C23	2.24	105.49	113.62	1	3
4	A	367	PX4	C5-N1-C3	2.24	103.23	108.97	8	1
4	A	410	PX4	C28-C27-C26	2.24	103.07	114.42	4	1
4	A	315	PX4	C34-C33-C32	2.23	103.08	114.42	11	1
4	A	389	PX4	C29-C28-C27	2.23	103.08	114.42	20	2
4	A	319	PX4	C25-C24-C23	2.23	105.50	113.62	2	2
4	A	326	PX4	C33-C32-C31	2.23	103.09	114.42	2	1
4	A	379	PX4	C30-C29-C28	2.23	103.09	114.42	9	2
4	A	328	PX4	C16-C15-C14	2.23	103.10	114.42	8	4
4	A	430	PX4	C16-C15-C14	2.23	103.10	114.42	6	1
4	A	431	PX4	C13-C12-C11	2.23	103.09	114.42	13	1
4	A	326	PX4	C26-C25-C24	2.23	105.17	113.19	3	2
4	A	378	PX4	C17-C16-C15	2.23	103.10	114.42	19	1
4	A	319	PX4	C19-C18-C17	2.23	103.11	114.42	14	1
4	A	352	PX4	C16-C15-C14	2.23	103.11	114.42	14	1
4	A	403	PX4	O8-C23-C24	2.23	115.04	123.73	13	2
4	A	405	PX4	C33-C32-C31	2.23	103.11	114.42	19	1
4	A	383	PX4	C19-C18-C17	2.23	103.11	114.42	14	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	411	PX4	O3-P1-O2	2.23	100.36	109.07	20	2
4	A	393	PX4	C20-C19-C18	2.23	103.11	114.42	12	1
4	A	394	PX4	C4-N1-C2	2.23	119.03	109.92	12	1
4	A	413	PX4	C29-C28-C27	2.23	103.11	114.42	11	1
4	A	424	PX4	C4-N1-C2	2.23	100.80	109.92	9	1
4	A	350	PX4	O6-C9-C10	2.23	115.04	123.73	20	2
4	A	371	PX4	C27-C26-C25	2.23	103.12	114.42	17	1
4	A	378	PX4	C34-C33-C32	2.23	103.13	114.42	2	2
4	A	408	PX4	C18-C17-C16	2.23	103.12	114.42	13	1
4	A	385	PX4	C14-C13-C12	2.23	103.12	114.42	4	2
4	A	418	PX4	O4-P1-O2	2.23	117.77	109.07	17	1
4	A	321	PX4	C11-C10-C9	2.23	105.53	113.62	5	2
4	A	365	PX4	C20-C19-C18	2.23	103.12	114.42	20	1
4	A	340	PX4	C17-C16-C15	2.22	103.14	114.42	18	1
4	A	344	PX4	C27-C26-C25	2.22	103.14	114.42	17	2
4	A	352	PX4	O5-C9-C10	2.22	118.89	111.91	12	2
4	A	401	PX4	C18-C17-C16	2.22	103.14	114.42	9	4
4	A	401	PX4	C20-C19-C18	2.22	103.14	114.42	19	3
4	A	382	PX4	C29-C28-C27	2.22	103.14	114.42	20	4
4	A	385	PX4	C5-N1-C2	2.22	119.02	109.92	10	1
4	A	394	PX4	C12-C11-C10	2.22	105.20	113.19	5	2
4	A	391	PX4	C31-C30-C29	2.22	103.14	114.42	18	1
4	A	395	PX4	C29-C28-C27	2.22	103.14	114.42	6	1
4	A	418	PX4	C15-C14-C13	2.22	103.13	114.42	15	1
4	A	419	PX4	C30-C29-C28	2.22	103.14	114.42	15	2
4	A	427	PX4	C13-C12-C11	2.22	103.14	114.42	14	1
4	A	430	PX4	C5-N1-C2	2.22	119.01	109.92	5	2
4	A	329	PX4	C17-C16-C15	2.22	103.15	114.42	13	1
4	A	353	PX4	C3-N1-C2	2.22	100.83	109.92	1	1
4	A	333	PX4	O5-C9-O6	2.22	117.99	123.59	1	2
4	A	417	PX4	C20-C19-C18	2.22	103.15	114.42	11	2
4	A	322	PX4	C15-C14-C13	2.22	103.16	114.42	15	2
4	A	427	PX4	C26-C25-C24	2.22	121.17	113.19	10	2
4	A	328	PX4	O1-P1-O3	2.22	97.44	107.75	17	2
4	A	311	PX4	C25-C24-C23	2.22	105.56	113.62	14	1
4	A	354	PX4	O1-P1-O4	2.22	118.05	107.75	15	1
4	A	373	PX4	C5-N1-C2	2.22	118.99	109.92	2	1
4	A	335	PX4	C27-C26-C25	2.22	103.18	114.42	11	3
4	A	349	PX4	C26-C25-C24	2.22	105.22	113.19	3	2
4	A	364	PX4	C31-C30-C29	2.22	103.17	114.42	5	3
4	A	419	PX4	C3-N1-C2	2.22	100.84	109.92	10	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	305	PX4	O1-P1-O3	2.21	118.03	107.75	10	1
4	A	332	PX4	C20-C19-C18	2.21	103.18	114.42	16	2
4	A	368	PX4	C29-C28-C27	2.21	103.19	114.42	12	1
4	A	369	PX4	C30-C29-C28	2.21	103.18	114.42	1	1
4	A	406	PX4	C5-N1-C3	2.21	114.67	108.97	4	1
4	A	397	PX4	C30-C29-C28	2.22	103.18	114.42	5	1
4	A	332	PX4	C33-C32-C31	2.21	103.19	114.42	12	1
4	A	409	PX4	C8-O5-C9	2.21	108.92	117.12	11	2
4	A	310	PX4	O8-C23-C24	2.21	115.10	123.73	10	1
4	A	355	PX4	C8-O5-C9	2.21	108.93	117.12	10	2
4	A	374	PX4	C27-C26-C25	2.21	103.20	114.42	12	1
4	A	387	PX4	C29-C28-C27	2.21	103.20	114.42	11	1
4	A	425	PX4	C33-C32-C31	2.21	103.20	114.42	16	1
4	A	406	PX4	C8-O5-C9	2.21	108.94	117.12	18	2
4	A	338	PX4	C27-C26-C25	2.21	103.21	114.42	9	1
4	A	345	PX4	C27-C26-C25	2.21	103.22	114.42	7	1
4	A	361	PX4	C29-C28-C27	2.21	103.21	114.42	2	1
4	A	362	PX4	C12-C11-C10	2.21	105.25	113.19	18	1
4	A	378	PX4	O3-C1-C2	2.21	120.78	109.16	7	1
4	A	395	PX4	C31-C30-C29	2.21	103.20	114.42	1	2
4	A	421	PX4	C20-C19-C18	2.21	103.20	114.42	10	1
4	A	308	PX4	C26-C25-C24	2.21	105.25	113.19	18	3
4	A	346	PX4	C29-C28-C27	2.21	103.22	114.42	18	2
4	A	347	PX4	C32-C31-C30	2.21	103.22	114.42	20	2
4	A	384	PX4	C33-C32-C31	2.21	103.21	114.42	3	1
4	A	386	PX4	C5-N1-C2	2.21	118.95	109.92	16	1
4	A	401	PX4	C16-C15-C14	2.21	103.22	114.42	20	1
4	A	372	PX4	O1-P1-O4	2.21	118.00	107.75	7	3
4	A	427	PX4	C15-C14-C13	2.21	103.21	114.42	9	2
4	A	360	PX4	C33-C32-C31	2.21	103.22	114.42	10	2
4	A	333	PX4	C12-C11-C10	2.21	105.26	113.19	10	1
4	A	364	PX4	C25-C24-C23	2.21	105.59	113.62	8	2
4	A	428	PX4	C29-C28-C27	2.21	103.22	114.42	17	4
4	A	372	PX4	C28-C27-C26	2.21	103.22	114.42	14	1
4	A	380	PX4	O1-P1-O3	2.21	97.50	107.75	1	1
4	A	410	PX4	C30-C29-C28	2.21	103.22	114.42	16	1
4	A	307	PX4	C29-C28-C27	2.20	103.23	114.42	14	2
4	A	341	PX4	C31-C30-C29	2.20	103.23	114.42	5	3
4	A	363	PX4	C33-C32-C31	2.20	103.23	114.42	1	2
4	A	354	PX4	C26-C25-C24	2.20	121.11	113.19	19	1
4	A	360	PX4	C32-C31-C30	2.20	103.23	114.42	10	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	413	PX4	C18-C17-C16	2.21	103.23	114.42	8	3
4	A	402	PX4	C5-N1-C2	2.20	100.90	109.92	7	2
4	A	375	PX4	C8-O5-C9	2.20	108.96	117.12	3	1
4	A	378	PX4	C29-C28-C27	2.20	103.24	114.42	6	2
4	A	425	PX4	C8-O5-C9	2.20	108.96	117.12	19	2
4	A	321	PX4	C25-C24-C23	2.20	105.61	113.62	16	2
4	A	355	PX4	C12-C11-C10	2.20	105.27	113.19	12	1
4	A	430	PX4	C13-C12-C11	2.20	103.25	114.42	5	2
4	A	346	PX4	C8-O5-C9	2.20	108.97	117.12	3	1
4	A	351	PX4	C4-N1-C2	2.20	100.91	109.92	16	1
4	A	315	PX4	C15-C14-C13	2.20	103.26	114.42	11	1
4	A	320	PX4	C27-C26-C25	2.20	103.26	114.42	14	1
4	A	323	PX4	C5-N1-C2	2.20	118.91	109.92	18	1
4	A	324	PX4	C27-C26-C25	2.20	103.26	114.42	14	1
4	A	328	PX4	O4-P1-O2	2.20	117.66	109.07	2	3
4	A	352	PX4	O1-P1-O4	2.20	117.96	107.75	12	1
4	A	358	PX4	C30-C29-C28	2.20	103.26	114.42	19	1
4	A	372	PX4	C11-C10-C9	2.20	105.62	113.62	6	2
4	A	416	PX4	C8-O5-C9	2.20	108.97	117.12	9	2
4	A	426	PX4	C30-C29-C28	2.20	103.26	114.42	18	1
4	A	429	PX4	C4-N1-C2	2.20	100.91	109.92	9	4
4	A	356	PX4	C27-C26-C25	2.20	103.27	114.42	13	1
4	A	410	PX4	O3-C1-C2	2.20	120.72	109.16	16	2
4	A	413	PX4	C15-C14-C13	2.20	103.26	114.42	6	1
4	A	395	PX4	C25-C24-C23	2.20	121.62	113.62	8	2
4	A	335	PX4	C13-C12-C11	2.20	103.28	114.42	18	1
4	A	342	PX4	O3-C1-C2	2.20	120.71	109.16	12	3
4	A	359	PX4	C27-C26-C25	2.20	103.27	114.42	5	1
4	A	412	PX4	C11-C10-C9	2.20	105.63	113.62	8	1
4	A	362	PX4	C32-C31-C30	2.20	103.28	114.42	8	1
4	A	426	PX4	C29-C28-C27	2.20	103.27	114.42	16	1
4	A	369	PX4	O3-C1-C2	2.19	120.70	109.16	12	2
4	A	370	PX4	C26-C25-C24	2.19	105.30	113.19	13	1
4	A	381	PX4	C11-C10-C9	2.19	105.64	113.62	18	2
4	A	364	PX4	C13-C12-C11	2.19	103.29	114.42	20	1
4	A	367	PX4	C11-C10-C9	2.19	105.64	113.62	15	3
4	A	412	PX4	C33-C32-C31	2.19	103.28	114.42	7	2
4	A	309	PX4	C17-C16-C15	2.19	103.30	114.42	13	1
4	A	318	PX4	C28-C27-C26	2.19	103.30	114.42	2	1
4	A	319	PX4	C27-C26-C25	2.19	103.30	114.42	6	1
4	A	403	PX4	C16-C15-C14	2.19	103.29	114.42	17	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	386	PX4	C13-C12-C11	2.19	103.29	114.42	19	2
4	A	392	PX4	O6-C9-C10	2.19	115.18	123.73	10	1
4	A	325	PX4	C29-C28-C27	2.19	103.30	114.42	8	1
4	A	353	PX4	C18-C17-C16	2.19	103.31	114.42	5	1
4	A	364	PX4	C15-C14-C13	2.19	103.30	114.42	2	2
4	A	350	PX4	C20-C19-C18	2.19	103.31	114.42	6	1
4	A	367	PX4	O8-C23-C24	2.19	115.19	123.73	17	2
4	A	368	PX4	O1-P1-O4	2.19	117.92	107.75	11	3
4	A	380	PX4	C17-C16-C15	2.19	103.31	114.42	11	2
4	A	415	PX4	O3-C1-C2	2.19	120.67	109.16	16	1
4	A	350	PX4	C16-C15-C14	2.19	103.32	114.42	6	1
4	A	354	PX4	C28-C27-C26	2.19	103.32	114.42	18	2
4	A	357	PX4	C33-C32-C31	2.19	103.32	114.42	1	2
4	A	405	PX4	C30-C29-C28	2.19	103.32	114.42	1	3
4	A	372	PX4	C14-C13-C12	2.19	103.33	114.42	9	1
4	A	313	PX4	C17-C16-C15	2.18	103.34	114.42	20	1
4	A	329	PX4	C14-C13-C12	2.18	103.33	114.42	14	2
4	A	356	PX4	O1-P1-O3	2.19	97.60	107.75	6	1
4	A	356	PX4	C30-C29-C28	2.19	103.33	114.42	11	2
4	A	373	PX4	C4-N1-C2	2.19	118.86	109.92	12	1
4	A	387	PX4	C17-C16-C15	2.19	103.33	114.42	5	2
4	A	424	PX4	C28-C27-C26	2.19	103.33	114.42	11	2
4	A	315	PX4	O1-P1-O4	2.18	117.88	107.75	11	1
4	A	319	PX4	C20-C19-C18	2.18	103.34	114.42	10	1
4	A	351	PX4	C33-C32-C31	2.18	103.34	114.42	8	1
4	A	355	PX4	O3-C1-C2	2.18	120.64	109.16	10	3
4	A	357	PX4	C30-C29-C28	2.18	103.34	114.42	17	2
4	A	378	PX4	C27-C26-C25	2.18	103.34	114.42	13	1
4	A	366	PX4	C30-C29-C28	2.18	103.35	114.42	1	2
4	A	366	PX4	C3-N1-C2	2.18	100.99	109.92	13	1
4	A	311	PX4	C34-C33-C32	2.18	103.36	114.42	13	3
4	A	305	PX4	C14-C13-C12	2.18	103.37	114.42	2	2
4	A	308	PX4	C28-C27-C26	2.18	103.36	114.42	10	1
4	A	333	PX4	C13-C12-C11	2.18	103.36	114.42	1	2
4	A	358	PX4	O6-C9-C10	2.18	115.23	123.73	18	2
4	A	404	PX4	O4-P1-O2	2.18	100.55	109.07	3	1
4	A	330	PX4	O3-C1-C2	2.18	120.61	109.16	7	3
4	A	351	PX4	C28-C27-C26	2.18	103.37	114.42	17	2
4	A	355	PX4	C29-C28-C27	2.18	103.37	114.42	6	1
4	A	362	PX4	C5-N1-C2	2.18	101.00	109.92	4	3
4	A	408	PX4	C4-N1-C2	2.18	118.82	109.92	5	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	387	PX4	C27-C26-C25	2.18	103.37	114.42	9	1
4	A	420	PX4	O6-C9-C10	2.18	132.23	123.73	3	1
4	A	307	PX4	C33-C32-C31	2.18	103.38	114.42	19	1
4	A	337	PX4	C15-C14-C13	2.18	103.38	114.42	2	1
4	A	351	PX4	C34-C33-C32	2.18	103.38	114.42	3	1
4	A	396	PX4	C11-C10-C9	2.18	105.70	113.62	9	4
4	A	351	PX4	C30-C29-C28	2.17	103.39	114.42	17	1
4	A	369	PX4	C4-N1-C2	2.17	101.03	109.92	15	1
4	A	378	PX4	C11-C10-C9	2.17	105.72	113.62	17	1
4	A	383	PX4	C18-C17-C16	2.17	103.39	114.42	12	1
4	A	387	PX4	O8-C23-C24	2.17	115.25	123.73	13	2
4	A	388	PX4	C28-C27-C26	2.17	103.39	114.42	18	2
4	A	394	PX4	C19-C18-C17	2.17	103.39	114.42	7	1
4	A	306	PX4	C31-C30-C29	2.17	103.40	114.42	6	1
4	A	347	PX4	C16-C15-C14	2.17	103.40	114.42	8	2
4	A	357	PX4	O1-P1-O4	2.17	117.84	107.75	13	1
4	A	406	PX4	O8-C23-C24	2.17	115.26	123.73	6	1
4	A	384	PX4	C16-C15-C14	2.17	103.40	114.42	5	1
4	A	430	PX4	O8-C23-C24	2.17	115.25	123.73	6	2
4	A	310	PX4	C31-C30-C29	2.17	103.40	114.42	18	1
4	A	332	PX4	C15-C14-C13	2.17	103.41	114.42	15	1
4	A	373	PX4	C11-C10-C9	2.17	105.73	113.62	4	2
4	A	375	PX4	C11-C10-C9	2.17	105.73	113.62	6	2
4	A	416	PX4	O3-C1-C2	2.17	120.58	109.16	14	3
4	A	321	PX4	C15-C14-C13	2.17	103.41	114.42	15	1
4	A	309	PX4	O6-C9-C10	2.17	115.28	123.73	16	1
4	A	308	PX4	C8-O5-C9	2.17	125.15	117.12	15	1
4	A	381	PX4	C29-C28-C27	2.17	103.42	114.42	15	1
4	A	407	PX4	C19-C18-C17	2.17	103.42	114.42	4	2
4	A	408	PX4	C13-C12-C11	2.17	103.42	114.42	8	1
4	A	390	PX4	O3-P1-O2	2.17	100.60	109.07	17	2
4	A	390	PX4	C14-C13-C12	2.17	103.42	114.42	16	1
4	A	354	PX4	C19-C18-C17	2.17	103.42	114.42	1	1
4	A	392	PX4	C16-C15-C14	2.17	103.43	114.42	14	1
4	A	395	PX4	C4-N1-C2	2.17	101.05	109.92	13	1
4	A	327	PX4	C28-C27-C26	2.17	103.43	114.42	1	1
4	A	379	PX4	C4-N1-C2	2.17	118.78	109.92	9	1
4	A	412	PX4	O8-C23-C24	2.17	115.28	123.73	20	1
4	A	313	PX4	C8-O5-C9	2.16	109.11	117.12	3	1
4	A	427	PX4	C19-C18-C17	2.16	103.44	114.42	1	2
4	A	336	PX4	C15-C14-C13	2.16	103.44	114.42	3	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	354	PX4	C27-C26-C25	2.16	103.44	114.42	3	1
4	A	373	PX4	O3-C1-C2	2.16	120.52	109.16	3	1
4	A	404	PX4	C14-C13-C12	2.16	103.45	114.42	14	1
4	A	380	PX4	C20-C19-C18	2.16	103.45	114.42	9	1
4	A	384	PX4	C17-C16-C15	2.16	103.45	114.42	9	1
4	A	388	PX4	O1-P1-O4	2.16	117.79	107.75	16	3
4	A	424	PX4	O1-P1-O3	2.16	97.70	107.75	12	1
4	A	431	PX4	O8-C23-C24	2.16	115.29	123.73	16	1
4	A	309	PX4	O1-P1-O4	2.16	117.78	107.75	17	1
4	A	350	PX4	C32-C31-C30	2.16	103.46	114.42	8	1
4	A	352	PX4	C31-C30-C29	2.16	103.45	114.42	12	2
4	A	362	PX4	C15-C14-C13	2.16	103.45	114.42	1	2
4	A	367	PX4	O3-C1-C2	2.16	120.53	109.16	13	1
4	A	389	PX4	C32-C31-C30	2.16	103.45	114.42	17	1
4	A	327	PX4	C34-C33-C32	2.16	103.46	114.42	2	1
4	A	382	PX4	C33-C32-C31	2.16	103.46	114.42	13	1
4	A	384	PX4	C5-N1-C3	2.16	103.42	108.97	9	2
4	A	390	PX4	C25-C24-C23	2.16	105.77	113.62	19	1
4	A	429	PX4	C28-C27-C26	2.16	103.46	114.42	5	1
4	A	325	PX4	C19-C18-C17	2.16	103.47	114.42	18	2
4	A	331	PX4	C34-C33-C32	2.16	103.47	114.42	1	1
4	A	353	PX4	C8-O5-C9	2.16	125.12	117.12	4	1
4	A	362	PX4	C11-C10-C9	2.16	105.77	113.62	20	1
4	A	398	PX4	C3-N1-C2	2.16	118.75	109.92	15	1
4	A	416	PX4	C33-C32-C31	2.16	103.47	114.42	14	1
4	A	307	PX4	C28-C27-C26	2.16	103.48	114.42	18	2
4	A	310	PX4	C29-C28-C27	2.16	103.48	114.42	7	1
4	A	345	PX4	C31-C30-C29	2.16	103.48	114.42	7	1
4	A	367	PX4	C3-N1-C2	2.16	118.74	109.92	14	1
4	A	403	PX4	C33-C32-C31	2.16	103.48	114.42	2	1
4	A	376	PX4	C30-C29-C28	2.16	103.48	114.42	13	1
4	A	387	PX4	C33-C32-C31	2.16	103.48	114.42	2	1
4	A	335	PX4	C3-N1-C2	2.15	118.72	109.92	12	1
4	A	363	PX4	C29-C28-C27	2.15	103.50	114.42	13	1
4	A	399	PX4	C31-C30-C29	2.15	103.50	114.42	7	1
4	A	407	PX4	C8-O5-C9	2.15	109.15	117.12	3	1
4	A	313	PX4	C18-C17-C16	2.15	103.51	114.42	11	2
4	A	308	PX4	O1-P1-O4	2.15	97.76	107.75	17	1
4	A	342	PX4	O6-C9-C10	2.15	115.35	123.73	9	2
4	A	355	PX4	C4-N1-C2	2.15	118.71	109.92	14	2
4	A	410	PX4	C18-C17-C16	2.15	103.51	114.42	16	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	415	PX4	C3-N1-C2	2.15	101.12	109.92	9	1
4	A	357	PX4	O4-P1-O2	2.15	117.46	109.07	7	2
4	A	371	PX4	C4-N1-C2	2.15	101.13	109.92	17	4
4	A	386	PX4	C19-C18-C17	2.15	103.52	114.42	15	3
4	A	398	PX4	C8-O5-C9	2.15	109.17	117.12	13	1
4	A	428	PX4	C20-C19-C18	2.15	103.52	114.42	7	1
4	A	317	PX4	C25-C24-C23	2.15	105.81	113.62	4	3
4	A	344	PX4	C29-C28-C27	2.15	103.53	114.42	9	1
4	A	360	PX4	C31-C30-C29	2.15	103.53	114.42	10	1
4	A	305	PX4	C5-N1-C2	2.15	118.69	109.92	8	1
4	A	322	PX4	C12-C11-C10	2.14	105.48	113.19	19	3
4	A	326	PX4	C34-C33-C32	2.14	103.54	114.42	19	1
4	A	329	PX4	C28-C27-C26	2.15	103.53	114.42	2	1
4	A	343	PX4	O8-C23-C24	2.15	132.10	123.73	17	1
4	A	347	PX4	C34-C33-C32	2.15	103.53	114.42	4	1
4	A	362	PX4	C28-C27-C26	2.15	103.53	114.42	10	1
4	A	407	PX4	C29-C28-C27	2.15	103.53	114.42	15	1
4	A	408	PX4	C20-C19-C18	2.15	103.53	114.42	10	2
4	A	414	PX4	O8-C23-C24	2.14	115.37	123.73	13	1
4	A	419	PX4	O1-P1-O3	2.15	97.78	107.75	13	1
4	A	398	PX4	O8-C23-C24	2.14	132.09	123.73	12	1
4	A	425	PX4	C32-C31-C30	2.14	103.54	114.42	1	1
4	A	309	PX4	O8-C23-C24	2.14	115.37	123.73	5	2
4	A	366	PX4	C32-C31-C30	2.14	103.55	114.42	17	1
4	A	426	PX4	C17-C16-C15	2.14	103.54	114.42	19	2
4	A	417	PX4	O1-P1-O3	2.14	97.79	107.75	4	1
4	A	421	PX4	C15-C14-C13	2.14	103.55	114.42	10	2
4	A	422	PX4	C27-C26-C25	2.14	103.55	114.42	15	2
4	A	309	PX4	C31-C30-C29	2.14	103.56	114.42	12	1
4	A	317	PX4	C20-C19-C18	2.14	103.56	114.42	17	1
4	A	330	PX4	C22-C21-C20	2.14	97.18	113.42	3	1
4	A	395	PX4	C26-C25-C24	2.14	105.50	113.19	13	3
4	A	422	PX4	C33-C32-C31	2.14	103.56	114.42	7	1
4	A	426	PX4	C13-C12-C11	2.14	103.56	114.42	13	2
4	A	429	PX4	C19-C18-C17	2.14	103.56	114.42	2	1
4	A	314	PX4	O8-C23-C24	2.14	115.39	123.73	9	1
4	A	325	PX4	O8-C23-C24	2.14	115.39	123.73	6	1
4	A	344	PX4	C33-C32-C31	2.14	103.57	114.42	18	1
4	A	363	PX4	O3-C1-C2	2.14	120.41	109.16	20	1
4	A	400	PX4	C32-C31-C30	2.14	103.57	114.42	2	1
4	A	378	PX4	C5-N1-C2	2.14	118.67	109.92	1	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	380	PX4	C32-C31-C30	2.14	103.57	114.42	15	1
4	A	325	PX4	C4-N1-C2	2.14	118.66	109.92	11	1
4	A	333	PX4	C27-C26-C25	2.14	103.58	114.42	3	1
4	A	377	PX4	C5-N1-C2	2.14	118.66	109.92	16	1
4	A	306	PX4	C13-C12-C11	2.13	103.59	114.42	18	2
4	A	314	PX4	C14-C13-C12	2.13	103.59	114.42	4	2
4	A	402	PX4	C18-C17-C16	2.14	103.58	114.42	5	2
4	A	324	PX4	C31-C30-C29	2.13	103.59	114.42	13	2
4	A	342	PX4	C32-C31-C30	2.13	103.59	114.42	3	2
4	A	352	PX4	C14-C13-C12	2.13	103.59	114.42	3	1
4	A	400	PX4	O3-C1-C2	2.13	120.37	109.16	11	1
4	A	379	PX4	C8-O5-C9	2.13	109.22	117.12	19	1
4	A	393	PX4	C34-C33-C32	2.13	103.59	114.42	9	1
4	A	398	PX4	O6-C9-C10	2.13	115.41	123.73	1	1
4	A	422	PX4	C18-C17-C16	2.13	103.59	114.42	20	1
4	A	431	PX4	C15-C14-C13	2.13	103.59	114.42	13	1
4	A	317	PX4	C34-C33-C32	2.13	103.60	114.42	4	1
4	A	325	PX4	C14-C13-C12	2.13	103.60	114.42	3	1
4	A	333	PX4	C26-C25-C24	2.13	120.86	113.19	9	1
4	A	373	PX4	C34-C33-C32	2.13	103.60	114.42	3	1
4	A	421	PX4	O1-P1-O4	2.13	117.65	107.75	7	2
4	A	315	PX4	C4-N1-C2	2.13	118.63	109.92	10	1
4	A	319	PX4	C28-C27-C26	2.13	103.61	114.42	9	1
4	A	404	PX4	C34-C33-C32	2.13	103.60	114.42	2	3
4	A	357	PX4	O1-P1-O3	2.13	117.64	107.75	9	1
4	A	406	PX4	O3-C1-C2	2.13	120.36	109.16	7	1
4	A	418	PX4	C8-O5-C9	2.13	109.23	117.12	19	1
4	A	422	PX4	C34-C33-C32	2.13	103.61	114.42	8	1
4	A	430	PX4	C8-O5-C9	2.13	109.23	117.12	7	1
4	A	305	PX4	C19-C18-C17	2.13	103.62	114.42	18	2
4	A	339	PX4	O1-P1-O3	2.13	117.63	107.75	20	1
4	A	363	PX4	C14-C13-C12	2.13	103.61	114.42	1	1
4	A	335	PX4	O6-C9-C10	2.13	115.43	123.73	9	2
4	A	338	PX4	C5-N1-C2	2.13	118.62	109.92	6	1
4	A	343	PX4	C19-C18-C17	2.13	103.62	114.42	19	2
4	A	399	PX4	C18-C17-C16	2.13	103.62	114.42	16	3
4	A	397	PX4	C15-C14-C13	2.13	103.62	114.42	9	1
4	A	426	PX4	C19-C18-C17	2.13	103.62	114.42	5	1
4	A	316	PX4	C25-C24-C23	2.13	105.89	113.62	17	1
4	A	330	PX4	C32-C31-C30	2.13	103.63	114.42	11	2
4	A	345	PX4	C16-C15-C14	2.13	103.63	114.42	17	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	369	PX4	C26-C25-C24	2.13	105.55	113.19	4	2
4	A	378	PX4	C33-C32-C31	2.13	103.62	114.42	18	1
4	A	379	PX4	O6-C9-C10	2.13	115.43	123.73	8	1
4	A	332	PX4	C31-C30-C29	2.13	103.63	114.42	11	1
4	A	363	PX4	C8-O5-C9	2.13	109.25	117.12	1	1
4	A	367	PX4	C29-C28-C27	2.13	103.63	114.42	2	1
4	A	305	PX4	O8-C23-C24	2.12	115.45	123.73	10	1
4	A	321	PX4	O6-C9-C10	2.12	132.02	123.73	14	1
4	A	355	PX4	C11-C10-C9	2.12	105.89	113.62	16	1
4	A	376	PX4	C32-C31-C30	2.13	103.64	114.42	19	1
4	A	411	PX4	O1-P1-O4	2.12	97.88	107.75	18	1
4	A	422	PX4	C14-C13-C12	2.13	103.64	114.42	20	1
4	A	352	PX4	C29-C28-C27	2.12	103.65	114.42	20	1
4	A	362	PX4	C31-C30-C29	2.12	103.65	114.42	15	1
4	A	422	PX4	C36-C35-C34	2.12	97.30	113.42	9	1
4	A	393	PX4	O3-C1-C2	2.12	120.32	109.16	16	1
4	A	419	PX4	C32-C31-C30	2.12	103.65	114.42	18	1
4	A	423	PX4	C20-C19-C18	2.12	103.65	114.42	4	1
4	A	319	PX4	C29-C28-C27	2.12	103.66	114.42	20	1
4	A	404	PX4	C16-C15-C14	2.12	103.65	114.42	10	1
4	A	326	PX4	O3-C1-C2	2.12	120.31	109.16	10	3
4	A	366	PX4	C4-N1-C2	2.12	101.24	109.92	7	1
4	A	307	PX4	O8-C23-C24	2.12	132.00	123.73	1	1
4	A	320	PX4	C32-C31-C30	2.12	103.67	114.42	9	1
4	A	371	PX4	C31-C30-C29	2.12	103.67	114.42	10	1
4	A	413	PX4	O4-P1-O2	2.12	117.35	109.07	8	2
4	A	420	PX4	C13-C12-C11	2.12	103.67	114.42	19	1
4	A	314	PX4	C3-N1-C2	2.12	101.25	109.92	14	1
4	A	429	PX4	C17-C16-C15	2.12	103.68	114.42	10	1
4	A	385	PX4	C28-C27-C26	2.11	103.69	114.42	8	2
4	A	389	PX4	C19-C18-C17	2.12	103.69	114.42	6	1
4	A	391	PX4	C16-C15-C14	2.12	103.69	114.42	14	1
4	A	413	PX4	C28-C27-C26	2.12	103.68	114.42	5	1
4	A	351	PX4	C20-C19-C18	2.11	103.69	114.42	6	1
4	A	390	PX4	C19-C18-C17	2.11	103.69	114.42	13	1
4	A	368	PX4	C4-N1-C2	2.11	118.56	109.92	11	1
4	A	310	PX4	C15-C14-C13	2.11	103.71	114.42	5	2
4	A	318	PX4	O8-C23-C24	2.11	131.97	123.73	15	1
4	A	346	PX4	O3-C1-C2	2.11	120.26	109.16	4	1
4	A	352	PX4	C8-O5-C9	2.11	109.30	117.12	4	2
4	A	401	PX4	C14-C13-C12	2.11	103.70	114.42	14	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	372	PX4	O6-C9-C10	2.11	115.49	123.73	10	1
4	A	391	PX4	C4-N1-C2	2.11	118.56	109.92	3	1
4	A	428	PX4	C27-C26-C25	2.11	103.70	114.42	13	1
4	A	365	PX4	C29-C28-C27	2.11	103.71	114.42	8	1
4	A	365	PX4	C15-C14-C13	2.11	103.71	114.42	20	1
4	A	372	PX4	C26-C25-C24	2.11	105.60	113.19	19	1
4	A	402	PX4	C28-C27-C26	2.11	103.71	114.42	20	2
4	A	325	PX4	C16-C15-C14	2.11	103.72	114.42	11	1
4	A	357	PX4	C31-C30-C29	2.11	103.72	114.42	5	1
4	A	376	PX4	C15-C14-C13	2.11	103.72	114.42	10	1
4	A	424	PX4	O6-C9-C10	2.11	115.50	123.73	14	1
4	A	305	PX4	C11-C10-C9	2.11	105.95	113.62	12	1
4	A	323	PX4	C30-C29-C28	2.11	103.73	114.42	6	1
4	A	338	PX4	C18-C17-C16	2.11	103.73	114.42	7	1
4	A	343	PX4	C27-C26-C25	2.11	103.73	114.42	11	1
4	A	393	PX4	C8-O5-C9	2.11	109.31	117.12	6	3
4	A	418	PX4	C14-C13-C12	2.11	103.72	114.42	17	2
4	A	329	PX4	C5-N1-C2	2.11	101.30	109.92	20	1
4	A	332	PX4	C29-C28-C27	2.11	103.73	114.42	1	1
4	A	336	PX4	C14-C13-C12	2.11	103.74	114.42	20	1
4	A	376	PX4	C11-C10-C9	2.11	105.96	113.62	16	1
4	A	390	PX4	C17-C16-C15	2.11	103.73	114.42	2	2
4	A	396	PX4	C8-O5-C9	2.11	124.92	117.12	3	1
4	A	377	PX4	C29-C28-C27	2.11	103.74	114.42	15	2
4	A	405	PX4	C13-C12-C11	2.11	103.74	114.42	7	1
4	A	382	PX4	C25-C24-C23	2.10	105.97	113.62	3	1
4	A	309	PX4	C15-C14-C13	2.10	103.75	114.42	14	1
4	A	317	PX4	C31-C30-C29	2.10	103.75	114.42	2	1
4	A	322	PX4	C16-C15-C14	2.10	103.75	114.42	3	1
4	A	344	PX4	C14-C13-C12	2.10	103.75	114.42	10	1
4	A	347	PX4	O4-P1-O2	2.10	117.28	109.07	1	1
4	A	354	PX4	C17-C16-C15	2.10	103.75	114.42	7	1
4	A	355	PX4	C27-C26-C25	2.10	103.75	114.42	19	1
4	A	414	PX4	C30-C29-C28	2.10	103.75	114.42	2	1
4	A	312	PX4	C3-N1-C2	2.10	118.52	109.92	9	1
4	A	331	PX4	C33-C32-C31	2.10	103.76	114.42	17	2
4	A	376	PX4	C18-C17-C16	2.10	103.76	114.42	11	2
4	A	392	PX4	C29-C28-C27	2.10	103.76	114.42	11	2
4	A	344	PX4	C32-C31-C30	2.10	103.77	114.42	11	1
4	A	360	PX4	C26-C25-C24	2.10	120.73	113.19	11	2
4	A	372	PX4	C13-C12-C11	2.10	103.77	114.42	16	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	382	PX4	O1-P1-O3	2.10	98.00	107.75	8	1
4	A	386	PX4	O6-C9-C10	2.10	115.55	123.73	9	1
4	A	429	PX4	C30-C29-C28	2.10	103.77	114.42	15	1
4	A	355	PX4	C5-N1-C2	2.10	101.34	109.92	16	1
4	A	357	PX4	O6-C9-C10	2.10	115.56	123.73	17	1
4	A	383	PX4	C12-C11-C10	2.10	105.66	113.19	13	1
4	A	410	PX4	C3-N1-C2	2.10	118.49	109.92	1	1
4	A	417	PX4	C18-C17-C16	2.10	103.78	114.42	6	1
4	A	313	PX4	C34-C33-C32	2.09	103.80	114.42	15	3
4	A	329	PX4	C18-C17-C16	2.09	103.80	114.42	12	1
4	A	336	PX4	C16-C15-C14	2.09	103.80	114.42	13	1
4	A	338	PX4	C4-N1-C2	2.09	118.48	109.92	13	1
4	A	379	PX4	C3-N1-C2	2.09	118.48	109.92	17	1
4	A	410	PX4	C15-C14-C13	2.09	103.80	114.42	7	1
4	A	394	PX4	O4-P1-O2	2.09	117.25	109.07	20	2
4	A	424	PX4	O8-C23-C24	2.09	115.56	123.73	9	1
4	A	399	PX4	O6-C9-C10	2.09	115.57	123.73	12	2
4	A	413	PX4	C27-C26-C25	2.09	103.80	114.42	20	1
4	A	416	PX4	O1-P1-O4	2.09	117.47	107.75	6	2
4	A	358	PX4	C20-C19-C18	2.09	103.81	114.42	15	1
4	A	373	PX4	C13-C12-C11	2.09	103.81	114.42	6	1
4	A	381	PX4	C3-N1-C2	2.09	118.47	109.92	13	1
4	A	305	PX4	C16-C15-C14	2.09	103.82	114.42	9	1
4	A	346	PX4	C34-C33-C32	2.09	103.82	114.42	9	1
4	A	369	PX4	C31-C30-C29	2.09	103.83	114.42	4	1
4	A	384	PX4	C19-C18-C17	2.09	103.82	114.42	3	1
4	A	409	PX4	C3-N1-C2	2.09	118.46	109.92	1	1
4	A	391	PX4	C33-C32-C31	2.09	103.82	114.42	3	2
4	A	341	PX4	C28-C27-C26	2.09	103.83	114.42	18	1
4	A	398	PX4	C32-C31-C30	2.09	103.83	114.42	1	1
4	A	426	PX4	O1-P1-O4	2.09	117.43	107.75	7	1
4	A	431	PX4	C31-C30-C29	2.09	103.83	114.42	10	1
4	A	400	PX4	C18-C17-C16	2.08	103.85	114.42	14	1
4	A	377	PX4	C27-C26-C25	2.08	103.85	114.42	18	2
4	A	382	PX4	O8-C23-C24	2.08	115.60	123.73	8	1
4	A	411	PX4	C11-C10-C9	2.08	106.04	113.62	15	2
4	A	414	PX4	C20-C19-C18	2.08	103.84	114.42	6	1
4	A	422	PX4	C4-N1-C2	2.08	101.39	109.92	16	1
4	A	324	PX4	C16-C15-C14	2.08	103.86	114.42	18	1
4	A	336	PX4	C17-C16-C15	2.08	103.86	114.42	9	1
4	A	377	PX4	C33-C32-C31	2.08	103.86	114.42	11	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	392	PX4	C13-C12-C11	2.08	103.86	114.42	6	1
4	A	430	PX4	C19-C18-C17	2.08	103.85	114.42	10	1
4	A	338	PX4	C8-O5-C9	2.08	109.42	117.12	5	2
4	A	351	PX4	C29-C28-C27	2.08	103.87	114.42	13	2
4	A	375	PX4	O3-C1-C2	2.08	120.09	109.16	11	1
4	A	429	PX4	O8-C23-C24	2.08	131.84	123.73	10	1
4	A	350	PX4	C5-N1-C2	2.08	101.42	109.92	1	1
4	A	366	PX4	O1-P1-O4	2.08	117.39	107.75	6	3
4	A	407	PX4	C27-C26-C25	2.08	103.87	114.42	20	1
4	A	307	PX4	C14-C13-C12	2.08	103.88	114.42	15	2
4	A	411	PX4	C15-C14-C13	2.08	103.88	114.42	3	2
4	A	314	PX4	C15-C14-C13	2.08	103.89	114.42	4	1
4	A	307	PX4	C34-C33-C32	2.07	103.90	114.42	18	1
4	A	315	PX4	O3-C1-C2	2.07	120.07	109.16	14	1
4	A	320	PX4	C19-C18-C17	2.08	103.89	114.42	8	1
4	A	320	PX4	O3-C1-C2	2.08	120.08	109.16	17	1
4	A	427	PX4	C31-C30-C29	2.08	103.89	114.42	19	2
4	A	311	PX4	O1-P1-O3	2.07	98.12	107.75	16	1
4	A	375	PX4	O6-C9-C10	2.07	115.64	123.73	7	2
4	A	370	PX4	C8-O5-C9	2.07	124.79	117.12	3	1
4	A	391	PX4	C17-C16-C15	2.07	103.90	114.42	6	1
4	A	322	PX4	C4-N1-C2	2.07	101.44	109.92	11	2
4	A	328	PX4	C8-O5-C9	2.07	109.45	117.12	9	3
4	A	403	PX4	C34-C33-C32	2.07	103.91	114.42	5	1
4	A	413	PX4	C32-C31-C30	2.07	103.91	114.42	8	1
4	A	395	PX4	C19-C18-C17	2.07	103.91	114.42	17	1
4	A	346	PX4	C33-C32-C31	2.07	103.91	114.42	6	2
4	A	397	PX4	C12-C11-C10	2.07	105.75	113.19	17	1
4	A	426	PX4	C4-N1-C3	2.07	114.30	108.97	3	1
4	A	338	PX4	O8-C23-C24	2.07	115.66	123.73	20	1
4	A	375	PX4	C12-C11-C10	2.07	105.75	113.19	10	1
4	A	319	PX4	O1-P1-O3	2.07	98.14	107.75	15	2
4	A	316	PX4	C18-C17-C16	2.07	103.93	114.42	9	1
4	A	336	PX4	C28-C27-C26	2.07	103.94	114.42	18	1
4	A	340	PX4	O1-P1-O4	2.07	117.34	107.75	2	2
4	A	369	PX4	C15-C14-C13	2.07	103.93	114.42	7	1
4	A	351	PX4	C3-N1-C2	2.07	118.37	109.92	14	1
4	A	422	PX4	C22-C21-C20	2.07	97.73	113.42	4	1
4	A	354	PX4	C33-C32-C31	2.07	103.94	114.42	20	1
4	A	381	PX4	C19-C18-C17	2.07	103.94	114.42	15	1
4	A	398	PX4	C29-C28-C27	2.07	103.93	114.42	11	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	317	PX4	C15-C14-C13	2.06	103.95	114.42	20	1
4	A	314	PX4	C27-C26-C25	2.06	103.95	114.42	4	1
4	A	320	PX4	C14-C13-C12	2.06	103.95	114.42	18	1
4	A	335	PX4	C34-C33-C32	2.06	103.95	114.42	18	1
4	A	365	PX4	O6-C9-C10	2.06	115.68	123.73	14	1
4	A	398	PX4	O1-P1-O4	2.06	117.33	107.75	11	1
4	A	334	PX4	O8-C23-C24	2.06	115.69	123.73	10	1
4	A	374	PX4	C19-C18-C17	2.06	124.89	114.42	11	1
4	A	374	PX4	O3-C1-C2	2.06	120.00	109.16	17	1
4	A	380	PX4	C33-C32-C31	2.06	103.95	114.42	2	1
4	A	412	PX4	C8-O5-C9	2.06	109.48	117.12	11	2
4	A	412	PX4	C27-C26-C25	2.06	103.95	114.42	12	1
4	A	416	PX4	O8-C23-C24	2.06	115.68	123.73	7	1
4	A	314	PX4	C33-C32-C31	2.06	103.96	114.42	5	1
4	A	322	PX4	C5-N1-C2	2.06	101.48	109.92	17	1
4	A	333	PX4	C4-N1-C2	2.06	118.34	109.92	7	1
4	A	334	PX4	C36-C35-C34	2.06	97.79	113.42	16	1
4	A	315	PX4	O6-C9-C10	2.06	115.70	123.73	20	1
4	A	353	PX4	O3-C1-C2	2.06	119.99	109.16	17	1
4	A	318	PX4	C30-C29-C28	2.06	103.98	114.42	14	2
4	A	369	PX4	C33-C32-C31	2.06	103.98	114.42	13	2
4	A	405	PX4	C5-N1-C2	2.06	101.50	109.92	15	1
4	A	382	PX4	O6-C9-C10	2.06	115.70	123.73	10	1
4	A	320	PX4	C31-C30-C29	2.06	103.99	114.42	14	1
4	A	324	PX4	C20-C19-C18	2.06	103.99	114.42	7	1
4	A	366	PX4	C31-C30-C29	2.06	103.99	114.42	20	1
4	A	407	PX4	C33-C32-C31	2.06	103.99	114.42	15	1
4	A	394	PX4	C8-O5-C9	2.06	124.74	117.12	12	1
4	A	385	PX4	C8-O5-C9	2.05	109.51	117.12	4	1
4	A	306	PX4	O6-C9-C10	2.05	115.73	123.73	19	1
4	A	339	PX4	C16-C15-C14	2.05	104.00	114.42	1	2
4	A	424	PX4	C34-C33-C32	2.05	104.00	114.42	20	2
4	A	387	PX4	C11-C10-C9	2.05	106.16	113.62	12	1
4	A	417	PX4	C29-C28-C27	2.05	104.01	114.42	18	1
4	A	427	PX4	C18-C17-C16	2.05	104.00	114.42	3	1
4	A	326	PX4	C5-N1-C2	2.05	118.31	109.92	20	1
4	A	328	PX4	C28-C27-C26	2.05	104.02	114.42	14	1
4	A	341	PX4	C25-C24-C23	2.05	106.16	113.62	8	1
4	A	409	PX4	C12-C11-C10	2.05	105.82	113.19	13	1
4	A	325	PX4	C32-C31-C30	2.05	104.03	114.42	2	1
4	A	327	PX4	C14-C13-C12	2.05	104.03	114.42	19	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	344	PX4	O1-P1-O3	2.05	98.23	107.75	18	1
4	A	363	PX4	C11-C10-C9	2.05	106.17	113.62	8	2
4	A	366	PX4	C28-C27-C26	2.05	104.02	114.42	10	2
4	A	389	PX4	C34-C33-C32	2.05	104.02	114.42	1	1
4	A	392	PX4	C31-C30-C29	2.05	104.02	114.42	14	1
4	A	426	PX4	O3-C1-C2	2.05	119.94	109.16	18	1
4	A	399	PX4	C17-C16-C15	2.05	104.03	114.42	17	1
4	A	378	PX4	C25-C24-C23	2.05	106.17	113.62	8	3
4	A	382	PX4	C17-C16-C15	2.05	104.02	114.42	4	1
4	A	347	PX4	C15-C14-C13	2.05	104.04	114.42	7	1
4	A	356	PX4	C33-C32-C31	2.05	124.82	114.42	10	2
4	A	385	PX4	O8-C23-C24	2.05	115.75	123.73	9	1
4	A	420	PX4	C20-C19-C18	2.05	104.03	114.42	7	1
4	A	373	PX4	C32-C31-C30	2.05	104.04	114.42	7	1
4	A	415	PX4	C26-C25-C24	2.05	105.83	113.19	6	1
4	A	365	PX4	C17-C16-C15	2.04	104.05	114.42	20	2
4	A	368	PX4	C16-C15-C14	2.04	104.05	114.42	8	1
4	A	374	PX4	C33-C32-C31	2.04	104.05	114.42	9	1
4	A	392	PX4	C18-C17-C16	2.04	104.04	114.42	10	1
4	A	407	PX4	C31-C30-C29	2.04	104.05	114.42	16	1
4	A	389	PX4	O8-C23-C24	2.04	115.76	123.73	18	1
4	A	413	PX4	C17-C16-C15	2.04	104.05	114.42	5	1
4	A	414	PX4	C29-C28-C27	2.04	104.05	114.42	4	1
4	A	309	PX4	C33-C32-C31	2.04	104.06	114.42	17	1
4	A	310	PX4	C14-C13-C12	2.04	104.05	114.42	19	1
4	A	311	PX4	O3-C1-C2	2.04	119.90	109.16	3	2
4	A	329	PX4	O3-C1-C2	2.04	119.90	109.16	7	2
4	A	363	PX4	C31-C30-C29	2.04	104.06	114.42	1	1
4	A	381	PX4	C13-C12-C11	2.04	104.06	114.42	10	1
4	A	408	PX4	C3-N1-C2	2.04	118.27	109.92	16	1
4	A	418	PX4	C17-C16-C15	2.04	104.05	114.42	17	1
4	A	311	PX4	C27-C26-C25	2.04	104.07	114.42	3	1
4	A	363	PX4	C20-C19-C18	2.04	104.06	114.42	18	1
4	A	379	PX4	C28-C27-C26	2.04	104.07	114.42	20	1
4	A	380	PX4	C3-N1-C2	2.04	101.56	109.92	3	1
4	A	409	PX4	C18-C17-C16	2.04	104.06	114.42	5	1
4	A	423	PX4	C3-N1-C2	2.04	118.27	109.92	6	1
4	A	323	PX4	C18-C17-C16	2.04	104.07	114.42	9	1
4	A	345	PX4	C13-C12-C11	2.04	104.07	114.42	14	1
4	A	428	PX4	C34-C33-C32	2.04	104.06	114.42	17	2
4	A	352	PX4	O3-C1-C2	2.04	119.89	109.16	2	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	309	PX4	C16-C15-C14	2.04	104.08	114.42	17	1
4	A	315	PX4	C22-C21-C20	2.04	97.95	113.42	1	1
4	A	351	PX4	C32-C31-C30	2.04	104.08	114.42	5	1
4	A	372	PX4	O3-C1-C2	2.04	119.87	109.16	11	1
4	A	390	PX4	C8-O5-C9	2.04	109.58	117.12	9	2
4	A	331	PX4	C25-C24-C23	2.04	106.22	113.62	16	1
4	A	348	PX4	C4-N1-C2	2.04	118.25	109.92	14	1
4	A	393	PX4	C3-N1-C2	2.04	118.25	109.92	17	1
4	A	349	PX4	C32-C31-C30	2.04	104.09	114.42	6	2
4	A	358	PX4	C28-C27-C26	2.03	104.09	114.42	15	2
4	A	368	PX4	C20-C19-C18	2.04	104.09	114.42	1	1
4	A	384	PX4	C8-O5-C9	2.03	124.66	117.12	6	1
4	A	390	PX4	C15-C14-C13	2.03	104.10	114.42	13	1
4	A	306	PX4	C33-C32-C31	2.03	104.11	114.42	14	1
4	A	318	PX4	O3-P1-O2	2.03	101.12	109.07	8	2
4	A	315	PX4	C25-C24-C23	2.03	106.23	113.62	18	1
4	A	324	PX4	C19-C18-C17	2.03	104.11	114.42	19	1
4	A	325	PX4	C11-C10-C9	2.03	106.23	113.62	6	1
4	A	409	PX4	O8-C23-C24	2.03	115.80	123.73	11	2
4	A	422	PX4	O4-P1-O2	2.03	117.01	109.07	8	1
4	A	356	PX4	C19-C18-C17	2.03	104.11	114.42	18	1
4	A	404	PX4	C33-C32-C31	2.03	104.11	114.42	18	2
4	A	354	PX4	C4-N1-C2	2.03	118.22	109.92	14	1
4	A	370	PX4	C33-C32-C31	2.03	104.12	114.42	15	1
4	A	382	PX4	C13-C12-C11	2.03	104.12	114.42	2	1
4	A	368	PX4	C36-C35-C34	2.03	98.03	113.42	18	1
4	A	385	PX4	C30-C29-C28	2.03	104.13	114.42	2	1
4	A	386	PX4	C30-C29-C28	2.03	104.12	114.42	17	1
4	A	430	PX4	C18-C17-C16	2.03	104.12	114.42	15	1
4	A	319	PX4	C34-C33-C32	2.03	104.13	114.42	14	1
4	A	326	PX4	C31-C30-C29	2.03	104.13	114.42	3	2
4	A	367	PX4	C19-C18-C17	2.03	104.13	114.42	2	1
4	A	339	PX4	O6-C9-C10	2.03	115.83	123.73	13	1
4	A	316	PX4	C5-N1-C2	2.03	118.20	109.92	3	1
4	A	364	PX4	C34-C33-C32	2.03	104.14	114.42	7	1
4	A	369	PX4	C28-C27-C26	2.03	104.14	114.42	15	1
4	A	403	PX4	O3-C1-C2	2.03	119.82	109.16	11	1
4	A	411	PX4	C16-C15-C14	2.03	124.71	114.42	3	1
4	A	397	PX4	C32-C31-C30	2.03	104.13	114.42	5	1
4	A	367	PX4	C22-C21-C20	2.03	98.05	113.42	17	1
4	A	377	PX4	O3-C1-C2	2.03	119.81	109.16	17	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	320	PX4	C30-C29-C28	2.02	104.15	114.42	7	1
4	A	321	PX4	C4-N1-C2	2.02	118.20	109.92	4	4
4	A	333	PX4	C32-C31-C30	2.02	104.15	114.42	12	1
4	A	380	PX4	C34-C33-C32	2.02	104.14	114.42	5	1
4	A	407	PX4	C28-C27-C26	2.02	104.15	114.42	15	1
4	A	341	PX4	C16-C15-C14	2.02	104.15	114.42	17	1
4	A	413	PX4	C20-C19-C18	2.02	104.15	114.42	2	1
4	A	333	PX4	C29-C28-C27	2.02	104.17	114.42	15	1
4	A	365	PX4	C28-C27-C26	2.02	124.69	114.42	11	1
4	A	374	PX4	C32-C31-C30	2.02	104.16	114.42	19	1
4	A	408	PX4	C34-C33-C32	2.02	104.16	114.42	20	1
4	A	393	PX4	C29-C28-C27	2.02	104.16	114.42	19	1
4	A	414	PX4	C5-N1-C2	2.02	118.19	109.92	18	1
4	A	362	PX4	O3-C1-C2	2.02	119.78	109.16	14	1
4	A	427	PX4	O6-C9-C10	2.02	115.85	123.73	5	1
4	A	324	PX4	C15-C14-C13	2.02	104.19	114.42	2	1
4	A	343	PX4	C5-N1-C2	2.02	118.17	109.92	12	1
4	A	349	PX4	C18-C17-C16	2.02	104.18	114.42	6	1
4	A	376	PX4	C8-O5-C9	2.02	109.65	117.12	18	1
4	A	389	PX4	C13-C12-C11	2.02	104.18	114.42	14	1
4	A	420	PX4	C31-C30-C29	2.02	104.19	114.42	13	1
4	A	423	PX4	O6-C9-C10	2.02	115.86	123.73	7	1
4	A	318	PX4	C31-C30-C29	2.02	104.19	114.42	8	1
4	A	331	PX4	C29-C28-C27	2.01	104.20	114.42	6	1
4	A	344	PX4	C17-C16-C15	2.02	104.19	114.42	13	1
4	A	354	PX4	O3-C1-C2	2.02	119.76	109.16	14	1
4	A	413	PX4	O8-C23-C24	2.02	115.86	123.73	8	1
4	A	352	PX4	O8-C23-C24	2.01	115.87	123.73	1	1
4	A	400	PX4	C11-C10-C9	2.01	120.95	113.62	11	1
4	A	405	PX4	C34-C33-C32	2.01	104.20	114.42	20	1
4	A	427	PX4	O1-P1-O4	2.02	117.10	107.75	12	1
4	A	380	PX4	C31-C30-C29	2.01	104.20	114.42	17	1
4	A	422	PX4	C13-C12-C11	2.01	104.20	114.42	5	1
4	A	428	PX4	C31-C30-C29	2.01	104.21	114.42	10	1
4	A	429	PX4	C14-C13-C12	2.01	104.20	114.42	2	1
4	A	327	PX4	C17-C16-C15	2.01	104.21	114.42	10	1
4	A	383	PX4	C4-N1-C2	2.01	118.15	109.92	14	1
4	A	422	PX4	C11-C10-C9	2.01	106.31	113.62	1	1
4	A	350	PX4	O1-P1-O3	2.01	98.41	107.75	4	1
4	A	305	PX4	C28-C27-C26	2.01	104.22	114.42	3	1
4	A	306	PX4	C22-C21-C20	2.01	98.19	113.42	5	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	320	PX4	C3-N1-C2	2.01	118.13	109.92	2	1
4	A	407	PX4	C32-C31-C30	2.01	104.23	114.42	13	1
4	A	388	PX4	C33-C32-C31	2.01	104.23	114.42	4	1
4	A	323	PX4	C32-C31-C30	2.01	104.24	114.42	17	1
4	A	328	PX4	C13-C12-C11	2.01	104.24	114.42	6	1
4	A	417	PX4	C25-C24-C23	2.01	106.32	113.62	13	1
4	A	329	PX4	C16-C15-C14	2.01	104.24	114.42	10	1
4	A	331	PX4	C19-C18-C17	2.01	104.24	114.42	11	1
4	A	372	PX4	O8-C23-C24	2.01	115.91	123.73	5	1
4	A	369	PX4	C3-N1-C2	2.00	118.12	109.92	15	1
4	A	380	PX4	C14-C13-C12	2.01	104.25	114.42	6	1
4	A	414	PX4	C14-C13-C12	2.01	104.24	114.42	19	1
4	A	334	PX4	C28-C27-C26	2.00	104.26	114.42	20	1
4	A	343	PX4	C33-C32-C31	2.00	104.26	114.42	15	1
4	A	324	PX4	C12-C11-C10	2.00	106.00	113.19	10	1
4	A	345	PX4	C5-N1-C2	2.00	118.11	109.92	18	1
4	A	354	PX4	C30-C29-C28	2.00	104.27	114.42	10	1
4	A	355	PX4	C3-N1-C2	2.00	118.10	109.92	5	1
4	A	366	PX4	C15-C14-C13	2.00	104.27	114.42	15	1
4	A	370	PX4	O6-C9-C10	2.00	115.93	123.73	4	1
4	A	392	PX4	C32-C31-C30	2.00	104.27	114.42	6	1

There are no chirality outliers.

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

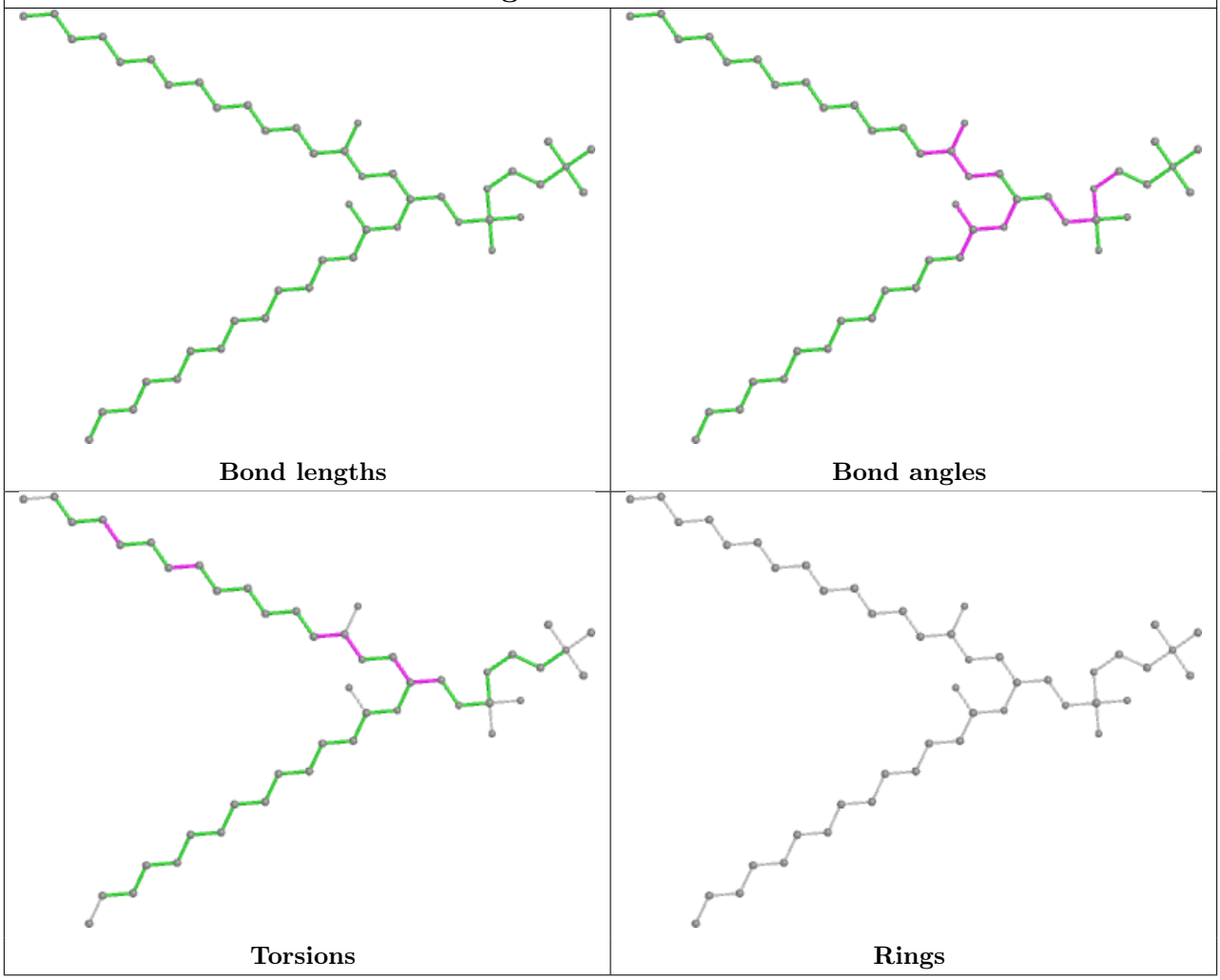
Mol	Chain	Res	Type	Atoms	Models (Total)
4	A	414	PX4	O8-C23-O7-C7	4
4	A	331	PX4	O8-C23-O7-C7	2
4	A	321	PX4	O8-C23-O7-C7	1
4	A	323	PX4	O8-C23-O7-C7	1

There are no ring outliers.

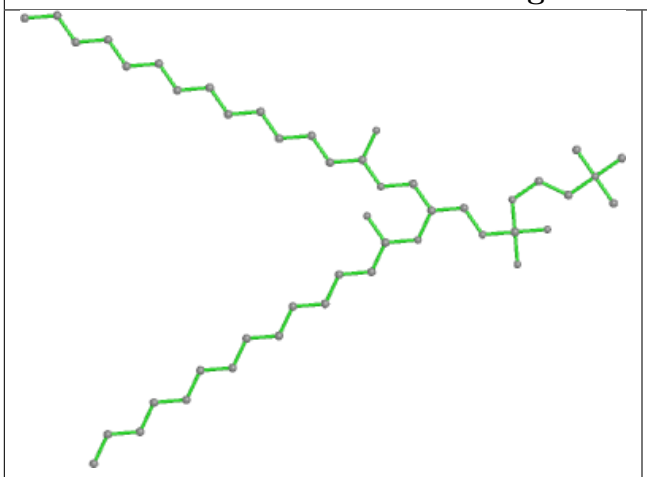
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

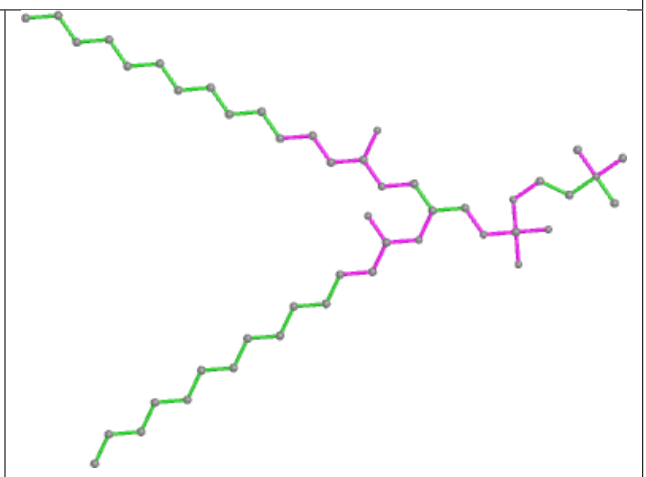
Ligand PX4 A 417



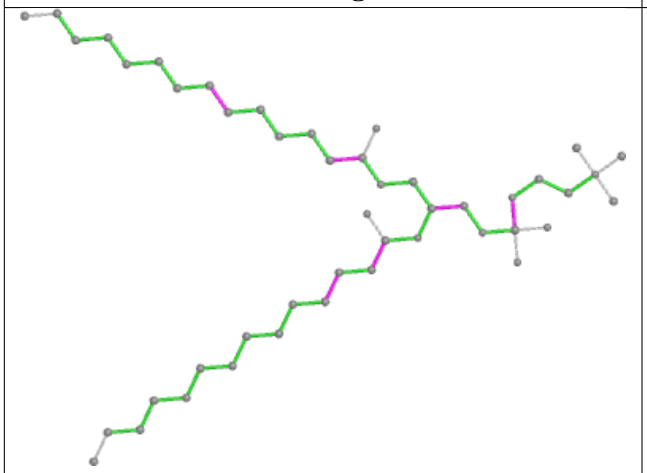
Ligand PX4 A 374



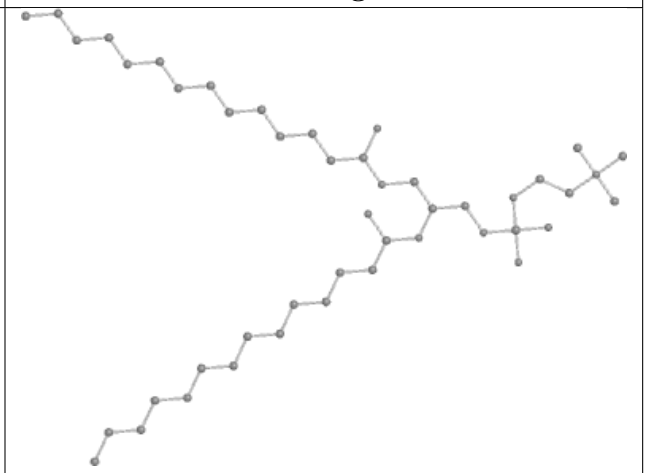
Bond lengths



Bond angles

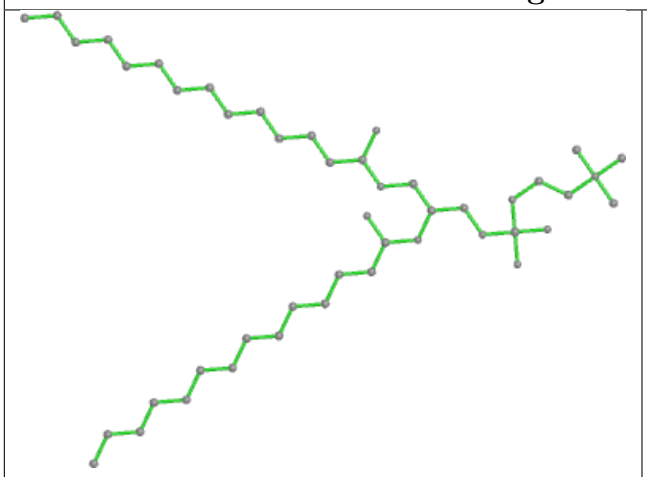


Torsions

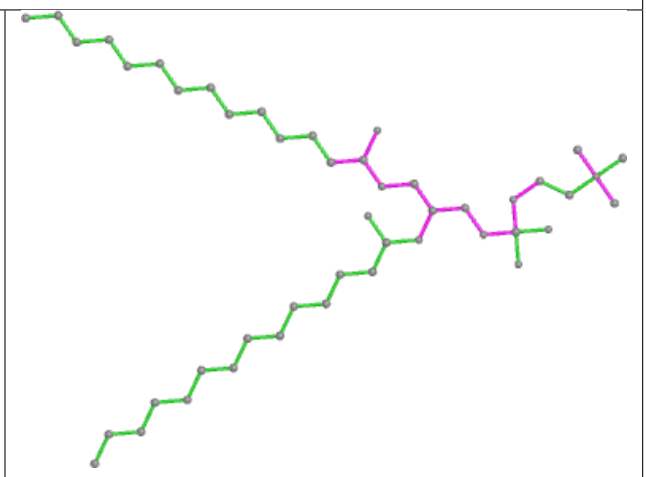


Rings

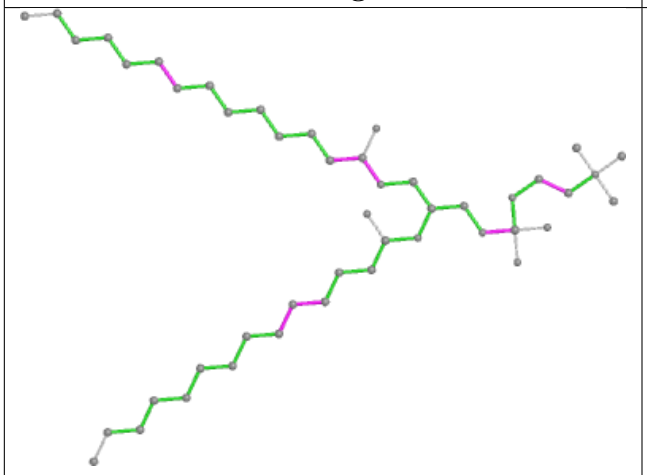
Ligand PX4 A 407



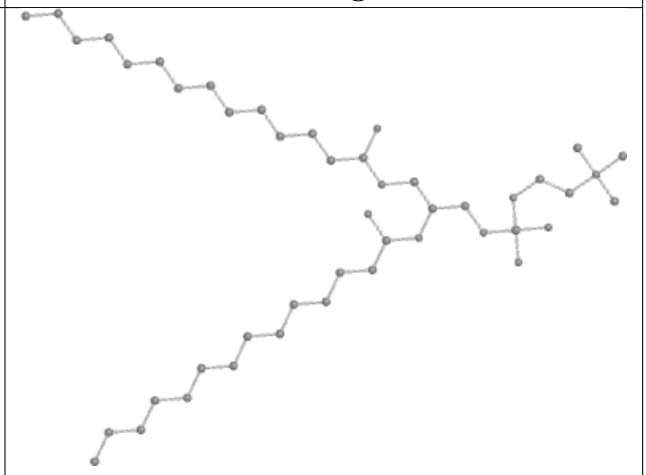
Bond lengths



Bond angles

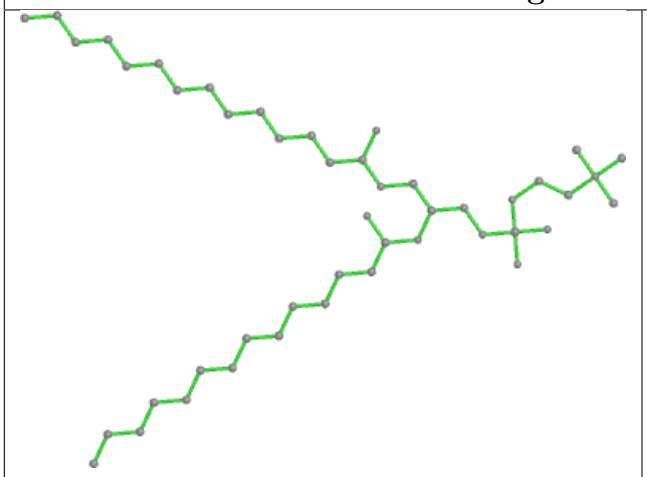


Torsions



Rings

Ligand PX4 A 375



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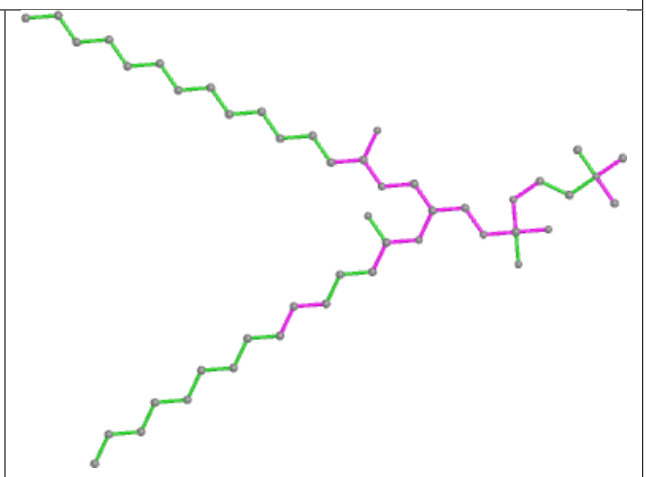

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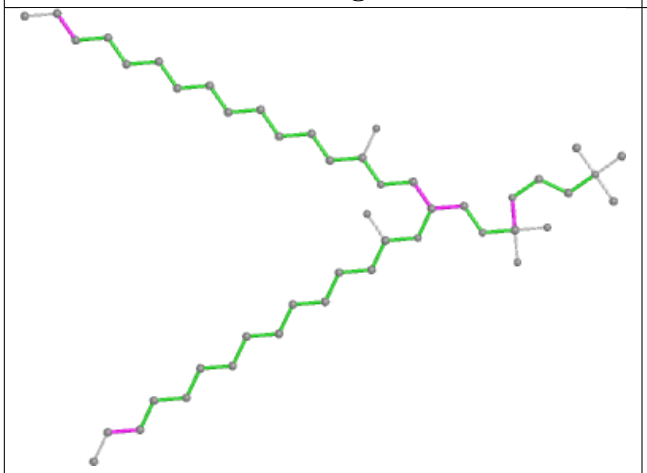

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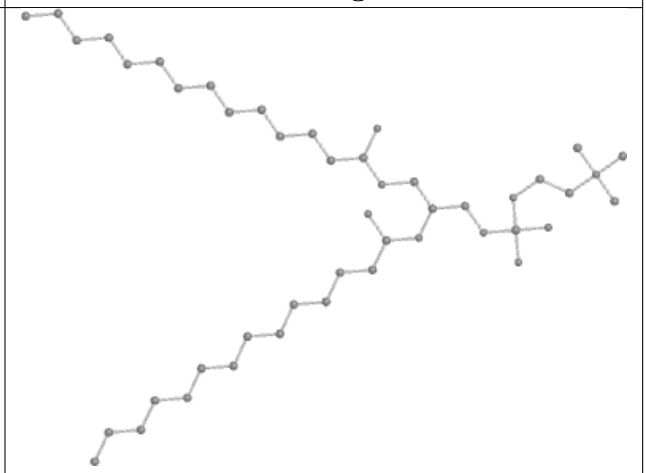
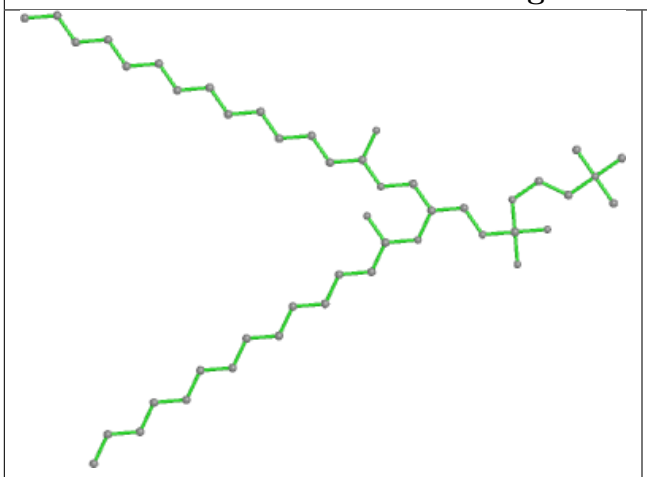


Rings

Ligand PX4 A 333



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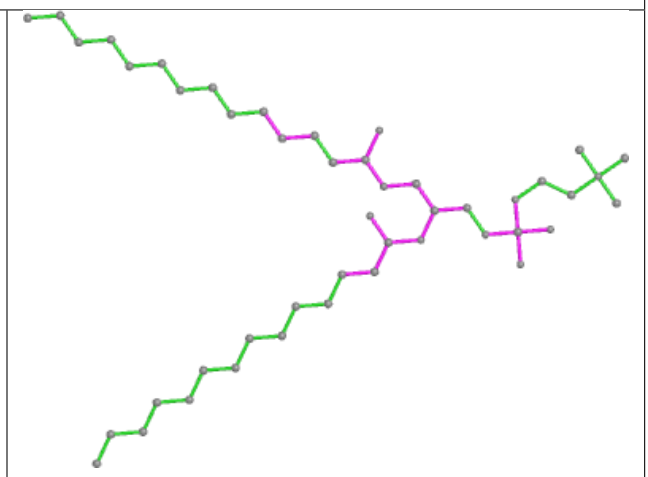

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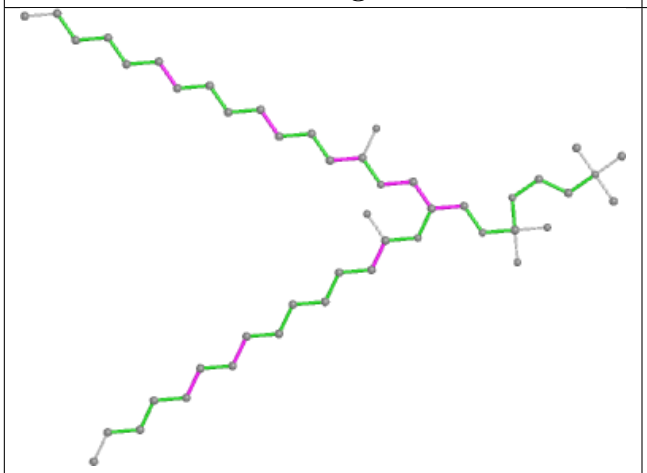

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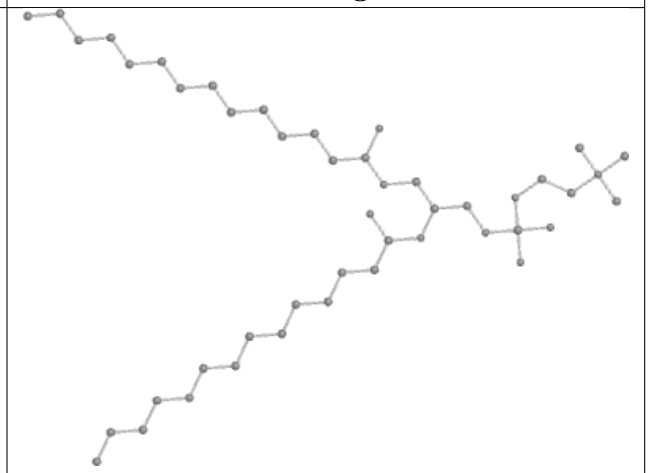
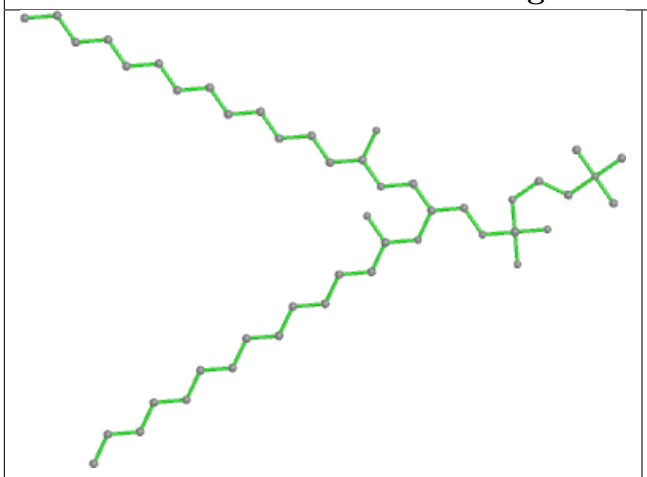


Rings

Ligand PX4 A 405



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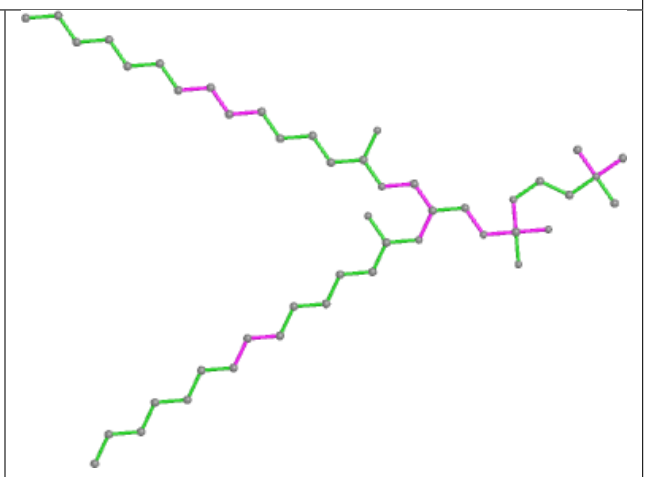

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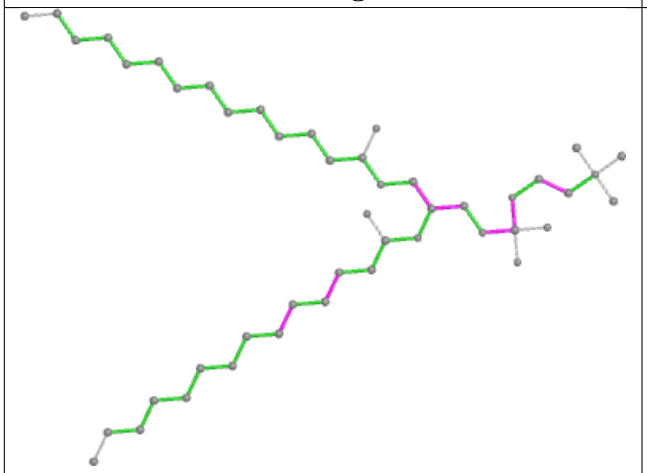

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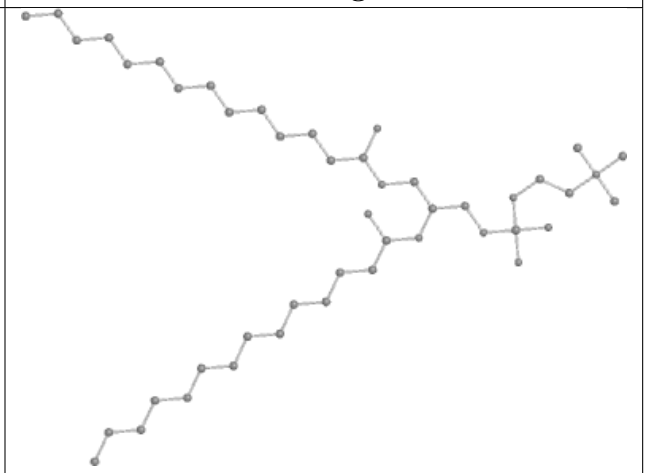
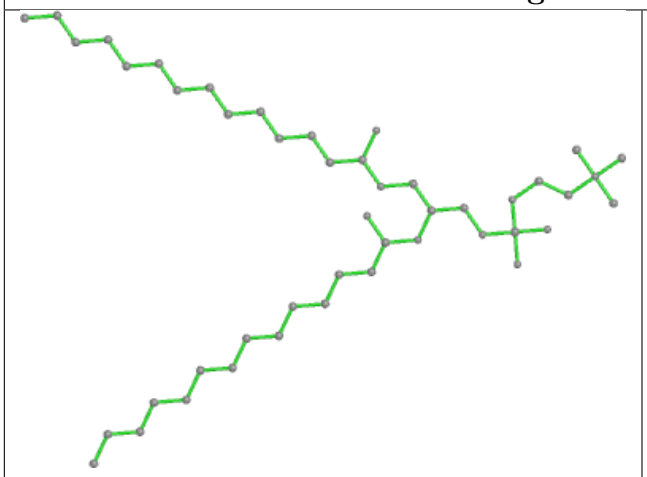


Rings

Ligand PX4 A 342



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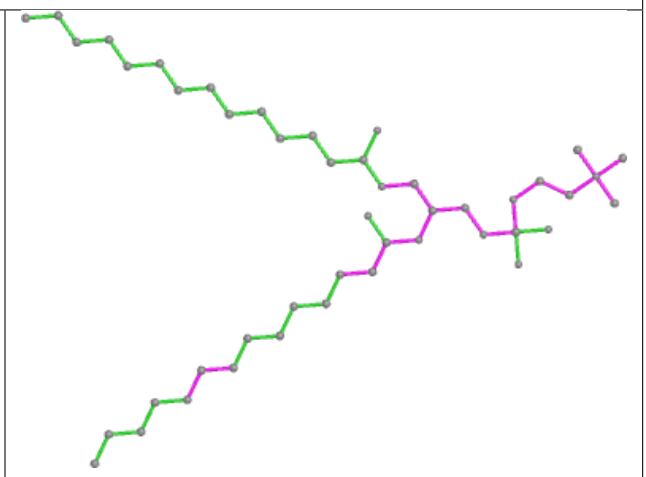

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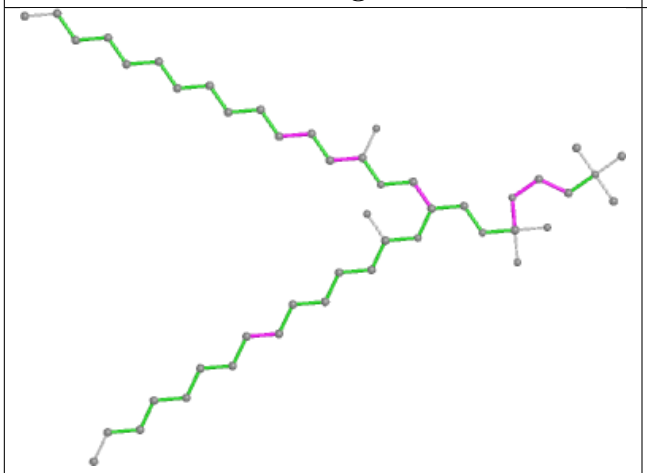

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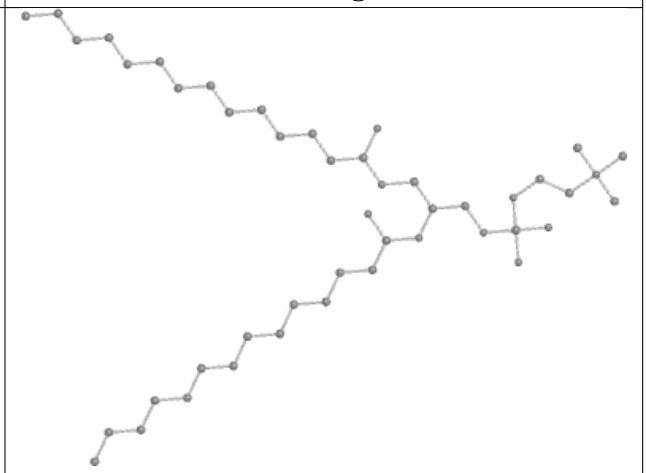
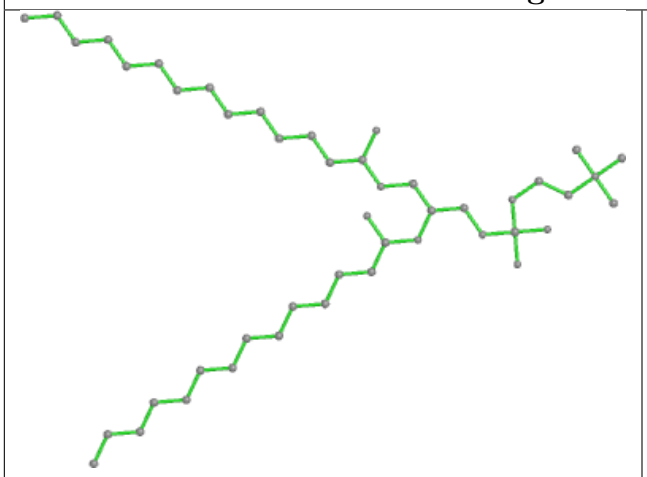


Rings

Ligand PX4 A 315



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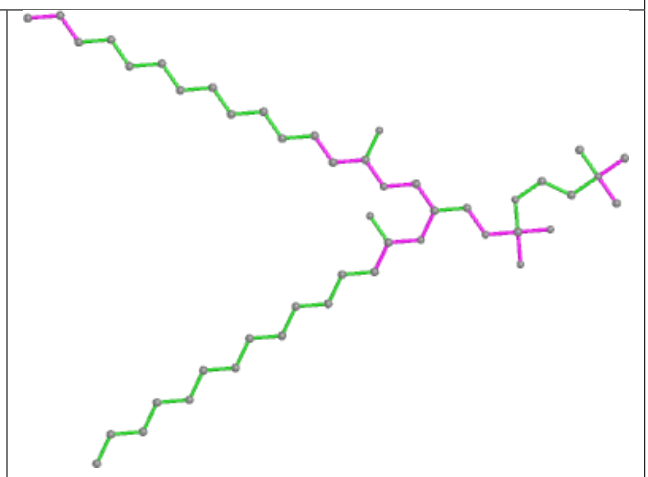

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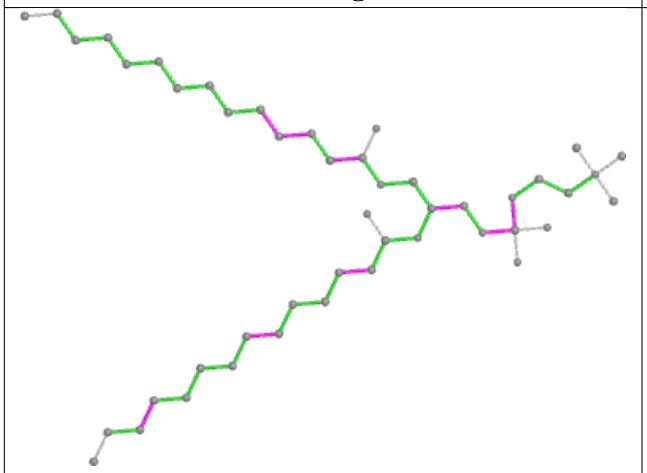

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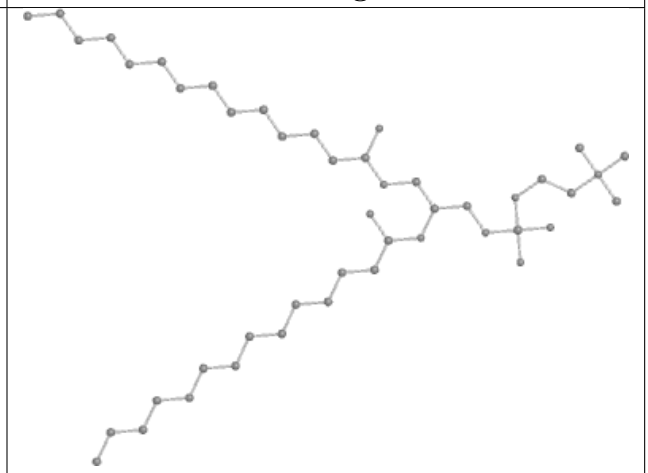
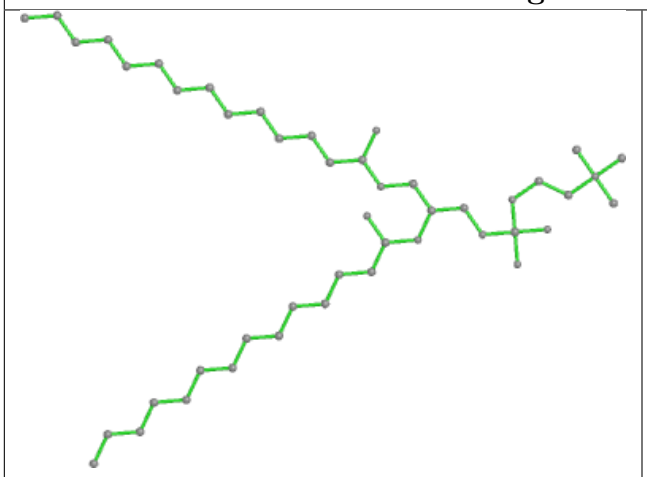


Rings

Ligand PX4 A 419



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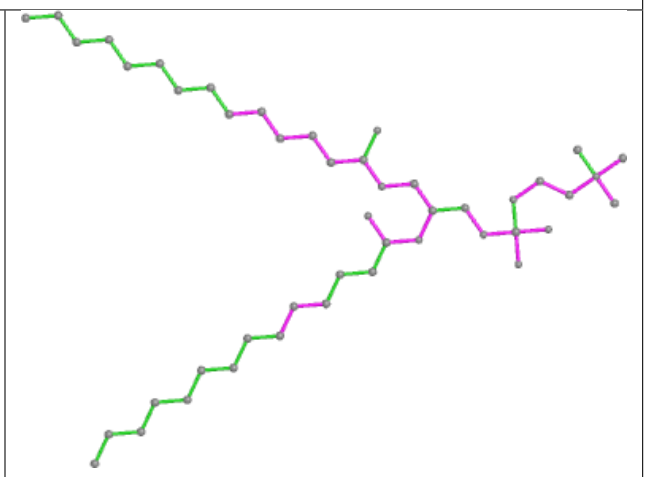

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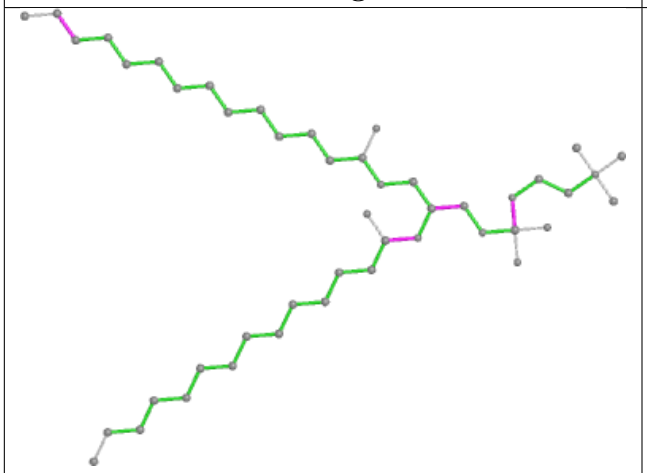

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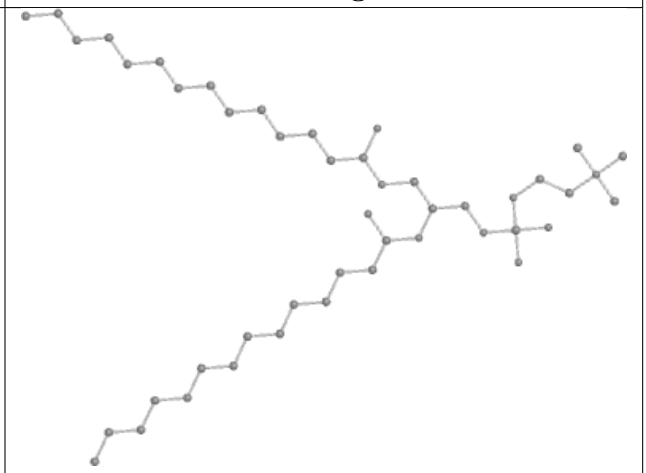
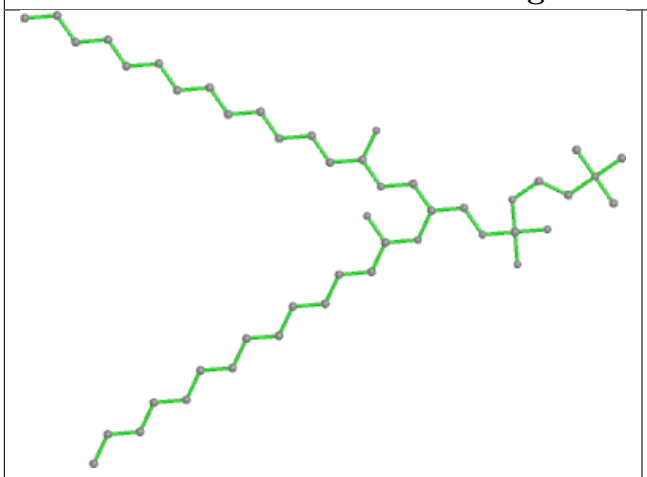


Rings

Ligand PX4 A 380



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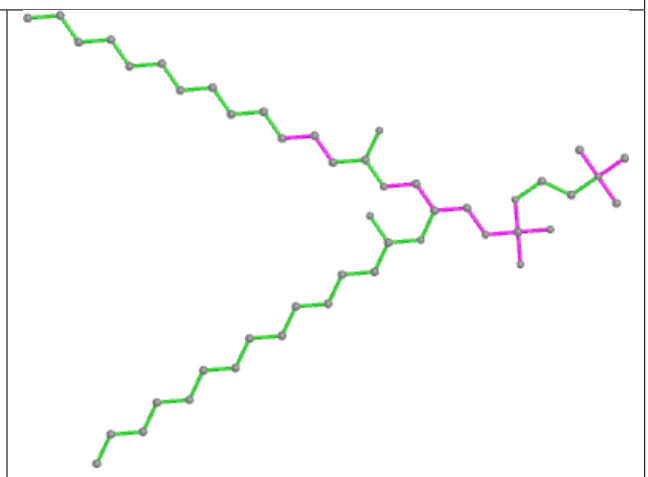

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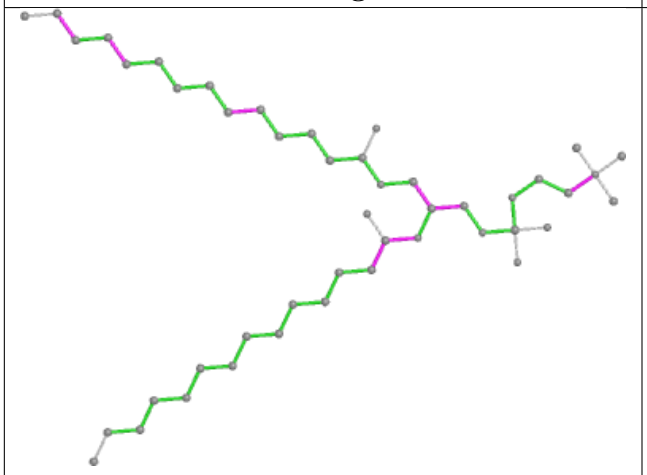

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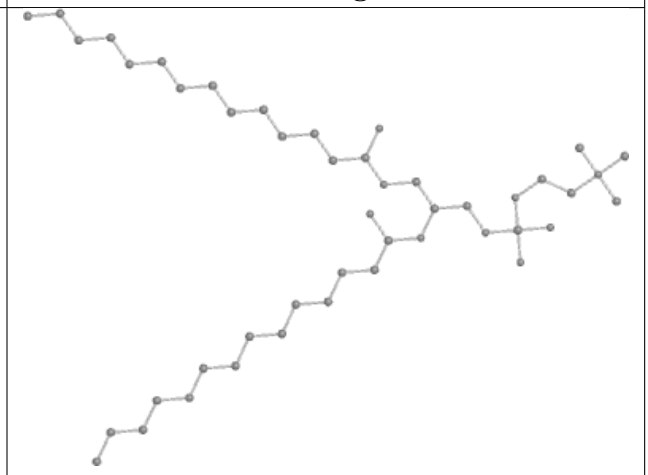
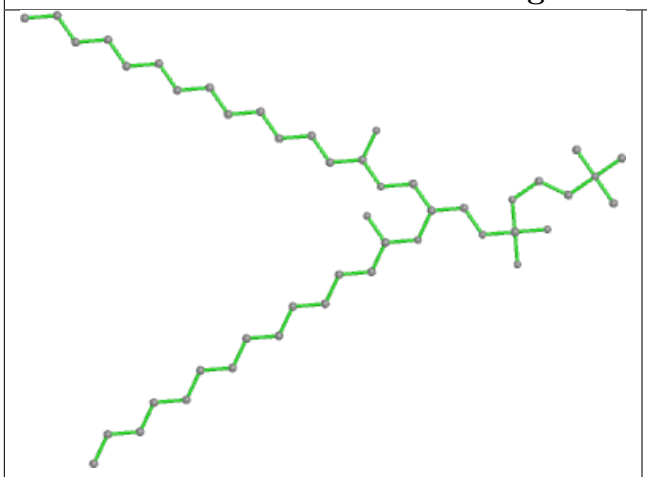


Rings

Ligand PX4 A 341



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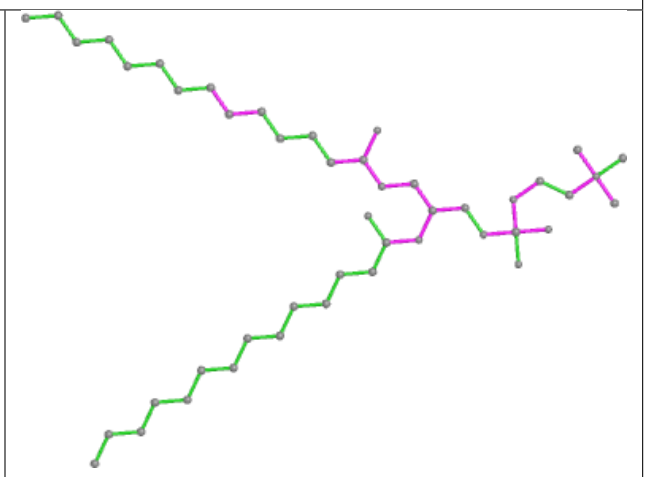

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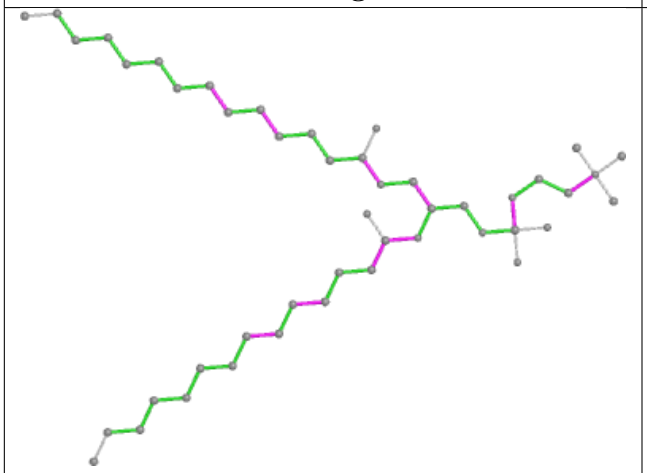

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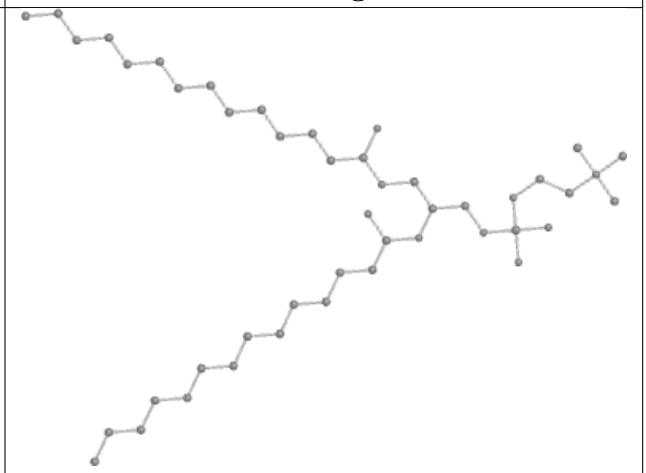
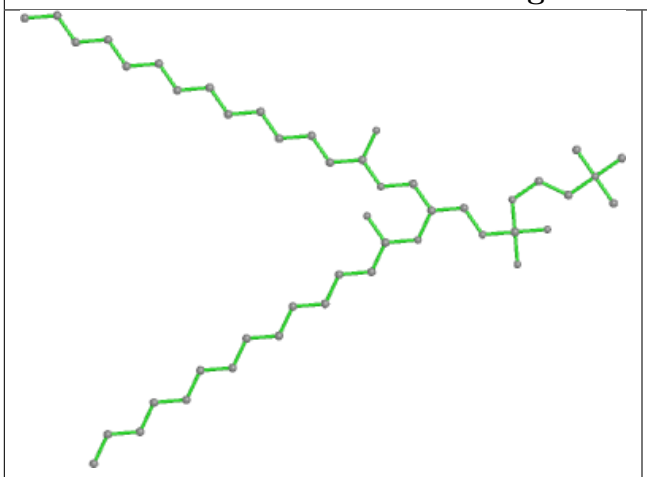


Rings

Ligand PX4 A 399



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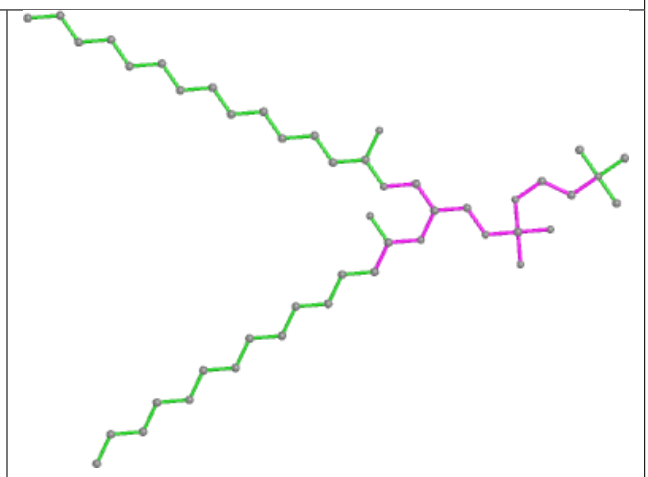

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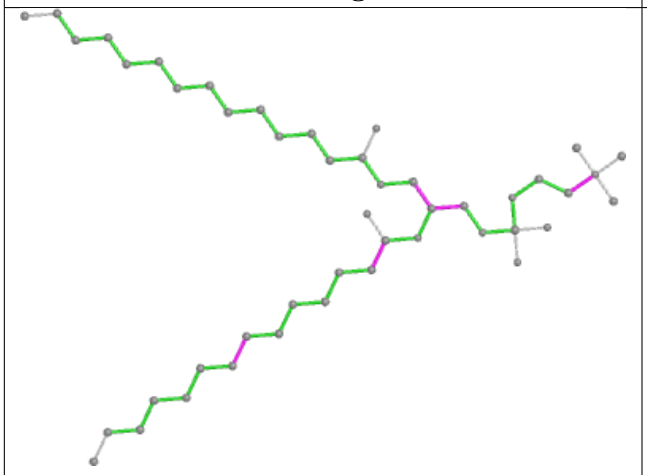

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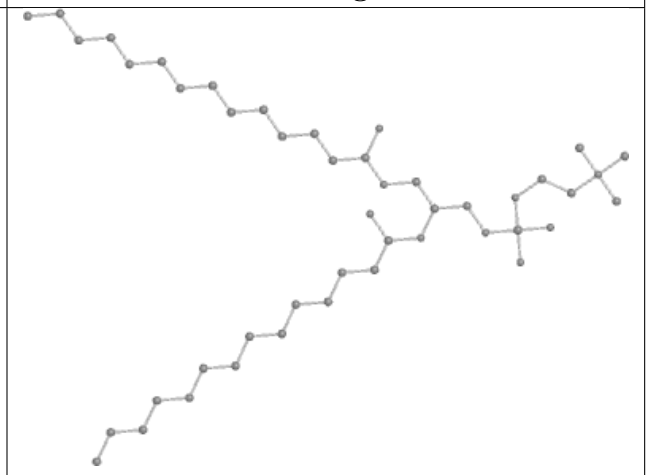
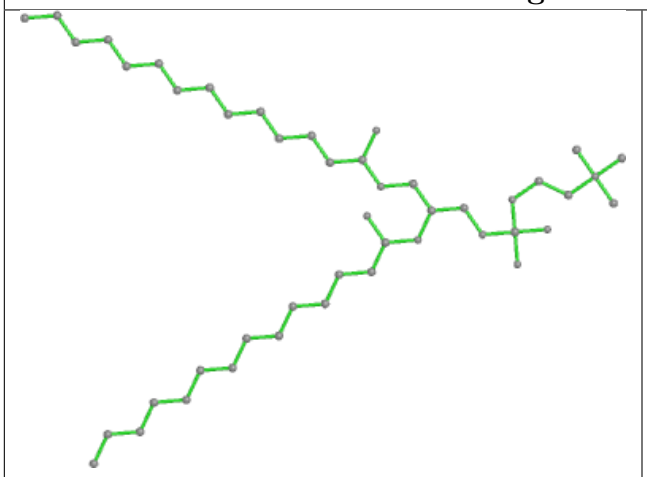


Rings

Ligand PX4 A 365



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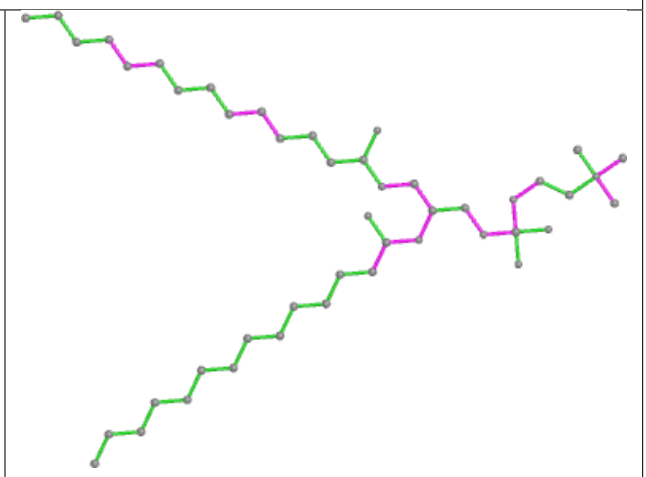
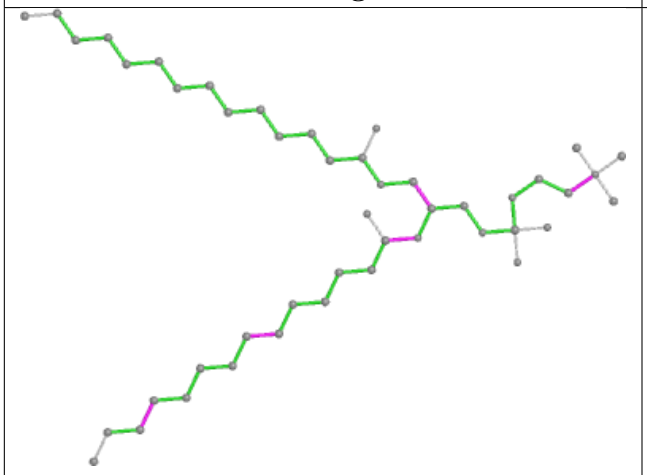


Bond angles



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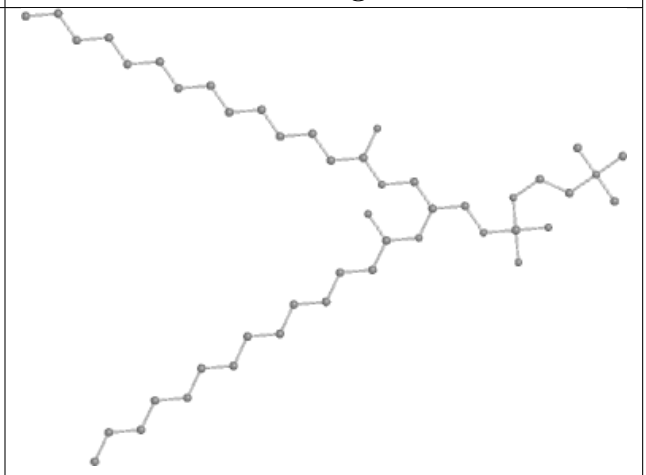
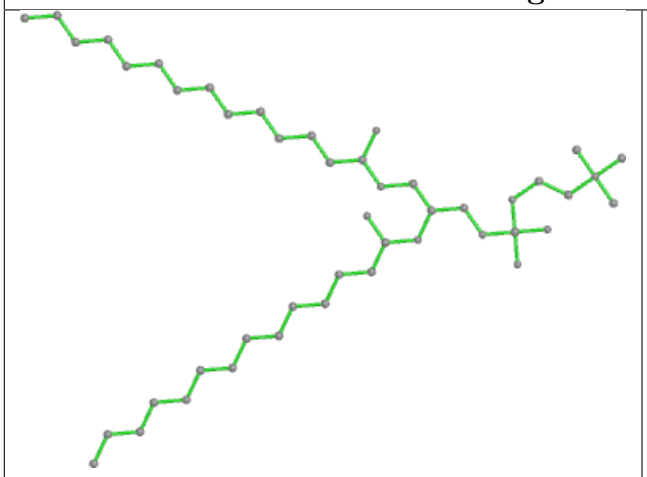


Rings

Ligand PX4 A 391



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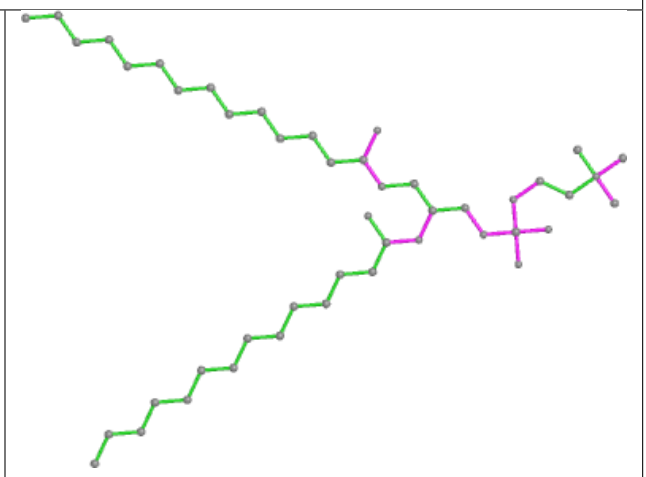
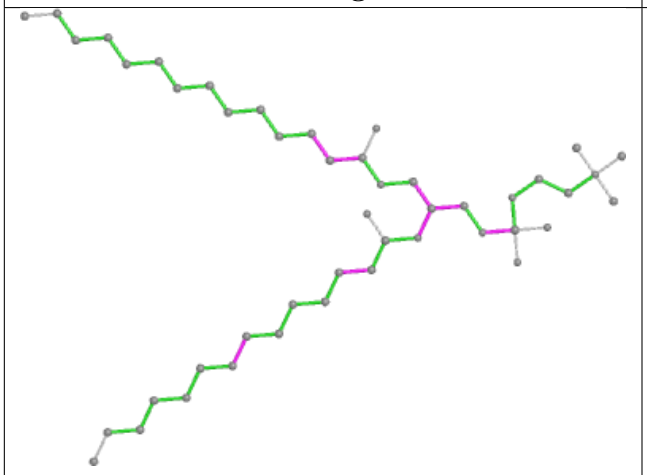


Bond angles



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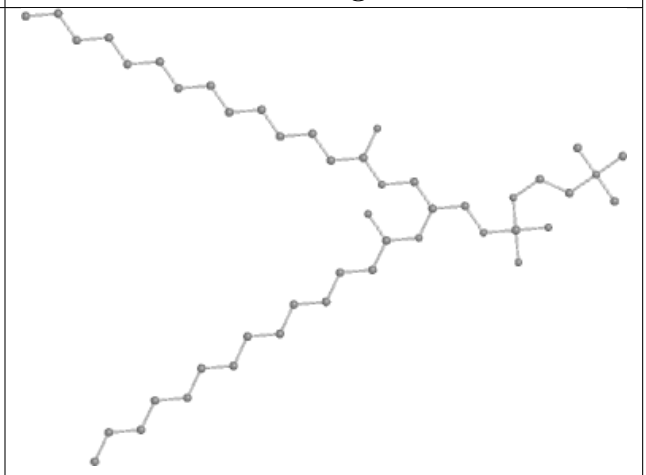
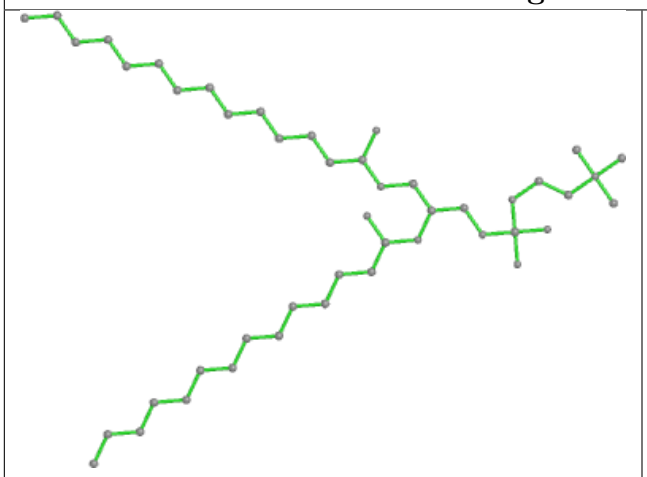


Rings

Ligand PX4 A 367



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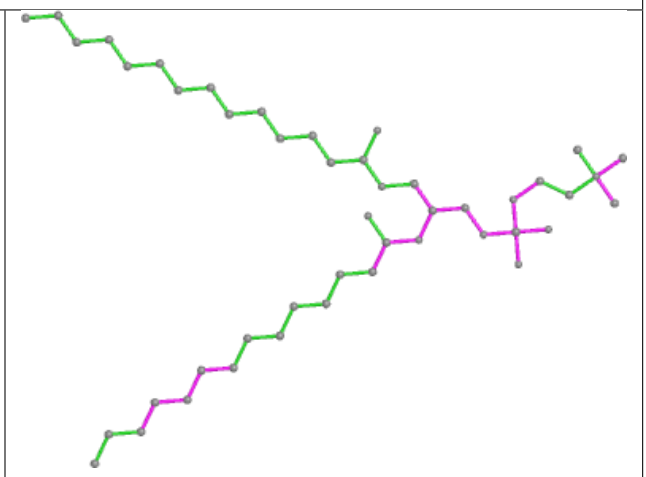
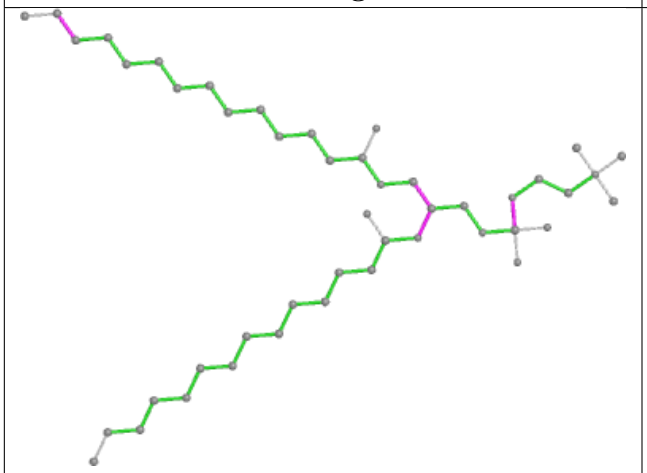


Bond angles



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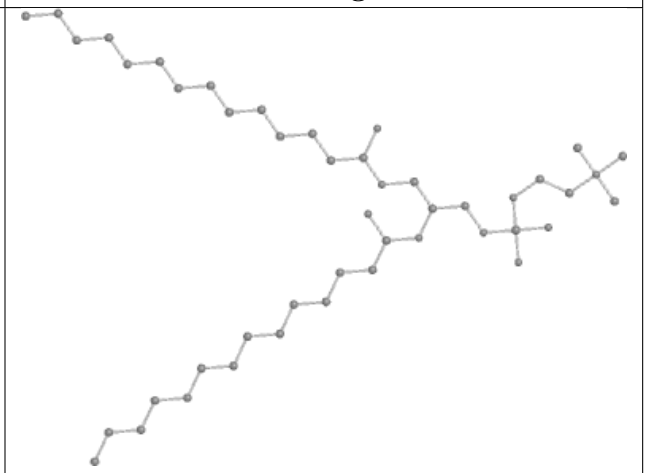
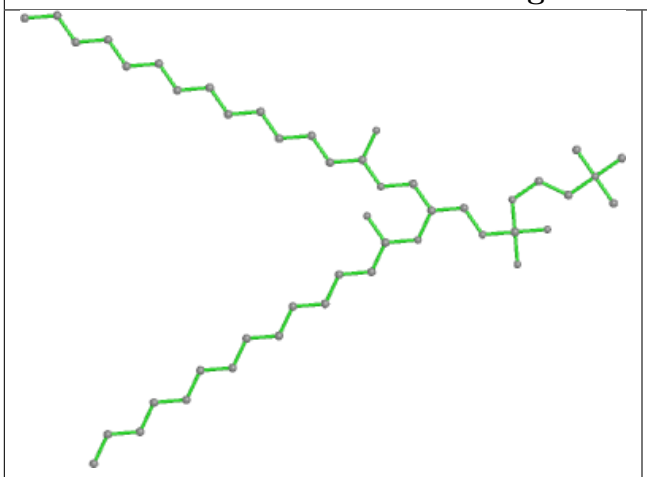


Rings

Ligand PX4 A 386



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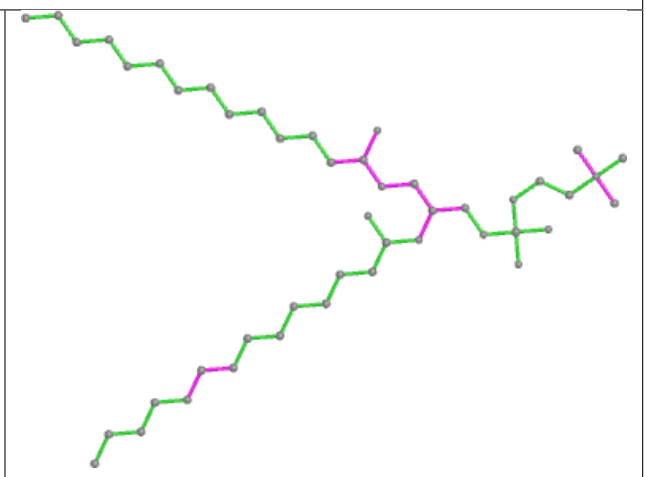
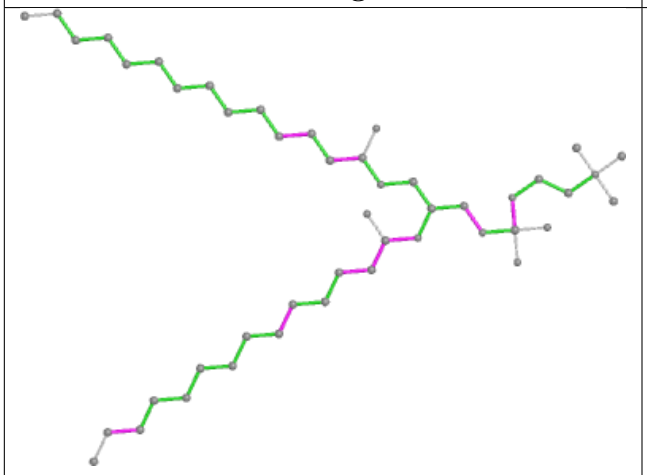
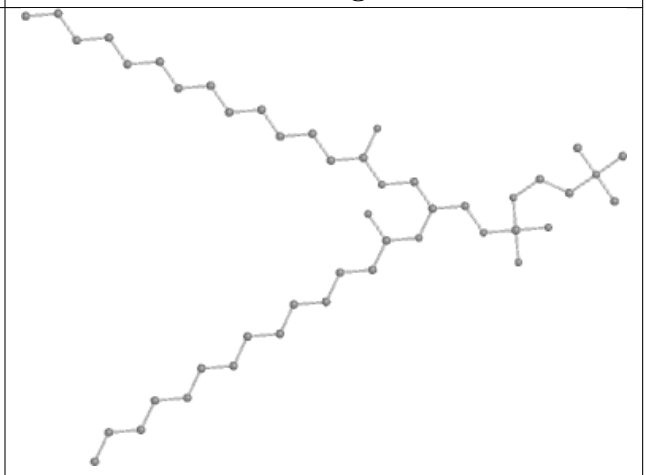


Bond angles

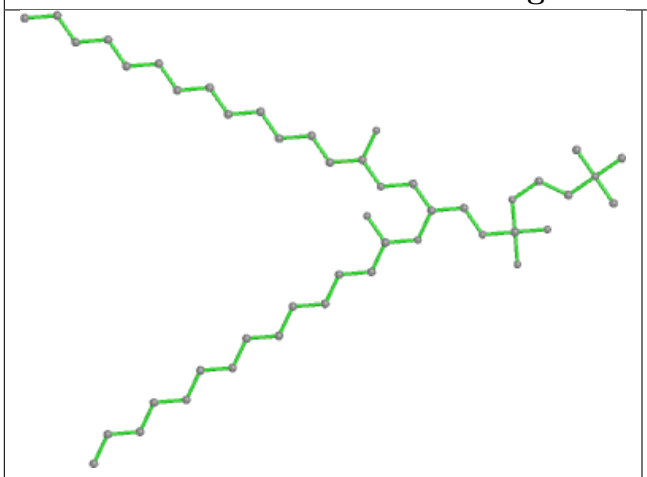


Torsions



Rings

Ligand PX4 A 429



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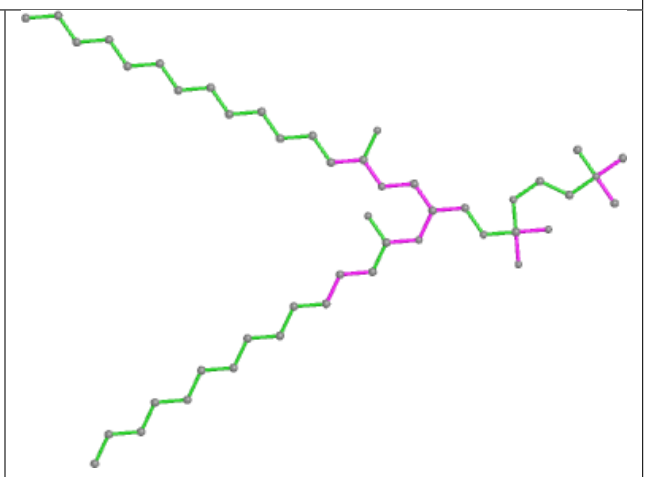
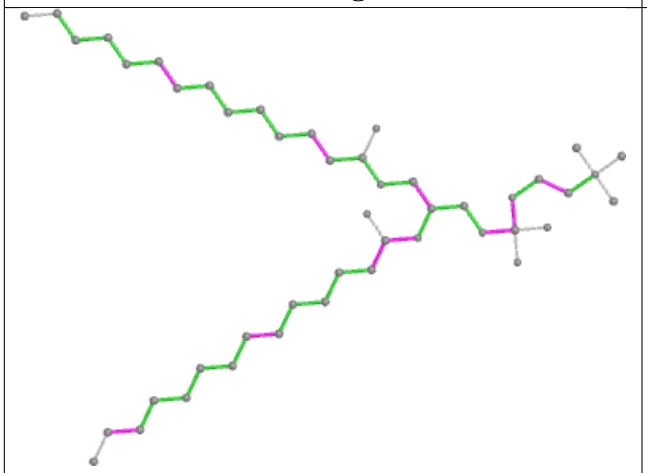


Bond angles



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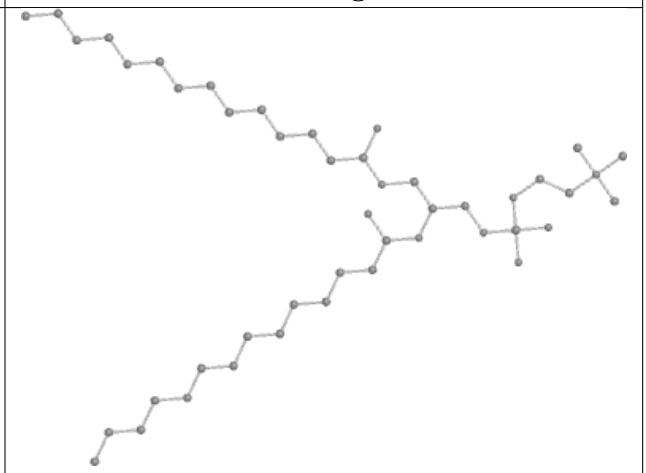
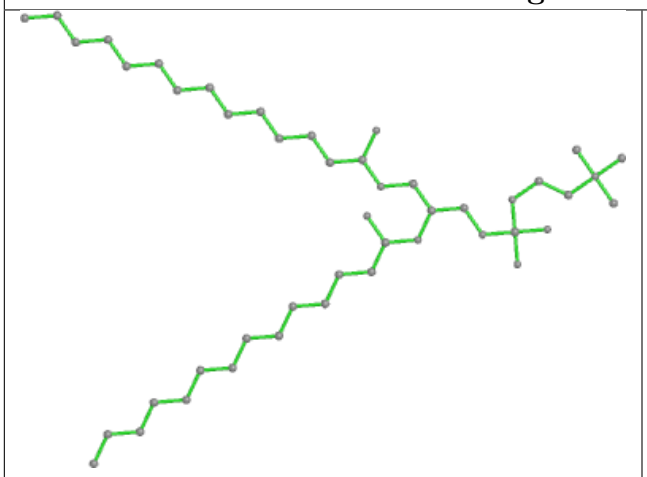


Rings

Ligand PX4 A 369



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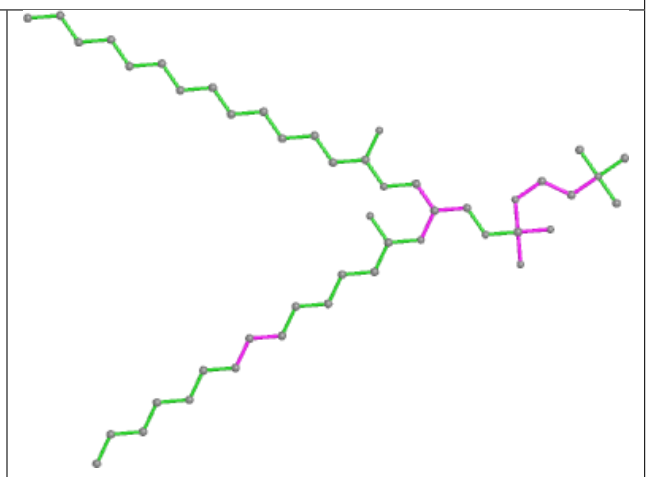
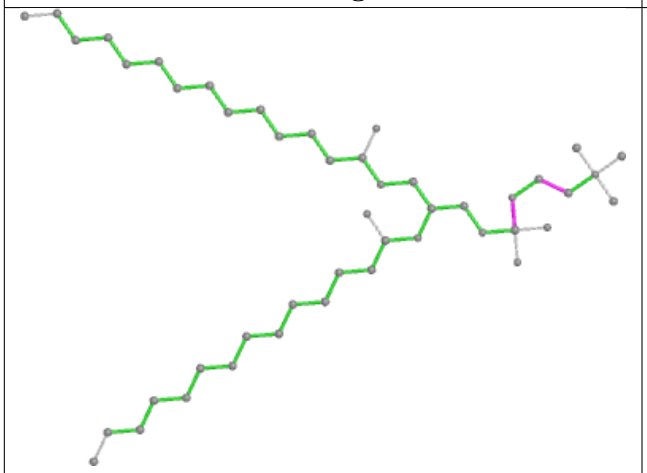


Bond angles



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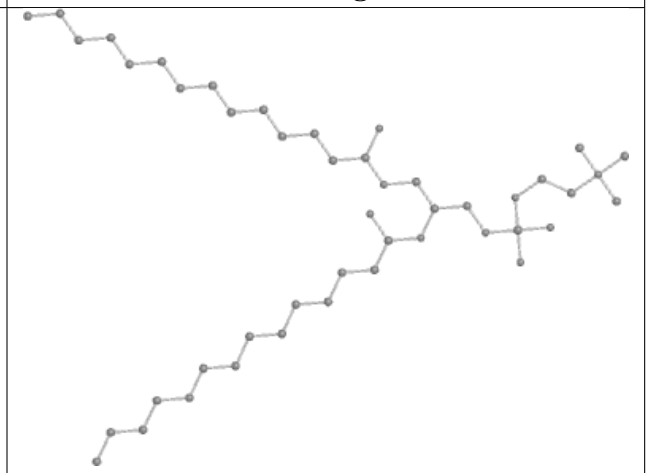
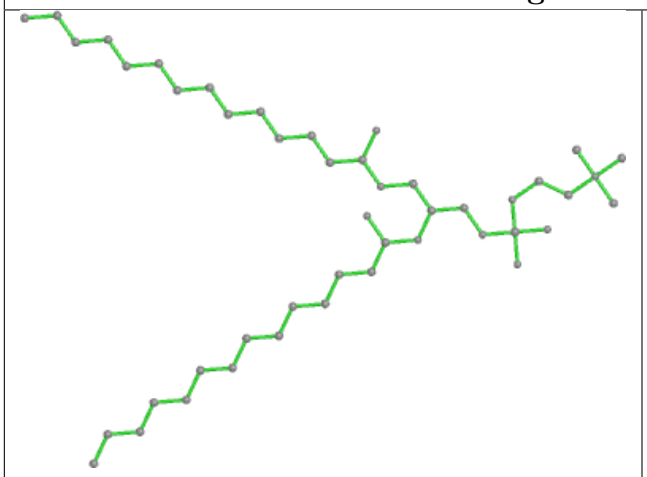


Rings

Ligand PX4 A 350



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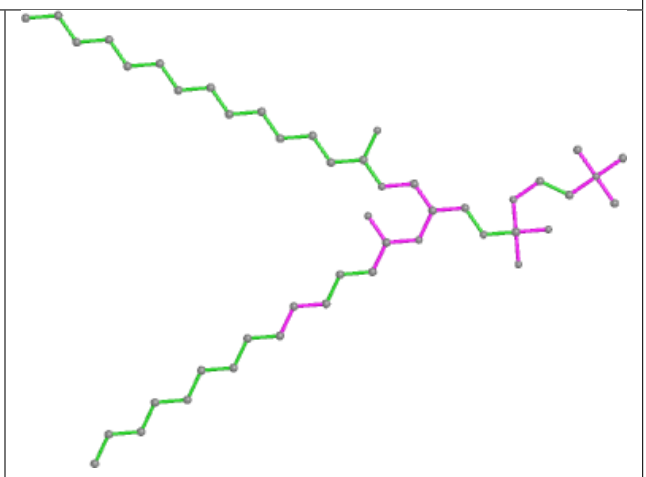
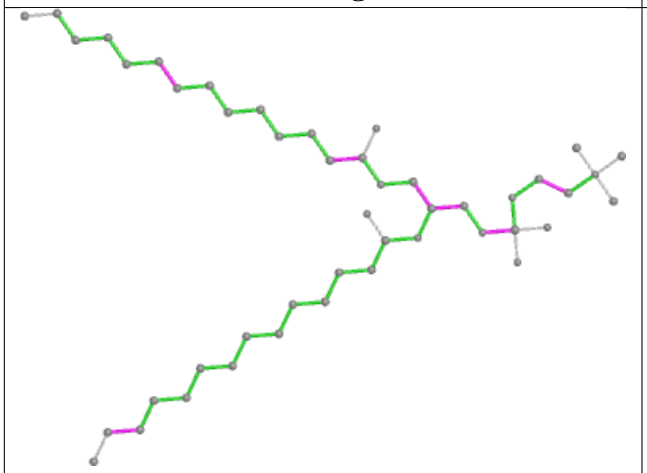


Bond angles



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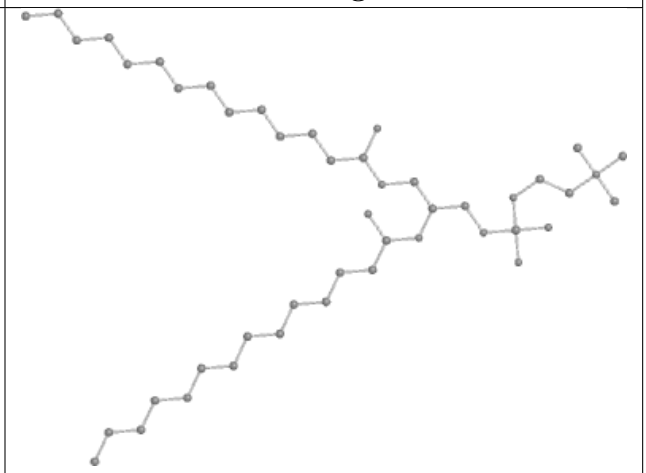
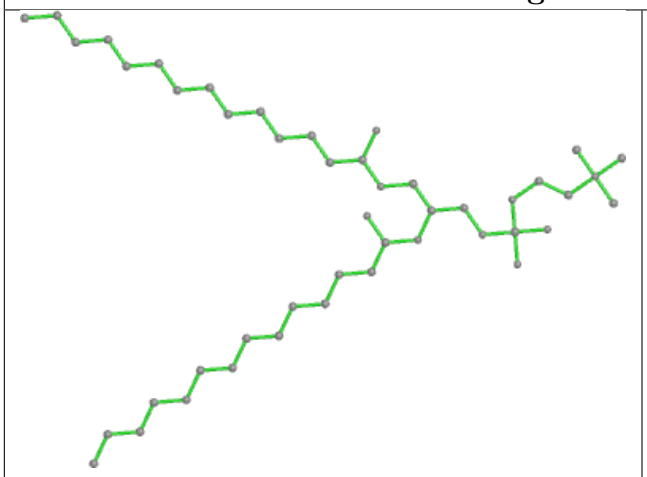


Rings

Ligand PX4 A 353



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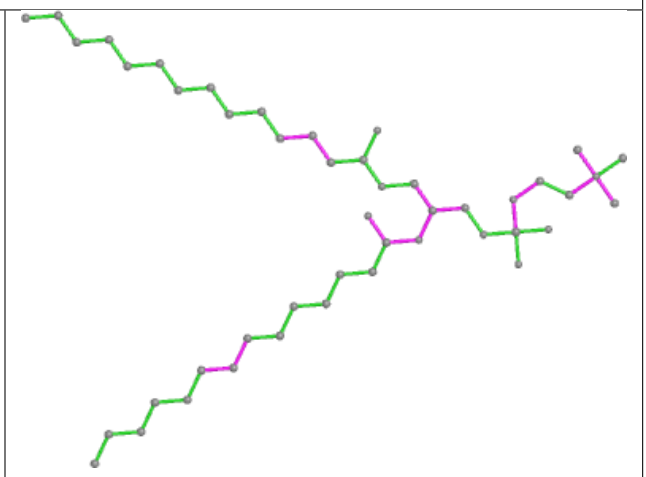
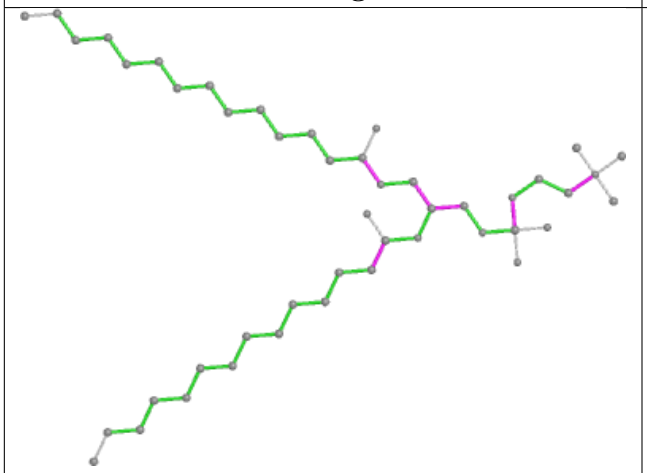


Bond angles



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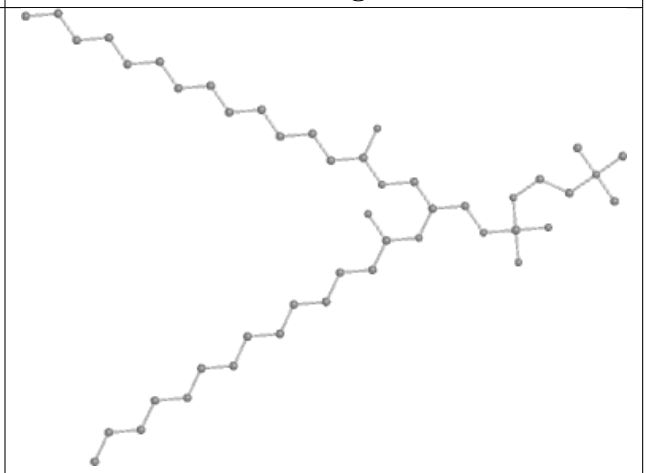
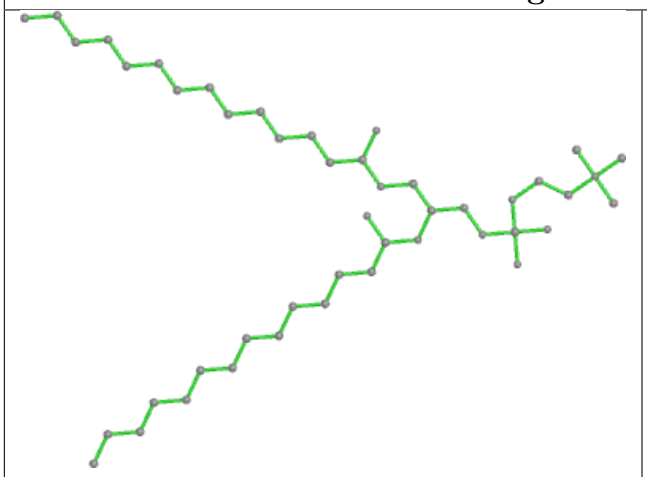


Rings

Ligand PX4 A 408



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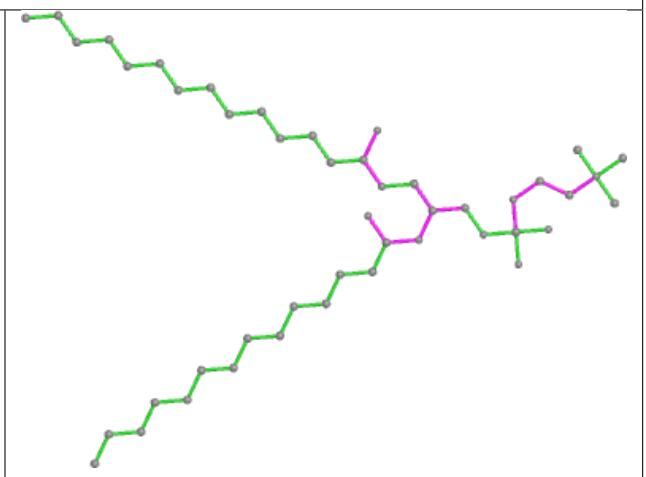
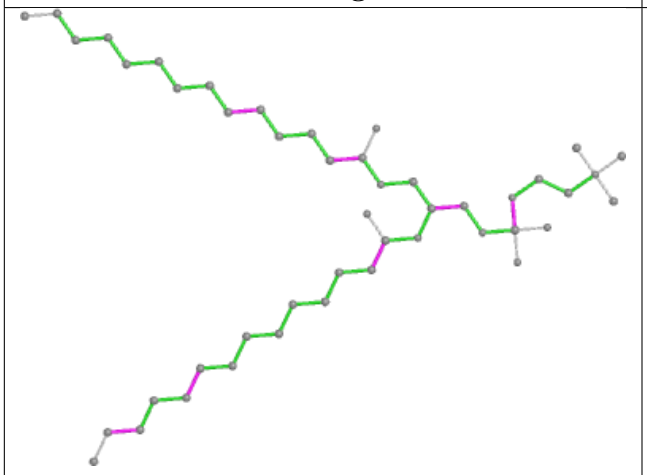


Bond angles



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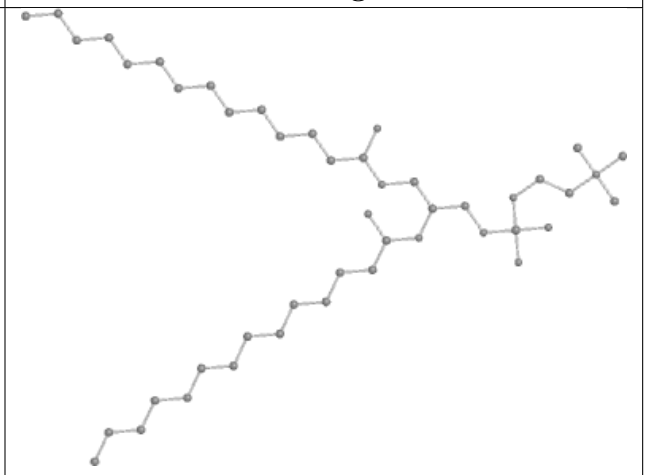
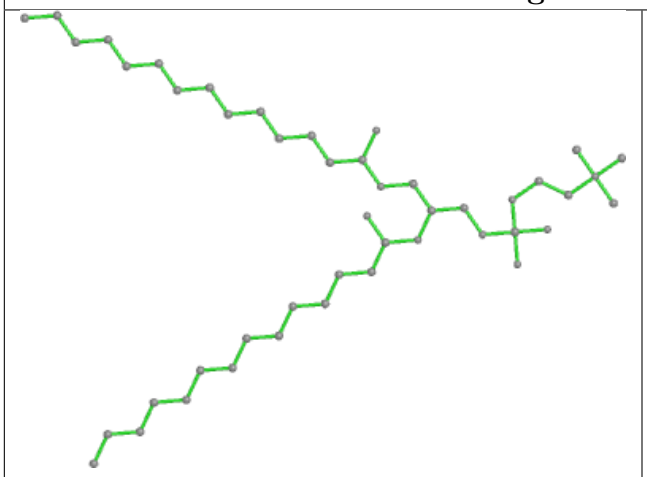


Rings

Ligand PX4 A 338



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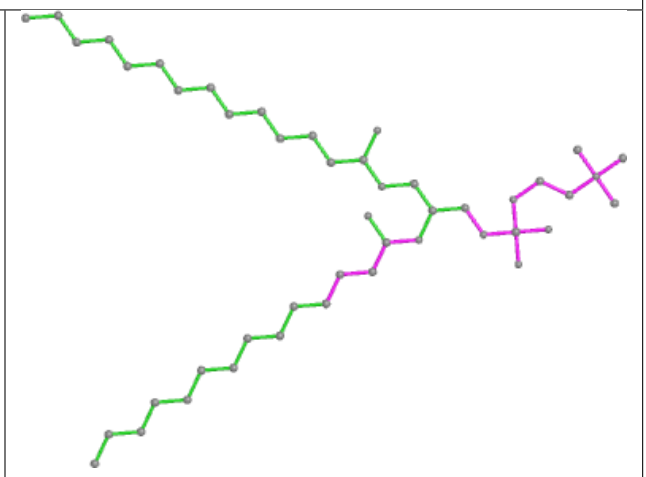

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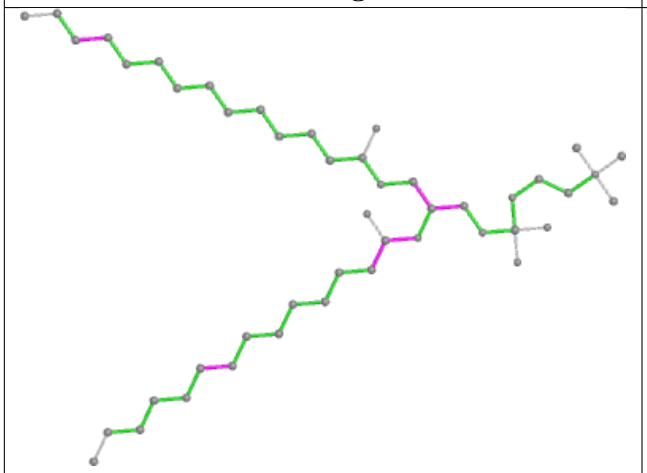

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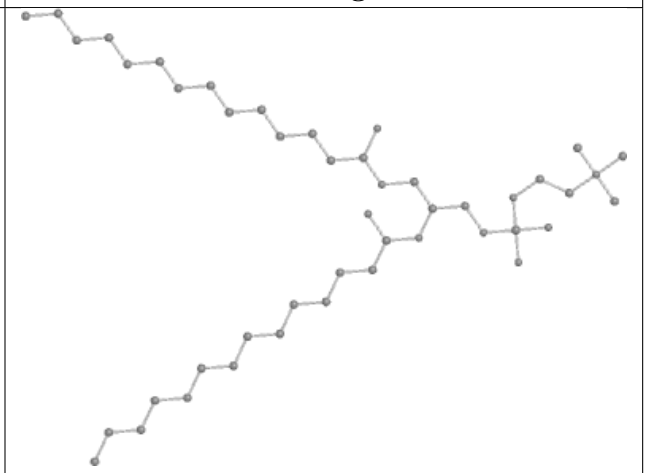
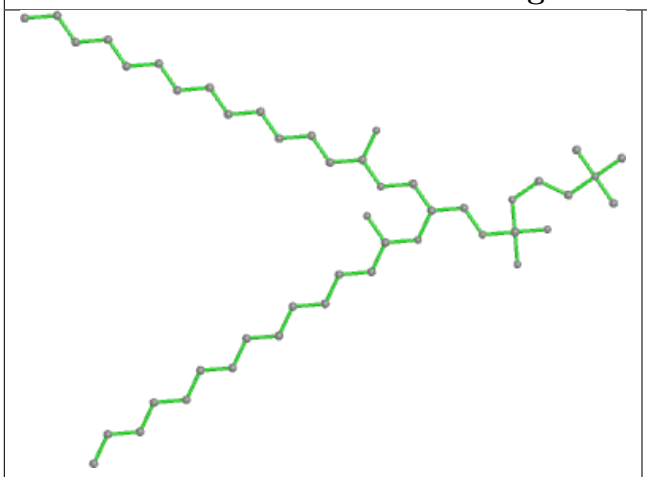


Rings

Ligand PX4 A 352



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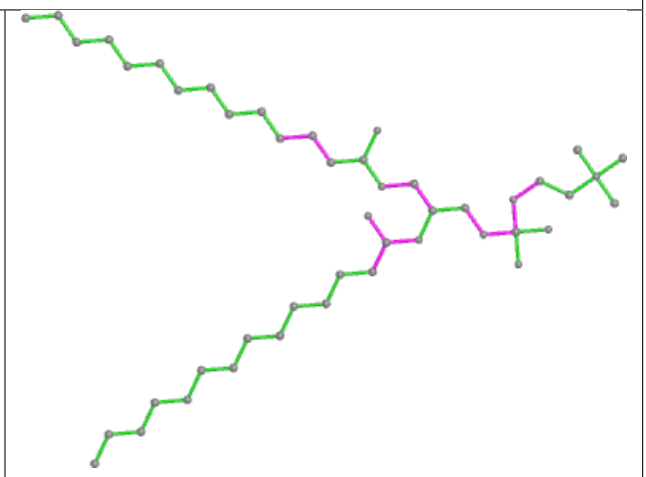

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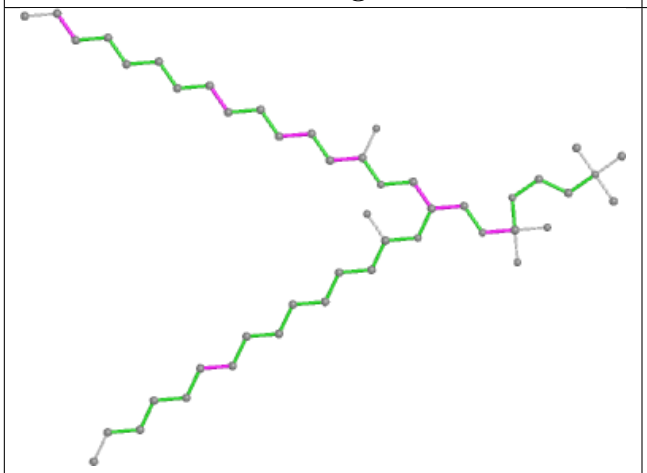

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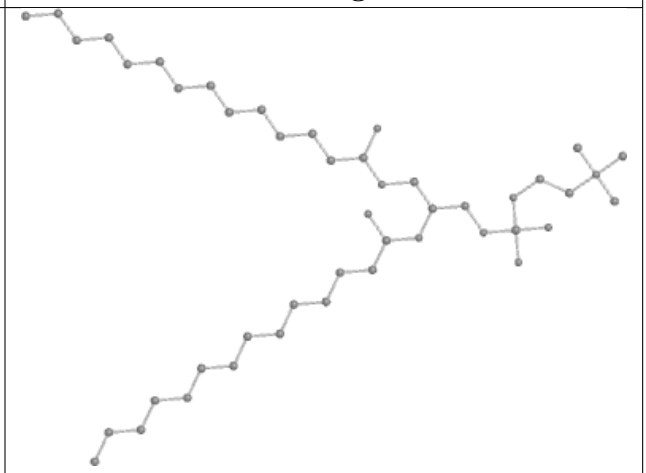
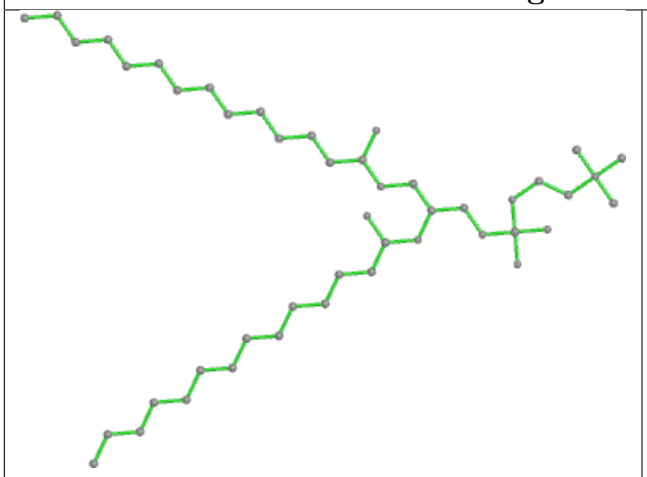


Rings

Ligand PX4 A 390



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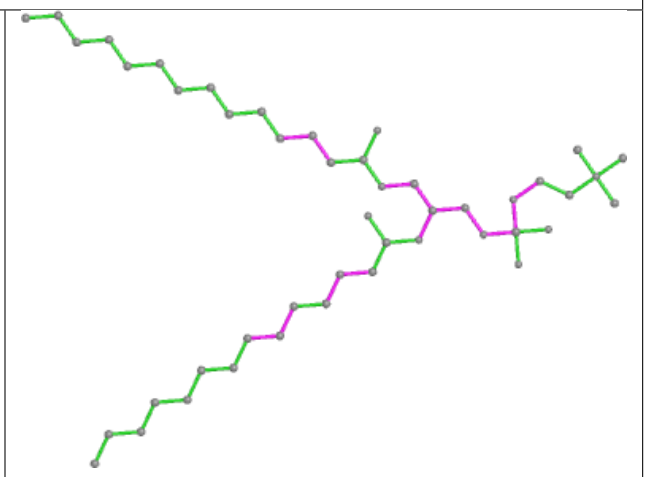
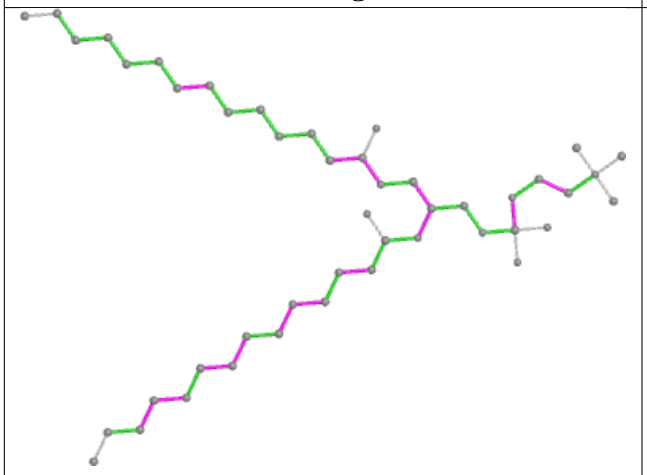


Bond angles



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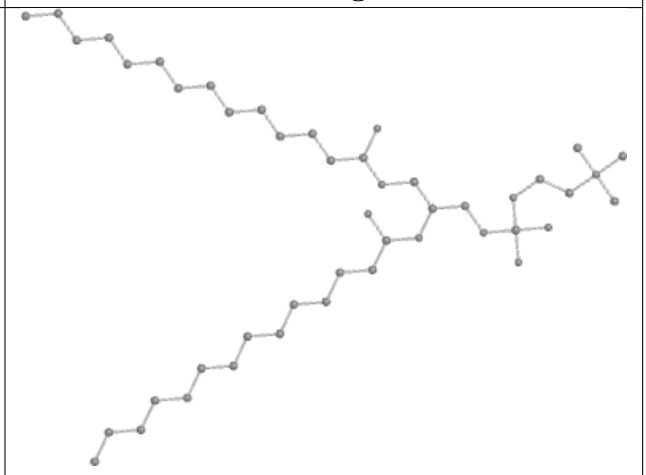
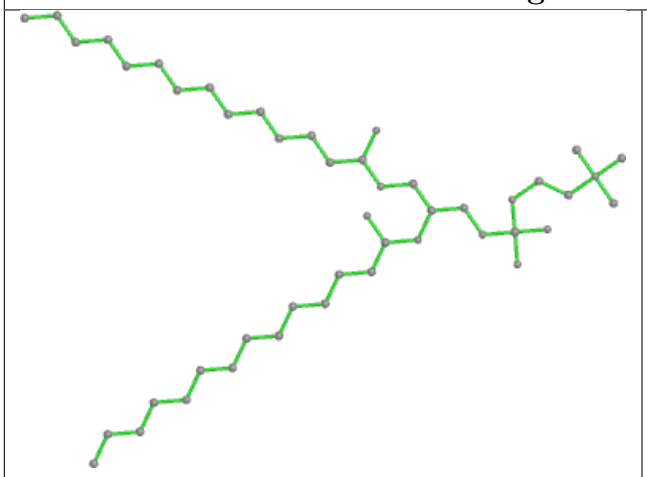


Rings

Ligand PX4 A 314



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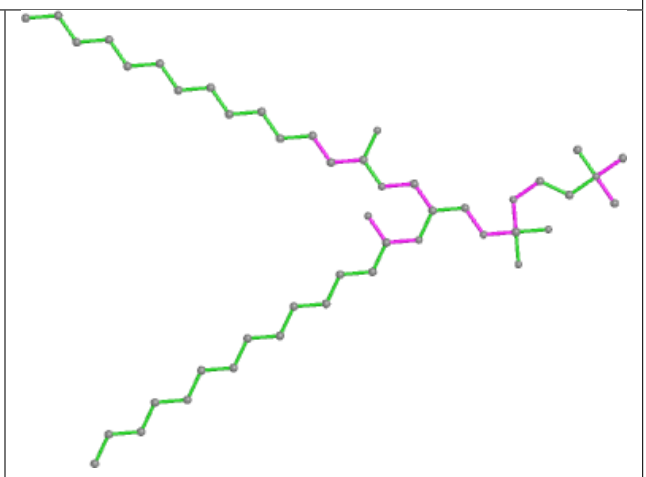

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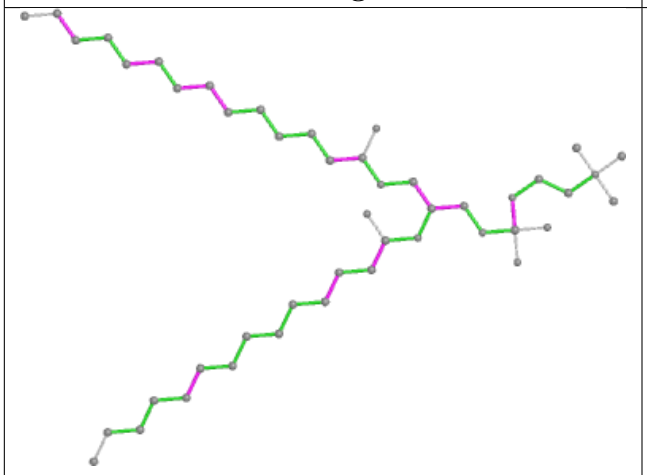

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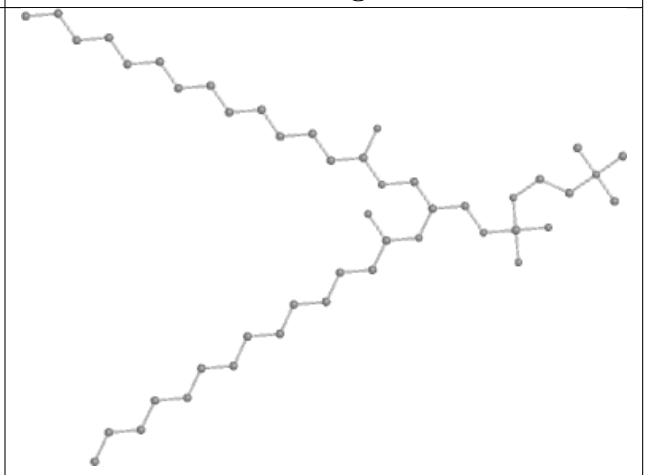
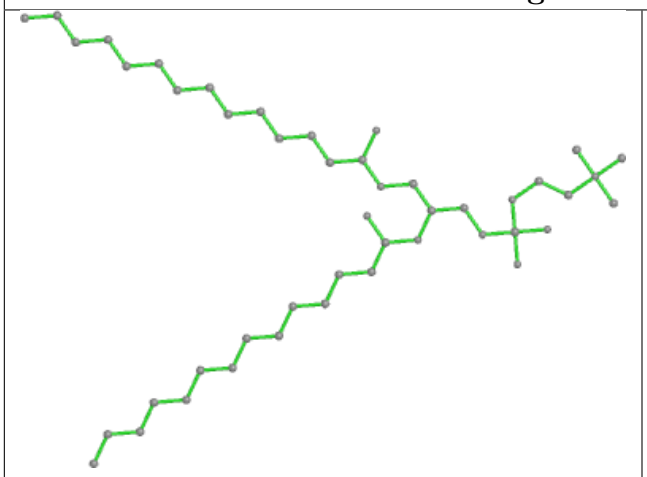


Rings

Ligand PX4 A 371



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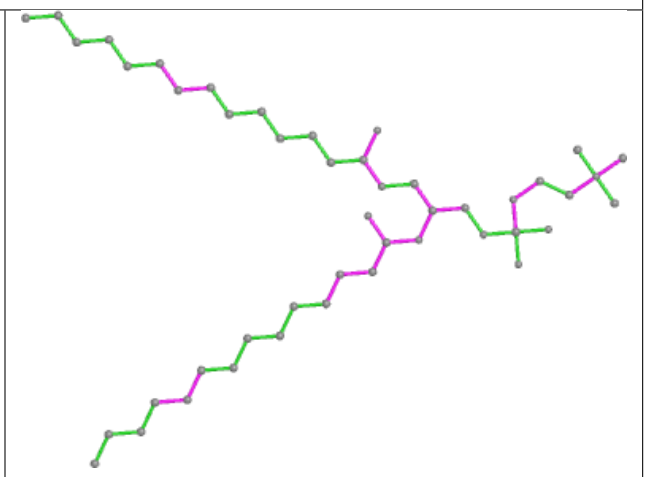
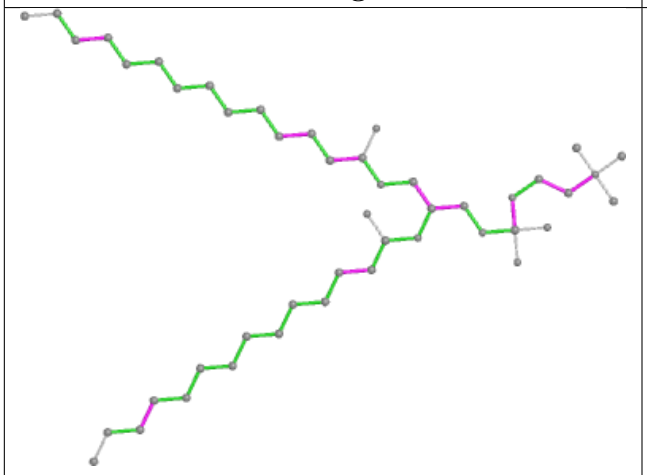


Bond angles



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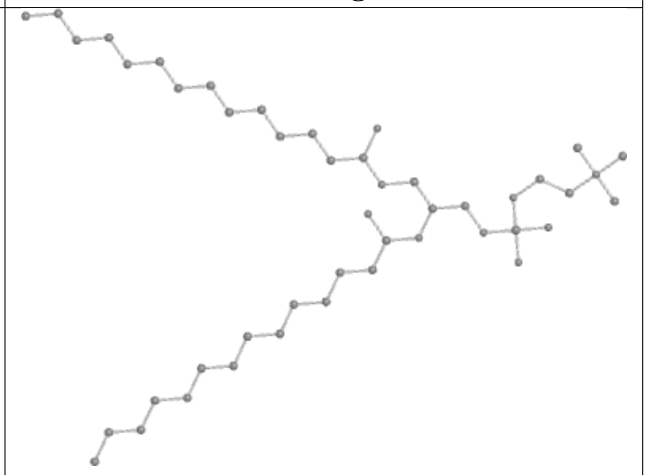
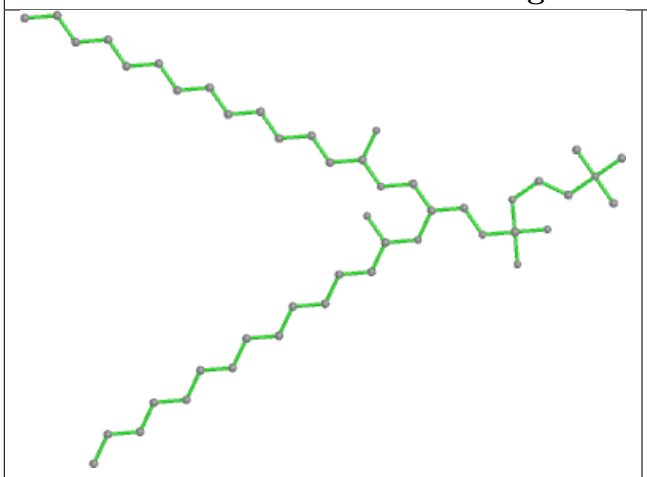


Rings

Ligand PX4 A 324



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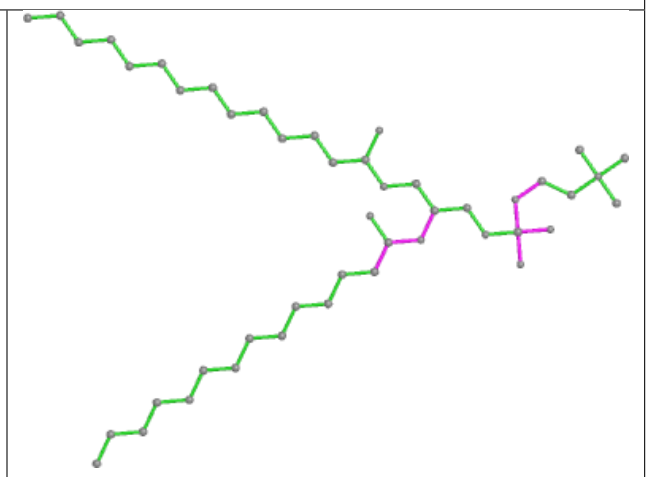
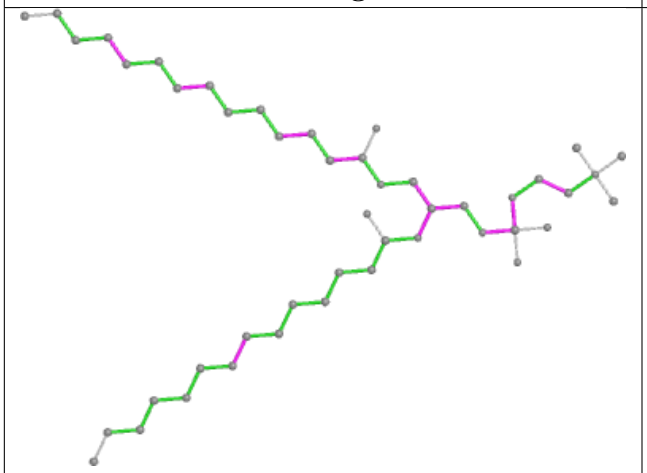


Bond angles



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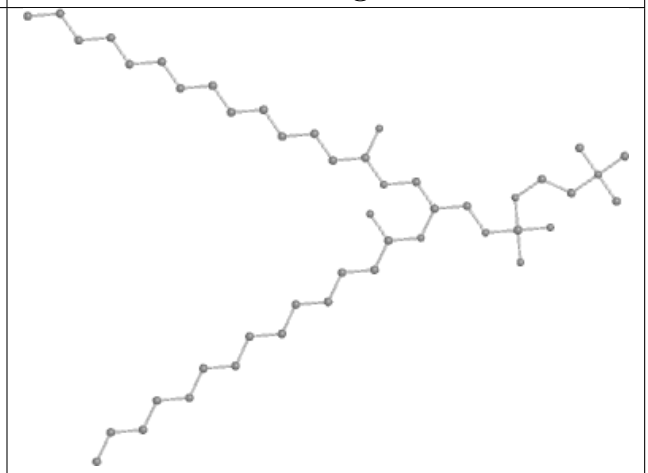
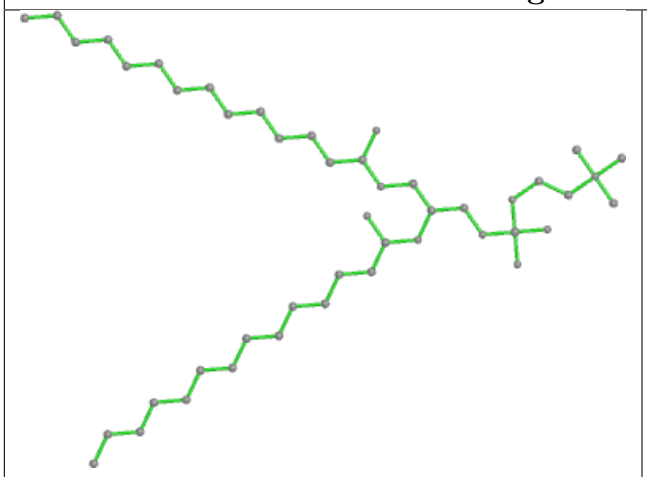


Rings

Ligand PX4 A 398



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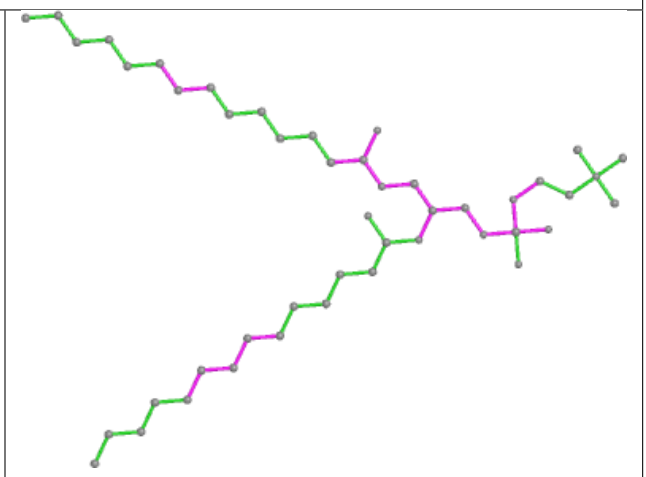
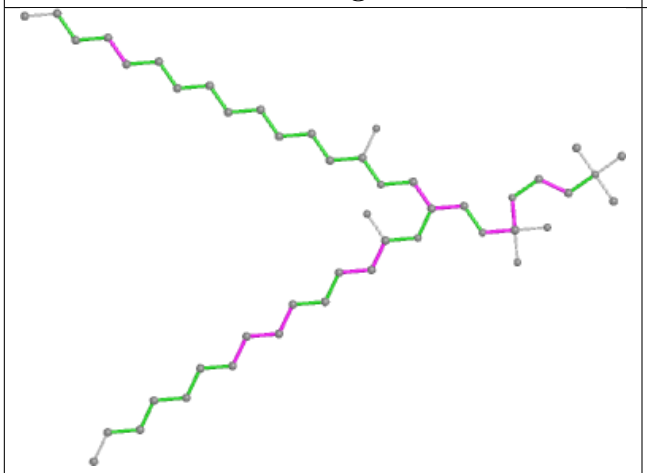


Bond angles



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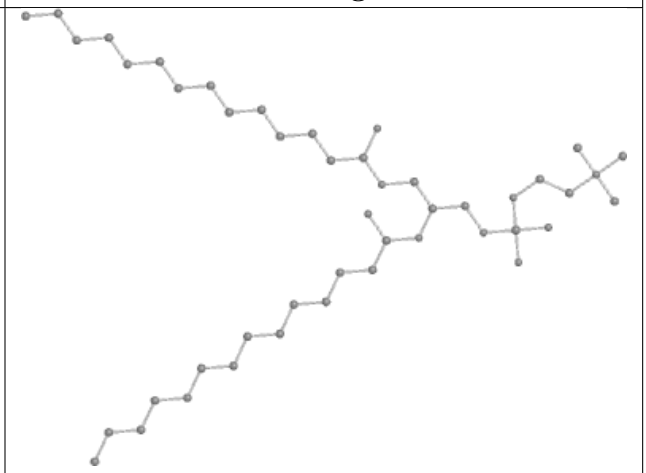
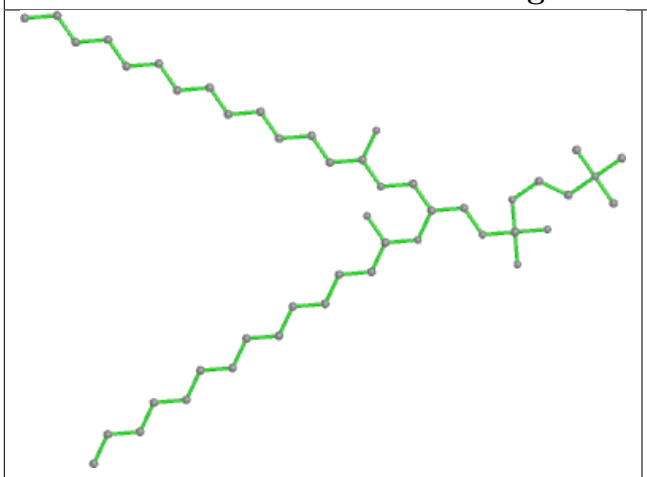


Rings

Ligand PX4 A 349



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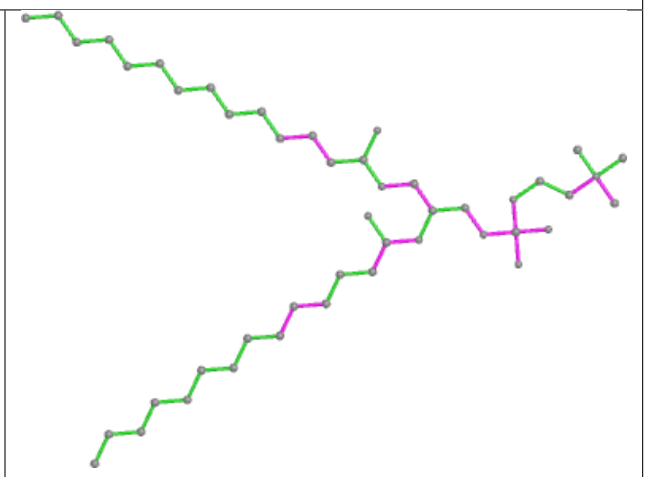
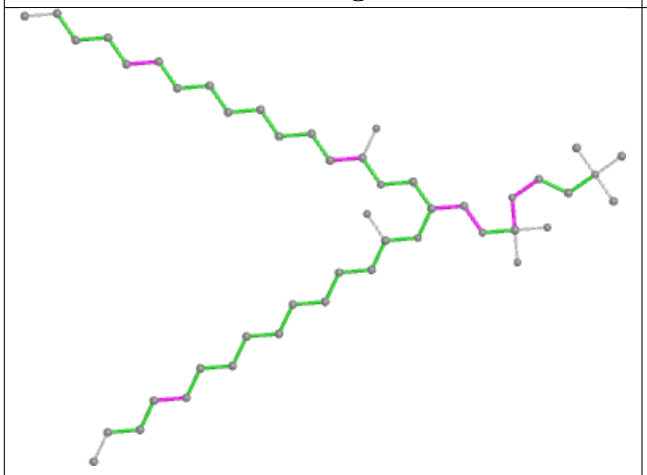
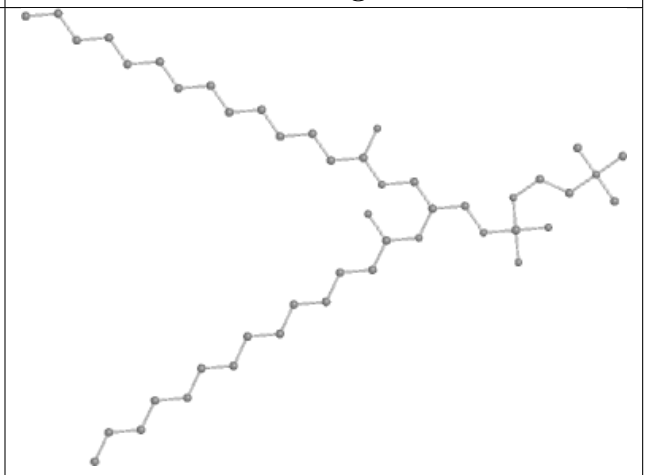


Bond angles

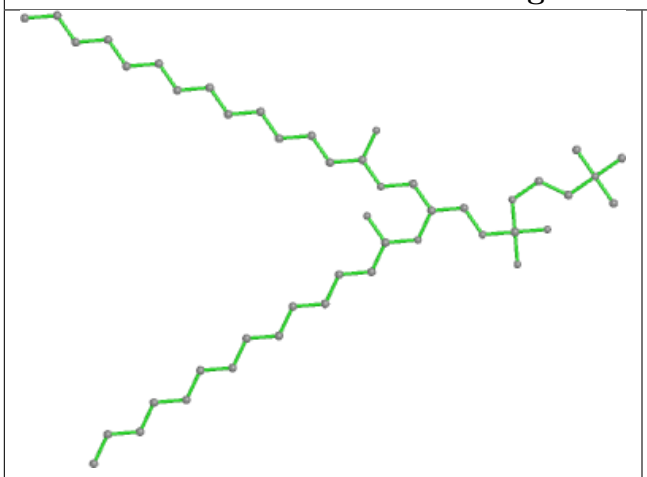


Torsions

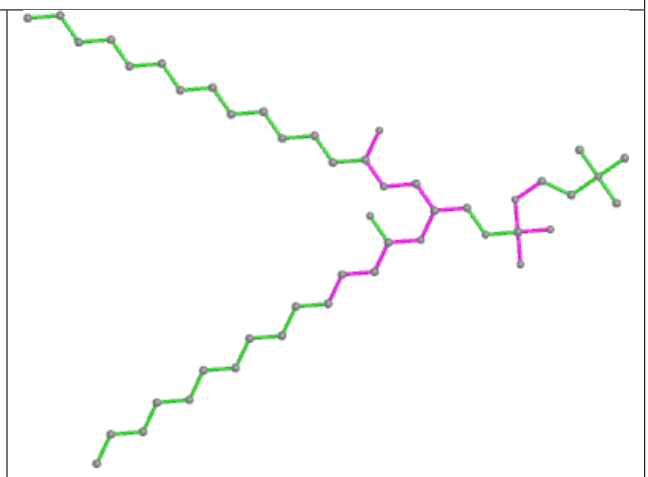


Rings

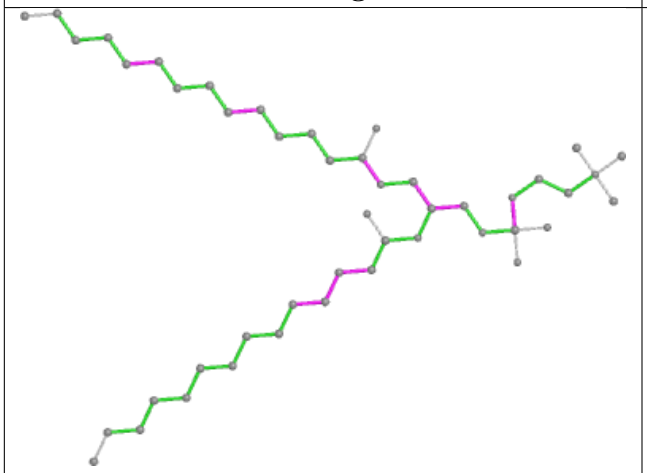
Ligand PX4 A 337



Bond lengths



Bond angles



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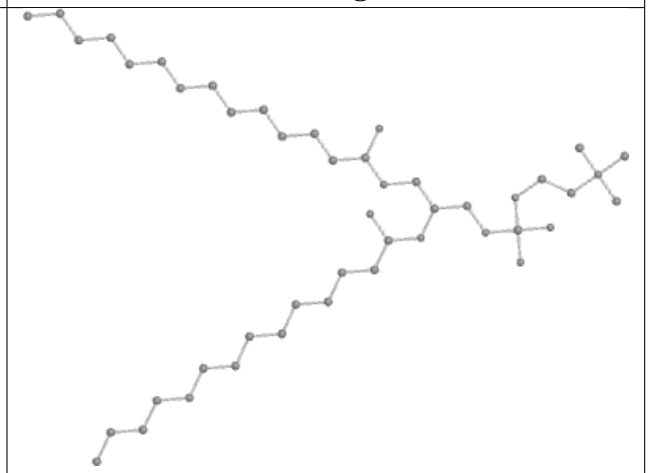
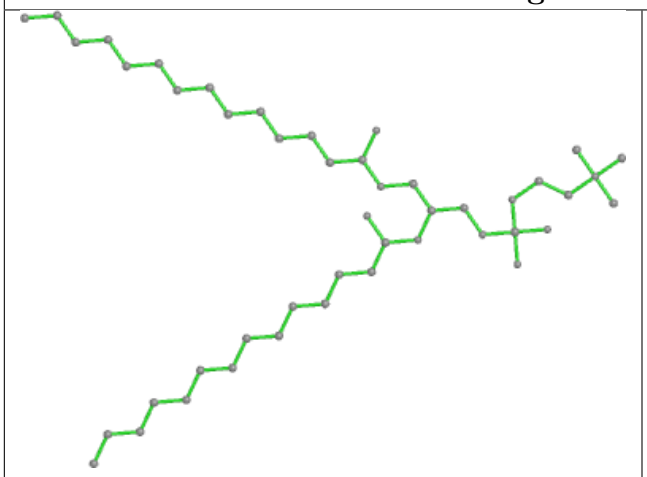


Rings

Ligand PX4 A 351



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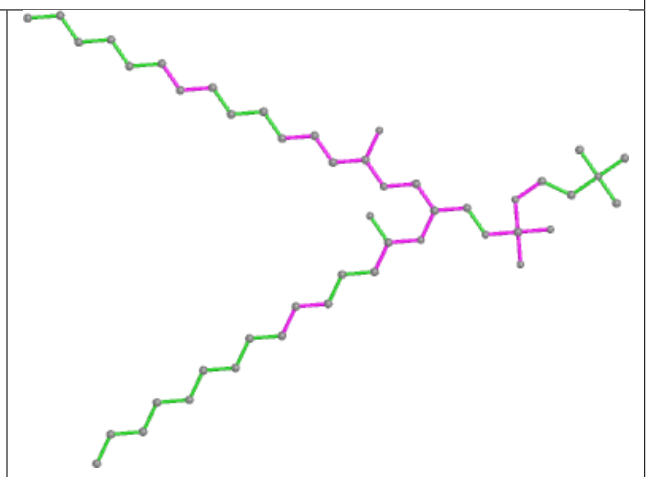

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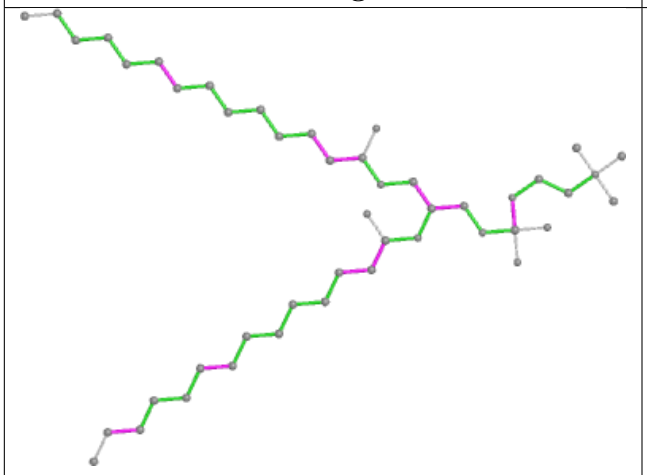

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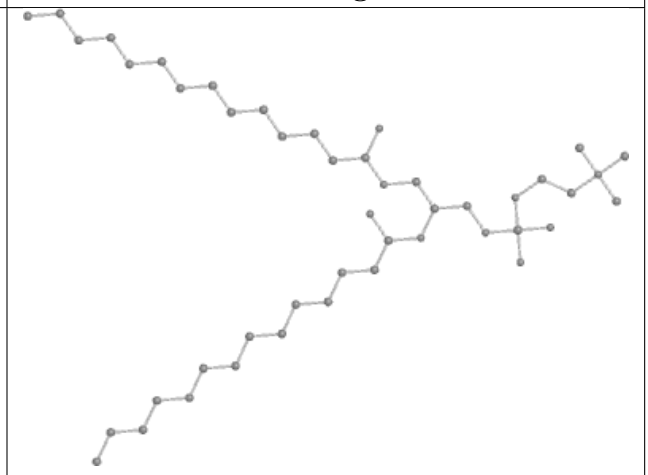
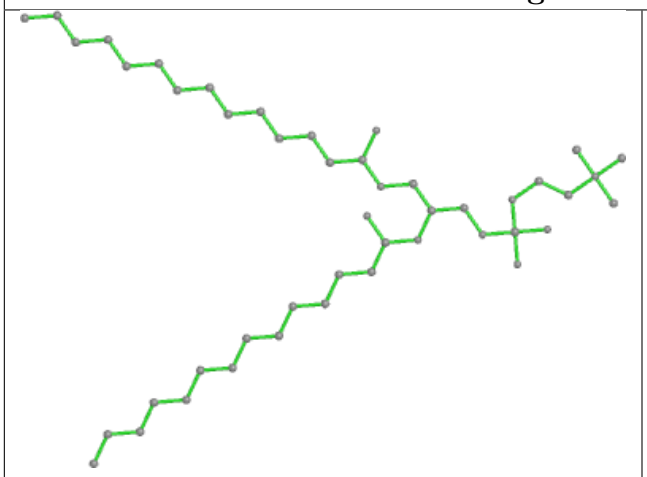


Rings

Ligand PX4 A 348



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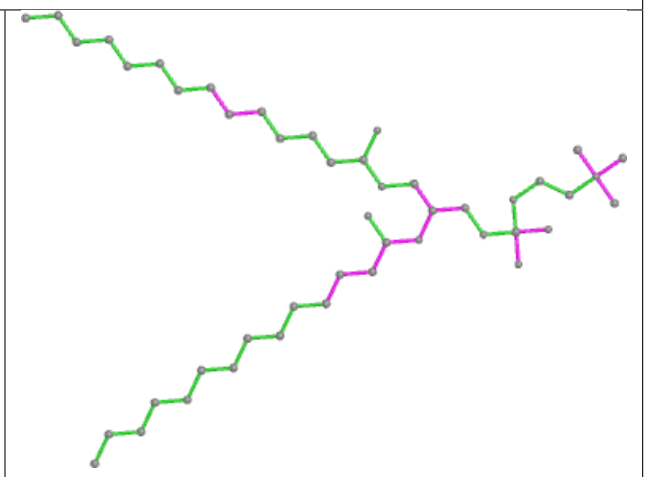

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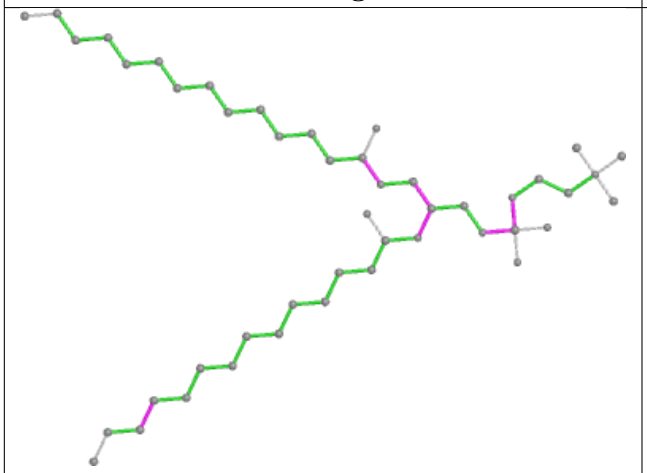

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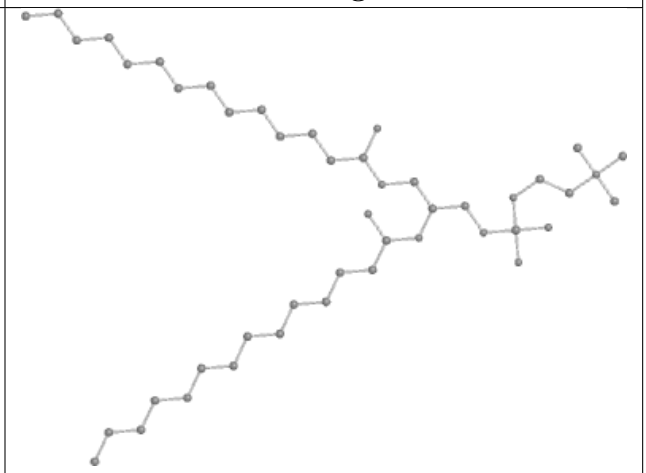
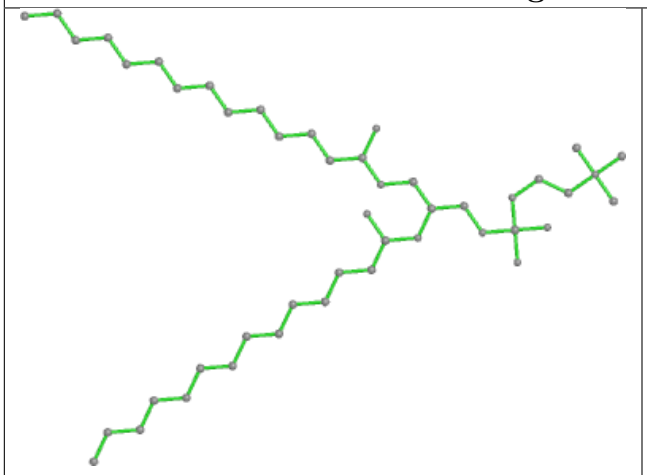


Rings

Ligand PX4 A 431



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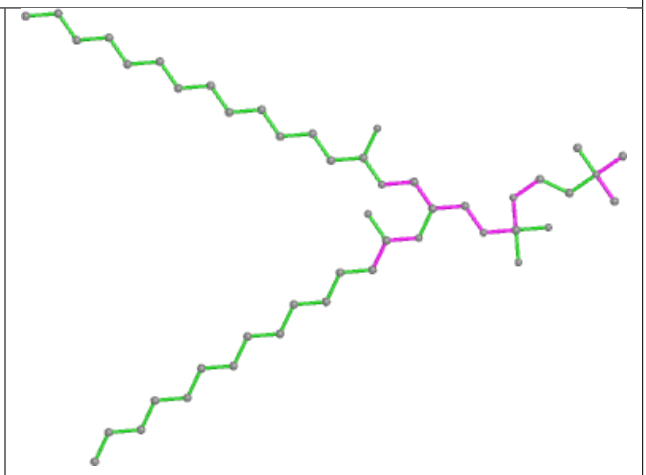
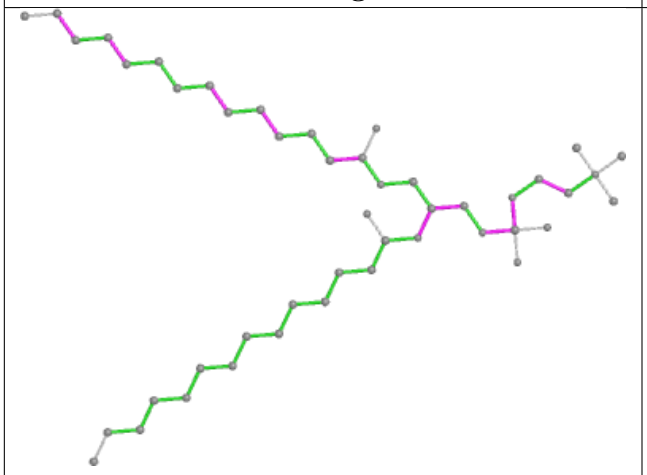


Bond angles



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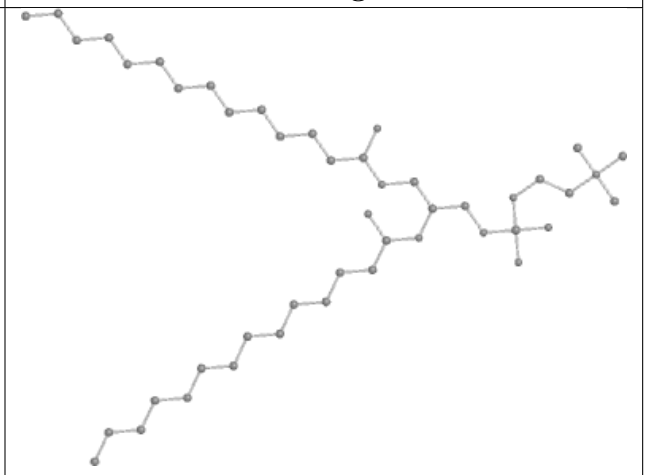
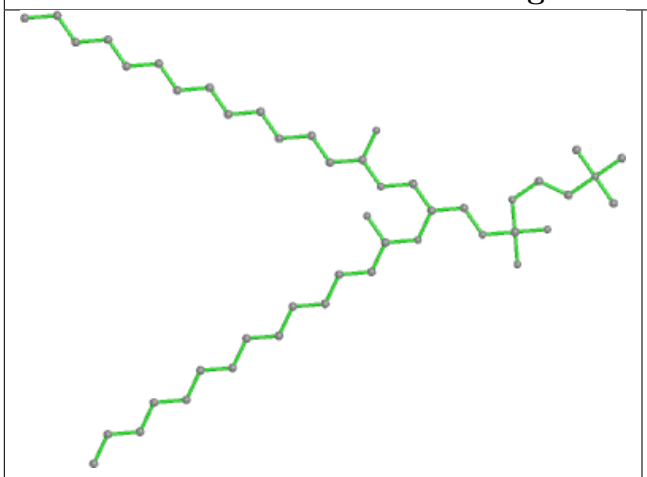


Rings

Ligand PX4 A 335



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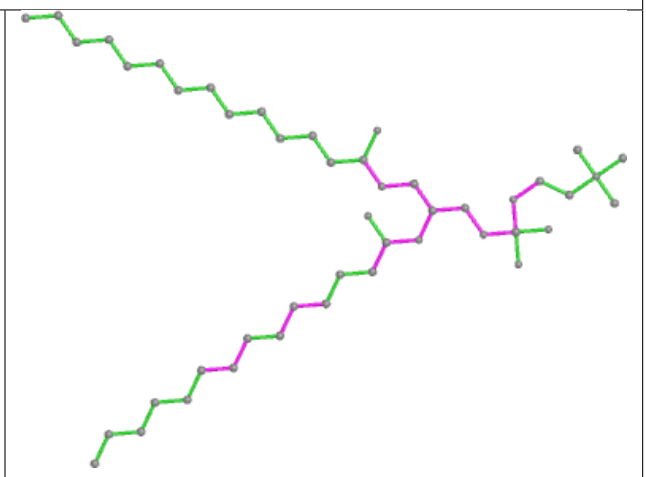

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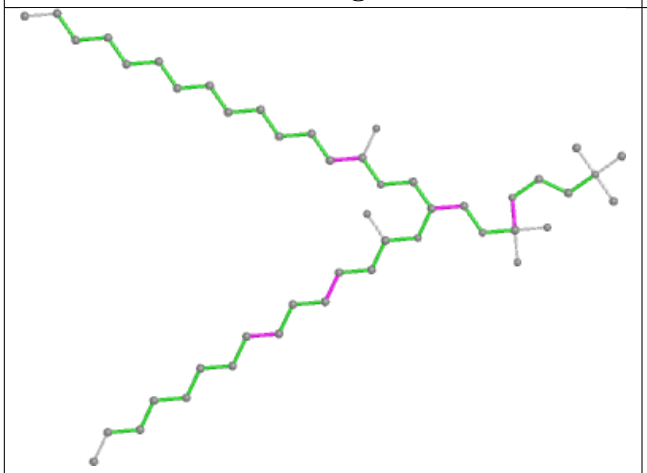

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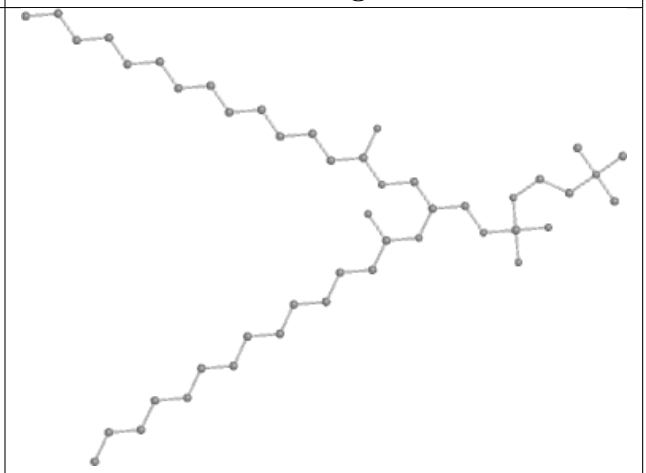
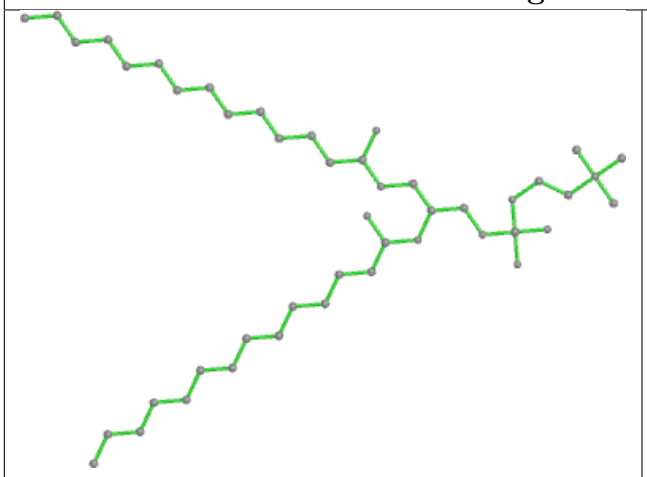


Rings

Ligand PX4 A 354



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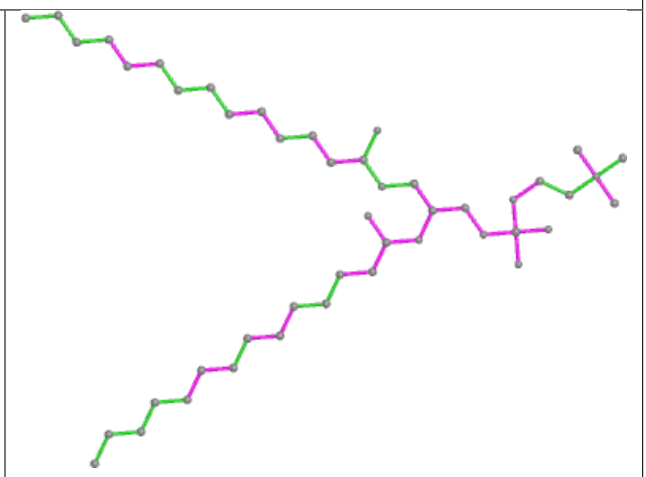

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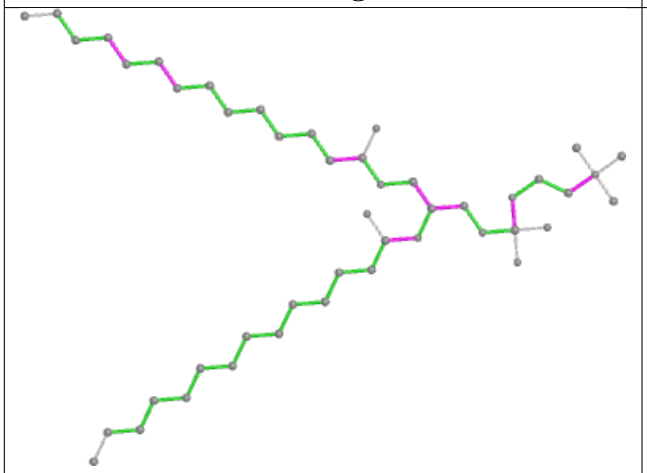

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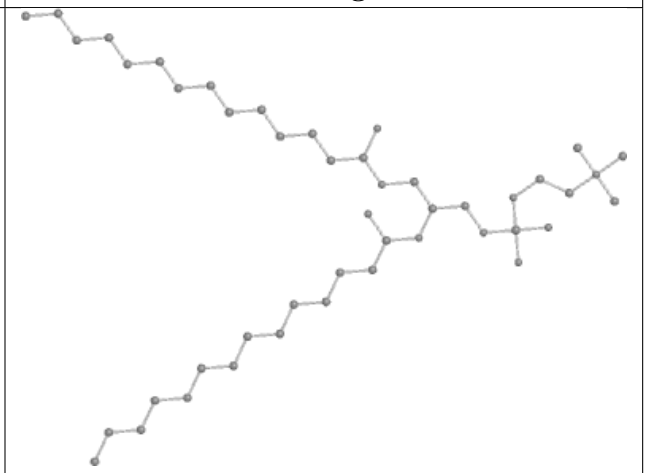
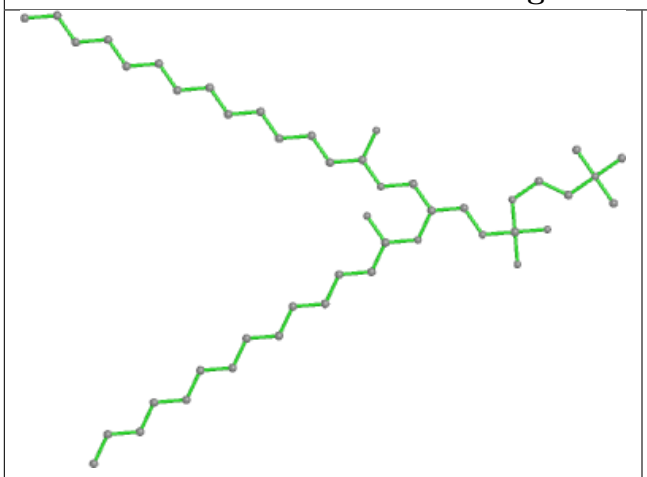


Rings

Ligand PX4 A 388



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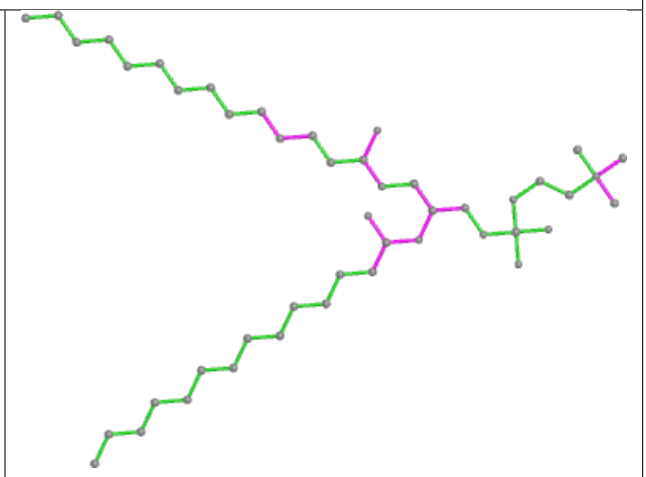

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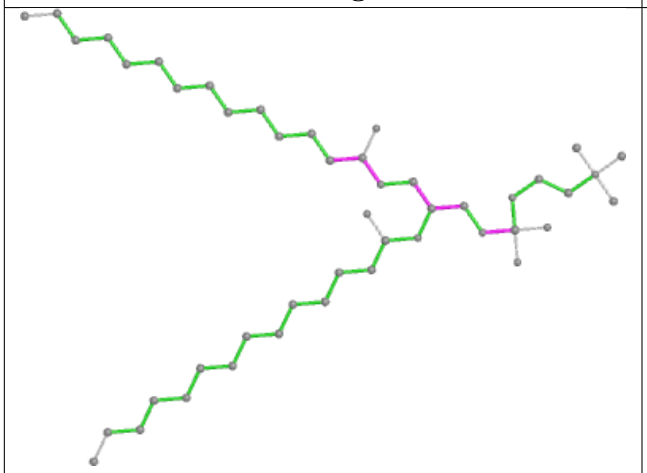

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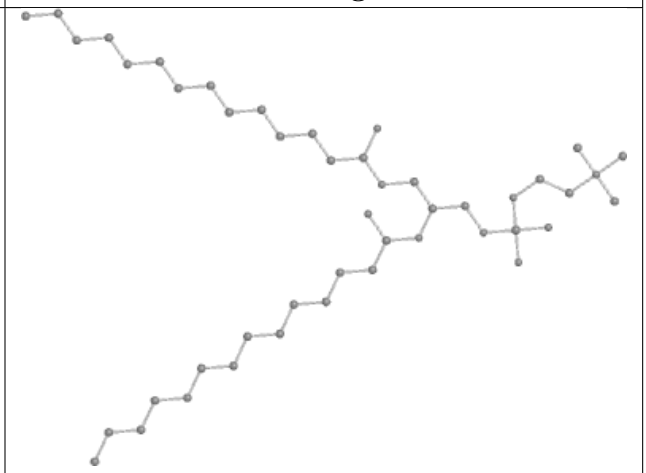
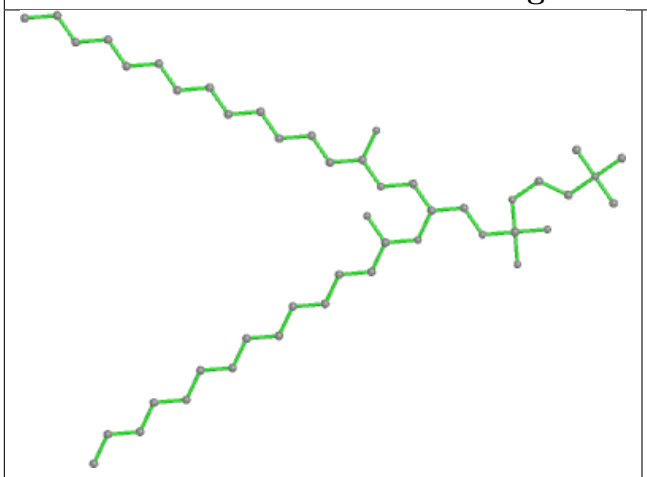


Rings

Ligand PX4 A 370



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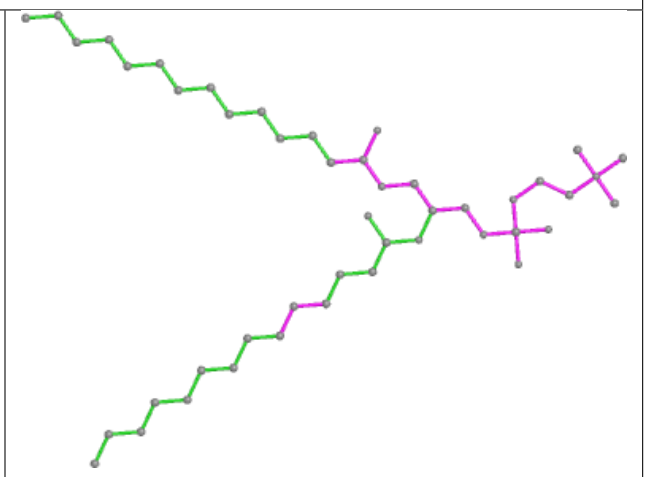
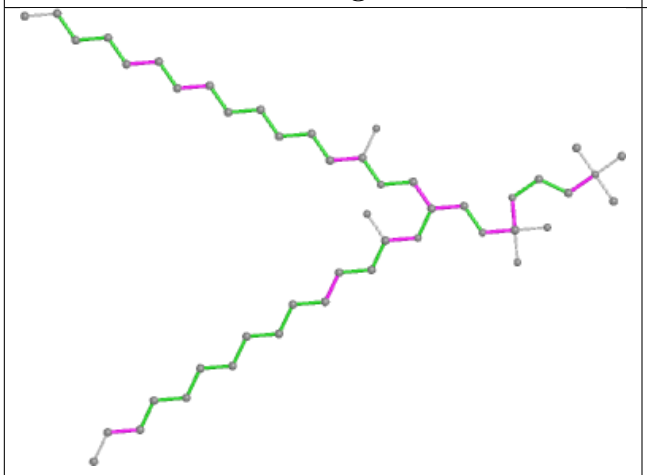


Bond angles



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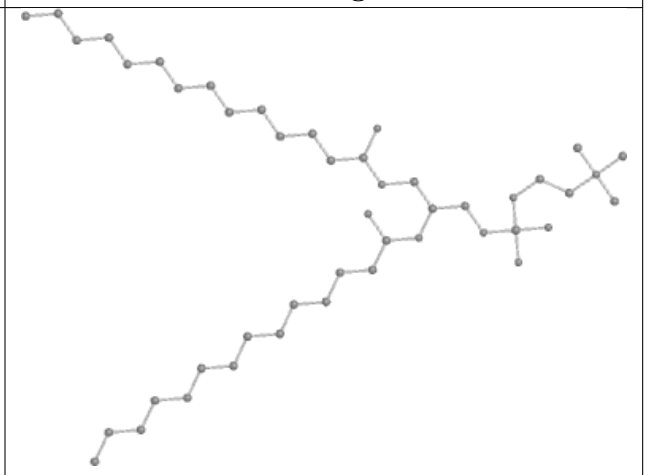
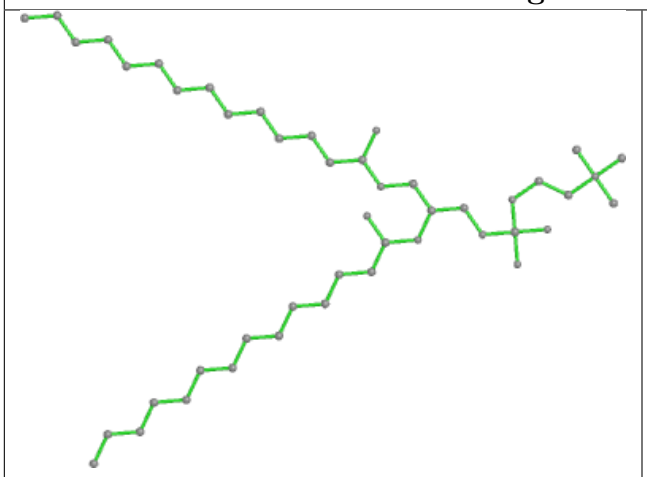


Rings

Ligand PX4 A 361



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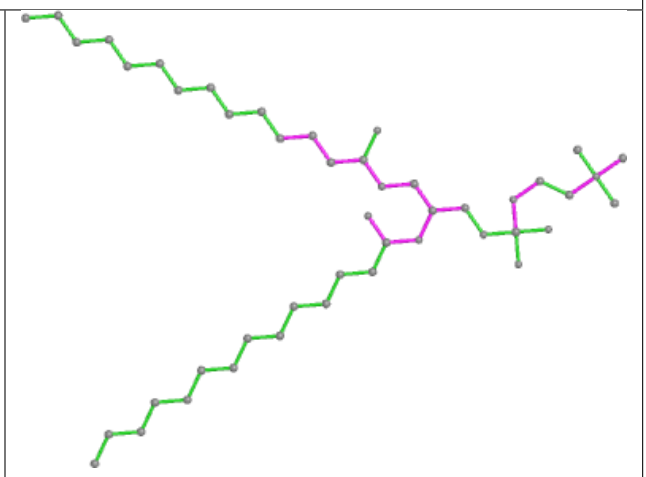

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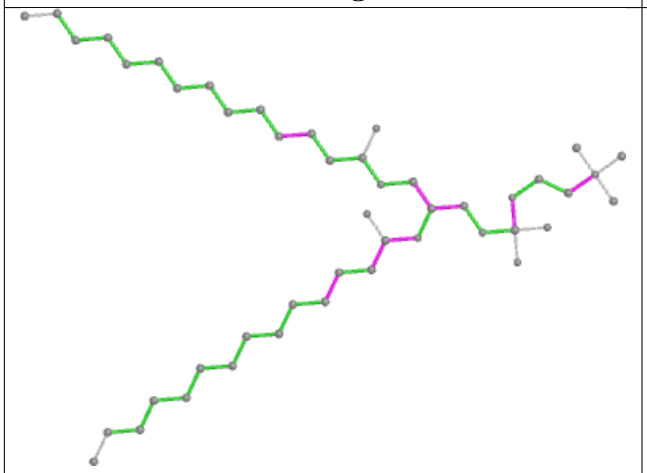

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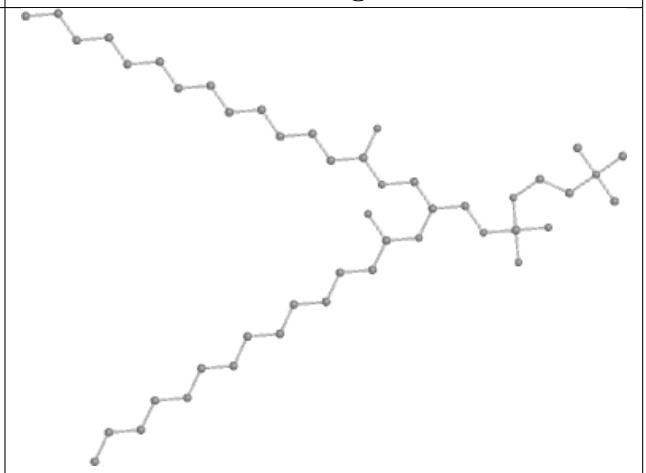
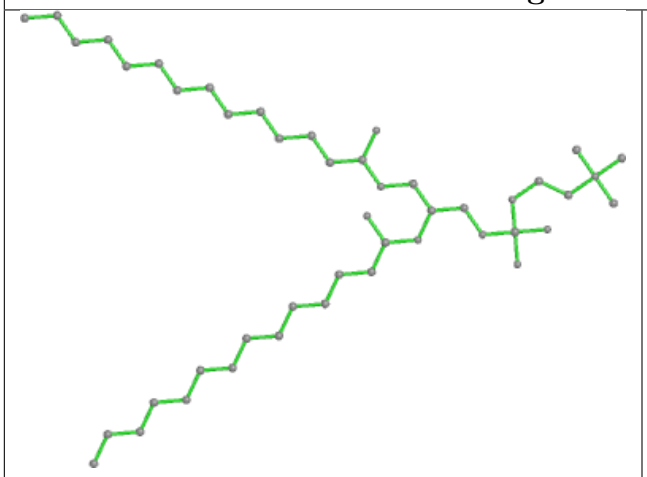


Rings

Ligand PX4 A 420



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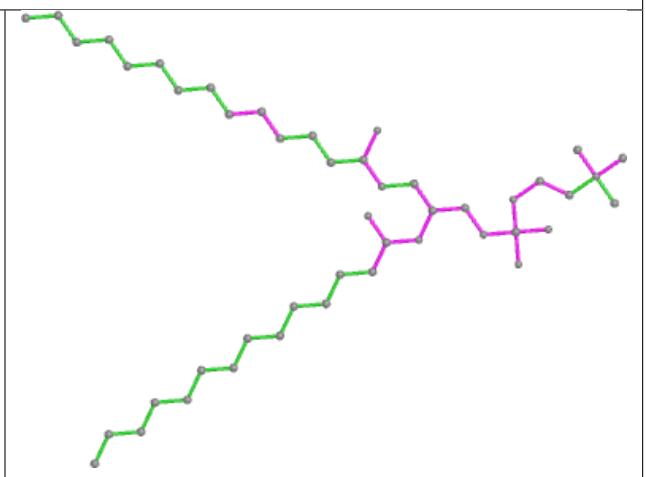

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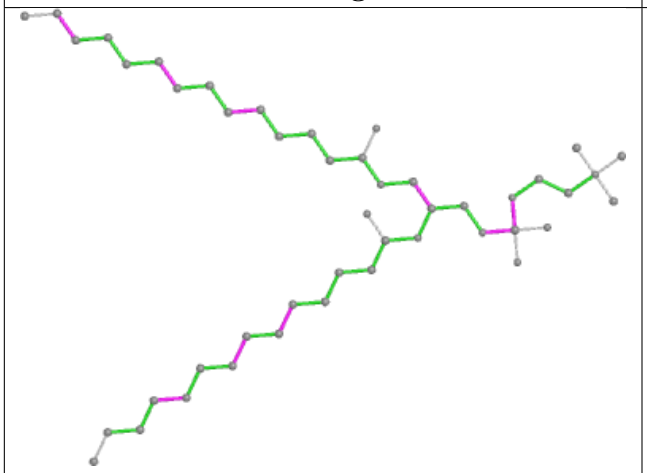

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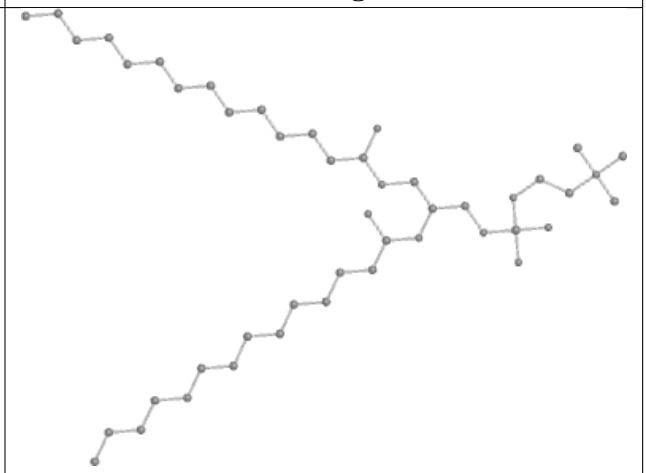
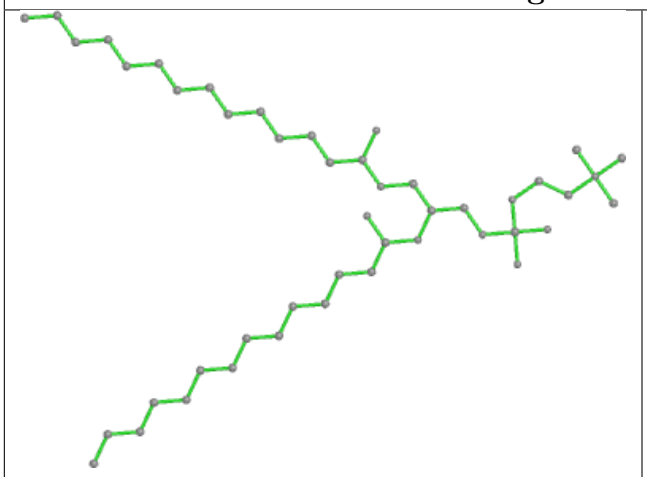


Rings

Ligand PX4 A 340



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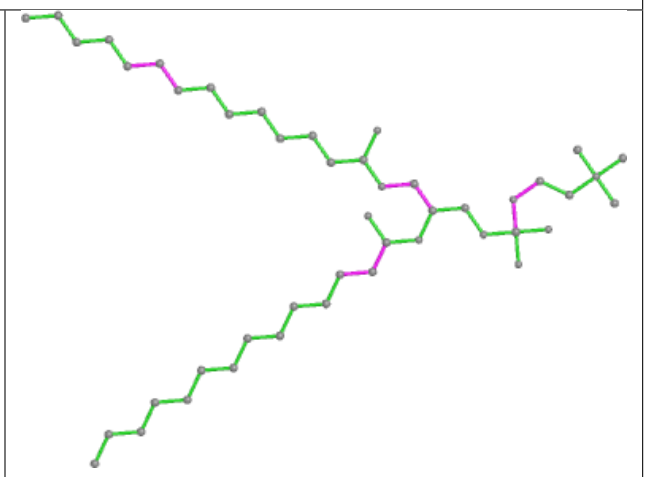

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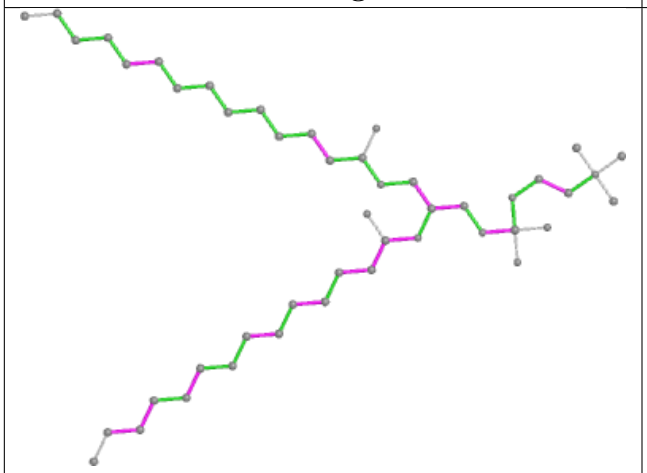

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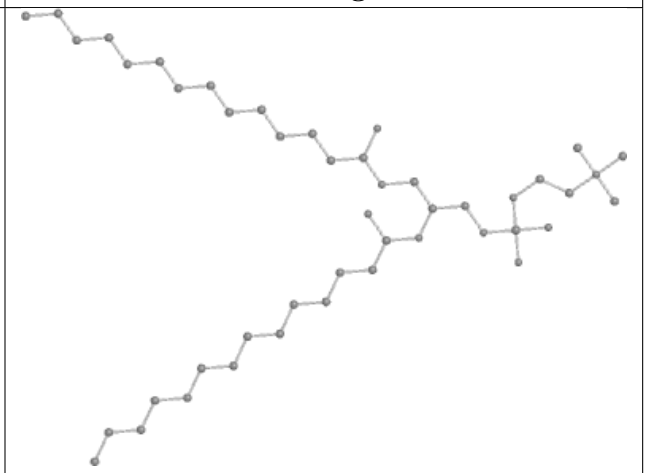
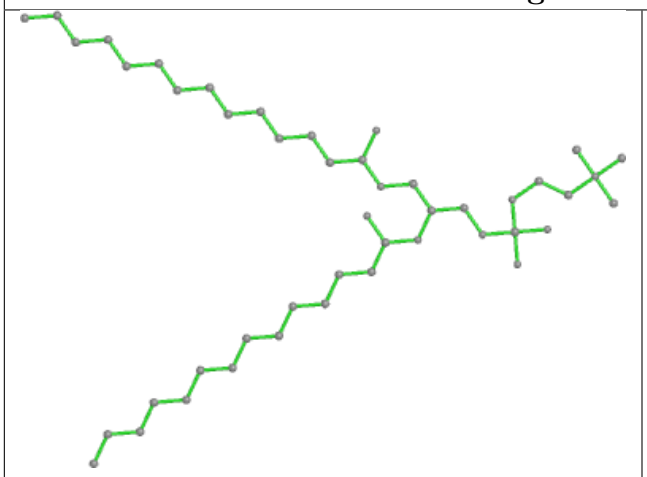


Rings

Ligand PX4 A 334



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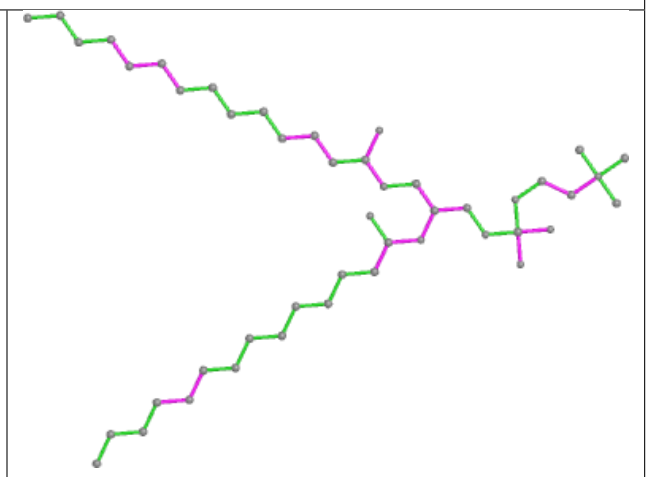
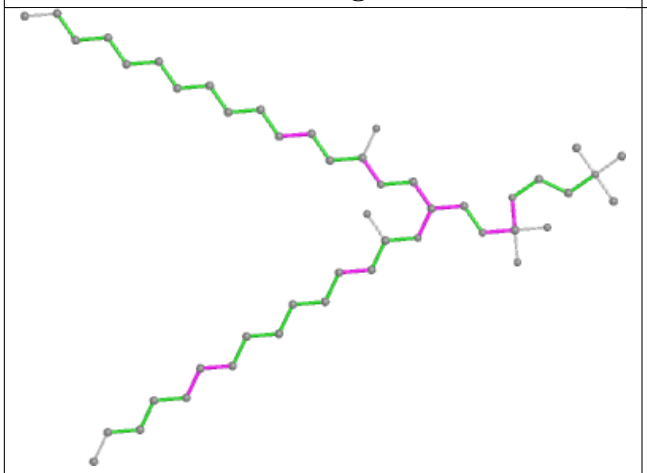


Bond angles



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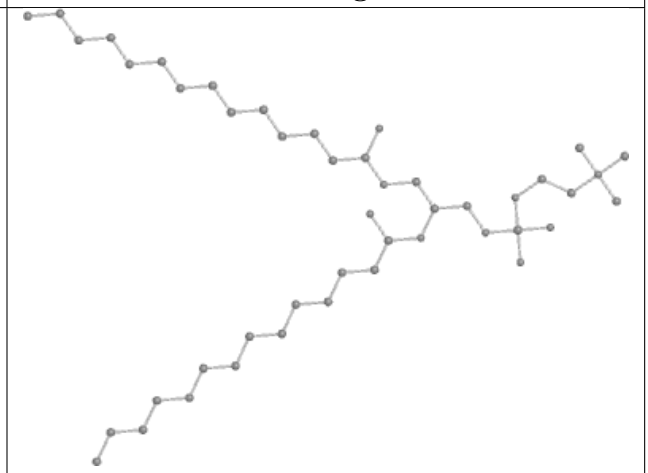
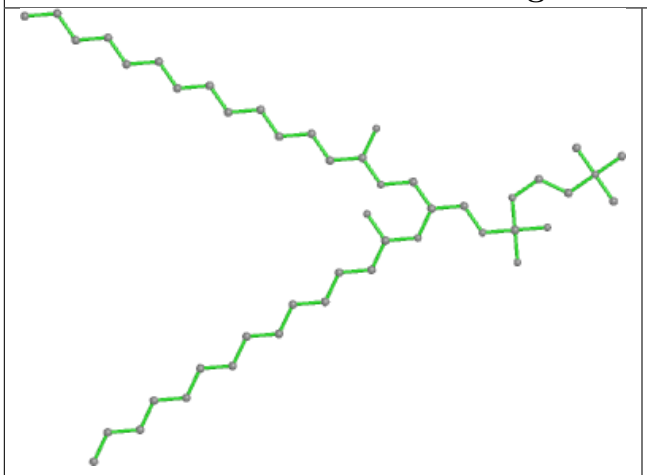


Rings

Ligand PX4 A 403



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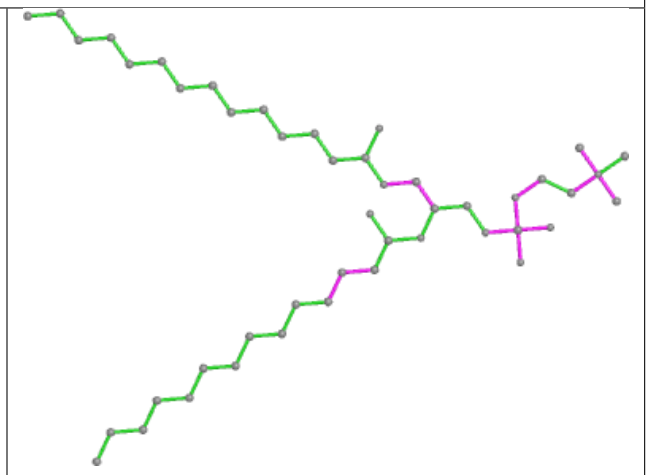
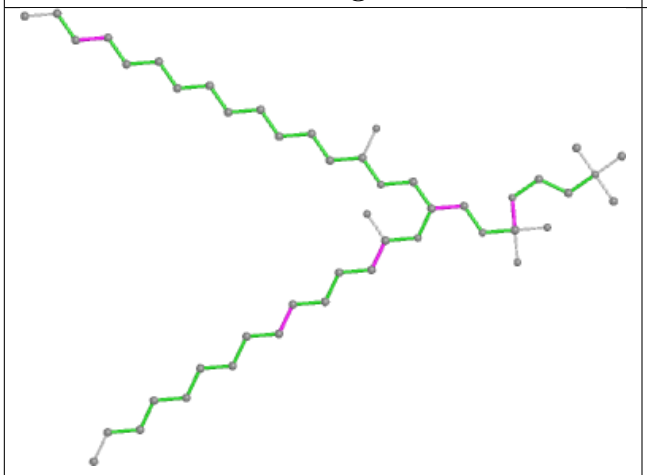


Bond angles



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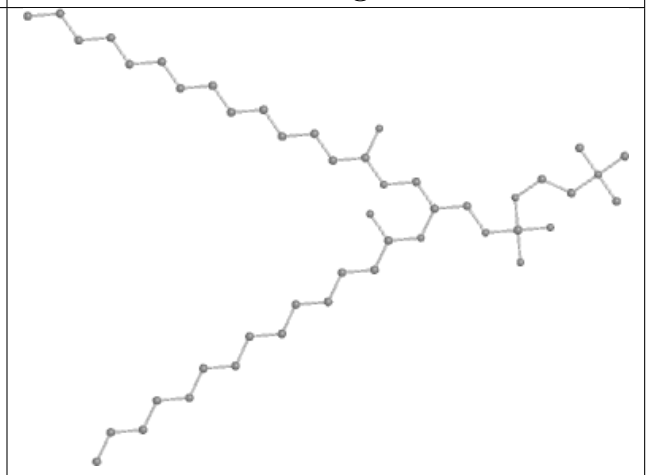
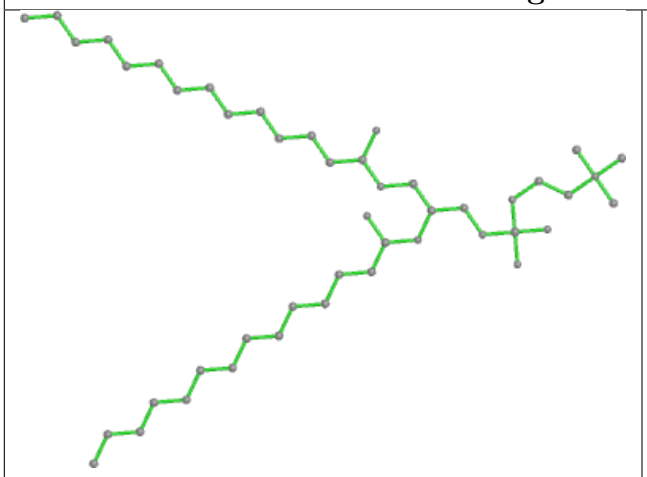
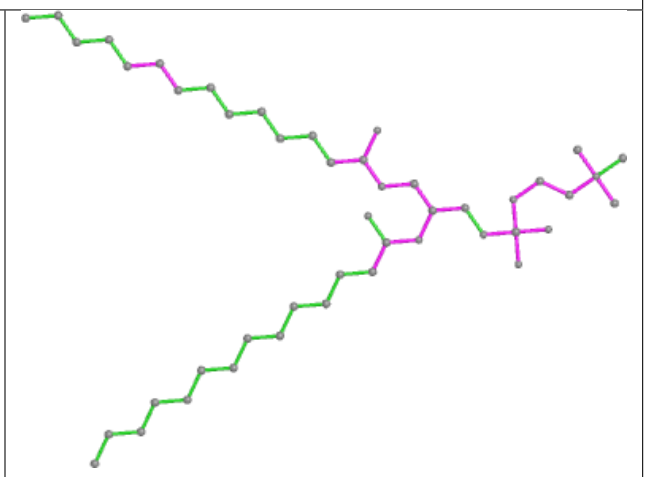


Rings

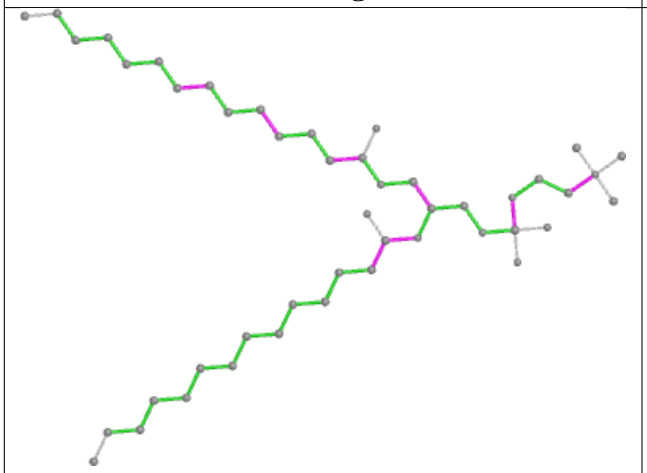
Ligand PX4 A 372



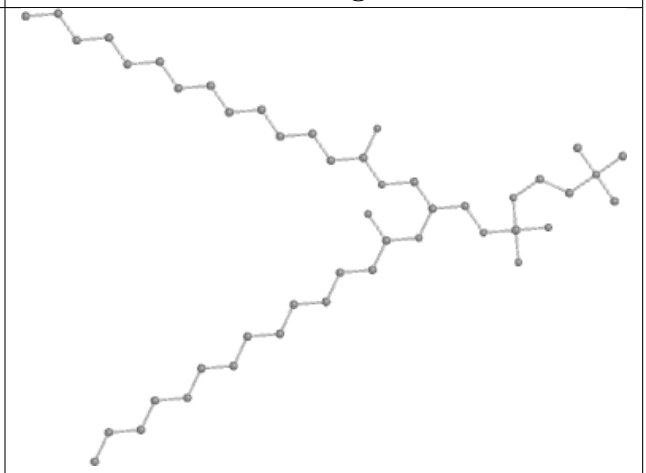
Bond lengths



Bond angles

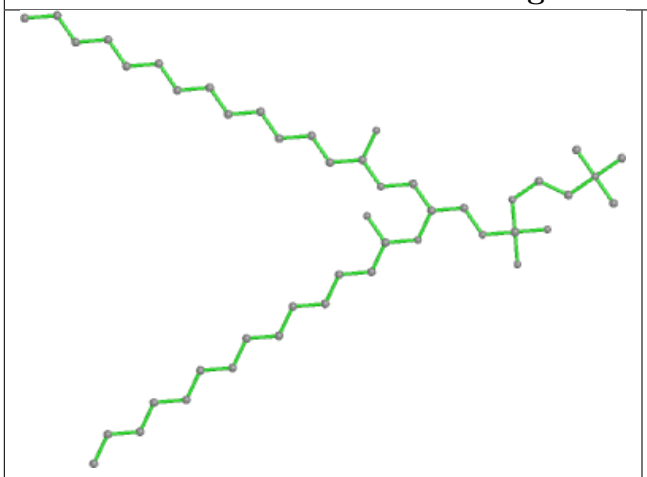


Torsions



Rings

Ligand PX4 A 309



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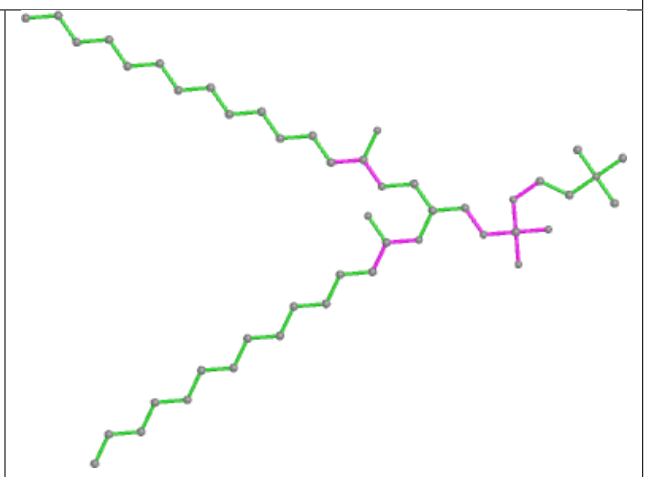

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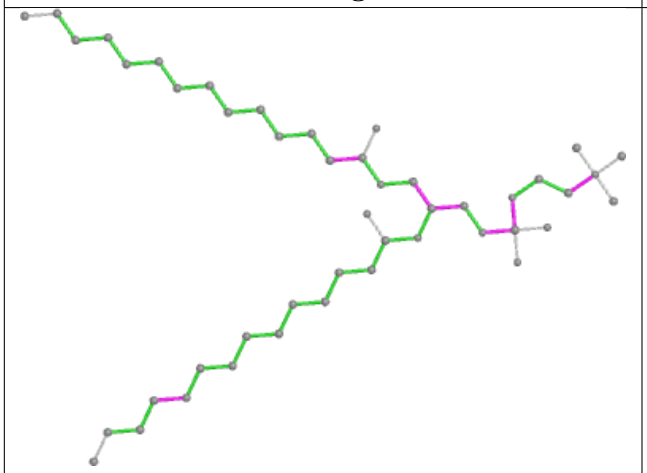

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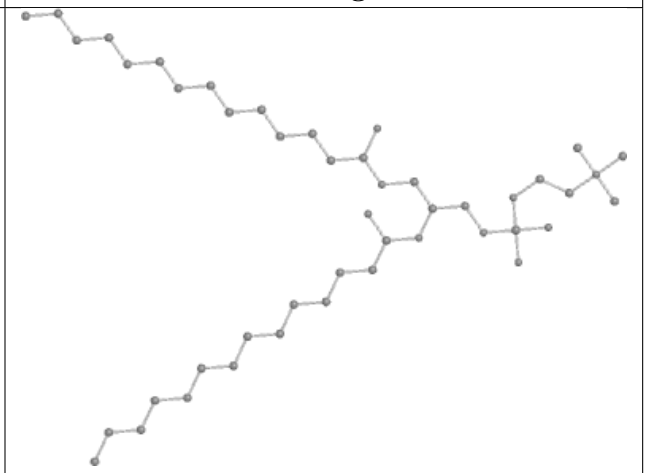
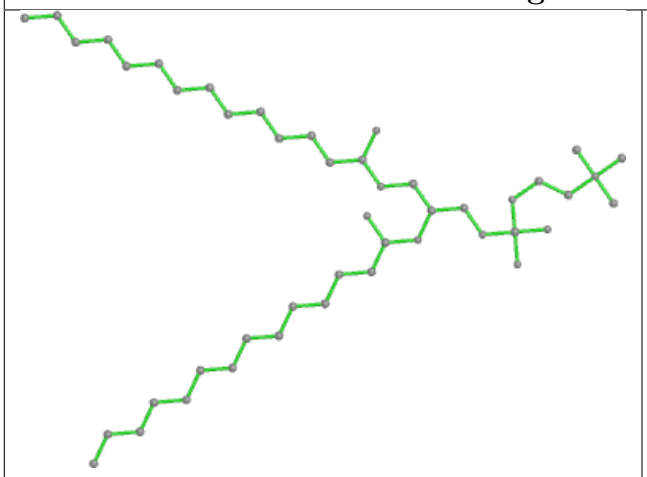


Rings

Ligand PX4 A 397



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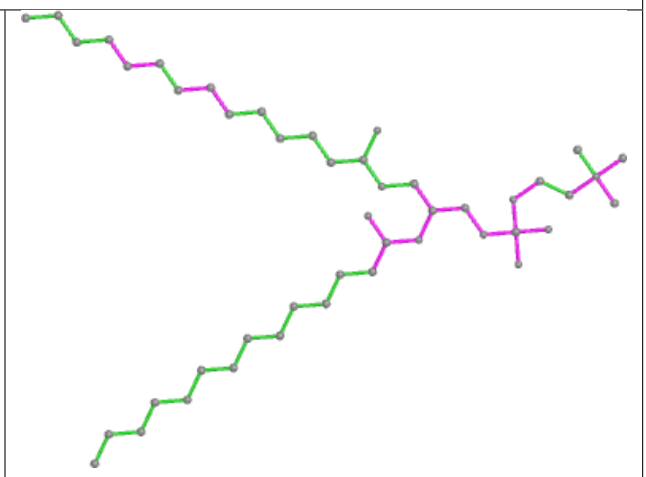

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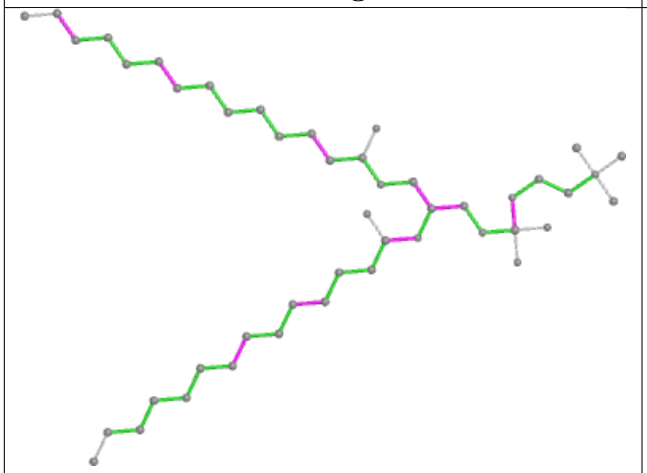

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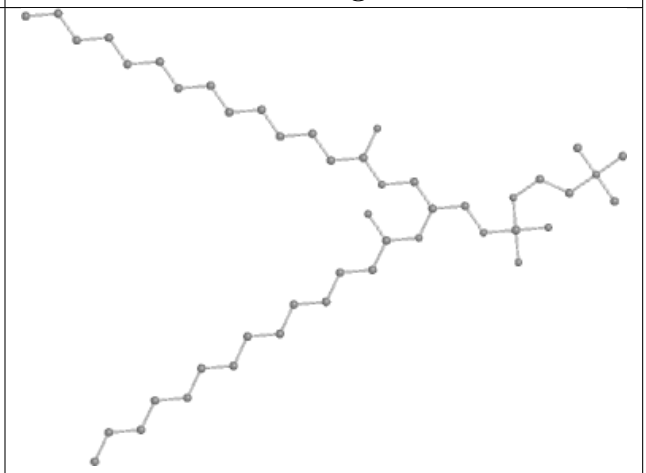
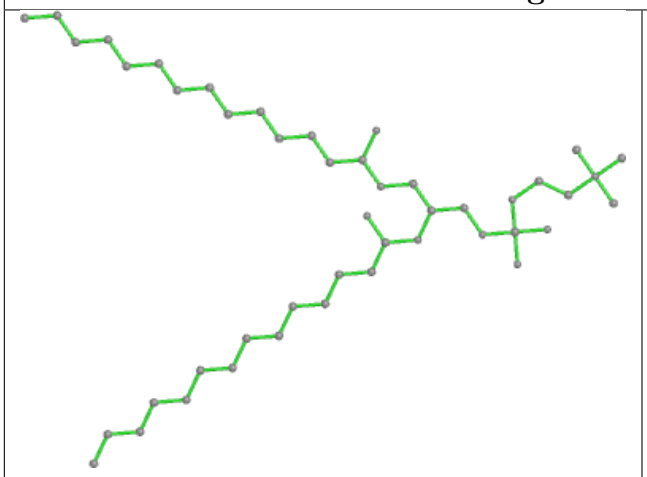


Rings

Ligand PX4 A 355



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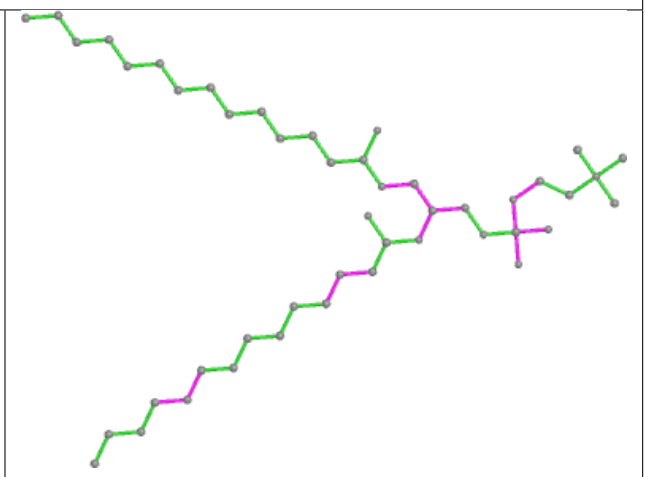

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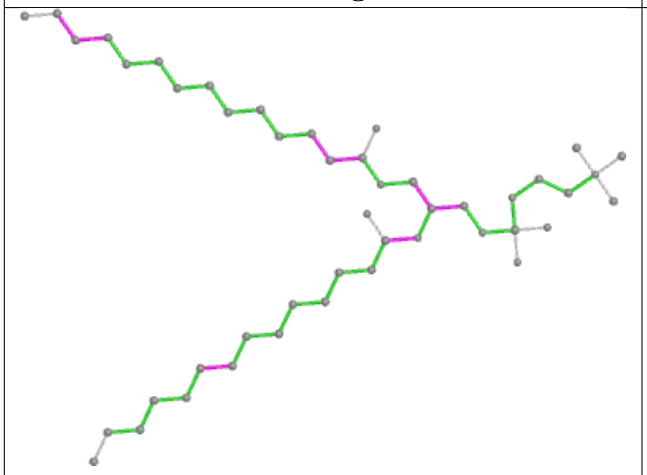

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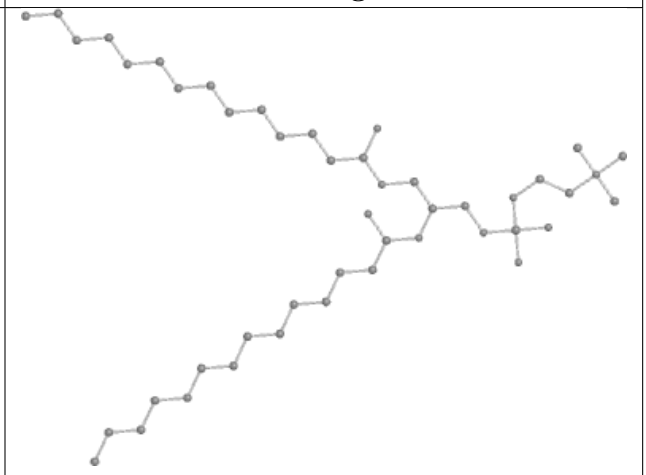
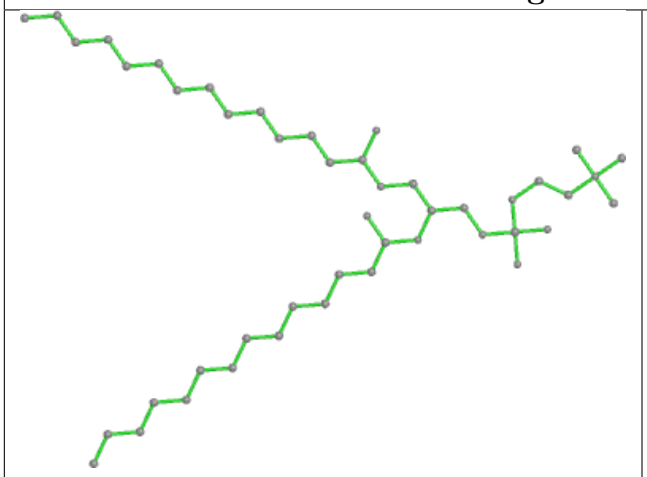


Rings

Ligand PX4 A 326



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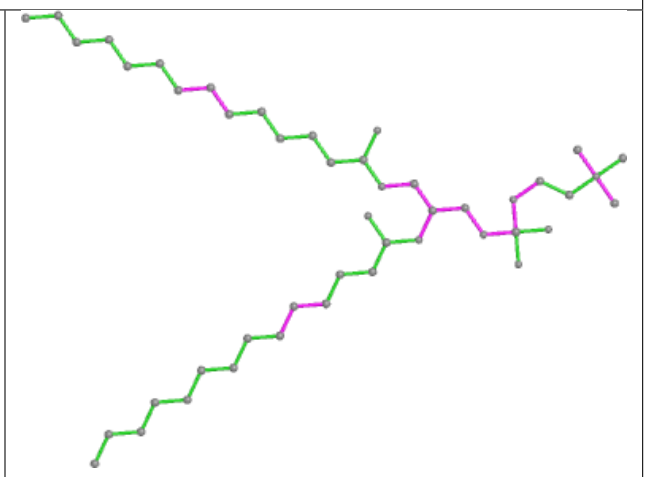

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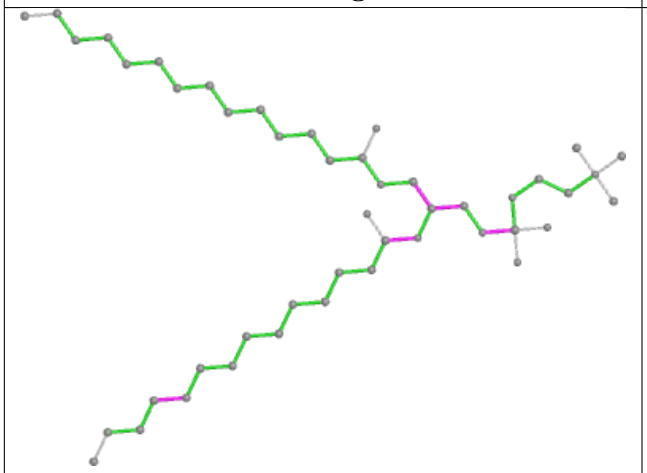

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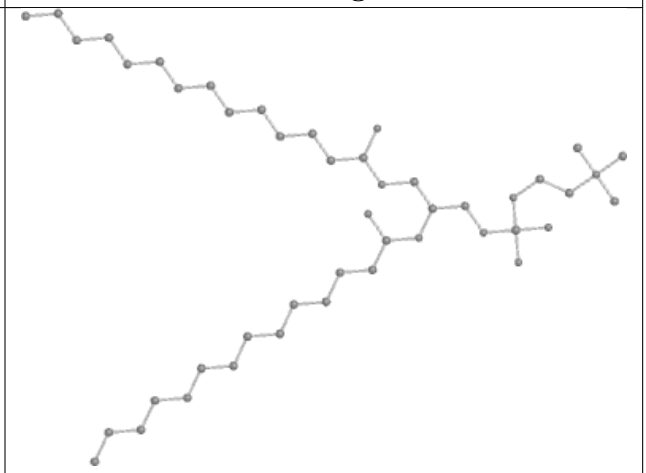
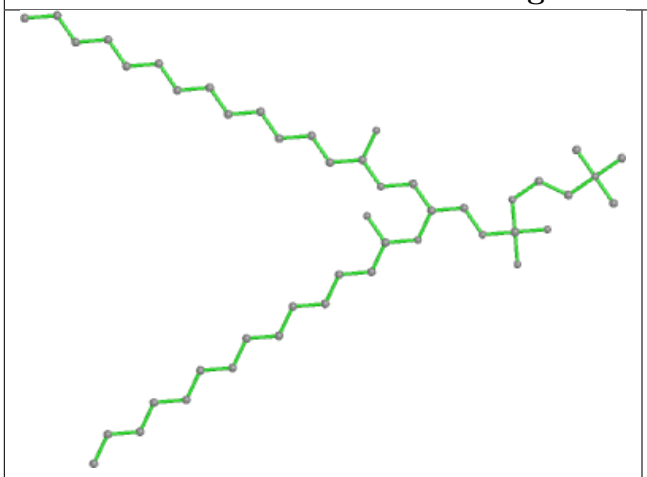


Rings

Ligand PX4 A 383



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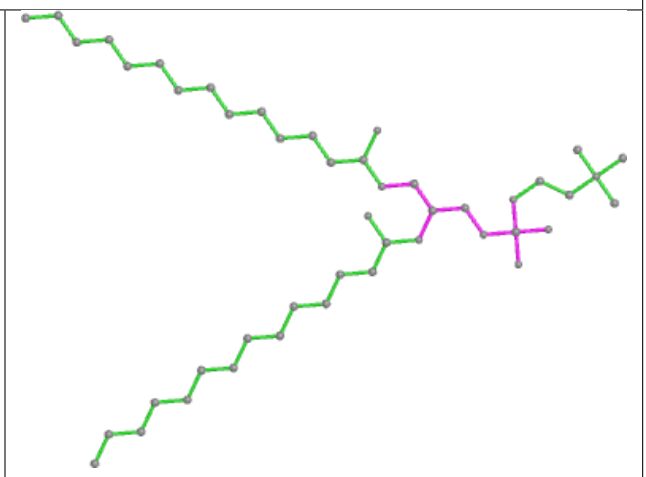

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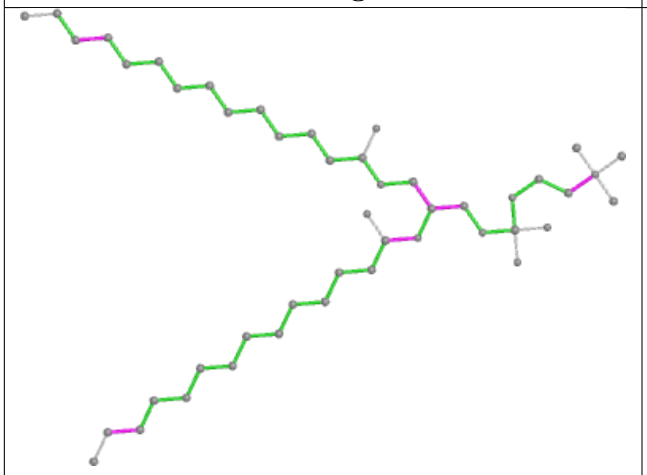

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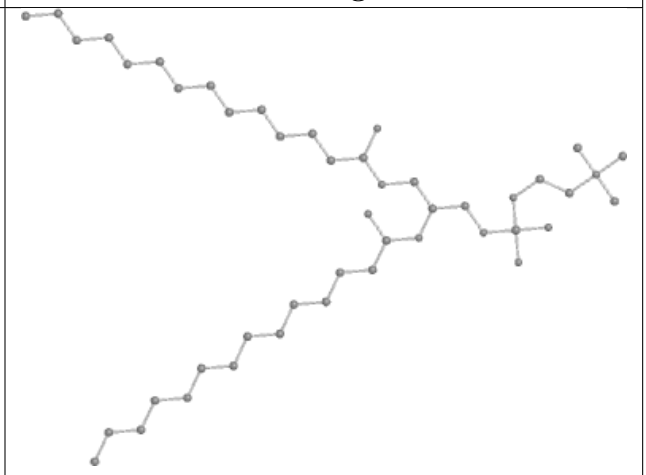
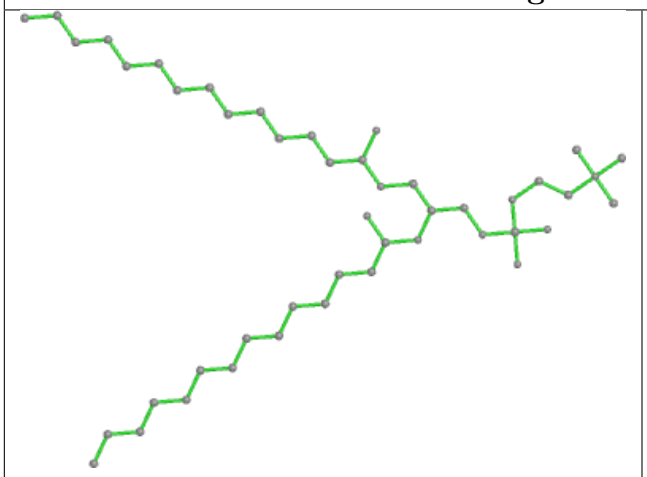


Rings

Ligand PX4 A 406



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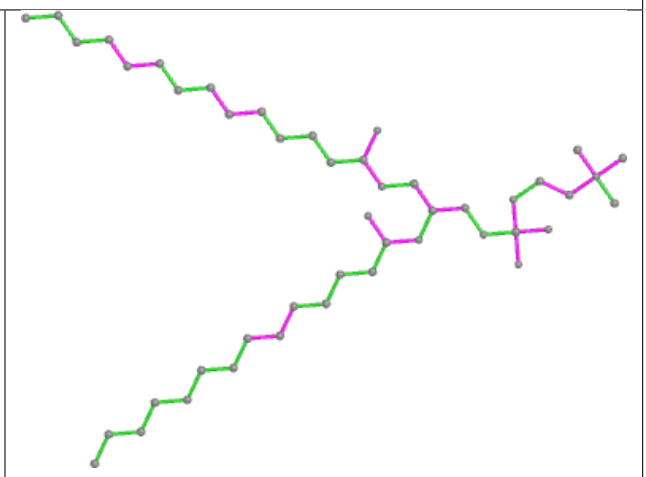

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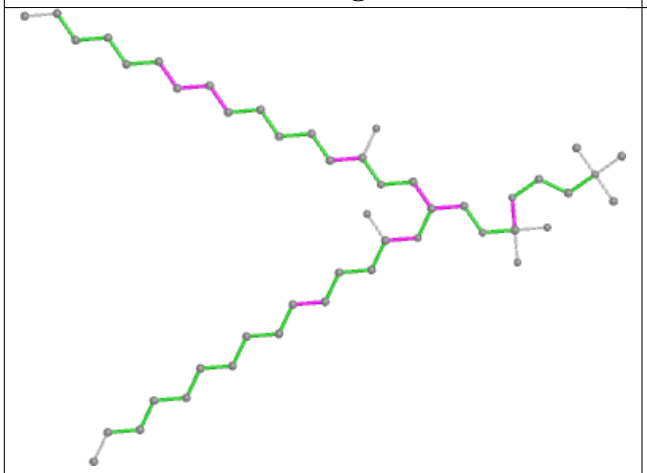

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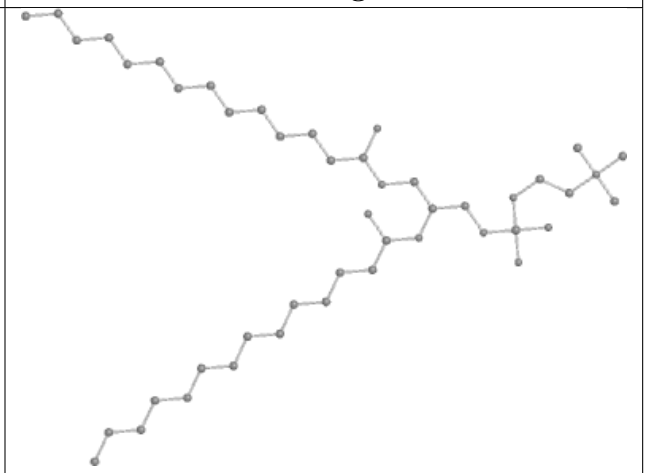
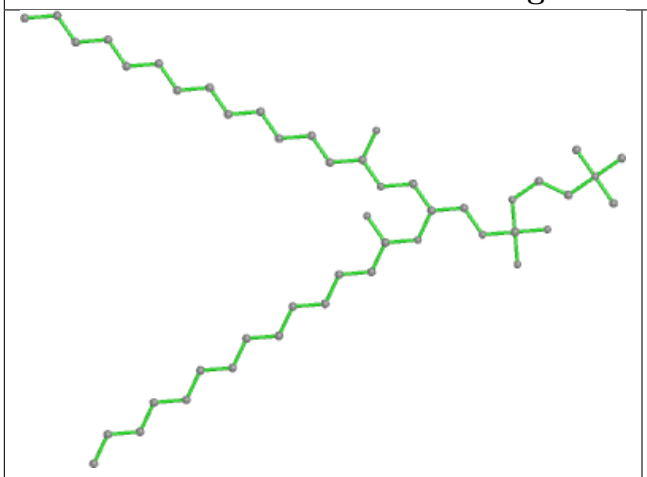


Rings

Ligand PX4 A 331



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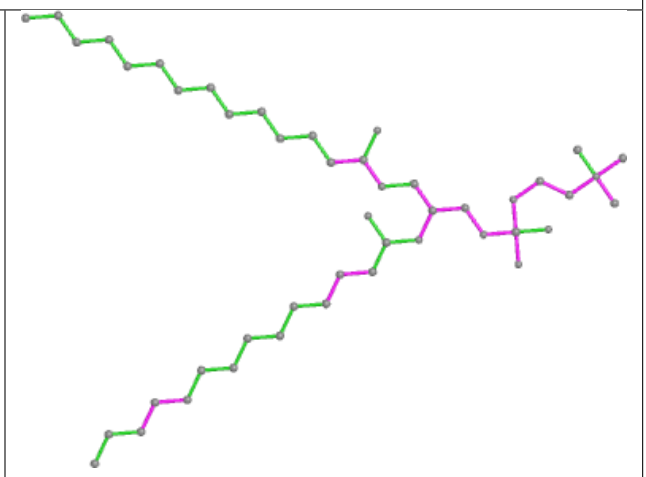

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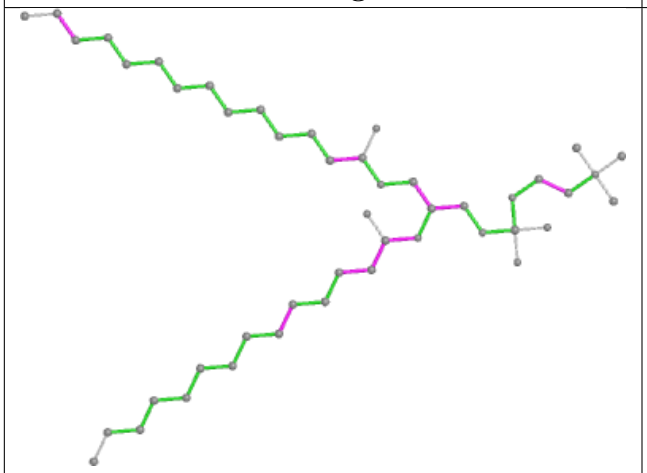

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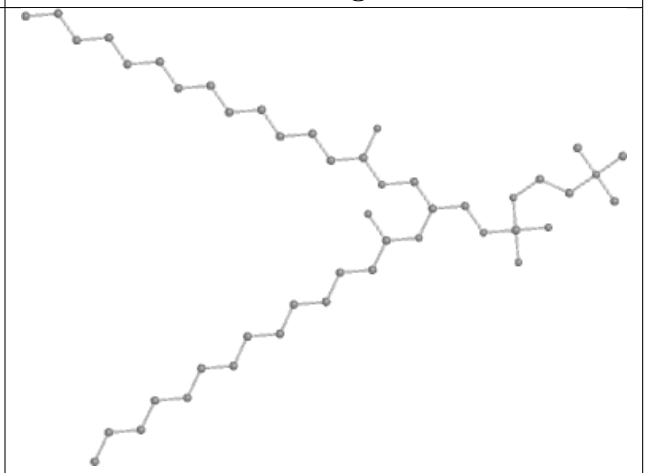
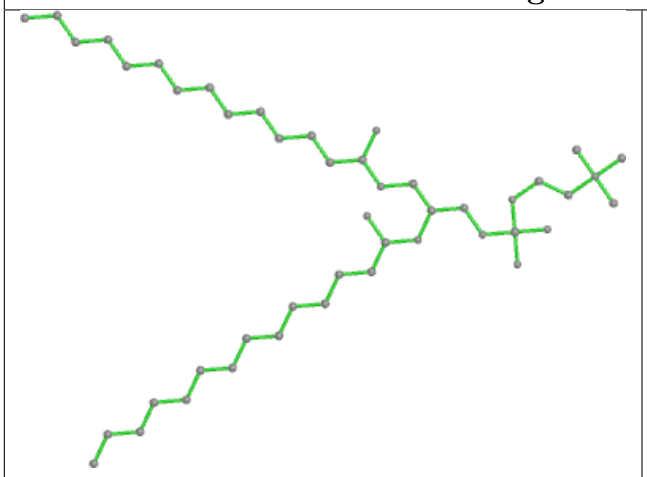


Rings

Ligand PX4 A 421



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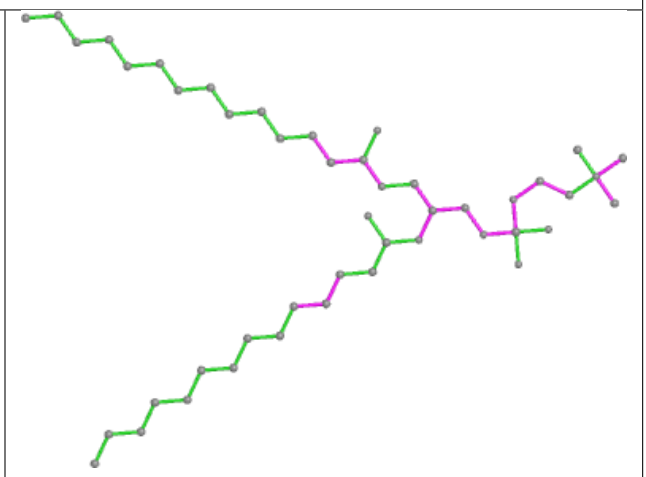

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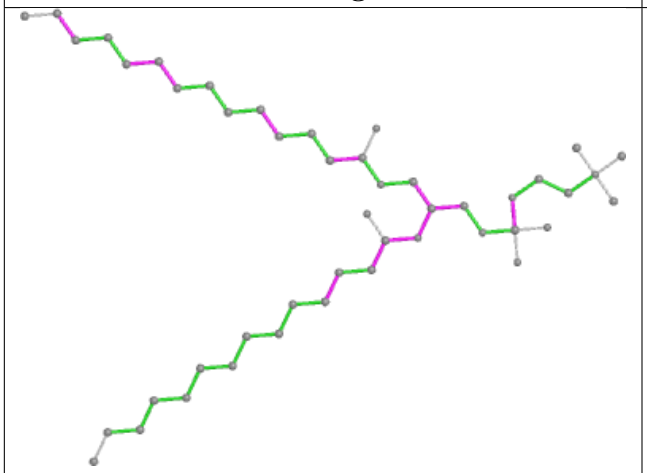

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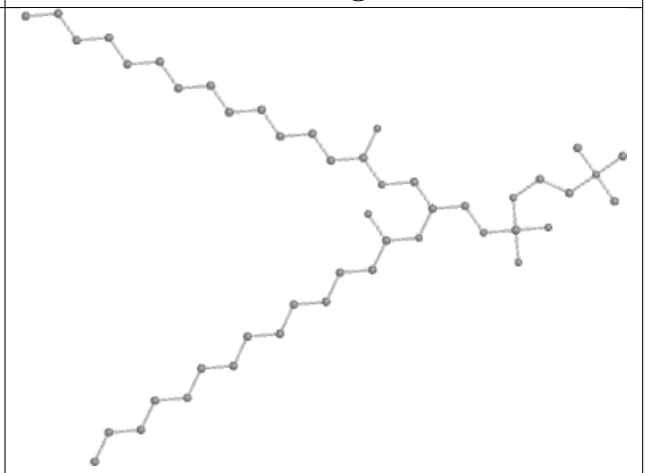
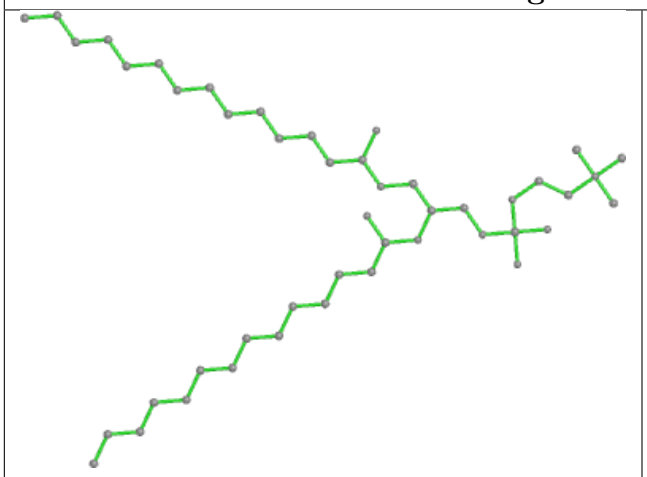


Rings

Ligand PX4 A 409



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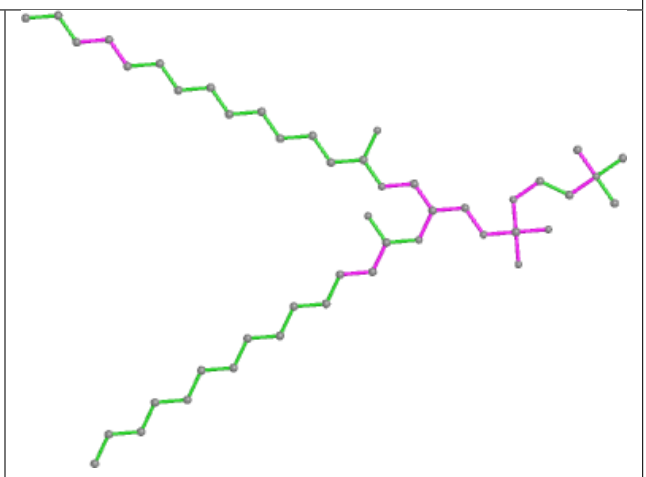

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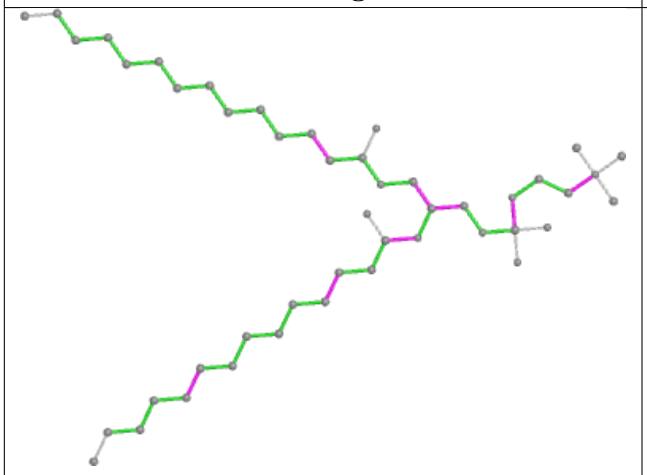

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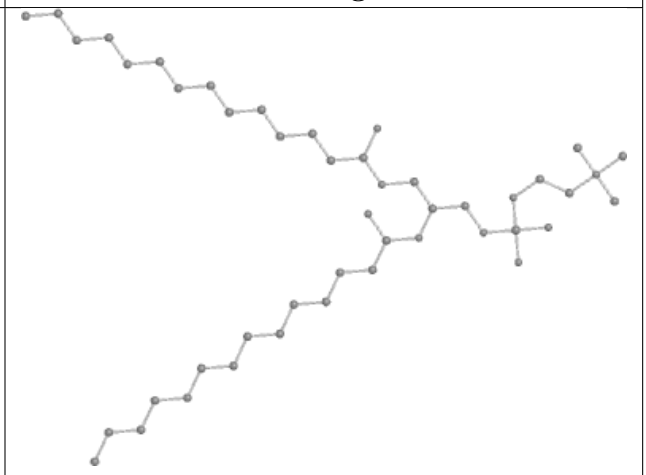
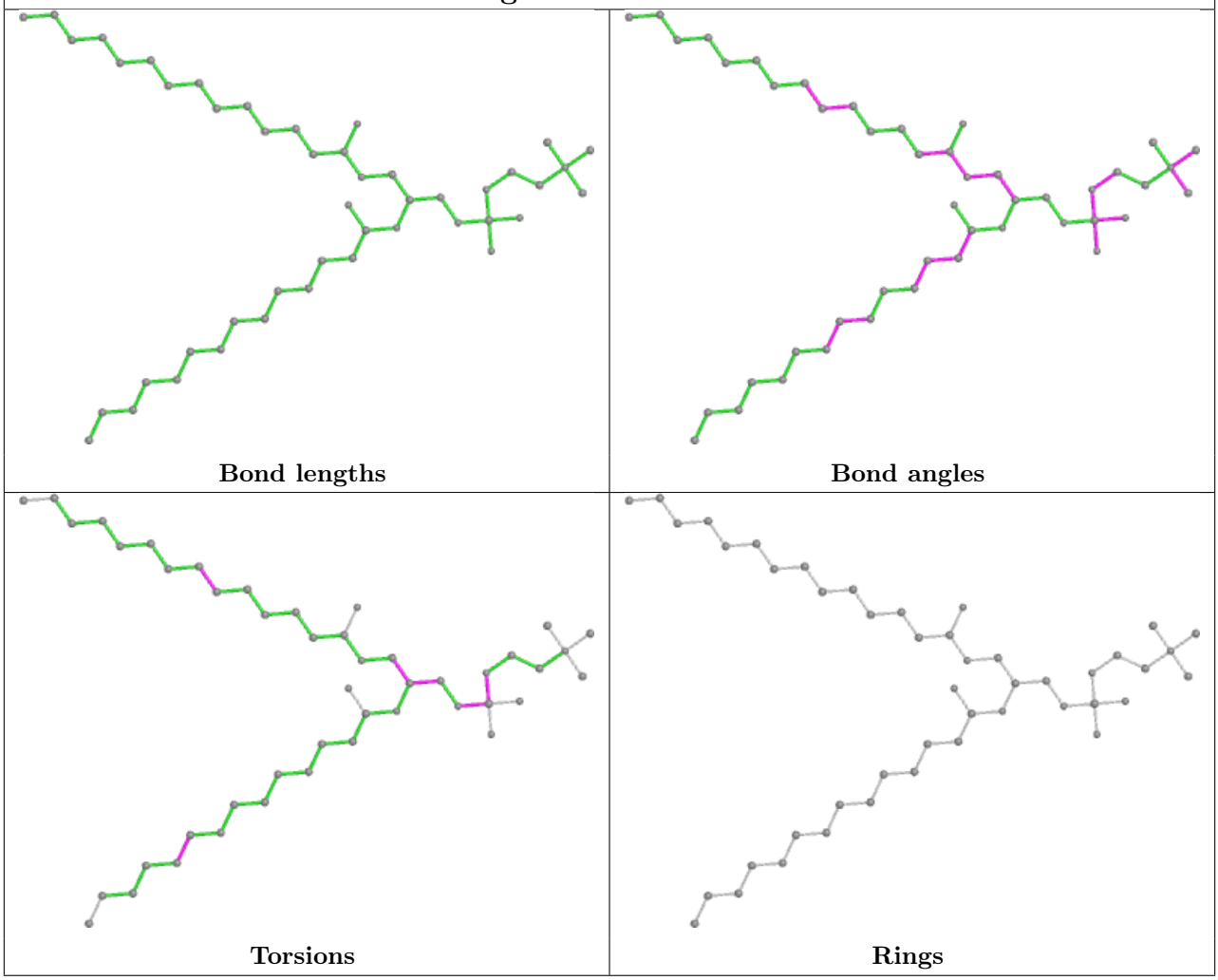
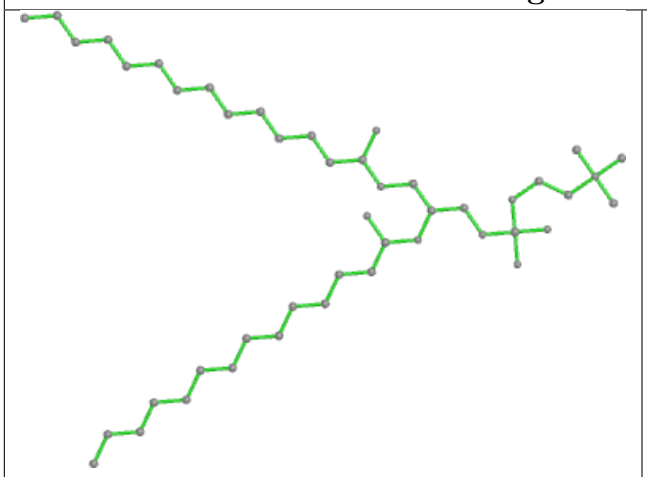


Rings

Ligand PX4 A 362



Ligand PX4 A 373



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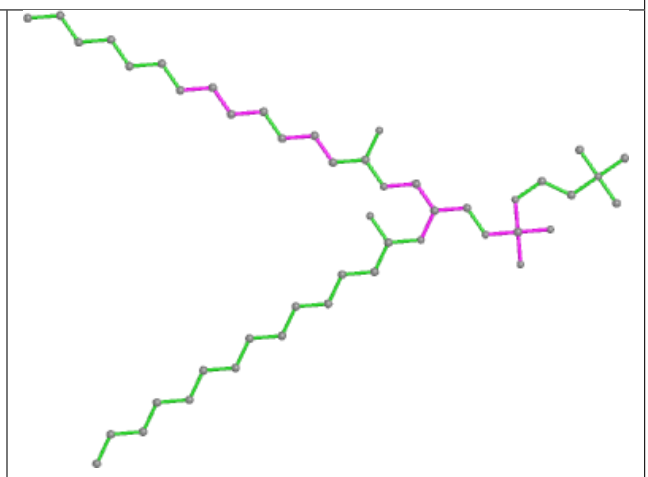
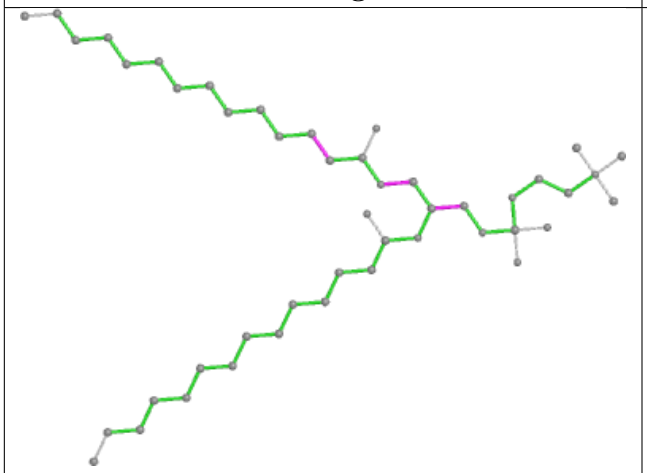


Bond angles



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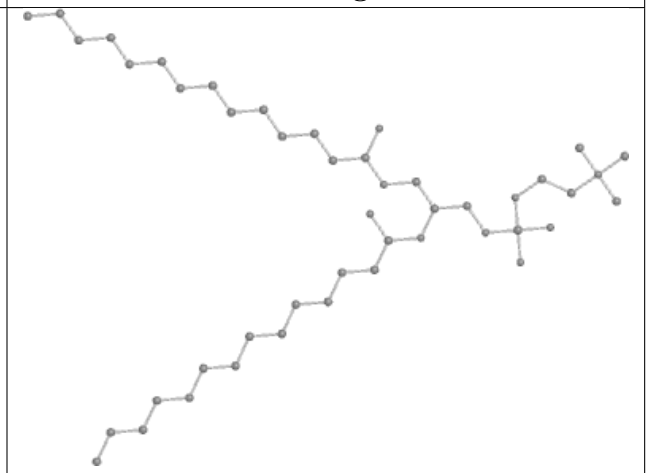
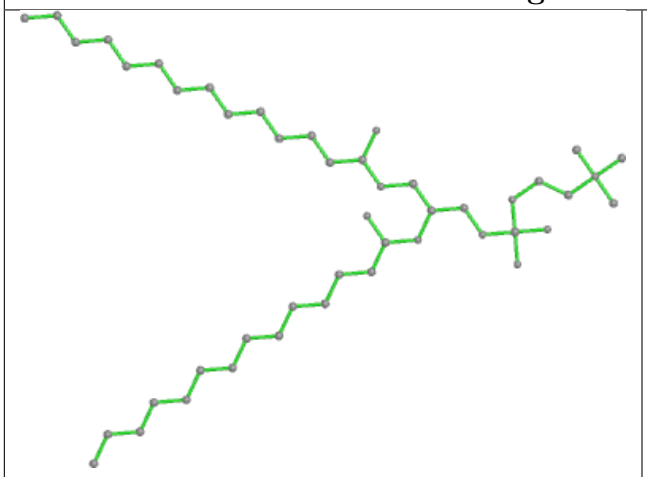


Rings

Ligand PX4 A 412



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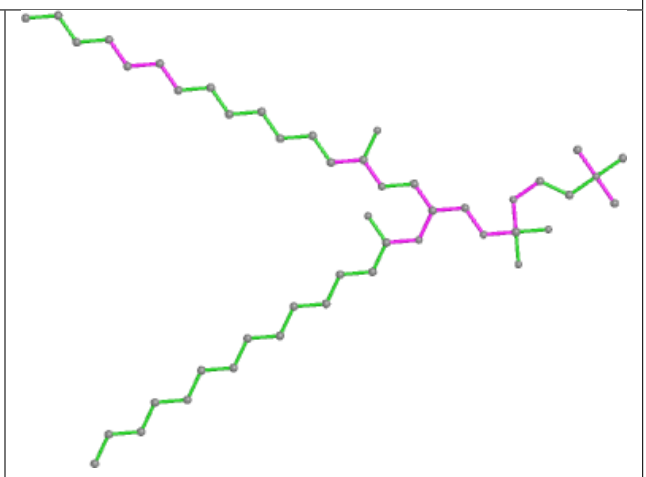
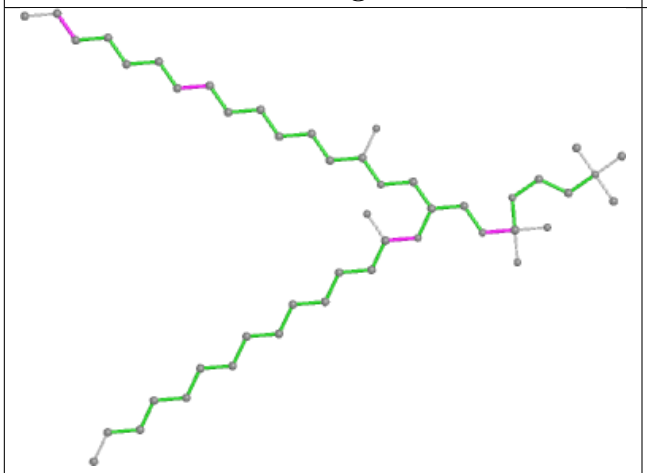


Bond angles



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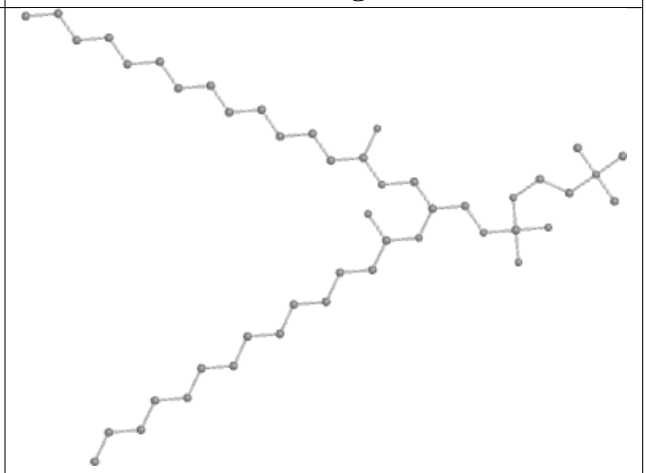
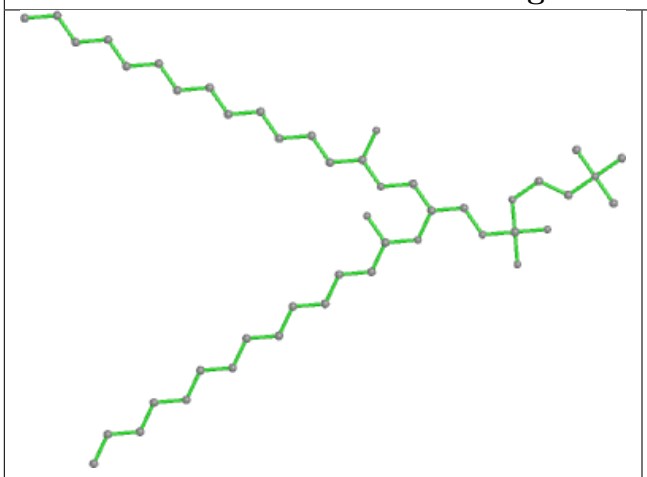


Rings

Ligand PX4 A 430



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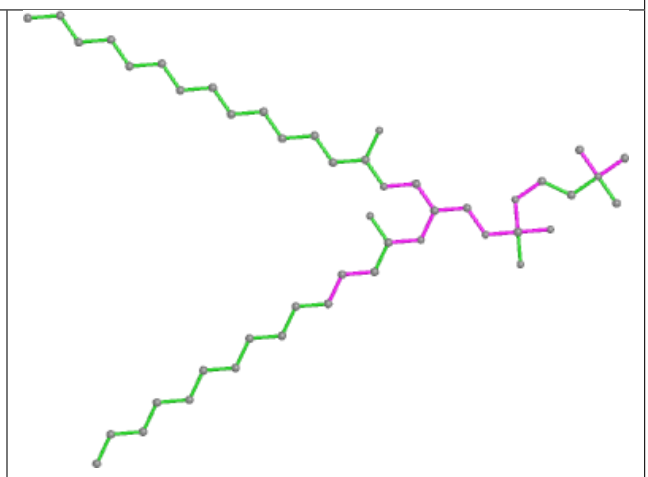
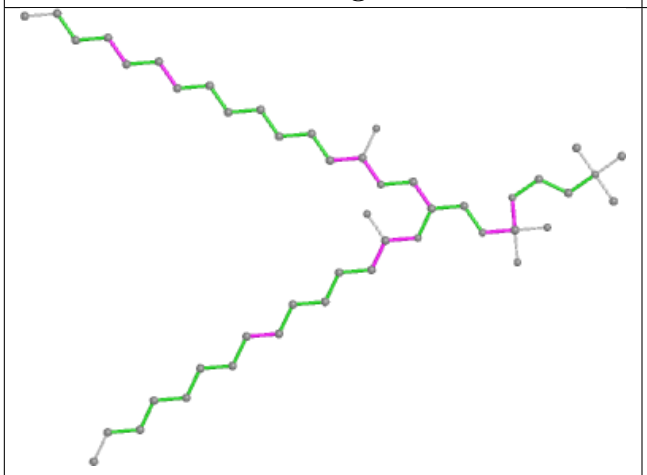


Bond angles



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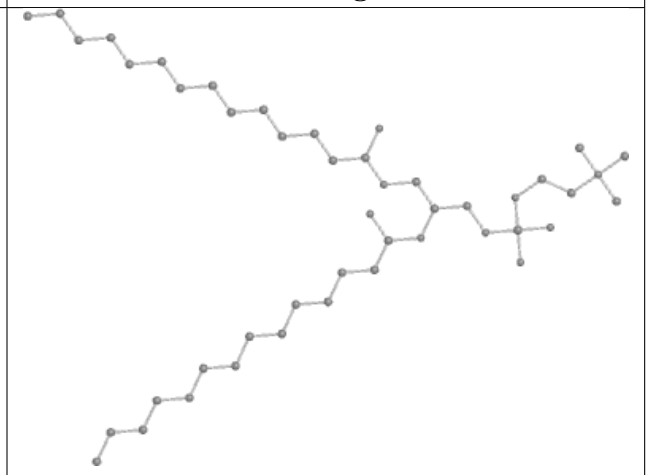
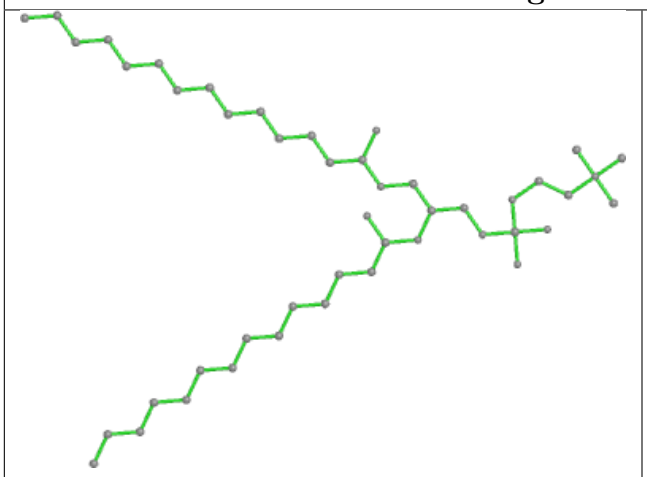
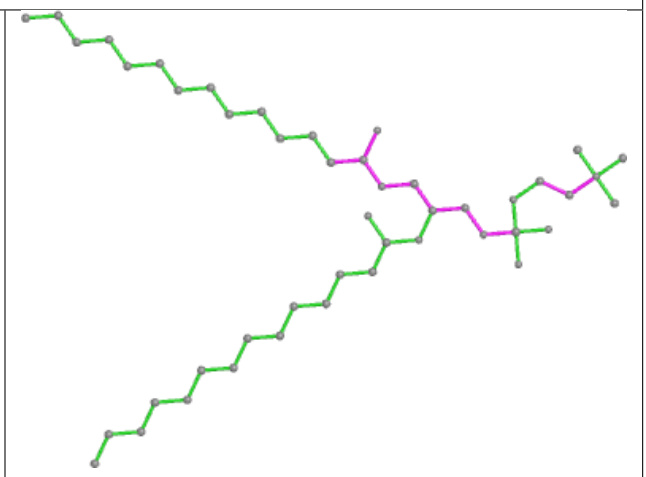


Rings

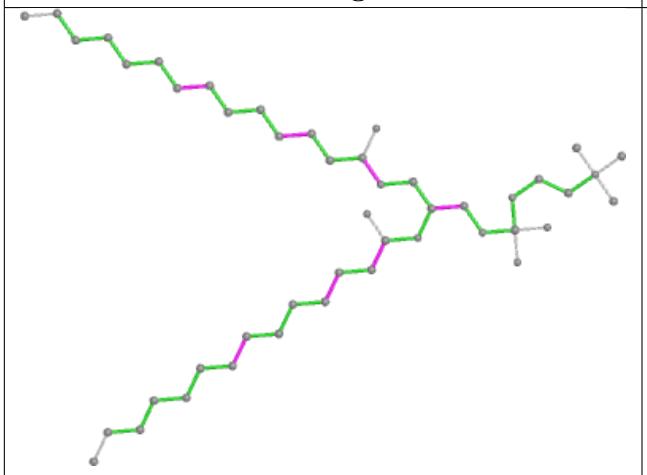
Ligand PX4 A 411



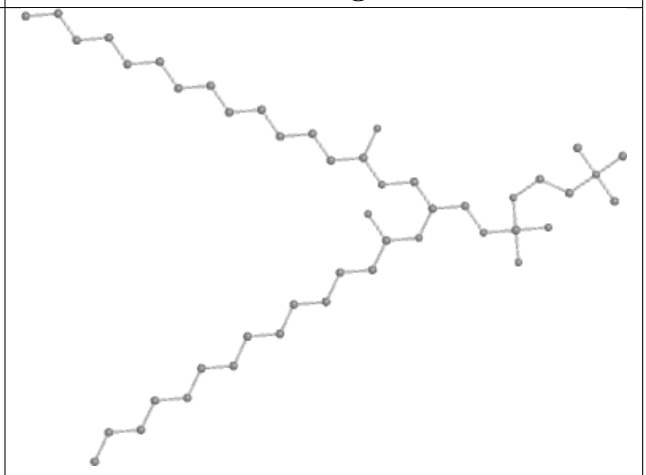
Bond lengths



Bond angles

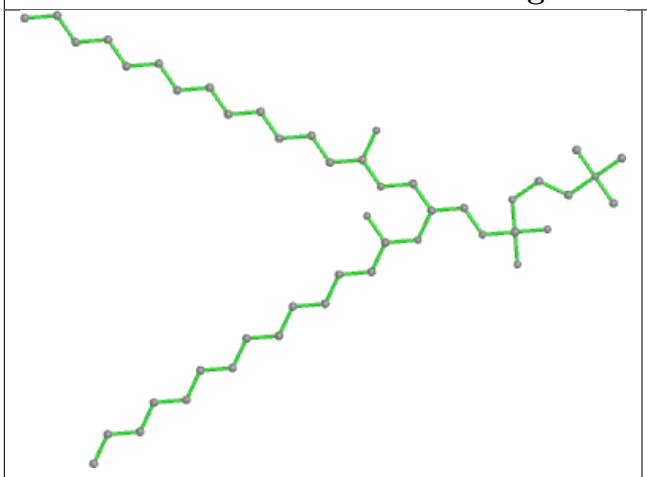


Torsions



Rings

Ligand PX4 A 316



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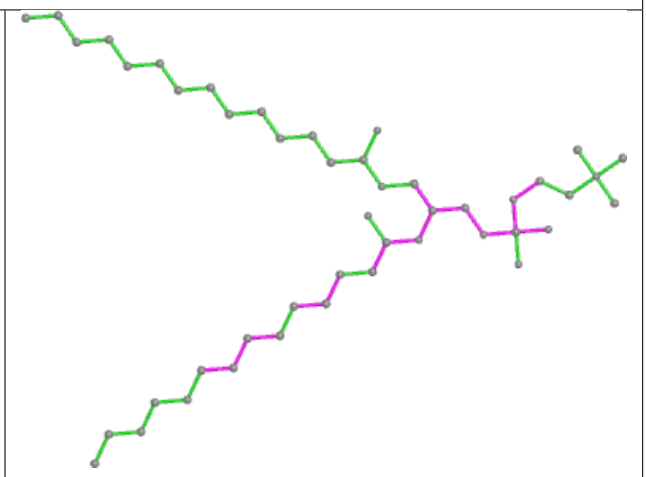

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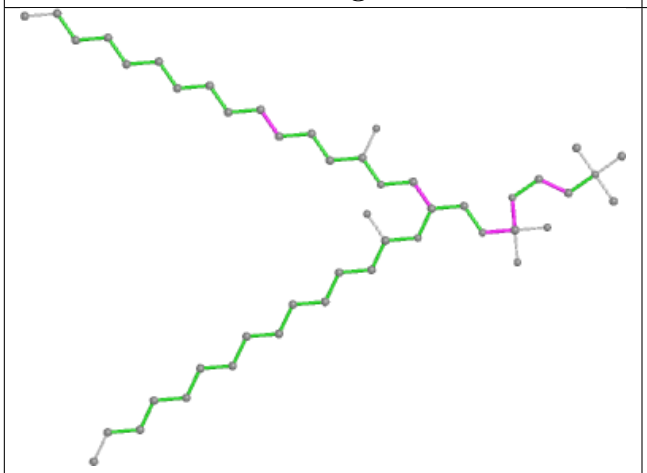

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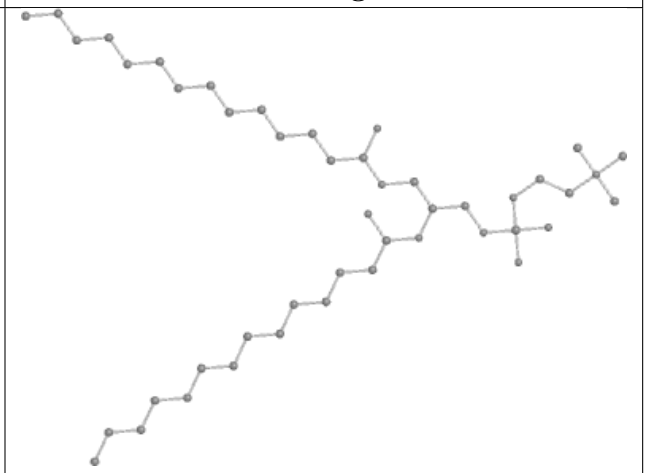
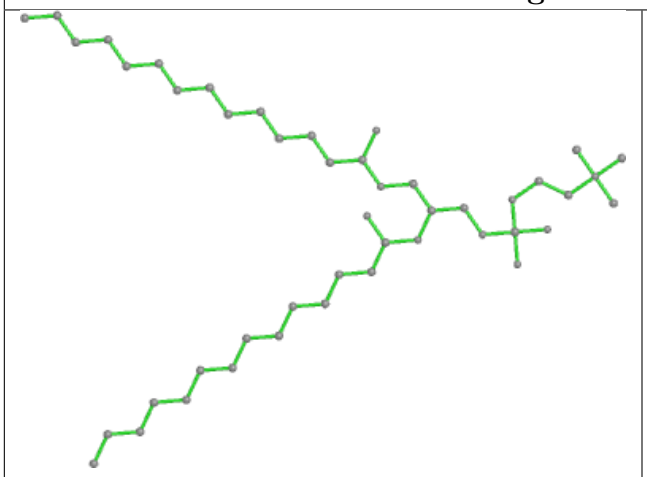


Rings

Ligand PX4 A 423



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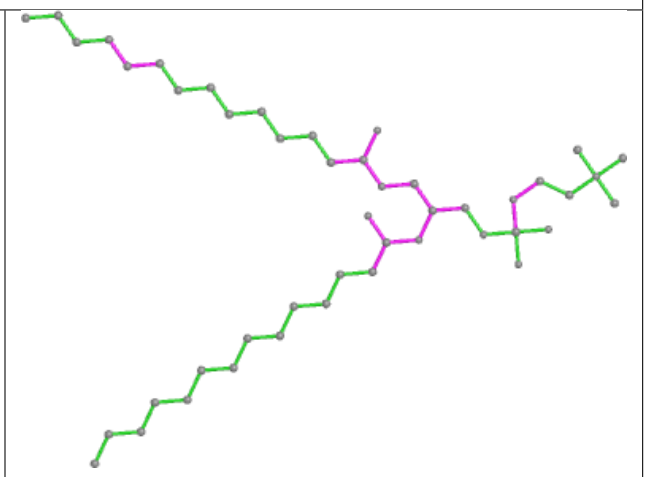

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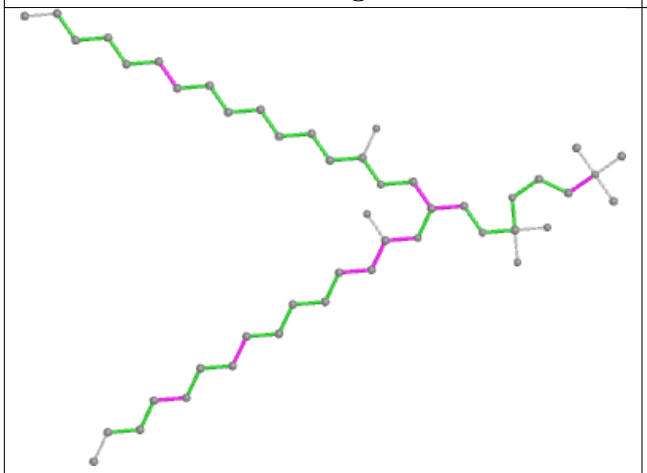

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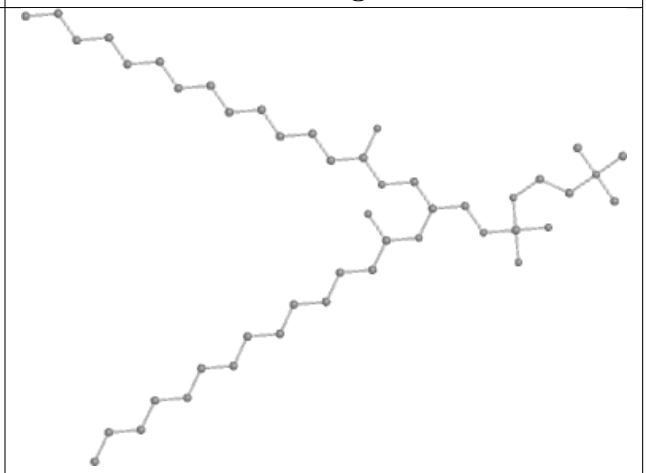
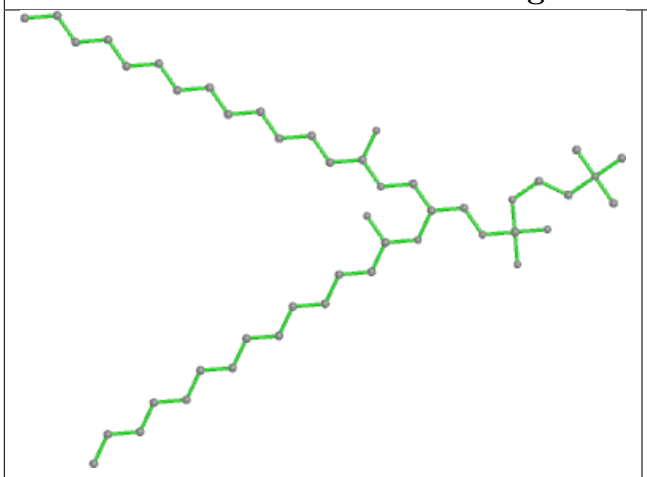


Rings

Ligand PX4 A 416



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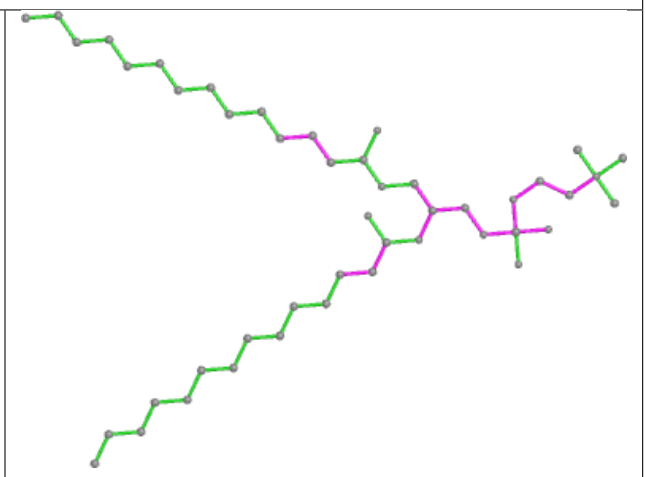

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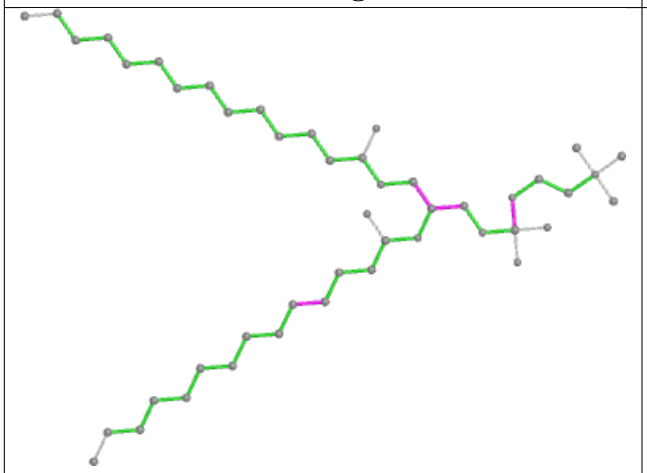

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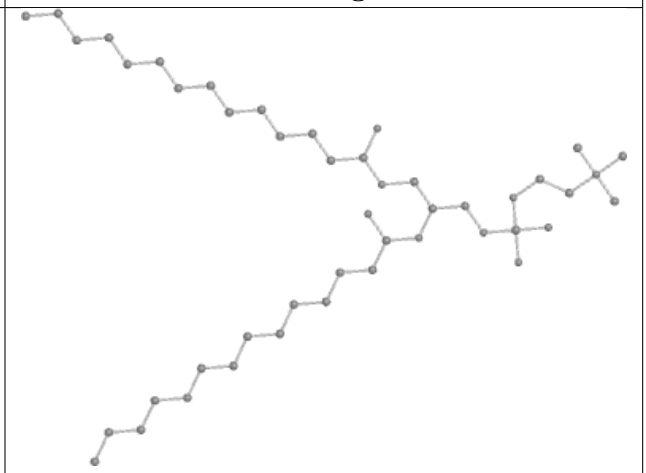
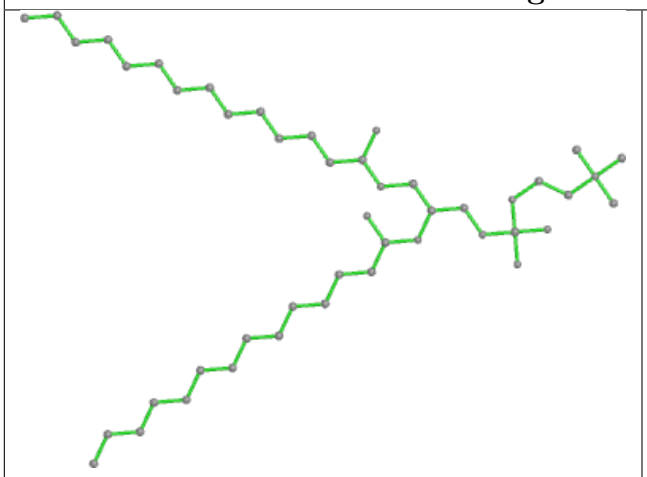


Rings

Ligand PX4 A 339



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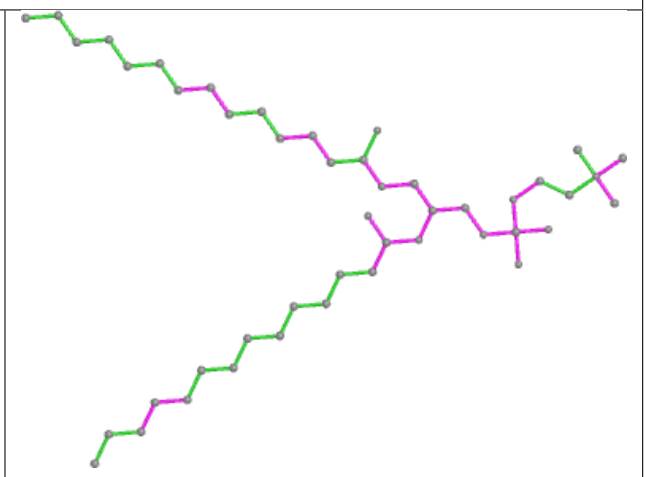

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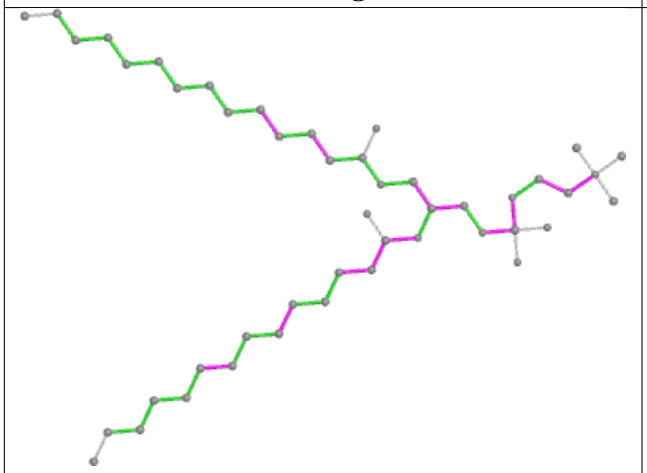

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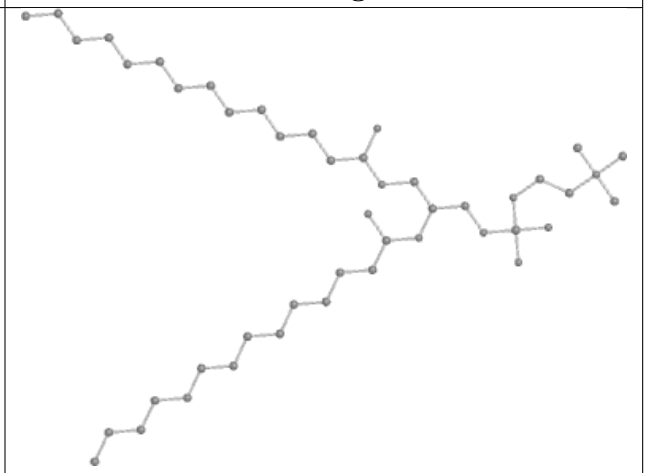
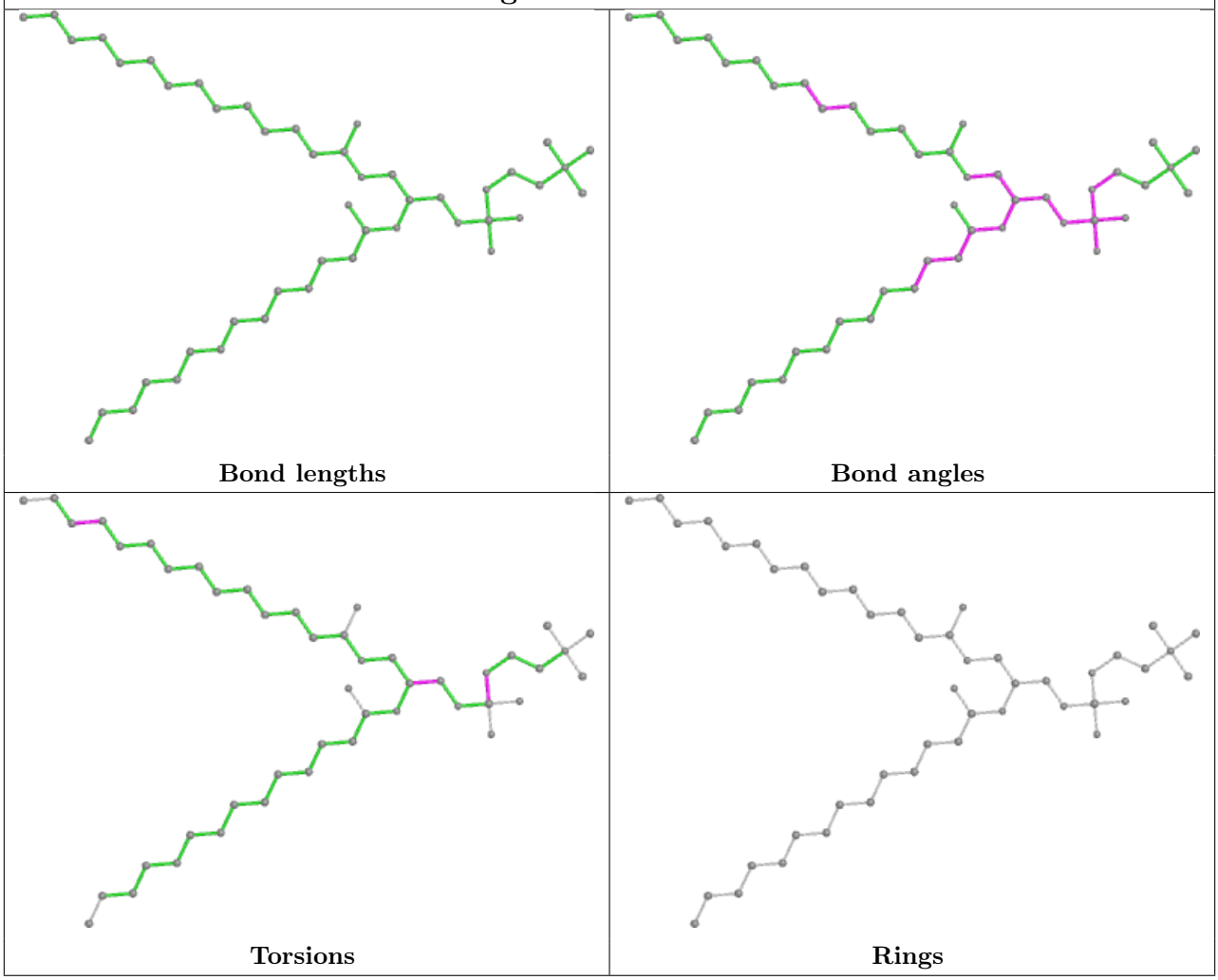
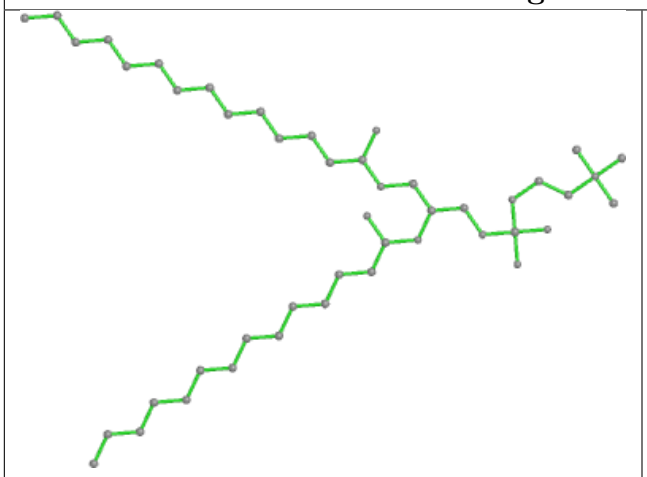


Rings

Ligand PX4 A 330



Ligand PX4 A 318



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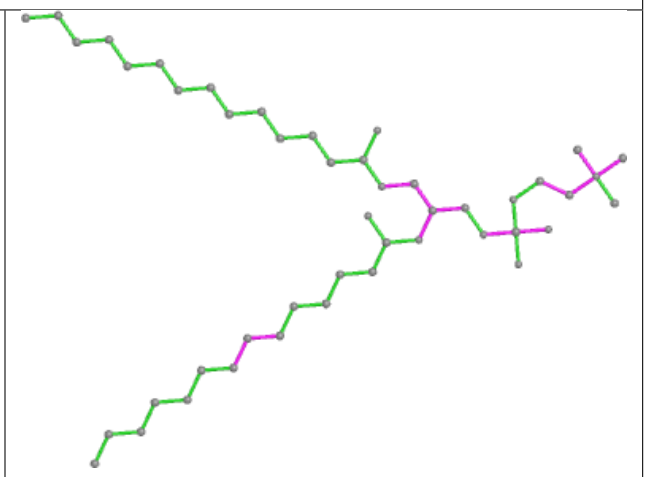
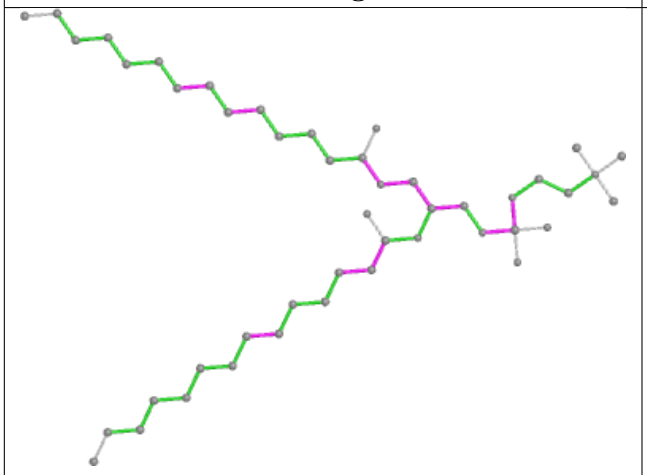


Bond angles



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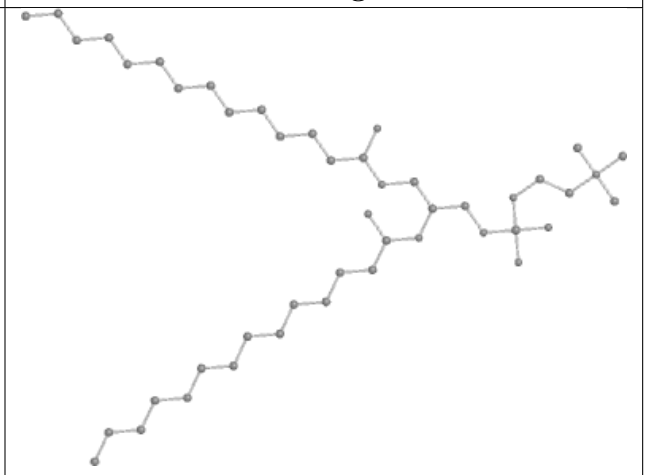
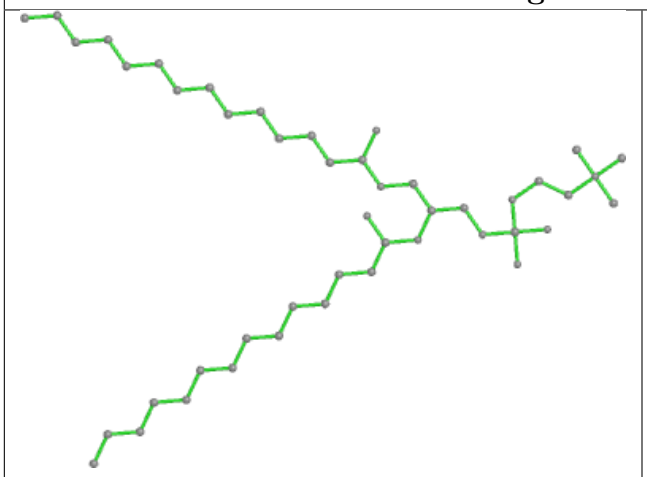


Rings

Ligand PX4 A 384



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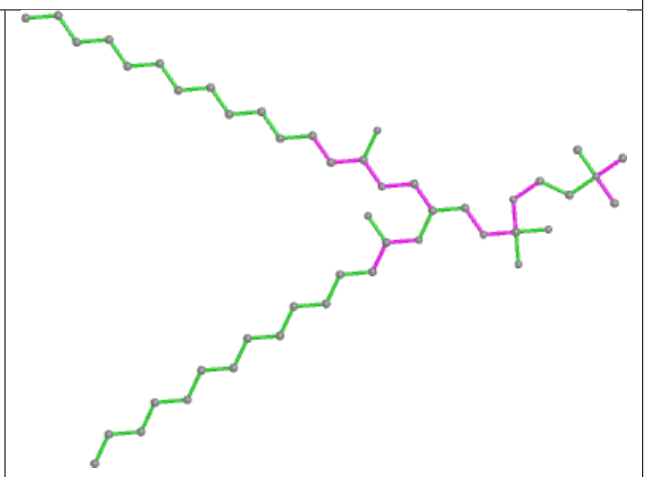

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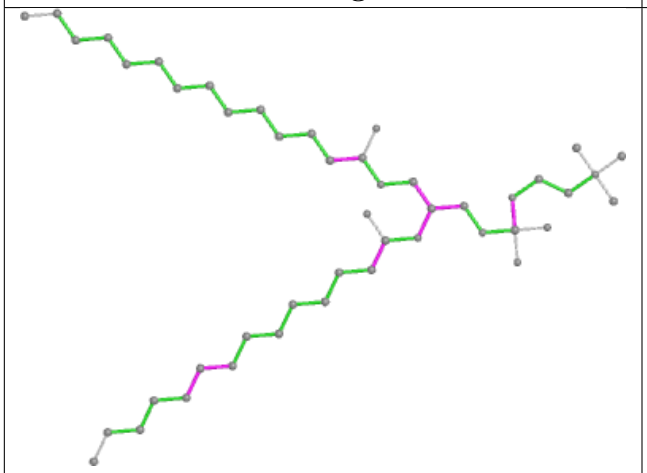

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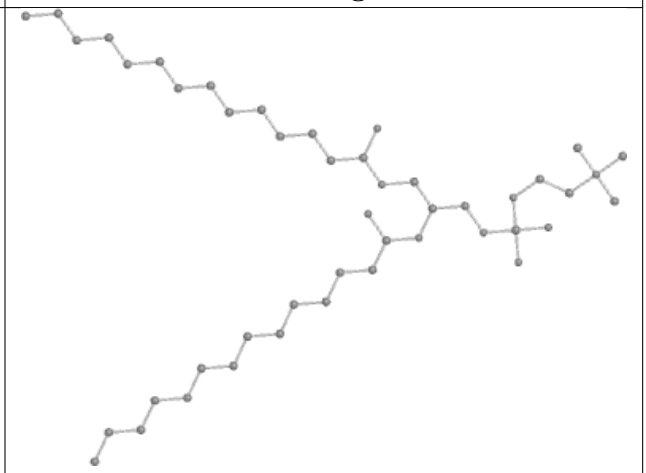
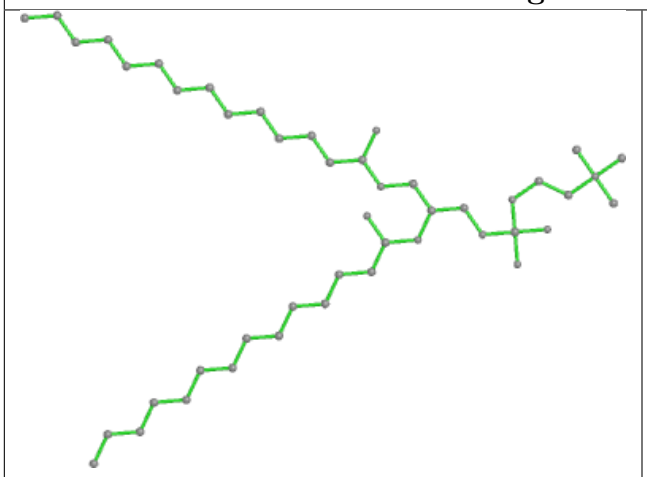


Rings

Ligand PX4 A 336



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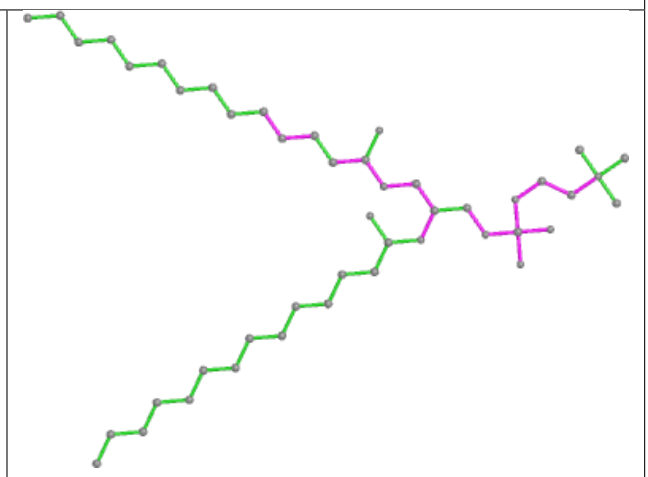
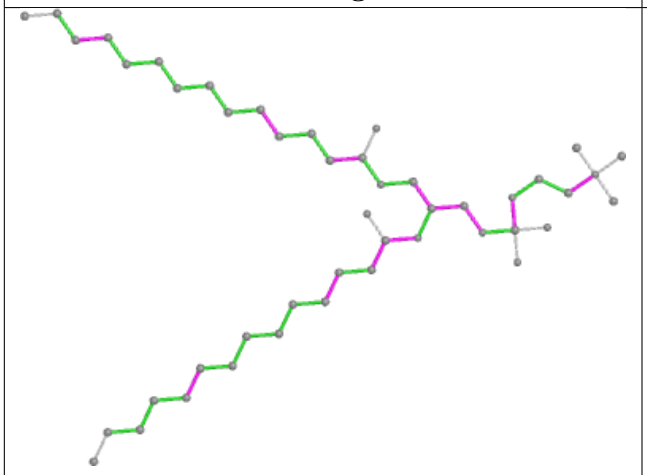


Bond angles



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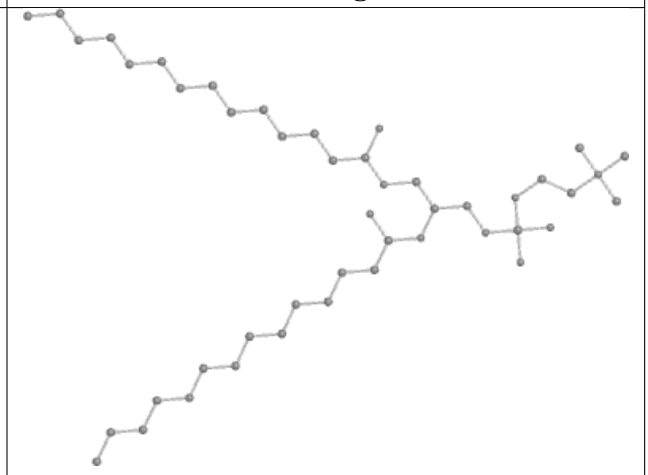
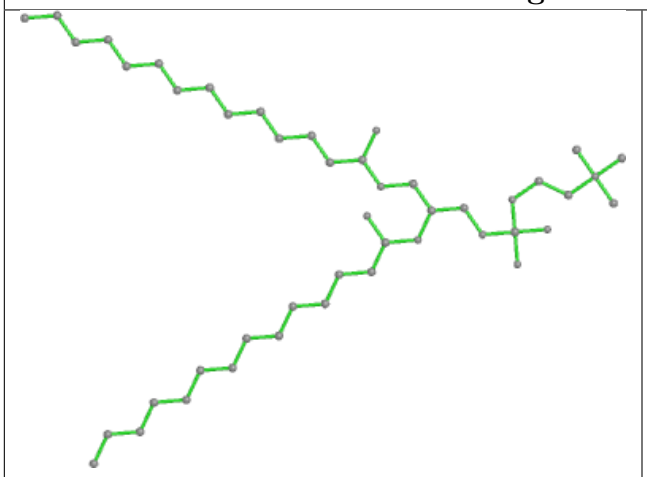


Rings

Ligand PX4 A 402



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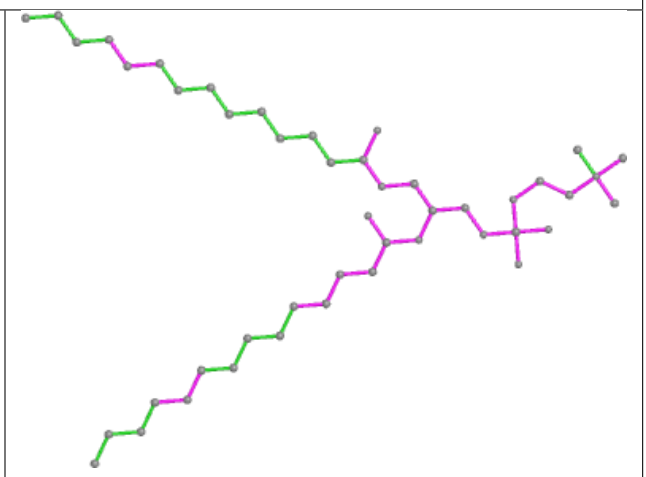
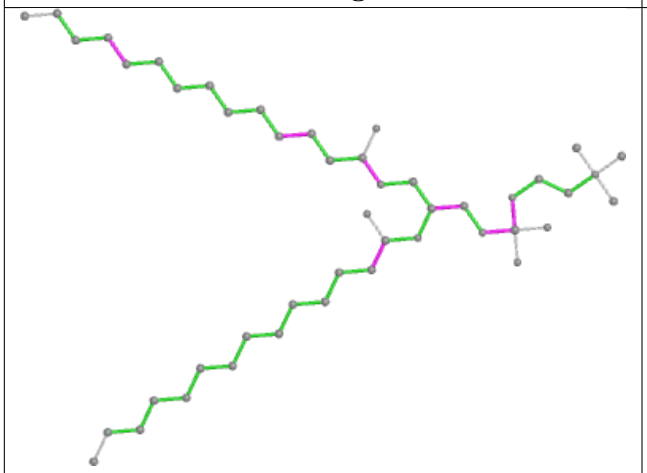


Bond angles



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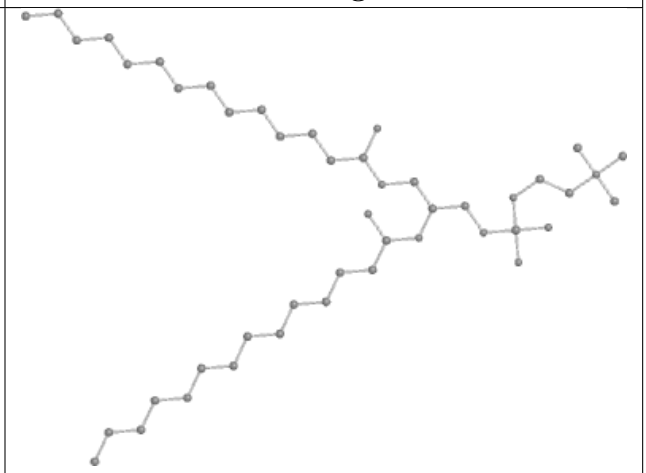
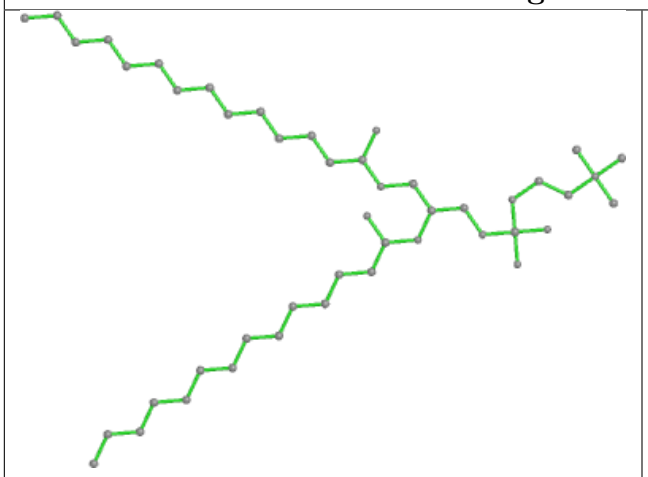


Rings

Ligand PX4 A 401



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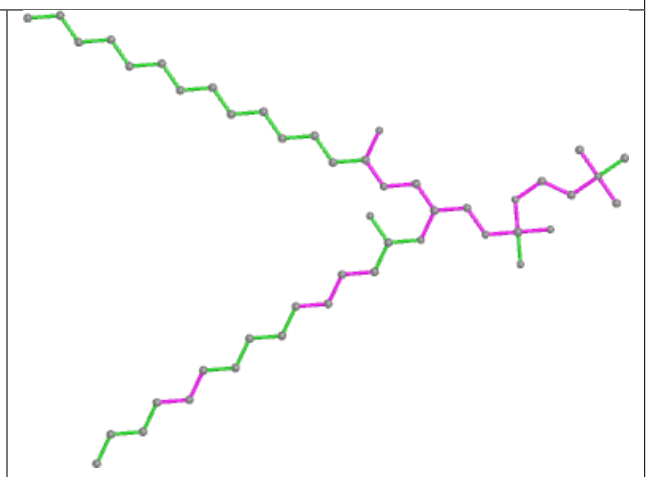

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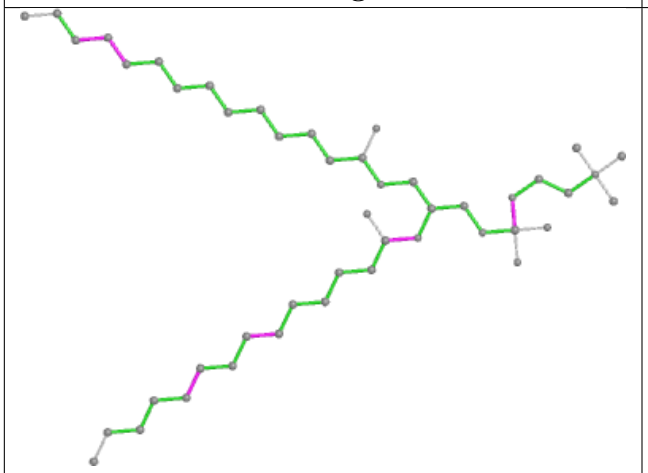

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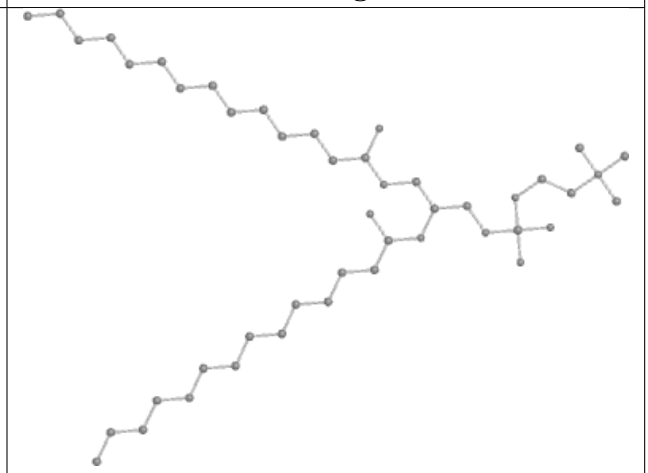
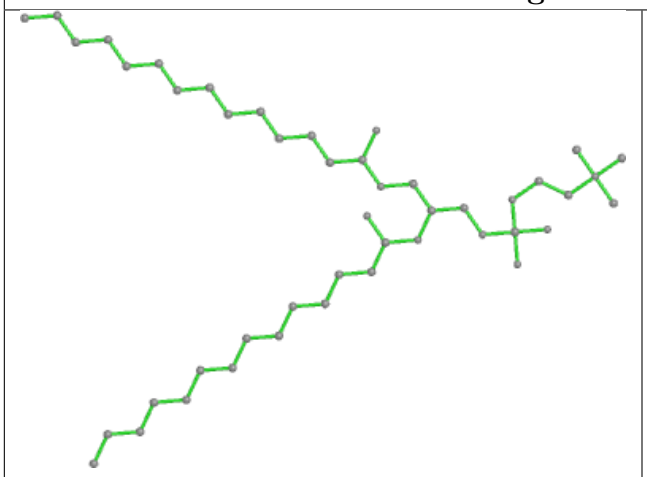


Rings

Ligand PX4 A 321



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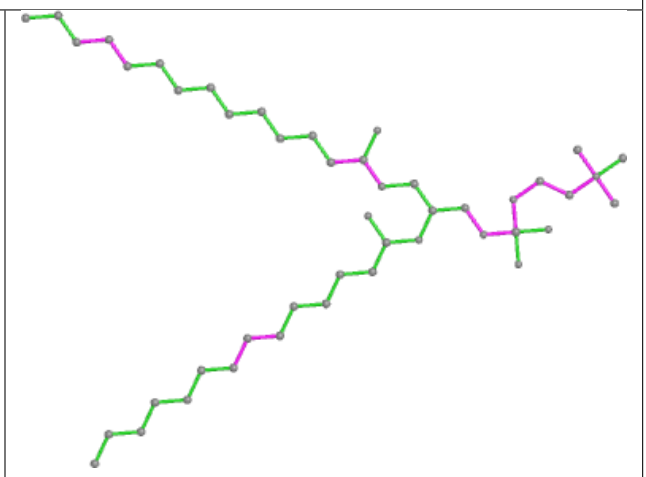

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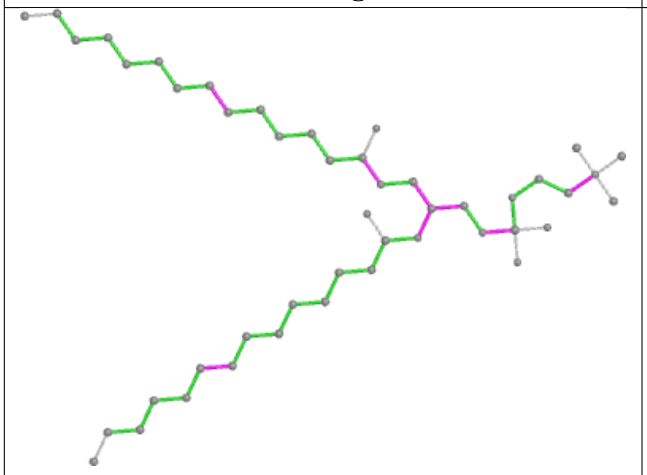

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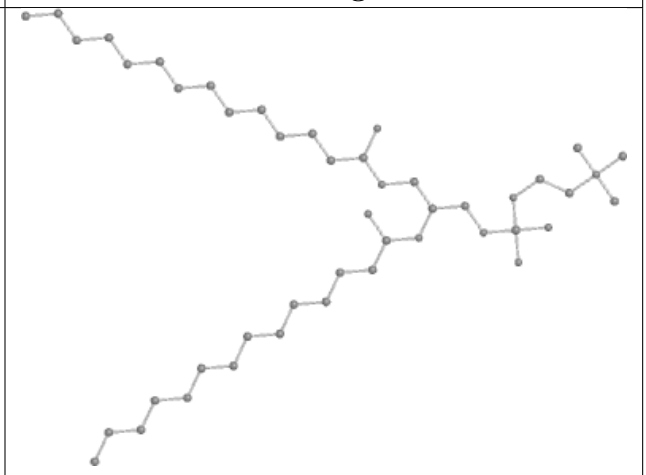
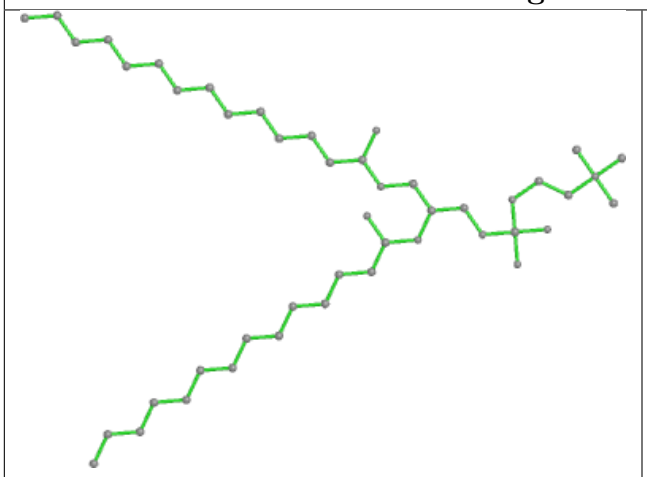


Rings

Ligand PX4 A 327



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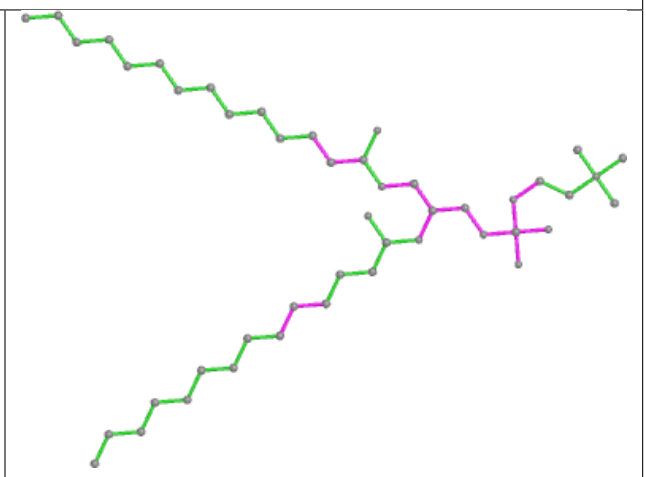

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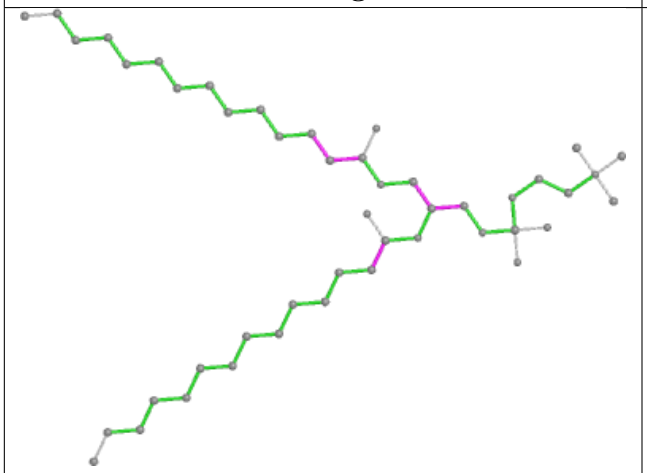

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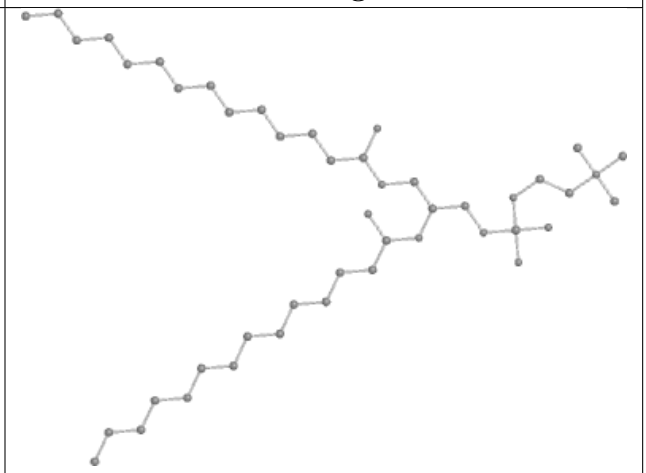
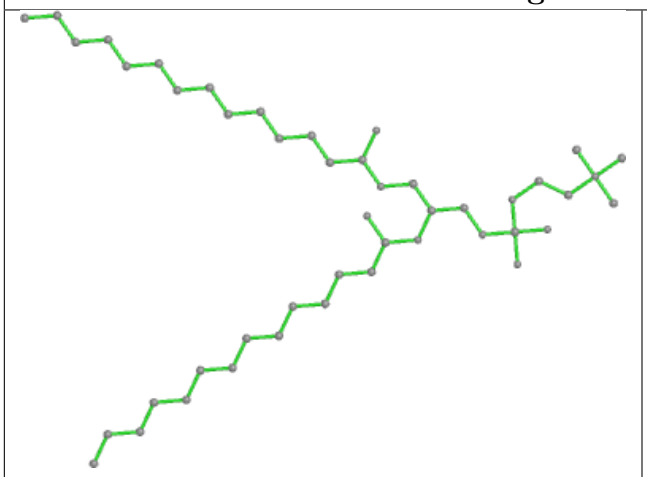


Rings

Ligand PX4 A 422



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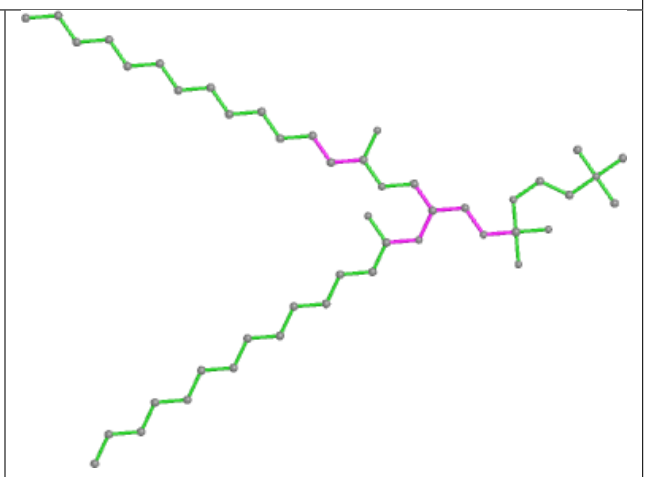
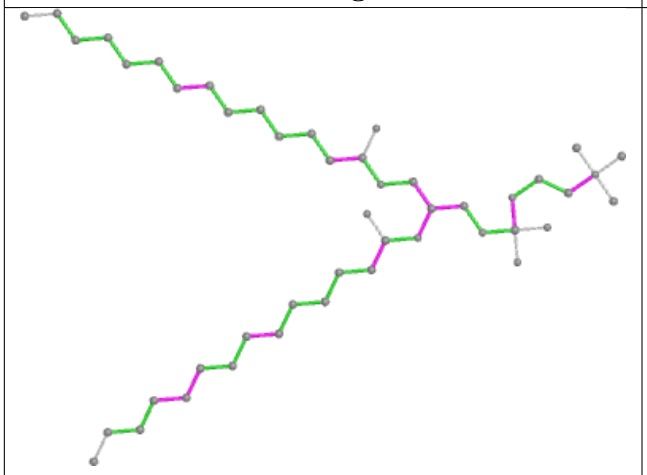
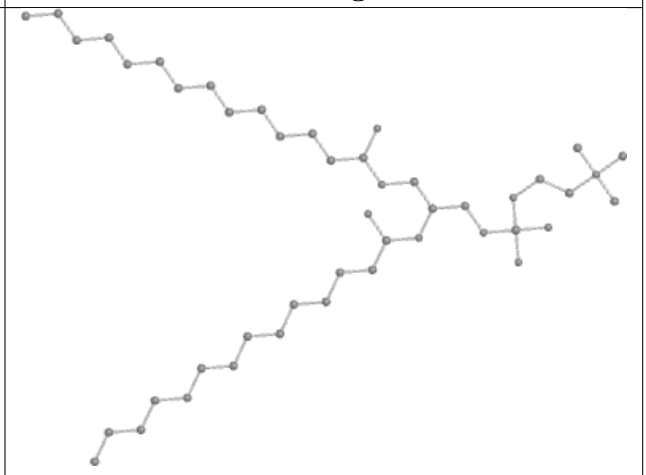


Bond angles

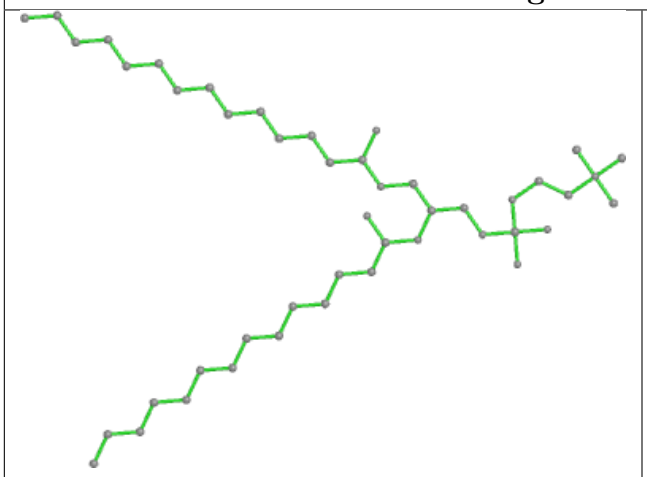


Torsions

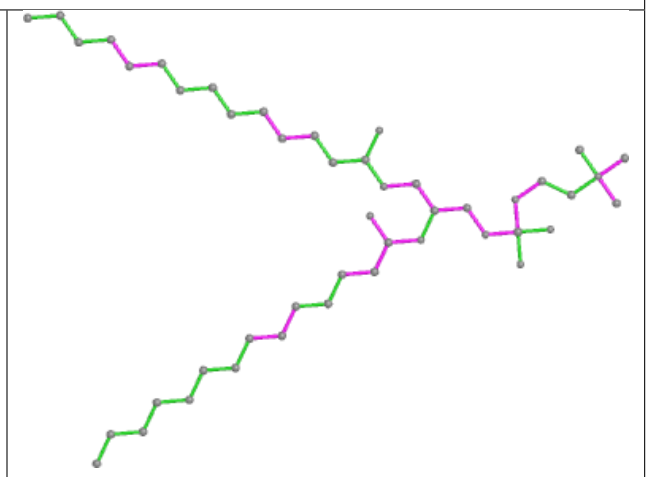


Rings

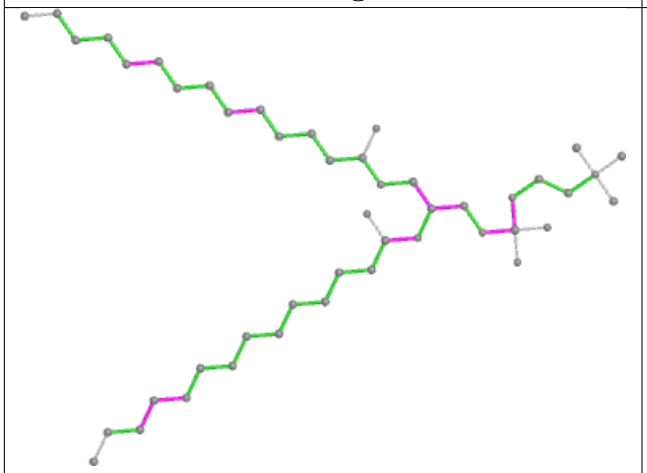
Ligand PX4 A 404



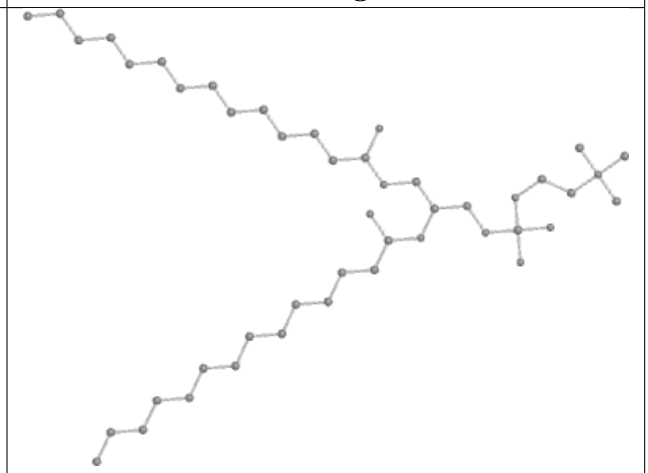
Bond lengths



Bond angles

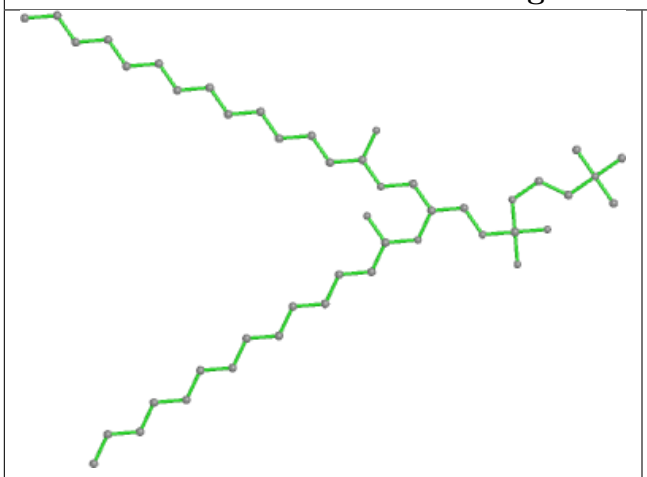


Torsions



Rings

Ligand PX4 A 394



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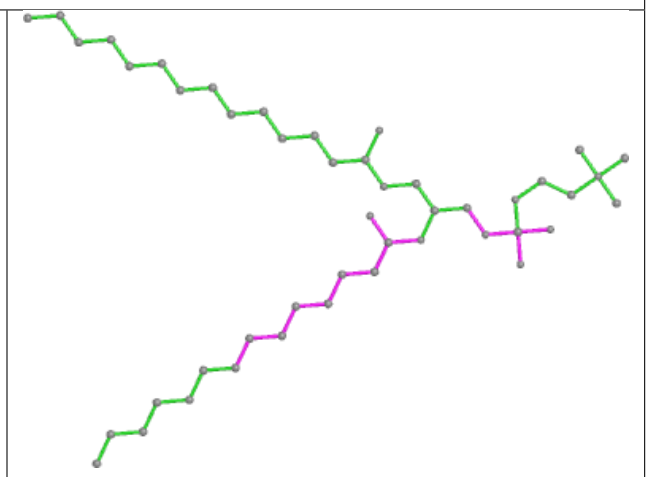

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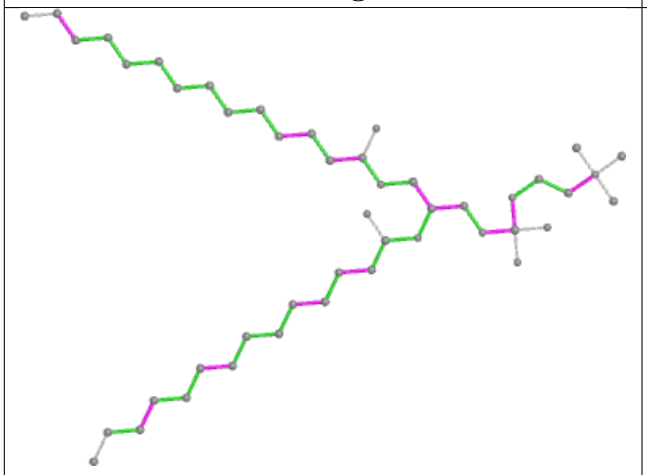

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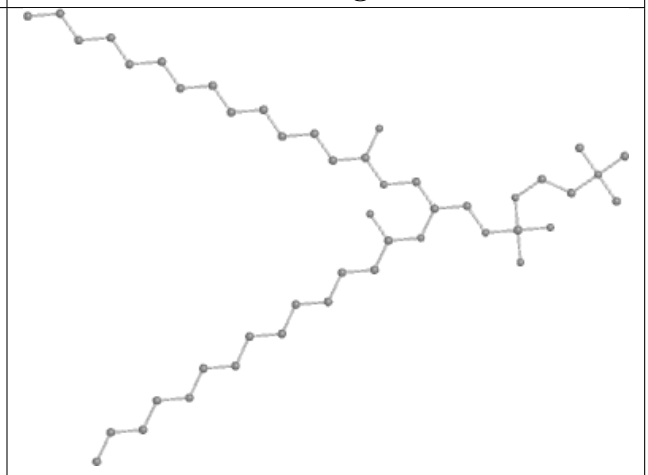
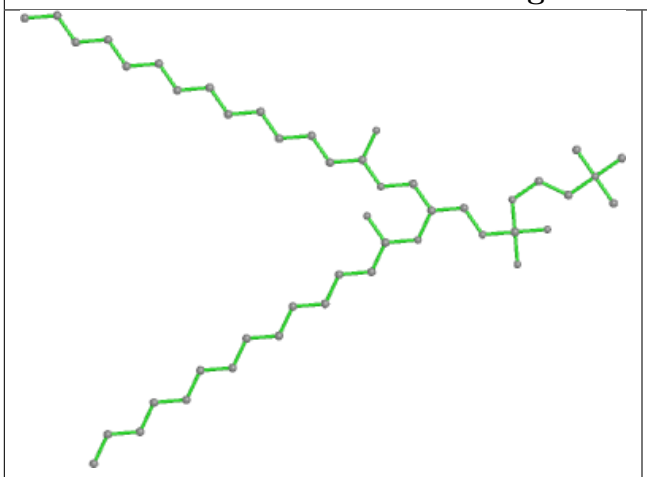


Rings

Ligand PX4 A 413



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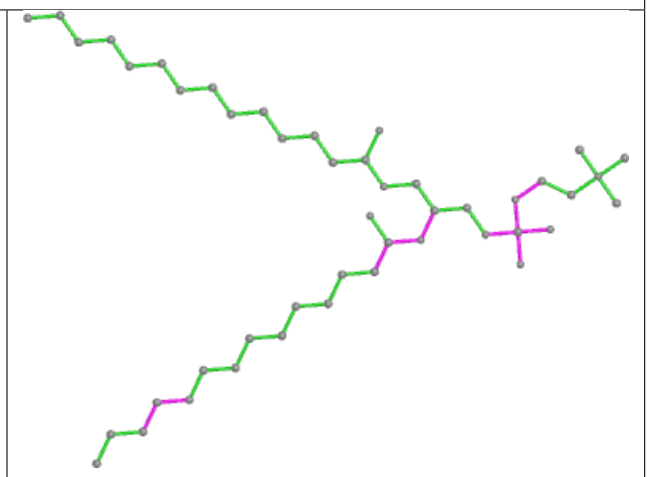

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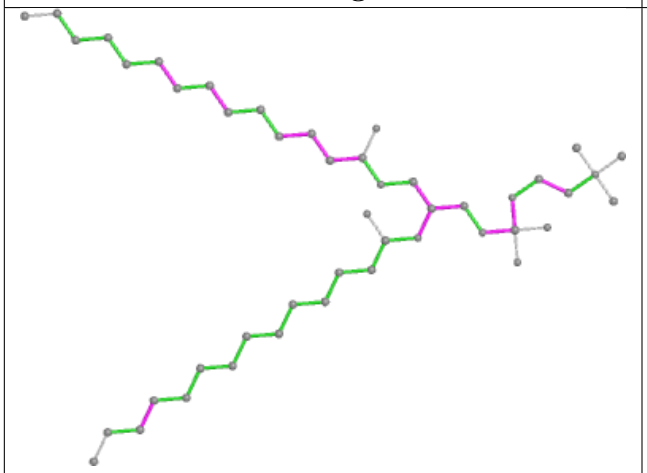

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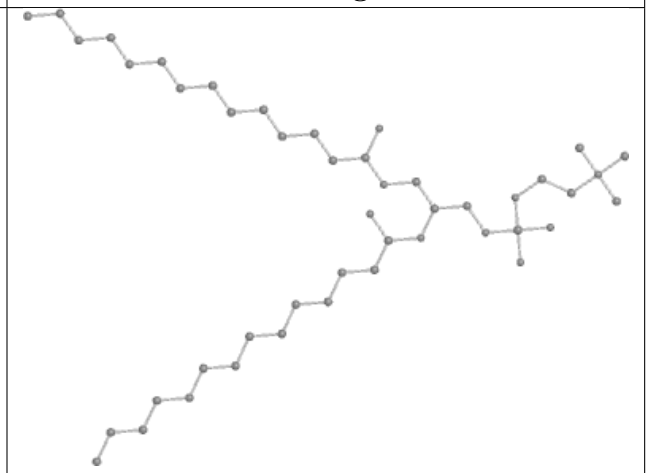
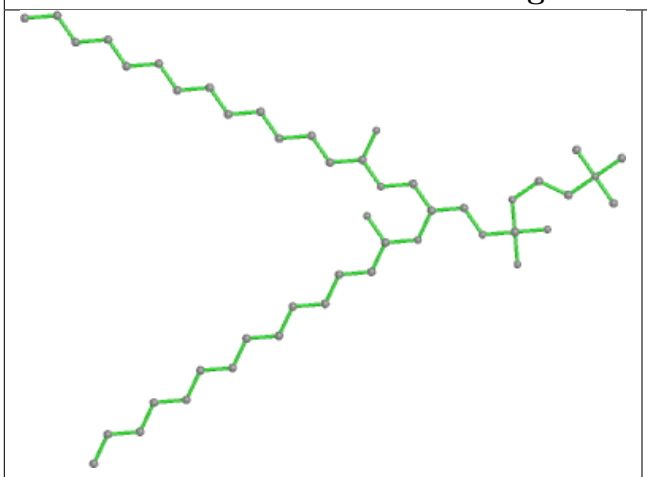


Rings

Ligand PX4 A 357



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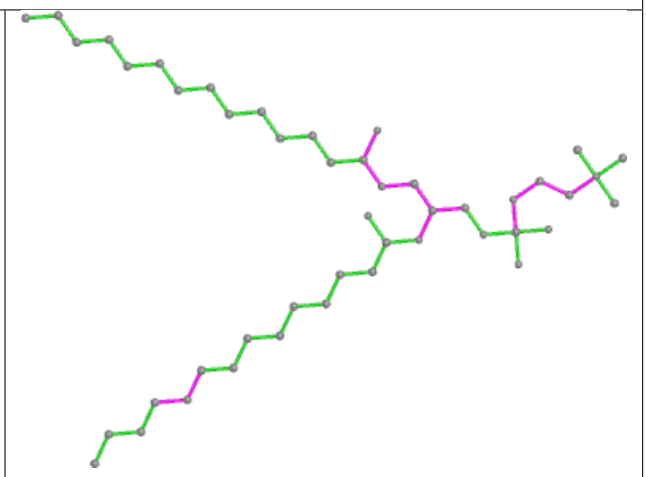

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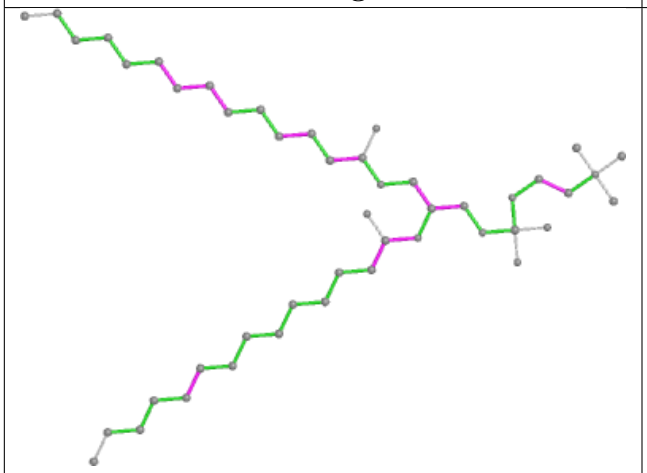

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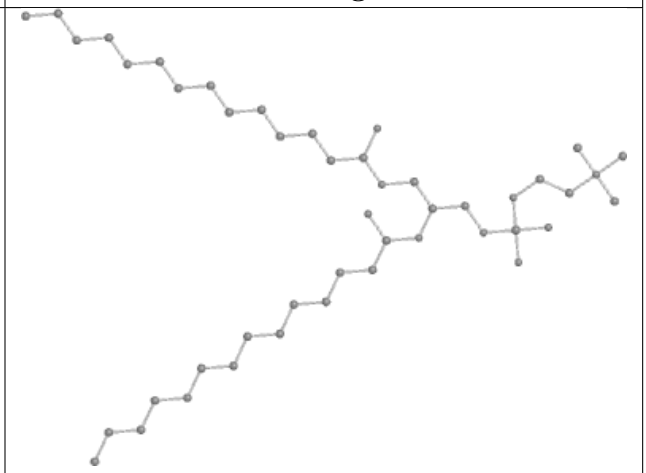
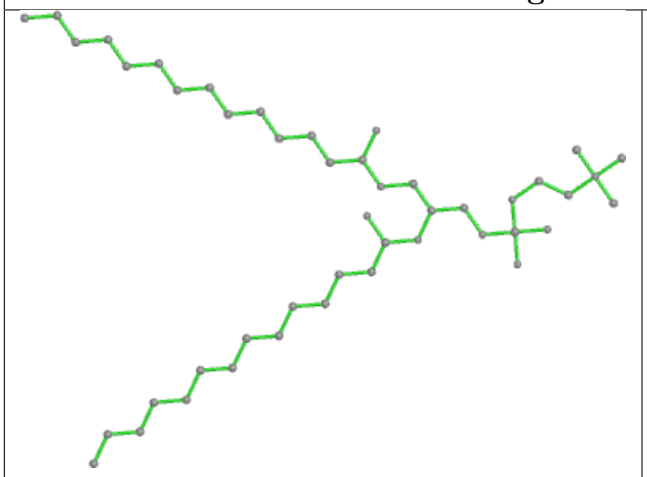


Rings

Ligand PX4 A 376



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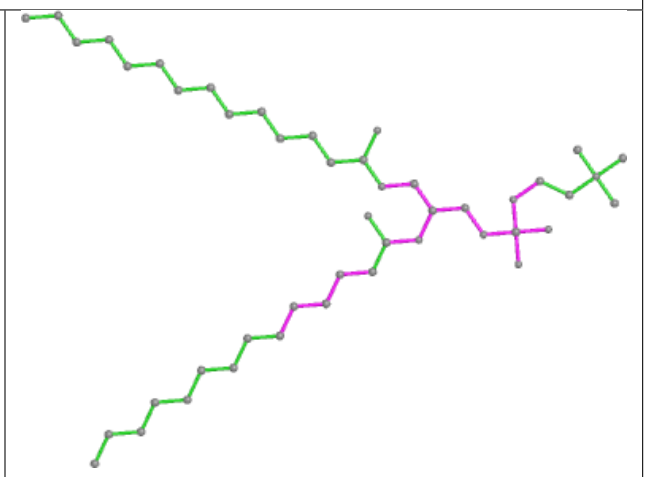

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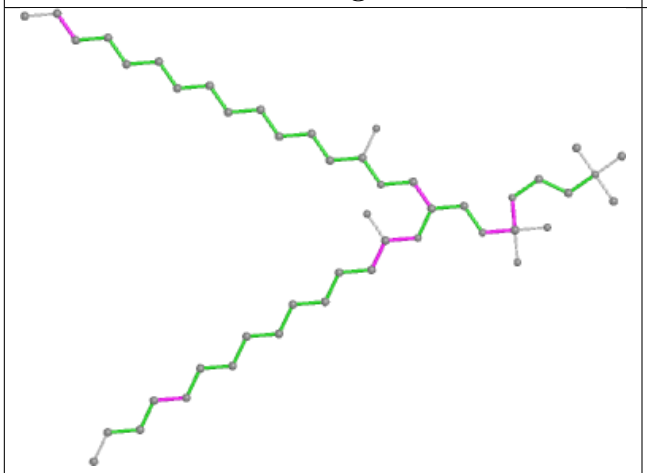

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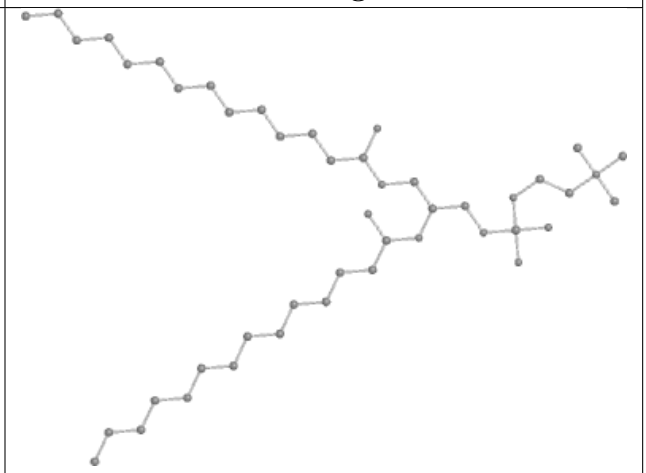
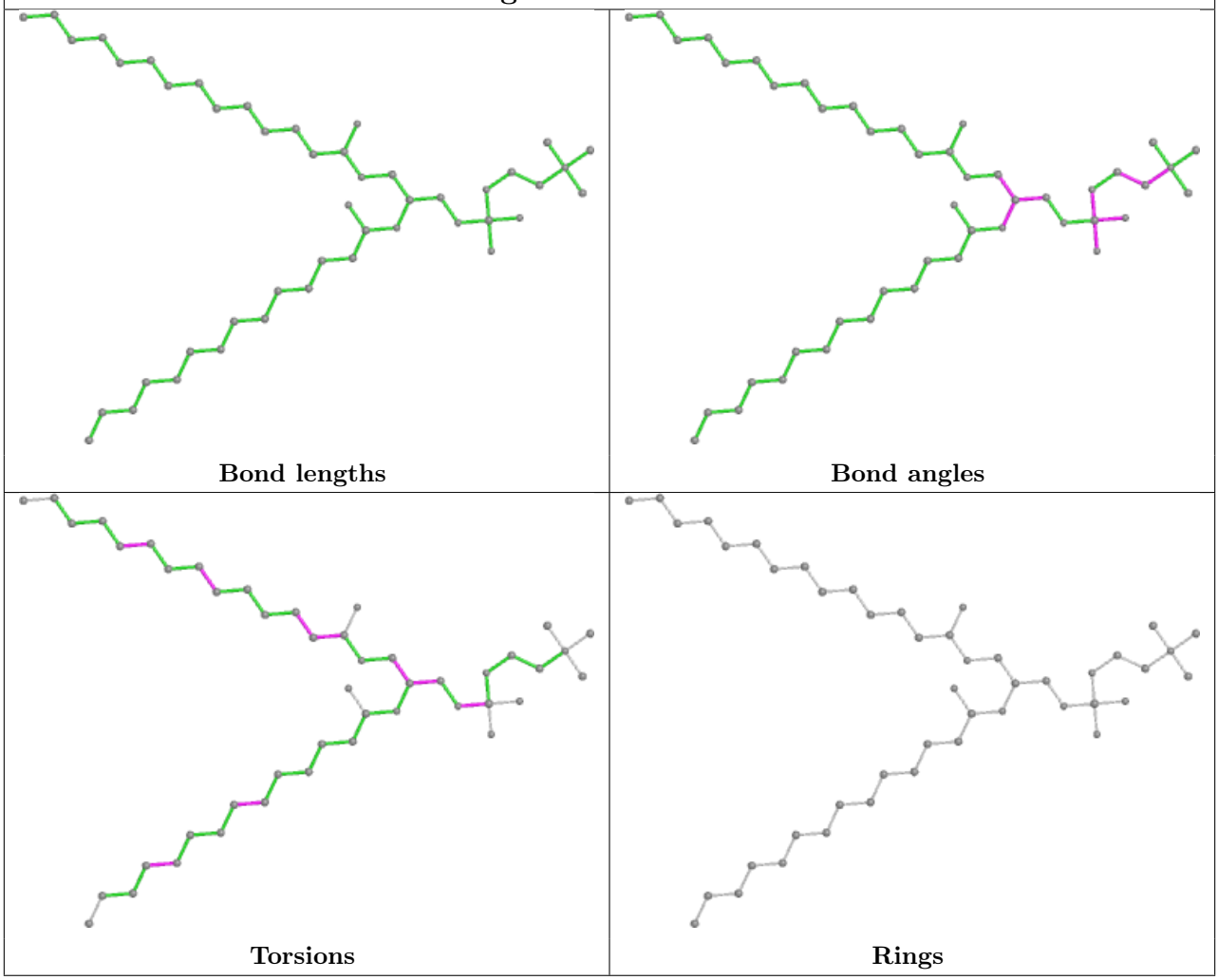
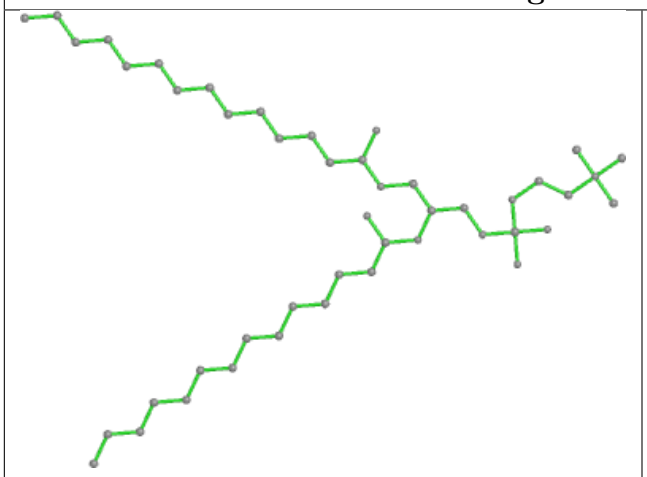


Rings

Ligand PX4 A 323



Ligand PX4 A 415



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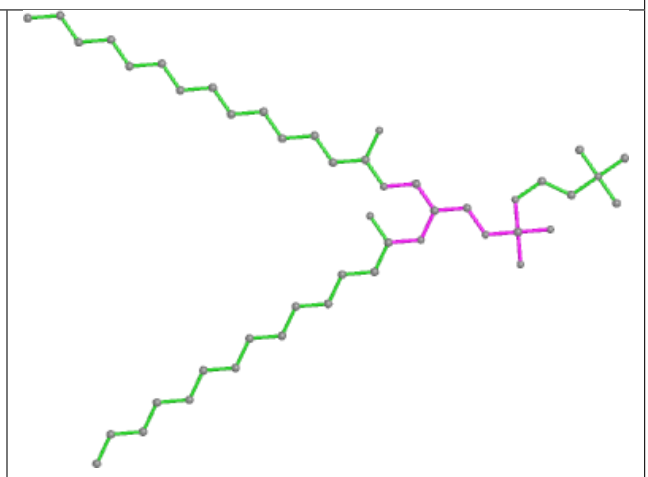
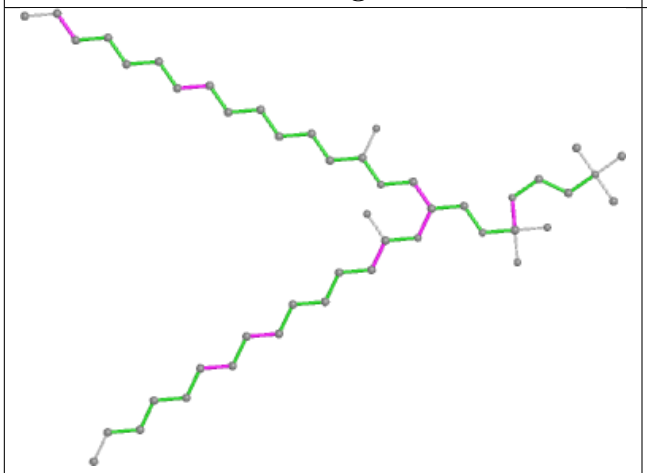


Bond angles



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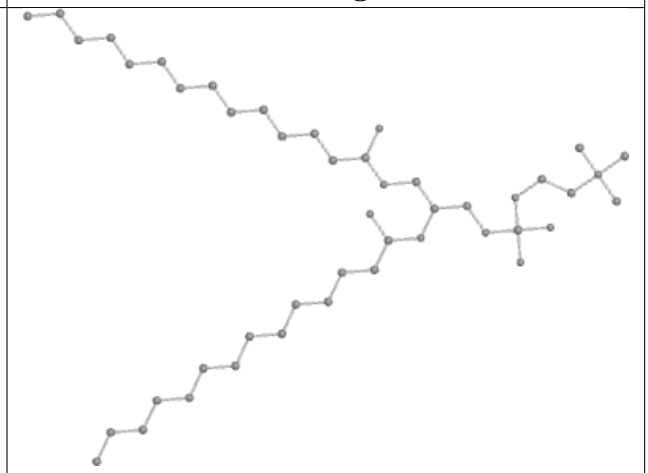
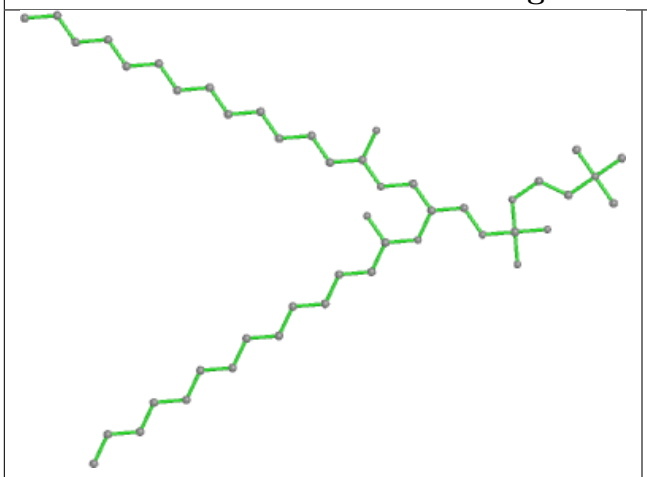


Rings

Ligand PX4 A 345



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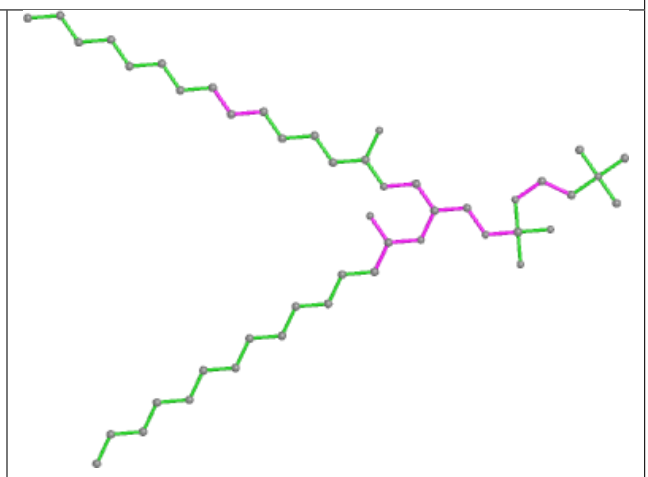
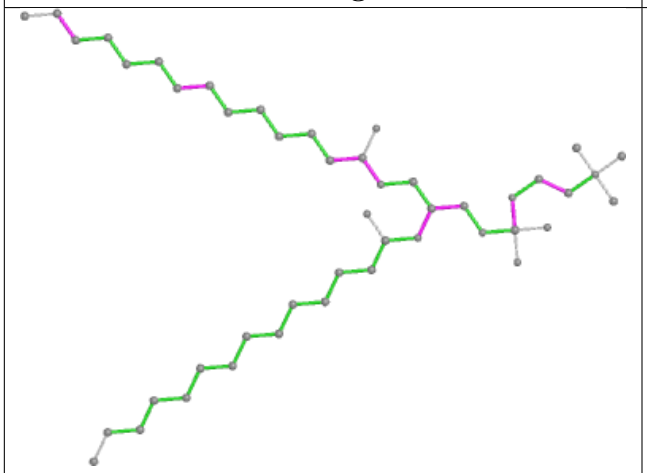


Bond angles



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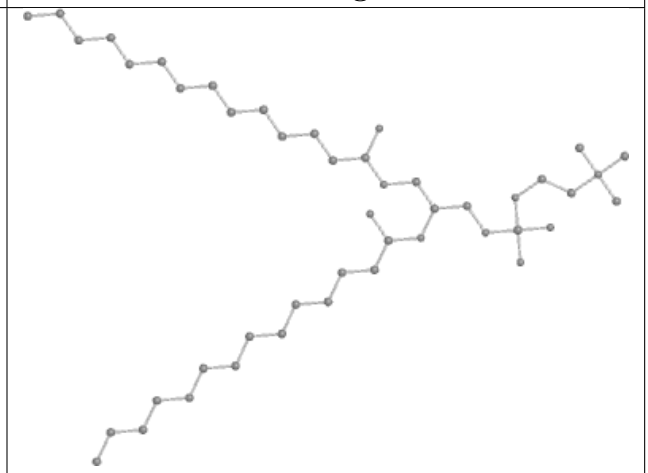
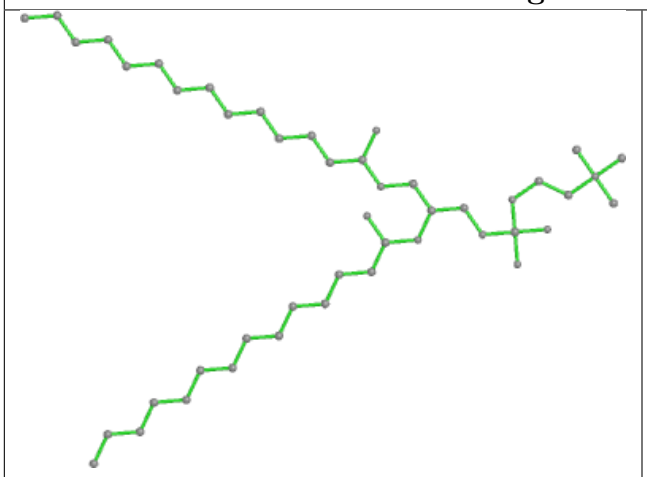


Rings

Ligand PX4 A 306



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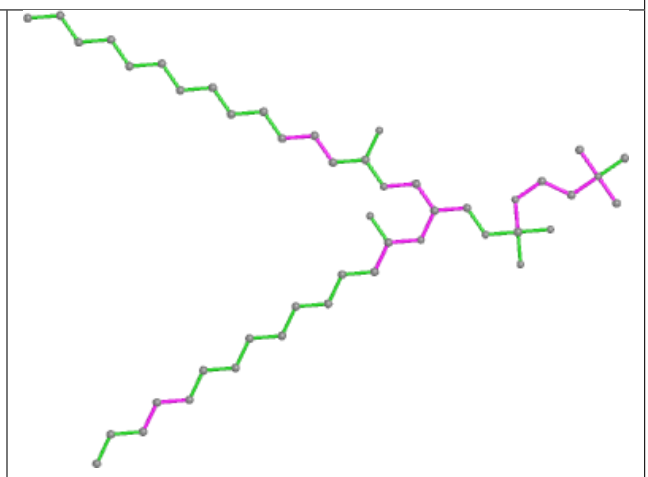
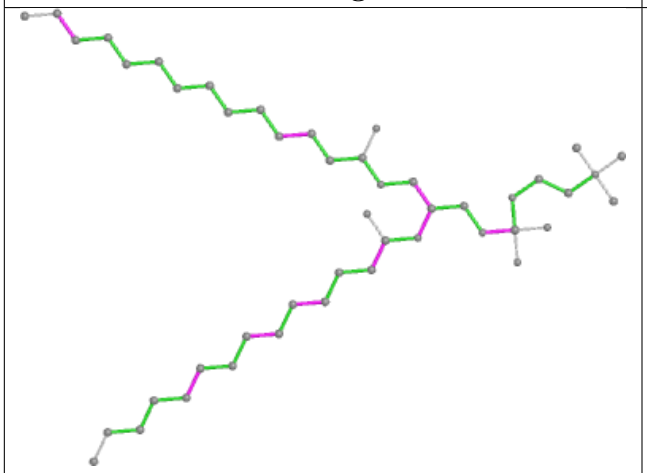


Bond angles



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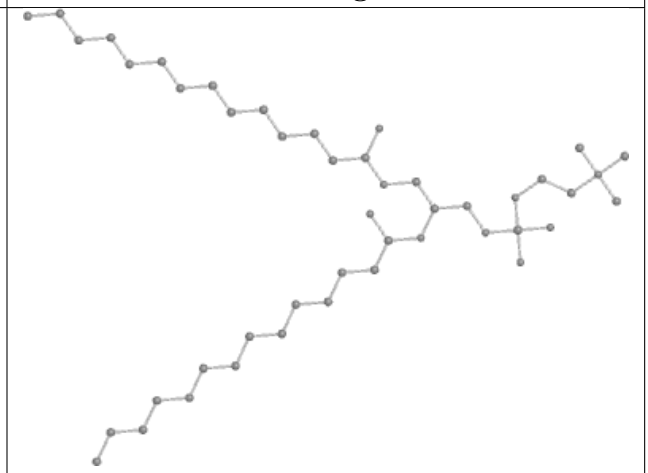
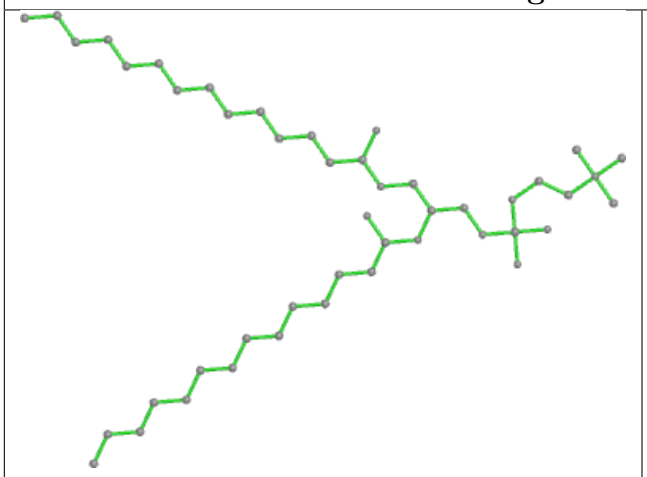


Rings

Ligand PX4 A 385



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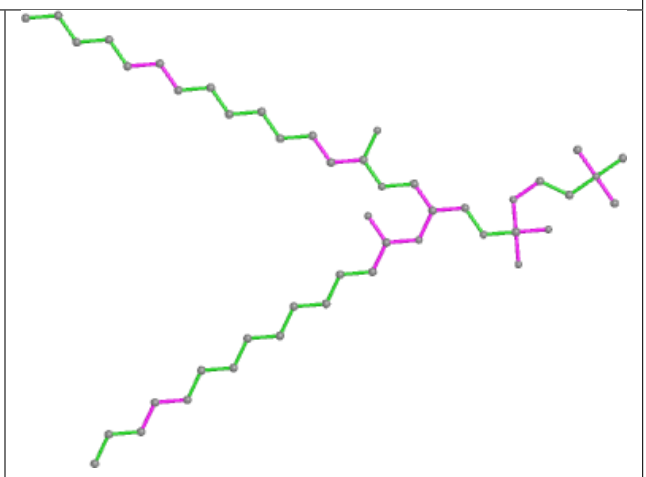
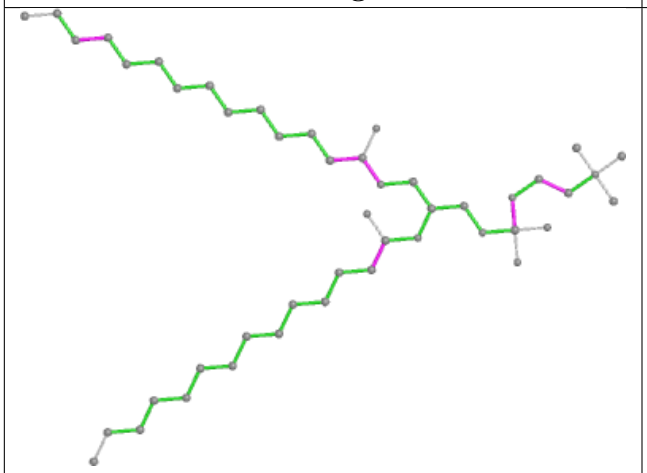


Bond angles



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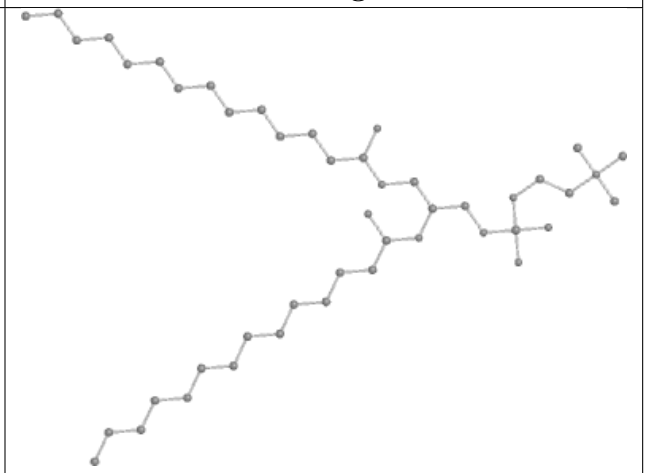
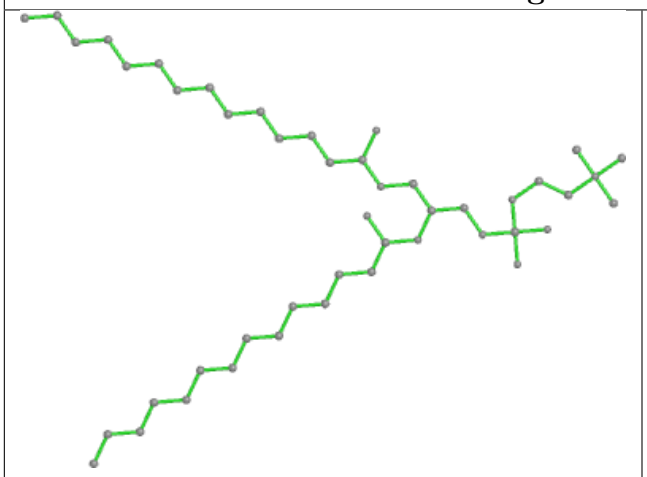


Rings

Ligand PX4 A 359



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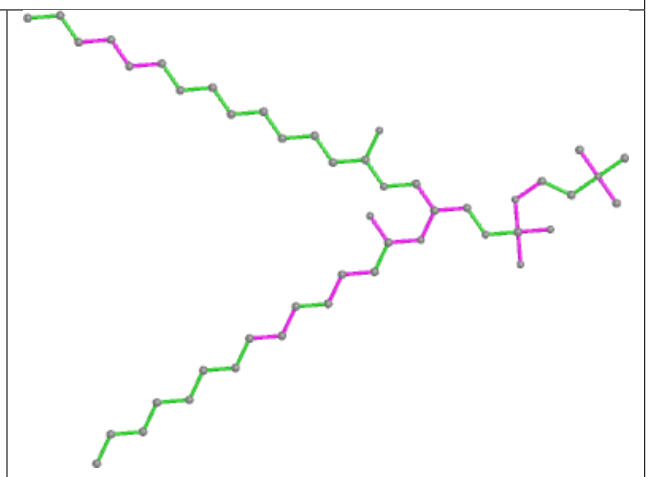

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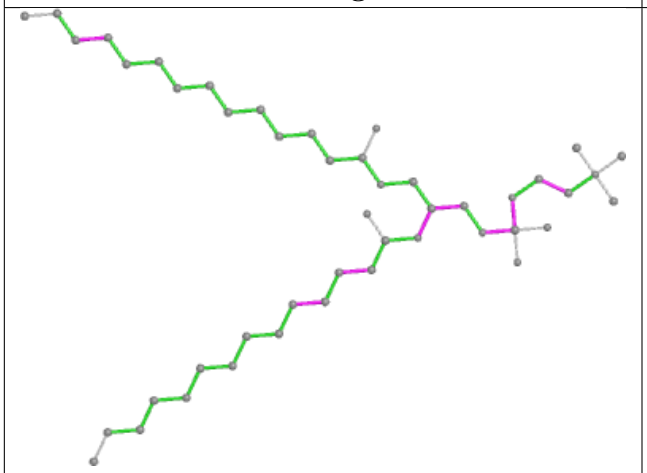

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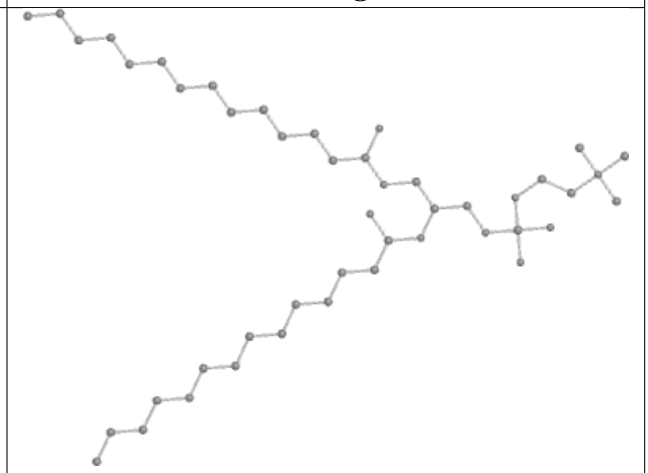
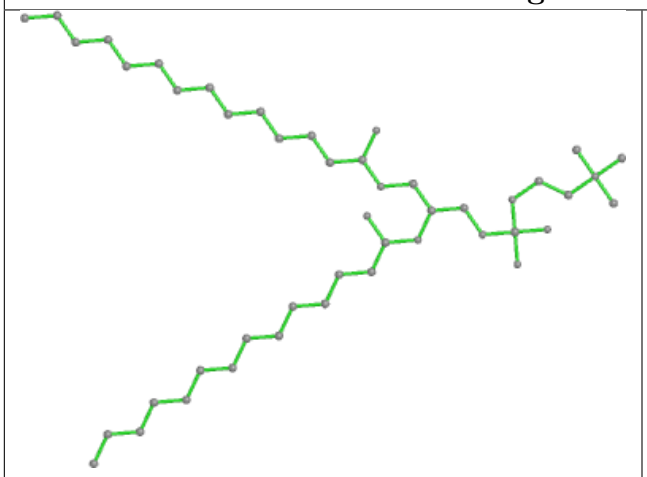


Rings

Ligand PX4 A 389



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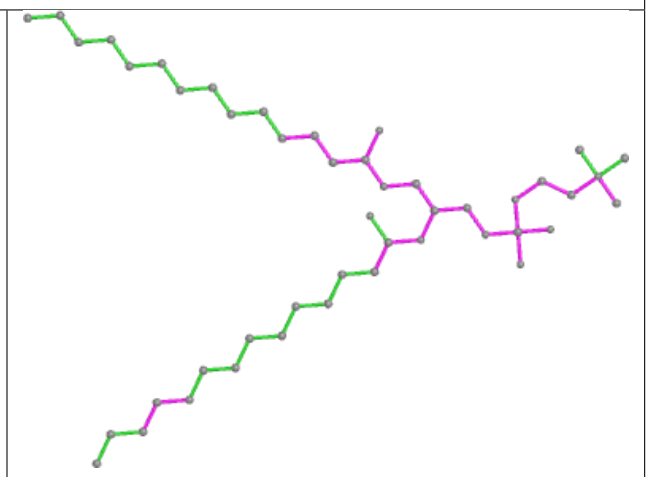

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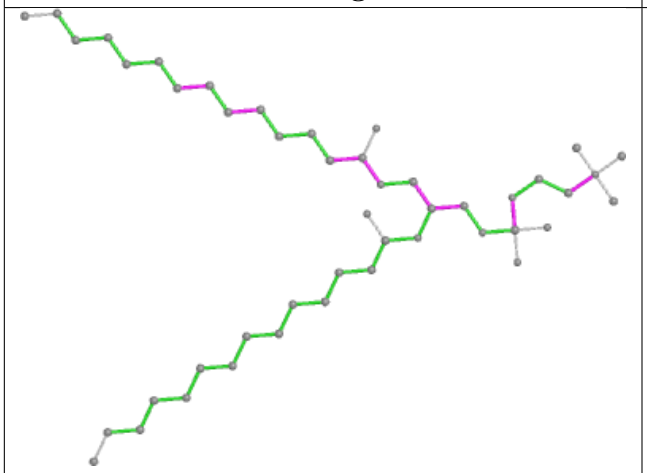

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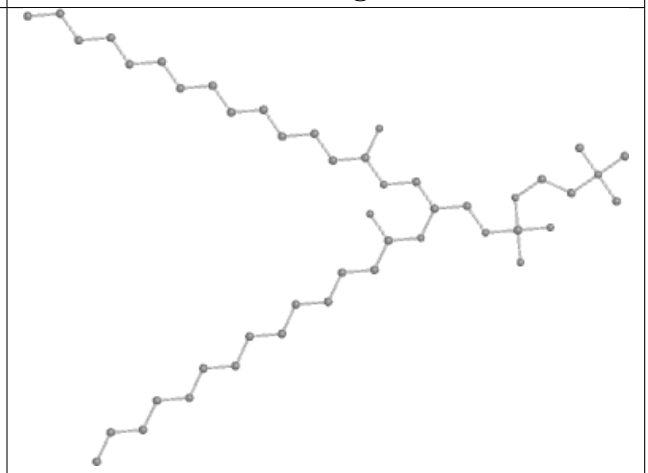
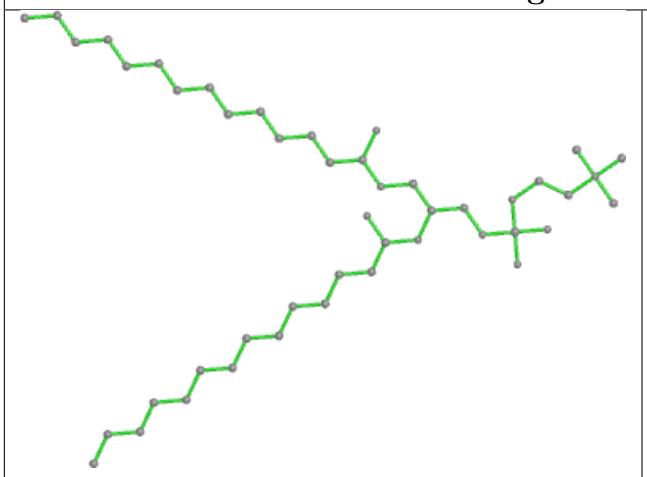


Rings

Ligand PX4 A 400



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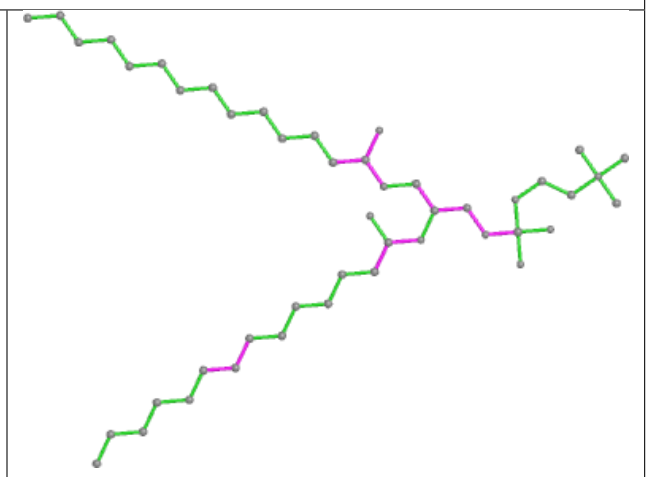
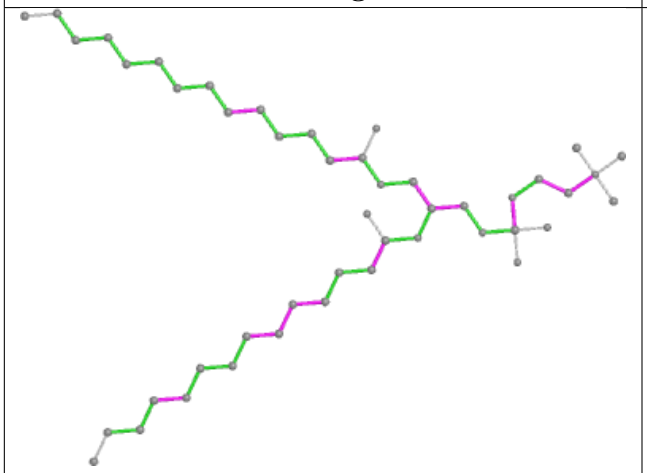


Bond angles



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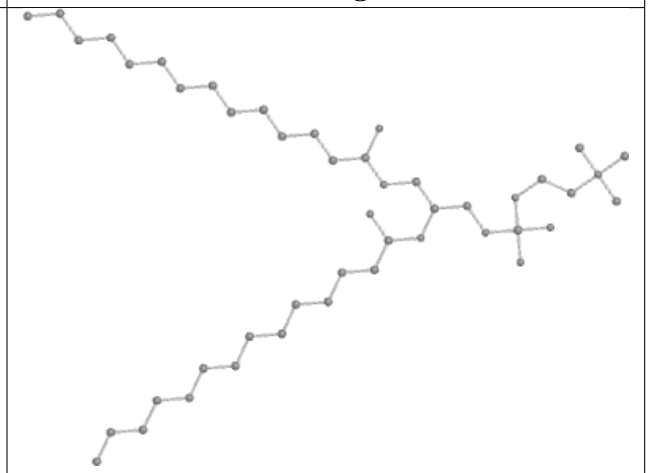
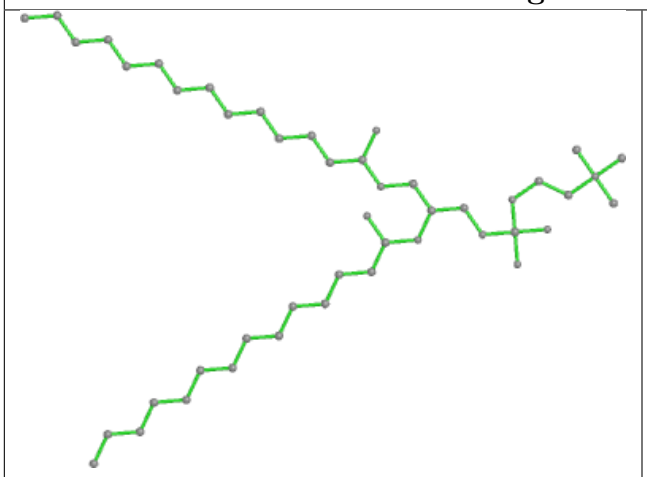


Rings

Ligand PX4 A 368



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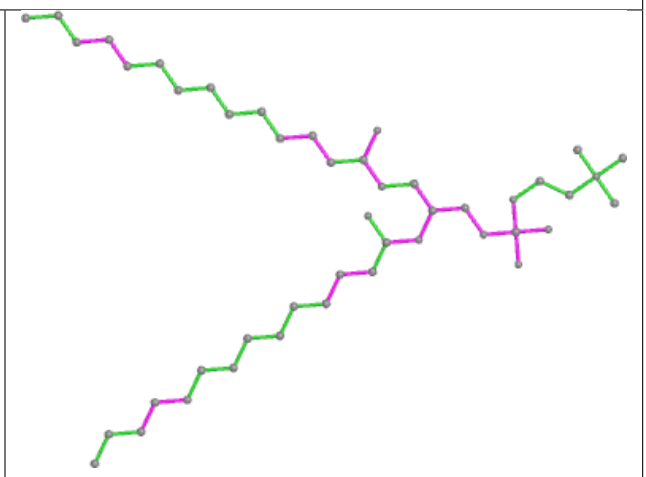
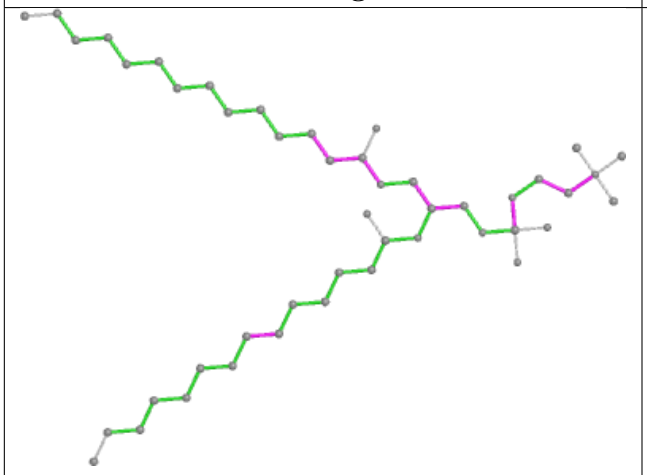


Bond angles



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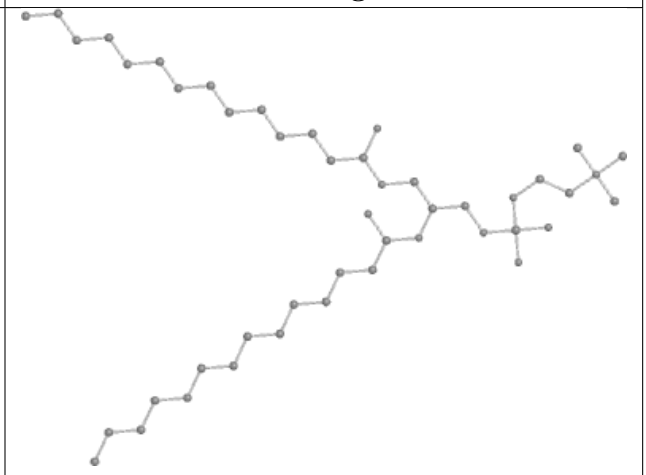
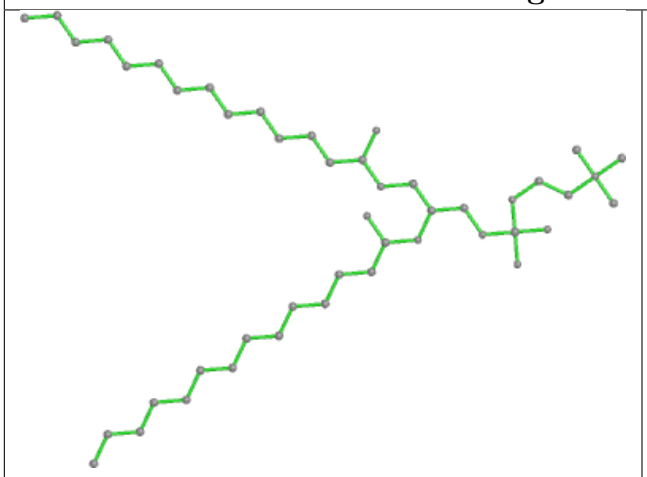
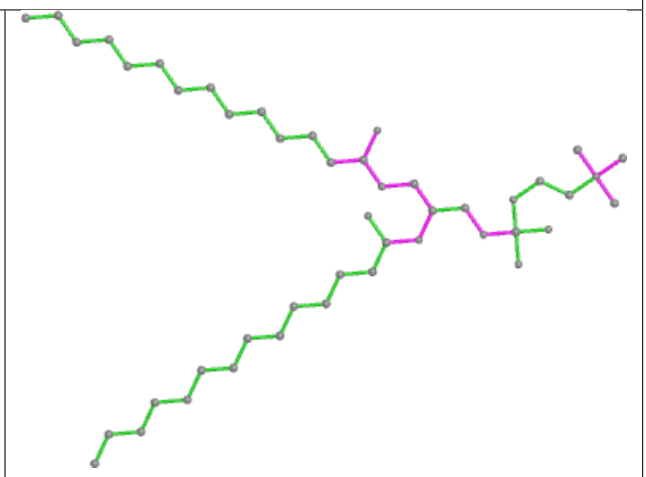


Rings

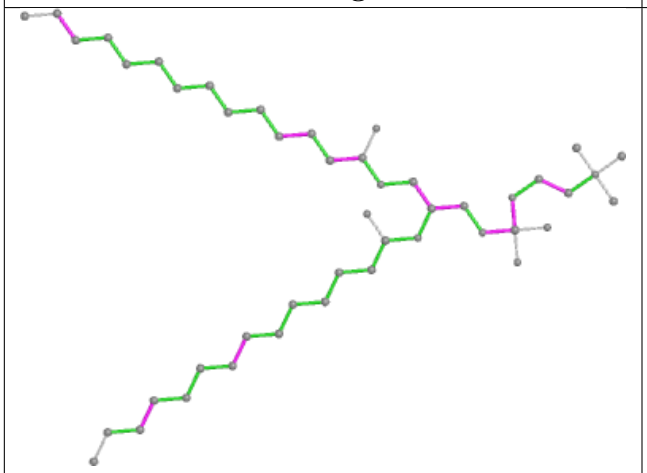
Ligand PX4 A 313



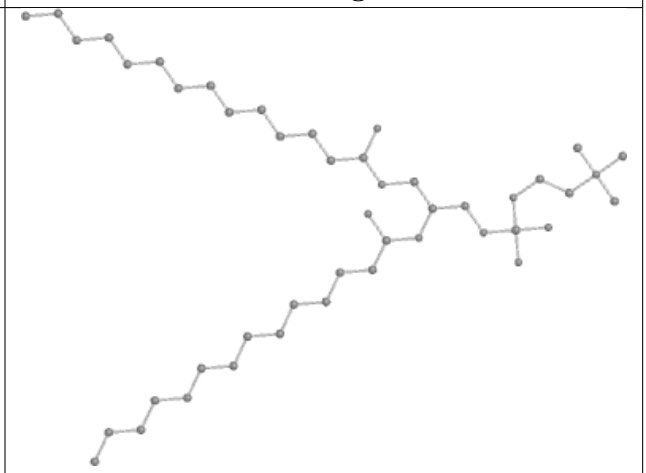
Bond lengths



Bond angles

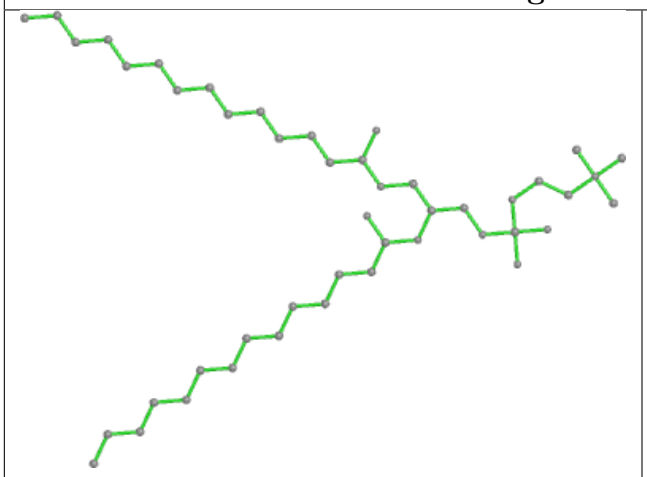


Torsions



Rings

Ligand PX4 A 343



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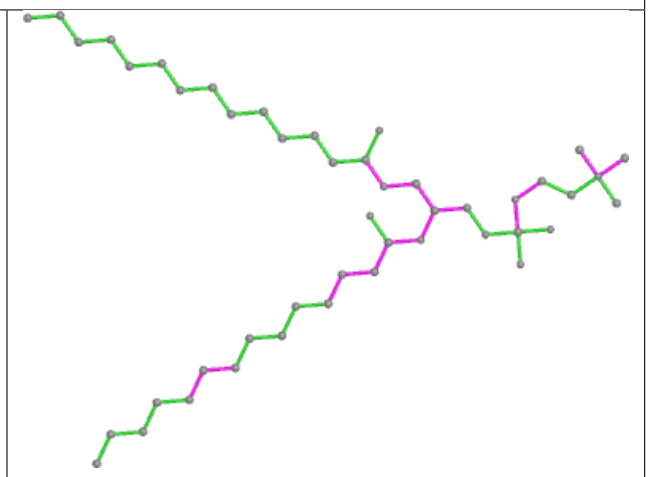

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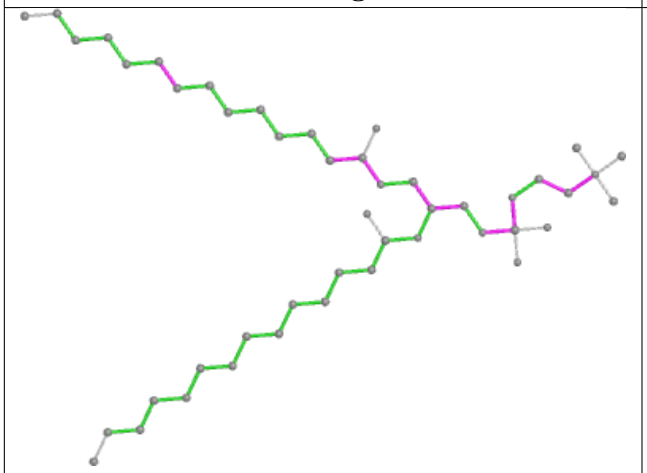

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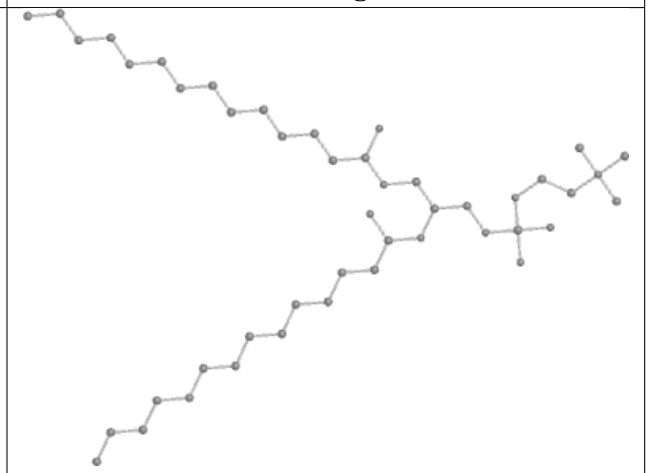
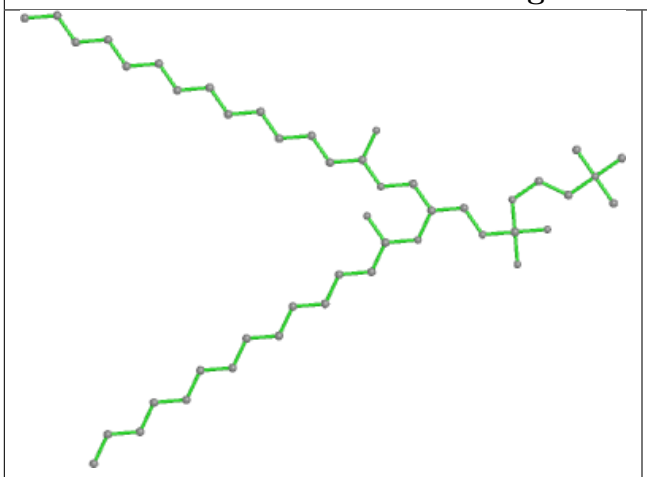


Rings

Ligand PX4 A 358



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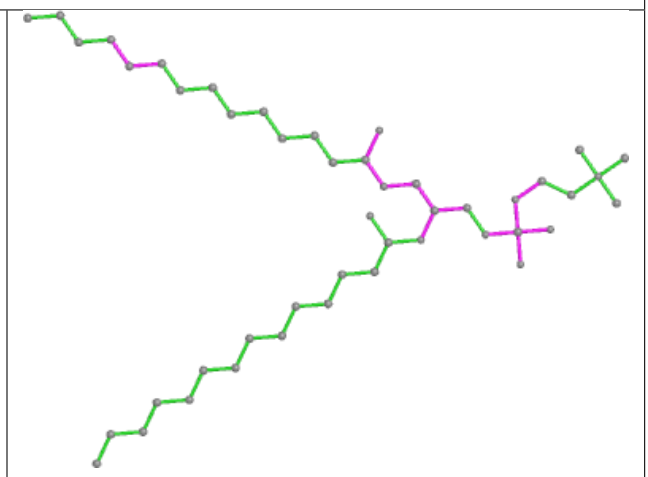

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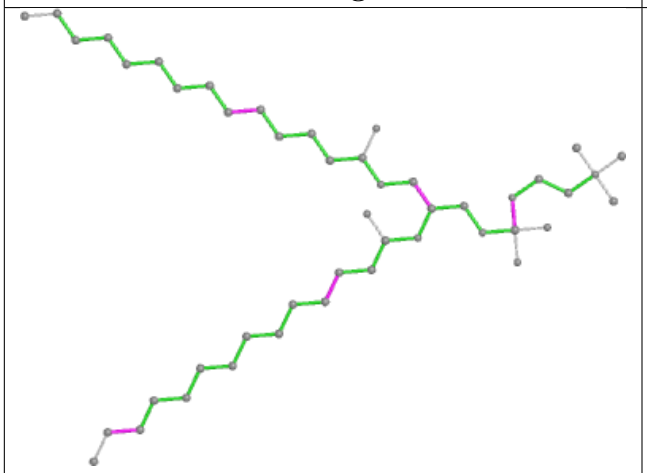

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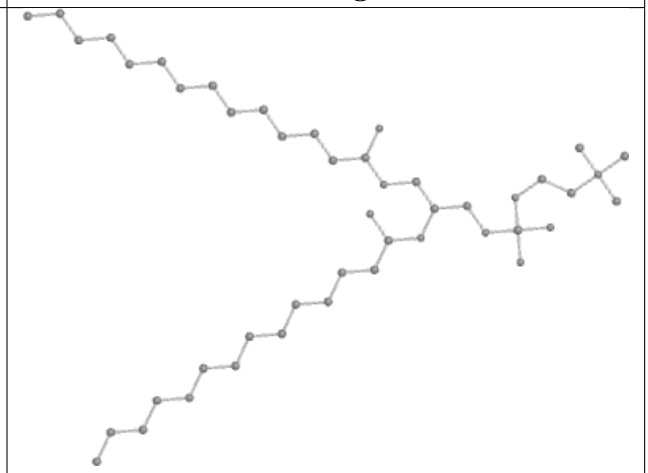
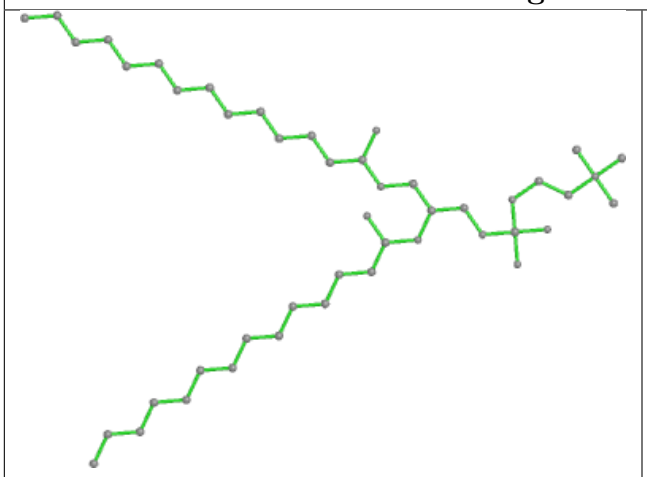


Rings

Ligand PX4 A 325



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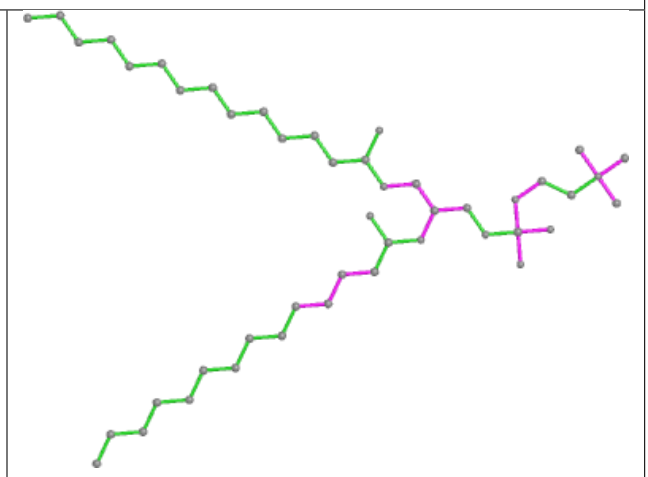

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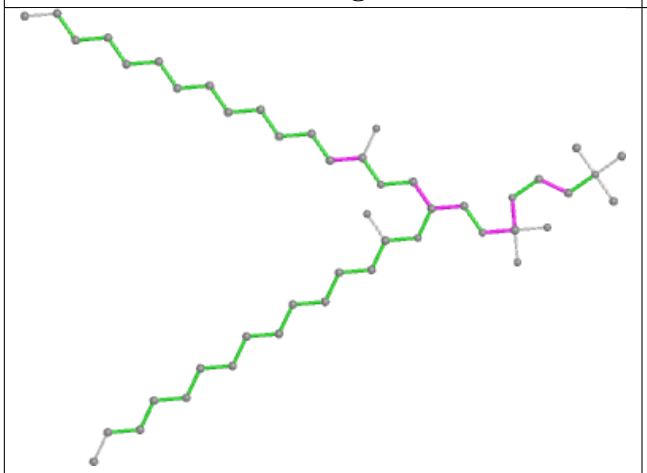

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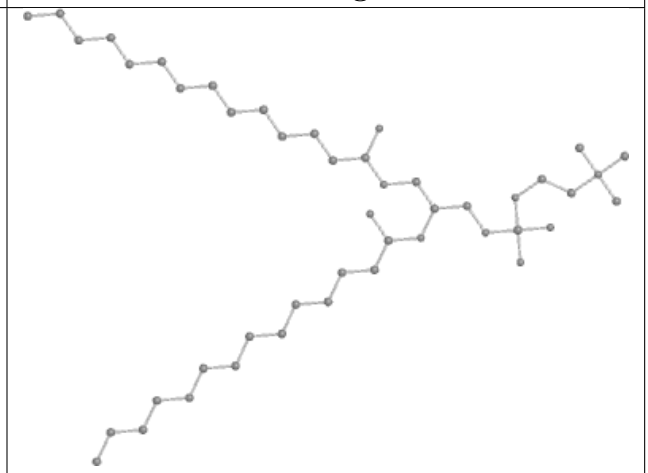
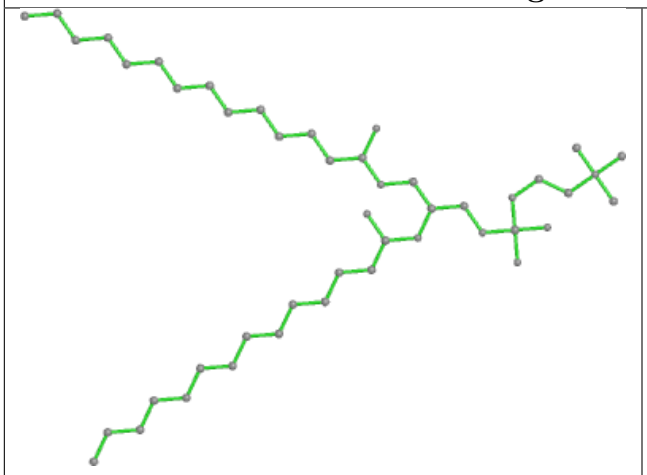


Rings

Ligand PX4 A 328



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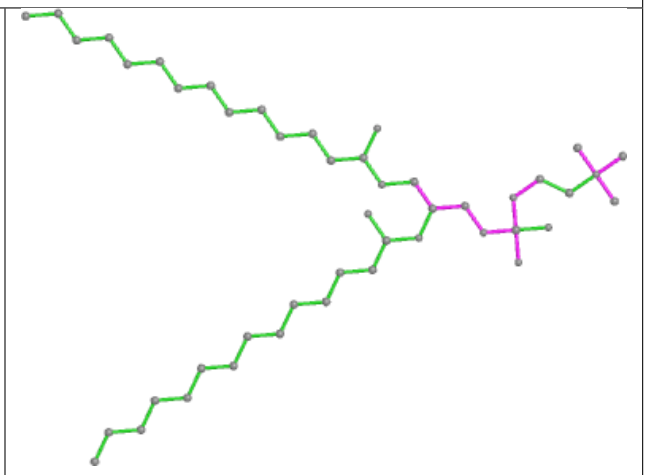
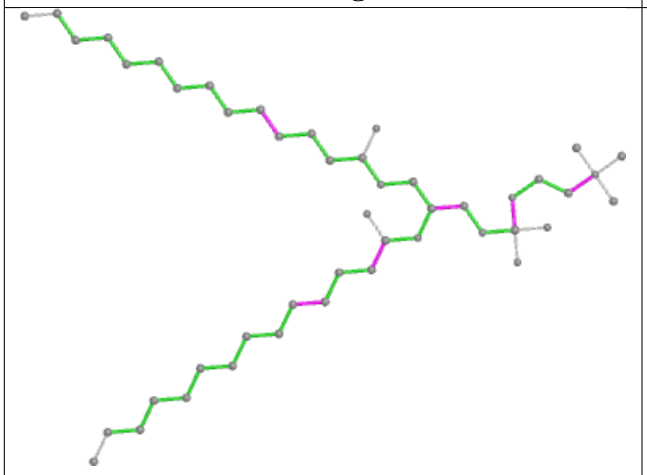


Bond angles



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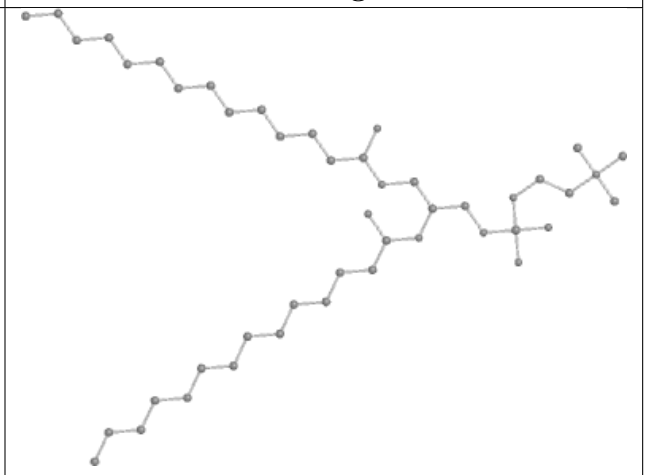
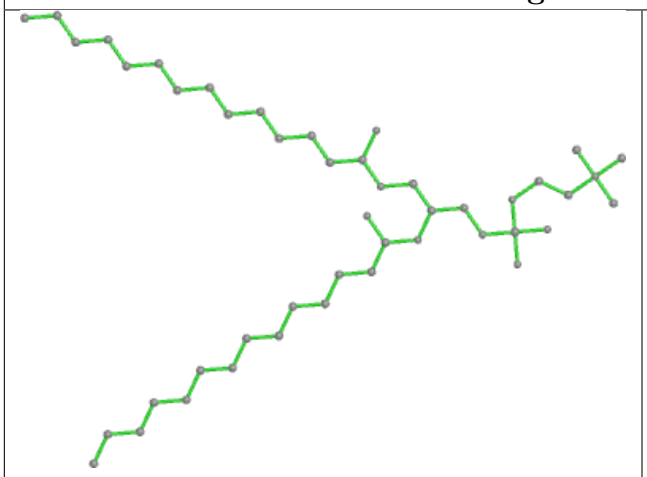


Rings

Ligand PX4 A 396



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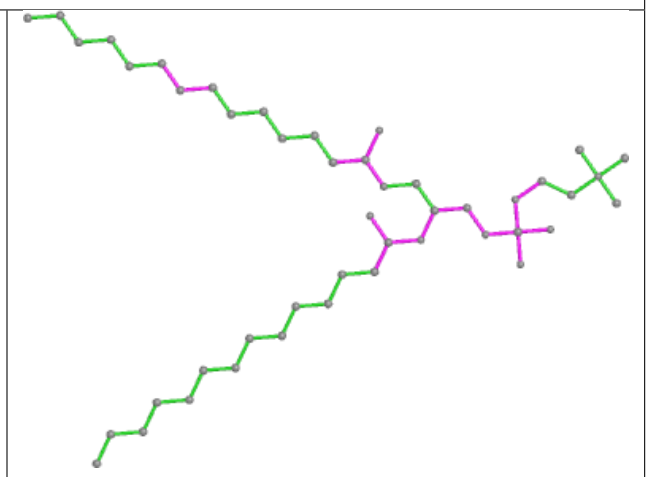
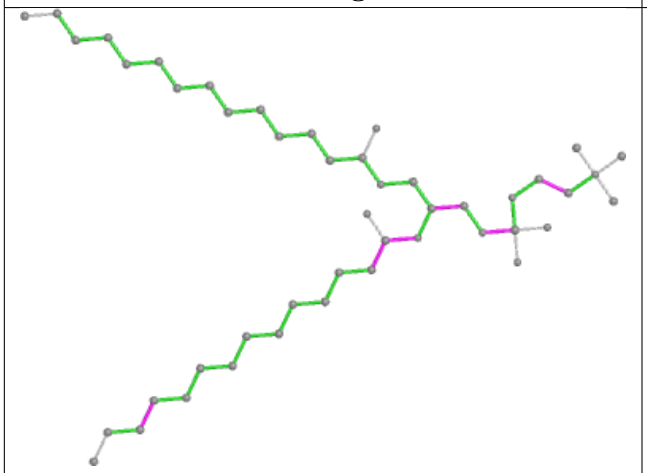


Bond angles



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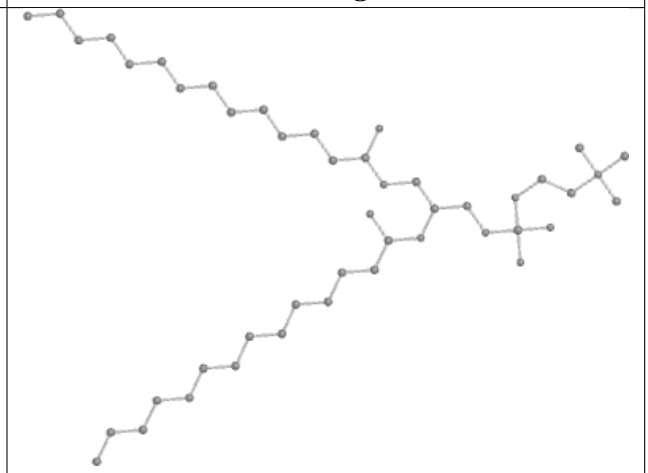
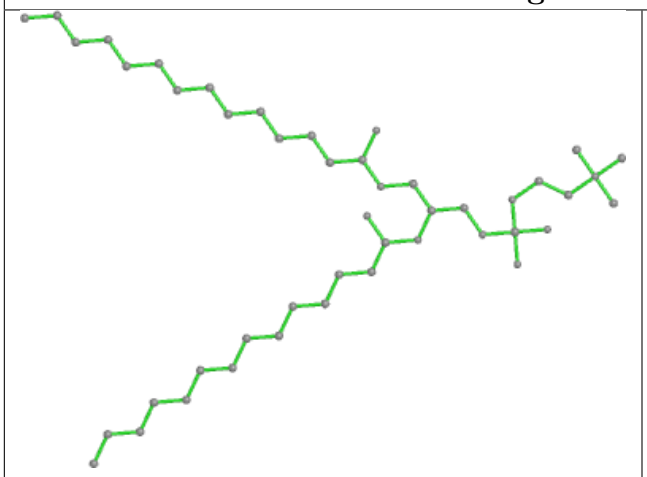


Rings

Ligand PX4 A 307



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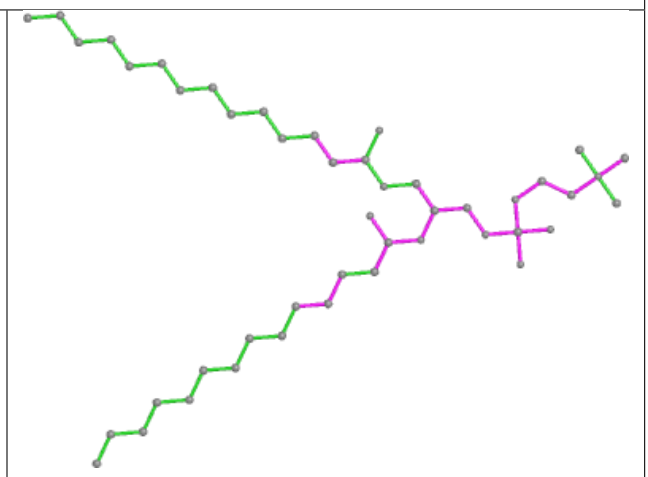
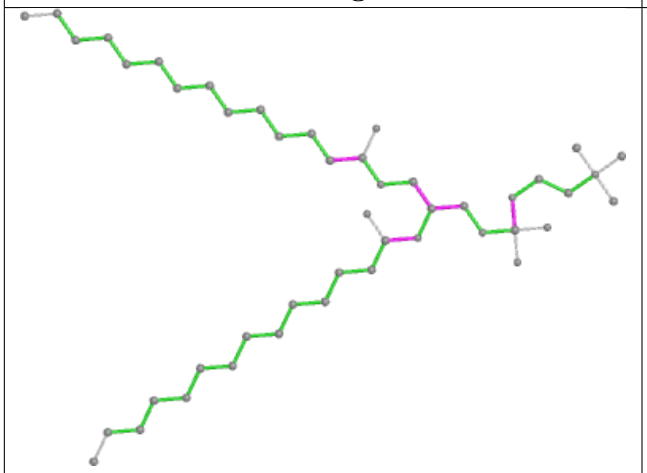


Bond angles



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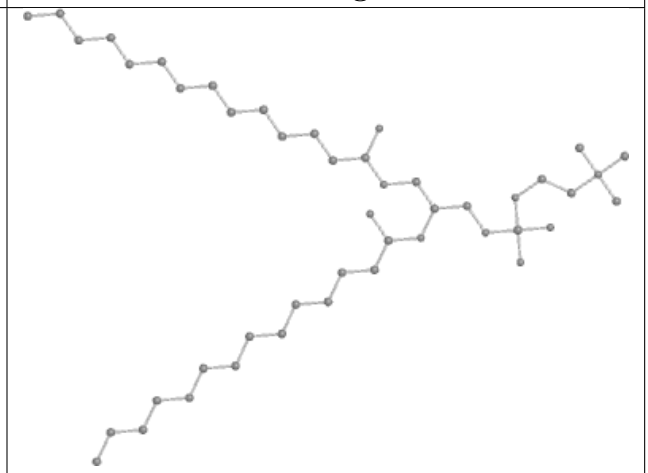
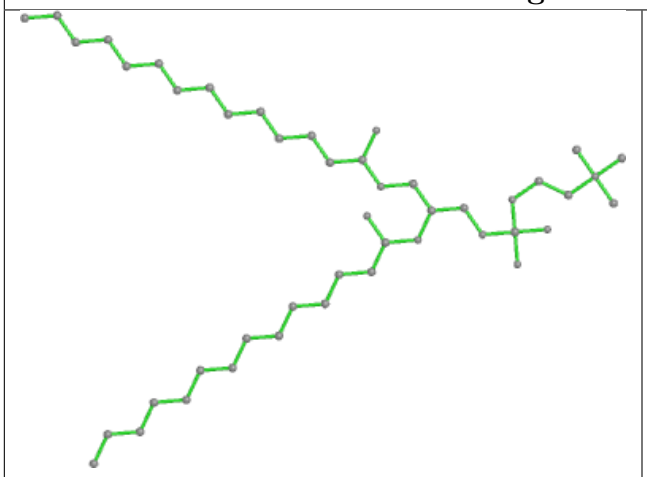


Rings

Ligand PX4 A 378



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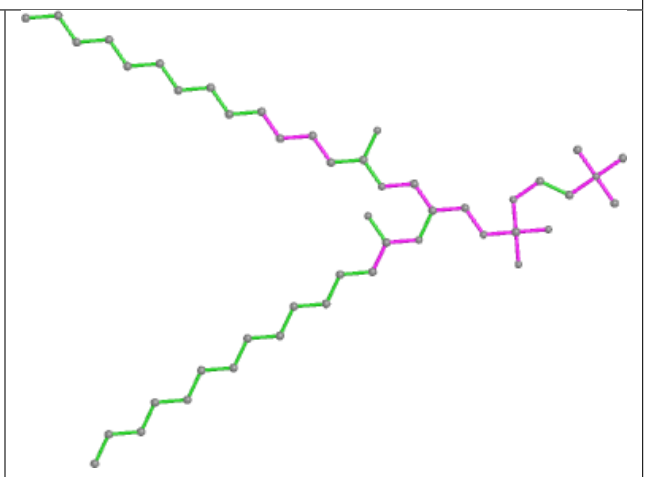

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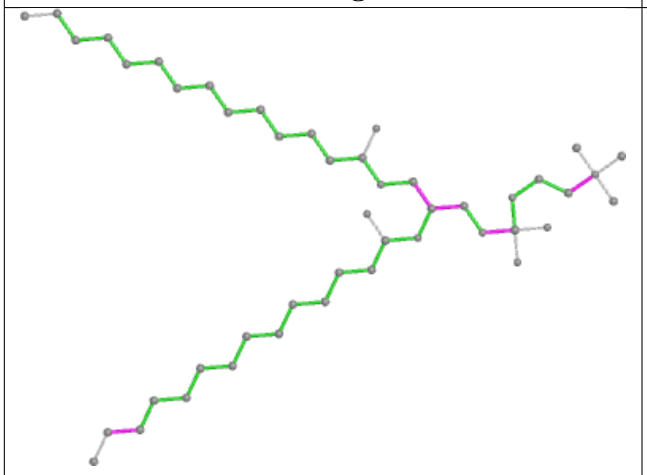

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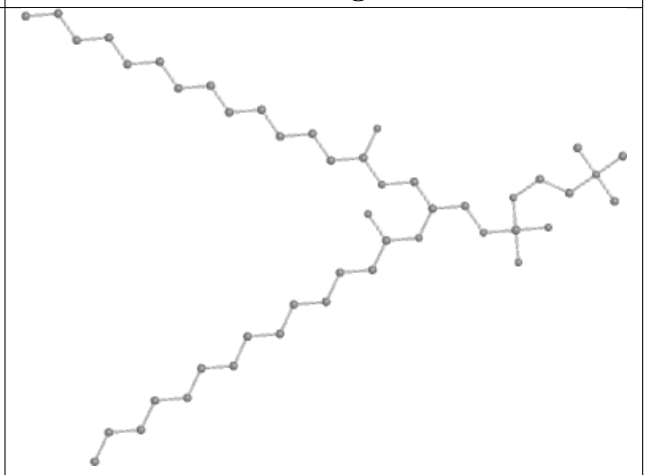
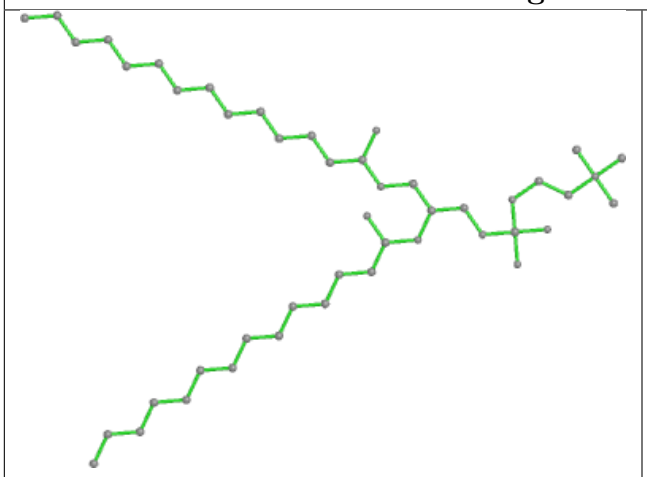


Rings

Ligand PX4 A 414



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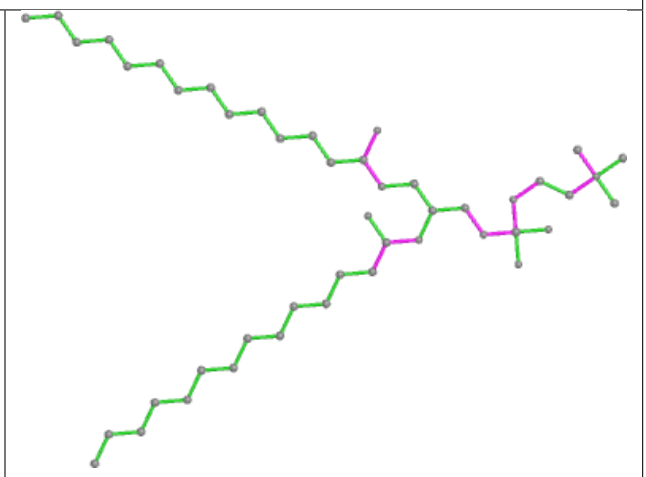
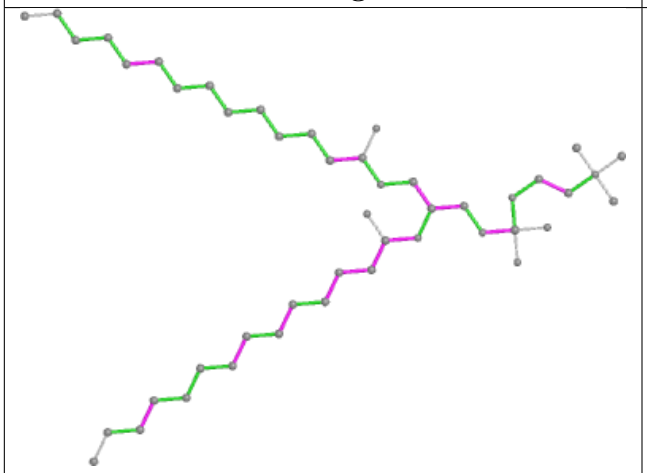


Bond angles



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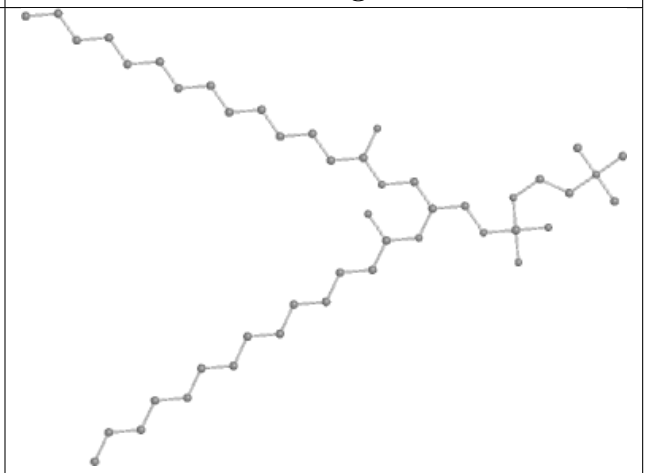
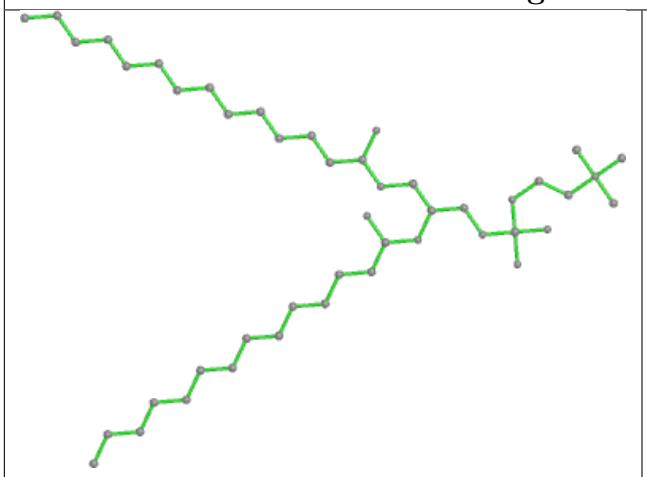


Rings

Ligand PX4 A 312



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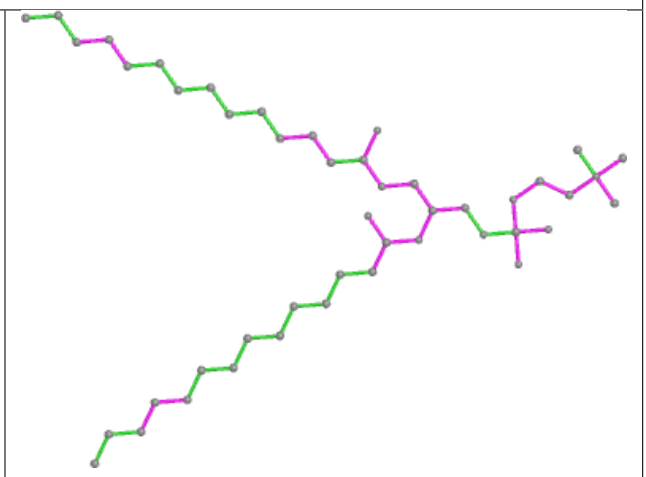

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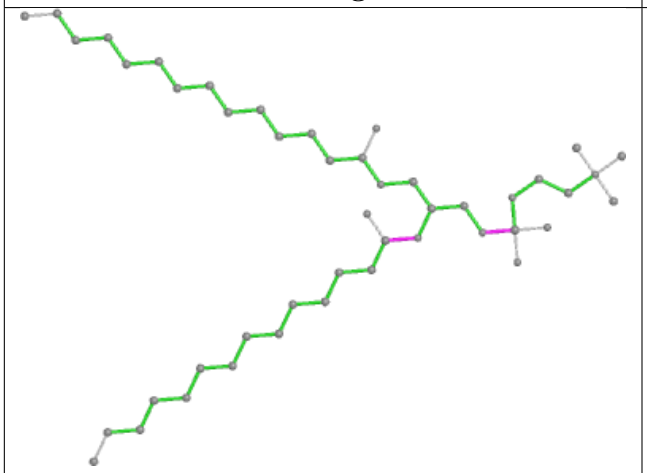

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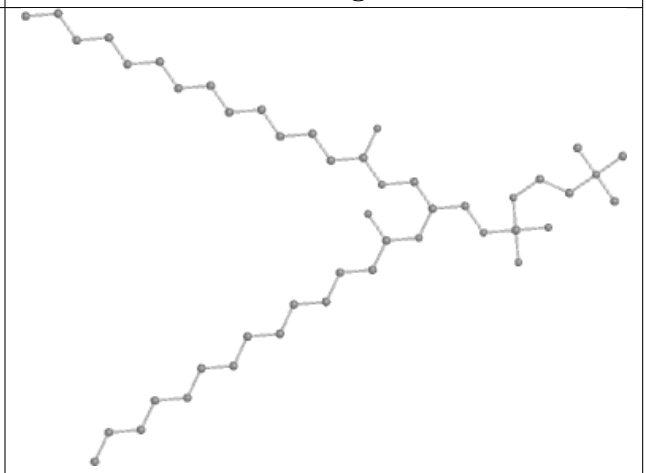
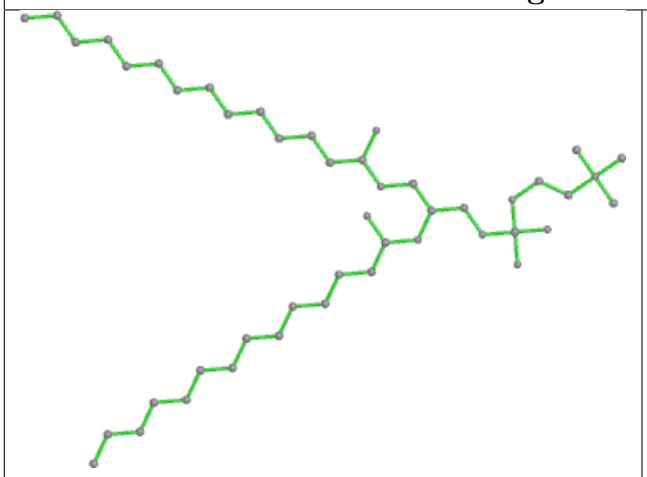


Rings

Ligand PX4 A 305



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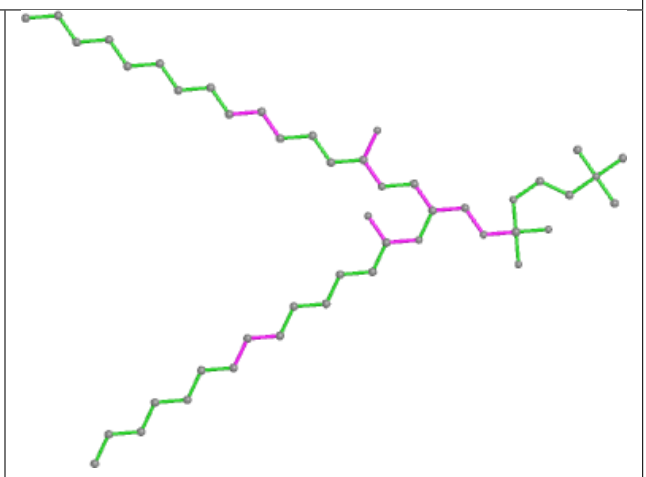
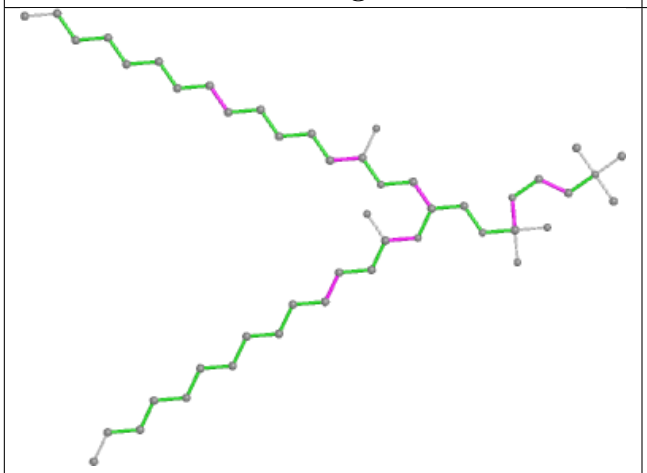


Bond angles



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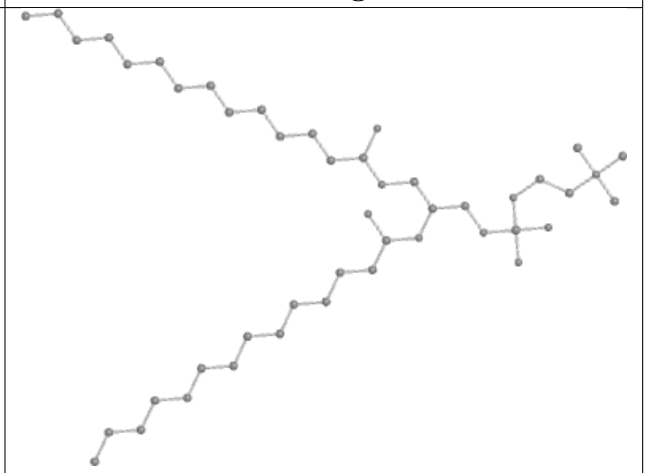
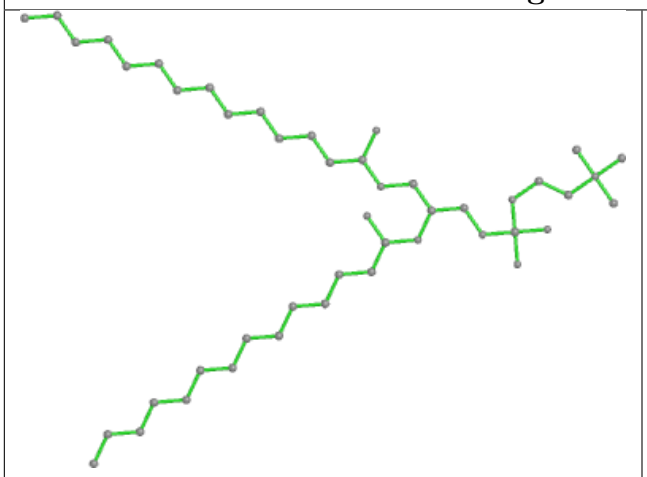


Rings

Ligand PX4 A 427



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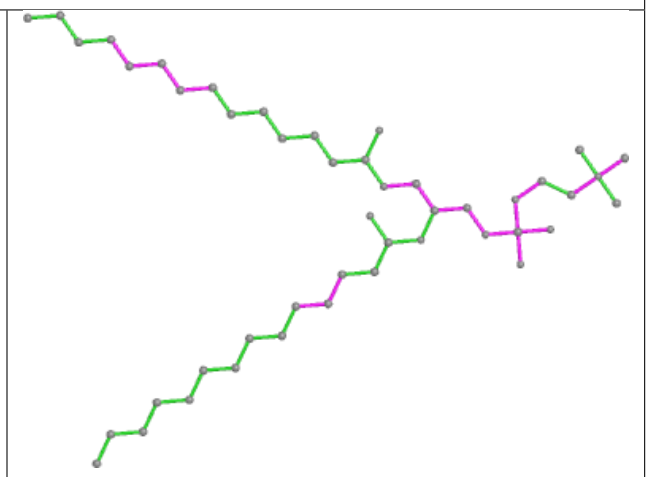
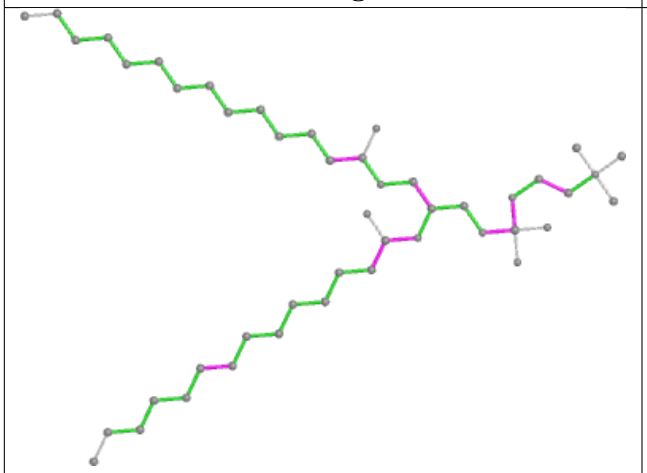


Bond angles



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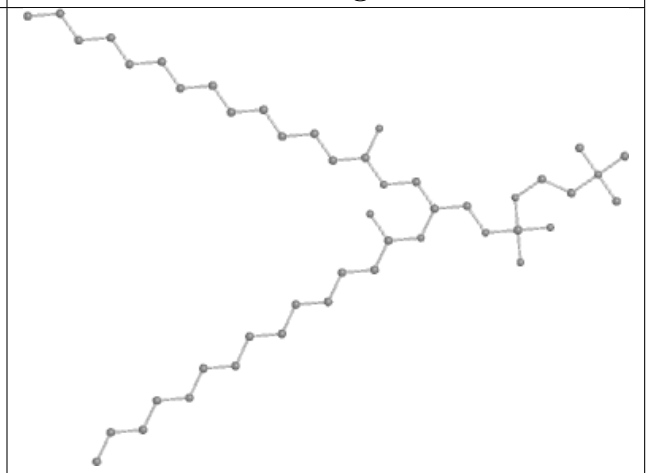
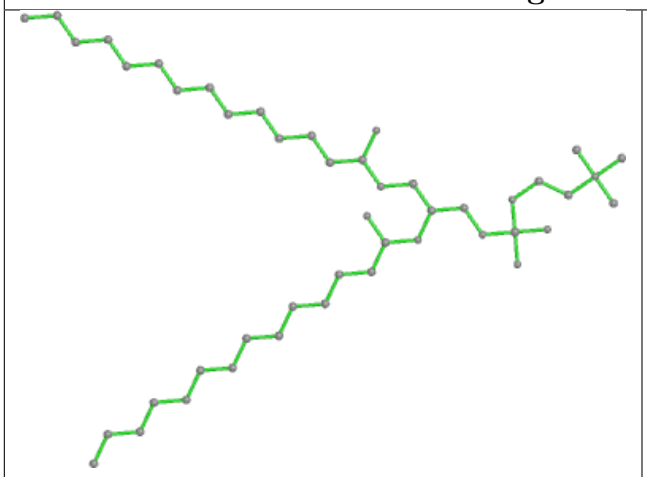


Rings

Ligand PX4 A 308



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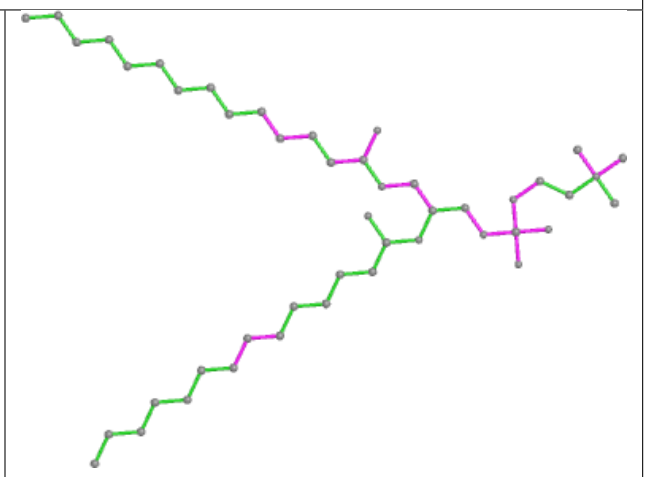
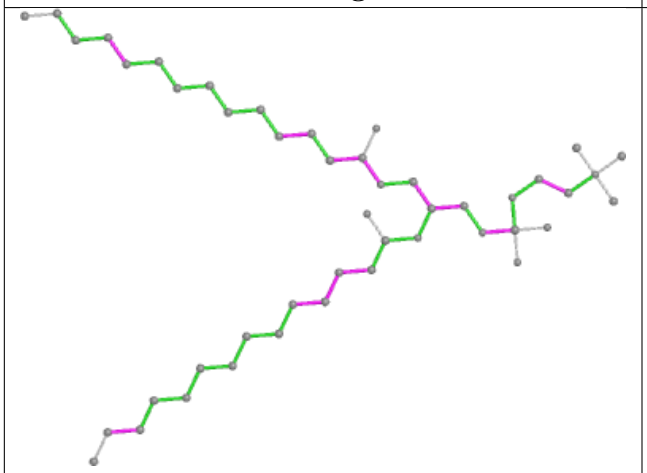


Bond angles



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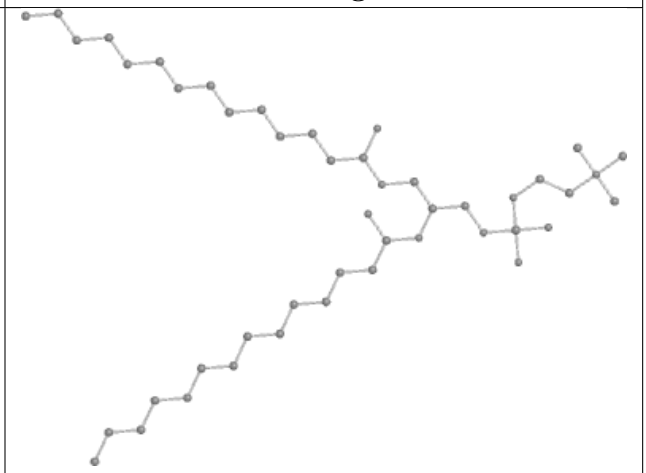
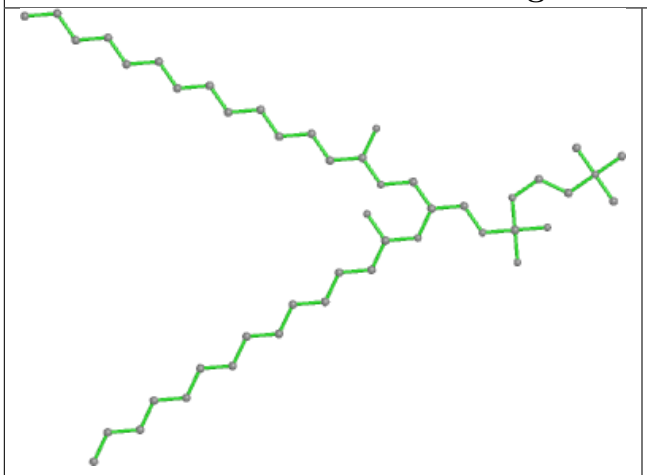


Rings

Ligand PX4 A 379



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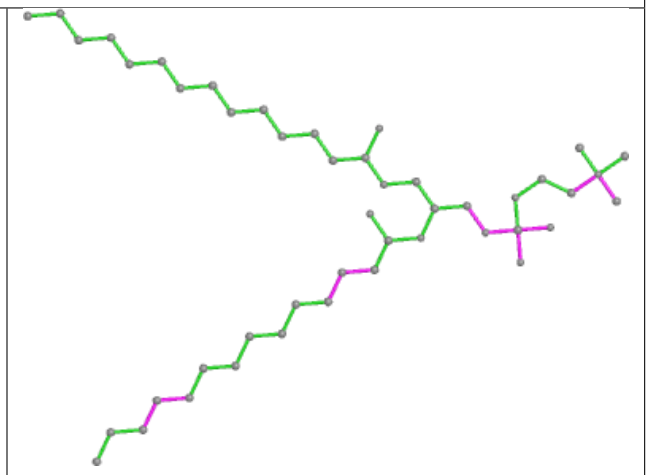
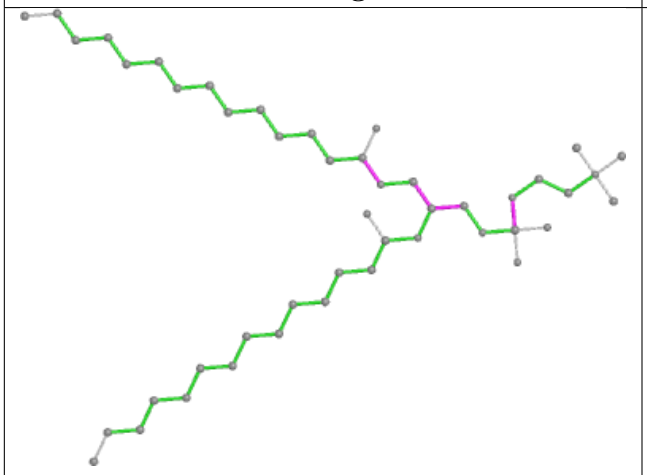
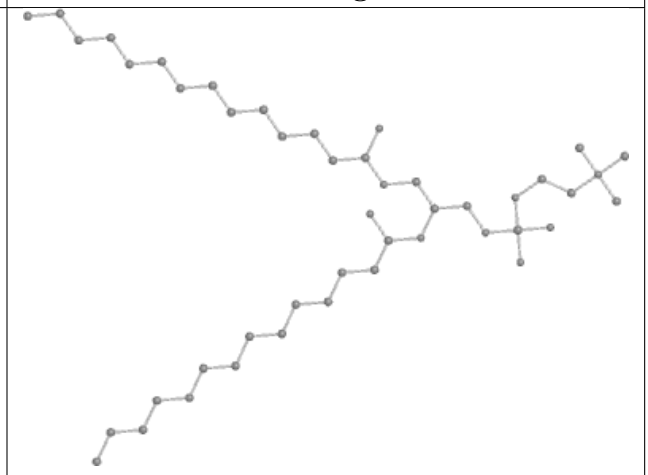


Bond angles

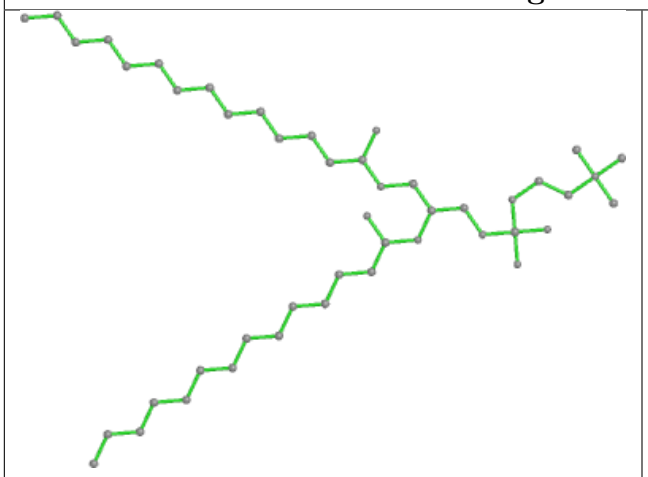


Torsions



Rings

Ligand PX4 A 418



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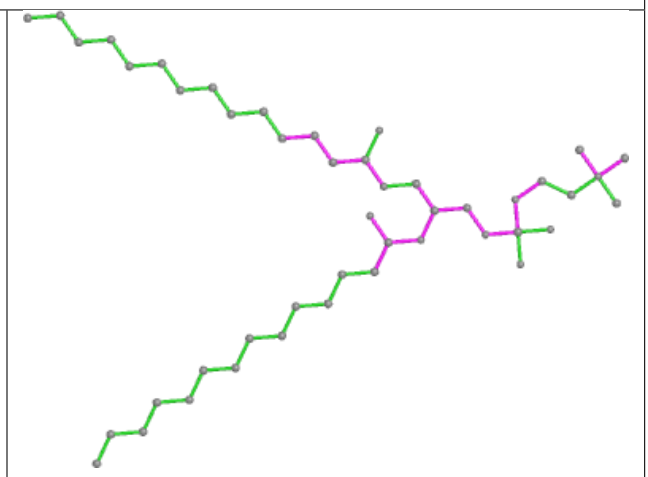

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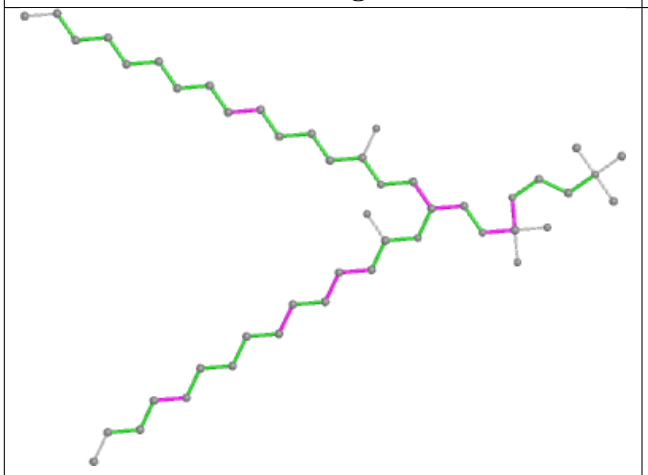

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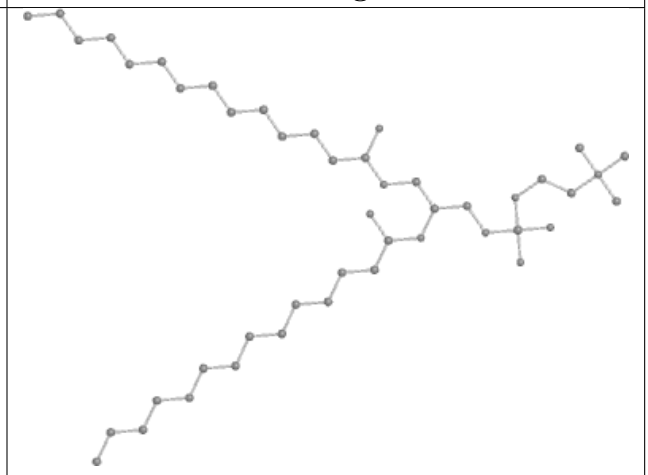
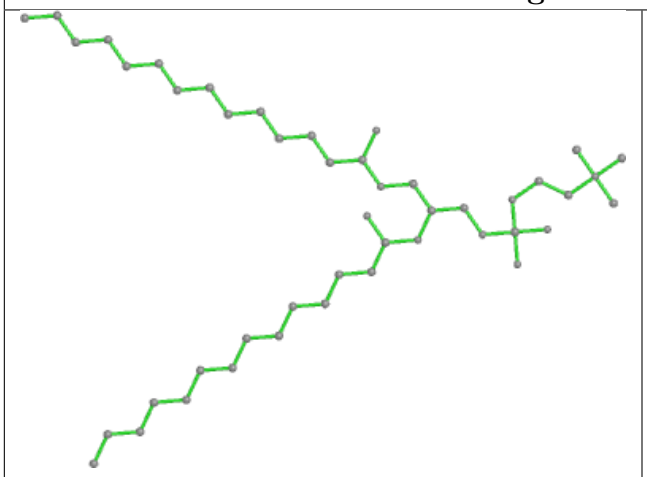


Rings

Ligand PX4 A 319



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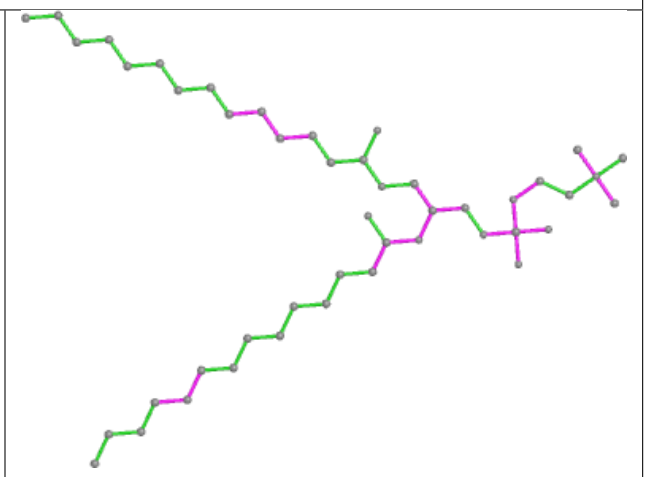
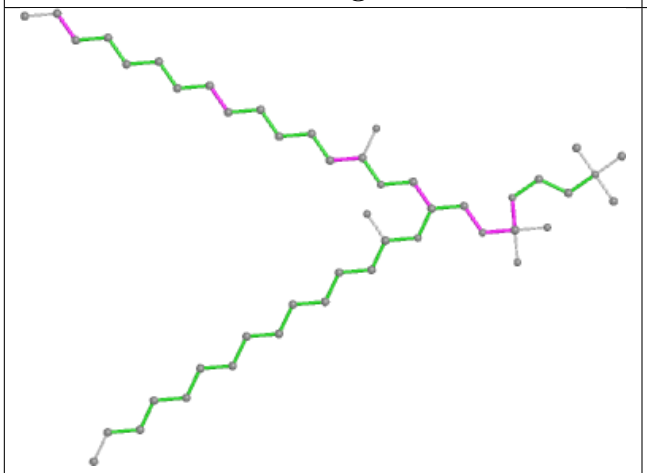


Bond angles



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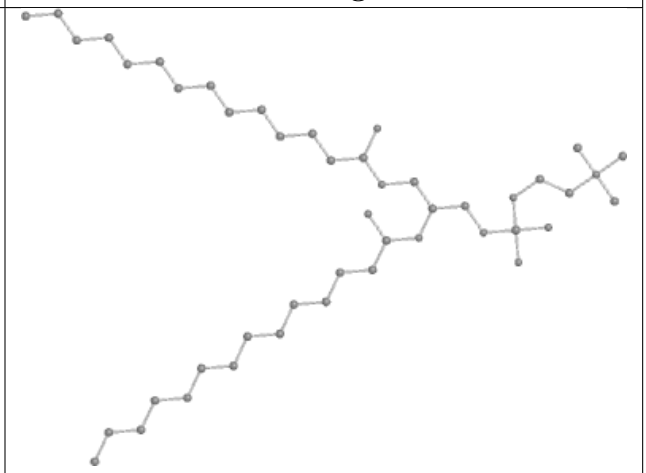
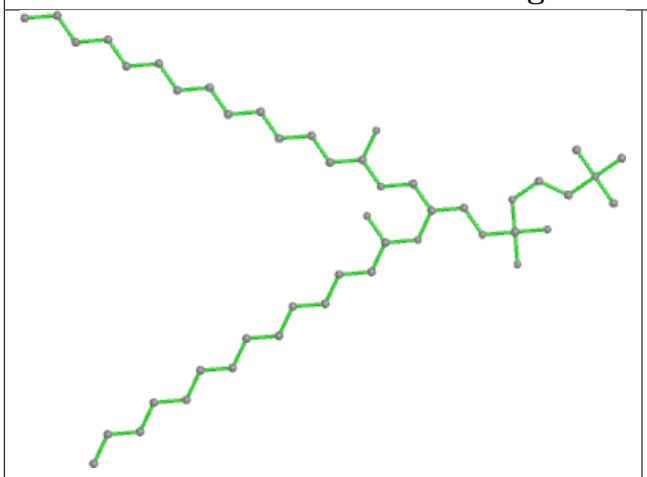


Rings

Ligand PX4 A 363



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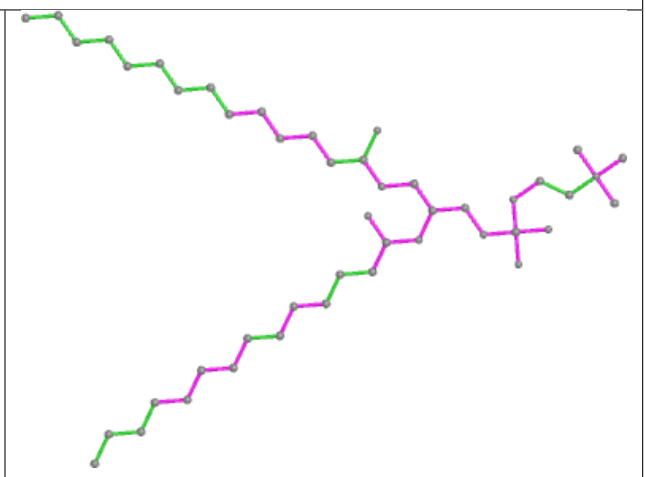

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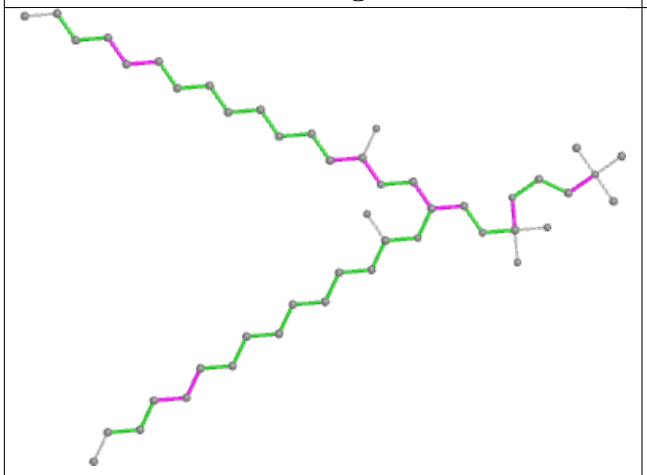

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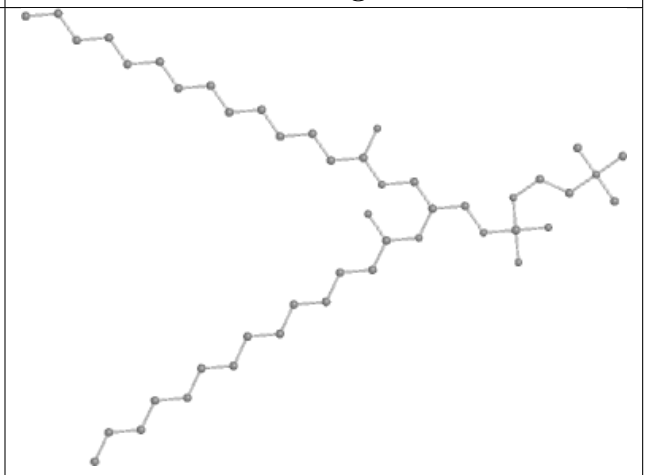
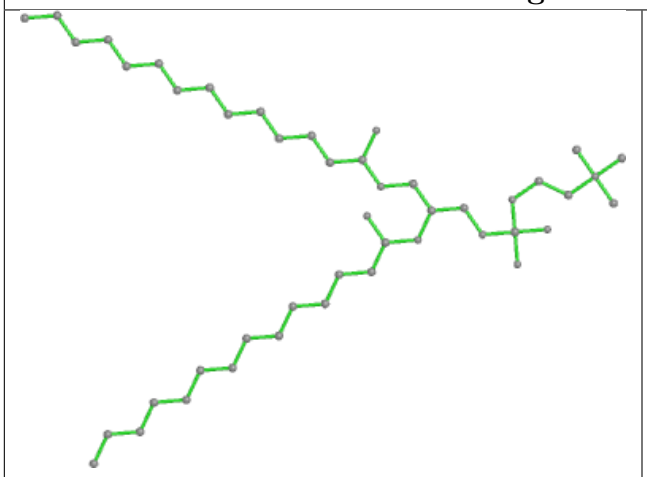


Rings

Ligand PX4 A 364



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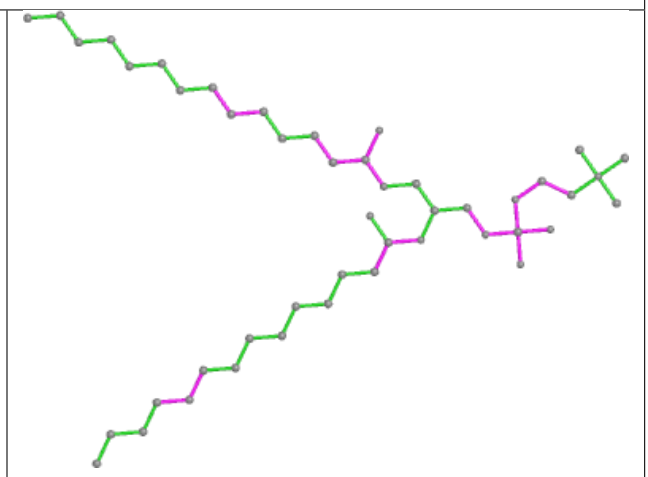

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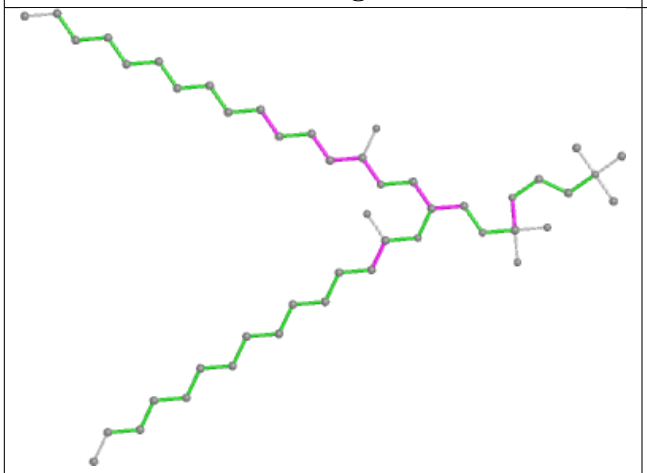

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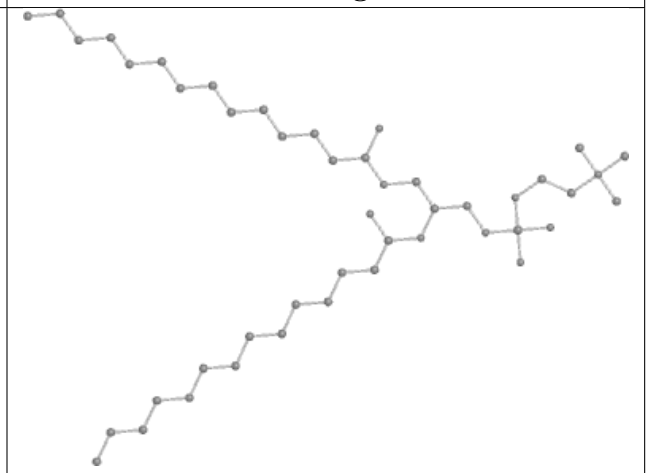
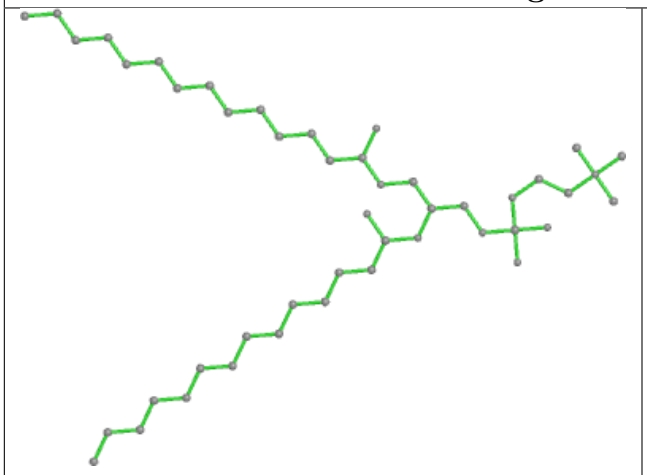


Rings

Ligand PX4 A 382



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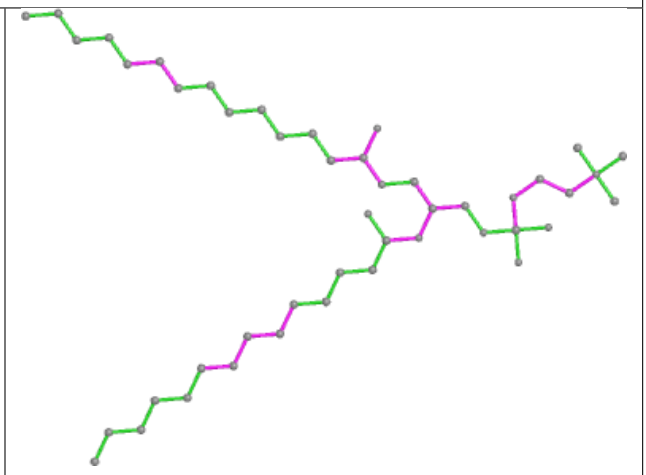

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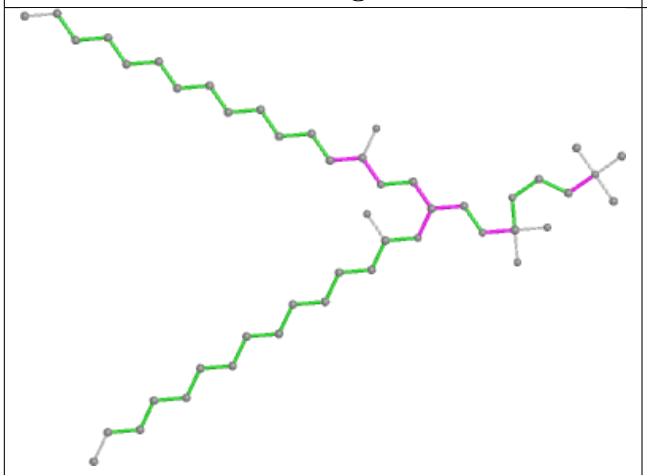

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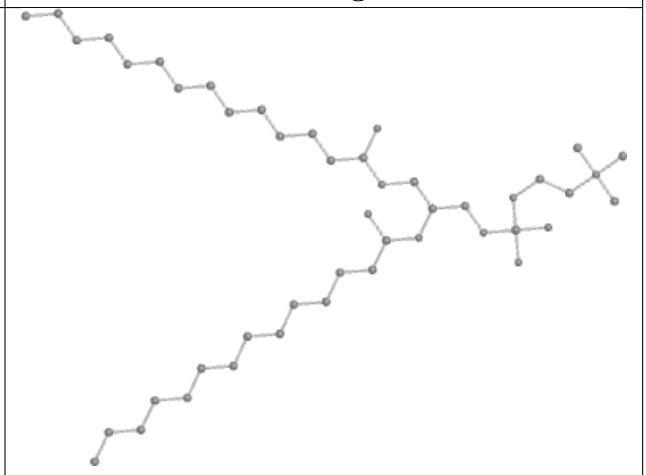
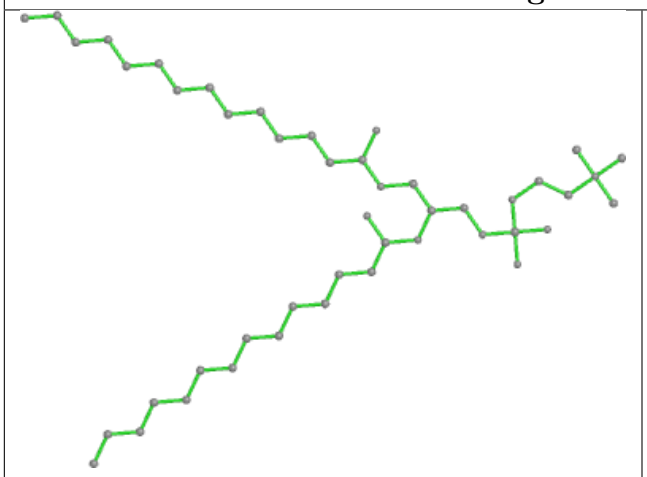


Rings

Ligand PX4 A 424



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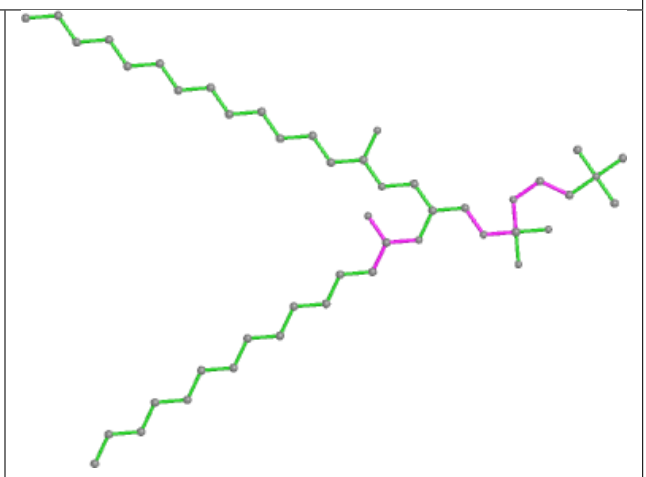
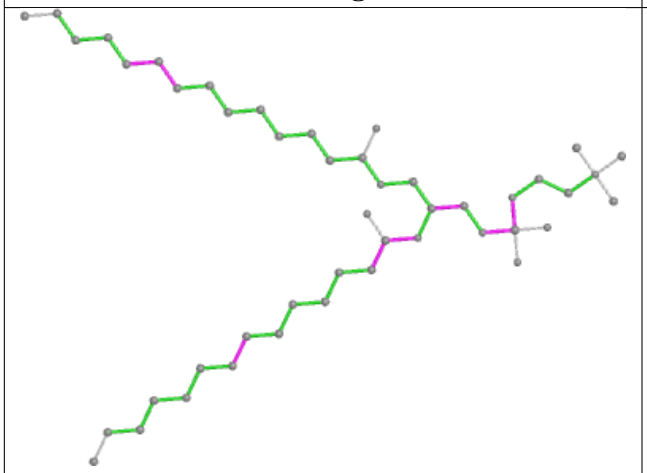


Bond angles



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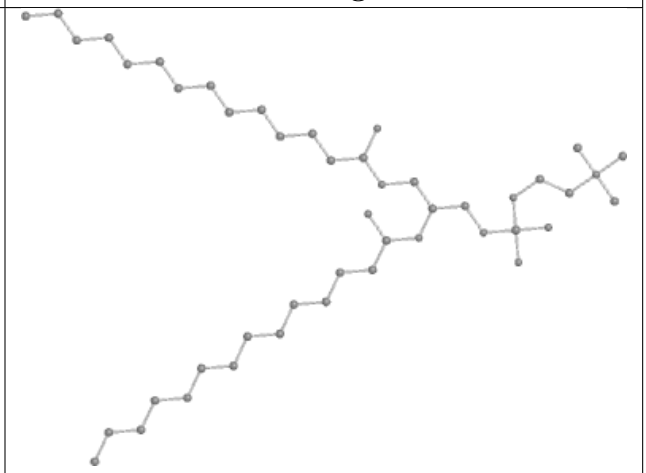
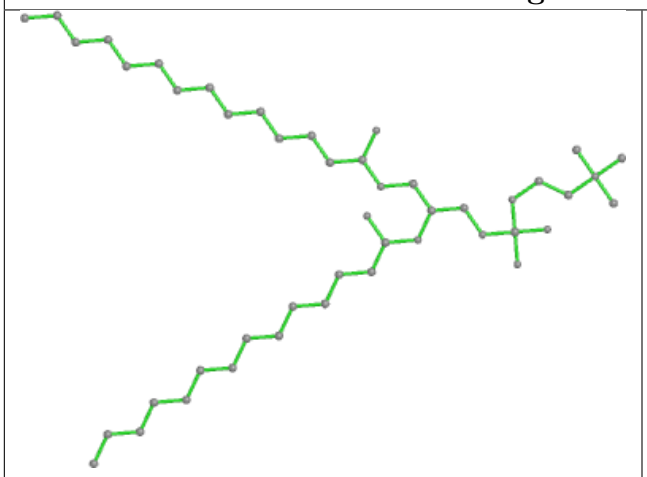


Rings

Ligand PX4 A 428



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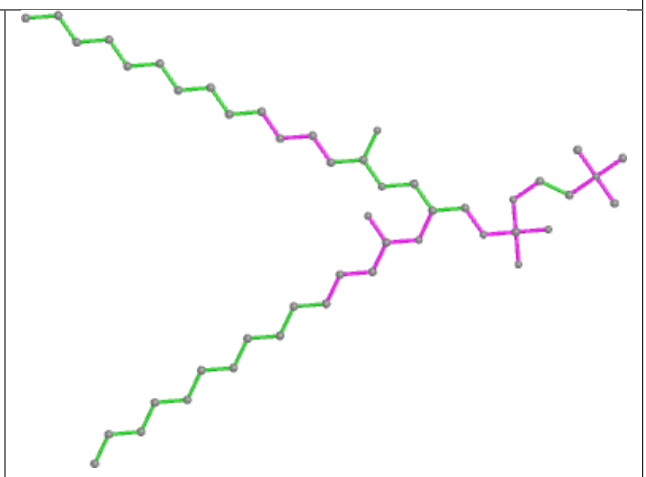

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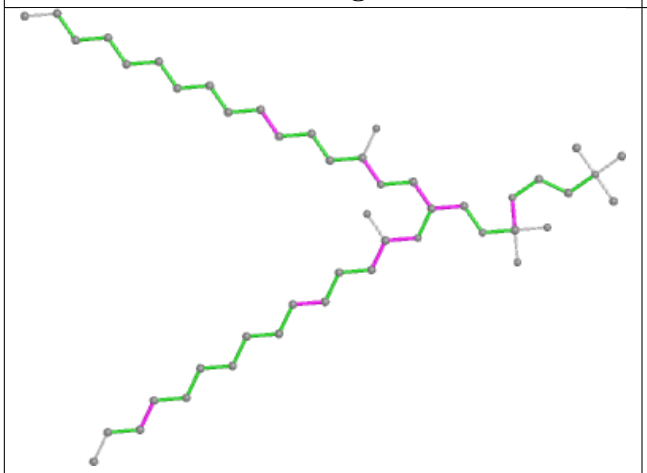

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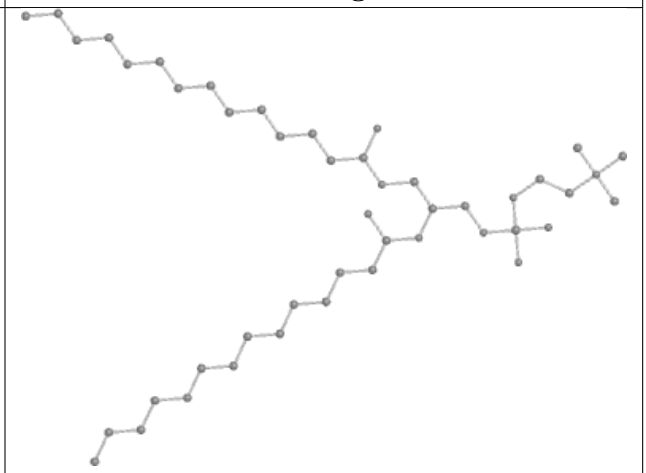
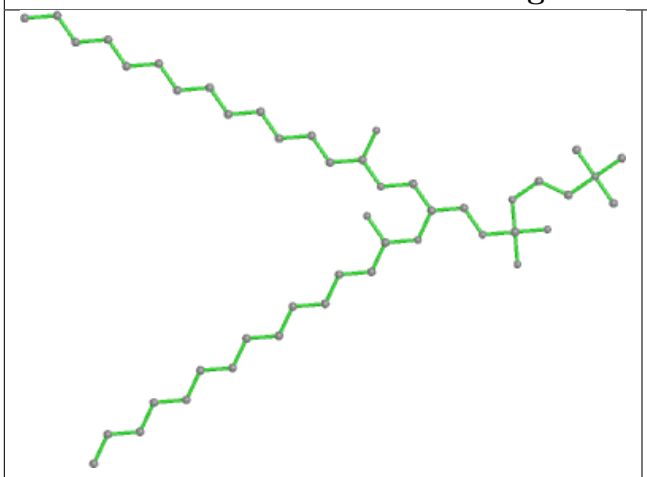


Rings

Ligand PX4 A 387



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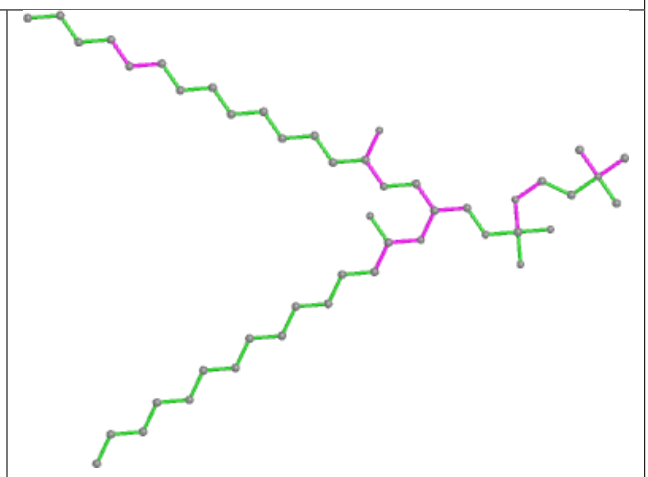
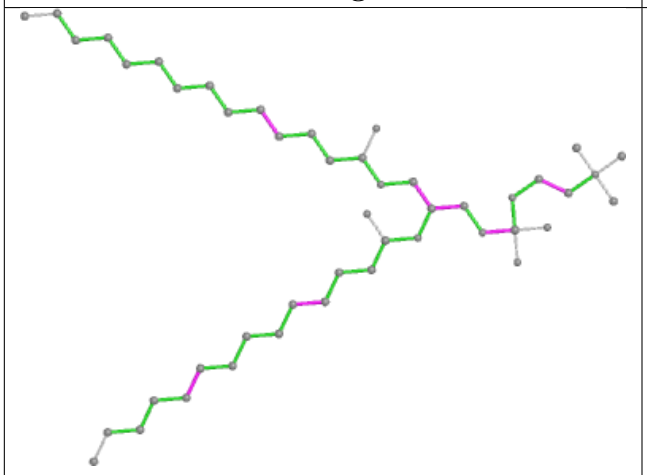


Bond angles



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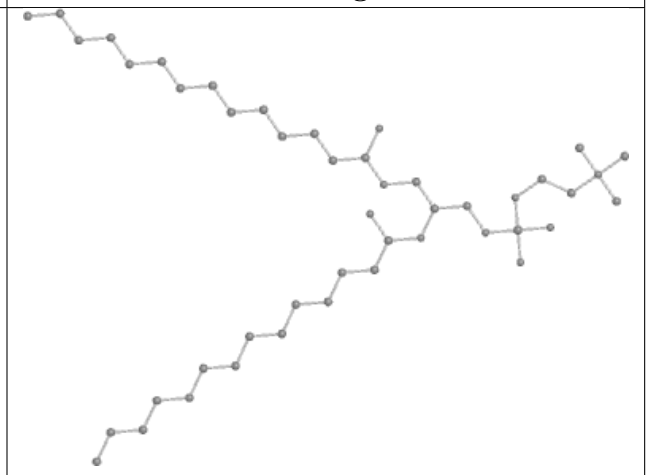
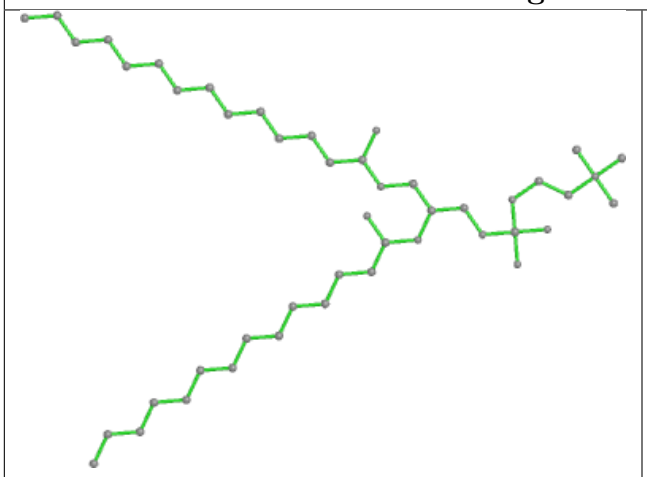


Rings

Ligand PX4 A 344



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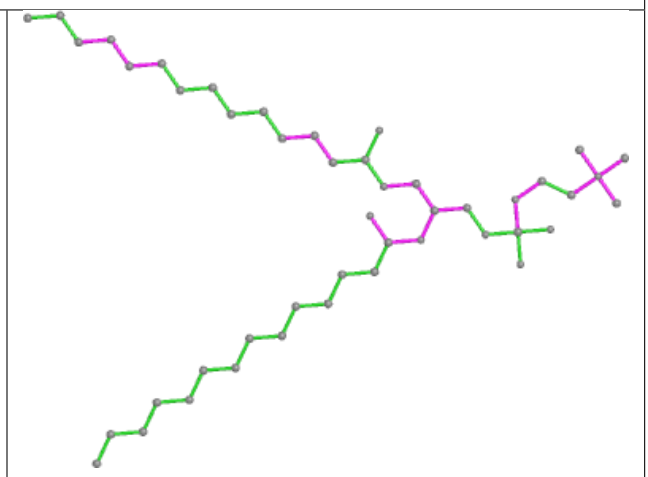

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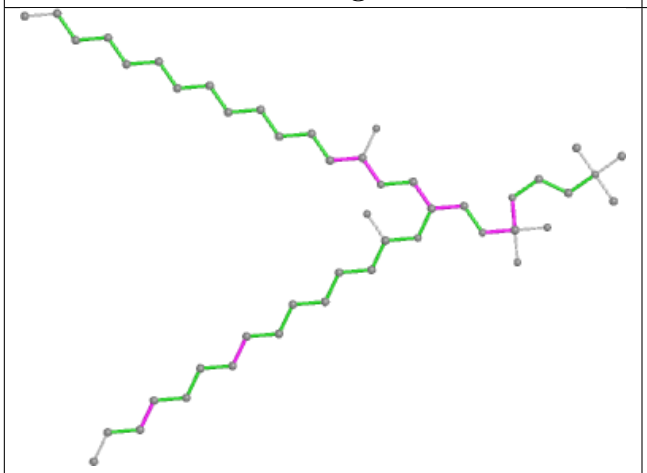

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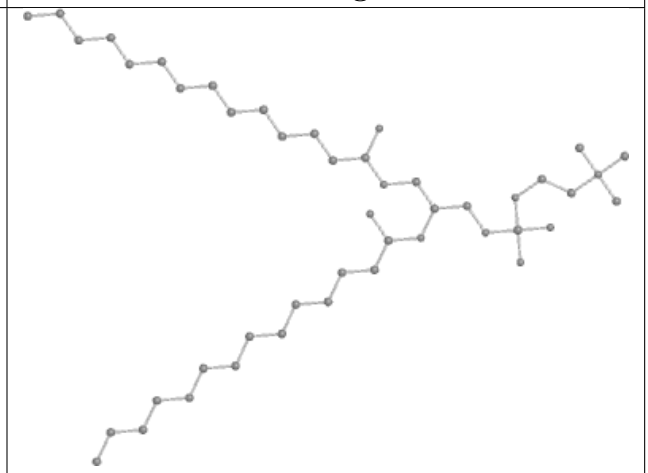
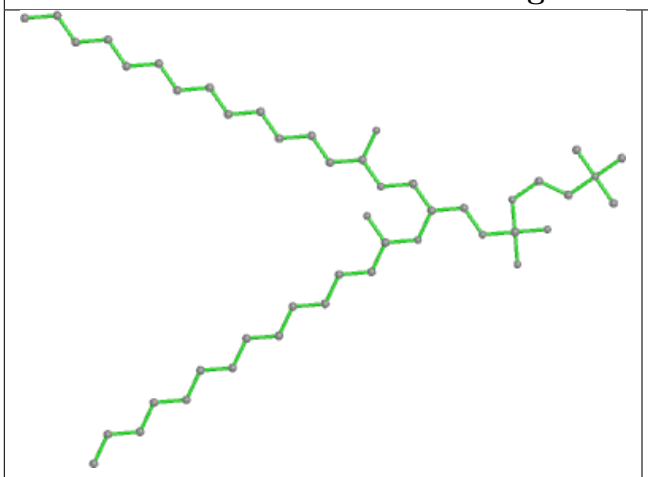


Rings

Ligand PX4 A 360



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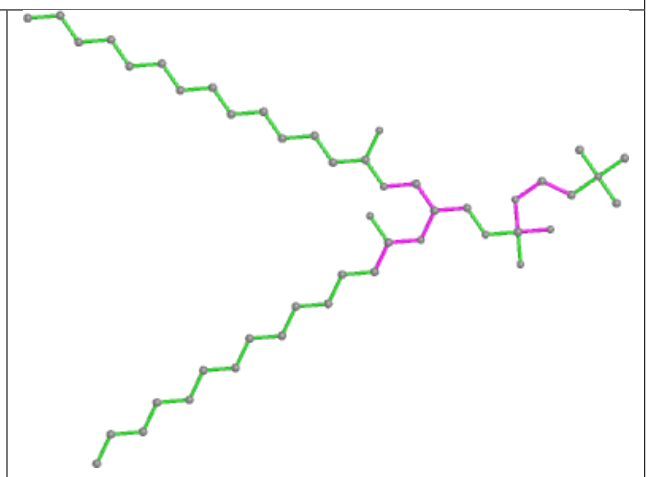
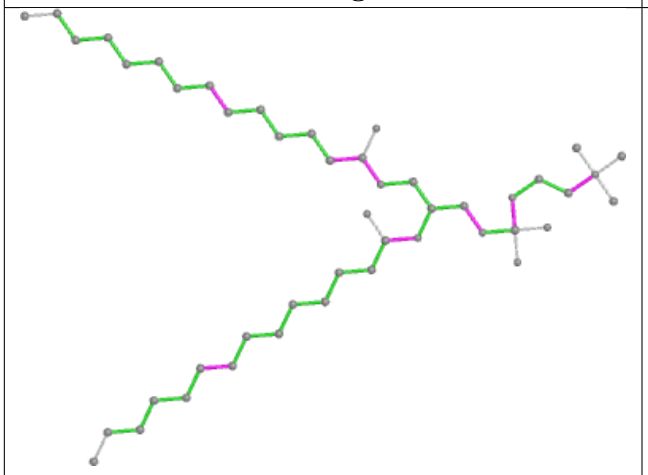


Bond angles



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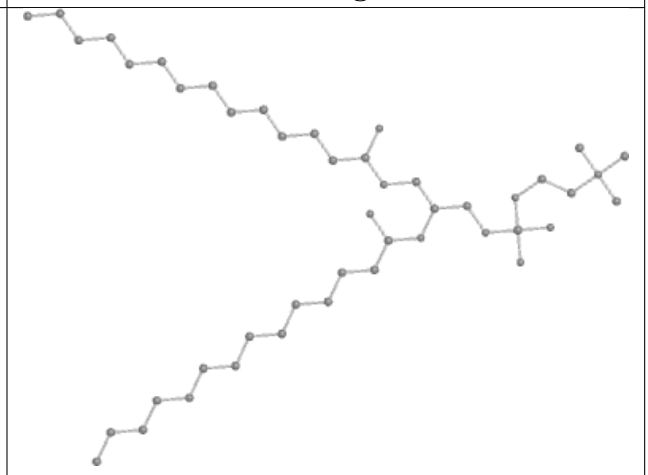
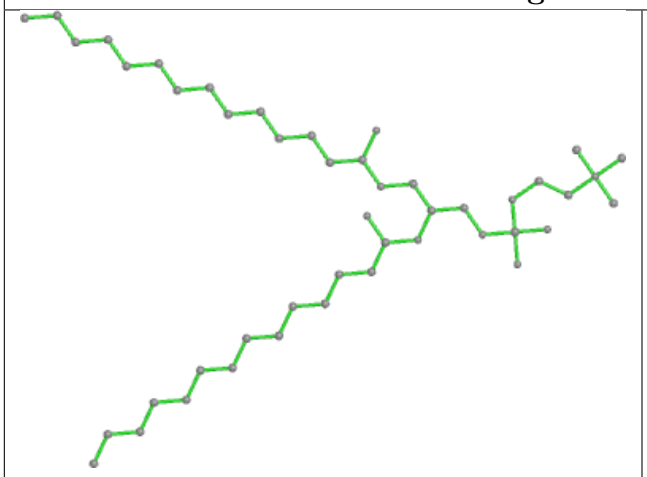


Rings

Ligand PX4 A 425



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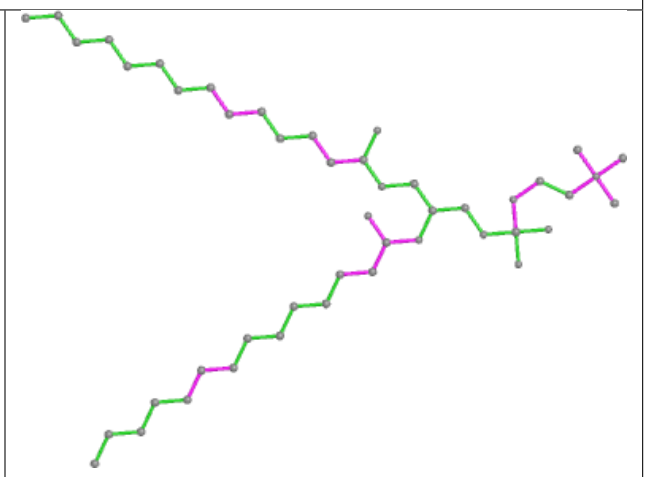
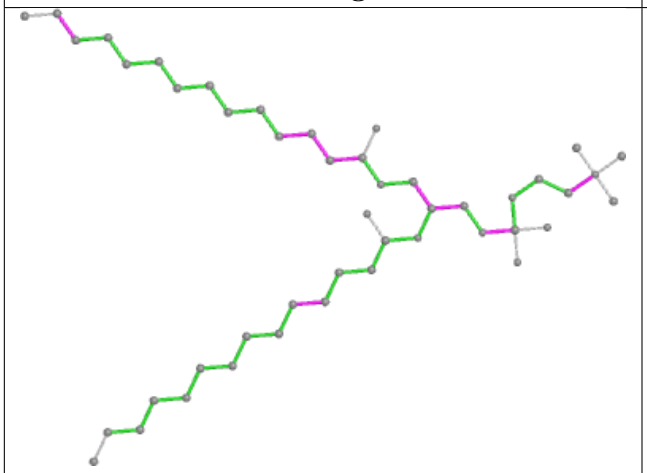


Bond angles



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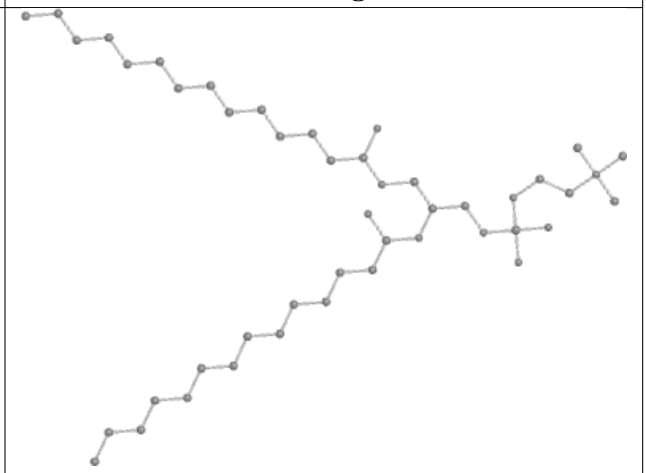
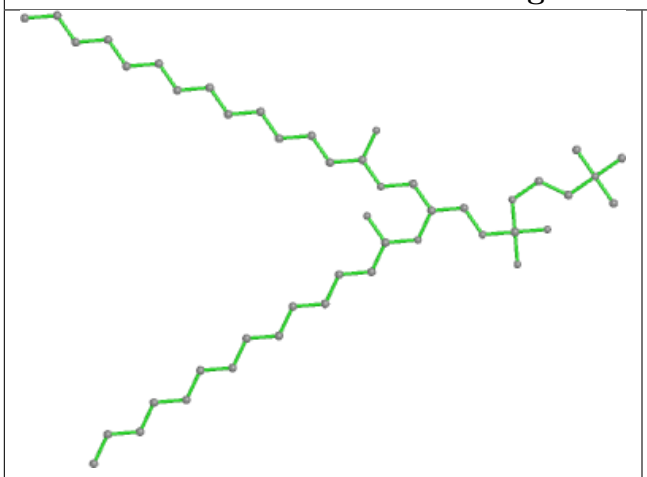


Rings

Ligand PX4 A 395



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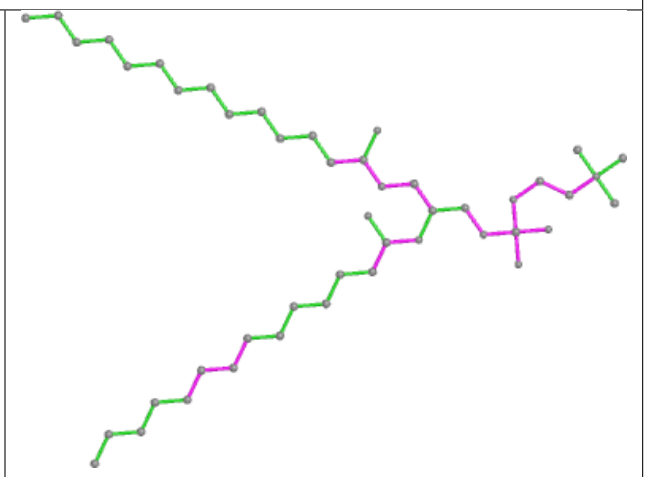
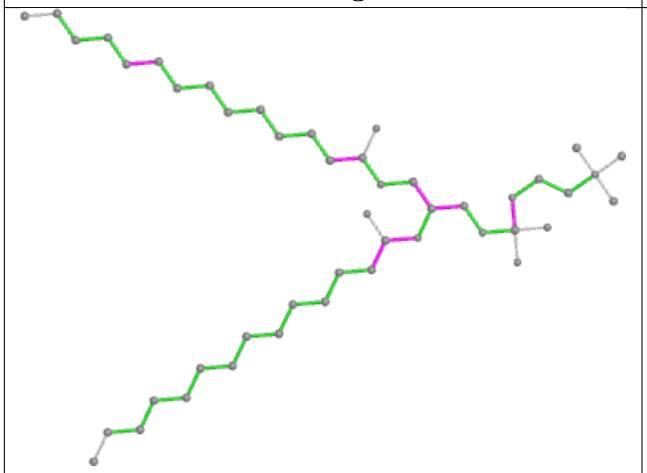


Bond angles



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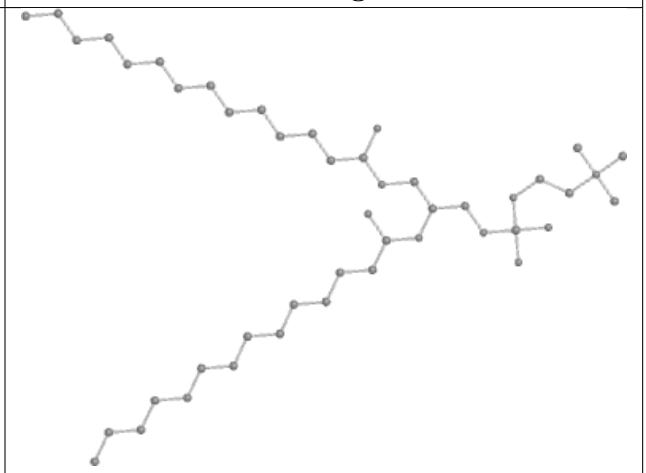
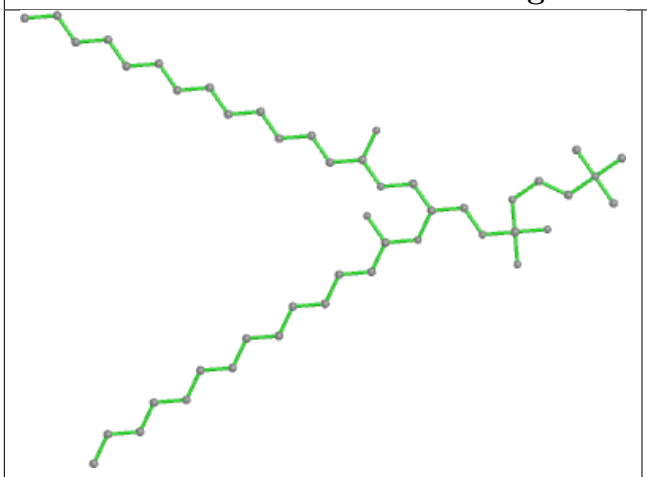


Rings

Ligand PX4 A 310



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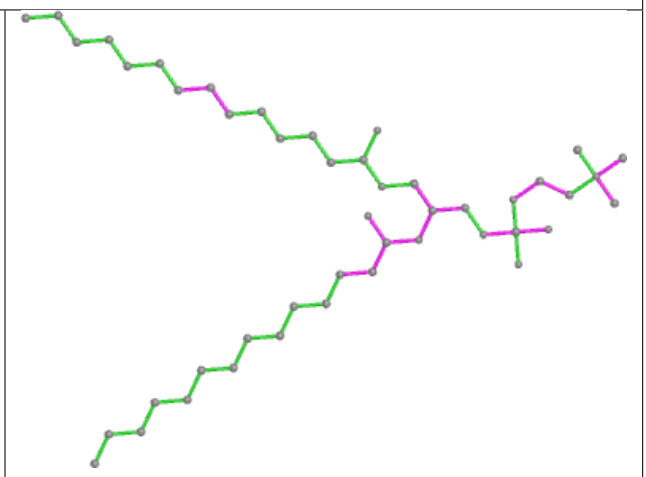
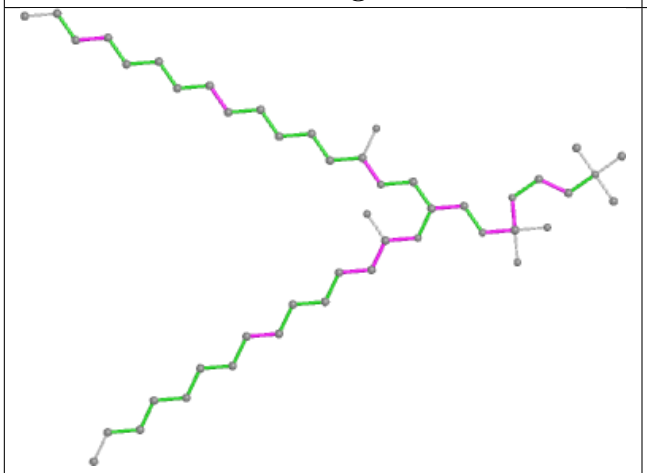
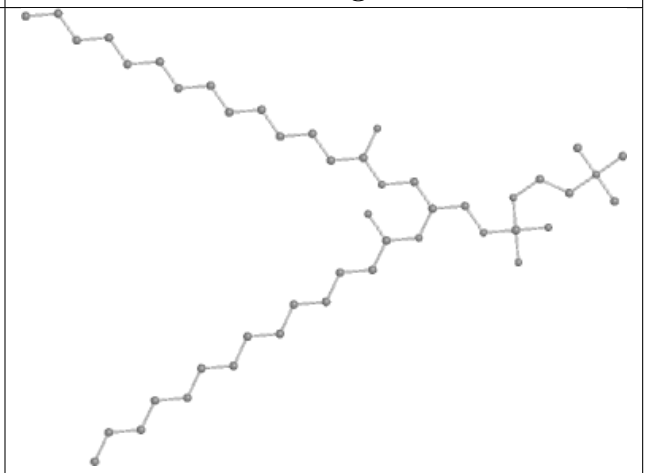


Bond angles

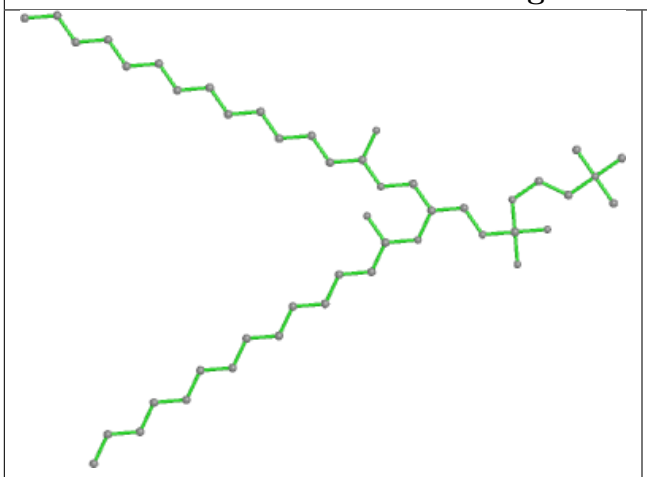


Torsions

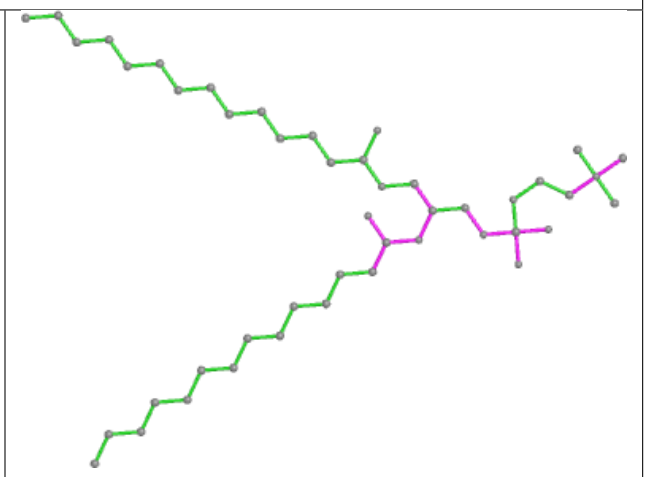


Rings

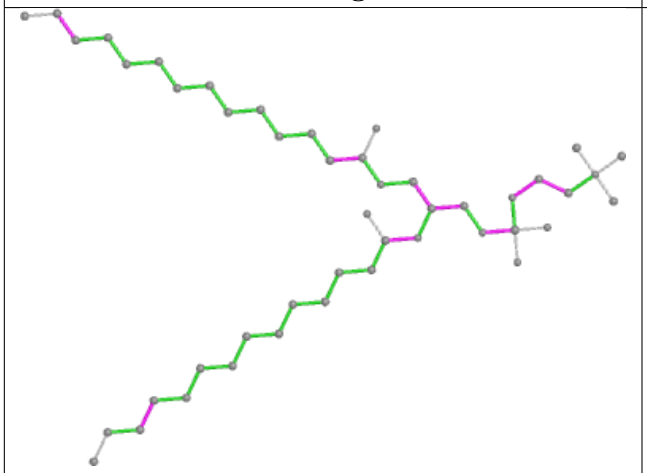
Ligand PX4 A 381



Bond lengths



Bond angles



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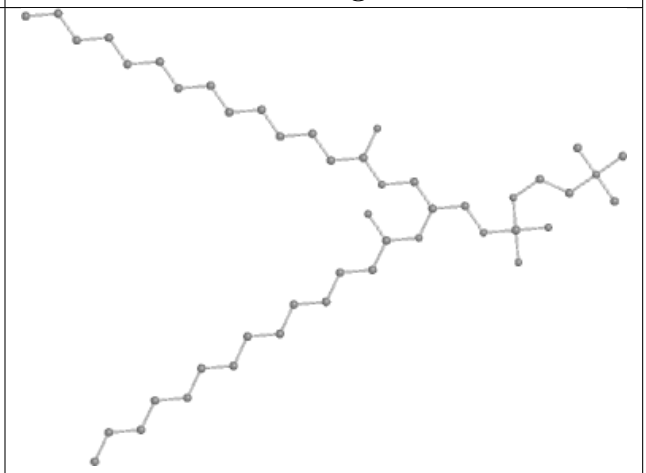
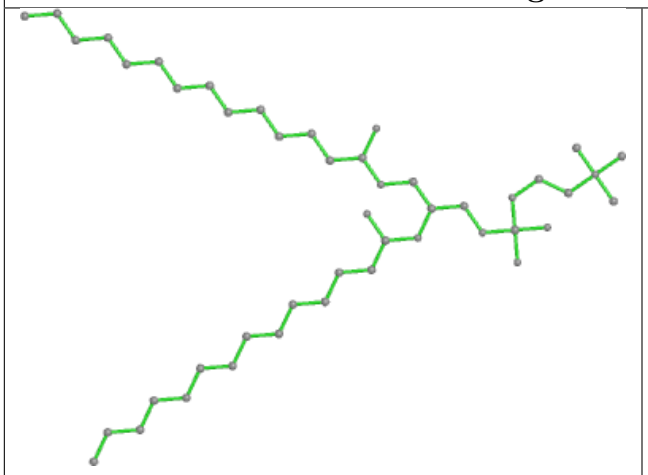


Rings

Ligand PX4 A 347



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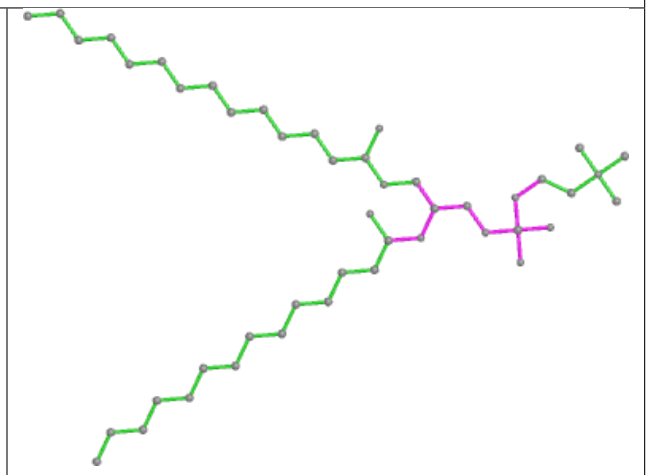

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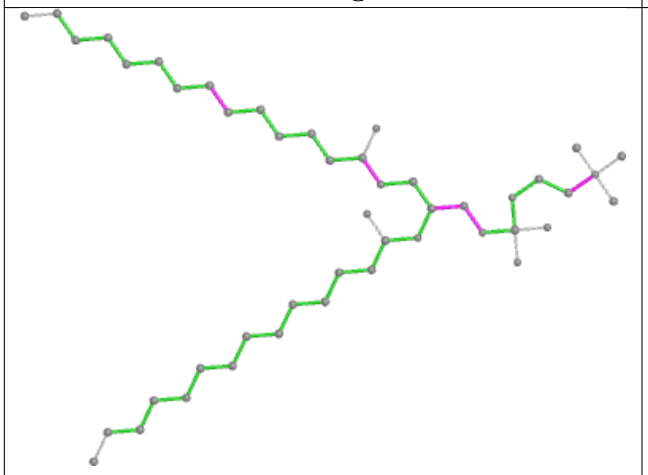

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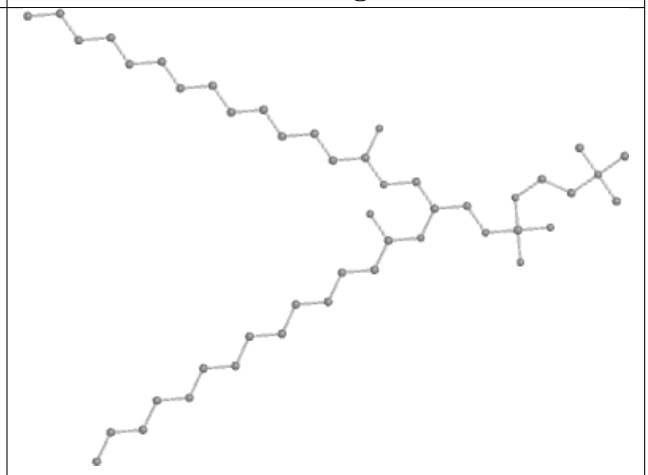
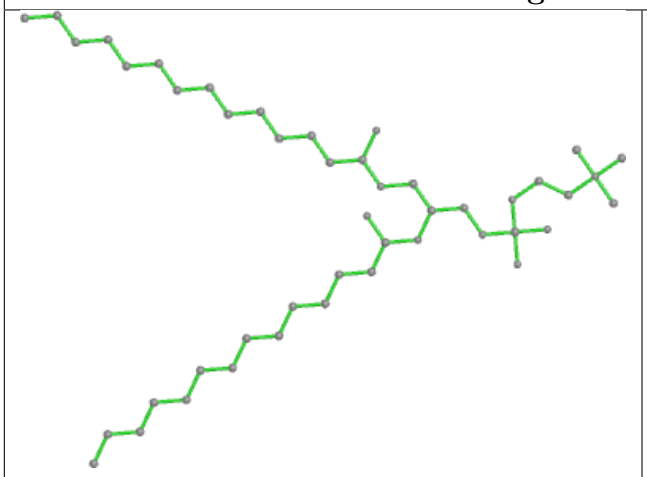


Rings

Ligand PX4 A 377



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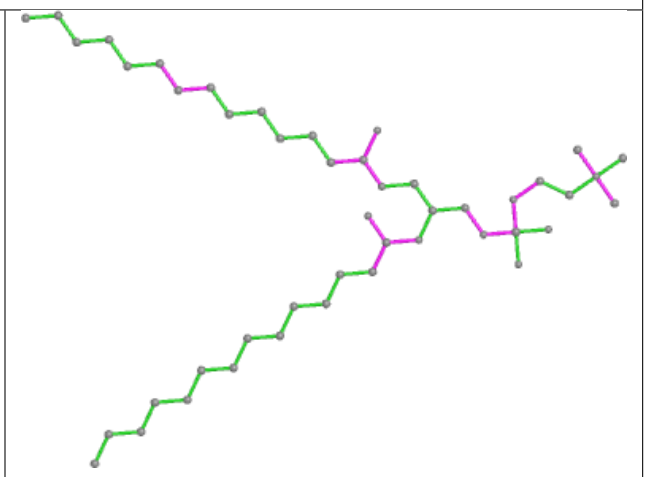

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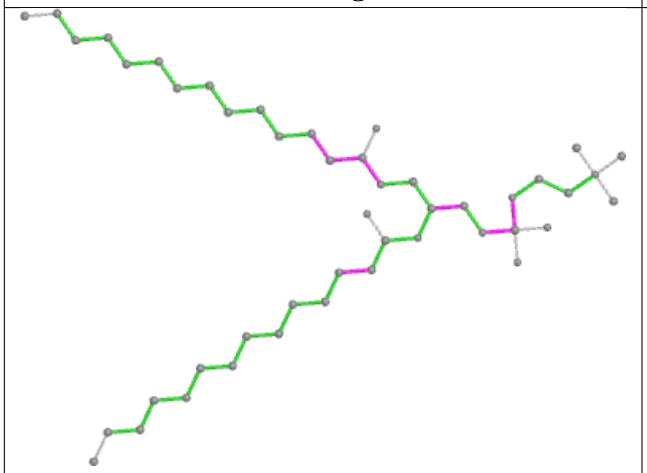

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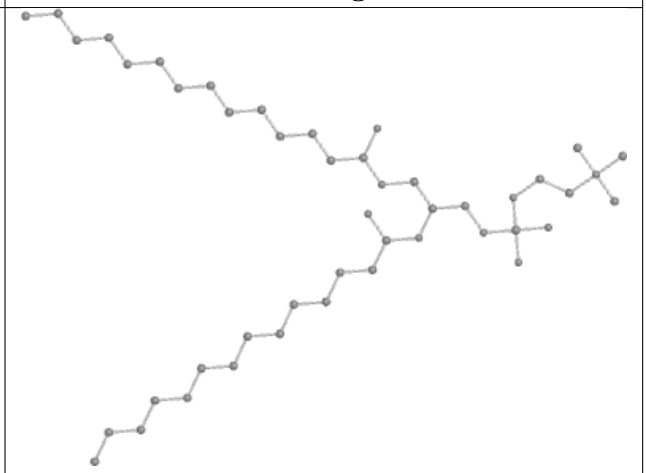
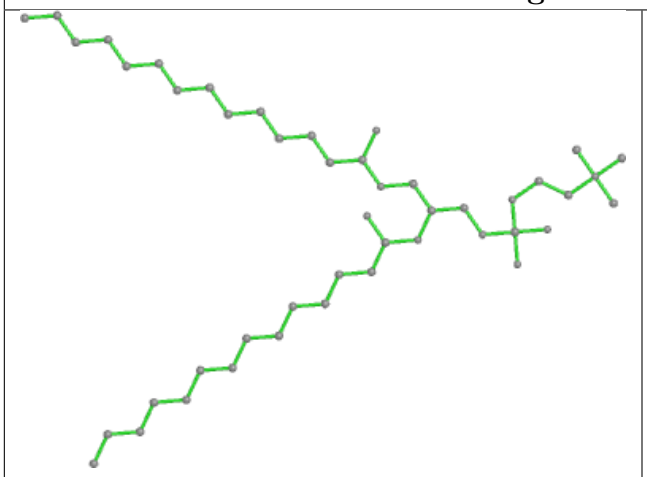


Rings

Ligand PX4 A 322



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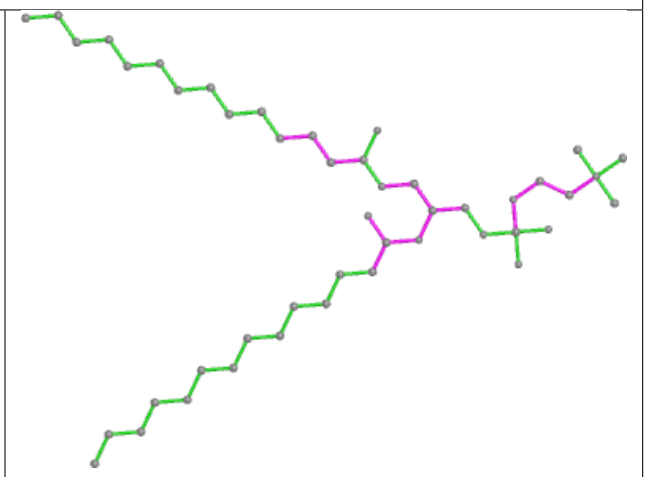
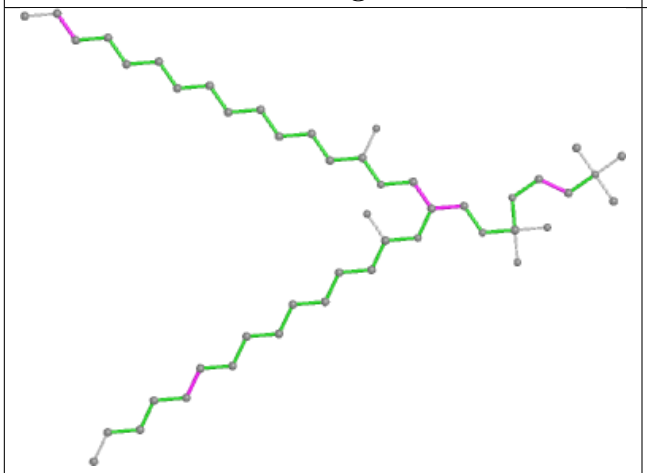


Bond angles



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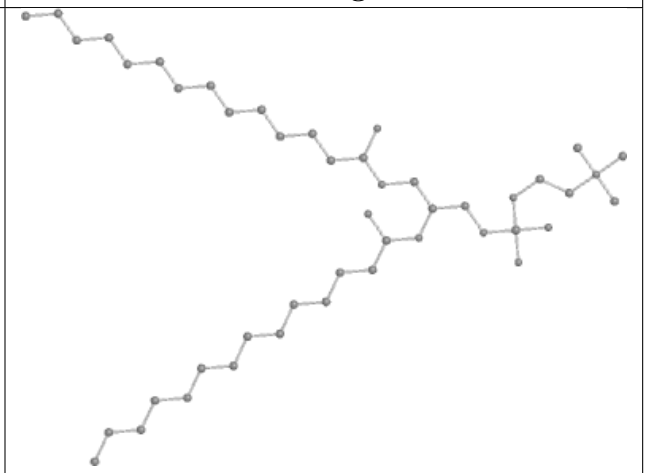
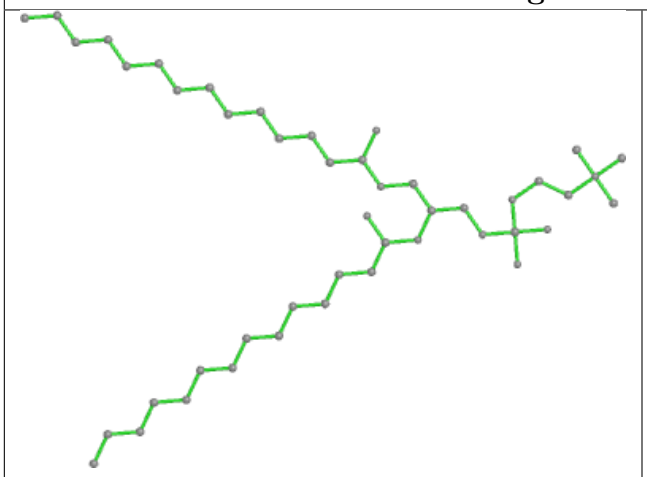


Rings

Ligand PX4 A 356



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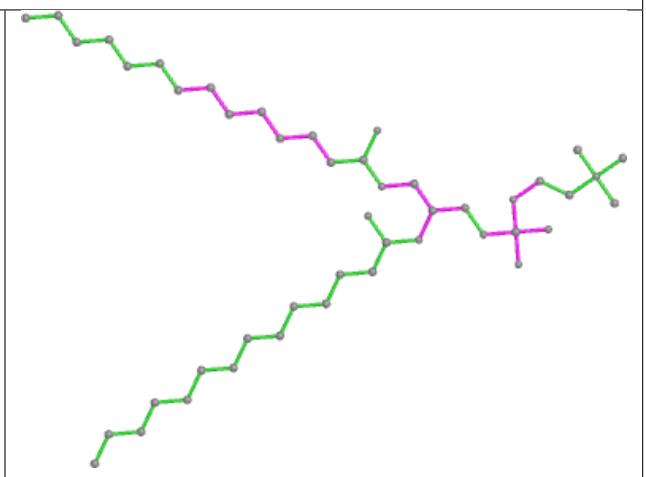

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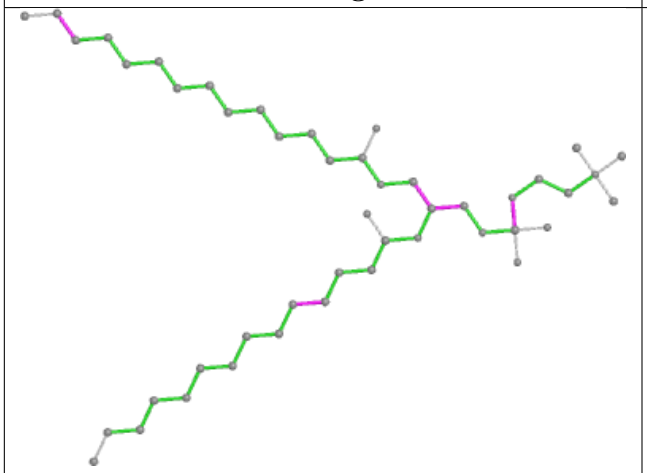

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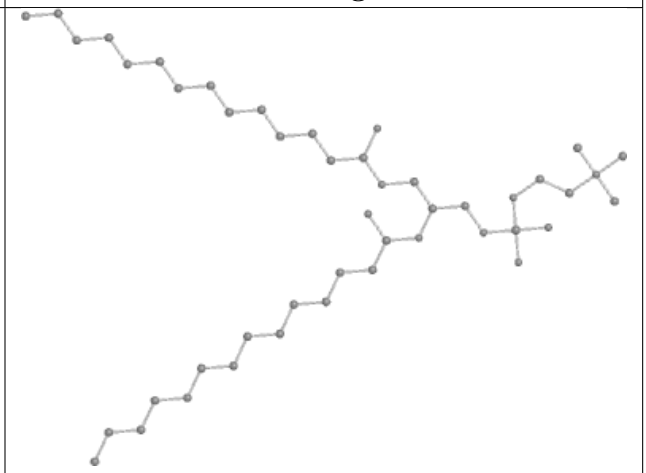
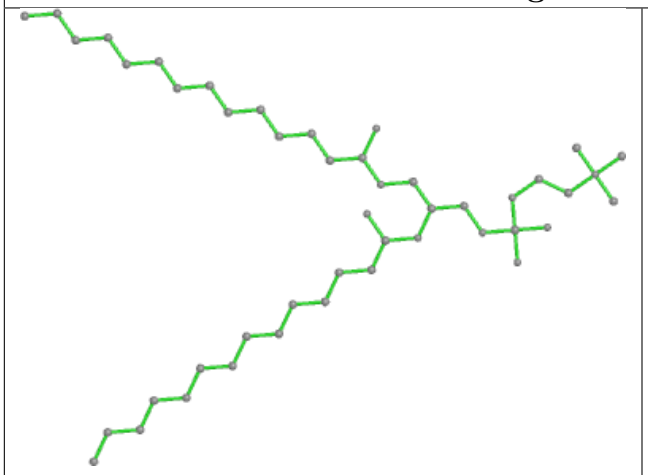


Rings

Ligand PX4 A 392



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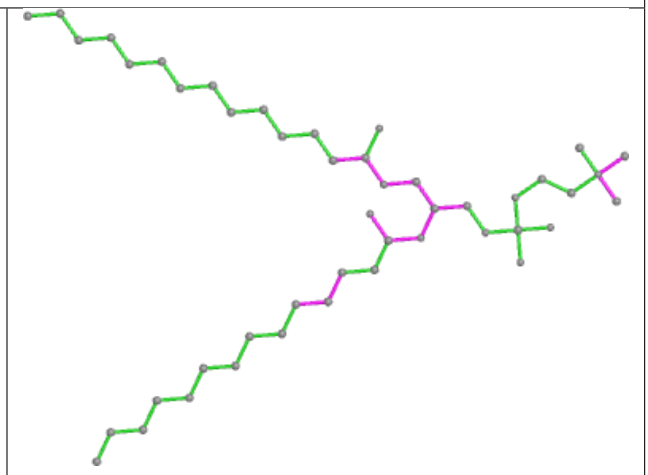

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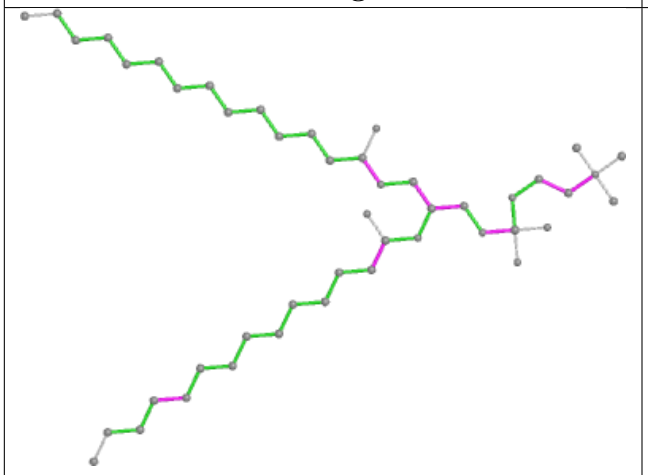

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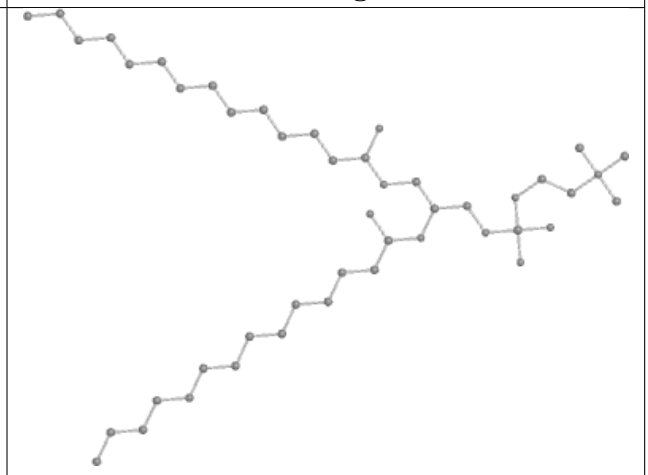
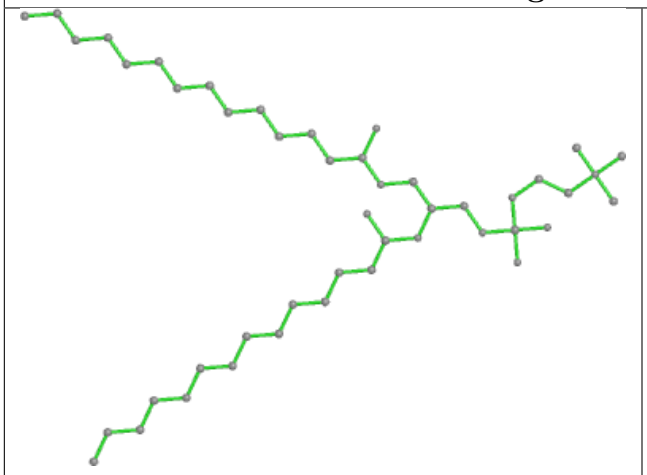


Rings

Ligand PX4 A 410



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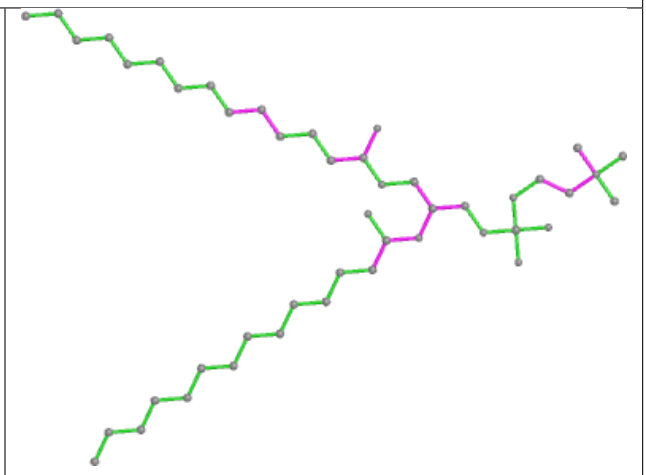

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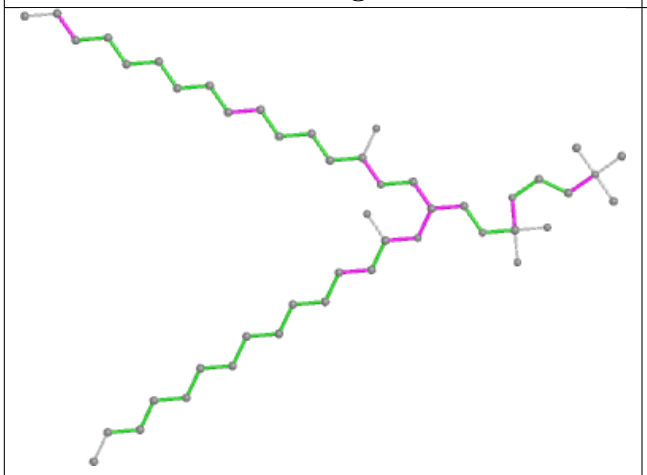

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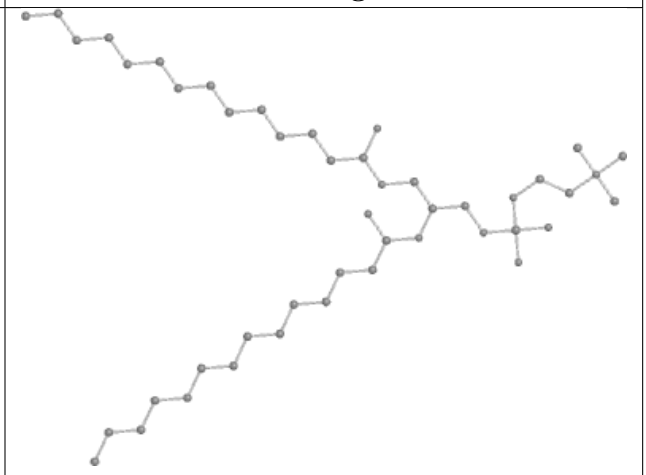
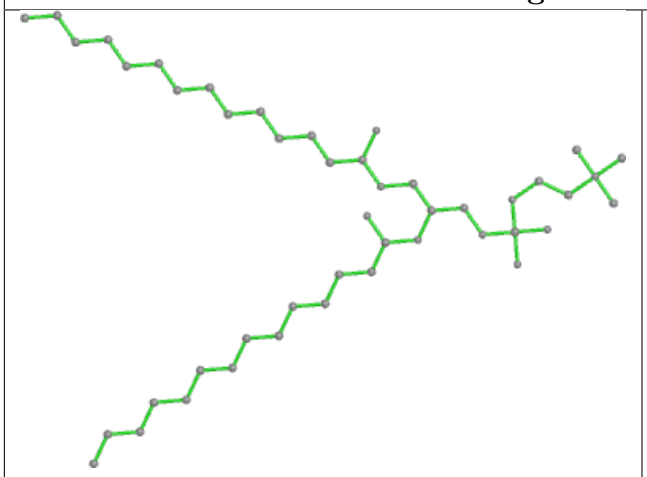


Rings

Ligand PX4 A 329



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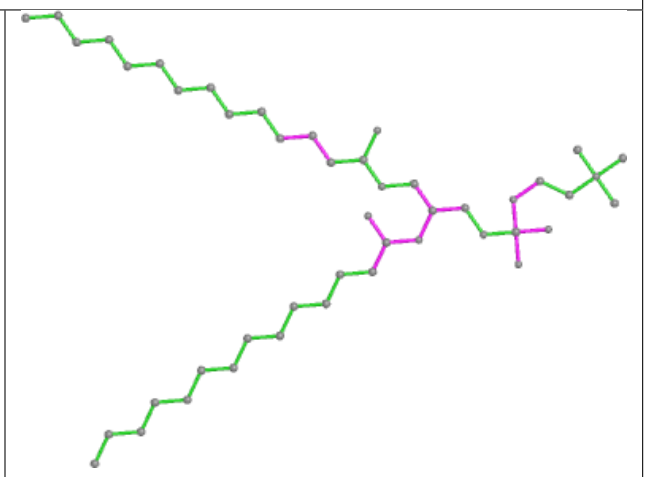

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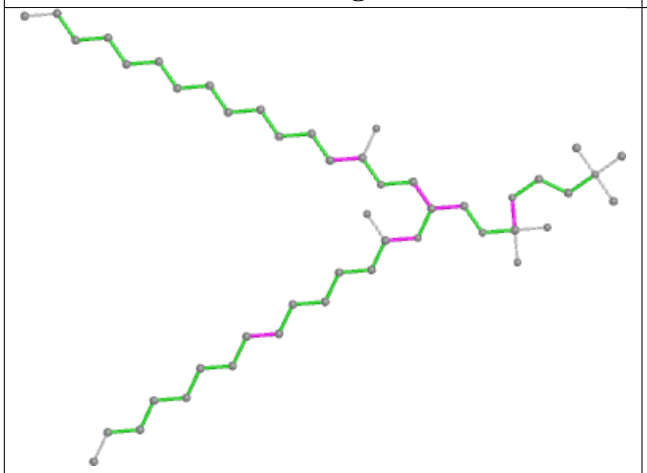

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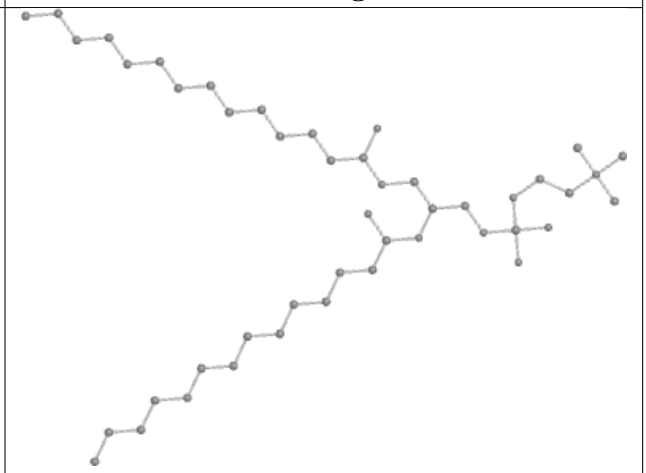
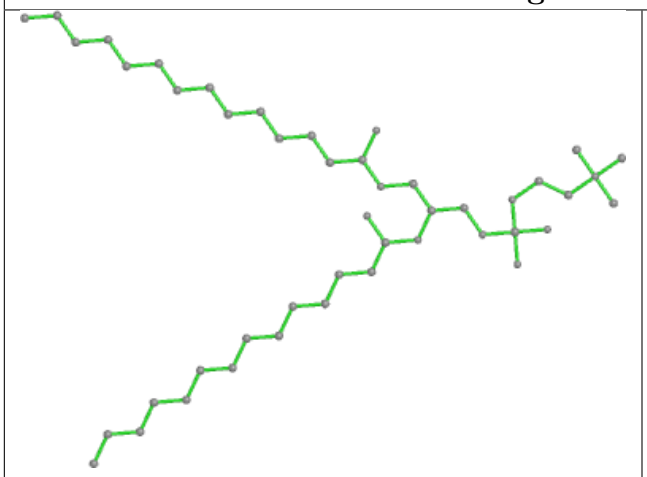


Rings

Ligand PX4 A 317



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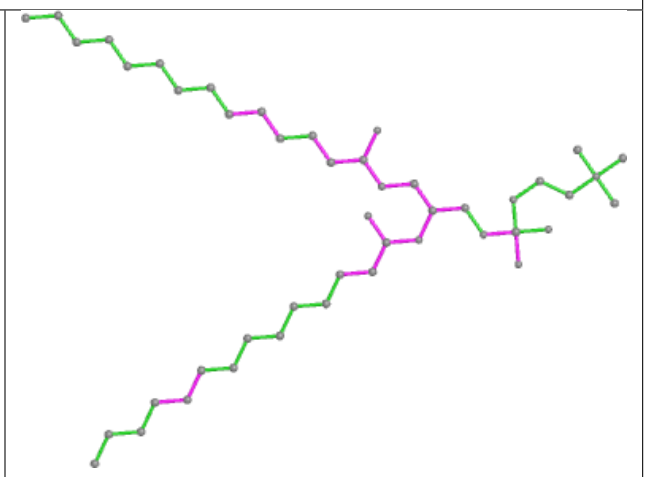

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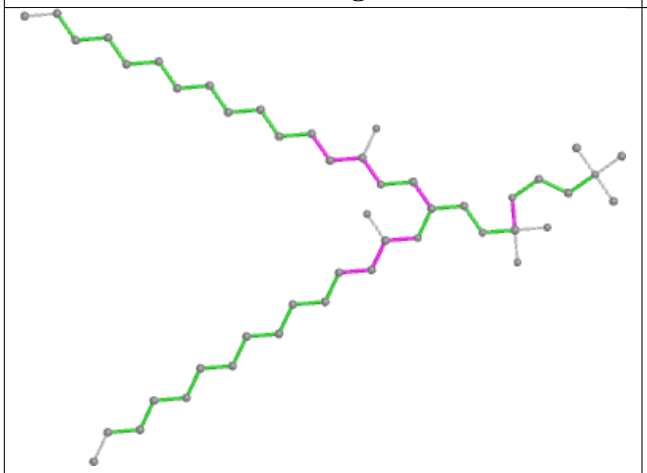

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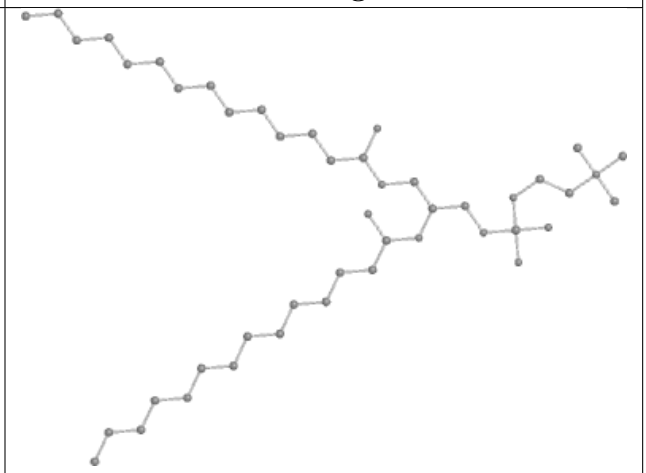
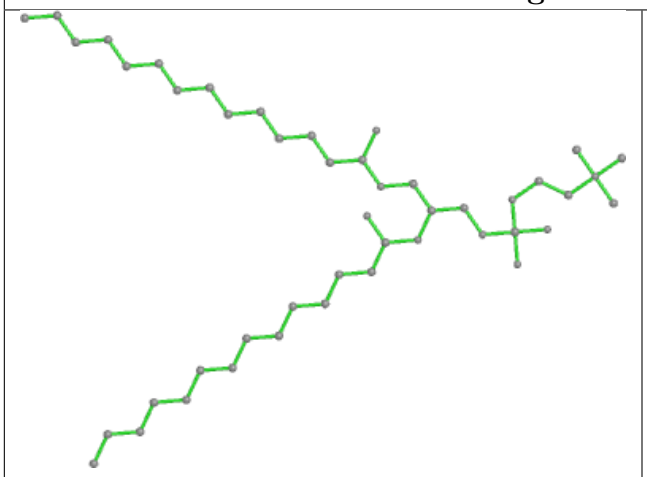


Rings

Ligand PX4 A 426



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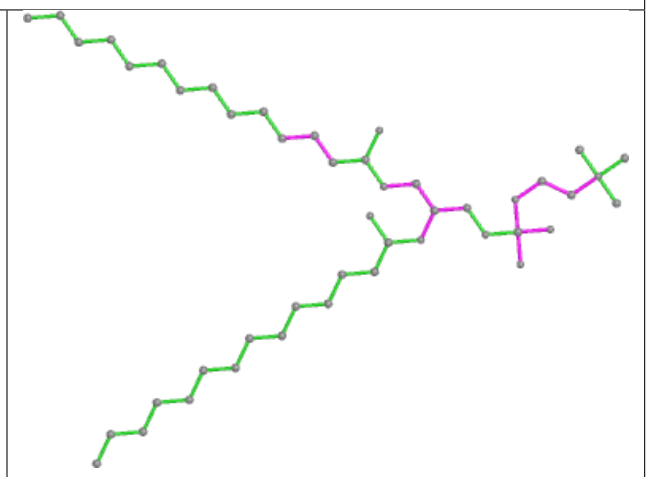

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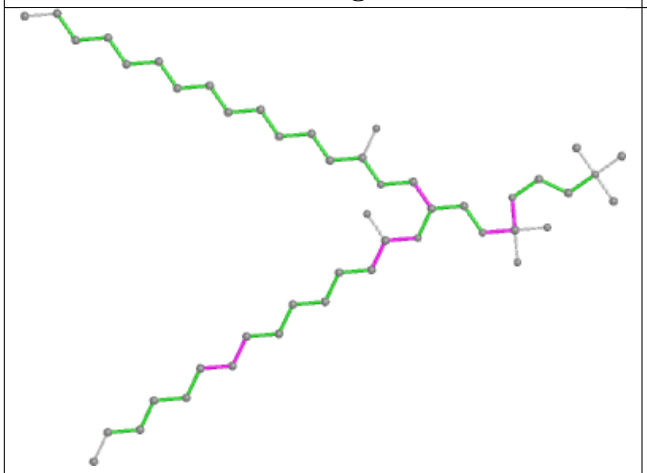

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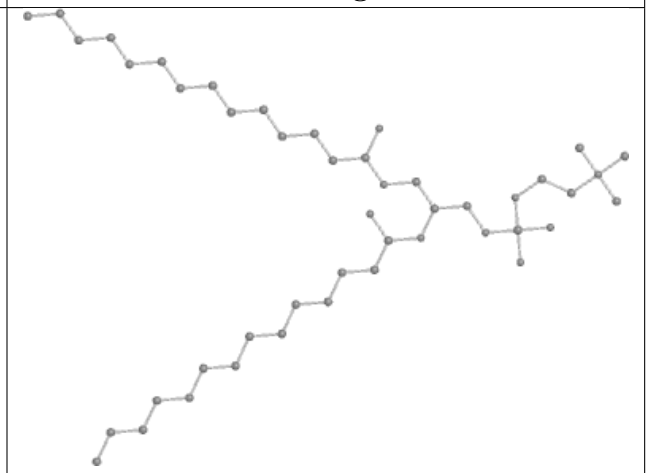
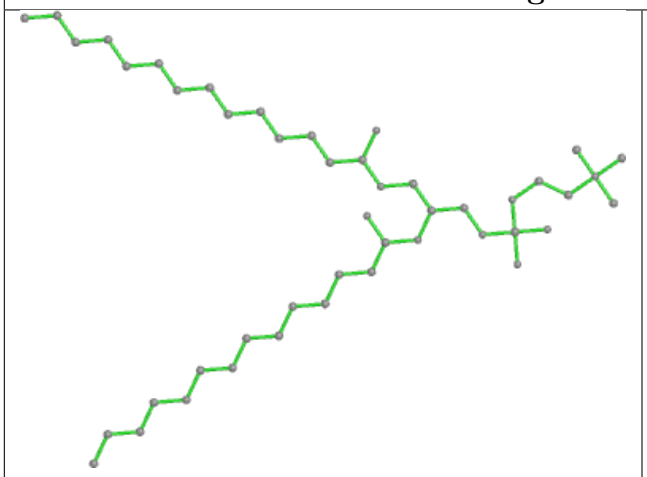


Rings

Ligand PX4 A 346



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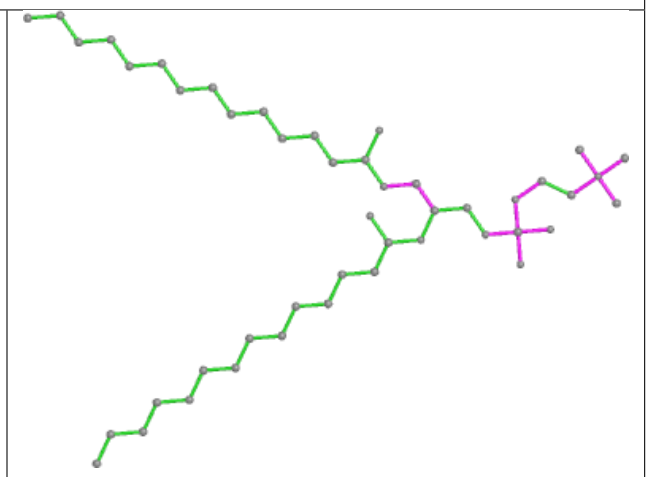
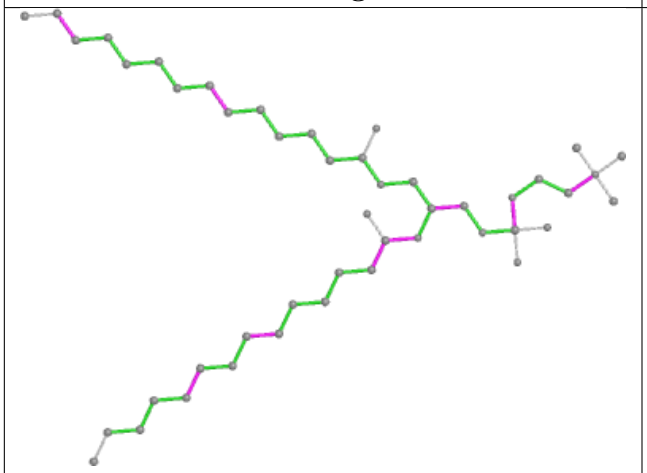


Bond angles



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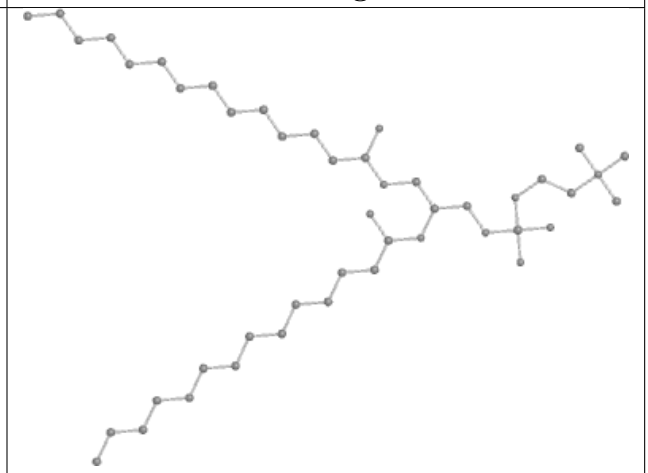
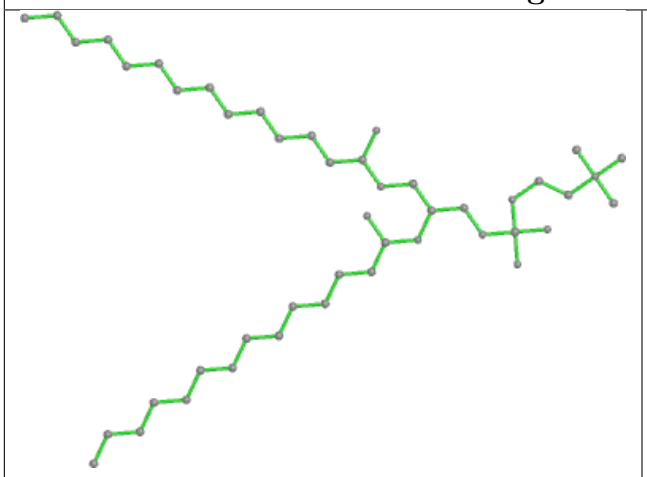


Rings

Ligand PX4 A 311



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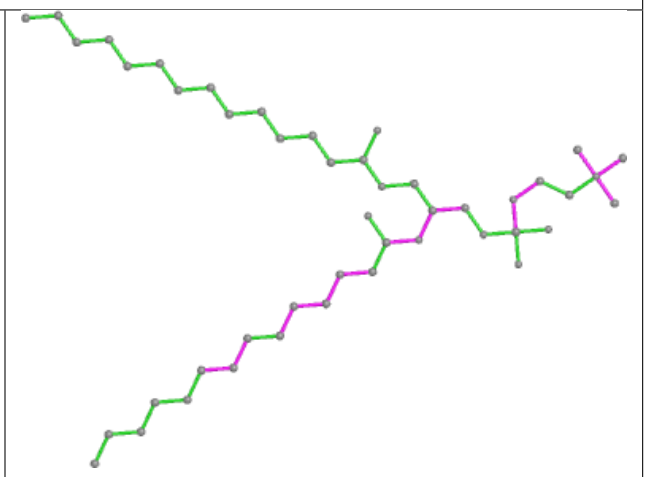
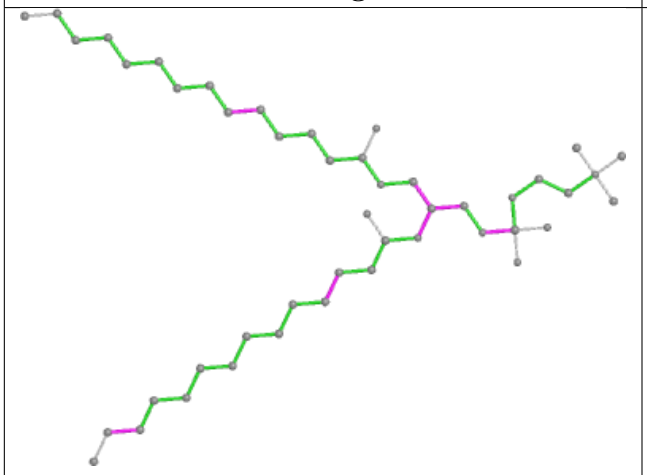


Bond angles



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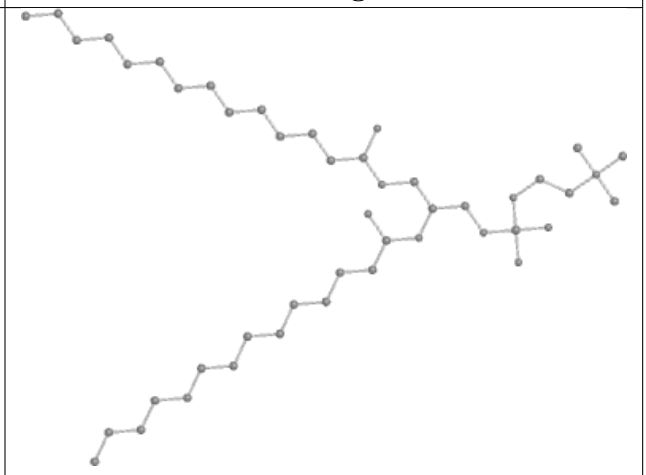
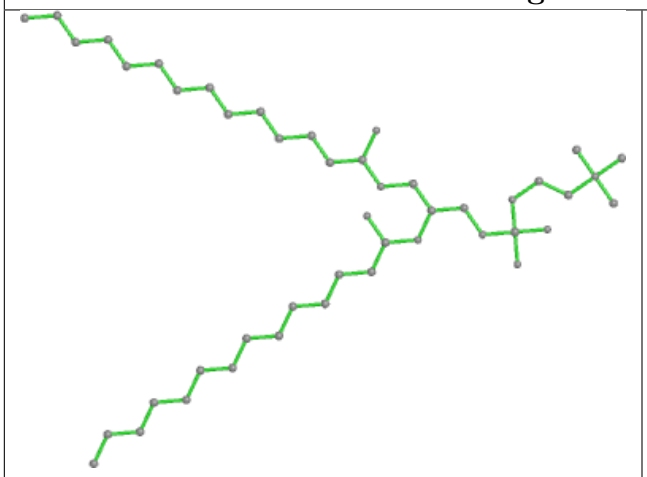


Rings

Ligand PX4 A 332



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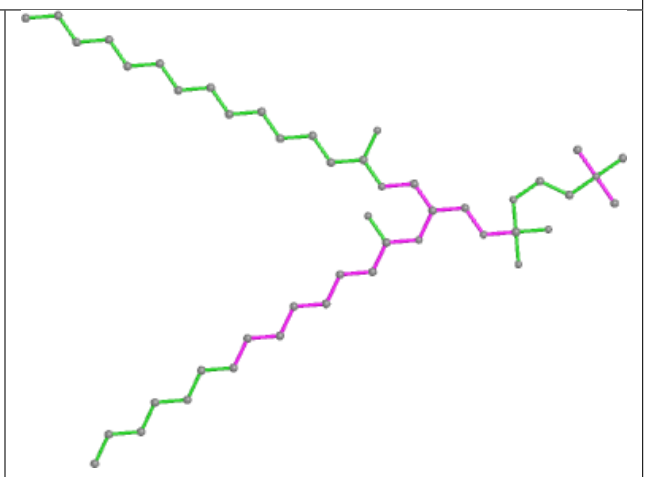
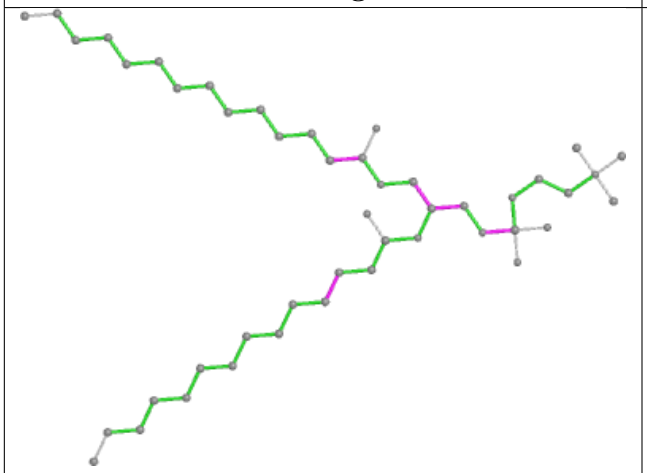


Bond angles



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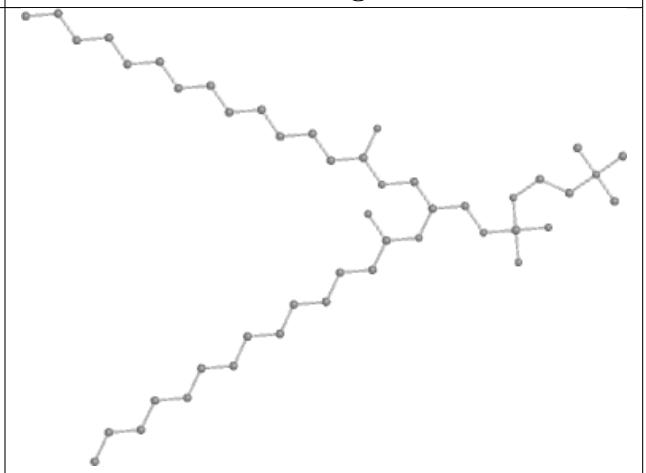
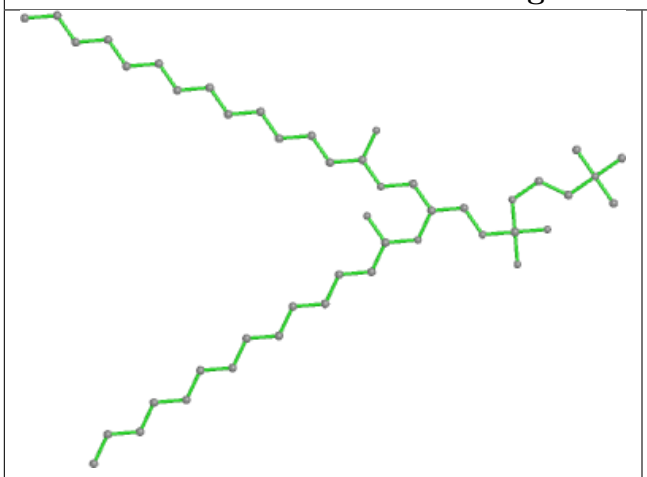
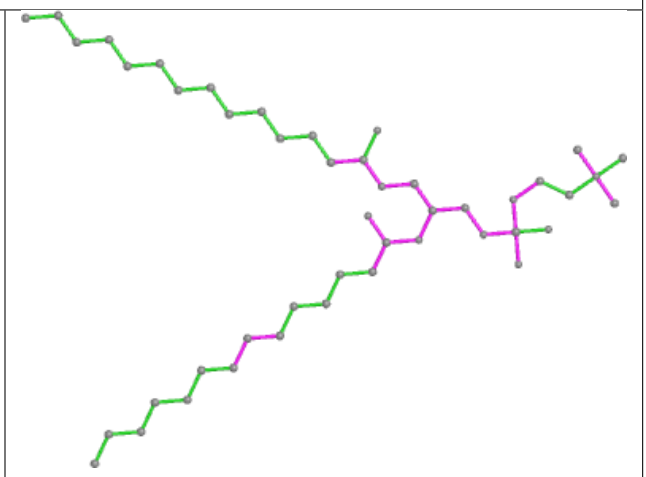


Rings

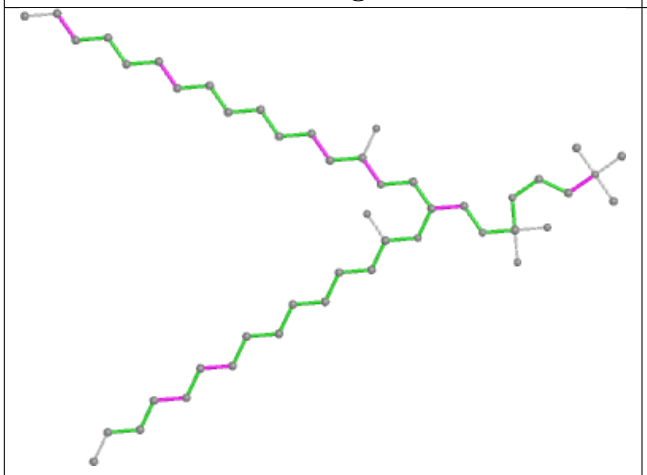
Ligand PX4 A 366



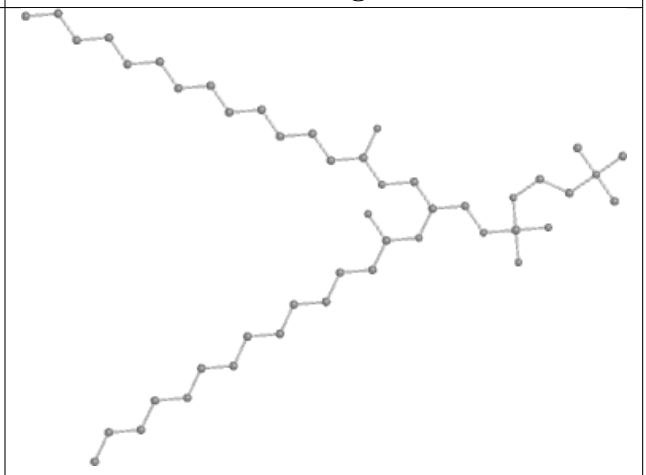
Bond lengths



Bond angles

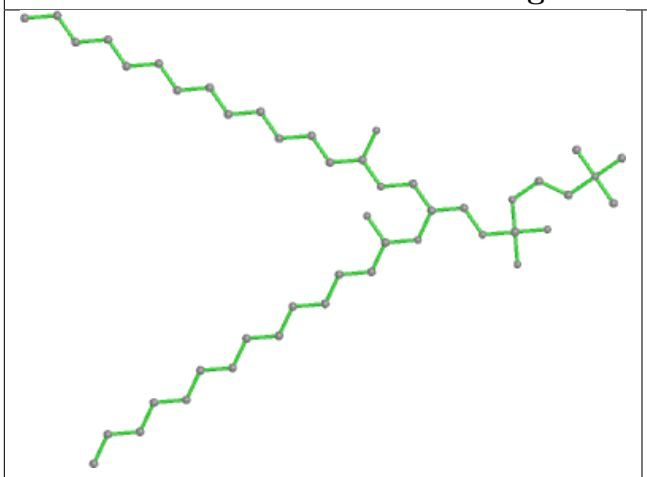


Torsions

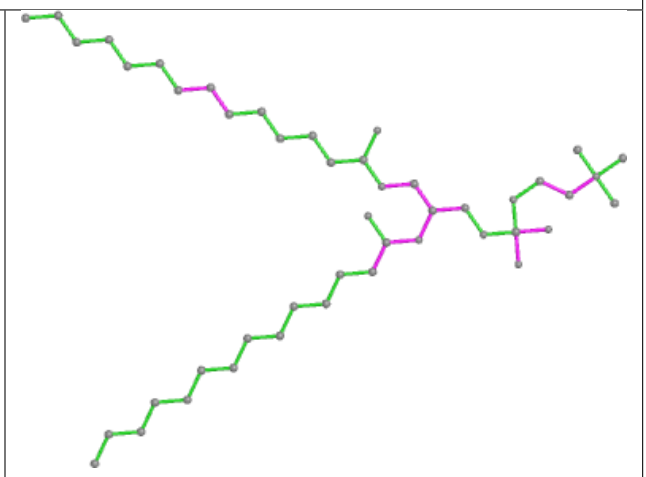


Rings

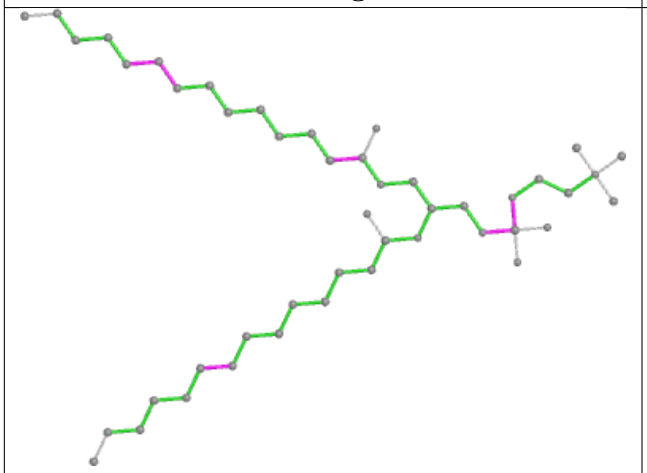
Ligand PX4 A 320



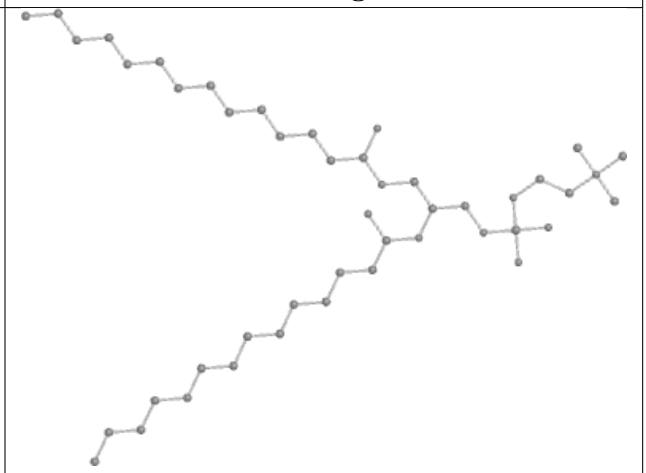
Bond lengths



Bond angles

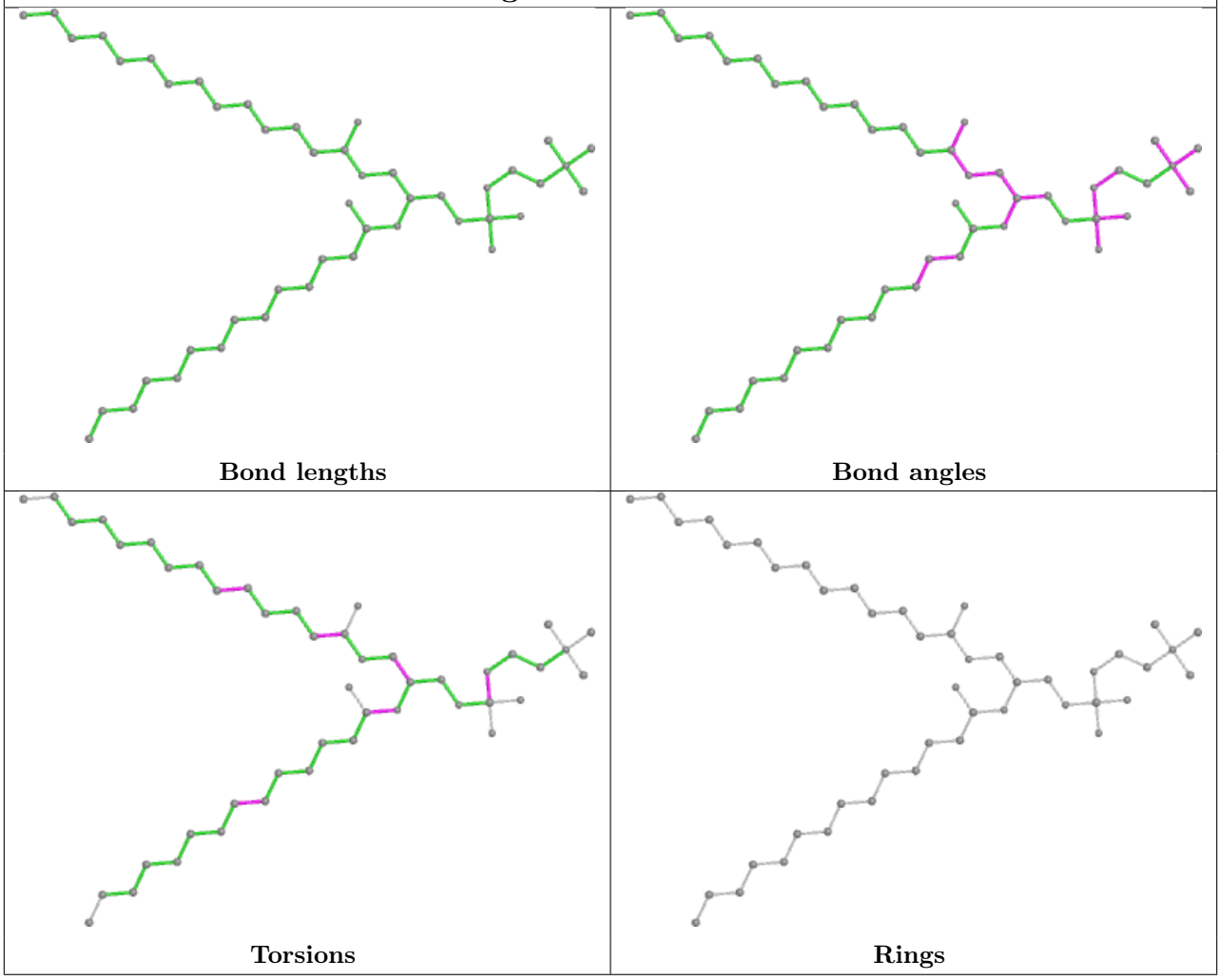


Torsions



Rings

Ligand PX4 A 393



6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

The completeness of assignment taking into account all chemical shift lists is 48% for the well-defined parts and 45% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping (i)

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	1503
Number of shifts mapped to atoms	1503
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	5

7.1.2 Chemical shift referencing (i)

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	212	-0.20 ± 0.38	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 48%, i.e. 1465 atoms were assigned a chemical shift out of a possible 3064. 0 out of 30 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	603/1142 (53%)	402/468 (86%)	0/458 (0%)	201/216 (93%)
Sidechain	796/1597 (50%)	728/1039 (70%)	62/499 (12%)	6/59 (10%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	66/325 (20%)	61/161 (38%)	0/151 (0%)	5/13 (38%)
Overall	1465/3064 (48%)	1191/1668 (71%)	62/1108 (6%)	212/288 (74%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 45%, i.e. 1503 atoms were assigned a chemical shift out of a possible 3323. 0 out of 32 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	632/1237 (51%)	420/507 (83%)	0/496 (0%)	212/234 (91%)
Sidechain	805/1761 (46%)	737/1143 (64%)	62/548 (11%)	6/70 (9%)
Aromatic	66/325 (20%)	61/161 (38%)	0/151 (0%)	5/13 (38%)
Overall	1503/3323 (45%)	1218/1811 (67%)	62/1195 (5%)	223/317 (70%)

7.1.4 Statistically unusual chemical shifts (i)

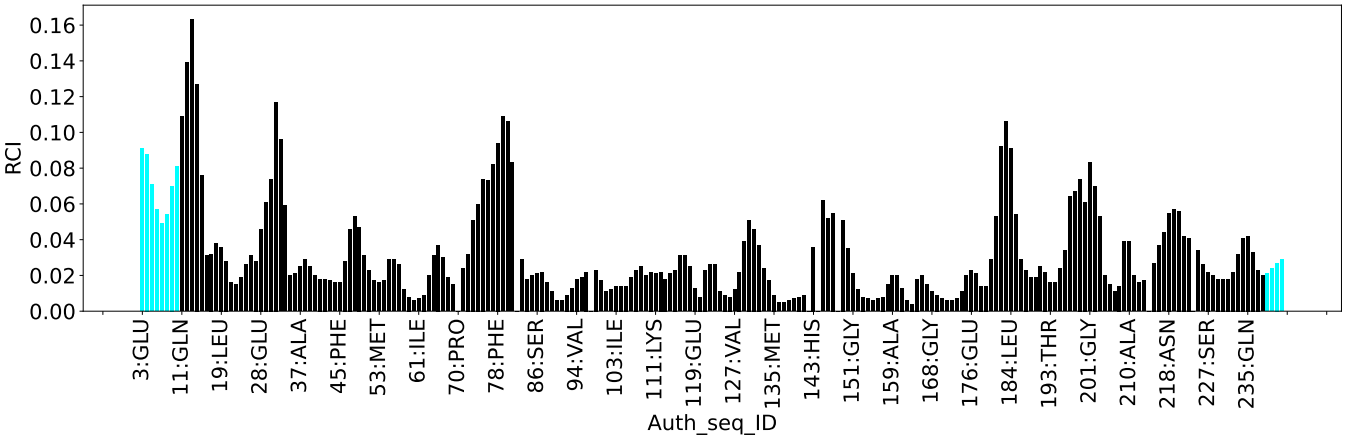
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	107	ARG	NE	119.47	76.53 – 92.65	21.6
1	A	162	PRO	HB3	-0.30	0.25 – 3.76	-6.6
1	A	242	SER	N	135.65	99.14 – 133.45	5.6
1	A	62	MET	HG3	0.34	0.54 – 4.26	-5.5
1	A	97	THR	HB	2.52	2.57 – 5.77	-5.2

7.1.5 Random Coil Index (RCI) plots (i)

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

Random coil index (RCI) for chain A:


RCI
0.16
0.14
0.12
0.10
0.08
0.06
0.04
0.02
0.00
3:GLU
11:GLN
19:LEU
28:GLU
37:ALA
45:PHE
53:MET
61:ILE
70:PRO
78:PHE
86:SER
94:VAL
103:ILE
111:LYS
119:GLU
127:VAL
135:MET
143:HIS
151:GLY
159:ALA
168:GLY
176:GLU
184:LEU
193:THR
201:GLY
210:ALA
218:ASN
227:SER
235:GLN
Auth_seq_ID

8 NMR restraints analysis (i)

8.1 Conformationally restricting restraints (i)

The following table provides the summary of experimentally observed NMR restraints in different categories. Restraints are classified into different categories based on the sequence separation of the atoms involved.

Description	Value
Total distance restraints	1064
Intra-residue (|i-j|=0)	197
Sequential (|i-j|=1)	383
Medium range (|i-j|>1 and |i-j|<5)	164
Long range (|i-j|≥5)	314
Inter-chain	0
Hydrogen bond restraints	6
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	77
Number of restraints per residue	4.3
Number of long range restraints per residue[1]	1.3

[1]Long range hydrogen bonds and disulfide bonds are counted as long range restraints while calculating the number of long range restraints per residue

8.2 Residual restraint violations (i)

This section provides the overview of the restraint violations analysis. The violations are binned as small, medium and large violations based on its absolute value. Average number of violations per model is calculated by dividing the total number of violations in each bin by the size of the ensemble.

8.2.1 Average number of distance violations per model (i)

Distance violations less than 0.1 Å are not included in the calculation.

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	27.2	0.2
0.2-0.5 (Medium)	47.0	0.5
>0.5 (Large)	88.9	20.41

8.2.2 Average number of dihedral-angle violations per model (i)

Dihedral-angle violations less than 1° are not included in the calculation.There are no dihedral-angle violations

9 Distance violation analysis (i)

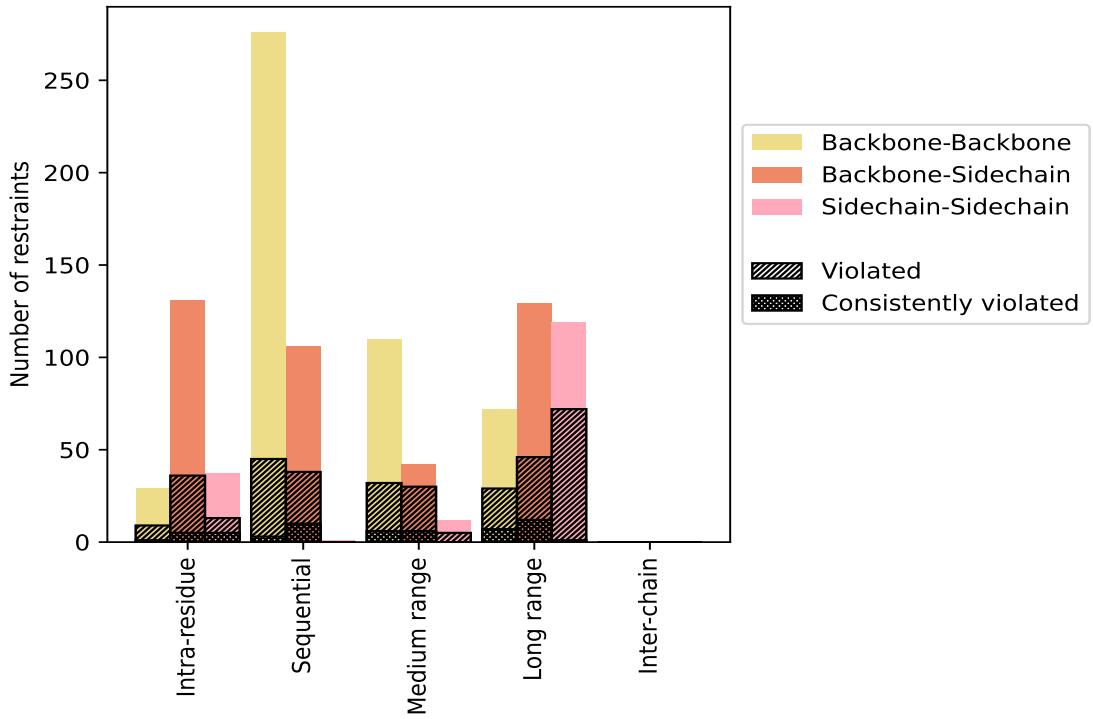
9.1 Summary of distance violations (i)

The following table shows the summary of distance violations in different restraint categories based on the sequence separation of the atoms involved. Each category is further sub-divided into three sub-categories based on the atoms involved. Violations less than 0.1 Å are not included in the statistics.

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	197	18.5	58	29.4	5.5	11	5.6	1.0
Backbone-Backbone	29	2.7	9	31.0	0.8	1	3.4	0.1
Backbone-Sidechain	131	12.3	36	27.5	3.4	5	3.8	0.5
Sidechain-Sidechain	37	3.5	13	35.1	1.2	5	13.5	0.5
Sequential (|i-j|=1)	383	36.0	83	21.7	7.8	13	3.4	1.2
Backbone-Backbone	276	25.9	45	16.3	4.2	3	1.1	0.3
Backbone-Sidechain	106	10.0	38	35.8	3.6	10	9.4	0.9
Sidechain-Sidechain	1	0.1	0	0.0	0.0	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	164	15.4	67	40.9	6.3	12	7.3	1.1
Backbone-Backbone	110	10.3	32	29.1	3.0	6	5.5	0.6
Backbone-Sidechain	42	3.9	30	71.4	2.8	6	14.3	0.6
Sidechain-Sidechain	12	1.1	5	41.7	0.5	0	0.0	0.0
Long range (|i-j|≥5)	314	29.5	147	46.8	13.8	20	6.4	1.9
Backbone-Backbone	66	6.2	29	43.9	2.7	7	10.6	0.7
Backbone-Sidechain	129	12.1	46	35.7	4.3	12	9.3	1.1
Sidechain-Sidechain	119	11.2	72	60.5	6.8	1	0.8	0.1
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	6	0.6	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1064	100.0	355	33.4	33.4	56	5.3	5.3
Backbone-Backbone	487	45.8	115	23.6	10.8	17	3.5	1.6
Backbone-Sidechain	408	38.3	150	36.8	14.1	33	8.1	3.1
Sidechain-Sidechain	169	15.9	90	53.3	8.5	6	3.6	0.6

[1] percentage calculated with respect to the total number of distance restraints, [2] percentage calculated with respect to the number of restraints in a particular restraint category, [3] violated in at least one model, [4] violated in all the models

9.1.1 Bar chart : Distribution of distance restraints and violations (i)



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfied bonds are counted in their appropriate category on the x-axis

9.2 Distance violation statistics for each model (i)

The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å are not included in the statistics.

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	29	39	34	67	0	169	1.69	18.85	3.14	0.64
2	26	35	40	54	0	155	1.62	18.36	3.22	0.52
3	29	42	30	50	0	151	1.68	18.95	3.3	0.67
4	23	42	30	62	0	157	1.55	19.12	3.2	0.59
5	25	38	38	62	0	163	1.65	18.57	3.16	0.67
6	34	42	31	73	0	180	1.56	18.8	3.1	0.56
7	30	47	35	61	0	173	1.59	19.47	3.16	0.55
8	33	42	32	63	0	170	1.56	18.51	3.13	0.52
9	25	36	27	72	0	160	1.66	18.94	3.26	0.58
10	29	42	28	69	0	168	1.56	18.87	3.2	0.48
11	25	30	29	53	0	137	1.85	19.63	3.44	0.74

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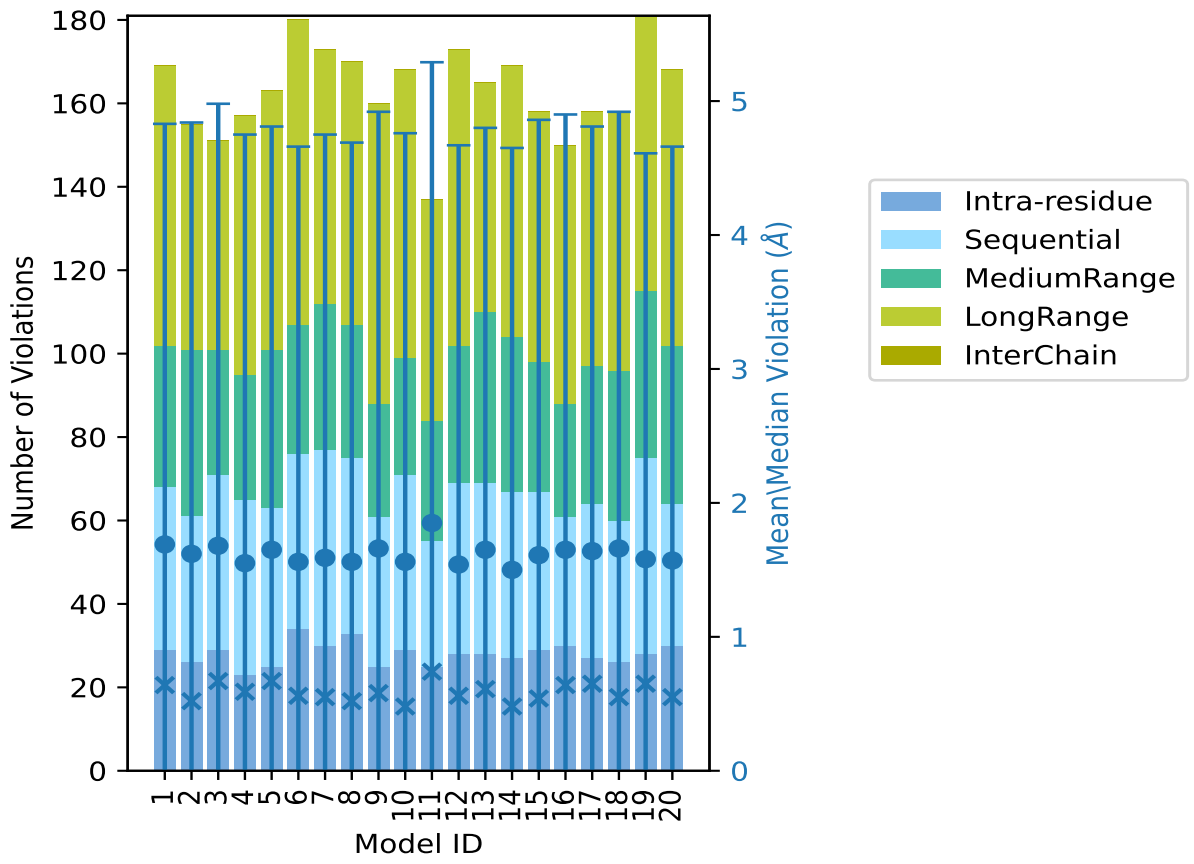
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	28	41	33	71	0	173	1.54	19.71	3.13	0.56
13	28	41	41	55	0	165	1.65	18.84	3.15	0.61
14	27	40	37	65	0	169	1.5	19.31	3.15	0.48
15	29	38	31	60	0	158	1.61	18.53	3.25	0.54
16	30	31	27	62	0	150	1.65	20.41	3.25	0.64
17	27	37	33	61	0	158	1.64	19.34	3.17	0.65
18	26	34	36	62	0	158	1.66	19.15	3.26	0.55
19	28	47	40	66	0	181	1.58	19.06	3.03	0.65
20	30	34	38	66	0	168	1.57	19.06	3.09	0.55

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints, [5]Inter-chain restraints, [6]Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model (i)



The mean(dot),median(x) and the standard deviation are shown in blue with respect to the y axis on the right

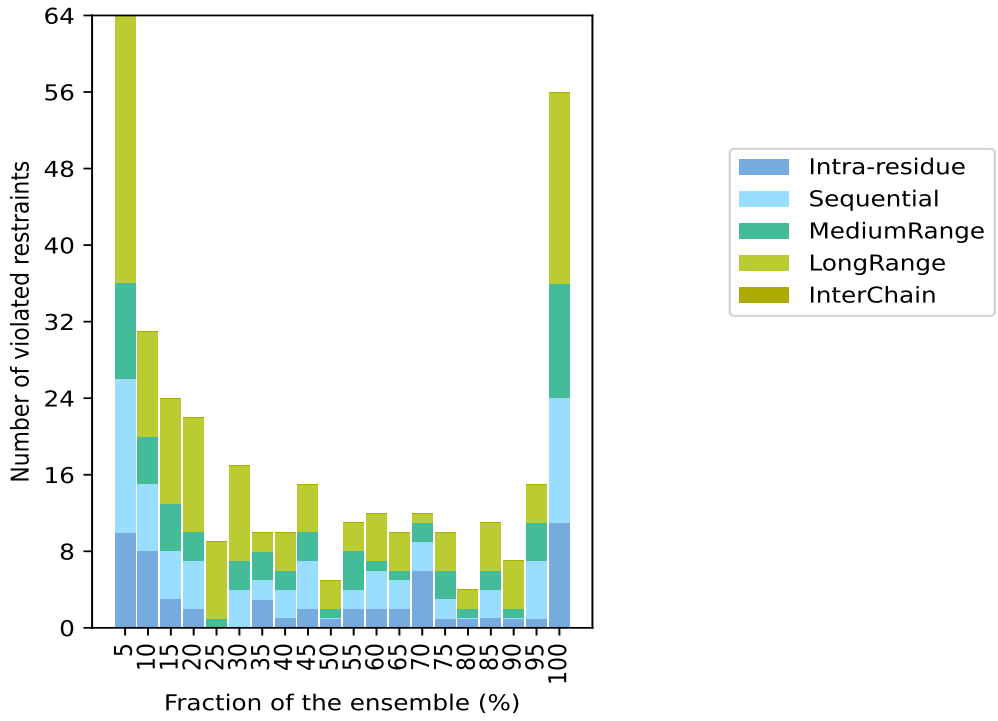
9.3 Distance violation statistics for the ensemble (i)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 703(IR:139, SQ:300, MR:97, LR:167, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
10	16	10	28	0	64	1	5.0
8	7	5	11	0	31	2	10.0
3	5	5	11	0	24	3	15.0
2	5	3	12	0	22	4	20.0
0	0	1	8	0	9	5	25.0
0	4	3	10	0	17	6	30.0
3	2	3	2	0	10	7	35.0
1	3	2	4	0	10	8	40.0
2	5	3	5	0	15	9	45.0
1	0	1	3	0	5	10	50.0
2	2	4	3	0	11	11	55.0
2	4	1	5	0	12	12	60.0
2	3	1	4	0	10	13	65.0
6	3	2	1	0	12	14	70.0
1	2	3	4	0	10	15	75.0
1	0	1	2	0	4	16	80.0
1	3	2	5	0	11	17	85.0
1	0	1	5	0	7	18	90.0
1	6	4	4	0	15	19	95.0
11	13	12	20	0	56	20	100.0

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints, [5]Inter-chain restraints, [6] Number of models with violations

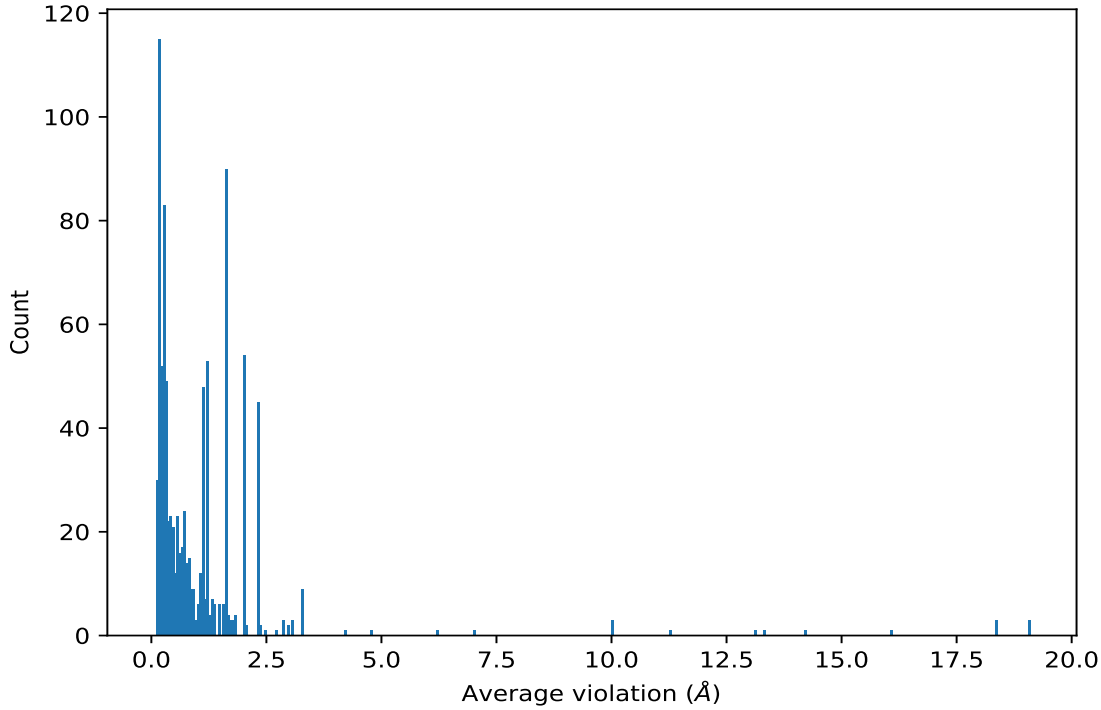
9.3.1 Bar graph : Distance violation statistics for the ensemble (i)



9.4 Most violated distance restraints in the ensemble (i)

9.4.1 Histogram : Distribution of mean distance violations (i)

The following histogram shows the distribution of the average value of the violation. The average is calculated for each restraint that is violated in more than one model over all the violated models in the ensemble



9.4.2 Table: Most violated distance restraints (i)

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,210)	1:A:105:VAL:HG21	1:A:237:LEU:H	20	19.06	0.48	19.0
(2,210)	1:A:105:VAL:HG22	1:A:237:LEU:H	20	19.06	0.48	19.0
(2,210)	1:A:105:VAL:HG23	1:A:237:LEU:H	20	19.06	0.48	19.0
(2,211)	1:A:120:ILE:HD11	1:A:100:LEU:H	20	18.36	0.45	18.39
(2,211)	1:A:120:ILE:HD12	1:A:100:LEU:H	20	18.36	0.45	18.39
(2,211)	1:A:120:ILE:HD13	1:A:100:LEU:H	20	18.36	0.45	18.39
(2,111)	1:A:11:GLN:H	1:A:26:ASP:H	20	16.08	0.97	16.42
(2,386)	1:A:156:LEU:H	1:A:182:SER:H	20	14.2	0.39	14.14
(2,112)	1:A:14:GLN:H	1:A:25:TYR:H	20	13.31	0.57	13.42
(2,389)	1:A:66:ARG:H	1:A:180:ASP:H	20	13.13	0.76	13.18
(2,532)	1:A:23:TYR:H	1:A:205:SER:H	20	11.29	0.57	11.21
(2,180)	1:A:92:ARG:H	1:A:69:VAL:HG11	20	10.0	0.48	9.93
(2,180)	1:A:92:ARG:H	1:A:69:VAL:HG12	20	10.0	0.48	9.93
(2,180)	1:A:92:ARG:H	1:A:69:VAL:HG13	20	10.0	0.48	9.93
(2,530)	1:A:204:HIS:HE1	1:A:24:LEU:H	20	7.04	1.06	6.72
(2,934)	1:A:72:VAL:HB	1:A:77:LEU:H	20	6.2	0.51	6.08

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,933)	1:A:72:VAL:HA	1:A:77:LEU:H	20	4.75	0.38	4.79
(2,318)	1:A:125:ARG:H	1:A:92:ARG:H	20	4.2	0.28	4.14
(2,882)	1:A:24:LEU:HD11	1:A:73:ALA:HB1	20	3.27	0.37	3.18
(2,882)	1:A:24:LEU:HD11	1:A:73:ALA:HB2	20	3.27	0.37	3.18
(2,882)	1:A:24:LEU:HD11	1:A:73:ALA:HB3	20	3.27	0.37	3.18
(2,882)	1:A:24:LEU:HD12	1:A:73:ALA:HB1	20	3.27	0.37	3.18
(2,882)	1:A:24:LEU:HD12	1:A:73:ALA:HB2	20	3.27	0.37	3.18
(2,882)	1:A:24:LEU:HD12	1:A:73:ALA:HB3	20	3.27	0.37	3.18
(2,882)	1:A:24:LEU:HD13	1:A:73:ALA:HB1	20	3.27	0.37	3.18
(2,882)	1:A:24:LEU:HD13	1:A:73:ALA:HB2	20	3.27	0.37	3.18
(2,882)	1:A:24:LEU:HD13	1:A:73:ALA:HB3	20	3.27	0.37	3.18
(2,177)	1:A:171:HIS:H	1:A:134:ILE:HD11	20	3.05	0.29	3.0
(2,177)	1:A:171:HIS:H	1:A:134:ILE:HD12	20	3.05	0.29	3.0
(2,177)	1:A:171:HIS:H	1:A:134:ILE:HD13	20	3.05	0.29	3.0
(2,531)	1:A:205:SER:H	1:A:204:HIS:HE1	20	2.97	0.47	3.01
(2,941)	1:A:73:ALA:HA	1:A:77:LEU:H	20	2.89	0.33	2.91
(2,472)	1:A:186:ILE:H	1:A:156:LEU:HD21	20	2.72	1.37	2.28
(2,471)	1:A:186:ILE:H	1:A:156:LEU:HD11	20	2.03	1.05	2.6
(2,471)	1:A:186:ILE:H	1:A:156:LEU:HD12	20	2.03	1.05	2.6
(2,471)	1:A:186:ILE:H	1:A:156:LEU:HD13	20	2.03	1.05	2.6
(3,21)	1:A:77:LEU:H	4:A:305:PX4:C35	20	2.0	0.86	1.84
(3,21)	1:A:77:LEU:H	4:A:307:PX4:C35	20	2.0	0.86	1.84
(3,21)	1:A:77:LEU:H	4:A:309:PX4:C35	20	2.0	0.86	1.84
(3,21)	1:A:77:LEU:H	4:A:311:PX4:C35	20	2.0	0.86	1.84
(3,21)	1:A:77:LEU:H	4:A:313:PX4:C35	20	2.0	0.86	1.84
(3,21)	1:A:77:LEU:H	4:A:315:PX4:C35	20	2.0	0.86	1.84
(3,21)	1:A:77:LEU:H	4:A:317:PX4:C35	20	2.0	0.86	1.84
(3,21)	1:A:77:LEU:H	4:A:319:PX4:C35	20	2.0	0.86	1.84
(3,21)	1:A:77:LEU:H	4:A:321:PX4:C35	20	2.0	0.86	1.84
(3,21)	1:A:77:LEU:H	4:A:323:PX4:C35	20	2.0	0.86	1.84
(3,21)	1:A:77:LEU:H	4:A:325:PX4:C35	20	2.0	0.86	1.84
(3,21)	1:A:77:LEU:H	4:A:327:PX4:C35	20	2.0	0.86	1.84
(3,21)	1:A:77:LEU:H	4:A:329:PX4:C35	20	2.0	0.86	1.84
(3,21)	1:A:77:LEU:H	4:A:331:PX4:C35	20	2.0	0.86	1.84
(3,21)	1:A:77:LEU:H	4:A:333:PX4:C35	20	2.0	0.86	1.84
(3,21)	1:A:77:LEU:H	4:A:335:PX4:C35	20	2.0	0.86	1.84
(3,21)	1:A:77:LEU:H	4:A:337:PX4:C35	20	2.0	0.86	1.84
(3,21)	1:A:77:LEU:H	4:A:339:PX4:C35	20	2.0	0.86	1.84
(3,21)	1:A:77:LEU:H	4:A:341:PX4:C35	20	2.0	0.86	1.84
(3,21)	1:A:77:LEU:H	4:A:343:PX4:C35	20	2.0	0.86	1.84
(3,21)	1:A:77:LEU:H	4:A:345:PX4:C35	20	2.0	0.86	1.84
(3,21)	1:A:77:LEU:H	4:A:347:PX4:C35	20	2.0	0.86	1.84

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(3,21)	1:A:77:LEU:H	4:A:349:PX4:C35	20	2.0	0.86	1.84
(3,21)	1:A:77:LEU:H	4:A:351:PX4:C35	20	2.0	0.86	1.84
(3,21)	1:A:77:LEU:H	4:A:353:PX4:C35	20	2.0	0.86	1.84
(3,21)	1:A:77:LEU:H	4:A:355:PX4:C35	20	2.0	0.86	1.84
(3,21)	1:A:77:LEU:H	4:A:357:PX4:C35	20	2.0	0.86	1.84
(3,21)	1:A:77:LEU:H	4:A:359:PX4:C35	20	2.0	0.86	1.84
(3,21)	1:A:77:LEU:H	4:A:361:PX4:C35	20	2.0	0.86	1.84
(3,21)	1:A:77:LEU:H	4:A:363:PX4:C35	20	2.0	0.86	1.84
(3,21)	1:A:77:LEU:H	4:A:402:PX4:C35	20	2.0	0.86	1.84
(3,21)	1:A:77:LEU:H	4:A:404:PX4:C35	20	2.0	0.86	1.84
(3,21)	1:A:77:LEU:H	4:A:406:PX4:C35	20	2.0	0.86	1.84
(3,21)	1:A:77:LEU:H	4:A:408:PX4:C35	20	2.0	0.86	1.84
(3,21)	1:A:77:LEU:H	4:A:410:PX4:C35	20	2.0	0.86	1.84
(3,21)	1:A:77:LEU:H	4:A:412:PX4:C35	20	2.0	0.86	1.84
(3,21)	1:A:77:LEU:H	4:A:414:PX4:C35	20	2.0	0.86	1.84
(3,21)	1:A:77:LEU:H	4:A:416:PX4:C35	20	2.0	0.86	1.84
(3,21)	1:A:77:LEU:H	4:A:418:PX4:C35	20	2.0	0.86	1.84
(3,21)	1:A:77:LEU:H	4:A:420:PX4:C35	20	2.0	0.86	1.84
(3,21)	1:A:77:LEU:H	4:A:422:PX4:C35	20	2.0	0.86	1.84
(3,21)	1:A:77:LEU:H	4:A:424:PX4:C35	20	2.0	0.86	1.84
(3,21)	1:A:77:LEU:H	4:A:426:PX4:C35	20	2.0	0.86	1.84
(3,21)	1:A:77:LEU:H	4:A:428:PX4:C35	20	2.0	0.86	1.84
(3,21)	1:A:77:LEU:H	4:A:430:PX4:C35	20	2.0	0.86	1.84
(2,473)	1:A:186:ILE:H	1:A:156:LEU:HD22	20	1.8	1.27	1.33
(2,473)	1:A:186:ILE:H	1:A:156:LEU:HD23	20	1.8	1.27	1.33
(2,932)	1:A:72:VAL:HG11	1:A:76:SER:H	20	1.67	0.36	1.77
(2,932)	1:A:72:VAL:HG12	1:A:76:SER:H	20	1.67	0.36	1.77
(2,932)	1:A:72:VAL:HG13	1:A:76:SER:H	20	1.67	0.36	1.77
(2,598)	1:A:235:GLN:H	1:A:238:TYR:HE1	20	1.57	0.49	1.64
(2,598)	1:A:235:GLN:H	1:A:238:TYR:HE2	20	1.57	0.49	1.64
(2,940)	1:A:73:ALA:HB1	1:A:75:TYR:H	20	1.39	0.1	1.4
(2,940)	1:A:73:ALA:HB2	1:A:75:TYR:H	20	1.39	0.1	1.4
(2,940)	1:A:73:ALA:HB3	1:A:75:TYR:H	20	1.39	0.1	1.4
(2,902)	1:A:66:ARG:HA	1:A:68:GLY:H	20	1.33	0.2	1.32
(2,981)	1:A:78:PHE:H	1:A:79:PRO:HG3	20	1.28	0.2	1.34
(2,981)	1:A:78:PHE:H	1:A:79:PRO:HG3	20	1.28	0.2	1.34
(2,954)	1:A:74:GLU:HB3	1:A:77:LEU:H	20	1.22	0.61	1.12
(2,954)	1:A:74:GLU:HB3	1:A:77:LEU:H	20	1.22	0.61	1.12
(2,542)	1:A:210:ALA:H	1:A:209:ASN:HD22	20	1.2	0.28	1.2
(2,948)	1:A:74:GLU:HG3	1:A:75:TYR:H	20	1.2	0.23	1.26
(2,948)	1:A:74:GLU:HG3	1:A:75:TYR:H	20	1.2	0.23	1.26
(2,928)	1:A:72:VAL:H	1:A:73:ALA:HB1	20	1.15	0.22	1.14

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(3,33)	1:A:155:THR:H	4:A:305:PX4:C35	20	1.1	0.36	1.15
(3,33)	1:A:155:THR:H	4:A:307:PX4:C35	20	1.1	0.36	1.15
(3,33)	1:A:155:THR:H	4:A:309:PX4:C35	20	1.1	0.36	1.15
(3,33)	1:A:155:THR:H	4:A:311:PX4:C35	20	1.1	0.36	1.15
(3,33)	1:A:155:THR:H	4:A:313:PX4:C35	20	1.1	0.36	1.15
(3,33)	1:A:155:THR:H	4:A:315:PX4:C35	20	1.1	0.36	1.15
(3,33)	1:A:155:THR:H	4:A:317:PX4:C35	20	1.1	0.36	1.15
(3,33)	1:A:155:THR:H	4:A:319:PX4:C35	20	1.1	0.36	1.15
(3,33)	1:A:155:THR:H	4:A:321:PX4:C35	20	1.1	0.36	1.15
(3,33)	1:A:155:THR:H	4:A:323:PX4:C35	20	1.1	0.36	1.15
(3,33)	1:A:155:THR:H	4:A:325:PX4:C35	20	1.1	0.36	1.15
(3,33)	1:A:155:THR:H	4:A:327:PX4:C35	20	1.1	0.36	1.15
(3,33)	1:A:155:THR:H	4:A:329:PX4:C35	20	1.1	0.36	1.15
(3,33)	1:A:155:THR:H	4:A:331:PX4:C35	20	1.1	0.36	1.15
(3,33)	1:A:155:THR:H	4:A:333:PX4:C35	20	1.1	0.36	1.15
(3,33)	1:A:155:THR:H	4:A:335:PX4:C35	20	1.1	0.36	1.15
(3,33)	1:A:155:THR:H	4:A:337:PX4:C35	20	1.1	0.36	1.15
(3,33)	1:A:155:THR:H	4:A:339:PX4:C35	20	1.1	0.36	1.15
(3,33)	1:A:155:THR:H	4:A:341:PX4:C35	20	1.1	0.36	1.15
(3,33)	1:A:155:THR:H	4:A:343:PX4:C35	20	1.1	0.36	1.15
(3,33)	1:A:155:THR:H	4:A:345:PX4:C35	20	1.1	0.36	1.15
(3,33)	1:A:155:THR:H	4:A:347:PX4:C35	20	1.1	0.36	1.15
(3,33)	1:A:155:THR:H	4:A:349:PX4:C35	20	1.1	0.36	1.15
(3,33)	1:A:155:THR:H	4:A:351:PX4:C35	20	1.1	0.36	1.15
(3,33)	1:A:155:THR:H	4:A:353:PX4:C35	20	1.1	0.36	1.15
(3,33)	1:A:155:THR:H	4:A:355:PX4:C35	20	1.1	0.36	1.15
(3,33)	1:A:155:THR:H	4:A:357:PX4:C35	20	1.1	0.36	1.15
(3,33)	1:A:155:THR:H	4:A:359:PX4:C35	20	1.1	0.36	1.15
(3,33)	1:A:155:THR:H	4:A:361:PX4:C35	20	1.1	0.36	1.15
(3,33)	1:A:155:THR:H	4:A:363:PX4:C35	20	1.1	0.36	1.15
(3,33)	1:A:155:THR:H	4:A:402:PX4:C35	20	1.1	0.36	1.15
(3,33)	1:A:155:THR:H	4:A:404:PX4:C35	20	1.1	0.36	1.15
(3,33)	1:A:155:THR:H	4:A:406:PX4:C35	20	1.1	0.36	1.15
(3,33)	1:A:155:THR:H	4:A:408:PX4:C35	20	1.1	0.36	1.15
(3,33)	1:A:155:THR:H	4:A:410:PX4:C35	20	1.1	0.36	1.15
(3,33)	1:A:155:THR:H	4:A:412:PX4:C35	20	1.1	0.36	1.15
(3,33)	1:A:155:THR:H	4:A:414:PX4:C35	20	1.1	0.36	1.15
(3,33)	1:A:155:THR:H	4:A:416:PX4:C35	20	1.1	0.36	1.15
(3,33)	1:A:155:THR:H	4:A:418:PX4:C35	20	1.1	0.36	1.15
(3,33)	1:A:155:THR:H	4:A:420:PX4:C35	20	1.1	0.36	1.15
(3,33)	1:A:155:THR:H	4:A:422:PX4:C35	20	1.1	0.36	1.15
(3,33)	1:A:155:THR:H	4:A:424:PX4:C35	20	1.1	0.36	1.15

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(3,33)	1:A:155:THR:H	4:A:426:PX4:C35	20	1.1	0.36	1.15
(3,33)	1:A:155:THR:H	4:A:428:PX4:C35	20	1.1	0.36	1.15
(3,33)	1:A:155:THR:H	4:A:430:PX4:C35	20	1.1	0.36	1.15
(2,178)	1:A:171:HIS:H	1:A:69:VAL:HG11	20	1.08	0.36	1.0
(2,178)	1:A:171:HIS:H	1:A:69:VAL:HG12	20	1.08	0.36	1.0
(2,178)	1:A:171:HIS:H	1:A:69:VAL:HG13	20	1.08	0.36	1.0
(2,516)	1:A:200:LEU:H	1:A:196:LEU:HD11	20	1.08	0.27	0.98
(2,516)	1:A:200:LEU:H	1:A:196:LEU:HD12	20	1.08	0.27	0.98
(2,516)	1:A:200:LEU:H	1:A:196:LEU:HD13	20	1.08	0.27	0.98
(2,974)	1:A:78:PHE:H	1:A:77:LEU:HD21	20	1.05	0.75	0.9
(2,110)	1:A:11:GLN:H	1:A:14:GLN:H	20	1.02	0.18	1.0
(2,229)	1:A:106:ASP:H	1:A:109:VAL:H	20	1.01	0.13	1.01
(2,899)	1:A:66:ARG:H	1:A:64:LYS:H	20	1.0	0.3	0.96
(2,891)	1:A:63:GLN:H	1:A:63:GLN:HB3	20	0.87	0.12	0.86
(2,891)	1:A:63:GLN:H	1:A:63:GLN:HB2	20	0.87	0.12	0.86
(2,891)	1:A:63:GLN:H	1:A:63:GLN:HB3	20	0.87	0.12	0.86
(2,891)	1:A:63:GLN:H	1:A:63:GLN:HB2	20	0.87	0.12	0.86
(2,936)	1:A:73:ALA:HB1	1:A:73:ALA:H	20	0.82	0.09	0.84
(2,936)	1:A:73:ALA:HB2	1:A:73:ALA:H	20	0.82	0.09	0.84
(2,936)	1:A:73:ALA:HB3	1:A:73:ALA:H	20	0.82	0.09	0.84
(2,983)	1:A:79:PRO:HD3	1:A:80:ASN:H	20	0.78	0.14	0.78
(2,983)	1:A:79:PRO:HD3	1:A:80:ASN:H	20	0.78	0.14	0.78
(2,925)	1:A:72:VAL:HG21	1:A:73:ALA:H	20	0.75	0.19	0.76
(2,925)	1:A:72:VAL:HG22	1:A:73:ALA:H	20	0.75	0.19	0.76
(2,925)	1:A:72:VAL:HG23	1:A:73:ALA:H	20	0.75	0.19	0.76
(2,925)	1:A:72:VAL:HG11	1:A:73:ALA:H	20	0.75	0.19	0.76
(2,925)	1:A:72:VAL:HG12	1:A:73:ALA:H	20	0.75	0.19	0.76
(2,925)	1:A:72:VAL:HG13	1:A:73:ALA:H	20	0.75	0.19	0.76
(2,905)	1:A:67:CYS:HA	1:A:68:GLY:H	20	0.74	0.17	0.74
(2,930)	1:A:72:VAL:HG11	1:A:75:TYR:H	20	0.69	0.2	0.7
(2,930)	1:A:72:VAL:HG12	1:A:75:TYR:H	20	0.69	0.2	0.7
(2,930)	1:A:72:VAL:HG13	1:A:75:TYR:H	20	0.69	0.2	0.7
(2,913)	1:A:71:ASP:H	1:A:70:PRO:HB3	20	0.68	0.12	0.68
(2,913)	1:A:71:ASP:H	1:A:70:PRO:HB2	20	0.68	0.12	0.68
(2,911)	1:A:69:VAL:HG21	1:A:69:VAL:H	20	0.65	0.2	0.62
(2,911)	1:A:69:VAL:HG22	1:A:69:VAL:H	20	0.65	0.2	0.62
(2,911)	1:A:69:VAL:HG23	1:A:69:VAL:H	20	0.65	0.2	0.62
(2,911)	1:A:69:VAL:HG11	1:A:69:VAL:H	20	0.65	0.2	0.62
(2,911)	1:A:69:VAL:HG12	1:A:69:VAL:H	20	0.65	0.2	0.62
(2,911)	1:A:69:VAL:HG13	1:A:69:VAL:H	20	0.65	0.2	0.62
(2,425)	1:A:170:ALA:H	1:A:169:ASP:H	20	0.55	0.1	0.57
(2,896)	1:A:64:LYS:H	1:A:64:LYS:HE3	20	0.52	0.16	0.49

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,896)	1:A:64:LYS:H	1:A:64:LYS:HE3	20	0.52	0.16	0.49
(2,384)	1:A:154:ASN:HD22	1:A:154:ASN:HD21	20	0.45	0.03	0.45
(2,384)	1:A:154:ASN:HD22	1:A:154:ASN:HD21	20	0.45	0.03	0.45
(2,540)	1:A:209:ASN:HD21	1:A:209:ASN:HD22	20	0.44	0.05	0.44
(2,540)	1:A:209:ASN:HD21	1:A:209:ASN:HD22	20	0.44	0.05	0.44
(2,919)	1:A:72:VAL:H	1:A:71:ASP:HA	20	0.44	0.17	0.38
(2,557)	1:A:21:ARG:H	1:A:23:TYR:H	20	0.34	0.13	0.32
(2,895)	1:A:64:LYS:H	1:A:64:LYS:HA	20	0.31	0.09	0.29
(2,357)	1:A:136:ILE:HD11	1:A:137:GLY:H	20	0.3	0.09	0.3
(2,357)	1:A:136:ILE:HD12	1:A:137:GLY:H	20	0.3	0.09	0.3
(2,357)	1:A:136:ILE:HD13	1:A:137:GLY:H	20	0.3	0.09	0.3
(2,945)	1:A:74:GLU:H	1:A:74:GLU:HG3	20	0.29	0.13	0.26
(2,945)	1:A:74:GLU:H	1:A:74:GLU:HG3	20	0.29	0.13	0.26
(2,655)	1:A:16:GLN:HE21	1:A:16:GLN:HE22	20	0.25	0.03	0.24
(2,653)	1:A:11:GLN:HE22	1:A:11:GLN:HE21	20	0.25	0.04	0.24
(2,39)	1:A:43:GLN:HE21	1:A:43:GLN:HE22	20	0.24	0.03	0.24
(2,832)	1:A:120:ILE:HD11	1:A:200:LEU:HD21	19	2.87	1.3	2.89
(2,879)	1:A:234:ILE:HD11	1:A:200:LEU:HB2	19	1.76	0.48	1.79
(2,879)	1:A:234:ILE:HD12	1:A:200:LEU:HB2	19	1.76	0.48	1.79
(2,879)	1:A:234:ILE:HD13	1:A:200:LEU:HB2	19	1.76	0.48	1.79
(2,517)	1:A:200:LEU:H	1:A:196:LEU:HD21	19	1.28	0.66	1.45
(2,804)	1:A:93:ILE:HD11	1:A:105:VAL:HG21	19	0.8	0.29	0.77
(2,804)	1:A:93:ILE:HD11	1:A:105:VAL:HG22	19	0.8	0.29	0.77
(2,804)	1:A:93:ILE:HD11	1:A:105:VAL:HG23	19	0.8	0.29	0.77
(2,804)	1:A:93:ILE:HD12	1:A:105:VAL:HG21	19	0.8	0.29	0.77
(2,804)	1:A:93:ILE:HD12	1:A:105:VAL:HG22	19	0.8	0.29	0.77
(2,804)	1:A:93:ILE:HD12	1:A:105:VAL:HG23	19	0.8	0.29	0.77
(2,804)	1:A:93:ILE:HD13	1:A:105:VAL:HG21	19	0.8	0.29	0.77
(2,804)	1:A:93:ILE:HD13	1:A:105:VAL:HG22	19	0.8	0.29	0.77
(2,804)	1:A:93:ILE:HD13	1:A:105:VAL:HG23	19	0.8	0.29	0.77
(2,424)	1:A:169:ASP:H	1:A:166:LEU:HB3	19	0.76	0.26	0.79
(2,185)	1:A:94:VAL:H	1:A:92:ARG:H	19	0.66	0.26	0.64
(2,959)	1:A:75:TYR:H	1:A:76:SER:H	19	0.53	0.22	0.57
(2,964)	1:A:75:TYR:H	1:A:76:SER:H	19	0.53	0.22	0.57
(2,912)	1:A:70:PRO:HB3	1:A:76:SER:H	19	0.51	0.27	0.45
(2,912)	1:A:70:PRO:HB2	1:A:76:SER:H	19	0.51	0.27	0.45
(2,961)	1:A:75:TYR:HD1	1:A:76:SER:H	19	0.5	0.16	0.5
(2,961)	1:A:75:TYR:HD2	1:A:76:SER:H	19	0.5	0.16	0.5
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG21	19	0.49	0.13	0.48
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG22	19	0.49	0.13	0.48
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG23	19	0.49	0.13	0.48
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG11	19	0.49	0.13	0.48

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG12	19	0.49	0.13	0.48
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG13	19	0.49	0.13	0.48
(2,903)	1:A:67:CYS:H	1:A:66:ARG:HA	19	0.46	0.15	0.46
(2,626)	1:A:12:TRP:H	1:A:10:LEU:H	19	0.42	0.18	0.37
(2,980)	1:A:78:PHE:H	1:A:79:PRO:HD3	19	0.39	0.12	0.43
(2,980)	1:A:78:PHE:H	1:A:79:PRO:HD3	19	0.39	0.12	0.43
(2,315)	1:A:125:ARG:H	1:A:126:LYS:H	19	0.34	0.12	0.34
(2,836)	1:A:120:ILE:HD13	1:A:200:LEU:HD21	18	2.86	1.29	3.14
(2,833)	1:A:120:ILE:HD11	1:A:200:LEU:HD22	18	2.03	0.78	2.1
(2,833)	1:A:120:ILE:HD11	1:A:200:LEU:HD23	18	2.03	0.78	2.1
(2,967)	1:A:77:LEU:H	1:A:77:LEU:HG	18	1.65	0.16	1.65
(2,765)	1:A:22:PHE:H	1:A:19:LEU:HD21	18	1.38	0.63	1.52
(2,264)	1:A:113:LEU:H	1:A:196:LEU:HD21	18	0.99	0.5	0.95
(2,392)	1:A:157:ALA:H	1:A:68:GLY:H	18	0.78	0.44	0.62
(2,212)	1:A:120:ILE:HD11	1:A:237:LEU:H	18	0.73	0.26	0.72
(2,212)	1:A:120:ILE:HD12	1:A:237:LEU:H	18	0.73	0.26	0.72
(2,212)	1:A:120:ILE:HD13	1:A:237:LEU:H	18	0.73	0.26	0.72
(2,837)	1:A:120:ILE:HD13	1:A:200:LEU:HD22	17	2.09	0.46	2.19
(2,837)	1:A:120:ILE:HD13	1:A:200:LEU:HD23	17	2.09	0.46	2.19
(2,759)	1:A:54:LEU:HD21	1:A:59:ILE:HD11	17	1.72	1.24	1.35
(2,759)	1:A:54:LEU:HD21	1:A:59:ILE:HD12	17	1.72	1.24	1.35
(2,759)	1:A:54:LEU:HD21	1:A:59:ILE:HD13	17	1.72	1.24	1.35
(3,6)	1:A:78:PHE:H	4:A:305:PX4:C27	17	1.24	0.6	1.21
(3,6)	1:A:78:PHE:H	4:A:307:PX4:C27	17	1.24	0.6	1.21
(3,6)	1:A:78:PHE:H	4:A:309:PX4:C27	17	1.24	0.6	1.21
(3,6)	1:A:78:PHE:H	4:A:311:PX4:C27	17	1.24	0.6	1.21
(3,6)	1:A:78:PHE:H	4:A:313:PX4:C27	17	1.24	0.6	1.21
(3,6)	1:A:78:PHE:H	4:A:315:PX4:C27	17	1.24	0.6	1.21
(3,6)	1:A:78:PHE:H	4:A:317:PX4:C27	17	1.24	0.6	1.21
(3,6)	1:A:78:PHE:H	4:A:319:PX4:C27	17	1.24	0.6	1.21
(3,6)	1:A:78:PHE:H	4:A:321:PX4:C27	17	1.24	0.6	1.21
(3,6)	1:A:78:PHE:H	4:A:323:PX4:C27	17	1.24	0.6	1.21
(3,6)	1:A:78:PHE:H	4:A:325:PX4:C27	17	1.24	0.6	1.21
(3,6)	1:A:78:PHE:H	4:A:327:PX4:C27	17	1.24	0.6	1.21
(3,6)	1:A:78:PHE:H	4:A:329:PX4:C27	17	1.24	0.6	1.21
(3,6)	1:A:78:PHE:H	4:A:331:PX4:C27	17	1.24	0.6	1.21
(3,6)	1:A:78:PHE:H	4:A:333:PX4:C27	17	1.24	0.6	1.21
(3,6)	1:A:78:PHE:H	4:A:335:PX4:C27	17	1.24	0.6	1.21
(3,6)	1:A:78:PHE:H	4:A:337:PX4:C27	17	1.24	0.6	1.21
(3,6)	1:A:78:PHE:H	4:A:339:PX4:C27	17	1.24	0.6	1.21
(3,6)	1:A:78:PHE:H	4:A:341:PX4:C27	17	1.24	0.6	1.21
(3,6)	1:A:78:PHE:H	4:A:343:PX4:C27	17	1.24	0.6	1.21

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(3,6)	1:A:78:PHE:H	4:A:345:PX4:C27	17	1.24	0.6	1.21
(3,6)	1:A:78:PHE:H	4:A:347:PX4:C27	17	1.24	0.6	1.21
(3,6)	1:A:78:PHE:H	4:A:349:PX4:C27	17	1.24	0.6	1.21
(3,6)	1:A:78:PHE:H	4:A:351:PX4:C27	17	1.24	0.6	1.21
(3,6)	1:A:78:PHE:H	4:A:353:PX4:C27	17	1.24	0.6	1.21
(3,6)	1:A:78:PHE:H	4:A:355:PX4:C27	17	1.24	0.6	1.21
(3,6)	1:A:78:PHE:H	4:A:357:PX4:C27	17	1.24	0.6	1.21
(3,6)	1:A:78:PHE:H	4:A:359:PX4:C27	17	1.24	0.6	1.21
(3,6)	1:A:78:PHE:H	4:A:361:PX4:C27	17	1.24	0.6	1.21
(3,6)	1:A:78:PHE:H	4:A:363:PX4:C27	17	1.24	0.6	1.21
(3,6)	1:A:78:PHE:H	4:A:402:PX4:C27	17	1.24	0.6	1.21
(3,6)	1:A:78:PHE:H	4:A:404:PX4:C27	17	1.24	0.6	1.21
(3,6)	1:A:78:PHE:H	4:A:406:PX4:C27	17	1.24	0.6	1.21
(3,6)	1:A:78:PHE:H	4:A:408:PX4:C27	17	1.24	0.6	1.21
(3,6)	1:A:78:PHE:H	4:A:410:PX4:C27	17	1.24	0.6	1.21
(3,6)	1:A:78:PHE:H	4:A:412:PX4:C27	17	1.24	0.6	1.21
(3,6)	1:A:78:PHE:H	4:A:414:PX4:C27	17	1.24	0.6	1.21
(3,6)	1:A:78:PHE:H	4:A:416:PX4:C27	17	1.24	0.6	1.21
(3,6)	1:A:78:PHE:H	4:A:418:PX4:C27	17	1.24	0.6	1.21
(3,6)	1:A:78:PHE:H	4:A:420:PX4:C27	17	1.24	0.6	1.21
(3,6)	1:A:78:PHE:H	4:A:422:PX4:C27	17	1.24	0.6	1.21
(3,6)	1:A:78:PHE:H	4:A:424:PX4:C27	17	1.24	0.6	1.21
(3,6)	1:A:78:PHE:H	4:A:426:PX4:C27	17	1.24	0.6	1.21
(3,6)	1:A:78:PHE:H	4:A:428:PX4:C27	17	1.24	0.6	1.21
(3,6)	1:A:78:PHE:H	4:A:430:PX4:C27	17	1.24	0.6	1.21
(2,510)	1:A:200:LEU:HD21	1:A:199:SER:H	17	1.12	0.58	1.07
(2,466)	1:A:84:TRP:H	1:A:200:LEU:HD21	17	1.0	0.67	0.92
(2,975)	1:A:78:PHE:H	1:A:77:LEU:HD22	17	0.73	0.61	0.58
(2,975)	1:A:78:PHE:H	1:A:77:LEU:HD23	17	0.73	0.61	0.58
(2,976)	1:A:78:PHE:H	1:A:78:PHE:HD1	17	0.7	0.29	0.65
(2,976)	1:A:78:PHE:H	1:A:78:PHE:HD2	17	0.7	0.29	0.65
(2,507)	1:A:199:SER:H	1:A:202:MET:H	17	0.62	0.26	0.55
(2,426)	1:A:170:ALA:H	1:A:136:ILE:HD11	17	0.37	0.22	0.37
(2,426)	1:A:170:ALA:H	1:A:136:ILE:HD12	17	0.37	0.22	0.37
(2,426)	1:A:170:ALA:H	1:A:136:ILE:HD13	17	0.37	0.22	0.37
(2,228)	1:A:106:ASP:H	1:A:108:LEU:H	17	0.35	0.11	0.34
(2,927)	1:A:72:VAL:H	1:A:73:ALA:H	17	0.27	0.09	0.28
(2,927)	1:A:72:VAL:H	1:A:73:ALA:H	17	0.27	0.09	0.28
(2,834)	1:A:120:ILE:HD12	1:A:200:LEU:HD21	16	2.01	1.01	2.44
(2,985)	1:A:80:ASN:H	1:A:78:PHE:HD1	16	1.84	1.26	1.6
(2,835)	1:A:120:ILE:HD12	1:A:200:LEU:HD22	16	1.08	0.41	1.08
(2,835)	1:A:120:ILE:HD12	1:A:200:LEU:HD23	16	1.08	0.41	1.08

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,977)	1:A:78:PHE:H	1:A:78:PHE:HA	16	0.2	0.06	0.21
(2,757)	1:A:54:LEU:HD21	1:A:39:LEU:HD11	15	2.02	1.08	1.96
(2,757)	1:A:54:LEU:HD21	1:A:39:LEU:HD12	15	2.02	1.08	1.96
(2,757)	1:A:54:LEU:HD21	1:A:39:LEU:HD13	15	2.02	1.08	1.96
(2,379)	1:A:10:LEU:H	1:A:10:LEU:HD21	15	0.75	0.42	0.7
(2,970)	1:A:77:LEU:HG	1:A:78:PHE:H	15	0.7	0.3	0.59
(2,627)	1:A:13:GLU:H	1:A:10:LEU:H	15	0.6	0.18	0.65
(2,75)	1:A:55:ASN:H	1:A:59:ILE:H	15	0.56	0.34	0.53
(2,951)	1:A:74:GLU:H	1:A:76:SER:H	15	0.51	0.23	0.49
(2,659)	1:A:42:MET:H	1:A:19:LEU:HD11	15	0.42	0.2	0.44
(2,659)	1:A:42:MET:H	1:A:19:LEU:HD12	15	0.42	0.2	0.44
(2,659)	1:A:42:MET:H	1:A:19:LEU:HD13	15	0.42	0.2	0.44
(2,809)	1:A:136:ILE:H	1:A:94:VAL:HG11	15	0.34	0.22	0.27
(2,809)	1:A:136:ILE:H	1:A:94:VAL:HG12	15	0.34	0.22	0.27
(2,809)	1:A:136:ILE:H	1:A:94:VAL:HG13	15	0.34	0.22	0.27
(2,423)	1:A:169:ASP:H	1:A:134:ILE:HD11	15	0.3	0.18	0.25
(2,423)	1:A:169:ASP:H	1:A:134:ILE:HD12	15	0.3	0.18	0.25
(2,423)	1:A:169:ASP:H	1:A:134:ILE:HD13	15	0.3	0.18	0.25
(2,113)	1:A:25:TYR:H	1:A:26:ASP:H	15	0.24	0.09	0.21
(2,656)	1:A:39:LEU:H	1:A:19:LEU:HD21	14	2.95	1.41	2.82
(2,979)	1:A:78:PHE:H	1:A:78:PHE:HD1	14	0.67	0.32	0.64
(2,898)	1:A:66:ARG:H	1:A:63:GLN:HB3	14	0.54	0.26	0.53
(2,898)	1:A:66:ARG:H	1:A:63:GLN:HB2	14	0.54	0.26	0.53
(2,786)	1:A:24:LEU:H	1:A:24:LEU:HD21	14	0.49	0.26	0.63
(2,917)	1:A:71:ASP:H	1:A:72:VAL:HB	14	0.39	0.18	0.34
(2,226)	1:A:104:THR:H	1:A:106:ASP:H	14	0.3	0.19	0.21
(2,810)	1:A:93:ILE:H	1:A:94:VAL:HG11	14	0.27	0.09	0.27
(2,810)	1:A:93:ILE:H	1:A:94:VAL:HG12	14	0.27	0.09	0.27
(2,810)	1:A:93:ILE:H	1:A:94:VAL:HG13	14	0.27	0.09	0.27
(2,969)	1:A:77:LEU:H	1:A:78:PHE:H	14	0.24	0.1	0.2
(2,921)	1:A:72:VAL:H	1:A:72:VAL:HA	14	0.2	0.04	0.2
(2,968)	1:A:77:LEU:H	1:A:77:LEU:HA	14	0.2	0.06	0.2
(2,865)	1:A:186:ILE:HD11	1:A:186:ILE:HG13	14	0.14	0.03	0.14
(2,865)	1:A:186:ILE:HD12	1:A:186:ILE:HG13	14	0.14	0.03	0.14
(2,865)	1:A:186:ILE:HD13	1:A:186:ILE:HG13	14	0.14	0.03	0.14
(2,865)	1:A:186:ILE:HD11	1:A:186:ILE:HG12	14	0.14	0.03	0.14
(2,865)	1:A:186:ILE:HD12	1:A:186:ILE:HG12	14	0.14	0.03	0.14
(2,865)	1:A:186:ILE:HD13	1:A:186:ILE:HG12	14	0.14	0.03	0.14
(2,811)	1:A:103:ILE:HD11	1:A:103:ILE:HG13	14	0.14	0.02	0.13
(2,811)	1:A:103:ILE:HD12	1:A:103:ILE:HG13	14	0.14	0.02	0.13
(2,811)	1:A:103:ILE:HD13	1:A:103:ILE:HG13	14	0.14	0.02	0.13
(2,811)	1:A:103:ILE:HD11	1:A:103:ILE:HG12	14	0.14	0.02	0.13

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,811)	1:A:103:ILE:HD12	1:A:103:ILE:HG12	14	0.14	0.02	0.13
(2,811)	1:A:103:ILE:HD13	1:A:103:ILE:HG12	14	0.14	0.02	0.13
(2,727)	1:A:211:VAL:HG11	1:A:226:LEU:HD21	13	1.35	0.84	1.36
(2,731)	1:A:211:VAL:HG13	1:A:226:LEU:HD21	13	1.31	1.03	1.01
(2,758)	1:A:54:LEU:HD22	1:A:39:LEU:HD11	13	0.94	0.44	1.07
(2,758)	1:A:54:LEU:HD22	1:A:39:LEU:HD12	13	0.94	0.44	1.07
(2,758)	1:A:54:LEU:HD22	1:A:39:LEU:HD13	13	0.94	0.44	1.07
(2,758)	1:A:54:LEU:HD23	1:A:39:LEU:HD11	13	0.94	0.44	1.07
(2,758)	1:A:54:LEU:HD23	1:A:39:LEU:HD12	13	0.94	0.44	1.07
(2,758)	1:A:54:LEU:HD23	1:A:39:LEU:HD13	13	0.94	0.44	1.07
(2,755)	1:A:54:LEU:HD21	1:A:58:VAL:HG11	13	0.8	0.55	0.8
(2,755)	1:A:54:LEU:HD21	1:A:58:VAL:HG12	13	0.8	0.55	0.8
(2,755)	1:A:54:LEU:HD21	1:A:58:VAL:HG13	13	0.8	0.55	0.8
(2,890)	1:A:63:GLN:H	1:A:63:GLN:HG3	13	0.58	0.12	0.61
(2,890)	1:A:63:GLN:H	1:A:63:GLN:HG3	13	0.58	0.12	0.61
(2,608)	1:A:238:TYR:H	1:A:120:ILE:HD11	13	0.47	0.23	0.42
(2,608)	1:A:238:TYR:H	1:A:120:ILE:HD12	13	0.47	0.23	0.42
(2,608)	1:A:238:TYR:H	1:A:120:ILE:HD13	13	0.47	0.23	0.42
(2,511)	1:A:200:LEU:HD22	1:A:199:SER:H	13	0.37	0.19	0.34
(2,511)	1:A:200:LEU:HD23	1:A:199:SER:H	13	0.37	0.19	0.34
(2,947)	1:A:74:GLU:HB3	1:A:75:TYR:H	13	0.32	0.14	0.29
(2,947)	1:A:74:GLU:HB3	1:A:75:TYR:H	13	0.32	0.14	0.29
(2,926)	1:A:72:VAL:HB	1:A:73:ALA:H	13	0.21	0.06	0.22
(2,909)	1:A:69:VAL:H	1:A:69:VAL:HA	13	0.16	0.04	0.14
(2,988)	1:A:129:TRP:HE1	4:A:305:PX4:C2	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:307:PX4:C2	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:309:PX4:C2	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:311:PX4:C2	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:313:PX4:C2	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:315:PX4:C2	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:317:PX4:C2	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:319:PX4:C2	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:321:PX4:C2	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:323:PX4:C2	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:325:PX4:C2	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:327:PX4:C2	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:329:PX4:C2	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:331:PX4:C2	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:333:PX4:C2	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:335:PX4:C2	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:337:PX4:C2	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:339:PX4:C2	12	1.6	1.23	1.34

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,988)	1:A:129:TRP:HE1	4:A:341:PX4:C2	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:343:PX4:C2	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:345:PX4:C2	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:347:PX4:C2	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:349:PX4:C2	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:351:PX4:C2	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:353:PX4:C2	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:355:PX4:C2	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:357:PX4:C2	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:359:PX4:C2	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:361:PX4:C2	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:363:PX4:C2	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:402:PX4:C2	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:404:PX4:C2	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:406:PX4:C2	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:408:PX4:C2	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:410:PX4:C2	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:412:PX4:C2	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:414:PX4:C2	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:416:PX4:C2	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:418:PX4:C2	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:420:PX4:C2	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:422:PX4:C2	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:424:PX4:C2	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:426:PX4:C2	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:428:PX4:C2	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:430:PX4:C2	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:305:PX4:C1	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:307:PX4:C1	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:309:PX4:C1	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:311:PX4:C1	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:313:PX4:C1	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:315:PX4:C1	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:317:PX4:C1	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:319:PX4:C1	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:321:PX4:C1	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:323:PX4:C1	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:325:PX4:C1	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:327:PX4:C1	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:329:PX4:C1	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:331:PX4:C1	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:333:PX4:C1	12	1.6	1.23	1.34

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,988)	1:A:129:TRP:HE1	4:A:335:PX4:C1	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:337:PX4:C1	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:339:PX4:C1	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:341:PX4:C1	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:343:PX4:C1	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:345:PX4:C1	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:347:PX4:C1	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:349:PX4:C1	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:351:PX4:C1	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:353:PX4:C1	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:355:PX4:C1	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:357:PX4:C1	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:359:PX4:C1	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:361:PX4:C1	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:363:PX4:C1	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:402:PX4:C1	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:404:PX4:C1	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:406:PX4:C1	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:408:PX4:C1	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:410:PX4:C1	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:412:PX4:C1	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:414:PX4:C1	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:416:PX4:C1	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:418:PX4:C1	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:420:PX4:C1	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:422:PX4:C1	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:424:PX4:C1	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:426:PX4:C1	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:428:PX4:C1	12	1.6	1.23	1.34
(2,988)	1:A:129:TRP:HE1	4:A:430:PX4:C1	12	1.6	1.23	1.34
(2,760)	1:A:54:LEU:HD22	1:A:59:ILE:HD11	12	1.49	0.47	1.56
(2,760)	1:A:54:LEU:HD22	1:A:59:ILE:HD12	12	1.49	0.47	1.56
(2,760)	1:A:54:LEU:HD22	1:A:59:ILE:HD13	12	1.49	0.47	1.56
(2,760)	1:A:54:LEU:HD23	1:A:59:ILE:HD11	12	1.49	0.47	1.56
(2,760)	1:A:54:LEU:HD23	1:A:59:ILE:HD12	12	1.49	0.47	1.56
(2,760)	1:A:54:LEU:HD23	1:A:59:ILE:HD13	12	1.49	0.47	1.56
(2,729)	1:A:211:VAL:HG12	1:A:226:LEU:HD21	12	1.2	0.86	1.2
(2,867)	1:A:186:ILE:HD11	1:A:156:LEU:HD21	12	1.05	0.75	0.97
(2,414)	1:A:167:GLY:H	1:A:166:LEU:HD21	12	0.63	0.28	0.63
(2,621)	1:A:200:LEU:HD21	1:A:201:GLY:H	12	0.42	0.17	0.38
(2,207)	1:A:98:ARG:H	1:A:100:LEU:H	12	0.38	0.09	0.42
(2,920)	1:A:72:VAL:H	1:A:71:ASP:H	12	0.33	0.24	0.26

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,920)	1:A:72:VAL:H	1:A:71:ASP:H	12	0.33	0.24	0.26
(2,74)	1:A:55:ASN:H	1:A:55:ASN:HD21	12	0.31	0.14	0.28
(2,538)	1:A:205:SER:H	1:A:213:TYR:H	12	0.28	0.12	0.28
(2,673)	1:A:77:LEU:H	1:A:78:PHE:H	12	0.23	0.1	0.2
(2,830)	1:A:120:ILE:HD11	1:A:120:ILE:HG13	12	0.14	0.02	0.14
(2,830)	1:A:120:ILE:HD12	1:A:120:ILE:HG13	12	0.14	0.02	0.14
(2,830)	1:A:120:ILE:HD13	1:A:120:ILE:HG13	12	0.14	0.02	0.14
(2,830)	1:A:120:ILE:HD11	1:A:120:ILE:HG12	12	0.14	0.02	0.14
(2,830)	1:A:120:ILE:HD12	1:A:120:ILE:HG12	12	0.14	0.02	0.14
(2,830)	1:A:120:ILE:HD13	1:A:120:ILE:HG12	12	0.14	0.02	0.14
(2,657)	1:A:39:LEU:H	1:A:19:LEU:HD22	11	2.39	0.94	1.99
(2,657)	1:A:39:LEU:H	1:A:19:LEU:HD23	11	2.39	0.94	1.99
(3,36)	1:A:129:TRP:HE1	4:A:305:PX4:N1	11	2.3	0.92	2.04
(3,36)	1:A:129:TRP:HE1	4:A:307:PX4:N1	11	2.3	0.92	2.04
(3,36)	1:A:129:TRP:HE1	4:A:309:PX4:N1	11	2.3	0.92	2.04
(3,36)	1:A:129:TRP:HE1	4:A:311:PX4:N1	11	2.3	0.92	2.04
(3,36)	1:A:129:TRP:HE1	4:A:313:PX4:N1	11	2.3	0.92	2.04
(3,36)	1:A:129:TRP:HE1	4:A:315:PX4:N1	11	2.3	0.92	2.04
(3,36)	1:A:129:TRP:HE1	4:A:317:PX4:N1	11	2.3	0.92	2.04
(3,36)	1:A:129:TRP:HE1	4:A:319:PX4:N1	11	2.3	0.92	2.04
(3,36)	1:A:129:TRP:HE1	4:A:321:PX4:N1	11	2.3	0.92	2.04
(3,36)	1:A:129:TRP:HE1	4:A:323:PX4:N1	11	2.3	0.92	2.04
(3,36)	1:A:129:TRP:HE1	4:A:325:PX4:N1	11	2.3	0.92	2.04
(3,36)	1:A:129:TRP:HE1	4:A:327:PX4:N1	11	2.3	0.92	2.04
(3,36)	1:A:129:TRP:HE1	4:A:329:PX4:N1	11	2.3	0.92	2.04
(3,36)	1:A:129:TRP:HE1	4:A:331:PX4:N1	11	2.3	0.92	2.04
(3,36)	1:A:129:TRP:HE1	4:A:333:PX4:N1	11	2.3	0.92	2.04
(3,36)	1:A:129:TRP:HE1	4:A:335:PX4:N1	11	2.3	0.92	2.04
(3,36)	1:A:129:TRP:HE1	4:A:337:PX4:N1	11	2.3	0.92	2.04
(3,36)	1:A:129:TRP:HE1	4:A:339:PX4:N1	11	2.3	0.92	2.04
(3,36)	1:A:129:TRP:HE1	4:A:341:PX4:N1	11	2.3	0.92	2.04
(3,36)	1:A:129:TRP:HE1	4:A:343:PX4:N1	11	2.3	0.92	2.04
(3,36)	1:A:129:TRP:HE1	4:A:345:PX4:N1	11	2.3	0.92	2.04
(3,36)	1:A:129:TRP:HE1	4:A:347:PX4:N1	11	2.3	0.92	2.04
(3,36)	1:A:129:TRP:HE1	4:A:349:PX4:N1	11	2.3	0.92	2.04
(3,36)	1:A:129:TRP:HE1	4:A:351:PX4:N1	11	2.3	0.92	2.04
(3,36)	1:A:129:TRP:HE1	4:A:353:PX4:N1	11	2.3	0.92	2.04
(3,36)	1:A:129:TRP:HE1	4:A:355:PX4:N1	11	2.3	0.92	2.04
(3,36)	1:A:129:TRP:HE1	4:A:357:PX4:N1	11	2.3	0.92	2.04
(3,36)	1:A:129:TRP:HE1	4:A:359:PX4:N1	11	2.3	0.92	2.04
(3,36)	1:A:129:TRP:HE1	4:A:361:PX4:N1	11	2.3	0.92	2.04
(3,36)	1:A:129:TRP:HE1	4:A:363:PX4:N1	11	2.3	0.92	2.04

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(3,36)	1:A:129:TRP:HE1	4:A:402:PX4:N1	11	2.3	0.92	2.04
(3,36)	1:A:129:TRP:HE1	4:A:404:PX4:N1	11	2.3	0.92	2.04
(3,36)	1:A:129:TRP:HE1	4:A:406:PX4:N1	11	2.3	0.92	2.04
(3,36)	1:A:129:TRP:HE1	4:A:408:PX4:N1	11	2.3	0.92	2.04
(3,36)	1:A:129:TRP:HE1	4:A:410:PX4:N1	11	2.3	0.92	2.04
(3,36)	1:A:129:TRP:HE1	4:A:412:PX4:N1	11	2.3	0.92	2.04
(3,36)	1:A:129:TRP:HE1	4:A:414:PX4:N1	11	2.3	0.92	2.04
(3,36)	1:A:129:TRP:HE1	4:A:416:PX4:N1	11	2.3	0.92	2.04
(3,36)	1:A:129:TRP:HE1	4:A:418:PX4:N1	11	2.3	0.92	2.04
(3,36)	1:A:129:TRP:HE1	4:A:420:PX4:N1	11	2.3	0.92	2.04
(3,36)	1:A:129:TRP:HE1	4:A:422:PX4:N1	11	2.3	0.92	2.04
(3,36)	1:A:129:TRP:HE1	4:A:424:PX4:N1	11	2.3	0.92	2.04
(3,36)	1:A:129:TRP:HE1	4:A:426:PX4:N1	11	2.3	0.92	2.04
(3,36)	1:A:129:TRP:HE1	4:A:428:PX4:N1	11	2.3	0.92	2.04
(3,36)	1:A:129:TRP:HE1	4:A:430:PX4:N1	11	2.3	0.92	2.04
(2,871)	1:A:186:ILE:HD13	1:A:156:LEU:HD21	11	1.38	0.92	1.52
(2,766)	1:A:22:PHE:H	1:A:19:LEU:HD22	11	0.85	0.38	0.95
(2,766)	1:A:22:PHE:H	1:A:19:LEU:HD23	11	0.85	0.38	0.95
(2,518)	1:A:200:LEU:H	1:A:196:LEU:HD22	11	0.64	0.38	0.5
(2,518)	1:A:200:LEU:H	1:A:196:LEU:HD23	11	0.64	0.38	0.5
(2,973)	1:A:78:PHE:H	1:A:77:LEU:HD11	11	0.55	0.25	0.61
(2,973)	1:A:78:PHE:H	1:A:77:LEU:HD12	11	0.55	0.25	0.61
(2,973)	1:A:78:PHE:H	1:A:77:LEU:HD13	11	0.55	0.25	0.61
(2,543)	1:A:210:ALA:H	1:A:213:TYR:H	11	0.48	0.24	0.48
(2,570)	1:A:226:LEU:H	1:A:226:LEU:HD21	11	0.35	0.19	0.38
(2,103)	1:A:39:LEU:H	1:A:37:ALA:H	11	0.23	0.05	0.21
(2,62)	1:A:50:ILE:HG12	1:A:50:ILE:H	11	0.21	0.07	0.2
(2,916)	1:A:71:ASP:H	1:A:72:VAL:HA	11	0.18	0.06	0.15
(2,773)	1:A:61:ILE:HD11	1:A:48:LEU:HD21	10	1.31	0.85	1.2
(2,748)	1:A:89:VAL:HG12	1:A:122:LEU:HD21	10	0.58	0.57	0.4
(2,369)	1:A:143:HIS:H	1:A:145:ASP:H	10	0.44	0.24	0.35
(2,680)	1:A:158:HIS:H	1:A:172:PHE:H	10	0.23	0.07	0.23
(2,803)	1:A:93:ILE:HD11	1:A:93:ILE:HG13	10	0.15	0.03	0.14
(2,803)	1:A:93:ILE:HD12	1:A:93:ILE:HG13	10	0.15	0.03	0.14
(2,803)	1:A:93:ILE:HD13	1:A:93:ILE:HG13	10	0.15	0.03	0.14
(2,803)	1:A:93:ILE:HD11	1:A:93:ILE:HG12	10	0.15	0.03	0.14
(2,803)	1:A:93:ILE:HD12	1:A:93:ILE:HG12	10	0.15	0.03	0.14
(2,803)	1:A:93:ILE:HD13	1:A:93:ILE:HG12	10	0.15	0.03	0.14
(2,982)	1:A:78:PHE:HD1	1:A:80:ASN:H	9	1.84	0.73	1.96
(2,257)	1:A:112:ALA:H	1:A:189:LEU:HD21	9	1.07	0.68	1.12
(2,732)	1:A:211:VAL:HG13	1:A:226:LEU:HD22	9	0.91	0.6	0.96
(2,732)	1:A:211:VAL:HG13	1:A:226:LEU:HD23	9	0.91	0.6	0.96

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,10)	1:A:92:ARG:H	1:A:93:ILE:HG13	9	0.46	0.24	0.51
(2,10)	1:A:92:ARG:H	1:A:93:ILE:HG12	9	0.46	0.24	0.51
(2,162)	1:A:125:ARG:H	1:A:89:VAL:H	9	0.4	0.22	0.34
(2,316)	1:A:125:ARG:H	1:A:89:VAL:H	9	0.4	0.22	0.34
(2,624)	1:A:11:GLN:H	1:A:8:SER:H	9	0.36	0.11	0.38
(2,693)	1:A:11:GLN:H	1:A:8:SER:H	9	0.36	0.11	0.38
(2,915)	1:A:71:ASP:H	1:A:72:VAL:HG21	9	0.28	0.17	0.2
(2,915)	1:A:71:ASP:H	1:A:72:VAL:HG22	9	0.28	0.17	0.2
(2,915)	1:A:71:ASP:H	1:A:72:VAL:HG23	9	0.28	0.17	0.2
(2,63)	1:A:52:GLY:H	1:A:51:THR:H	9	0.23	0.15	0.14
(2,8)	1:A:135:MET:H	1:A:92:ARG:H	9	0.22	0.08	0.2
(2,904)	1:A:67:CYS:H	1:A:67:CYS:HA	9	0.18	0.06	0.16
(2,324)	1:A:128:VAL:H	1:A:129:TRP:H	9	0.16	0.03	0.16
(2,326)	1:A:128:VAL:H	1:A:129:TRP:H	9	0.16	0.03	0.16
(2,935)	1:A:73:ALA:H	1:A:73:ALA:HA	9	0.14	0.03	0.13
(2,869)	1:A:186:ILE:HD12	1:A:156:LEU:HD21	8	1.03	0.41	1.14
(2,775)	1:A:61:ILE:HD12	1:A:48:LEU:HD21	8	1.03	0.56	0.88
(2,746)	1:A:89:VAL:HG11	1:A:122:LEU:HD21	8	0.85	0.51	0.83
(2,661)	1:A:4:ALA:H	1:A:59:ILE:HG21	8	0.6	0.28	0.49
(2,661)	1:A:4:ALA:H	1:A:59:ILE:HG22	8	0.6	0.28	0.49
(2,661)	1:A:4:ALA:H	1:A:59:ILE:HG23	8	0.6	0.28	0.49
(2,504)	1:A:198:HIS:H	1:A:202:MET:H	8	0.38	0.2	0.32
(2,741)	1:A:114:ASN:H	1:A:113:LEU:HD21	8	0.37	0.08	0.36
(2,303)	1:A:122:LEU:H	1:A:120:ILE:HG13	8	0.31	0.09	0.28
(2,303)	1:A:122:LEU:H	1:A:120:ILE:HG12	8	0.31	0.09	0.28
(2,60)	1:A:50:ILE:H	1:A:50:ILE:HD11	8	0.3	0.1	0.32
(2,60)	1:A:50:ILE:H	1:A:50:ILE:HD12	8	0.3	0.1	0.32
(2,60)	1:A:50:ILE:H	1:A:50:ILE:HD13	8	0.3	0.1	0.32
(2,304)	1:A:123:HIS:H	1:A:122:LEU:HD11	8	0.29	0.16	0.26
(2,304)	1:A:123:HIS:H	1:A:122:LEU:HD12	8	0.29	0.16	0.26
(2,304)	1:A:123:HIS:H	1:A:122:LEU:HD13	8	0.29	0.16	0.26
(2,839)	1:A:123:HIS:H	1:A:122:LEU:HD11	8	0.29	0.16	0.26
(2,839)	1:A:123:HIS:H	1:A:122:LEU:HD12	8	0.29	0.16	0.26
(2,839)	1:A:123:HIS:H	1:A:122:LEU:HD13	8	0.29	0.16	0.26
(2,984)	1:A:78:PHE:HD1	1:A:80:ASN:HD21	7	1.58	0.78	1.79
(2,984)	1:A:78:PHE:HD1	1:A:80:ASN:HD22	7	1.58	0.78	1.79
(2,984)	1:A:78:PHE:HD1	1:A:80:ASN:HD21	7	1.58	0.78	1.79
(2,984)	1:A:78:PHE:HD1	1:A:80:ASN:HD22	7	1.58	0.78	1.79
(2,777)	1:A:61:ILE:HD13	1:A:48:LEU:HD21	7	0.99	0.48	1.03
(2,931)	1:A:72:VAL:H	1:A:75:TYR:HB3	7	0.57	0.42	0.37
(2,931)	1:A:72:VAL:H	1:A:75:TYR:HB3	7	0.57	0.42	0.37
(2,467)	1:A:84:TRP:H	1:A:200:LEU:HD22	7	0.46	0.28	0.3

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,467)	1:A:84:TRP:H	1:A:200:LEU:HD23	7	0.46	0.28	0.3
(2,501)	1:A:198:HIS:H	1:A:195:ALA:H	7	0.24	0.1	0.21
(2,368)	1:A:151:GLY:H	1:A:150:ASP:H	7	0.24	0.05	0.25
(2,381)	1:A:151:GLY:H	1:A:150:ASP:H	7	0.24	0.05	0.25
(2,454)	1:A:178:TRP:HE1	1:A:178:TRP:H	7	0.23	0.06	0.23
(2,239)	1:A:108:LEU:H	1:A:108:LEU:HD21	7	0.22	0.13	0.17
(2,547)	1:A:211:VAL:H	1:A:211:VAL:HG11	7	0.16	0.05	0.15
(2,547)	1:A:211:VAL:H	1:A:211:VAL:HG12	7	0.16	0.05	0.15
(2,547)	1:A:211:VAL:H	1:A:211:VAL:HG13	7	0.16	0.05	0.15
(2,547)	1:A:211:VAL:H	1:A:211:VAL:HG21	7	0.16	0.05	0.15
(2,547)	1:A:211:VAL:H	1:A:211:VAL:HG22	7	0.16	0.05	0.15
(2,547)	1:A:211:VAL:H	1:A:211:VAL:HG23	7	0.16	0.05	0.15
(2,728)	1:A:211:VAL:HG11	1:A:226:LEU:HD22	6	1.23	0.54	1.17
(2,728)	1:A:211:VAL:HG11	1:A:226:LEU:HD23	6	1.23	0.54	1.17
(2,861)	1:A:186:ILE:HD13	1:A:156:LEU:HD21	6	1.17	0.4	1.15
(2,321)	1:A:128:VAL:HG11	1:A:126:LYS:H	6	1.16	0.9	1.14
(2,321)	1:A:128:VAL:HG12	1:A:126:LYS:H	6	1.16	0.9	1.14
(2,321)	1:A:128:VAL:HG13	1:A:126:LYS:H	6	1.16	0.9	1.14
(2,750)	1:A:89:VAL:HG13	1:A:122:LEU:HD21	6	0.76	0.35	0.72
(2,857)	1:A:186:ILE:HD11	1:A:156:LEU:HD21	6	0.61	0.65	0.34
(2,717)	1:A:54:LEU:HD11	1:A:39:LEU:HD11	6	0.57	0.3	0.64
(2,717)	1:A:54:LEU:HD11	1:A:39:LEU:HD12	6	0.57	0.3	0.64
(2,717)	1:A:54:LEU:HD11	1:A:39:LEU:HD13	6	0.57	0.3	0.64
(2,717)	1:A:54:LEU:HD12	1:A:39:LEU:HD11	6	0.57	0.3	0.64
(2,717)	1:A:54:LEU:HD12	1:A:39:LEU:HD12	6	0.57	0.3	0.64
(2,717)	1:A:54:LEU:HD12	1:A:39:LEU:HD13	6	0.57	0.3	0.64
(2,717)	1:A:54:LEU:HD13	1:A:39:LEU:HD11	6	0.57	0.3	0.64
(2,717)	1:A:54:LEU:HD13	1:A:39:LEU:HD12	6	0.57	0.3	0.64
(2,717)	1:A:54:LEU:HD13	1:A:39:LEU:HD13	6	0.57	0.3	0.64
(2,907)	1:A:68:GLY:H	1:A:69:VAL:H	6	0.36	0.24	0.29
(2,317)	1:A:125:ARG:H	1:A:91:TYR:H	6	0.32	0.16	0.3
(2,442)	1:A:175:ASP:H	1:A:178:TRP:HE1	6	0.31	0.13	0.34
(2,453)	1:A:178:TRP:HE1	1:A:175:ASP:H	6	0.31	0.13	0.34
(2,120)	1:A:66:ARG:H	1:A:156:LEU:H	6	0.31	0.11	0.3
(2,388)	1:A:66:ARG:H	1:A:156:LEU:H	6	0.31	0.11	0.3
(2,14)	1:A:159:ALA:H	1:A:171:HIS:H	6	0.19	0.04	0.2
(2,949)	1:A:74:GLU:H	1:A:75:TYR:H	6	0.18	0.05	0.18
(2,683)	1:A:179:THR:HG21	1:A:185:GLY:H	6	0.18	0.03	0.17
(2,683)	1:A:179:THR:HG22	1:A:185:GLY:H	6	0.18	0.03	0.17
(2,683)	1:A:179:THR:HG23	1:A:185:GLY:H	6	0.18	0.03	0.17
(2,385)	1:A:157:ALA:H	1:A:156:LEU:H	6	0.18	0.04	0.18
(2,391)	1:A:157:ALA:H	1:A:156:LEU:H	6	0.18	0.04	0.18

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,872)	1:A:186:ILE:HD13	1:A:156:LEU:HD22	5	1.31	0.63	0.9
(2,872)	1:A:186:ILE:HD13	1:A:156:LEU:HD23	5	1.31	0.63	0.9
(2,671)	1:A:66:ARG:H	1:A:156:LEU:HD21	5	0.92	0.75	0.55
(2,868)	1:A:186:ILE:HD11	1:A:156:LEU:HD22	5	0.85	1.06	0.33
(2,868)	1:A:186:ILE:HD11	1:A:156:LEU:HD23	5	0.85	1.06	0.33
(2,953)	1:A:74:GLU:HB3	1:A:76:SER:H	5	0.28	0.07	0.31
(2,953)	1:A:74:GLU:HB3	1:A:76:SER:H	5	0.28	0.07	0.31
(2,275)	1:A:116:TRP:HE1	1:A:196:LEU:H	5	0.28	0.09	0.31
(2,489)	1:A:116:TRP:HE1	1:A:196:LEU:H	5	0.28	0.09	0.31
(2,13)	1:A:135:MET:H	1:A:170:ALA:H	5	0.23	0.18	0.14
(2,744)	1:A:134:ILE:HD11	1:A:89:VAL:HG11	5	0.22	0.07	0.19
(2,744)	1:A:134:ILE:HD11	1:A:89:VAL:HG12	5	0.22	0.07	0.19
(2,744)	1:A:134:ILE:HD11	1:A:89:VAL:HG13	5	0.22	0.07	0.19
(2,744)	1:A:134:ILE:HD12	1:A:89:VAL:HG11	5	0.22	0.07	0.19
(2,744)	1:A:134:ILE:HD12	1:A:89:VAL:HG12	5	0.22	0.07	0.19
(2,744)	1:A:134:ILE:HD12	1:A:89:VAL:HG13	5	0.22	0.07	0.19
(2,744)	1:A:134:ILE:HD13	1:A:89:VAL:HG11	5	0.22	0.07	0.19
(2,744)	1:A:134:ILE:HD13	1:A:89:VAL:HG12	5	0.22	0.07	0.19
(2,744)	1:A:134:ILE:HD13	1:A:89:VAL:HG13	5	0.22	0.07	0.19
(2,885)	1:A:134:ILE:HD11	1:A:89:VAL:HG11	5	0.22	0.07	0.19
(2,885)	1:A:134:ILE:HD11	1:A:89:VAL:HG12	5	0.22	0.07	0.19
(2,885)	1:A:134:ILE:HD11	1:A:89:VAL:HG13	5	0.22	0.07	0.19
(2,885)	1:A:134:ILE:HD12	1:A:89:VAL:HG11	5	0.22	0.07	0.19
(2,885)	1:A:134:ILE:HD12	1:A:89:VAL:HG12	5	0.22	0.07	0.19
(2,885)	1:A:134:ILE:HD12	1:A:89:VAL:HG13	5	0.22	0.07	0.19
(2,885)	1:A:134:ILE:HD13	1:A:89:VAL:HG11	5	0.22	0.07	0.19
(2,885)	1:A:134:ILE:HD13	1:A:89:VAL:HG12	5	0.22	0.07	0.19
(2,885)	1:A:134:ILE:HD13	1:A:89:VAL:HG13	5	0.22	0.07	0.19
(2,82)	1:A:58:VAL:H	1:A:48:LEU:HD21	4	2.45	0.41	2.28
(2,842)	1:A:200:LEU:HD21	1:A:122:LEU:HD21	4	1.27	0.71	1.0
(2,730)	1:A:211:VAL:HG12	1:A:226:LEU:HD22	4	1.18	0.61	1.1
(2,730)	1:A:211:VAL:HG12	1:A:226:LEU:HD23	4	1.18	0.61	1.1
(2,756)	1:A:54:LEU:HD22	1:A:58:VAL:HG11	4	0.71	0.34	0.76
(2,756)	1:A:54:LEU:HD22	1:A:58:VAL:HG12	4	0.71	0.34	0.76
(2,756)	1:A:54:LEU:HD22	1:A:58:VAL:HG13	4	0.71	0.34	0.76
(2,756)	1:A:54:LEU:HD23	1:A:58:VAL:HG11	4	0.71	0.34	0.76
(2,756)	1:A:54:LEU:HD23	1:A:58:VAL:HG12	4	0.71	0.34	0.76
(2,756)	1:A:54:LEU:HD23	1:A:58:VAL:HG13	4	0.71	0.34	0.76
(2,870)	1:A:186:ILE:HD12	1:A:156:LEU:HD22	4	0.68	0.56	0.52
(2,870)	1:A:186:ILE:HD12	1:A:156:LEU:HD23	4	0.68	0.56	0.52
(2,733)	1:A:196:LEU:HD21	1:A:113:LEU:HD21	4	0.56	0.38	0.38
(2,125)	1:A:157:ALA:H	1:A:68:GLY:H	4	0.52	0.26	0.5

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,866)	1:A:186:ILE:HD11	1:A:156:LEU:HD11	4	0.4	0.31	0.29
(2,866)	1:A:186:ILE:HD11	1:A:156:LEU:HD12	4	0.4	0.31	0.29
(2,866)	1:A:186:ILE:HD11	1:A:156:LEU:HD13	4	0.4	0.31	0.29
(2,866)	1:A:186:ILE:HD12	1:A:156:LEU:HD11	4	0.4	0.31	0.29
(2,866)	1:A:186:ILE:HD12	1:A:156:LEU:HD12	4	0.4	0.31	0.29
(2,866)	1:A:186:ILE:HD12	1:A:156:LEU:HD13	4	0.4	0.31	0.29
(2,866)	1:A:186:ILE:HD13	1:A:156:LEU:HD11	4	0.4	0.31	0.29
(2,866)	1:A:186:ILE:HD13	1:A:156:LEU:HD12	4	0.4	0.31	0.29
(2,866)	1:A:186:ILE:HD13	1:A:156:LEU:HD13	4	0.4	0.31	0.29
(2,265)	1:A:113:LEU:H	1:A:196:LEU:HD22	4	0.38	0.12	0.38
(2,265)	1:A:113:LEU:H	1:A:196:LEU:HD23	4	0.38	0.12	0.38
(2,305)	1:A:123:HIS:H	1:A:122:LEU:HD21	4	0.34	0.22	0.28
(2,859)	1:A:186:ILE:HD12	1:A:156:LEU:HD21	4	0.34	0.14	0.31
(2,445)	1:A:178:TRP:HE1	1:A:176:GLU:H	4	0.32	0.15	0.28
(2,456)	1:A:178:TRP:HE1	1:A:176:GLU:H	4	0.32	0.15	0.28
(2,380)	1:A:10:LEU:H	1:A:10:LEU:HD22	4	0.31	0.09	0.34
(2,380)	1:A:10:LEU:H	1:A:10:LEU:HD23	4	0.31	0.09	0.34
(2,500)	1:A:116:TRP:HE1	1:A:198:HIS:H	4	0.28	0.07	0.29
(3,32)	1:A:154:ASN:ND2	4:A:305:PX4:C35	4	0.26	0.16	0.17
(3,32)	1:A:154:ASN:ND2	4:A:307:PX4:C35	4	0.26	0.16	0.17
(3,32)	1:A:154:ASN:ND2	4:A:309:PX4:C35	4	0.26	0.16	0.17
(3,32)	1:A:154:ASN:ND2	4:A:311:PX4:C35	4	0.26	0.16	0.17
(3,32)	1:A:154:ASN:ND2	4:A:313:PX4:C35	4	0.26	0.16	0.17
(3,32)	1:A:154:ASN:ND2	4:A:315:PX4:C35	4	0.26	0.16	0.17
(3,32)	1:A:154:ASN:ND2	4:A:317:PX4:C35	4	0.26	0.16	0.17
(3,32)	1:A:154:ASN:ND2	4:A:319:PX4:C35	4	0.26	0.16	0.17
(3,32)	1:A:154:ASN:ND2	4:A:321:PX4:C35	4	0.26	0.16	0.17
(3,32)	1:A:154:ASN:ND2	4:A:323:PX4:C35	4	0.26	0.16	0.17
(3,32)	1:A:154:ASN:ND2	4:A:325:PX4:C35	4	0.26	0.16	0.17
(3,32)	1:A:154:ASN:ND2	4:A:327:PX4:C35	4	0.26	0.16	0.17
(3,32)	1:A:154:ASN:ND2	4:A:329:PX4:C35	4	0.26	0.16	0.17
(3,32)	1:A:154:ASN:ND2	4:A:331:PX4:C35	4	0.26	0.16	0.17
(3,32)	1:A:154:ASN:ND2	4:A:333:PX4:C35	4	0.26	0.16	0.17
(3,32)	1:A:154:ASN:ND2	4:A:335:PX4:C35	4	0.26	0.16	0.17
(3,32)	1:A:154:ASN:ND2	4:A:337:PX4:C35	4	0.26	0.16	0.17
(3,32)	1:A:154:ASN:ND2	4:A:339:PX4:C35	4	0.26	0.16	0.17
(3,32)	1:A:154:ASN:ND2	4:A:341:PX4:C35	4	0.26	0.16	0.17
(3,32)	1:A:154:ASN:ND2	4:A:343:PX4:C35	4	0.26	0.16	0.17
(3,32)	1:A:154:ASN:ND2	4:A:345:PX4:C35	4	0.26	0.16	0.17
(3,32)	1:A:154:ASN:ND2	4:A:347:PX4:C35	4	0.26	0.16	0.17
(3,32)	1:A:154:ASN:ND2	4:A:349:PX4:C35	4	0.26	0.16	0.17
(3,32)	1:A:154:ASN:ND2	4:A:351:PX4:C35	4	0.26	0.16	0.17

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(3,32)	1:A:154:ASN:ND2	4:A:353:PX4:C35	4	0.26	0.16	0.17
(3,32)	1:A:154:ASN:ND2	4:A:355:PX4:C35	4	0.26	0.16	0.17
(3,32)	1:A:154:ASN:ND2	4:A:357:PX4:C35	4	0.26	0.16	0.17
(3,32)	1:A:154:ASN:ND2	4:A:359:PX4:C35	4	0.26	0.16	0.17
(3,32)	1:A:154:ASN:ND2	4:A:361:PX4:C35	4	0.26	0.16	0.17
(3,32)	1:A:154:ASN:ND2	4:A:363:PX4:C35	4	0.26	0.16	0.17
(3,32)	1:A:154:ASN:ND2	4:A:402:PX4:C35	4	0.26	0.16	0.17
(3,32)	1:A:154:ASN:ND2	4:A:404:PX4:C35	4	0.26	0.16	0.17
(3,32)	1:A:154:ASN:ND2	4:A:406:PX4:C35	4	0.26	0.16	0.17
(3,32)	1:A:154:ASN:ND2	4:A:408:PX4:C35	4	0.26	0.16	0.17
(3,32)	1:A:154:ASN:ND2	4:A:410:PX4:C35	4	0.26	0.16	0.17
(3,32)	1:A:154:ASN:ND2	4:A:412:PX4:C35	4	0.26	0.16	0.17
(3,32)	1:A:154:ASN:ND2	4:A:414:PX4:C35	4	0.26	0.16	0.17
(3,32)	1:A:154:ASN:ND2	4:A:416:PX4:C35	4	0.26	0.16	0.17
(3,32)	1:A:154:ASN:ND2	4:A:418:PX4:C35	4	0.26	0.16	0.17
(3,32)	1:A:154:ASN:ND2	4:A:420:PX4:C35	4	0.26	0.16	0.17
(3,32)	1:A:154:ASN:ND2	4:A:422:PX4:C35	4	0.26	0.16	0.17
(3,32)	1:A:154:ASN:ND2	4:A:424:PX4:C35	4	0.26	0.16	0.17
(3,32)	1:A:154:ASN:ND2	4:A:426:PX4:C35	4	0.26	0.16	0.17
(3,32)	1:A:154:ASN:ND2	4:A:428:PX4:C35	4	0.26	0.16	0.17
(3,32)	1:A:154:ASN:ND2	4:A:430:PX4:C35	4	0.26	0.16	0.17
(2,274)	1:A:116:TRP:HE1	1:A:197:GLY:H	4	0.25	0.07	0.24
(2,64)	1:A:52:GLY:H	1:A:53:MET:H	4	0.24	0.1	0.24
(2,67)	1:A:53:MET:H	1:A:52:GLY:H	4	0.24	0.1	0.24
(2,533)	1:A:23:TYR:H	1:A:24:LEU:H	4	0.18	0.04	0.16
(2,558)	1:A:23:TYR:H	1:A:24:LEU:H	4	0.18	0.04	0.16
(2,215)	1:A:103:ILE:H	1:A:103:ILE:HG13	4	0.17	0.05	0.15
(2,215)	1:A:103:ILE:H	1:A:103:ILE:HG12	4	0.17	0.05	0.15
(2,83)	1:A:58:VAL:H	1:A:48:LEU:HD22	3	1.3	0.39	1.39
(2,83)	1:A:58:VAL:H	1:A:48:LEU:HD23	3	1.3	0.39	1.39
(2,774)	1:A:61:ILE:HD11	1:A:48:LEU:HD22	3	1.13	0.12	1.08
(2,774)	1:A:61:ILE:HD11	1:A:48:LEU:HD23	3	1.13	0.12	1.08
(2,844)	1:A:200:LEU:HD22	1:A:122:LEU:HD21	3	1.06	0.75	0.72
(2,846)	1:A:200:LEU:HD23	1:A:122:LEU:HD21	3	0.96	0.22	1.11
(2,735)	1:A:196:LEU:HD22	1:A:113:LEU:HD21	3	0.79	0.23	0.82
(2,718)	1:A:54:LEU:HD11	1:A:59:ILE:HD11	3	0.71	0.16	0.68
(2,718)	1:A:54:LEU:HD11	1:A:59:ILE:HD12	3	0.71	0.16	0.68
(2,718)	1:A:54:LEU:HD11	1:A:59:ILE:HD13	3	0.71	0.16	0.68
(2,718)	1:A:54:LEU:HD12	1:A:59:ILE:HD11	3	0.71	0.16	0.68
(2,718)	1:A:54:LEU:HD12	1:A:59:ILE:HD12	3	0.71	0.16	0.68
(2,718)	1:A:54:LEU:HD12	1:A:59:ILE:HD13	3	0.71	0.16	0.68
(2,718)	1:A:54:LEU:HD13	1:A:59:ILE:HD11	3	0.71	0.16	0.68

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,718)	1:A:54:LEU:HD13	1:A:59:ILE:HD12	3	0.71	0.16	0.68
(2,718)	1:A:54:LEU:HD13	1:A:59:ILE:HD13	3	0.71	0.16	0.68
(2,737)	1:A:196:LEU:HD23	1:A:113:LEU:HD21	3	0.63	0.33	0.86
(2,634)	1:A:54:LEU:HD11	1:A:12:TRP:HE1	3	0.56	0.15	0.45
(2,634)	1:A:54:LEU:HD12	1:A:12:TRP:HE1	3	0.56	0.15	0.45
(2,634)	1:A:54:LEU:HD13	1:A:12:TRP:HE1	3	0.56	0.15	0.45
(2,258)	1:A:112:ALA:H	1:A:189:LEU:HD22	3	0.46	0.26	0.44
(2,258)	1:A:112:ALA:H	1:A:189:LEU:HD23	3	0.46	0.26	0.44
(2,788)	1:A:58:VAL:HG11	1:A:39:LEU:HD21	3	0.46	0.26	0.29
(2,894)	1:A:64:LYS:H	1:A:64:LYS:HG3	3	0.36	0.32	0.16
(2,894)	1:A:64:LYS:H	1:A:64:LYS:HG3	3	0.36	0.32	0.16
(2,71)	1:A:55:ASN:H	1:A:54:LEU:HD21	3	0.35	0.15	0.27
(2,986)	1:A:80:ASN:H	1:A:79:PRO:HB3	3	0.34	0.08	0.36
(2,986)	1:A:80:ASN:H	1:A:79:PRO:HB2	3	0.34	0.08	0.36
(2,986)	1:A:80:ASN:H	1:A:79:PRO:HB3	3	0.34	0.08	0.36
(2,986)	1:A:80:ASN:H	1:A:79:PRO:HB2	3	0.34	0.08	0.36
(2,503)	1:A:198:HIS:H	1:A:201:GLY:H	3	0.31	0.09	0.26
(2,716)	1:A:54:LEU:HD11	1:A:58:VAL:HG11	3	0.26	0.12	0.18
(2,716)	1:A:54:LEU:HD11	1:A:58:VAL:HG12	3	0.26	0.12	0.18
(2,716)	1:A:54:LEU:HD11	1:A:58:VAL:HG13	3	0.26	0.12	0.18
(2,716)	1:A:54:LEU:HD12	1:A:58:VAL:HG11	3	0.26	0.12	0.18
(2,716)	1:A:54:LEU:HD12	1:A:58:VAL:HG12	3	0.26	0.12	0.18
(2,716)	1:A:54:LEU:HD12	1:A:58:VAL:HG13	3	0.26	0.12	0.18
(2,716)	1:A:54:LEU:HD13	1:A:58:VAL:HG11	3	0.26	0.12	0.18
(2,716)	1:A:54:LEU:HD13	1:A:58:VAL:HG12	3	0.26	0.12	0.18
(2,716)	1:A:54:LEU:HD13	1:A:58:VAL:HG13	3	0.26	0.12	0.18
(2,301)	1:A:120:ILE:HD11	1:A:122:LEU:H	3	0.22	0.05	0.26
(2,301)	1:A:120:ILE:HD12	1:A:122:LEU:H	3	0.22	0.05	0.26
(2,301)	1:A:120:ILE:HD13	1:A:122:LEU:H	3	0.22	0.05	0.26
(2,764)	1:A:120:ILE:HD11	1:A:122:LEU:H	3	0.22	0.05	0.26
(2,764)	1:A:120:ILE:HD12	1:A:122:LEU:H	3	0.22	0.05	0.26
(2,764)	1:A:120:ILE:HD13	1:A:122:LEU:H	3	0.22	0.05	0.26
(2,564)	1:A:231:ILE:H	1:A:231:ILE:HG13	3	0.21	0.04	0.23
(2,564)	1:A:231:ILE:H	1:A:231:ILE:HG12	3	0.21	0.04	0.23
(2,462)	1:A:182:SER:H	1:A:181:GLY:H	3	0.19	0.05	0.2
(2,462)	1:A:182:SER:H	1:A:181:GLY:H	3	0.19	0.05	0.2
(2,677)	1:A:125:ARG:H	1:A:90:THR:H	3	0.18	0.05	0.2
(2,539)	1:A:206:SER:H	1:A:207:ASP:H	3	0.17	0.03	0.19
(2,539)	1:A:206:SER:H	1:A:207:ASP:H	3	0.17	0.03	0.19
(2,235)	1:A:104:THR:H	1:A:107:ARG:H	3	0.17	0.04	0.18
(2,889)	1:A:63:GLN:HA	1:A:63:GLN:H	3	0.16	0.03	0.16
(2,938)	1:A:73:ALA:HA	1:A:74:GLU:H	3	0.13	0.02	0.11

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,725)	1:A:113:LEU:HD13	1:A:196:LEU:HD21	2	0.77	0.35	0.77
(2,971)	1:A:77:LEU:HB3	1:A:78:PHE:H	2	0.65	0.48	0.65
(2,971)	1:A:77:LEU:HB3	1:A:78:PHE:H	2	0.65	0.48	0.65
(2,708)	1:A:226:LEU:HD11	1:A:231:ILE:HG13	2	0.62	0.36	0.62
(2,708)	1:A:226:LEU:HD12	1:A:231:ILE:HG13	2	0.62	0.36	0.62
(2,708)	1:A:226:LEU:HD13	1:A:231:ILE:HG13	2	0.62	0.36	0.62
(2,708)	1:A:226:LEU:HD11	1:A:231:ILE:HG12	2	0.62	0.36	0.62
(2,708)	1:A:226:LEU:HD12	1:A:231:ILE:HG12	2	0.62	0.36	0.62
(2,708)	1:A:226:LEU:HD13	1:A:231:ILE:HG12	2	0.62	0.36	0.62
(2,278)	1:A:116:TRP:HE1	1:A:211:VAL:HG11	2	0.42	0.2	0.42
(2,278)	1:A:116:TRP:HE1	1:A:211:VAL:HG12	2	0.42	0.2	0.42
(2,278)	1:A:116:TRP:HE1	1:A:211:VAL:HG13	2	0.42	0.2	0.42
(2,410)	1:A:167:GLY:H	1:A:165:GLY:H	2	0.37	0.06	0.37
(2,966)	1:A:77:LEU:H	1:A:77:LEU:HB3	2	0.34	0.07	0.34
(2,966)	1:A:77:LEU:H	1:A:77:LEU:HB3	2	0.34	0.07	0.34
(2,302)	1:A:120:ILE:HG21	1:A:122:LEU:H	2	0.33	0.04	0.33
(2,302)	1:A:120:ILE:HG22	1:A:122:LEU:H	2	0.33	0.04	0.33
(2,302)	1:A:120:ILE:HG23	1:A:122:LEU:H	2	0.33	0.04	0.33
(2,776)	1:A:61:ILE:HD12	1:A:48:LEU:HD22	2	0.32	0.12	0.32
(2,776)	1:A:61:ILE:HD12	1:A:48:LEU:HD23	2	0.32	0.12	0.32
(2,378)	1:A:10:LEU:H	1:A:10:LEU:HD11	2	0.31	0.04	0.31
(2,378)	1:A:10:LEU:H	1:A:10:LEU:HD12	2	0.31	0.04	0.31
(2,378)	1:A:10:LEU:H	1:A:10:LEU:HD13	2	0.31	0.04	0.31
(2,843)	1:A:200:LEU:HD21	1:A:122:LEU:HD22	2	0.29	0.16	0.29
(2,843)	1:A:200:LEU:HD21	1:A:122:LEU:HD23	2	0.29	0.16	0.29
(2,672)	1:A:66:ARG:H	1:A:156:LEU:HD22	2	0.27	0.09	0.27
(2,672)	1:A:66:ARG:H	1:A:156:LEU:HD23	2	0.27	0.09	0.27
(2,397)	1:A:169:ASP:H	1:A:160:PHE:H	2	0.23	0.07	0.23
(2,587)	1:A:232:LYS:H	1:A:231:ILE:HD11	2	0.2	0.09	0.2
(2,587)	1:A:232:LYS:H	1:A:231:ILE:HD12	2	0.2	0.09	0.2
(2,587)	1:A:232:LYS:H	1:A:231:ILE:HD13	2	0.2	0.09	0.2
(2,568)	1:A:235:GLN:H	1:A:233:GLY:H	2	0.2	0.09	0.2
(2,499)	1:A:197:GLY:H	1:A:198:HIS:H	2	0.19	0.06	0.19
(2,499)	1:A:197:GLY:H	1:A:198:HIS:H	2	0.19	0.06	0.19
(2,901)	1:A:66:ARG:H	1:A:66:ARG:HB3	2	0.18	0.06	0.18
(2,901)	1:A:66:ARG:H	1:A:66:ARG:HB3	2	0.18	0.06	0.18
(2,887)	1:A:134:ILE:HD11	1:A:134:ILE:HG21	2	0.18	0.02	0.18
(2,887)	1:A:134:ILE:HD11	1:A:134:ILE:HG22	2	0.18	0.02	0.18
(2,887)	1:A:134:ILE:HD11	1:A:134:ILE:HG23	2	0.18	0.02	0.18
(2,887)	1:A:134:ILE:HD12	1:A:134:ILE:HG21	2	0.18	0.02	0.18
(2,887)	1:A:134:ILE:HD12	1:A:134:ILE:HG22	2	0.18	0.02	0.18
(2,887)	1:A:134:ILE:HD12	1:A:134:ILE:HG23	2	0.18	0.02	0.18

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,887)	1:A:134:ILE:HD13	1:A:134:ILE:HG21	2	0.18	0.02	0.18
(2,887)	1:A:134:ILE:HD13	1:A:134:ILE:HG22	2	0.18	0.02	0.18
(2,887)	1:A:134:ILE:HD13	1:A:134:ILE:HG23	2	0.18	0.02	0.18
(2,670)	1:A:66:ARG:H	1:A:156:LEU:HD11	2	0.17	0.03	0.17
(2,670)	1:A:66:ARG:H	1:A:156:LEU:HD12	2	0.17	0.03	0.17
(2,670)	1:A:66:ARG:H	1:A:156:LEU:HD13	2	0.17	0.03	0.17
(3,35)	1:A:194:HIS:H	4:A:305:PX4:C35	2	0.17	0.06	0.17
(3,35)	1:A:194:HIS:H	4:A:307:PX4:C35	2	0.17	0.06	0.17
(3,35)	1:A:194:HIS:H	4:A:309:PX4:C35	2	0.17	0.06	0.17
(3,35)	1:A:194:HIS:H	4:A:311:PX4:C35	2	0.17	0.06	0.17
(3,35)	1:A:194:HIS:H	4:A:313:PX4:C35	2	0.17	0.06	0.17
(3,35)	1:A:194:HIS:H	4:A:315:PX4:C35	2	0.17	0.06	0.17
(3,35)	1:A:194:HIS:H	4:A:317:PX4:C35	2	0.17	0.06	0.17
(3,35)	1:A:194:HIS:H	4:A:319:PX4:C35	2	0.17	0.06	0.17
(3,35)	1:A:194:HIS:H	4:A:321:PX4:C35	2	0.17	0.06	0.17
(3,35)	1:A:194:HIS:H	4:A:323:PX4:C35	2	0.17	0.06	0.17
(3,35)	1:A:194:HIS:H	4:A:325:PX4:C35	2	0.17	0.06	0.17
(3,35)	1:A:194:HIS:H	4:A:327:PX4:C35	2	0.17	0.06	0.17
(3,35)	1:A:194:HIS:H	4:A:329:PX4:C35	2	0.17	0.06	0.17
(3,35)	1:A:194:HIS:H	4:A:331:PX4:C35	2	0.17	0.06	0.17
(3,35)	1:A:194:HIS:H	4:A:333:PX4:C35	2	0.17	0.06	0.17
(3,35)	1:A:194:HIS:H	4:A:335:PX4:C35	2	0.17	0.06	0.17
(3,35)	1:A:194:HIS:H	4:A:337:PX4:C35	2	0.17	0.06	0.17
(3,35)	1:A:194:HIS:H	4:A:339:PX4:C35	2	0.17	0.06	0.17
(3,35)	1:A:194:HIS:H	4:A:341:PX4:C35	2	0.17	0.06	0.17
(3,35)	1:A:194:HIS:H	4:A:343:PX4:C35	2	0.17	0.06	0.17
(3,35)	1:A:194:HIS:H	4:A:345:PX4:C35	2	0.17	0.06	0.17
(3,35)	1:A:194:HIS:H	4:A:347:PX4:C35	2	0.17	0.06	0.17
(3,35)	1:A:194:HIS:H	4:A:349:PX4:C35	2	0.17	0.06	0.17
(3,35)	1:A:194:HIS:H	4:A:351:PX4:C35	2	0.17	0.06	0.17
(3,35)	1:A:194:HIS:H	4:A:353:PX4:C35	2	0.17	0.06	0.17
(3,35)	1:A:194:HIS:H	4:A:355:PX4:C35	2	0.17	0.06	0.17
(3,35)	1:A:194:HIS:H	4:A:357:PX4:C35	2	0.17	0.06	0.17
(3,35)	1:A:194:HIS:H	4:A:359:PX4:C35	2	0.17	0.06	0.17
(3,35)	1:A:194:HIS:H	4:A:361:PX4:C35	2	0.17	0.06	0.17
(3,35)	1:A:194:HIS:H	4:A:363:PX4:C35	2	0.17	0.06	0.17
(3,35)	1:A:194:HIS:H	4:A:402:PX4:C35	2	0.17	0.06	0.17
(3,35)	1:A:194:HIS:H	4:A:404:PX4:C35	2	0.17	0.06	0.17
(3,35)	1:A:194:HIS:H	4:A:406:PX4:C35	2	0.17	0.06	0.17
(3,35)	1:A:194:HIS:H	4:A:408:PX4:C35	2	0.17	0.06	0.17
(3,35)	1:A:194:HIS:H	4:A:410:PX4:C35	2	0.17	0.06	0.17
(3,35)	1:A:194:HIS:H	4:A:412:PX4:C35	2	0.17	0.06	0.17

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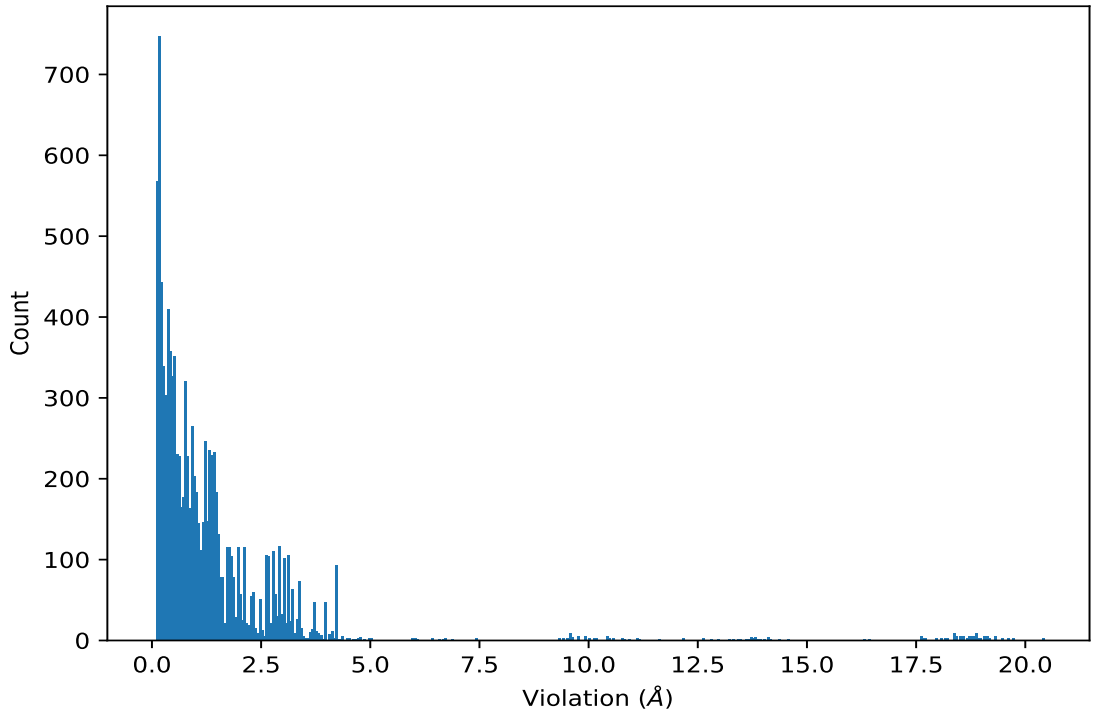
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(3,35)	1:A:194:HIS:H	4:A:414:PX4:C35	2	0.17	0.06	0.17
(3,35)	1:A:194:HIS:H	4:A:416:PX4:C35	2	0.17	0.06	0.17
(3,35)	1:A:194:HIS:H	4:A:418:PX4:C35	2	0.17	0.06	0.17
(3,35)	1:A:194:HIS:H	4:A:420:PX4:C35	2	0.17	0.06	0.17
(3,35)	1:A:194:HIS:H	4:A:422:PX4:C35	2	0.17	0.06	0.17
(3,35)	1:A:194:HIS:H	4:A:424:PX4:C35	2	0.17	0.06	0.17
(3,35)	1:A:194:HIS:H	4:A:426:PX4:C35	2	0.17	0.06	0.17
(3,35)	1:A:194:HIS:H	4:A:428:PX4:C35	2	0.17	0.06	0.17
(3,35)	1:A:194:HIS:H	4:A:430:PX4:C35	2	0.17	0.06	0.17
(2,17)	1:A:93:ILE:H	1:A:93:ILE:HD11	2	0.17	0.01	0.17
(2,17)	1:A:93:ILE:H	1:A:93:ILE:HD12	2	0.17	0.01	0.17
(2,17)	1:A:93:ILE:H	1:A:93:ILE:HD13	2	0.17	0.01	0.17
(2,801)	1:A:93:ILE:H	1:A:93:ILE:HD11	2	0.17	0.01	0.17
(2,801)	1:A:93:ILE:H	1:A:93:ILE:HD12	2	0.17	0.01	0.17
(2,801)	1:A:93:ILE:H	1:A:93:ILE:HD13	2	0.17	0.01	0.17
(2,632)	1:A:25:TYR:H	1:A:24:LEU:HD21	2	0.16	0.04	0.16
(2,353)	1:A:136:ILE:H	1:A:136:ILE:HD11	2	0.16	0.02	0.16
(2,353)	1:A:136:ILE:H	1:A:136:ILE:HD12	2	0.16	0.02	0.16
(2,353)	1:A:136:ILE:H	1:A:136:ILE:HD13	2	0.16	0.02	0.16
(2,137)	1:A:73:ALA:H	1:A:72:VAL:HG11	2	0.16	0.05	0.16
(2,137)	1:A:73:ALA:H	1:A:72:VAL:HG12	2	0.16	0.05	0.16
(2,137)	1:A:73:ALA:H	1:A:72:VAL:HG13	2	0.16	0.05	0.16
(2,137)	1:A:73:ALA:H	1:A:72:VAL:HG21	2	0.16	0.05	0.16
(2,137)	1:A:73:ALA:H	1:A:72:VAL:HG22	2	0.16	0.05	0.16
(2,137)	1:A:73:ALA:H	1:A:72:VAL:HG23	2	0.16	0.05	0.16
(2,602)	1:A:237:LEU:H	1:A:239:GLY:H	2	0.16	0.05	0.16
(2,36)	1:A:46:PHE:H	1:A:43:GLN:H	2	0.16	0.04	0.16
(2,157)	1:A:88:VAL:H	1:A:123:HIS:H	2	0.16	0.05	0.16
(2,767)	1:A:61:ILE:HD11	1:A:60:GLU:H	2	0.14	0.03	0.14
(2,767)	1:A:61:ILE:HD12	1:A:60:GLU:H	2	0.14	0.03	0.14
(2,767)	1:A:61:ILE:HD13	1:A:60:GLU:H	2	0.14	0.03	0.14
(2,623)	1:A:6:GLY:H	1:A:7:MET:H	2	0.14	0.01	0.14
(2,179)	1:A:92:ARG:H	1:A:134:ILE:HD11	2	0.12	0.01	0.12
(2,179)	1:A:92:ARG:H	1:A:134:ILE:HD12	2	0.12	0.01	0.12
(2,179)	1:A:92:ARG:H	1:A:134:ILE:HD13	2	0.12	0.01	0.12
(2,404)	1:A:161:ALA:H	1:A:161:ALA:HB1	2	0.12	0.02	0.12
(2,404)	1:A:161:ALA:H	1:A:161:ALA:HB2	2	0.12	0.02	0.12
(2,404)	1:A:161:ALA:H	1:A:161:ALA:HB3	2	0.12	0.02	0.12

[1]Number of violated models, [2]Standard deviation

9.5 All violated distance restraints (i)

9.5.1 Histogram : Distribution of distance violations (i)

The following histogram shows the distribution of the absolute value of the violation for all violated restraints in the ensemble.



9.5.2 Table : All distance violations (i)

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,210)	1:A:105:VAL:HG21	1:A:237:LEU:H	16	20.41
(2,210)	1:A:105:VAL:HG22	1:A:237:LEU:H	16	20.41
(2,210)	1:A:105:VAL:HG23	1:A:237:LEU:H	16	20.41
(2,210)	1:A:105:VAL:HG21	1:A:237:LEU:H	12	19.71
(2,210)	1:A:105:VAL:HG22	1:A:237:LEU:H	12	19.71
(2,210)	1:A:105:VAL:HG23	1:A:237:LEU:H	12	19.71
(2,210)	1:A:105:VAL:HG21	1:A:237:LEU:H	11	19.63
(2,210)	1:A:105:VAL:HG22	1:A:237:LEU:H	11	19.63
(2,210)	1:A:105:VAL:HG23	1:A:237:LEU:H	11	19.63
(2,210)	1:A:105:VAL:HG21	1:A:237:LEU:H	7	19.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,210)	1:A:105:VAL:HG22	1:A:237:LEU:H	7	19.47
(2,210)	1:A:105:VAL:HG23	1:A:237:LEU:H	7	19.47
(2,210)	1:A:105:VAL:HG21	1:A:237:LEU:H	17	19.34
(2,210)	1:A:105:VAL:HG22	1:A:237:LEU:H	17	19.34
(2,210)	1:A:105:VAL:HG23	1:A:237:LEU:H	17	19.34
(2,210)	1:A:105:VAL:HG21	1:A:237:LEU:H	14	19.31
(2,210)	1:A:105:VAL:HG22	1:A:237:LEU:H	14	19.31
(2,210)	1:A:105:VAL:HG23	1:A:237:LEU:H	14	19.31
(2,210)	1:A:105:VAL:HG21	1:A:237:LEU:H	18	19.15
(2,210)	1:A:105:VAL:HG22	1:A:237:LEU:H	18	19.15
(2,210)	1:A:105:VAL:HG23	1:A:237:LEU:H	18	19.15
(2,211)	1:A:120:ILE:HD11	1:A:100:LEU:H	11	19.12
(2,211)	1:A:120:ILE:HD12	1:A:100:LEU:H	11	19.12
(2,211)	1:A:120:ILE:HD13	1:A:100:LEU:H	11	19.12
(2,210)	1:A:105:VAL:HG21	1:A:237:LEU:H	4	19.12
(2,210)	1:A:105:VAL:HG22	1:A:237:LEU:H	4	19.12
(2,210)	1:A:105:VAL:HG23	1:A:237:LEU:H	4	19.12
(2,210)	1:A:105:VAL:HG21	1:A:237:LEU:H	19	19.06
(2,210)	1:A:105:VAL:HG22	1:A:237:LEU:H	19	19.06
(2,210)	1:A:105:VAL:HG23	1:A:237:LEU:H	19	19.06
(2,210)	1:A:105:VAL:HG21	1:A:237:LEU:H	20	19.06
(2,210)	1:A:105:VAL:HG22	1:A:237:LEU:H	20	19.06
(2,210)	1:A:105:VAL:HG23	1:A:237:LEU:H	20	19.06
(2,210)	1:A:105:VAL:HG21	1:A:237:LEU:H	3	18.95
(2,210)	1:A:105:VAL:HG22	1:A:237:LEU:H	3	18.95
(2,210)	1:A:105:VAL:HG23	1:A:237:LEU:H	3	18.95
(2,210)	1:A:105:VAL:HG21	1:A:237:LEU:H	9	18.94
(2,210)	1:A:105:VAL:HG22	1:A:237:LEU:H	9	18.94
(2,210)	1:A:105:VAL:HG23	1:A:237:LEU:H	9	18.94
(2,210)	1:A:105:VAL:HG21	1:A:237:LEU:H	10	18.87
(2,210)	1:A:105:VAL:HG22	1:A:237:LEU:H	10	18.87
(2,210)	1:A:105:VAL:HG23	1:A:237:LEU:H	10	18.87
(2,211)	1:A:120:ILE:HD11	1:A:100:LEU:H	19	18.86
(2,211)	1:A:120:ILE:HD12	1:A:100:LEU:H	19	18.86
(2,211)	1:A:120:ILE:HD13	1:A:100:LEU:H	19	18.86
(2,210)	1:A:105:VAL:HG21	1:A:237:LEU:H	1	18.85
(2,210)	1:A:105:VAL:HG22	1:A:237:LEU:H	1	18.85
(2,210)	1:A:105:VAL:HG23	1:A:237:LEU:H	1	18.85
(2,211)	1:A:120:ILE:HD11	1:A:100:LEU:H	13	18.84
(2,211)	1:A:120:ILE:HD12	1:A:100:LEU:H	13	18.84
(2,211)	1:A:120:ILE:HD13	1:A:100:LEU:H	13	18.84
(2,211)	1:A:120:ILE:HD11	1:A:100:LEU:H	6	18.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,211)	1:A:120:ILE:HD12	1:A:100:LEU:H	6	18.8
(2,211)	1:A:120:ILE:HD13	1:A:100:LEU:H	6	18.8
(2,211)	1:A:120:ILE:HD11	1:A:100:LEU:H	4	18.79
(2,211)	1:A:120:ILE:HD12	1:A:100:LEU:H	4	18.79
(2,211)	1:A:120:ILE:HD13	1:A:100:LEU:H	4	18.79
(2,211)	1:A:120:ILE:HD11	1:A:100:LEU:H	7	18.75
(2,211)	1:A:120:ILE:HD12	1:A:100:LEU:H	7	18.75
(2,211)	1:A:120:ILE:HD13	1:A:100:LEU:H	7	18.75
(2,210)	1:A:105:VAL:HG21	1:A:237:LEU:H	6	18.74
(2,210)	1:A:105:VAL:HG22	1:A:237:LEU:H	6	18.74
(2,210)	1:A:105:VAL:HG23	1:A:237:LEU:H	6	18.74
(2,211)	1:A:120:ILE:HD11	1:A:100:LEU:H	17	18.73
(2,211)	1:A:120:ILE:HD12	1:A:100:LEU:H	17	18.73
(2,211)	1:A:120:ILE:HD13	1:A:100:LEU:H	17	18.73
(2,211)	1:A:120:ILE:HD11	1:A:100:LEU:H	3	18.68
(2,211)	1:A:120:ILE:HD12	1:A:100:LEU:H	3	18.68
(2,211)	1:A:120:ILE:HD13	1:A:100:LEU:H	3	18.68
(2,210)	1:A:105:VAL:HG21	1:A:237:LEU:H	5	18.57
(2,210)	1:A:105:VAL:HG22	1:A:237:LEU:H	5	18.57
(2,210)	1:A:105:VAL:HG23	1:A:237:LEU:H	5	18.57
(2,210)	1:A:105:VAL:HG21	1:A:237:LEU:H	13	18.56
(2,210)	1:A:105:VAL:HG22	1:A:237:LEU:H	13	18.56
(2,210)	1:A:105:VAL:HG23	1:A:237:LEU:H	13	18.56
(2,210)	1:A:105:VAL:HG21	1:A:237:LEU:H	15	18.53
(2,210)	1:A:105:VAL:HG22	1:A:237:LEU:H	15	18.53
(2,210)	1:A:105:VAL:HG23	1:A:237:LEU:H	15	18.53
(2,210)	1:A:105:VAL:HG21	1:A:237:LEU:H	8	18.51
(2,210)	1:A:105:VAL:HG22	1:A:237:LEU:H	8	18.51
(2,210)	1:A:105:VAL:HG23	1:A:237:LEU:H	8	18.51
(2,211)	1:A:120:ILE:HD11	1:A:100:LEU:H	12	18.44
(2,211)	1:A:120:ILE:HD12	1:A:100:LEU:H	12	18.44
(2,211)	1:A:120:ILE:HD13	1:A:100:LEU:H	12	18.44
(2,211)	1:A:120:ILE:HD11	1:A:100:LEU:H	5	18.4
(2,211)	1:A:120:ILE:HD12	1:A:100:LEU:H	5	18.4
(2,211)	1:A:120:ILE:HD13	1:A:100:LEU:H	5	18.4
(2,211)	1:A:120:ILE:HD11	1:A:100:LEU:H	9	18.38
(2,211)	1:A:120:ILE:HD12	1:A:100:LEU:H	9	18.38
(2,211)	1:A:120:ILE:HD13	1:A:100:LEU:H	9	18.38
(2,210)	1:A:105:VAL:HG21	1:A:237:LEU:H	2	18.36
(2,210)	1:A:105:VAL:HG22	1:A:237:LEU:H	2	18.36
(2,210)	1:A:105:VAL:HG23	1:A:237:LEU:H	2	18.36
(2,211)	1:A:120:ILE:HD11	1:A:100:LEU:H	10	18.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,211)	1:A:120:ILE:HD12	1:A:100:LEU:H	10	18.35
(2,211)	1:A:120:ILE:HD13	1:A:100:LEU:H	10	18.35
(2,211)	1:A:120:ILE:HD11	1:A:100:LEU:H	2	18.23
(2,211)	1:A:120:ILE:HD12	1:A:100:LEU:H	2	18.23
(2,211)	1:A:120:ILE:HD13	1:A:100:LEU:H	2	18.23
(2,211)	1:A:120:ILE:HD11	1:A:100:LEU:H	8	18.15
(2,211)	1:A:120:ILE:HD12	1:A:100:LEU:H	8	18.15
(2,211)	1:A:120:ILE:HD13	1:A:100:LEU:H	8	18.15
(2,211)	1:A:120:ILE:HD11	1:A:100:LEU:H	15	18.07
(2,211)	1:A:120:ILE:HD12	1:A:100:LEU:H	15	18.07
(2,211)	1:A:120:ILE:HD13	1:A:100:LEU:H	15	18.07
(2,211)	1:A:120:ILE:HD11	1:A:100:LEU:H	1	17.96
(2,211)	1:A:120:ILE:HD12	1:A:100:LEU:H	1	17.96
(2,211)	1:A:120:ILE:HD13	1:A:100:LEU:H	1	17.96
(2,211)	1:A:120:ILE:HD11	1:A:100:LEU:H	20	17.74
(2,211)	1:A:120:ILE:HD12	1:A:100:LEU:H	20	17.74
(2,211)	1:A:120:ILE:HD13	1:A:100:LEU:H	20	17.74
(2,211)	1:A:120:ILE:HD11	1:A:100:LEU:H	14	17.69
(2,211)	1:A:120:ILE:HD12	1:A:100:LEU:H	14	17.69
(2,211)	1:A:120:ILE:HD13	1:A:100:LEU:H	14	17.69
(2,211)	1:A:120:ILE:HD11	1:A:100:LEU:H	18	17.64
(2,211)	1:A:120:ILE:HD12	1:A:100:LEU:H	18	17.64
(2,211)	1:A:120:ILE:HD13	1:A:100:LEU:H	18	17.64
(2,211)	1:A:120:ILE:HD11	1:A:100:LEU:H	16	17.6
(2,211)	1:A:120:ILE:HD12	1:A:100:LEU:H	16	17.6
(2,211)	1:A:120:ILE:HD13	1:A:100:LEU:H	16	17.6
(2,111)	1:A:11:GLN:H	1:A:26:ASP:H	7	17.35
(2,111)	1:A:11:GLN:H	1:A:26:ASP:H	2	16.92
(2,111)	1:A:11:GLN:H	1:A:26:ASP:H	14	16.89
(2,111)	1:A:11:GLN:H	1:A:26:ASP:H	10	16.75
(2,111)	1:A:11:GLN:H	1:A:26:ASP:H	1	16.72
(2,111)	1:A:11:GLN:H	1:A:26:ASP:H	8	16.62
(2,111)	1:A:11:GLN:H	1:A:26:ASP:H	19	16.58
(2,111)	1:A:11:GLN:H	1:A:26:ASP:H	5	16.54
(2,111)	1:A:11:GLN:H	1:A:26:ASP:H	12	16.48
(2,111)	1:A:11:GLN:H	1:A:26:ASP:H	6	16.44
(2,111)	1:A:11:GLN:H	1:A:26:ASP:H	4	16.4
(2,111)	1:A:11:GLN:H	1:A:26:ASP:H	11	16.34
(2,111)	1:A:11:GLN:H	1:A:26:ASP:H	15	16.33
(2,111)	1:A:11:GLN:H	1:A:26:ASP:H	13	16.26
(2,111)	1:A:11:GLN:H	1:A:26:ASP:H	3	15.85
(2,111)	1:A:11:GLN:H	1:A:26:ASP:H	17	15.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,111)	1:A:11:GLN:H	1:A:26:ASP:H	9	15.48
(2,386)	1:A:156:LEU:H	1:A:182:SER:H	3	15.17
(2,386)	1:A:156:LEU:H	1:A:182:SER:H	9	14.73
(2,386)	1:A:156:LEU:H	1:A:182:SER:H	15	14.68
(2,386)	1:A:156:LEU:H	1:A:182:SER:H	6	14.58
(2,111)	1:A:11:GLN:H	1:A:26:ASP:H	18	14.55
(2,386)	1:A:156:LEU:H	1:A:182:SER:H	10	14.52
(2,386)	1:A:156:LEU:H	1:A:182:SER:H	13	14.38
(2,386)	1:A:156:LEU:H	1:A:182:SER:H	20	14.36
(2,386)	1:A:156:LEU:H	1:A:182:SER:H	1	14.26
(2,386)	1:A:156:LEU:H	1:A:182:SER:H	8	14.22
(2,386)	1:A:156:LEU:H	1:A:182:SER:H	4	14.18
(2,112)	1:A:14:GLN:H	1:A:25:TYR:H	7	14.17
(2,389)	1:A:66:ARG:H	1:A:180:ASP:H	9	14.13
(2,112)	1:A:14:GLN:H	1:A:25:TYR:H	1	14.13
(2,386)	1:A:156:LEU:H	1:A:182:SER:H	12	14.1
(2,386)	1:A:156:LEU:H	1:A:182:SER:H	16	14.1
(2,386)	1:A:156:LEU:H	1:A:182:SER:H	11	14.08
(2,389)	1:A:66:ARG:H	1:A:180:ASP:H	20	14.03
(2,389)	1:A:66:ARG:H	1:A:180:ASP:H	6	14.01
(2,386)	1:A:156:LEU:H	1:A:182:SER:H	18	13.93
(2,389)	1:A:66:ARG:H	1:A:180:ASP:H	7	13.91
(2,386)	1:A:156:LEU:H	1:A:182:SER:H	5	13.89
(2,386)	1:A:156:LEU:H	1:A:182:SER:H	7	13.86
(2,389)	1:A:66:ARG:H	1:A:180:ASP:H	18	13.84
(2,386)	1:A:156:LEU:H	1:A:182:SER:H	14	13.82
(2,389)	1:A:66:ARG:H	1:A:180:ASP:H	16	13.8
(2,112)	1:A:14:GLN:H	1:A:25:TYR:H	4	13.8
(2,111)	1:A:11:GLN:H	1:A:26:ASP:H	16	13.78
(2,386)	1:A:156:LEU:H	1:A:182:SER:H	2	13.77
(2,389)	1:A:66:ARG:H	1:A:180:ASP:H	15	13.76
(2,111)	1:A:11:GLN:H	1:A:26:ASP:H	20	13.74
(2,112)	1:A:14:GLN:H	1:A:25:TYR:H	10	13.73
(2,112)	1:A:14:GLN:H	1:A:25:TYR:H	19	13.72
(2,386)	1:A:156:LEU:H	1:A:182:SER:H	19	13.7
(2,389)	1:A:66:ARG:H	1:A:180:ASP:H	10	13.69
(2,112)	1:A:14:GLN:H	1:A:25:TYR:H	17	13.65
(2,112)	1:A:14:GLN:H	1:A:25:TYR:H	11	13.64
(2,386)	1:A:156:LEU:H	1:A:182:SER:H	17	13.63
(2,112)	1:A:14:GLN:H	1:A:25:TYR:H	8	13.55
(2,389)	1:A:66:ARG:H	1:A:180:ASP:H	1	13.47
(2,112)	1:A:14:GLN:H	1:A:25:TYR:H	2	13.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,112)	1:A:14:GLN:H	1:A:25:TYR:H	13	13.44
(2,112)	1:A:14:GLN:H	1:A:25:TYR:H	6	13.4
(2,389)	1:A:66:ARG:H	1:A:180:ASP:H	12	13.34
(2,112)	1:A:14:GLN:H	1:A:25:TYR:H	15	13.33
(2,112)	1:A:14:GLN:H	1:A:25:TYR:H	12	13.25
(2,112)	1:A:14:GLN:H	1:A:25:TYR:H	5	13.23
(2,112)	1:A:14:GLN:H	1:A:25:TYR:H	3	13.21
(2,389)	1:A:66:ARG:H	1:A:180:ASP:H	4	13.01
(2,112)	1:A:14:GLN:H	1:A:25:TYR:H	14	12.98
(2,389)	1:A:66:ARG:H	1:A:180:ASP:H	13	12.97
(2,389)	1:A:66:ARG:H	1:A:180:ASP:H	11	12.84
(2,112)	1:A:14:GLN:H	1:A:25:TYR:H	18	12.84
(2,389)	1:A:66:ARG:H	1:A:180:ASP:H	5	12.62
(2,112)	1:A:14:GLN:H	1:A:25:TYR:H	9	12.62
(2,389)	1:A:66:ARG:H	1:A:180:ASP:H	3	12.6
(2,389)	1:A:66:ARG:H	1:A:180:ASP:H	2	12.53
(2,389)	1:A:66:ARG:H	1:A:180:ASP:H	8	12.4
(2,532)	1:A:23:TYR:H	1:A:205:SER:H	14	12.29
(2,389)	1:A:66:ARG:H	1:A:180:ASP:H	19	12.19
(2,532)	1:A:23:TYR:H	1:A:205:SER:H	6	12.18
(2,389)	1:A:66:ARG:H	1:A:180:ASP:H	14	12.17
(2,112)	1:A:14:GLN:H	1:A:25:TYR:H	16	12.05
(2,112)	1:A:14:GLN:H	1:A:25:TYR:H	20	12.0
(2,532)	1:A:23:TYR:H	1:A:205:SER:H	3	11.96
(2,532)	1:A:23:TYR:H	1:A:205:SER:H	5	11.89
(2,532)	1:A:23:TYR:H	1:A:205:SER:H	18	11.72
(2,532)	1:A:23:TYR:H	1:A:205:SER:H	8	11.61
(2,532)	1:A:23:TYR:H	1:A:205:SER:H	20	11.61
(2,532)	1:A:23:TYR:H	1:A:205:SER:H	16	11.56
(2,532)	1:A:23:TYR:H	1:A:205:SER:H	10	11.37
(2,389)	1:A:66:ARG:H	1:A:180:ASP:H	17	11.32
(2,532)	1:A:23:TYR:H	1:A:205:SER:H	15	11.23
(2,532)	1:A:23:TYR:H	1:A:205:SER:H	13	11.19
(2,532)	1:A:23:TYR:H	1:A:205:SER:H	2	11.17
(2,180)	1:A:92:ARG:H	1:A:69:VAL:HG11	15	11.11
(2,180)	1:A:92:ARG:H	1:A:69:VAL:HG12	15	11.11
(2,180)	1:A:92:ARG:H	1:A:69:VAL:HG13	15	11.11
(2,532)	1:A:23:TYR:H	1:A:205:SER:H	12	11.08
(2,532)	1:A:23:TYR:H	1:A:205:SER:H	1	10.99
(2,532)	1:A:23:TYR:H	1:A:205:SER:H	19	10.93
(2,532)	1:A:23:TYR:H	1:A:205:SER:H	17	10.91
(2,532)	1:A:23:TYR:H	1:A:205:SER:H	9	10.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,532)	1:A:23:TYR:H	1:A:205:SER:H	7	10.8
(2,180)	1:A:92:ARG:H	1:A:69:VAL:HG11	18	10.76
(2,180)	1:A:92:ARG:H	1:A:69:VAL:HG12	18	10.76
(2,180)	1:A:92:ARG:H	1:A:69:VAL:HG13	18	10.76
(2,532)	1:A:23:TYR:H	1:A:205:SER:H	11	10.68
(2,180)	1:A:92:ARG:H	1:A:69:VAL:HG11	16	10.56
(2,180)	1:A:92:ARG:H	1:A:69:VAL:HG12	16	10.56
(2,180)	1:A:92:ARG:H	1:A:69:VAL:HG13	16	10.56
(2,180)	1:A:92:ARG:H	1:A:69:VAL:HG11	17	10.49
(2,180)	1:A:92:ARG:H	1:A:69:VAL:HG12	17	10.49
(2,180)	1:A:92:ARG:H	1:A:69:VAL:HG13	17	10.49
(2,180)	1:A:92:ARG:H	1:A:69:VAL:HG11	20	10.43
(2,180)	1:A:92:ARG:H	1:A:69:VAL:HG12	20	10.43
(2,180)	1:A:92:ARG:H	1:A:69:VAL:HG13	20	10.43
(2,180)	1:A:92:ARG:H	1:A:69:VAL:HG11	9	10.41
(2,180)	1:A:92:ARG:H	1:A:69:VAL:HG12	9	10.41
(2,180)	1:A:92:ARG:H	1:A:69:VAL:HG13	9	10.41
(2,530)	1:A:204:HIS:HE1	1:A:24:LEU:H	18	10.25
(2,180)	1:A:92:ARG:H	1:A:69:VAL:HG11	10	10.15
(2,180)	1:A:92:ARG:H	1:A:69:VAL:HG12	10	10.15
(2,180)	1:A:92:ARG:H	1:A:69:VAL:HG13	10	10.15
(2,180)	1:A:92:ARG:H	1:A:69:VAL:HG11	14	10.11
(2,180)	1:A:92:ARG:H	1:A:69:VAL:HG12	14	10.11
(2,180)	1:A:92:ARG:H	1:A:69:VAL:HG13	14	10.11
(2,180)	1:A:92:ARG:H	1:A:69:VAL:HG11	3	10.02
(2,180)	1:A:92:ARG:H	1:A:69:VAL:HG12	3	10.02
(2,180)	1:A:92:ARG:H	1:A:69:VAL:HG13	3	10.02
(2,180)	1:A:92:ARG:H	1:A:69:VAL:HG11	8	9.93
(2,180)	1:A:92:ARG:H	1:A:69:VAL:HG12	8	9.93
(2,180)	1:A:92:ARG:H	1:A:69:VAL:HG13	8	9.93
(2,180)	1:A:92:ARG:H	1:A:69:VAL:HG11	12	9.92
(2,180)	1:A:92:ARG:H	1:A:69:VAL:HG12	12	9.92
(2,180)	1:A:92:ARG:H	1:A:69:VAL:HG13	12	9.92
(2,532)	1:A:23:TYR:H	1:A:205:SER:H	4	9.81
(2,180)	1:A:92:ARG:H	1:A:69:VAL:HG11	11	9.79
(2,180)	1:A:92:ARG:H	1:A:69:VAL:HG12	11	9.79
(2,180)	1:A:92:ARG:H	1:A:69:VAL:HG13	11	9.79
(2,180)	1:A:92:ARG:H	1:A:69:VAL:HG11	13	9.77
(2,180)	1:A:92:ARG:H	1:A:69:VAL:HG12	13	9.77
(2,180)	1:A:92:ARG:H	1:A:69:VAL:HG13	13	9.77
(2,180)	1:A:92:ARG:H	1:A:69:VAL:HG11	1	9.61
(2,180)	1:A:92:ARG:H	1:A:69:VAL:HG12	1	9.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,180)	1:A:92:ARG:H	1:A:69:VAL:HG13	1	9.61
(2,530)	1:A:204:HIS:HE1	1:A:24:LEU:H	9	9.6
(2,180)	1:A:92:ARG:H	1:A:69:VAL:HG11	4	9.59
(2,180)	1:A:92:ARG:H	1:A:69:VAL:HG12	4	9.59
(2,180)	1:A:92:ARG:H	1:A:69:VAL:HG13	4	9.59
(2,180)	1:A:92:ARG:H	1:A:69:VAL:HG11	7	9.59
(2,180)	1:A:92:ARG:H	1:A:69:VAL:HG12	7	9.59
(2,180)	1:A:92:ARG:H	1:A:69:VAL:HG13	7	9.59
(2,180)	1:A:92:ARG:H	1:A:69:VAL:HG11	19	9.55
(2,180)	1:A:92:ARG:H	1:A:69:VAL:HG12	19	9.55
(2,180)	1:A:92:ARG:H	1:A:69:VAL:HG13	19	9.55
(2,180)	1:A:92:ARG:H	1:A:69:VAL:HG11	5	9.5
(2,180)	1:A:92:ARG:H	1:A:69:VAL:HG12	5	9.5
(2,180)	1:A:92:ARG:H	1:A:69:VAL:HG13	5	9.5
(2,180)	1:A:92:ARG:H	1:A:69:VAL:HG11	2	9.44
(2,180)	1:A:92:ARG:H	1:A:69:VAL:HG12	2	9.44
(2,180)	1:A:92:ARG:H	1:A:69:VAL:HG13	2	9.44
(2,180)	1:A:92:ARG:H	1:A:69:VAL:HG11	6	9.34
(2,180)	1:A:92:ARG:H	1:A:69:VAL:HG12	6	9.34
(2,180)	1:A:92:ARG:H	1:A:69:VAL:HG13	6	9.34
(2,530)	1:A:204:HIS:HE1	1:A:24:LEU:H	20	7.43
(2,934)	1:A:72:VAL:HB	1:A:77:LEU:H	18	7.41
(2,530)	1:A:204:HIS:HE1	1:A:24:LEU:H	14	7.41
(2,530)	1:A:204:HIS:HE1	1:A:24:LEU:H	5	7.39
(2,530)	1:A:204:HIS:HE1	1:A:24:LEU:H	12	7.24
(2,934)	1:A:72:VAL:HB	1:A:77:LEU:H	9	7.19
(2,530)	1:A:204:HIS:HE1	1:A:24:LEU:H	2	6.98
(2,530)	1:A:204:HIS:HE1	1:A:24:LEU:H	10	6.89
(2,530)	1:A:204:HIS:HE1	1:A:24:LEU:H	8	6.85
(2,530)	1:A:204:HIS:HE1	1:A:24:LEU:H	3	6.74
(2,530)	1:A:204:HIS:HE1	1:A:24:LEU:H	11	6.71
(2,530)	1:A:204:HIS:HE1	1:A:24:LEU:H	19	6.7
(2,934)	1:A:72:VAL:HB	1:A:77:LEU:H	15	6.69
(2,530)	1:A:204:HIS:HE1	1:A:24:LEU:H	13	6.66
(2,530)	1:A:204:HIS:HE1	1:A:24:LEU:H	1	6.64
(2,934)	1:A:72:VAL:HB	1:A:77:LEU:H	20	6.56
(2,530)	1:A:204:HIS:HE1	1:A:24:LEU:H	6	6.55
(2,934)	1:A:72:VAL:HB	1:A:77:LEU:H	1	6.45
(2,934)	1:A:72:VAL:HB	1:A:77:LEU:H	7	6.44
(2,934)	1:A:72:VAL:HB	1:A:77:LEU:H	10	6.44
(2,530)	1:A:204:HIS:HE1	1:A:24:LEU:H	7	6.4
(2,934)	1:A:72:VAL:HB	1:A:77:LEU:H	2	6.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,530)	1:A:204:HIS:HE1	1:A:24:LEU:H	17	6.29
(2,934)	1:A:72:VAL:HB	1:A:77:LEU:H	13	6.19
(2,934)	1:A:72:VAL:HB	1:A:77:LEU:H	3	6.12
(2,530)	1:A:204:HIS:HE1	1:A:24:LEU:H	4	6.09
(2,934)	1:A:72:VAL:HB	1:A:77:LEU:H	19	6.05
(2,934)	1:A:72:VAL:HB	1:A:77:LEU:H	12	6.03
(2,530)	1:A:204:HIS:HE1	1:A:24:LEU:H	15	6.03
(2,934)	1:A:72:VAL:HB	1:A:77:LEU:H	5	6.0
(2,934)	1:A:72:VAL:HB	1:A:77:LEU:H	16	5.97
(2,530)	1:A:204:HIS:HE1	1:A:24:LEU:H	16	5.97
(2,934)	1:A:72:VAL:HB	1:A:77:LEU:H	11	5.96
(2,934)	1:A:72:VAL:HB	1:A:77:LEU:H	8	5.93
(2,934)	1:A:72:VAL:HB	1:A:77:LEU:H	14	5.75
(2,934)	1:A:72:VAL:HB	1:A:77:LEU:H	17	5.72
(2,656)	1:A:39:LEU:H	1:A:19:LEU:HD21	16	5.66
(2,934)	1:A:72:VAL:HB	1:A:77:LEU:H	6	5.61
(2,933)	1:A:72:VAL:HA	1:A:77:LEU:H	9	5.58
(2,933)	1:A:72:VAL:HA	1:A:77:LEU:H	18	5.35
(2,934)	1:A:72:VAL:HB	1:A:77:LEU:H	4	5.19
(2,933)	1:A:72:VAL:HA	1:A:77:LEU:H	15	5.01
(2,836)	1:A:120:ILE:HD13	1:A:200:LEU:HD21	10	5.01
(2,472)	1:A:186:ILE:H	1:A:156:LEU:HD21	19	5.01
(2,933)	1:A:72:VAL:HA	1:A:77:LEU:H	2	4.99
(2,933)	1:A:72:VAL:HA	1:A:77:LEU:H	10	4.99
(2,933)	1:A:72:VAL:HA	1:A:77:LEU:H	20	4.97
(2,933)	1:A:72:VAL:HA	1:A:77:LEU:H	1	4.93
(2,933)	1:A:72:VAL:HA	1:A:77:LEU:H	12	4.89
(2,933)	1:A:72:VAL:HA	1:A:77:LEU:H	16	4.87
(2,933)	1:A:72:VAL:HA	1:A:77:LEU:H	7	4.8
(2,933)	1:A:72:VAL:HA	1:A:77:LEU:H	17	4.78
(2,472)	1:A:186:ILE:H	1:A:156:LEU:HD21	6	4.78
(2,933)	1:A:72:VAL:HA	1:A:77:LEU:H	14	4.77
(2,318)	1:A:125:ARG:H	1:A:92:ARG:H	2	4.77
(2,656)	1:A:39:LEU:H	1:A:19:LEU:HD21	18	4.74
(2,472)	1:A:186:ILE:H	1:A:156:LEU:HD21	8	4.74
(2,656)	1:A:39:LEU:H	1:A:19:LEU:HD21	20	4.73
(2,318)	1:A:125:ARG:H	1:A:92:ARG:H	9	4.69
(2,933)	1:A:72:VAL:HA	1:A:77:LEU:H	19	4.66
(2,933)	1:A:72:VAL:HA	1:A:77:LEU:H	13	4.63
(2,933)	1:A:72:VAL:HA	1:A:77:LEU:H	5	4.62
(2,472)	1:A:186:ILE:H	1:A:156:LEU:HD21	12	4.55
(2,832)	1:A:120:ILE:HD11	1:A:200:LEU:HD21	17	4.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,318)	1:A:125:ARG:H	1:A:92:ARG:H	4	4.51
(2,318)	1:A:125:ARG:H	1:A:92:ARG:H	1	4.5
(2,933)	1:A:72:VAL:HA	1:A:77:LEU:H	8	4.49
(2,318)	1:A:125:ARG:H	1:A:92:ARG:H	18	4.49
(2,472)	1:A:186:ILE:H	1:A:156:LEU:HD21	14	4.48
(2,832)	1:A:120:ILE:HD11	1:A:200:LEU:HD21	10	4.39
(2,933)	1:A:72:VAL:HA	1:A:77:LEU:H	11	4.38
(2,472)	1:A:186:ILE:H	1:A:156:LEU:HD21	1	4.37
(2,836)	1:A:120:ILE:HD13	1:A:200:LEU:HD21	8	4.36
(2,318)	1:A:125:ARG:H	1:A:92:ARG:H	8	4.35
(2,318)	1:A:125:ARG:H	1:A:92:ARG:H	11	4.34
(2,318)	1:A:125:ARG:H	1:A:92:ARG:H	5	4.31
(2,832)	1:A:120:ILE:HD11	1:A:200:LEU:HD21	6	4.29
(2,318)	1:A:125:ARG:H	1:A:92:ARG:H	7	4.25
(2,836)	1:A:120:ILE:HD13	1:A:200:LEU:HD21	11	4.24
(2,933)	1:A:72:VAL:HA	1:A:77:LEU:H	3	4.23
(2,988)	1:A:129:TRP:HE1	4:A:305:PX4:C2	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:307:PX4:C2	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:309:PX4:C2	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:311:PX4:C2	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:313:PX4:C2	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:315:PX4:C2	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:317:PX4:C2	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:319:PX4:C2	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:321:PX4:C2	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:323:PX4:C2	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:325:PX4:C2	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:327:PX4:C2	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:329:PX4:C2	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:331:PX4:C2	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:333:PX4:C2	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:335:PX4:C2	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:337:PX4:C2	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:339:PX4:C2	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:341:PX4:C2	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:343:PX4:C2	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:345:PX4:C2	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:347:PX4:C2	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:349:PX4:C2	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:351:PX4:C2	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:353:PX4:C2	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:355:PX4:C2	3	4.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,988)	1:A:129:TRP:HE1	4:A:357:PX4:C2	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:359:PX4:C2	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:361:PX4:C2	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:363:PX4:C2	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:402:PX4:C2	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:404:PX4:C2	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:406:PX4:C2	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:408:PX4:C2	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:410:PX4:C2	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:412:PX4:C2	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:414:PX4:C2	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:416:PX4:C2	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:418:PX4:C2	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:420:PX4:C2	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:422:PX4:C2	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:424:PX4:C2	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:426:PX4:C2	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:428:PX4:C2	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:430:PX4:C2	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:305:PX4:C1	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:307:PX4:C1	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:309:PX4:C1	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:311:PX4:C1	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:313:PX4:C1	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:315:PX4:C1	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:317:PX4:C1	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:319:PX4:C1	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:321:PX4:C1	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:323:PX4:C1	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:325:PX4:C1	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:327:PX4:C1	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:329:PX4:C1	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:331:PX4:C1	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:333:PX4:C1	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:335:PX4:C1	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:337:PX4:C1	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:339:PX4:C1	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:341:PX4:C1	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:343:PX4:C1	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:345:PX4:C1	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:347:PX4:C1	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:349:PX4:C1	3	4.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,988)	1:A:129:TRP:HE1	4:A:351:PX4:C1	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:353:PX4:C1	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:355:PX4:C1	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:357:PX4:C1	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:359:PX4:C1	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:361:PX4:C1	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:363:PX4:C1	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:402:PX4:C1	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:404:PX4:C1	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:406:PX4:C1	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:408:PX4:C1	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:410:PX4:C1	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:412:PX4:C1	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:414:PX4:C1	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:416:PX4:C1	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:418:PX4:C1	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:420:PX4:C1	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:422:PX4:C1	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:424:PX4:C1	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:426:PX4:C1	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:428:PX4:C1	3	4.22
(2,988)	1:A:129:TRP:HE1	4:A:430:PX4:C1	3	4.22
(2,836)	1:A:120:ILE:HD13	1:A:200:LEU:HD21	5	4.21
(2,836)	1:A:120:ILE:HD13	1:A:200:LEU:HD21	2	4.17
(2,318)	1:A:125:ARG:H	1:A:92:ARG:H	12	4.17
(2,832)	1:A:120:ILE:HD11	1:A:200:LEU:HD21	14	4.15
(2,318)	1:A:125:ARG:H	1:A:92:ARG:H	3	4.11
(2,985)	1:A:80:ASN:H	1:A:78:PHE:HD1	5	4.1
(2,882)	1:A:24:LEU:HD11	1:A:73:ALA:HB1	16	4.1
(2,882)	1:A:24:LEU:HD11	1:A:73:ALA:HB2	16	4.1
(2,882)	1:A:24:LEU:HD11	1:A:73:ALA:HB3	16	4.1
(2,882)	1:A:24:LEU:HD12	1:A:73:ALA:HB1	16	4.1
(2,882)	1:A:24:LEU:HD12	1:A:73:ALA:HB2	16	4.1
(2,882)	1:A:24:LEU:HD12	1:A:73:ALA:HB3	16	4.1
(2,882)	1:A:24:LEU:HD13	1:A:73:ALA:HB1	16	4.1
(2,882)	1:A:24:LEU:HD13	1:A:73:ALA:HB2	16	4.1
(2,882)	1:A:24:LEU:HD13	1:A:73:ALA:HB3	16	4.1
(2,318)	1:A:125:ARG:H	1:A:92:ARG:H	17	4.1
(2,832)	1:A:120:ILE:HD11	1:A:200:LEU:HD21	11	4.09
(2,933)	1:A:72:VAL:HA	1:A:77:LEU:H	6	4.07
(2,657)	1:A:39:LEU:H	1:A:19:LEU:HD22	18	4.06
(2,657)	1:A:39:LEU:H	1:A:19:LEU:HD23	18	4.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,531)	1:A:205:SER:H	1:A:204:HIS:HE1	6	4.06
(2,318)	1:A:125:ARG:H	1:A:92:ARG:H	10	4.06
(2,933)	1:A:72:VAL:HA	1:A:77:LEU:H	4	4.05
(2,832)	1:A:120:ILE:HD11	1:A:200:LEU:HD21	5	4.05
(2,318)	1:A:125:ARG:H	1:A:92:ARG:H	19	4.02
(3,36)	1:A:129:TRP:HE1	4:A:305:PX4:N1	3	3.98
(3,36)	1:A:129:TRP:HE1	4:A:307:PX4:N1	3	3.98
(3,36)	1:A:129:TRP:HE1	4:A:309:PX4:N1	3	3.98
(3,36)	1:A:129:TRP:HE1	4:A:311:PX4:N1	3	3.98
(3,36)	1:A:129:TRP:HE1	4:A:313:PX4:N1	3	3.98
(3,36)	1:A:129:TRP:HE1	4:A:315:PX4:N1	3	3.98
(3,36)	1:A:129:TRP:HE1	4:A:317:PX4:N1	3	3.98
(3,36)	1:A:129:TRP:HE1	4:A:319:PX4:N1	3	3.98
(3,36)	1:A:129:TRP:HE1	4:A:321:PX4:N1	3	3.98
(3,36)	1:A:129:TRP:HE1	4:A:323:PX4:N1	3	3.98
(3,36)	1:A:129:TRP:HE1	4:A:325:PX4:N1	3	3.98
(3,36)	1:A:129:TRP:HE1	4:A:327:PX4:N1	3	3.98
(3,36)	1:A:129:TRP:HE1	4:A:329:PX4:N1	3	3.98
(3,36)	1:A:129:TRP:HE1	4:A:331:PX4:N1	3	3.98
(3,36)	1:A:129:TRP:HE1	4:A:333:PX4:N1	3	3.98
(3,36)	1:A:129:TRP:HE1	4:A:335:PX4:N1	3	3.98
(3,36)	1:A:129:TRP:HE1	4:A:337:PX4:N1	3	3.98
(3,36)	1:A:129:TRP:HE1	4:A:339:PX4:N1	3	3.98
(3,36)	1:A:129:TRP:HE1	4:A:341:PX4:N1	3	3.98
(3,36)	1:A:129:TRP:HE1	4:A:343:PX4:N1	3	3.98
(3,36)	1:A:129:TRP:HE1	4:A:345:PX4:N1	3	3.98
(3,36)	1:A:129:TRP:HE1	4:A:347:PX4:N1	3	3.98
(3,36)	1:A:129:TRP:HE1	4:A:349:PX4:N1	3	3.98
(3,36)	1:A:129:TRP:HE1	4:A:351:PX4:N1	3	3.98
(3,36)	1:A:129:TRP:HE1	4:A:353:PX4:N1	3	3.98
(3,36)	1:A:129:TRP:HE1	4:A:355:PX4:N1	3	3.98
(3,36)	1:A:129:TRP:HE1	4:A:357:PX4:N1	3	3.98
(3,36)	1:A:129:TRP:HE1	4:A:359:PX4:N1	3	3.98
(3,36)	1:A:129:TRP:HE1	4:A:361:PX4:N1	3	3.98
(3,36)	1:A:129:TRP:HE1	4:A:363:PX4:N1	3	3.98
(3,36)	1:A:129:TRP:HE1	4:A:402:PX4:N1	3	3.98
(3,36)	1:A:129:TRP:HE1	4:A:404:PX4:N1	3	3.98
(3,36)	1:A:129:TRP:HE1	4:A:406:PX4:N1	3	3.98
(3,36)	1:A:129:TRP:HE1	4:A:408:PX4:N1	3	3.98
(3,36)	1:A:129:TRP:HE1	4:A:410:PX4:N1	3	3.98
(3,36)	1:A:129:TRP:HE1	4:A:412:PX4:N1	3	3.98
(3,36)	1:A:129:TRP:HE1	4:A:414:PX4:N1	3	3.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,36)	1:A:129:TRP:HE1	4:A:416:PX4:N1	3	3.98
(3,36)	1:A:129:TRP:HE1	4:A:418:PX4:N1	3	3.98
(3,36)	1:A:129:TRP:HE1	4:A:420:PX4:N1	3	3.98
(3,36)	1:A:129:TRP:HE1	4:A:422:PX4:N1	3	3.98
(3,36)	1:A:129:TRP:HE1	4:A:424:PX4:N1	3	3.98
(3,36)	1:A:129:TRP:HE1	4:A:426:PX4:N1	3	3.98
(3,36)	1:A:129:TRP:HE1	4:A:428:PX4:N1	3	3.98
(3,36)	1:A:129:TRP:HE1	4:A:430:PX4:N1	3	3.98
(2,318)	1:A:125:ARG:H	1:A:92:ARG:H	16	3.96
(2,318)	1:A:125:ARG:H	1:A:92:ARG:H	14	3.95
(2,318)	1:A:125:ARG:H	1:A:92:ARG:H	15	3.93
(2,318)	1:A:125:ARG:H	1:A:92:ARG:H	13	3.92
(2,757)	1:A:54:LEU:HD21	1:A:39:LEU:HD11	15	3.87
(2,757)	1:A:54:LEU:HD21	1:A:39:LEU:HD12	15	3.87
(2,757)	1:A:54:LEU:HD21	1:A:39:LEU:HD13	15	3.87
(2,473)	1:A:186:ILE:H	1:A:156:LEU:HD22	1	3.86
(2,473)	1:A:186:ILE:H	1:A:156:LEU:HD23	1	3.86
(2,473)	1:A:186:ILE:H	1:A:156:LEU:HD22	12	3.85
(2,473)	1:A:186:ILE:H	1:A:156:LEU:HD23	12	3.85
(2,882)	1:A:24:LEU:HD11	1:A:73:ALA:HB1	18	3.81
(2,882)	1:A:24:LEU:HD11	1:A:73:ALA:HB2	18	3.81
(2,882)	1:A:24:LEU:HD11	1:A:73:ALA:HB3	18	3.81
(2,882)	1:A:24:LEU:HD12	1:A:73:ALA:HB1	18	3.81
(2,882)	1:A:24:LEU:HD12	1:A:73:ALA:HB2	18	3.81
(2,882)	1:A:24:LEU:HD12	1:A:73:ALA:HB3	18	3.81
(2,882)	1:A:24:LEU:HD13	1:A:73:ALA:HB1	18	3.81
(2,882)	1:A:24:LEU:HD13	1:A:73:ALA:HB2	18	3.81
(2,882)	1:A:24:LEU:HD13	1:A:73:ALA:HB3	18	3.81
(2,832)	1:A:120:ILE:HD11	1:A:200:LEU:HD21	2	3.79
(2,318)	1:A:125:ARG:H	1:A:92:ARG:H	6	3.79
(2,882)	1:A:24:LEU:HD11	1:A:73:ALA:HB1	19	3.77
(2,882)	1:A:24:LEU:HD11	1:A:73:ALA:HB2	19	3.77
(2,882)	1:A:24:LEU:HD11	1:A:73:ALA:HB3	19	3.77
(2,882)	1:A:24:LEU:HD12	1:A:73:ALA:HB1	19	3.77
(2,882)	1:A:24:LEU:HD12	1:A:73:ALA:HB2	19	3.77
(2,882)	1:A:24:LEU:HD12	1:A:73:ALA:HB3	19	3.77
(2,882)	1:A:24:LEU:HD13	1:A:73:ALA:HB1	19	3.77
(2,882)	1:A:24:LEU:HD13	1:A:73:ALA:HB2	19	3.77
(2,882)	1:A:24:LEU:HD13	1:A:73:ALA:HB3	19	3.77
(2,836)	1:A:120:ILE:HD13	1:A:200:LEU:HD21	14	3.77
(3,36)	1:A:129:TRP:HE1	4:A:305:PX4:N1	8	3.74
(3,36)	1:A:129:TRP:HE1	4:A:307:PX4:N1	8	3.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,36)	1:A:129:TRP:HE1	4:A:309:PX4:N1	8	3.74
(3,36)	1:A:129:TRP:HE1	4:A:311:PX4:N1	8	3.74
(3,36)	1:A:129:TRP:HE1	4:A:313:PX4:N1	8	3.74
(3,36)	1:A:129:TRP:HE1	4:A:315:PX4:N1	8	3.74
(3,36)	1:A:129:TRP:HE1	4:A:317:PX4:N1	8	3.74
(3,36)	1:A:129:TRP:HE1	4:A:319:PX4:N1	8	3.74
(3,36)	1:A:129:TRP:HE1	4:A:321:PX4:N1	8	3.74
(3,36)	1:A:129:TRP:HE1	4:A:323:PX4:N1	8	3.74
(3,36)	1:A:129:TRP:HE1	4:A:325:PX4:N1	8	3.74
(3,36)	1:A:129:TRP:HE1	4:A:327:PX4:N1	8	3.74
(3,36)	1:A:129:TRP:HE1	4:A:329:PX4:N1	8	3.74
(3,36)	1:A:129:TRP:HE1	4:A:331:PX4:N1	8	3.74
(3,36)	1:A:129:TRP:HE1	4:A:333:PX4:N1	8	3.74
(3,36)	1:A:129:TRP:HE1	4:A:335:PX4:N1	8	3.74
(3,36)	1:A:129:TRP:HE1	4:A:337:PX4:N1	8	3.74
(3,36)	1:A:129:TRP:HE1	4:A:339:PX4:N1	8	3.74
(3,36)	1:A:129:TRP:HE1	4:A:341:PX4:N1	8	3.74
(3,36)	1:A:129:TRP:HE1	4:A:343:PX4:N1	8	3.74
(3,36)	1:A:129:TRP:HE1	4:A:345:PX4:N1	8	3.74
(3,36)	1:A:129:TRP:HE1	4:A:347:PX4:N1	8	3.74
(3,36)	1:A:129:TRP:HE1	4:A:349:PX4:N1	8	3.74
(3,36)	1:A:129:TRP:HE1	4:A:351:PX4:N1	8	3.74
(3,36)	1:A:129:TRP:HE1	4:A:353:PX4:N1	8	3.74
(3,36)	1:A:129:TRP:HE1	4:A:355:PX4:N1	8	3.74
(3,36)	1:A:129:TRP:HE1	4:A:357:PX4:N1	8	3.74
(3,36)	1:A:129:TRP:HE1	4:A:359:PX4:N1	8	3.74
(3,36)	1:A:129:TRP:HE1	4:A:361:PX4:N1	8	3.74
(3,36)	1:A:129:TRP:HE1	4:A:363:PX4:N1	8	3.74
(3,36)	1:A:129:TRP:HE1	4:A:402:PX4:N1	8	3.74
(3,36)	1:A:129:TRP:HE1	4:A:404:PX4:N1	8	3.74
(3,36)	1:A:129:TRP:HE1	4:A:406:PX4:N1	8	3.74
(3,36)	1:A:129:TRP:HE1	4:A:408:PX4:N1	8	3.74
(3,36)	1:A:129:TRP:HE1	4:A:410:PX4:N1	8	3.74
(3,36)	1:A:129:TRP:HE1	4:A:412:PX4:N1	8	3.74
(3,36)	1:A:129:TRP:HE1	4:A:414:PX4:N1	8	3.74
(3,36)	1:A:129:TRP:HE1	4:A:416:PX4:N1	8	3.74
(3,36)	1:A:129:TRP:HE1	4:A:418:PX4:N1	8	3.74
(3,36)	1:A:129:TRP:HE1	4:A:420:PX4:N1	8	3.74
(3,36)	1:A:129:TRP:HE1	4:A:422:PX4:N1	8	3.74
(3,36)	1:A:129:TRP:HE1	4:A:424:PX4:N1	8	3.74
(3,36)	1:A:129:TRP:HE1	4:A:426:PX4:N1	8	3.74
(3,36)	1:A:129:TRP:HE1	4:A:428:PX4:N1	8	3.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,36)	1:A:129:TRP:HE1	4:A:430:PX4:N1	8	3.74
(2,318)	1:A:125:ARG:H	1:A:92:ARG:H	20	3.74
(2,473)	1:A:186:ILE:H	1:A:156:LEU:HD22	6	3.71
(2,473)	1:A:186:ILE:H	1:A:156:LEU:HD23	6	3.71
(2,882)	1:A:24:LEU:HD11	1:A:73:ALA:HB1	4	3.68
(2,882)	1:A:24:LEU:HD11	1:A:73:ALA:HB2	4	3.68
(2,882)	1:A:24:LEU:HD11	1:A:73:ALA:HB3	4	3.68
(2,882)	1:A:24:LEU:HD12	1:A:73:ALA:HB1	4	3.68
(2,882)	1:A:24:LEU:HD12	1:A:73:ALA:HB2	4	3.68
(2,882)	1:A:24:LEU:HD12	1:A:73:ALA:HB3	4	3.68
(2,882)	1:A:24:LEU:HD13	1:A:73:ALA:HB1	4	3.68
(2,882)	1:A:24:LEU:HD13	1:A:73:ALA:HB2	4	3.68
(2,882)	1:A:24:LEU:HD13	1:A:73:ALA:HB3	4	3.68
(2,832)	1:A:120:ILE:HD11	1:A:200:LEU:HD21	8	3.68
(2,656)	1:A:39:LEU:H	1:A:19:LEU:HD21	10	3.68
(2,832)	1:A:120:ILE:HD11	1:A:200:LEU:HD21	20	3.67
(2,657)	1:A:39:LEU:H	1:A:19:LEU:HD22	20	3.65
(2,657)	1:A:39:LEU:H	1:A:19:LEU:HD23	20	3.65
(2,836)	1:A:120:ILE:HD13	1:A:200:LEU:HD21	6	3.64
(2,882)	1:A:24:LEU:HD11	1:A:73:ALA:HB1	15	3.63
(2,882)	1:A:24:LEU:HD11	1:A:73:ALA:HB2	15	3.63
(2,882)	1:A:24:LEU:HD11	1:A:73:ALA:HB3	15	3.63
(2,882)	1:A:24:LEU:HD12	1:A:73:ALA:HB1	15	3.63
(2,882)	1:A:24:LEU:HD12	1:A:73:ALA:HB2	15	3.63
(2,882)	1:A:24:LEU:HD12	1:A:73:ALA:HB3	15	3.63
(2,882)	1:A:24:LEU:HD13	1:A:73:ALA:HB1	15	3.63
(2,882)	1:A:24:LEU:HD13	1:A:73:ALA:HB2	15	3.63
(2,882)	1:A:24:LEU:HD13	1:A:73:ALA:HB3	15	3.63
(2,177)	1:A:171:HIS:H	1:A:134:ILE:HD11	18	3.57
(2,177)	1:A:171:HIS:H	1:A:134:ILE:HD12	18	3.57
(2,177)	1:A:171:HIS:H	1:A:134:ILE:HD13	18	3.57
(2,531)	1:A:205:SER:H	1:A:204:HIS:HE1	8	3.54
(2,531)	1:A:205:SER:H	1:A:204:HIS:HE1	16	3.53
(2,656)	1:A:39:LEU:H	1:A:19:LEU:HD21	9	3.52
(2,473)	1:A:186:ILE:H	1:A:156:LEU:HD22	14	3.49
(2,473)	1:A:186:ILE:H	1:A:156:LEU:HD23	14	3.49
(2,177)	1:A:171:HIS:H	1:A:134:ILE:HD11	9	3.46
(2,177)	1:A:171:HIS:H	1:A:134:ILE:HD12	9	3.46
(2,177)	1:A:171:HIS:H	1:A:134:ILE:HD13	9	3.46
(2,834)	1:A:120:ILE:HD12	1:A:200:LEU:HD21	10	3.45
(2,473)	1:A:186:ILE:H	1:A:156:LEU:HD22	8	3.44
(2,473)	1:A:186:ILE:H	1:A:156:LEU:HD23	8	3.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,941)	1:A:73:ALA:HA	1:A:77:LEU:H	2	3.43
(2,759)	1:A:54:LEU:HD21	1:A:59:ILE:HD11	7	3.43
(2,759)	1:A:54:LEU:HD21	1:A:59:ILE:HD12	7	3.43
(2,759)	1:A:54:LEU:HD21	1:A:59:ILE:HD13	7	3.43
(2,882)	1:A:24:LEU:HD11	1:A:73:ALA:HB1	1	3.42
(2,882)	1:A:24:LEU:HD11	1:A:73:ALA:HB2	1	3.42
(2,882)	1:A:24:LEU:HD11	1:A:73:ALA:HB3	1	3.42
(2,882)	1:A:24:LEU:HD12	1:A:73:ALA:HB1	1	3.42
(2,882)	1:A:24:LEU:HD12	1:A:73:ALA:HB2	1	3.42
(2,882)	1:A:24:LEU:HD12	1:A:73:ALA:HB3	1	3.42
(2,882)	1:A:24:LEU:HD13	1:A:73:ALA:HB1	1	3.42
(2,882)	1:A:24:LEU:HD13	1:A:73:ALA:HB2	1	3.42
(2,882)	1:A:24:LEU:HD13	1:A:73:ALA:HB3	1	3.42
(2,656)	1:A:39:LEU:H	1:A:19:LEU:HD21	15	3.42
(2,657)	1:A:39:LEU:H	1:A:19:LEU:HD22	16	3.39
(2,657)	1:A:39:LEU:H	1:A:19:LEU:HD23	16	3.39
(3,21)	1:A:77:LEU:H	4:A:305:PX4:C35	20	3.38
(3,21)	1:A:77:LEU:H	4:A:307:PX4:C35	20	3.38
(3,21)	1:A:77:LEU:H	4:A:309:PX4:C35	20	3.38
(3,21)	1:A:77:LEU:H	4:A:311:PX4:C35	20	3.38
(3,21)	1:A:77:LEU:H	4:A:313:PX4:C35	20	3.38
(3,21)	1:A:77:LEU:H	4:A:315:PX4:C35	20	3.38
(3,21)	1:A:77:LEU:H	4:A:317:PX4:C35	20	3.38
(3,21)	1:A:77:LEU:H	4:A:319:PX4:C35	20	3.38
(3,21)	1:A:77:LEU:H	4:A:321:PX4:C35	20	3.38
(3,21)	1:A:77:LEU:H	4:A:323:PX4:C35	20	3.38
(3,21)	1:A:77:LEU:H	4:A:325:PX4:C35	20	3.38
(3,21)	1:A:77:LEU:H	4:A:327:PX4:C35	20	3.38
(3,21)	1:A:77:LEU:H	4:A:329:PX4:C35	20	3.38
(3,21)	1:A:77:LEU:H	4:A:331:PX4:C35	20	3.38
(3,21)	1:A:77:LEU:H	4:A:333:PX4:C35	20	3.38
(3,21)	1:A:77:LEU:H	4:A:335:PX4:C35	20	3.38
(3,21)	1:A:77:LEU:H	4:A:337:PX4:C35	20	3.38
(3,21)	1:A:77:LEU:H	4:A:339:PX4:C35	20	3.38
(3,21)	1:A:77:LEU:H	4:A:341:PX4:C35	20	3.38
(3,21)	1:A:77:LEU:H	4:A:343:PX4:C35	20	3.38
(3,21)	1:A:77:LEU:H	4:A:345:PX4:C35	20	3.38
(3,21)	1:A:77:LEU:H	4:A:347:PX4:C35	20	3.38
(3,21)	1:A:77:LEU:H	4:A:349:PX4:C35	20	3.38
(3,21)	1:A:77:LEU:H	4:A:351:PX4:C35	20	3.38
(3,21)	1:A:77:LEU:H	4:A:353:PX4:C35	20	3.38
(3,21)	1:A:77:LEU:H	4:A:355:PX4:C35	20	3.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,21)	1:A:77:LEU:H	4:A:357:PX4:C35	20	3.38
(3,21)	1:A:77:LEU:H	4:A:359:PX4:C35	20	3.38
(3,21)	1:A:77:LEU:H	4:A:361:PX4:C35	20	3.38
(3,21)	1:A:77:LEU:H	4:A:363:PX4:C35	20	3.38
(3,21)	1:A:77:LEU:H	4:A:402:PX4:C35	20	3.38
(3,21)	1:A:77:LEU:H	4:A:404:PX4:C35	20	3.38
(3,21)	1:A:77:LEU:H	4:A:406:PX4:C35	20	3.38
(3,21)	1:A:77:LEU:H	4:A:408:PX4:C35	20	3.38
(3,21)	1:A:77:LEU:H	4:A:410:PX4:C35	20	3.38
(3,21)	1:A:77:LEU:H	4:A:412:PX4:C35	20	3.38
(3,21)	1:A:77:LEU:H	4:A:414:PX4:C35	20	3.38
(3,21)	1:A:77:LEU:H	4:A:416:PX4:C35	20	3.38
(3,21)	1:A:77:LEU:H	4:A:418:PX4:C35	20	3.38
(3,21)	1:A:77:LEU:H	4:A:420:PX4:C35	20	3.38
(3,21)	1:A:77:LEU:H	4:A:422:PX4:C35	20	3.38
(3,21)	1:A:77:LEU:H	4:A:424:PX4:C35	20	3.38
(3,21)	1:A:77:LEU:H	4:A:426:PX4:C35	20	3.38
(3,21)	1:A:77:LEU:H	4:A:428:PX4:C35	20	3.38
(3,21)	1:A:77:LEU:H	4:A:430:PX4:C35	20	3.38
(2,882)	1:A:24:LEU:HD11	1:A:73:ALA:HB1	2	3.38
(2,882)	1:A:24:LEU:HD11	1:A:73:ALA:HB2	2	3.38
(2,882)	1:A:24:LEU:HD11	1:A:73:ALA:HB3	2	3.38
(2,882)	1:A:24:LEU:HD12	1:A:73:ALA:HB1	2	3.38
(2,882)	1:A:24:LEU:HD12	1:A:73:ALA:HB2	2	3.38
(2,882)	1:A:24:LEU:HD12	1:A:73:ALA:HB3	2	3.38
(2,882)	1:A:24:LEU:HD13	1:A:73:ALA:HB1	2	3.38
(2,882)	1:A:24:LEU:HD13	1:A:73:ALA:HB2	2	3.38
(2,882)	1:A:24:LEU:HD13	1:A:73:ALA:HB3	2	3.38
(2,941)	1:A:73:ALA:HA	1:A:77:LEU:H	15	3.37
(2,759)	1:A:54:LEU:HD21	1:A:59:ILE:HD11	13	3.37
(2,759)	1:A:54:LEU:HD21	1:A:59:ILE:HD12	13	3.37
(2,759)	1:A:54:LEU:HD21	1:A:59:ILE:HD13	13	3.37
(2,757)	1:A:54:LEU:HD21	1:A:39:LEU:HD11	13	3.37
(2,757)	1:A:54:LEU:HD21	1:A:39:LEU:HD12	13	3.37
(2,757)	1:A:54:LEU:HD21	1:A:39:LEU:HD13	13	3.37
(2,177)	1:A:171:HIS:H	1:A:134:ILE:HD11	19	3.37
(2,177)	1:A:171:HIS:H	1:A:134:ILE:HD12	19	3.37
(2,177)	1:A:171:HIS:H	1:A:134:ILE:HD13	19	3.37
(2,177)	1:A:171:HIS:H	1:A:134:ILE:HD11	4	3.36
(2,177)	1:A:171:HIS:H	1:A:134:ILE:HD12	4	3.36
(2,177)	1:A:171:HIS:H	1:A:134:ILE:HD13	4	3.36
(2,985)	1:A:80:ASN:H	1:A:78:PHE:HD1	6	3.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,759)	1:A:54:LEU:HD21	1:A:59:ILE:HD11	19	3.35
(2,759)	1:A:54:LEU:HD21	1:A:59:ILE:HD12	19	3.35
(2,759)	1:A:54:LEU:HD21	1:A:59:ILE:HD13	19	3.35
(2,882)	1:A:24:LEU:HD11	1:A:73:ALA:HB1	5	3.34
(2,882)	1:A:24:LEU:HD11	1:A:73:ALA:HB2	5	3.34
(2,882)	1:A:24:LEU:HD11	1:A:73:ALA:HB3	5	3.34
(2,882)	1:A:24:LEU:HD12	1:A:73:ALA:HB1	5	3.34
(2,882)	1:A:24:LEU:HD12	1:A:73:ALA:HB2	5	3.34
(2,882)	1:A:24:LEU:HD12	1:A:73:ALA:HB3	5	3.34
(2,882)	1:A:24:LEU:HD13	1:A:73:ALA:HB1	5	3.34
(2,882)	1:A:24:LEU:HD13	1:A:73:ALA:HB2	5	3.34
(2,882)	1:A:24:LEU:HD13	1:A:73:ALA:HB3	5	3.34
(2,882)	1:A:24:LEU:HD11	1:A:73:ALA:HB1	17	3.34
(2,882)	1:A:24:LEU:HD11	1:A:73:ALA:HB2	17	3.34
(2,882)	1:A:24:LEU:HD11	1:A:73:ALA:HB3	17	3.34
(2,882)	1:A:24:LEU:HD12	1:A:73:ALA:HB1	17	3.34
(2,882)	1:A:24:LEU:HD12	1:A:73:ALA:HB2	17	3.34
(2,882)	1:A:24:LEU:HD12	1:A:73:ALA:HB3	17	3.34
(2,882)	1:A:24:LEU:HD13	1:A:73:ALA:HB1	17	3.34
(2,882)	1:A:24:LEU:HD13	1:A:73:ALA:HB2	17	3.34
(2,882)	1:A:24:LEU:HD13	1:A:73:ALA:HB3	17	3.34
(2,177)	1:A:171:HIS:H	1:A:134:ILE:HD11	1	3.34
(2,177)	1:A:171:HIS:H	1:A:134:ILE:HD12	1	3.34
(2,177)	1:A:171:HIS:H	1:A:134:ILE:HD13	1	3.34
(2,177)	1:A:171:HIS:H	1:A:134:ILE:HD11	3	3.32
(2,177)	1:A:171:HIS:H	1:A:134:ILE:HD12	3	3.32
(2,177)	1:A:171:HIS:H	1:A:134:ILE:HD13	3	3.32
(2,473)	1:A:186:ILE:H	1:A:156:LEU:HD22	19	3.31
(2,473)	1:A:186:ILE:H	1:A:156:LEU:HD23	19	3.31
(2,836)	1:A:120:ILE:HD13	1:A:200:LEU:HD21	17	3.28
(2,757)	1:A:54:LEU:HD21	1:A:39:LEU:HD11	19	3.28
(2,757)	1:A:54:LEU:HD21	1:A:39:LEU:HD12	19	3.28
(2,757)	1:A:54:LEU:HD21	1:A:39:LEU:HD13	19	3.28
(2,531)	1:A:205:SER:H	1:A:204:HIS:HE1	3	3.26
(2,177)	1:A:171:HIS:H	1:A:134:ILE:HD11	11	3.26
(2,177)	1:A:171:HIS:H	1:A:134:ILE:HD12	11	3.26
(2,177)	1:A:171:HIS:H	1:A:134:ILE:HD13	11	3.26
(2,974)	1:A:78:PHE:H	1:A:77:LEU:HD21	18	3.25
(3,21)	1:A:77:LEU:H	4:A:305:PX4:C35	9	3.24
(3,21)	1:A:77:LEU:H	4:A:307:PX4:C35	9	3.24
(3,21)	1:A:77:LEU:H	4:A:309:PX4:C35	9	3.24
(3,21)	1:A:77:LEU:H	4:A:311:PX4:C35	9	3.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,21)	1:A:77:LEU:H	4:A:313:PX4:C35	9	3.24
(3,21)	1:A:77:LEU:H	4:A:315:PX4:C35	9	3.24
(3,21)	1:A:77:LEU:H	4:A:317:PX4:C35	9	3.24
(3,21)	1:A:77:LEU:H	4:A:319:PX4:C35	9	3.24
(3,21)	1:A:77:LEU:H	4:A:321:PX4:C35	9	3.24
(3,21)	1:A:77:LEU:H	4:A:323:PX4:C35	9	3.24
(3,21)	1:A:77:LEU:H	4:A:325:PX4:C35	9	3.24
(3,21)	1:A:77:LEU:H	4:A:327:PX4:C35	9	3.24
(3,21)	1:A:77:LEU:H	4:A:329:PX4:C35	9	3.24
(3,21)	1:A:77:LEU:H	4:A:331:PX4:C35	9	3.24
(3,21)	1:A:77:LEU:H	4:A:333:PX4:C35	9	3.24
(3,21)	1:A:77:LEU:H	4:A:335:PX4:C35	9	3.24
(3,21)	1:A:77:LEU:H	4:A:337:PX4:C35	9	3.24
(3,21)	1:A:77:LEU:H	4:A:339:PX4:C35	9	3.24
(3,21)	1:A:77:LEU:H	4:A:341:PX4:C35	9	3.24
(3,21)	1:A:77:LEU:H	4:A:343:PX4:C35	9	3.24
(3,21)	1:A:77:LEU:H	4:A:345:PX4:C35	9	3.24
(3,21)	1:A:77:LEU:H	4:A:347:PX4:C35	9	3.24
(3,21)	1:A:77:LEU:H	4:A:349:PX4:C35	9	3.24
(3,21)	1:A:77:LEU:H	4:A:351:PX4:C35	9	3.24
(3,21)	1:A:77:LEU:H	4:A:353:PX4:C35	9	3.24
(3,21)	1:A:77:LEU:H	4:A:355:PX4:C35	9	3.24
(3,21)	1:A:77:LEU:H	4:A:357:PX4:C35	9	3.24
(3,21)	1:A:77:LEU:H	4:A:359:PX4:C35	9	3.24
(3,21)	1:A:77:LEU:H	4:A:361:PX4:C35	9	3.24
(3,21)	1:A:77:LEU:H	4:A:363:PX4:C35	9	3.24
(3,21)	1:A:77:LEU:H	4:A:402:PX4:C35	9	3.24
(3,21)	1:A:77:LEU:H	4:A:404:PX4:C35	9	3.24
(3,21)	1:A:77:LEU:H	4:A:406:PX4:C35	9	3.24
(3,21)	1:A:77:LEU:H	4:A:408:PX4:C35	9	3.24
(3,21)	1:A:77:LEU:H	4:A:410:PX4:C35	9	3.24
(3,21)	1:A:77:LEU:H	4:A:412:PX4:C35	9	3.24
(3,21)	1:A:77:LEU:H	4:A:414:PX4:C35	9	3.24
(3,21)	1:A:77:LEU:H	4:A:416:PX4:C35	9	3.24
(3,21)	1:A:77:LEU:H	4:A:418:PX4:C35	9	3.24
(3,21)	1:A:77:LEU:H	4:A:420:PX4:C35	9	3.24
(3,21)	1:A:77:LEU:H	4:A:422:PX4:C35	9	3.24
(3,21)	1:A:77:LEU:H	4:A:424:PX4:C35	9	3.24
(3,21)	1:A:77:LEU:H	4:A:426:PX4:C35	9	3.24
(3,21)	1:A:77:LEU:H	4:A:428:PX4:C35	9	3.24
(3,21)	1:A:77:LEU:H	4:A:430:PX4:C35	9	3.24
(2,941)	1:A:73:ALA:HA	1:A:77:LEU:H	1	3.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,759)	1:A:54:LEU:HD21	1:A:59:ILE:HD11	11	3.22
(2,759)	1:A:54:LEU:HD21	1:A:59:ILE:HD12	11	3.22
(2,759)	1:A:54:LEU:HD21	1:A:59:ILE:HD13	11	3.22
(2,882)	1:A:24:LEU:HD11	1:A:73:ALA:HB1	14	3.21
(2,882)	1:A:24:LEU:HD11	1:A:73:ALA:HB2	14	3.21
(2,882)	1:A:24:LEU:HD11	1:A:73:ALA:HB3	14	3.21
(2,882)	1:A:24:LEU:HD12	1:A:73:ALA:HB1	14	3.21
(2,882)	1:A:24:LEU:HD12	1:A:73:ALA:HB2	14	3.21
(2,882)	1:A:24:LEU:HD12	1:A:73:ALA:HB3	14	3.21
(2,882)	1:A:24:LEU:HD13	1:A:73:ALA:HB1	14	3.21
(2,882)	1:A:24:LEU:HD13	1:A:73:ALA:HB2	14	3.21
(2,882)	1:A:24:LEU:HD13	1:A:73:ALA:HB3	14	3.21
(2,759)	1:A:54:LEU:HD21	1:A:59:ILE:HD11	1	3.2
(2,759)	1:A:54:LEU:HD21	1:A:59:ILE:HD12	1	3.2
(2,759)	1:A:54:LEU:HD21	1:A:59:ILE:HD13	1	3.2
(2,177)	1:A:171:HIS:H	1:A:134:ILE:HD11	15	3.2
(2,177)	1:A:171:HIS:H	1:A:134:ILE:HD12	15	3.2
(2,177)	1:A:171:HIS:H	1:A:134:ILE:HD13	15	3.2
(2,836)	1:A:120:ILE:HD13	1:A:200:LEU:HD21	15	3.19
(2,471)	1:A:186:ILE:H	1:A:156:LEU:HD11	9	3.19
(2,471)	1:A:186:ILE:H	1:A:156:LEU:HD12	9	3.19
(2,471)	1:A:186:ILE:H	1:A:156:LEU:HD13	9	3.19
(2,941)	1:A:73:ALA:HA	1:A:77:LEU:H	9	3.18
(2,531)	1:A:205:SER:H	1:A:204:HIS:HE1	5	3.18
(2,531)	1:A:205:SER:H	1:A:204:HIS:HE1	19	3.18
(2,882)	1:A:24:LEU:HD11	1:A:73:ALA:HB1	9	3.16
(2,882)	1:A:24:LEU:HD11	1:A:73:ALA:HB2	9	3.16
(2,882)	1:A:24:LEU:HD11	1:A:73:ALA:HB3	9	3.16
(2,882)	1:A:24:LEU:HD12	1:A:73:ALA:HB1	9	3.16
(2,882)	1:A:24:LEU:HD12	1:A:73:ALA:HB2	9	3.16
(2,882)	1:A:24:LEU:HD12	1:A:73:ALA:HB3	9	3.16
(2,882)	1:A:24:LEU:HD13	1:A:73:ALA:HB1	9	3.16
(2,882)	1:A:24:LEU:HD13	1:A:73:ALA:HB2	9	3.16
(2,882)	1:A:24:LEU:HD13	1:A:73:ALA:HB3	9	3.16
(2,177)	1:A:171:HIS:H	1:A:134:ILE:HD11	8	3.16
(2,177)	1:A:171:HIS:H	1:A:134:ILE:HD12	8	3.16
(2,177)	1:A:171:HIS:H	1:A:134:ILE:HD13	8	3.16
(2,941)	1:A:73:ALA:HA	1:A:77:LEU:H	7	3.15
(2,941)	1:A:73:ALA:HA	1:A:77:LEU:H	10	3.15
(2,941)	1:A:73:ALA:HA	1:A:77:LEU:H	18	3.15
(2,82)	1:A:58:VAL:H	1:A:48:LEU:HD21	18	3.15
(2,531)	1:A:205:SER:H	1:A:204:HIS:HE1	17	3.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,882)	1:A:24:LEU:HD11	1:A:73:ALA:HB1	3	3.14
(2,882)	1:A:24:LEU:HD11	1:A:73:ALA:HB2	3	3.14
(2,882)	1:A:24:LEU:HD11	1:A:73:ALA:HB3	3	3.14
(2,882)	1:A:24:LEU:HD12	1:A:73:ALA:HB1	3	3.14
(2,882)	1:A:24:LEU:HD12	1:A:73:ALA:HB2	3	3.14
(2,882)	1:A:24:LEU:HD12	1:A:73:ALA:HB3	3	3.14
(2,882)	1:A:24:LEU:HD13	1:A:73:ALA:HB1	3	3.14
(2,882)	1:A:24:LEU:HD13	1:A:73:ALA:HB2	3	3.14
(2,882)	1:A:24:LEU:HD13	1:A:73:ALA:HB3	3	3.14
(2,941)	1:A:73:ALA:HA	1:A:77:LEU:H	12	3.13
(2,731)	1:A:211:VAL:HG13	1:A:226:LEU:HD21	1	3.13
(3,36)	1:A:129:TRP:HE1	4:A:305:PX4:N1	6	3.12
(3,36)	1:A:129:TRP:HE1	4:A:307:PX4:N1	6	3.12
(3,36)	1:A:129:TRP:HE1	4:A:309:PX4:N1	6	3.12
(3,36)	1:A:129:TRP:HE1	4:A:311:PX4:N1	6	3.12
(3,36)	1:A:129:TRP:HE1	4:A:313:PX4:N1	6	3.12
(3,36)	1:A:129:TRP:HE1	4:A:315:PX4:N1	6	3.12
(3,36)	1:A:129:TRP:HE1	4:A:317:PX4:N1	6	3.12
(3,36)	1:A:129:TRP:HE1	4:A:319:PX4:N1	6	3.12
(3,36)	1:A:129:TRP:HE1	4:A:321:PX4:N1	6	3.12
(3,36)	1:A:129:TRP:HE1	4:A:323:PX4:N1	6	3.12
(3,36)	1:A:129:TRP:HE1	4:A:325:PX4:N1	6	3.12
(3,36)	1:A:129:TRP:HE1	4:A:327:PX4:N1	6	3.12
(3,36)	1:A:129:TRP:HE1	4:A:329:PX4:N1	6	3.12
(3,36)	1:A:129:TRP:HE1	4:A:331:PX4:N1	6	3.12
(3,36)	1:A:129:TRP:HE1	4:A:333:PX4:N1	6	3.12
(3,36)	1:A:129:TRP:HE1	4:A:335:PX4:N1	6	3.12
(3,36)	1:A:129:TRP:HE1	4:A:337:PX4:N1	6	3.12
(3,36)	1:A:129:TRP:HE1	4:A:339:PX4:N1	6	3.12
(3,36)	1:A:129:TRP:HE1	4:A:341:PX4:N1	6	3.12
(3,36)	1:A:129:TRP:HE1	4:A:343:PX4:N1	6	3.12
(3,36)	1:A:129:TRP:HE1	4:A:345:PX4:N1	6	3.12
(3,36)	1:A:129:TRP:HE1	4:A:347:PX4:N1	6	3.12
(3,36)	1:A:129:TRP:HE1	4:A:349:PX4:N1	6	3.12
(3,36)	1:A:129:TRP:HE1	4:A:351:PX4:N1	6	3.12
(3,36)	1:A:129:TRP:HE1	4:A:353:PX4:N1	6	3.12
(3,36)	1:A:129:TRP:HE1	4:A:355:PX4:N1	6	3.12
(3,36)	1:A:129:TRP:HE1	4:A:357:PX4:N1	6	3.12
(3,36)	1:A:129:TRP:HE1	4:A:359:PX4:N1	6	3.12
(3,36)	1:A:129:TRP:HE1	4:A:361:PX4:N1	6	3.12
(3,36)	1:A:129:TRP:HE1	4:A:363:PX4:N1	6	3.12
(3,36)	1:A:129:TRP:HE1	4:A:402:PX4:N1	6	3.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,36)	1:A:129:TRP:HE1	4:A:404:PX4:N1	6	3.12
(3,36)	1:A:129:TRP:HE1	4:A:406:PX4:N1	6	3.12
(3,36)	1:A:129:TRP:HE1	4:A:408:PX4:N1	6	3.12
(3,36)	1:A:129:TRP:HE1	4:A:410:PX4:N1	6	3.12
(3,36)	1:A:129:TRP:HE1	4:A:412:PX4:N1	6	3.12
(3,36)	1:A:129:TRP:HE1	4:A:414:PX4:N1	6	3.12
(3,36)	1:A:129:TRP:HE1	4:A:416:PX4:N1	6	3.12
(3,36)	1:A:129:TRP:HE1	4:A:418:PX4:N1	6	3.12
(3,36)	1:A:129:TRP:HE1	4:A:420:PX4:N1	6	3.12
(3,36)	1:A:129:TRP:HE1	4:A:422:PX4:N1	6	3.12
(3,36)	1:A:129:TRP:HE1	4:A:424:PX4:N1	6	3.12
(3,36)	1:A:129:TRP:HE1	4:A:426:PX4:N1	6	3.12
(3,36)	1:A:129:TRP:HE1	4:A:428:PX4:N1	6	3.12
(3,36)	1:A:129:TRP:HE1	4:A:430:PX4:N1	6	3.12
(3,21)	1:A:77:LEU:H	4:A:305:PX4:C35	7	3.12
(3,21)	1:A:77:LEU:H	4:A:307:PX4:C35	7	3.12
(3,21)	1:A:77:LEU:H	4:A:309:PX4:C35	7	3.12
(3,21)	1:A:77:LEU:H	4:A:311:PX4:C35	7	3.12
(3,21)	1:A:77:LEU:H	4:A:313:PX4:C35	7	3.12
(3,21)	1:A:77:LEU:H	4:A:315:PX4:C35	7	3.12
(3,21)	1:A:77:LEU:H	4:A:317:PX4:C35	7	3.12
(3,21)	1:A:77:LEU:H	4:A:319:PX4:C35	7	3.12
(3,21)	1:A:77:LEU:H	4:A:321:PX4:C35	7	3.12
(3,21)	1:A:77:LEU:H	4:A:323:PX4:C35	7	3.12
(3,21)	1:A:77:LEU:H	4:A:325:PX4:C35	7	3.12
(3,21)	1:A:77:LEU:H	4:A:327:PX4:C35	7	3.12
(3,21)	1:A:77:LEU:H	4:A:329:PX4:C35	7	3.12
(3,21)	1:A:77:LEU:H	4:A:331:PX4:C35	7	3.12
(3,21)	1:A:77:LEU:H	4:A:333:PX4:C35	7	3.12
(3,21)	1:A:77:LEU:H	4:A:335:PX4:C35	7	3.12
(3,21)	1:A:77:LEU:H	4:A:337:PX4:C35	7	3.12
(3,21)	1:A:77:LEU:H	4:A:339:PX4:C35	7	3.12
(3,21)	1:A:77:LEU:H	4:A:341:PX4:C35	7	3.12
(3,21)	1:A:77:LEU:H	4:A:343:PX4:C35	7	3.12
(3,21)	1:A:77:LEU:H	4:A:345:PX4:C35	7	3.12
(3,21)	1:A:77:LEU:H	4:A:347:PX4:C35	7	3.12
(3,21)	1:A:77:LEU:H	4:A:349:PX4:C35	7	3.12
(3,21)	1:A:77:LEU:H	4:A:351:PX4:C35	7	3.12
(3,21)	1:A:77:LEU:H	4:A:353:PX4:C35	7	3.12
(3,21)	1:A:77:LEU:H	4:A:355:PX4:C35	7	3.12
(3,21)	1:A:77:LEU:H	4:A:357:PX4:C35	7	3.12
(3,21)	1:A:77:LEU:H	4:A:359:PX4:C35	7	3.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,21)	1:A:77:LEU:H	4:A:361:PX4:C35	7	3.12
(3,21)	1:A:77:LEU:H	4:A:363:PX4:C35	7	3.12
(3,21)	1:A:77:LEU:H	4:A:402:PX4:C35	7	3.12
(3,21)	1:A:77:LEU:H	4:A:404:PX4:C35	7	3.12
(3,21)	1:A:77:LEU:H	4:A:406:PX4:C35	7	3.12
(3,21)	1:A:77:LEU:H	4:A:408:PX4:C35	7	3.12
(3,21)	1:A:77:LEU:H	4:A:410:PX4:C35	7	3.12
(3,21)	1:A:77:LEU:H	4:A:412:PX4:C35	7	3.12
(3,21)	1:A:77:LEU:H	4:A:414:PX4:C35	7	3.12
(3,21)	1:A:77:LEU:H	4:A:416:PX4:C35	7	3.12
(3,21)	1:A:77:LEU:H	4:A:418:PX4:C35	7	3.12
(3,21)	1:A:77:LEU:H	4:A:420:PX4:C35	7	3.12
(3,21)	1:A:77:LEU:H	4:A:422:PX4:C35	7	3.12
(3,21)	1:A:77:LEU:H	4:A:424:PX4:C35	7	3.12
(3,21)	1:A:77:LEU:H	4:A:426:PX4:C35	7	3.12
(3,21)	1:A:77:LEU:H	4:A:428:PX4:C35	7	3.12
(3,21)	1:A:77:LEU:H	4:A:430:PX4:C35	7	3.12
(2,985)	1:A:80:ASN:H	1:A:78:PHE:HD1	20	3.12
(2,731)	1:A:211:VAL:HG13	1:A:226:LEU:HD21	5	3.12
(2,982)	1:A:78:PHE:HD1	1:A:80:ASN:H	5	3.1
(2,836)	1:A:120:ILE:HD13	1:A:200:LEU:HD21	20	3.1
(2,531)	1:A:205:SER:H	1:A:204:HIS:HE1	14	3.1
(2,954)	1:A:74:GLU:HB3	1:A:77:LEU:H	18	3.09
(2,954)	1:A:74:GLU:HB3	1:A:77:LEU:H	18	3.09
(2,882)	1:A:24:LEU:HD11	1:A:73:ALA:HB1	20	3.09
(2,882)	1:A:24:LEU:HD11	1:A:73:ALA:HB2	20	3.09
(2,882)	1:A:24:LEU:HD11	1:A:73:ALA:HB3	20	3.09
(2,882)	1:A:24:LEU:HD12	1:A:73:ALA:HB1	20	3.09
(2,882)	1:A:24:LEU:HD12	1:A:73:ALA:HB2	20	3.09
(2,882)	1:A:24:LEU:HD12	1:A:73:ALA:HB3	20	3.09
(2,882)	1:A:24:LEU:HD13	1:A:73:ALA:HB1	20	3.09
(2,882)	1:A:24:LEU:HD13	1:A:73:ALA:HB2	20	3.09
(2,882)	1:A:24:LEU:HD13	1:A:73:ALA:HB3	20	3.09
(2,657)	1:A:39:LEU:H	1:A:19:LEU:HD22	9	3.09
(2,657)	1:A:39:LEU:H	1:A:19:LEU:HD23	9	3.09
(2,531)	1:A:205:SER:H	1:A:204:HIS:HE1	7	3.08
(2,833)	1:A:120:ILE:HD11	1:A:200:LEU:HD22	13	3.06
(2,833)	1:A:120:ILE:HD11	1:A:200:LEU:HD23	13	3.06
(2,833)	1:A:120:ILE:HD11	1:A:200:LEU:HD22	19	3.06
(2,833)	1:A:120:ILE:HD11	1:A:200:LEU:HD23	19	3.06
(2,177)	1:A:171:HIS:H	1:A:134:ILE:HD11	13	3.05
(2,177)	1:A:171:HIS:H	1:A:134:ILE:HD12	13	3.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,177)	1:A:171:HIS:H	1:A:134:ILE:HD13	13	3.05
(2,471)	1:A:186:ILE:H	1:A:156:LEU:HD11	17	3.04
(2,471)	1:A:186:ILE:H	1:A:156:LEU:HD12	17	3.04
(2,471)	1:A:186:ILE:H	1:A:156:LEU:HD13	17	3.04
(2,471)	1:A:186:ILE:H	1:A:156:LEU:HD11	20	3.04
(2,471)	1:A:186:ILE:H	1:A:156:LEU:HD12	20	3.04
(2,471)	1:A:186:ILE:H	1:A:156:LEU:HD13	20	3.04
(2,985)	1:A:80:ASN:H	1:A:78:PHE:HD1	2	3.03
(2,867)	1:A:186:ILE:HD11	1:A:156:LEU:HD21	1	3.03
(2,531)	1:A:205:SER:H	1:A:204:HIS:HE1	15	3.02
(2,988)	1:A:129:TRP:HE1	4:A:305:PX4:C2	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:307:PX4:C2	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:309:PX4:C2	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:311:PX4:C2	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:313:PX4:C2	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:315:PX4:C2	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:317:PX4:C2	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:319:PX4:C2	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:321:PX4:C2	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:323:PX4:C2	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:325:PX4:C2	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:327:PX4:C2	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:329:PX4:C2	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:331:PX4:C2	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:333:PX4:C2	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:335:PX4:C2	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:337:PX4:C2	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:339:PX4:C2	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:341:PX4:C2	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:343:PX4:C2	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:345:PX4:C2	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:347:PX4:C2	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:349:PX4:C2	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:351:PX4:C2	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:353:PX4:C2	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:355:PX4:C2	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:357:PX4:C2	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:359:PX4:C2	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:361:PX4:C2	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:363:PX4:C2	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:402:PX4:C2	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:404:PX4:C2	6	3.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,988)	1:A:129:TRP:HE1	4:A:406:PX4:C2	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:408:PX4:C2	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:410:PX4:C2	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:412:PX4:C2	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:414:PX4:C2	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:416:PX4:C2	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:418:PX4:C2	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:420:PX4:C2	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:422:PX4:C2	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:424:PX4:C2	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:426:PX4:C2	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:428:PX4:C2	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:430:PX4:C2	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:305:PX4:C1	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:307:PX4:C1	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:309:PX4:C1	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:311:PX4:C1	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:313:PX4:C1	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:315:PX4:C1	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:317:PX4:C1	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:319:PX4:C1	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:321:PX4:C1	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:323:PX4:C1	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:325:PX4:C1	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:327:PX4:C1	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:329:PX4:C1	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:331:PX4:C1	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:333:PX4:C1	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:335:PX4:C1	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:337:PX4:C1	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:339:PX4:C1	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:341:PX4:C1	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:343:PX4:C1	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:345:PX4:C1	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:347:PX4:C1	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:349:PX4:C1	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:351:PX4:C1	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:353:PX4:C1	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:355:PX4:C1	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:357:PX4:C1	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:359:PX4:C1	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:361:PX4:C1	6	3.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,988)	1:A:129:TRP:HE1	4:A:363:PX4:C1	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:402:PX4:C1	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:404:PX4:C1	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:406:PX4:C1	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:408:PX4:C1	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:410:PX4:C1	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:412:PX4:C1	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:414:PX4:C1	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:416:PX4:C1	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:418:PX4:C1	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:420:PX4:C1	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:422:PX4:C1	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:424:PX4:C1	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:426:PX4:C1	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:428:PX4:C1	6	3.0
(2,988)	1:A:129:TRP:HE1	4:A:430:PX4:C1	6	3.0
(2,531)	1:A:205:SER:H	1:A:204:HIS:HE1	12	3.0
(2,531)	1:A:205:SER:H	1:A:204:HIS:HE1	20	3.0
(2,472)	1:A:186:ILE:H	1:A:156:LEU:HD21	9	3.0
(2,941)	1:A:73:ALA:HA	1:A:77:LEU:H	16	2.99
(2,882)	1:A:24:LEU:HD11	1:A:73:ALA:HB1	7	2.99
(2,882)	1:A:24:LEU:HD11	1:A:73:ALA:HB2	7	2.99
(2,882)	1:A:24:LEU:HD11	1:A:73:ALA:HB3	7	2.99
(2,882)	1:A:24:LEU:HD12	1:A:73:ALA:HB1	7	2.99
(2,882)	1:A:24:LEU:HD12	1:A:73:ALA:HB2	7	2.99
(2,882)	1:A:24:LEU:HD12	1:A:73:ALA:HB3	7	2.99
(2,882)	1:A:24:LEU:HD13	1:A:73:ALA:HB1	7	2.99
(2,882)	1:A:24:LEU:HD13	1:A:73:ALA:HB2	7	2.99
(2,882)	1:A:24:LEU:HD13	1:A:73:ALA:HB3	7	2.99
(2,834)	1:A:120:ILE:HD12	1:A:200:LEU:HD21	17	2.99
(2,834)	1:A:120:ILE:HD12	1:A:200:LEU:HD21	11	2.97
(2,471)	1:A:186:ILE:H	1:A:156:LEU:HD11	10	2.97
(2,471)	1:A:186:ILE:H	1:A:156:LEU:HD12	10	2.97
(2,471)	1:A:186:ILE:H	1:A:156:LEU:HD13	10	2.97
(2,985)	1:A:80:ASN:H	1:A:78:PHE:HD1	13	2.96
(2,882)	1:A:24:LEU:HD11	1:A:73:ALA:HB1	6	2.96
(2,882)	1:A:24:LEU:HD11	1:A:73:ALA:HB2	6	2.96
(2,882)	1:A:24:LEU:HD11	1:A:73:ALA:HB3	6	2.96
(2,882)	1:A:24:LEU:HD12	1:A:73:ALA:HB1	6	2.96
(2,882)	1:A:24:LEU:HD12	1:A:73:ALA:HB2	6	2.96
(2,882)	1:A:24:LEU:HD12	1:A:73:ALA:HB3	6	2.96
(2,882)	1:A:24:LEU:HD13	1:A:73:ALA:HB1	6	2.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,882)	1:A:24:LEU:HD13	1:A:73:ALA:HB2	6	2.96
(2,882)	1:A:24:LEU:HD13	1:A:73:ALA:HB3	6	2.96
(2,833)	1:A:120:ILE:HD11	1:A:200:LEU:HD22	17	2.96
(2,833)	1:A:120:ILE:HD11	1:A:200:LEU:HD23	17	2.96
(2,773)	1:A:61:ILE:HD11	1:A:48:LEU:HD21	18	2.96
(2,177)	1:A:171:HIS:H	1:A:134:ILE:HD11	20	2.96
(2,177)	1:A:171:HIS:H	1:A:134:ILE:HD12	20	2.96
(2,177)	1:A:171:HIS:H	1:A:134:ILE:HD13	20	2.96
(2,868)	1:A:186:ILE:HD11	1:A:156:LEU:HD22	1	2.95
(2,868)	1:A:186:ILE:HD11	1:A:156:LEU:HD23	1	2.95
(2,985)	1:A:80:ASN:H	1:A:78:PHE:HD1	19	2.94
(2,882)	1:A:24:LEU:HD11	1:A:73:ALA:HB1	13	2.94
(2,882)	1:A:24:LEU:HD11	1:A:73:ALA:HB2	13	2.94
(2,882)	1:A:24:LEU:HD11	1:A:73:ALA:HB3	13	2.94
(2,882)	1:A:24:LEU:HD12	1:A:73:ALA:HB1	13	2.94
(2,882)	1:A:24:LEU:HD12	1:A:73:ALA:HB2	13	2.94
(2,882)	1:A:24:LEU:HD12	1:A:73:ALA:HB3	13	2.94
(2,882)	1:A:24:LEU:HD13	1:A:73:ALA:HB1	13	2.94
(2,882)	1:A:24:LEU:HD13	1:A:73:ALA:HB2	13	2.94
(2,882)	1:A:24:LEU:HD13	1:A:73:ALA:HB3	13	2.94
(2,471)	1:A:186:ILE:H	1:A:156:LEU:HD11	2	2.94
(2,471)	1:A:186:ILE:H	1:A:156:LEU:HD12	2	2.94
(2,471)	1:A:186:ILE:H	1:A:156:LEU:HD13	2	2.94
(2,941)	1:A:73:ALA:HA	1:A:77:LEU:H	20	2.93
(2,882)	1:A:24:LEU:HD11	1:A:73:ALA:HB1	8	2.93
(2,882)	1:A:24:LEU:HD11	1:A:73:ALA:HB2	8	2.93
(2,882)	1:A:24:LEU:HD11	1:A:73:ALA:HB3	8	2.93
(2,882)	1:A:24:LEU:HD12	1:A:73:ALA:HB1	8	2.93
(2,882)	1:A:24:LEU:HD12	1:A:73:ALA:HB2	8	2.93
(2,882)	1:A:24:LEU:HD12	1:A:73:ALA:HB3	8	2.93
(2,882)	1:A:24:LEU:HD13	1:A:73:ALA:HB1	8	2.93
(2,882)	1:A:24:LEU:HD13	1:A:73:ALA:HB2	8	2.93
(2,882)	1:A:24:LEU:HD13	1:A:73:ALA:HB3	8	2.93
(3,21)	1:A:77:LEU:H	4:A:305:PX4:C35	1	2.92
(3,21)	1:A:77:LEU:H	4:A:307:PX4:C35	1	2.92
(3,21)	1:A:77:LEU:H	4:A:309:PX4:C35	1	2.92
(3,21)	1:A:77:LEU:H	4:A:311:PX4:C35	1	2.92
(3,21)	1:A:77:LEU:H	4:A:313:PX4:C35	1	2.92
(3,21)	1:A:77:LEU:H	4:A:315:PX4:C35	1	2.92
(3,21)	1:A:77:LEU:H	4:A:317:PX4:C35	1	2.92
(3,21)	1:A:77:LEU:H	4:A:319:PX4:C35	1	2.92
(3,21)	1:A:77:LEU:H	4:A:321:PX4:C35	1	2.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,21)	1:A:77:LEU:H	4:A:323:PX4:C35	1	2.92
(3,21)	1:A:77:LEU:H	4:A:325:PX4:C35	1	2.92
(3,21)	1:A:77:LEU:H	4:A:327:PX4:C35	1	2.92
(3,21)	1:A:77:LEU:H	4:A:329:PX4:C35	1	2.92
(3,21)	1:A:77:LEU:H	4:A:331:PX4:C35	1	2.92
(3,21)	1:A:77:LEU:H	4:A:333:PX4:C35	1	2.92
(3,21)	1:A:77:LEU:H	4:A:335:PX4:C35	1	2.92
(3,21)	1:A:77:LEU:H	4:A:337:PX4:C35	1	2.92
(3,21)	1:A:77:LEU:H	4:A:339:PX4:C35	1	2.92
(3,21)	1:A:77:LEU:H	4:A:341:PX4:C35	1	2.92
(3,21)	1:A:77:LEU:H	4:A:343:PX4:C35	1	2.92
(3,21)	1:A:77:LEU:H	4:A:345:PX4:C35	1	2.92
(3,21)	1:A:77:LEU:H	4:A:347:PX4:C35	1	2.92
(3,21)	1:A:77:LEU:H	4:A:349:PX4:C35	1	2.92
(3,21)	1:A:77:LEU:H	4:A:351:PX4:C35	1	2.92
(3,21)	1:A:77:LEU:H	4:A:353:PX4:C35	1	2.92
(3,21)	1:A:77:LEU:H	4:A:355:PX4:C35	1	2.92
(3,21)	1:A:77:LEU:H	4:A:357:PX4:C35	1	2.92
(3,21)	1:A:77:LEU:H	4:A:359:PX4:C35	1	2.92
(3,21)	1:A:77:LEU:H	4:A:361:PX4:C35	1	2.92
(3,21)	1:A:77:LEU:H	4:A:363:PX4:C35	1	2.92
(3,21)	1:A:77:LEU:H	4:A:402:PX4:C35	1	2.92
(3,21)	1:A:77:LEU:H	4:A:404:PX4:C35	1	2.92
(3,21)	1:A:77:LEU:H	4:A:406:PX4:C35	1	2.92
(3,21)	1:A:77:LEU:H	4:A:408:PX4:C35	1	2.92
(3,21)	1:A:77:LEU:H	4:A:410:PX4:C35	1	2.92
(3,21)	1:A:77:LEU:H	4:A:412:PX4:C35	1	2.92
(3,21)	1:A:77:LEU:H	4:A:414:PX4:C35	1	2.92
(3,21)	1:A:77:LEU:H	4:A:416:PX4:C35	1	2.92
(3,21)	1:A:77:LEU:H	4:A:418:PX4:C35	1	2.92
(3,21)	1:A:77:LEU:H	4:A:420:PX4:C35	1	2.92
(3,21)	1:A:77:LEU:H	4:A:422:PX4:C35	1	2.92
(3,21)	1:A:77:LEU:H	4:A:424:PX4:C35	1	2.92
(3,21)	1:A:77:LEU:H	4:A:426:PX4:C35	1	2.92
(3,21)	1:A:77:LEU:H	4:A:428:PX4:C35	1	2.92
(3,21)	1:A:77:LEU:H	4:A:430:PX4:C35	1	2.92
(2,834)	1:A:120:ILE:HD12	1:A:200:LEU:HD21	5	2.92
(2,471)	1:A:186:ILE:H	1:A:156:LEU:HD11	4	2.92
(2,471)	1:A:186:ILE:H	1:A:156:LEU:HD12	4	2.92
(2,471)	1:A:186:ILE:H	1:A:156:LEU:HD13	4	2.92
(3,21)	1:A:77:LEU:H	4:A:305:PX4:C35	18	2.9
(3,21)	1:A:77:LEU:H	4:A:307:PX4:C35	18	2.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,21)	1:A:77:LEU:H	4:A:309:PX4:C35	18	2.9
(3,21)	1:A:77:LEU:H	4:A:311:PX4:C35	18	2.9
(3,21)	1:A:77:LEU:H	4:A:313:PX4:C35	18	2.9
(3,21)	1:A:77:LEU:H	4:A:315:PX4:C35	18	2.9
(3,21)	1:A:77:LEU:H	4:A:317:PX4:C35	18	2.9
(3,21)	1:A:77:LEU:H	4:A:319:PX4:C35	18	2.9
(3,21)	1:A:77:LEU:H	4:A:321:PX4:C35	18	2.9
(3,21)	1:A:77:LEU:H	4:A:323:PX4:C35	18	2.9
(3,21)	1:A:77:LEU:H	4:A:325:PX4:C35	18	2.9
(3,21)	1:A:77:LEU:H	4:A:327:PX4:C35	18	2.9
(3,21)	1:A:77:LEU:H	4:A:329:PX4:C35	18	2.9
(3,21)	1:A:77:LEU:H	4:A:331:PX4:C35	18	2.9
(3,21)	1:A:77:LEU:H	4:A:333:PX4:C35	18	2.9
(3,21)	1:A:77:LEU:H	4:A:335:PX4:C35	18	2.9
(3,21)	1:A:77:LEU:H	4:A:337:PX4:C35	18	2.9
(3,21)	1:A:77:LEU:H	4:A:339:PX4:C35	18	2.9
(3,21)	1:A:77:LEU:H	4:A:341:PX4:C35	18	2.9
(3,21)	1:A:77:LEU:H	4:A:343:PX4:C35	18	2.9
(3,21)	1:A:77:LEU:H	4:A:345:PX4:C35	18	2.9
(3,21)	1:A:77:LEU:H	4:A:347:PX4:C35	18	2.9
(3,21)	1:A:77:LEU:H	4:A:349:PX4:C35	18	2.9
(3,21)	1:A:77:LEU:H	4:A:351:PX4:C35	18	2.9
(3,21)	1:A:77:LEU:H	4:A:353:PX4:C35	18	2.9
(3,21)	1:A:77:LEU:H	4:A:355:PX4:C35	18	2.9
(3,21)	1:A:77:LEU:H	4:A:357:PX4:C35	18	2.9
(3,21)	1:A:77:LEU:H	4:A:359:PX4:C35	18	2.9
(3,21)	1:A:77:LEU:H	4:A:361:PX4:C35	18	2.9
(3,21)	1:A:77:LEU:H	4:A:363:PX4:C35	18	2.9
(3,21)	1:A:77:LEU:H	4:A:402:PX4:C35	18	2.9
(3,21)	1:A:77:LEU:H	4:A:404:PX4:C35	18	2.9
(3,21)	1:A:77:LEU:H	4:A:406:PX4:C35	18	2.9
(3,21)	1:A:77:LEU:H	4:A:408:PX4:C35	18	2.9
(3,21)	1:A:77:LEU:H	4:A:410:PX4:C35	18	2.9
(3,21)	1:A:77:LEU:H	4:A:412:PX4:C35	18	2.9
(3,21)	1:A:77:LEU:H	4:A:414:PX4:C35	18	2.9
(3,21)	1:A:77:LEU:H	4:A:416:PX4:C35	18	2.9
(3,21)	1:A:77:LEU:H	4:A:418:PX4:C35	18	2.9
(3,21)	1:A:77:LEU:H	4:A:420:PX4:C35	18	2.9
(3,21)	1:A:77:LEU:H	4:A:422:PX4:C35	18	2.9
(3,21)	1:A:77:LEU:H	4:A:424:PX4:C35	18	2.9
(3,21)	1:A:77:LEU:H	4:A:426:PX4:C35	18	2.9
(3,21)	1:A:77:LEU:H	4:A:428:PX4:C35	18	2.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,21)	1:A:77:LEU:H	4:A:430:PX4:C35	18	2.9
(2,941)	1:A:73:ALA:HA	1:A:77:LEU:H	14	2.89
(2,832)	1:A:120:ILE:HD11	1:A:200:LEU:HD21	19	2.89
(2,882)	1:A:24:LEU:HD11	1:A:73:ALA:HB1	10	2.88
(2,882)	1:A:24:LEU:HD11	1:A:73:ALA:HB2	10	2.88
(2,882)	1:A:24:LEU:HD11	1:A:73:ALA:HB3	10	2.88
(2,882)	1:A:24:LEU:HD12	1:A:73:ALA:HB1	10	2.88
(2,882)	1:A:24:LEU:HD12	1:A:73:ALA:HB2	10	2.88
(2,882)	1:A:24:LEU:HD12	1:A:73:ALA:HB3	10	2.88
(2,882)	1:A:24:LEU:HD13	1:A:73:ALA:HB1	10	2.88
(2,882)	1:A:24:LEU:HD13	1:A:73:ALA:HB2	10	2.88
(2,882)	1:A:24:LEU:HD13	1:A:73:ALA:HB3	10	2.88
(2,882)	1:A:24:LEU:HD11	1:A:73:ALA:HB1	12	2.88
(2,882)	1:A:24:LEU:HD11	1:A:73:ALA:HB2	12	2.88
(2,882)	1:A:24:LEU:HD11	1:A:73:ALA:HB3	12	2.88
(2,882)	1:A:24:LEU:HD12	1:A:73:ALA:HB1	12	2.88
(2,882)	1:A:24:LEU:HD12	1:A:73:ALA:HB2	12	2.88
(2,882)	1:A:24:LEU:HD12	1:A:73:ALA:HB3	12	2.88
(2,882)	1:A:24:LEU:HD13	1:A:73:ALA:HB1	12	2.88
(2,882)	1:A:24:LEU:HD13	1:A:73:ALA:HB2	12	2.88
(2,882)	1:A:24:LEU:HD13	1:A:73:ALA:HB3	12	2.88
(2,757)	1:A:54:LEU:HD21	1:A:39:LEU:HD11	3	2.88
(2,757)	1:A:54:LEU:HD21	1:A:39:LEU:HD12	3	2.88
(2,757)	1:A:54:LEU:HD21	1:A:39:LEU:HD13	3	2.88
(2,656)	1:A:39:LEU:H	1:A:19:LEU:HD21	1	2.87
(2,531)	1:A:205:SER:H	1:A:204:HIS:HE1	13	2.87
(2,177)	1:A:171:HIS:H	1:A:134:ILE:HD11	12	2.87
(2,177)	1:A:171:HIS:H	1:A:134:ILE:HD12	12	2.87
(2,177)	1:A:171:HIS:H	1:A:134:ILE:HD13	12	2.87
(2,834)	1:A:120:ILE:HD12	1:A:200:LEU:HD21	8	2.86
(2,832)	1:A:120:ILE:HD11	1:A:200:LEU:HD21	15	2.85
(2,941)	1:A:73:ALA:HA	1:A:77:LEU:H	17	2.84
(2,871)	1:A:186:ILE:HD13	1:A:156:LEU:HD21	12	2.84
(2,833)	1:A:120:ILE:HD11	1:A:200:LEU:HD22	6	2.84
(2,833)	1:A:120:ILE:HD11	1:A:200:LEU:HD23	6	2.84
(2,531)	1:A:205:SER:H	1:A:204:HIS:HE1	11	2.84
(2,177)	1:A:171:HIS:H	1:A:134:ILE:HD11	16	2.84
(2,177)	1:A:171:HIS:H	1:A:134:ILE:HD12	16	2.84
(2,177)	1:A:171:HIS:H	1:A:134:ILE:HD13	16	2.84
(3,21)	1:A:77:LEU:H	4:A:305:PX4:C35	8	2.83
(3,21)	1:A:77:LEU:H	4:A:307:PX4:C35	8	2.83
(3,21)	1:A:77:LEU:H	4:A:309:PX4:C35	8	2.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,21)	1:A:77:LEU:H	4:A:311:PX4:C35	8	2.83
(3,21)	1:A:77:LEU:H	4:A:313:PX4:C35	8	2.83
(3,21)	1:A:77:LEU:H	4:A:315:PX4:C35	8	2.83
(3,21)	1:A:77:LEU:H	4:A:317:PX4:C35	8	2.83
(3,21)	1:A:77:LEU:H	4:A:319:PX4:C35	8	2.83
(3,21)	1:A:77:LEU:H	4:A:321:PX4:C35	8	2.83
(3,21)	1:A:77:LEU:H	4:A:323:PX4:C35	8	2.83
(3,21)	1:A:77:LEU:H	4:A:325:PX4:C35	8	2.83
(3,21)	1:A:77:LEU:H	4:A:327:PX4:C35	8	2.83
(3,21)	1:A:77:LEU:H	4:A:329:PX4:C35	8	2.83
(3,21)	1:A:77:LEU:H	4:A:331:PX4:C35	8	2.83
(3,21)	1:A:77:LEU:H	4:A:333:PX4:C35	8	2.83
(3,21)	1:A:77:LEU:H	4:A:335:PX4:C35	8	2.83
(3,21)	1:A:77:LEU:H	4:A:337:PX4:C35	8	2.83
(3,21)	1:A:77:LEU:H	4:A:339:PX4:C35	8	2.83
(3,21)	1:A:77:LEU:H	4:A:341:PX4:C35	8	2.83
(3,21)	1:A:77:LEU:H	4:A:343:PX4:C35	8	2.83
(3,21)	1:A:77:LEU:H	4:A:345:PX4:C35	8	2.83
(3,21)	1:A:77:LEU:H	4:A:347:PX4:C35	8	2.83
(3,21)	1:A:77:LEU:H	4:A:349:PX4:C35	8	2.83
(3,21)	1:A:77:LEU:H	4:A:351:PX4:C35	8	2.83
(3,21)	1:A:77:LEU:H	4:A:353:PX4:C35	8	2.83
(3,21)	1:A:77:LEU:H	4:A:355:PX4:C35	8	2.83
(3,21)	1:A:77:LEU:H	4:A:357:PX4:C35	8	2.83
(3,21)	1:A:77:LEU:H	4:A:359:PX4:C35	8	2.83
(3,21)	1:A:77:LEU:H	4:A:361:PX4:C35	8	2.83
(3,21)	1:A:77:LEU:H	4:A:363:PX4:C35	8	2.83
(3,21)	1:A:77:LEU:H	4:A:402:PX4:C35	8	2.83
(3,21)	1:A:77:LEU:H	4:A:404:PX4:C35	8	2.83
(3,21)	1:A:77:LEU:H	4:A:406:PX4:C35	8	2.83
(3,21)	1:A:77:LEU:H	4:A:408:PX4:C35	8	2.83
(3,21)	1:A:77:LEU:H	4:A:410:PX4:C35	8	2.83
(3,21)	1:A:77:LEU:H	4:A:412:PX4:C35	8	2.83
(3,21)	1:A:77:LEU:H	4:A:414:PX4:C35	8	2.83
(3,21)	1:A:77:LEU:H	4:A:416:PX4:C35	8	2.83
(3,21)	1:A:77:LEU:H	4:A:418:PX4:C35	8	2.83
(3,21)	1:A:77:LEU:H	4:A:420:PX4:C35	8	2.83
(3,21)	1:A:77:LEU:H	4:A:422:PX4:C35	8	2.83
(3,21)	1:A:77:LEU:H	4:A:424:PX4:C35	8	2.83
(3,21)	1:A:77:LEU:H	4:A:426:PX4:C35	8	2.83
(3,21)	1:A:77:LEU:H	4:A:428:PX4:C35	8	2.83
(3,21)	1:A:77:LEU:H	4:A:430:PX4:C35	8	2.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,727)	1:A:211:VAL:HG11	1:A:226:LEU:HD21	1	2.83
(2,177)	1:A:171:HIS:H	1:A:134:ILE:HD11	6	2.83
(2,177)	1:A:171:HIS:H	1:A:134:ILE:HD12	6	2.83
(2,177)	1:A:171:HIS:H	1:A:134:ILE:HD13	6	2.83
(2,531)	1:A:205:SER:H	1:A:204:HIS:HE1	1	2.8
(2,941)	1:A:73:ALA:HA	1:A:77:LEU:H	5	2.79
(2,879)	1:A:234:ILE:HD11	1:A:200:LEU:HB2	13	2.79
(2,879)	1:A:234:ILE:HD12	1:A:200:LEU:HB2	13	2.79
(2,879)	1:A:234:ILE:HD13	1:A:200:LEU:HB2	13	2.79
(2,177)	1:A:171:HIS:H	1:A:134:ILE:HD11	7	2.79
(2,177)	1:A:171:HIS:H	1:A:134:ILE:HD12	7	2.79
(2,177)	1:A:171:HIS:H	1:A:134:ILE:HD13	7	2.79
(2,757)	1:A:54:LEU:HD21	1:A:39:LEU:HD11	1	2.78
(2,757)	1:A:54:LEU:HD21	1:A:39:LEU:HD12	1	2.78
(2,757)	1:A:54:LEU:HD21	1:A:39:LEU:HD13	1	2.78
(2,471)	1:A:186:ILE:H	1:A:156:LEU:HD11	5	2.77
(2,471)	1:A:186:ILE:H	1:A:156:LEU:HD12	5	2.77
(2,471)	1:A:186:ILE:H	1:A:156:LEU:HD13	5	2.77
(2,988)	1:A:129:TRP:HE1	4:A:305:PX4:C2	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:307:PX4:C2	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:309:PX4:C2	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:311:PX4:C2	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:313:PX4:C2	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:315:PX4:C2	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:317:PX4:C2	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:319:PX4:C2	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:321:PX4:C2	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:323:PX4:C2	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:325:PX4:C2	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:327:PX4:C2	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:329:PX4:C2	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:331:PX4:C2	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:333:PX4:C2	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:335:PX4:C2	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:337:PX4:C2	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:339:PX4:C2	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:341:PX4:C2	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:343:PX4:C2	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:345:PX4:C2	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:347:PX4:C2	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:349:PX4:C2	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:351:PX4:C2	7	2.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,988)	1:A:129:TRP:HE1	4:A:353:PX4:C2	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:355:PX4:C2	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:357:PX4:C2	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:359:PX4:C2	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:361:PX4:C2	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:363:PX4:C2	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:402:PX4:C2	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:404:PX4:C2	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:406:PX4:C2	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:408:PX4:C2	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:410:PX4:C2	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:412:PX4:C2	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:414:PX4:C2	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:416:PX4:C2	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:418:PX4:C2	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:420:PX4:C2	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:422:PX4:C2	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:424:PX4:C2	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:426:PX4:C2	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:428:PX4:C2	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:430:PX4:C2	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:305:PX4:C1	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:307:PX4:C1	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:309:PX4:C1	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:311:PX4:C1	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:313:PX4:C1	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:315:PX4:C1	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:317:PX4:C1	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:319:PX4:C1	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:321:PX4:C1	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:323:PX4:C1	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:325:PX4:C1	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:327:PX4:C1	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:329:PX4:C1	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:331:PX4:C1	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:333:PX4:C1	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:335:PX4:C1	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:337:PX4:C1	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:339:PX4:C1	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:341:PX4:C1	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:343:PX4:C1	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:345:PX4:C1	7	2.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,988)	1:A:129:TRP:HE1	4:A:347:PX4:C1	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:349:PX4:C1	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:351:PX4:C1	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:353:PX4:C1	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:355:PX4:C1	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:357:PX4:C1	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:359:PX4:C1	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:361:PX4:C1	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:363:PX4:C1	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:402:PX4:C1	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:404:PX4:C1	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:406:PX4:C1	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:408:PX4:C1	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:410:PX4:C1	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:412:PX4:C1	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:414:PX4:C1	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:416:PX4:C1	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:418:PX4:C1	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:420:PX4:C1	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:422:PX4:C1	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:424:PX4:C1	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:426:PX4:C1	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:428:PX4:C1	7	2.76
(2,988)	1:A:129:TRP:HE1	4:A:430:PX4:C1	7	2.76
(2,656)	1:A:39:LEU:H	1:A:19:LEU:HD21	3	2.76
(2,177)	1:A:171:HIS:H	1:A:134:ILE:HD11	2	2.76
(2,177)	1:A:171:HIS:H	1:A:134:ILE:HD12	2	2.76
(2,177)	1:A:171:HIS:H	1:A:134:ILE:HD13	2	2.76
(2,177)	1:A:171:HIS:H	1:A:134:ILE:HD11	14	2.76
(2,177)	1:A:171:HIS:H	1:A:134:ILE:HD12	14	2.76
(2,177)	1:A:171:HIS:H	1:A:134:ILE:HD13	14	2.76
(2,974)	1:A:78:PHE:H	1:A:77:LEU:HD21	9	2.75
(2,941)	1:A:73:ALA:HA	1:A:77:LEU:H	13	2.74
(2,466)	1:A:84:TRP:H	1:A:200:LEU:HD21	17	2.74
(2,177)	1:A:171:HIS:H	1:A:134:ILE:HD11	10	2.74
(2,177)	1:A:171:HIS:H	1:A:134:ILE:HD12	10	2.74
(2,177)	1:A:171:HIS:H	1:A:134:ILE:HD13	10	2.74
(2,471)	1:A:186:ILE:H	1:A:156:LEU:HD11	3	2.73
(2,471)	1:A:186:ILE:H	1:A:156:LEU:HD12	3	2.73
(2,471)	1:A:186:ILE:H	1:A:156:LEU:HD13	3	2.73
(2,837)	1:A:120:ILE:HD13	1:A:200:LEU:HD22	10	2.72
(2,837)	1:A:120:ILE:HD13	1:A:200:LEU:HD23	10	2.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,531)	1:A:205:SER:H	1:A:204:HIS:HE1	2	2.72
(2,941)	1:A:73:ALA:HA	1:A:77:LEU:H	19	2.71
(2,882)	1:A:24:LEU:HD11	1:A:73:ALA:HB1	11	2.7
(2,882)	1:A:24:LEU:HD11	1:A:73:ALA:HB2	11	2.7
(2,882)	1:A:24:LEU:HD11	1:A:73:ALA:HB3	11	2.7
(2,882)	1:A:24:LEU:HD12	1:A:73:ALA:HB1	11	2.7
(2,882)	1:A:24:LEU:HD12	1:A:73:ALA:HB2	11	2.7
(2,882)	1:A:24:LEU:HD12	1:A:73:ALA:HB3	11	2.7
(2,882)	1:A:24:LEU:HD13	1:A:73:ALA:HB1	11	2.7
(2,882)	1:A:24:LEU:HD13	1:A:73:ALA:HB2	11	2.7
(2,882)	1:A:24:LEU:HD13	1:A:73:ALA:HB3	11	2.7
(2,834)	1:A:120:ILE:HD12	1:A:200:LEU:HD21	2	2.69
(2,471)	1:A:186:ILE:H	1:A:156:LEU:HD11	15	2.69
(2,471)	1:A:186:ILE:H	1:A:156:LEU:HD12	15	2.69
(2,471)	1:A:186:ILE:H	1:A:156:LEU:HD13	15	2.69
(3,36)	1:A:129:TRP:HE1	4:A:305:PX4:N1	7	2.68
(3,36)	1:A:129:TRP:HE1	4:A:307:PX4:N1	7	2.68
(3,36)	1:A:129:TRP:HE1	4:A:309:PX4:N1	7	2.68
(3,36)	1:A:129:TRP:HE1	4:A:311:PX4:N1	7	2.68
(3,36)	1:A:129:TRP:HE1	4:A:313:PX4:N1	7	2.68
(3,36)	1:A:129:TRP:HE1	4:A:315:PX4:N1	7	2.68
(3,36)	1:A:129:TRP:HE1	4:A:317:PX4:N1	7	2.68
(3,36)	1:A:129:TRP:HE1	4:A:319:PX4:N1	7	2.68
(3,36)	1:A:129:TRP:HE1	4:A:321:PX4:N1	7	2.68
(3,36)	1:A:129:TRP:HE1	4:A:323:PX4:N1	7	2.68
(3,36)	1:A:129:TRP:HE1	4:A:325:PX4:N1	7	2.68
(3,36)	1:A:129:TRP:HE1	4:A:327:PX4:N1	7	2.68
(3,36)	1:A:129:TRP:HE1	4:A:329:PX4:N1	7	2.68
(3,36)	1:A:129:TRP:HE1	4:A:331:PX4:N1	7	2.68
(3,36)	1:A:129:TRP:HE1	4:A:333:PX4:N1	7	2.68
(3,36)	1:A:129:TRP:HE1	4:A:335:PX4:N1	7	2.68
(3,36)	1:A:129:TRP:HE1	4:A:337:PX4:N1	7	2.68
(3,36)	1:A:129:TRP:HE1	4:A:339:PX4:N1	7	2.68
(3,36)	1:A:129:TRP:HE1	4:A:341:PX4:N1	7	2.68
(3,36)	1:A:129:TRP:HE1	4:A:343:PX4:N1	7	2.68
(3,36)	1:A:129:TRP:HE1	4:A:345:PX4:N1	7	2.68
(3,36)	1:A:129:TRP:HE1	4:A:347:PX4:N1	7	2.68
(3,36)	1:A:129:TRP:HE1	4:A:349:PX4:N1	7	2.68
(3,36)	1:A:129:TRP:HE1	4:A:351:PX4:N1	7	2.68
(3,36)	1:A:129:TRP:HE1	4:A:353:PX4:N1	7	2.68
(3,36)	1:A:129:TRP:HE1	4:A:355:PX4:N1	7	2.68
(3,36)	1:A:129:TRP:HE1	4:A:357:PX4:N1	7	2.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,36)	1:A:129:TRP:HE1	4:A:359:PX4:N1	7	2.68
(3,36)	1:A:129:TRP:HE1	4:A:361:PX4:N1	7	2.68
(3,36)	1:A:129:TRP:HE1	4:A:363:PX4:N1	7	2.68
(3,36)	1:A:129:TRP:HE1	4:A:402:PX4:N1	7	2.68
(3,36)	1:A:129:TRP:HE1	4:A:404:PX4:N1	7	2.68
(3,36)	1:A:129:TRP:HE1	4:A:406:PX4:N1	7	2.68
(3,36)	1:A:129:TRP:HE1	4:A:408:PX4:N1	7	2.68
(3,36)	1:A:129:TRP:HE1	4:A:410:PX4:N1	7	2.68
(3,36)	1:A:129:TRP:HE1	4:A:412:PX4:N1	7	2.68
(3,36)	1:A:129:TRP:HE1	4:A:414:PX4:N1	7	2.68
(3,36)	1:A:129:TRP:HE1	4:A:416:PX4:N1	7	2.68
(3,36)	1:A:129:TRP:HE1	4:A:418:PX4:N1	7	2.68
(3,36)	1:A:129:TRP:HE1	4:A:420:PX4:N1	7	2.68
(3,36)	1:A:129:TRP:HE1	4:A:422:PX4:N1	7	2.68
(3,36)	1:A:129:TRP:HE1	4:A:424:PX4:N1	7	2.68
(3,36)	1:A:129:TRP:HE1	4:A:426:PX4:N1	7	2.68
(3,36)	1:A:129:TRP:HE1	4:A:428:PX4:N1	7	2.68
(3,36)	1:A:129:TRP:HE1	4:A:430:PX4:N1	7	2.68
(2,757)	1:A:54:LEU:HD21	1:A:39:LEU:HD11	7	2.68
(2,757)	1:A:54:LEU:HD21	1:A:39:LEU:HD12	7	2.68
(2,757)	1:A:54:LEU:HD21	1:A:39:LEU:HD13	7	2.68
(2,656)	1:A:39:LEU:H	1:A:19:LEU:HD21	17	2.68
(2,471)	1:A:186:ILE:H	1:A:156:LEU:HD11	13	2.66
(2,471)	1:A:186:ILE:H	1:A:156:LEU:HD12	13	2.66
(2,471)	1:A:186:ILE:H	1:A:156:LEU:HD13	13	2.66
(2,177)	1:A:171:HIS:H	1:A:134:ILE:HD11	5	2.66
(2,177)	1:A:171:HIS:H	1:A:134:ILE:HD12	5	2.66
(2,177)	1:A:171:HIS:H	1:A:134:ILE:HD13	5	2.66
(3,21)	1:A:77:LEU:H	4:A:305:PX4:C35	13	2.65
(3,21)	1:A:77:LEU:H	4:A:307:PX4:C35	13	2.65
(3,21)	1:A:77:LEU:H	4:A:309:PX4:C35	13	2.65
(3,21)	1:A:77:LEU:H	4:A:311:PX4:C35	13	2.65
(3,21)	1:A:77:LEU:H	4:A:313:PX4:C35	13	2.65
(3,21)	1:A:77:LEU:H	4:A:315:PX4:C35	13	2.65
(3,21)	1:A:77:LEU:H	4:A:317:PX4:C35	13	2.65
(3,21)	1:A:77:LEU:H	4:A:319:PX4:C35	13	2.65
(3,21)	1:A:77:LEU:H	4:A:321:PX4:C35	13	2.65
(3,21)	1:A:77:LEU:H	4:A:323:PX4:C35	13	2.65
(3,21)	1:A:77:LEU:H	4:A:325:PX4:C35	13	2.65
(3,21)	1:A:77:LEU:H	4:A:327:PX4:C35	13	2.65
(3,21)	1:A:77:LEU:H	4:A:329:PX4:C35	13	2.65
(3,21)	1:A:77:LEU:H	4:A:331:PX4:C35	13	2.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,21)	1:A:77:LEU:H	4:A:333:PX4:C35	13	2.65
(3,21)	1:A:77:LEU:H	4:A:335:PX4:C35	13	2.65
(3,21)	1:A:77:LEU:H	4:A:337:PX4:C35	13	2.65
(3,21)	1:A:77:LEU:H	4:A:339:PX4:C35	13	2.65
(3,21)	1:A:77:LEU:H	4:A:341:PX4:C35	13	2.65
(3,21)	1:A:77:LEU:H	4:A:343:PX4:C35	13	2.65
(3,21)	1:A:77:LEU:H	4:A:345:PX4:C35	13	2.65
(3,21)	1:A:77:LEU:H	4:A:347:PX4:C35	13	2.65
(3,21)	1:A:77:LEU:H	4:A:349:PX4:C35	13	2.65
(3,21)	1:A:77:LEU:H	4:A:351:PX4:C35	13	2.65
(3,21)	1:A:77:LEU:H	4:A:353:PX4:C35	13	2.65
(3,21)	1:A:77:LEU:H	4:A:355:PX4:C35	13	2.65
(3,21)	1:A:77:LEU:H	4:A:357:PX4:C35	13	2.65
(3,21)	1:A:77:LEU:H	4:A:359:PX4:C35	13	2.65
(3,21)	1:A:77:LEU:H	4:A:361:PX4:C35	13	2.65
(3,21)	1:A:77:LEU:H	4:A:363:PX4:C35	13	2.65
(3,21)	1:A:77:LEU:H	4:A:402:PX4:C35	13	2.65
(3,21)	1:A:77:LEU:H	4:A:404:PX4:C35	13	2.65
(3,21)	1:A:77:LEU:H	4:A:406:PX4:C35	13	2.65
(3,21)	1:A:77:LEU:H	4:A:408:PX4:C35	13	2.65
(3,21)	1:A:77:LEU:H	4:A:410:PX4:C35	13	2.65
(3,21)	1:A:77:LEU:H	4:A:412:PX4:C35	13	2.65
(3,21)	1:A:77:LEU:H	4:A:414:PX4:C35	13	2.65
(3,21)	1:A:77:LEU:H	4:A:416:PX4:C35	13	2.65
(3,21)	1:A:77:LEU:H	4:A:418:PX4:C35	13	2.65
(3,21)	1:A:77:LEU:H	4:A:420:PX4:C35	13	2.65
(3,21)	1:A:77:LEU:H	4:A:422:PX4:C35	13	2.65
(3,21)	1:A:77:LEU:H	4:A:424:PX4:C35	13	2.65
(3,21)	1:A:77:LEU:H	4:A:426:PX4:C35	13	2.65
(3,21)	1:A:77:LEU:H	4:A:428:PX4:C35	13	2.65
(3,21)	1:A:77:LEU:H	4:A:430:PX4:C35	13	2.65
(2,834)	1:A:120:ILE:HD12	1:A:200:LEU:HD21	6	2.65
(2,954)	1:A:74:GLU:HB3	1:A:77:LEU:H	9	2.64
(2,954)	1:A:74:GLU:HB3	1:A:77:LEU:H	9	2.64
(2,837)	1:A:120:ILE:HD13	1:A:200:LEU:HD22	13	2.64
(2,837)	1:A:120:ILE:HD13	1:A:200:LEU:HD23	13	2.64
(2,988)	1:A:129:TRP:HE1	4:A:305:PX4:C2	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:307:PX4:C2	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:309:PX4:C2	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:311:PX4:C2	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:313:PX4:C2	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:315:PX4:C2	8	2.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,988)	1:A:129:TRP:HE1	4:A:317:PX4:C2	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:319:PX4:C2	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:321:PX4:C2	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:323:PX4:C2	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:325:PX4:C2	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:327:PX4:C2	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:329:PX4:C2	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:331:PX4:C2	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:333:PX4:C2	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:335:PX4:C2	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:337:PX4:C2	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:339:PX4:C2	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:341:PX4:C2	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:343:PX4:C2	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:345:PX4:C2	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:347:PX4:C2	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:349:PX4:C2	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:351:PX4:C2	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:353:PX4:C2	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:355:PX4:C2	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:357:PX4:C2	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:359:PX4:C2	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:361:PX4:C2	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:363:PX4:C2	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:402:PX4:C2	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:404:PX4:C2	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:406:PX4:C2	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:408:PX4:C2	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:410:PX4:C2	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:412:PX4:C2	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:414:PX4:C2	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:416:PX4:C2	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:418:PX4:C2	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:420:PX4:C2	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:422:PX4:C2	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:424:PX4:C2	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:426:PX4:C2	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:428:PX4:C2	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:430:PX4:C2	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:305:PX4:C1	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:307:PX4:C1	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:309:PX4:C1	8	2.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,988)	1:A:129:TRP:HE1	4:A:311:PX4:C1	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:313:PX4:C1	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:315:PX4:C1	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:317:PX4:C1	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:319:PX4:C1	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:321:PX4:C1	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:323:PX4:C1	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:325:PX4:C1	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:327:PX4:C1	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:329:PX4:C1	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:331:PX4:C1	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:333:PX4:C1	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:335:PX4:C1	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:337:PX4:C1	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:339:PX4:C1	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:341:PX4:C1	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:343:PX4:C1	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:345:PX4:C1	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:347:PX4:C1	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:349:PX4:C1	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:351:PX4:C1	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:353:PX4:C1	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:355:PX4:C1	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:357:PX4:C1	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:359:PX4:C1	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:361:PX4:C1	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:363:PX4:C1	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:402:PX4:C1	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:404:PX4:C1	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:406:PX4:C1	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:408:PX4:C1	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:410:PX4:C1	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:412:PX4:C1	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:414:PX4:C1	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:416:PX4:C1	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:418:PX4:C1	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:420:PX4:C1	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:422:PX4:C1	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:424:PX4:C1	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:426:PX4:C1	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:428:PX4:C1	8	2.63
(2,988)	1:A:129:TRP:HE1	4:A:430:PX4:C1	8	2.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,833)	1:A:120:ILE:HD11	1:A:200:LEU:HD22	14	2.63
(2,833)	1:A:120:ILE:HD11	1:A:200:LEU:HD23	14	2.63
(2,177)	1:A:171:HIS:H	1:A:134:ILE:HD11	17	2.61
(2,177)	1:A:171:HIS:H	1:A:134:ILE:HD12	17	2.61
(2,177)	1:A:171:HIS:H	1:A:134:ILE:HD13	17	2.61
(2,984)	1:A:78:PHE:HD1	1:A:80:ASN:HD21	19	2.6
(2,984)	1:A:78:PHE:HD1	1:A:80:ASN:HD22	19	2.6
(2,984)	1:A:78:PHE:HD1	1:A:80:ASN:HD21	19	2.6
(2,984)	1:A:78:PHE:HD1	1:A:80:ASN:HD22	19	2.6
(2,832)	1:A:120:ILE:HD11	1:A:200:LEU:HD21	13	2.6
(2,729)	1:A:211:VAL:HG12	1:A:226:LEU:HD21	17	2.6
(2,531)	1:A:205:SER:H	1:A:204:HIS:HE1	4	2.6
(2,941)	1:A:73:ALA:HA	1:A:77:LEU:H	8	2.59
(2,759)	1:A:54:LEU:HD21	1:A:59:ILE:HD11	12	2.58
(2,759)	1:A:54:LEU:HD21	1:A:59:ILE:HD12	12	2.58
(2,759)	1:A:54:LEU:HD21	1:A:59:ILE:HD13	12	2.58
(2,729)	1:A:211:VAL:HG12	1:A:226:LEU:HD21	12	2.58
(2,837)	1:A:120:ILE:HD13	1:A:200:LEU:HD22	14	2.54
(2,837)	1:A:120:ILE:HD13	1:A:200:LEU:HD23	14	2.54
(2,471)	1:A:186:ILE:H	1:A:156:LEU:HD11	16	2.54
(2,471)	1:A:186:ILE:H	1:A:156:LEU:HD12	16	2.54
(2,471)	1:A:186:ILE:H	1:A:156:LEU:HD13	16	2.54
(2,834)	1:A:120:ILE:HD12	1:A:200:LEU:HD21	14	2.53
(2,984)	1:A:78:PHE:HD1	1:A:80:ASN:HD21	13	2.52
(2,984)	1:A:78:PHE:HD1	1:A:80:ASN:HD22	13	2.52
(2,984)	1:A:78:PHE:HD1	1:A:80:ASN:HD21	13	2.52
(2,984)	1:A:78:PHE:HD1	1:A:80:ASN:HD22	13	2.52
(2,837)	1:A:120:ILE:HD13	1:A:200:LEU:HD22	6	2.52
(2,837)	1:A:120:ILE:HD13	1:A:200:LEU:HD23	6	2.52
(2,472)	1:A:186:ILE:H	1:A:156:LEU:HD21	17	2.52
(2,833)	1:A:120:ILE:HD11	1:A:200:LEU:HD22	7	2.49
(2,833)	1:A:120:ILE:HD11	1:A:200:LEU:HD23	7	2.49
(2,985)	1:A:80:ASN:H	1:A:78:PHE:HD1	7	2.47
(3,6)	1:A:78:PHE:H	4:A:305:PX4:C27	20	2.46
(3,6)	1:A:78:PHE:H	4:A:307:PX4:C27	20	2.46
(3,6)	1:A:78:PHE:H	4:A:309:PX4:C27	20	2.46
(3,6)	1:A:78:PHE:H	4:A:311:PX4:C27	20	2.46
(3,6)	1:A:78:PHE:H	4:A:313:PX4:C27	20	2.46
(3,6)	1:A:78:PHE:H	4:A:315:PX4:C27	20	2.46
(3,6)	1:A:78:PHE:H	4:A:317:PX4:C27	20	2.46
(3,6)	1:A:78:PHE:H	4:A:319:PX4:C27	20	2.46
(3,6)	1:A:78:PHE:H	4:A:321:PX4:C27	20	2.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,6)	1:A:78:PHE:H	4:A:323:PX4:C27	20	2.46
(3,6)	1:A:78:PHE:H	4:A:325:PX4:C27	20	2.46
(3,6)	1:A:78:PHE:H	4:A:327:PX4:C27	20	2.46
(3,6)	1:A:78:PHE:H	4:A:329:PX4:C27	20	2.46
(3,6)	1:A:78:PHE:H	4:A:331:PX4:C27	20	2.46
(3,6)	1:A:78:PHE:H	4:A:333:PX4:C27	20	2.46
(3,6)	1:A:78:PHE:H	4:A:335:PX4:C27	20	2.46
(3,6)	1:A:78:PHE:H	4:A:337:PX4:C27	20	2.46
(3,6)	1:A:78:PHE:H	4:A:339:PX4:C27	20	2.46
(3,6)	1:A:78:PHE:H	4:A:341:PX4:C27	20	2.46
(3,6)	1:A:78:PHE:H	4:A:343:PX4:C27	20	2.46
(3,6)	1:A:78:PHE:H	4:A:345:PX4:C27	20	2.46
(3,6)	1:A:78:PHE:H	4:A:347:PX4:C27	20	2.46
(3,6)	1:A:78:PHE:H	4:A:349:PX4:C27	20	2.46
(3,6)	1:A:78:PHE:H	4:A:351:PX4:C27	20	2.46
(3,6)	1:A:78:PHE:H	4:A:353:PX4:C27	20	2.46
(3,6)	1:A:78:PHE:H	4:A:355:PX4:C27	20	2.46
(3,6)	1:A:78:PHE:H	4:A:357:PX4:C27	20	2.46
(3,6)	1:A:78:PHE:H	4:A:359:PX4:C27	20	2.46
(3,6)	1:A:78:PHE:H	4:A:361:PX4:C27	20	2.46
(3,6)	1:A:78:PHE:H	4:A:363:PX4:C27	20	2.46
(3,6)	1:A:78:PHE:H	4:A:402:PX4:C27	20	2.46
(3,6)	1:A:78:PHE:H	4:A:404:PX4:C27	20	2.46
(3,6)	1:A:78:PHE:H	4:A:406:PX4:C27	20	2.46
(3,6)	1:A:78:PHE:H	4:A:408:PX4:C27	20	2.46
(3,6)	1:A:78:PHE:H	4:A:410:PX4:C27	20	2.46
(3,6)	1:A:78:PHE:H	4:A:412:PX4:C27	20	2.46
(3,6)	1:A:78:PHE:H	4:A:414:PX4:C27	20	2.46
(3,6)	1:A:78:PHE:H	4:A:416:PX4:C27	20	2.46
(3,6)	1:A:78:PHE:H	4:A:418:PX4:C27	20	2.46
(3,6)	1:A:78:PHE:H	4:A:420:PX4:C27	20	2.46
(3,6)	1:A:78:PHE:H	4:A:422:PX4:C27	20	2.46
(3,6)	1:A:78:PHE:H	4:A:424:PX4:C27	20	2.46
(3,6)	1:A:78:PHE:H	4:A:426:PX4:C27	20	2.46
(3,6)	1:A:78:PHE:H	4:A:428:PX4:C27	20	2.46
(3,6)	1:A:78:PHE:H	4:A:430:PX4:C27	20	2.46
(2,941)	1:A:73:ALA:HA	1:A:77:LEU:H	4	2.46
(2,517)	1:A:200:LEU:H	1:A:196:LEU:HD21	20	2.46
(2,531)	1:A:205:SER:H	1:A:204:HIS:HE1	10	2.45
(2,842)	1:A:200:LEU:HD21	1:A:122:LEU:HD21	9	2.44
(2,837)	1:A:120:ILE:HD13	1:A:200:LEU:HD22	11	2.44
(2,837)	1:A:120:ILE:HD13	1:A:200:LEU:HD23	11	2.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,833)	1:A:120:ILE:HD11	1:A:200:LEU:HD22	11	2.43
(2,833)	1:A:120:ILE:HD11	1:A:200:LEU:HD23	11	2.43
(2,466)	1:A:84:TRP:H	1:A:200:LEU:HD21	18	2.43
(2,755)	1:A:54:LEU:HD21	1:A:58:VAL:HG11	12	2.4
(2,755)	1:A:54:LEU:HD21	1:A:58:VAL:HG12	12	2.4
(2,755)	1:A:54:LEU:HD21	1:A:58:VAL:HG13	12	2.4
(2,941)	1:A:73:ALA:HA	1:A:77:LEU:H	3	2.39
(2,941)	1:A:73:ALA:HA	1:A:77:LEU:H	11	2.39
(2,760)	1:A:54:LEU:HD22	1:A:59:ILE:HD11	11	2.39
(2,760)	1:A:54:LEU:HD22	1:A:59:ILE:HD12	11	2.39
(2,760)	1:A:54:LEU:HD22	1:A:59:ILE:HD13	11	2.39
(2,760)	1:A:54:LEU:HD23	1:A:59:ILE:HD11	11	2.39
(2,760)	1:A:54:LEU:HD23	1:A:59:ILE:HD12	11	2.39
(2,760)	1:A:54:LEU:HD23	1:A:59:ILE:HD13	11	2.39
(2,731)	1:A:211:VAL:HG13	1:A:226:LEU:HD21	7	2.39
(2,472)	1:A:186:ILE:H	1:A:156:LEU:HD21	11	2.39
(2,257)	1:A:112:ALA:H	1:A:189:LEU:HD21	19	2.38
(2,871)	1:A:186:ILE:HD13	1:A:156:LEU:HD21	8	2.37
(2,473)	1:A:186:ILE:H	1:A:156:LEU:HD22	13	2.36
(2,473)	1:A:186:ILE:H	1:A:156:LEU:HD23	13	2.36
(2,982)	1:A:78:PHE:HD1	1:A:80:ASN:H	6	2.35
(2,834)	1:A:120:ILE:HD12	1:A:200:LEU:HD21	20	2.35
(3,21)	1:A:77:LEU:H	4:A:305:PX4:C35	14	2.34
(3,21)	1:A:77:LEU:H	4:A:307:PX4:C35	14	2.34
(3,21)	1:A:77:LEU:H	4:A:309:PX4:C35	14	2.34
(3,21)	1:A:77:LEU:H	4:A:311:PX4:C35	14	2.34
(3,21)	1:A:77:LEU:H	4:A:313:PX4:C35	14	2.34
(3,21)	1:A:77:LEU:H	4:A:315:PX4:C35	14	2.34
(3,21)	1:A:77:LEU:H	4:A:317:PX4:C35	14	2.34
(3,21)	1:A:77:LEU:H	4:A:319:PX4:C35	14	2.34
(3,21)	1:A:77:LEU:H	4:A:321:PX4:C35	14	2.34
(3,21)	1:A:77:LEU:H	4:A:323:PX4:C35	14	2.34
(3,21)	1:A:77:LEU:H	4:A:325:PX4:C35	14	2.34
(3,21)	1:A:77:LEU:H	4:A:327:PX4:C35	14	2.34
(3,21)	1:A:77:LEU:H	4:A:329:PX4:C35	14	2.34
(3,21)	1:A:77:LEU:H	4:A:331:PX4:C35	14	2.34
(3,21)	1:A:77:LEU:H	4:A:333:PX4:C35	14	2.34
(3,21)	1:A:77:LEU:H	4:A:335:PX4:C35	14	2.34
(3,21)	1:A:77:LEU:H	4:A:337:PX4:C35	14	2.34
(3,21)	1:A:77:LEU:H	4:A:339:PX4:C35	14	2.34
(3,21)	1:A:77:LEU:H	4:A:341:PX4:C35	14	2.34
(3,21)	1:A:77:LEU:H	4:A:343:PX4:C35	14	2.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,21)	1:A:77:LEU:H	4:A:345:PX4:C35	14	2.34
(3,21)	1:A:77:LEU:H	4:A:347:PX4:C35	14	2.34
(3,21)	1:A:77:LEU:H	4:A:349:PX4:C35	14	2.34
(3,21)	1:A:77:LEU:H	4:A:351:PX4:C35	14	2.34
(3,21)	1:A:77:LEU:H	4:A:353:PX4:C35	14	2.34
(3,21)	1:A:77:LEU:H	4:A:355:PX4:C35	14	2.34
(3,21)	1:A:77:LEU:H	4:A:357:PX4:C35	14	2.34
(3,21)	1:A:77:LEU:H	4:A:359:PX4:C35	14	2.34
(3,21)	1:A:77:LEU:H	4:A:361:PX4:C35	14	2.34
(3,21)	1:A:77:LEU:H	4:A:363:PX4:C35	14	2.34
(3,21)	1:A:77:LEU:H	4:A:402:PX4:C35	14	2.34
(3,21)	1:A:77:LEU:H	4:A:404:PX4:C35	14	2.34
(3,21)	1:A:77:LEU:H	4:A:406:PX4:C35	14	2.34
(3,21)	1:A:77:LEU:H	4:A:408:PX4:C35	14	2.34
(3,21)	1:A:77:LEU:H	4:A:410:PX4:C35	14	2.34
(3,21)	1:A:77:LEU:H	4:A:412:PX4:C35	14	2.34
(3,21)	1:A:77:LEU:H	4:A:414:PX4:C35	14	2.34
(3,21)	1:A:77:LEU:H	4:A:416:PX4:C35	14	2.34
(3,21)	1:A:77:LEU:H	4:A:418:PX4:C35	14	2.34
(3,21)	1:A:77:LEU:H	4:A:420:PX4:C35	14	2.34
(3,21)	1:A:77:LEU:H	4:A:422:PX4:C35	14	2.34
(3,21)	1:A:77:LEU:H	4:A:424:PX4:C35	14	2.34
(3,21)	1:A:77:LEU:H	4:A:426:PX4:C35	14	2.34
(3,21)	1:A:77:LEU:H	4:A:428:PX4:C35	14	2.34
(3,21)	1:A:77:LEU:H	4:A:430:PX4:C35	14	2.34
(2,837)	1:A:120:ILE:HD13	1:A:200:LEU:HD22	19	2.34
(2,837)	1:A:120:ILE:HD13	1:A:200:LEU:HD23	19	2.34
(2,472)	1:A:186:ILE:H	1:A:156:LEU:HD21	20	2.33
(2,837)	1:A:120:ILE:HD13	1:A:200:LEU:HD22	8	2.32
(2,837)	1:A:120:ILE:HD13	1:A:200:LEU:HD23	8	2.32
(2,82)	1:A:58:VAL:H	1:A:48:LEU:HD21	9	2.32
(2,759)	1:A:54:LEU:HD21	1:A:59:ILE:HD11	8	2.32
(2,759)	1:A:54:LEU:HD21	1:A:59:ILE:HD12	8	2.32
(2,759)	1:A:54:LEU:HD21	1:A:59:ILE:HD13	8	2.32
(2,471)	1:A:186:ILE:H	1:A:156:LEU:HD11	11	2.32
(2,471)	1:A:186:ILE:H	1:A:156:LEU:HD12	11	2.32
(2,471)	1:A:186:ILE:H	1:A:156:LEU:HD13	11	2.32
(2,773)	1:A:61:ILE:HD11	1:A:48:LEU:HD21	16	2.31
(2,731)	1:A:211:VAL:HG13	1:A:226:LEU:HD21	12	2.3
(2,656)	1:A:39:LEU:H	1:A:19:LEU:HD21	6	2.3
(2,657)	1:A:39:LEU:H	1:A:19:LEU:HD22	3	2.29
(2,657)	1:A:39:LEU:H	1:A:19:LEU:HD23	3	2.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,598)	1:A:235:GLN:H	1:A:238:TYR:HE1	7	2.29
(2,598)	1:A:235:GLN:H	1:A:238:TYR:HE2	7	2.29
(3,36)	1:A:129:TRP:HE1	4:A:305:PX4:N1	14	2.28
(3,36)	1:A:129:TRP:HE1	4:A:307:PX4:N1	14	2.28
(3,36)	1:A:129:TRP:HE1	4:A:309:PX4:N1	14	2.28
(3,36)	1:A:129:TRP:HE1	4:A:311:PX4:N1	14	2.28
(3,36)	1:A:129:TRP:HE1	4:A:313:PX4:N1	14	2.28
(3,36)	1:A:129:TRP:HE1	4:A:315:PX4:N1	14	2.28
(3,36)	1:A:129:TRP:HE1	4:A:317:PX4:N1	14	2.28
(3,36)	1:A:129:TRP:HE1	4:A:319:PX4:N1	14	2.28
(3,36)	1:A:129:TRP:HE1	4:A:321:PX4:N1	14	2.28
(3,36)	1:A:129:TRP:HE1	4:A:323:PX4:N1	14	2.28
(3,36)	1:A:129:TRP:HE1	4:A:325:PX4:N1	14	2.28
(3,36)	1:A:129:TRP:HE1	4:A:327:PX4:N1	14	2.28
(3,36)	1:A:129:TRP:HE1	4:A:329:PX4:N1	14	2.28
(3,36)	1:A:129:TRP:HE1	4:A:331:PX4:N1	14	2.28
(3,36)	1:A:129:TRP:HE1	4:A:333:PX4:N1	14	2.28
(3,36)	1:A:129:TRP:HE1	4:A:335:PX4:N1	14	2.28
(3,36)	1:A:129:TRP:HE1	4:A:337:PX4:N1	14	2.28
(3,36)	1:A:129:TRP:HE1	4:A:339:PX4:N1	14	2.28
(3,36)	1:A:129:TRP:HE1	4:A:341:PX4:N1	14	2.28
(3,36)	1:A:129:TRP:HE1	4:A:343:PX4:N1	14	2.28
(3,36)	1:A:129:TRP:HE1	4:A:345:PX4:N1	14	2.28
(3,36)	1:A:129:TRP:HE1	4:A:347:PX4:N1	14	2.28
(3,36)	1:A:129:TRP:HE1	4:A:349:PX4:N1	14	2.28
(3,36)	1:A:129:TRP:HE1	4:A:351:PX4:N1	14	2.28
(3,36)	1:A:129:TRP:HE1	4:A:353:PX4:N1	14	2.28
(3,36)	1:A:129:TRP:HE1	4:A:355:PX4:N1	14	2.28
(3,36)	1:A:129:TRP:HE1	4:A:357:PX4:N1	14	2.28
(3,36)	1:A:129:TRP:HE1	4:A:359:PX4:N1	14	2.28
(3,36)	1:A:129:TRP:HE1	4:A:361:PX4:N1	14	2.28
(3,36)	1:A:129:TRP:HE1	4:A:363:PX4:N1	14	2.28
(3,36)	1:A:129:TRP:HE1	4:A:402:PX4:N1	14	2.28
(3,36)	1:A:129:TRP:HE1	4:A:404:PX4:N1	14	2.28
(3,36)	1:A:129:TRP:HE1	4:A:406:PX4:N1	14	2.28
(3,36)	1:A:129:TRP:HE1	4:A:408:PX4:N1	14	2.28
(3,36)	1:A:129:TRP:HE1	4:A:410:PX4:N1	14	2.28
(3,36)	1:A:129:TRP:HE1	4:A:412:PX4:N1	14	2.28
(3,36)	1:A:129:TRP:HE1	4:A:414:PX4:N1	14	2.28
(3,36)	1:A:129:TRP:HE1	4:A:416:PX4:N1	14	2.28
(3,36)	1:A:129:TRP:HE1	4:A:418:PX4:N1	14	2.28
(3,36)	1:A:129:TRP:HE1	4:A:420:PX4:N1	14	2.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,36)	1:A:129:TRP:HE1	4:A:422:PX4:N1	14	2.28
(3,36)	1:A:129:TRP:HE1	4:A:424:PX4:N1	14	2.28
(3,36)	1:A:129:TRP:HE1	4:A:426:PX4:N1	14	2.28
(3,36)	1:A:129:TRP:HE1	4:A:428:PX4:N1	14	2.28
(3,36)	1:A:129:TRP:HE1	4:A:430:PX4:N1	14	2.28
(2,985)	1:A:80:ASN:H	1:A:78:PHE:HD1	1	2.28
(2,837)	1:A:120:ILE:HD13	1:A:200:LEU:HD22	2	2.27
(2,837)	1:A:120:ILE:HD13	1:A:200:LEU:HD23	2	2.27
(2,671)	1:A:66:ARG:H	1:A:156:LEU:HD21	16	2.27
(2,941)	1:A:73:ALA:HA	1:A:77:LEU:H	6	2.26
(2,82)	1:A:58:VAL:H	1:A:48:LEU:HD21	19	2.25
(2,975)	1:A:78:PHE:H	1:A:77:LEU:HD22	9	2.24
(2,975)	1:A:78:PHE:H	1:A:77:LEU:HD23	9	2.24
(2,879)	1:A:234:ILE:HD11	1:A:200:LEU:HB2	11	2.23
(2,879)	1:A:234:ILE:HD12	1:A:200:LEU:HB2	11	2.23
(2,879)	1:A:234:ILE:HD13	1:A:200:LEU:HB2	11	2.23
(2,598)	1:A:235:GLN:H	1:A:238:TYR:HE1	15	2.23
(2,598)	1:A:235:GLN:H	1:A:238:TYR:HE2	15	2.23
(2,472)	1:A:186:ILE:H	1:A:156:LEU:HD21	10	2.23
(2,765)	1:A:22:PHE:H	1:A:19:LEU:HD21	5	2.22
(2,765)	1:A:22:PHE:H	1:A:19:LEU:HD21	11	2.22
(2,727)	1:A:211:VAL:HG11	1:A:226:LEU:HD21	17	2.22
(2,872)	1:A:186:ILE:HD13	1:A:156:LEU:HD22	1	2.21
(2,872)	1:A:186:ILE:HD13	1:A:156:LEU:HD23	1	2.21
(2,833)	1:A:120:ILE:HD11	1:A:200:LEU:HD22	10	2.21
(2,833)	1:A:120:ILE:HD11	1:A:200:LEU:HD23	10	2.21
(2,879)	1:A:234:ILE:HD11	1:A:200:LEU:HB2	19	2.2
(2,879)	1:A:234:ILE:HD12	1:A:200:LEU:HB2	19	2.2
(2,879)	1:A:234:ILE:HD13	1:A:200:LEU:HB2	19	2.2
(2,871)	1:A:186:ILE:HD13	1:A:156:LEU:HD21	6	2.2
(2,932)	1:A:72:VAL:HG11	1:A:76:SER:H	15	2.19
(2,932)	1:A:72:VAL:HG12	1:A:76:SER:H	15	2.19
(2,932)	1:A:72:VAL:HG13	1:A:76:SER:H	15	2.19
(2,837)	1:A:120:ILE:HD13	1:A:200:LEU:HD22	7	2.19
(2,837)	1:A:120:ILE:HD13	1:A:200:LEU:HD23	7	2.19
(2,932)	1:A:72:VAL:HG11	1:A:76:SER:H	7	2.17
(2,932)	1:A:72:VAL:HG12	1:A:76:SER:H	7	2.17
(2,932)	1:A:72:VAL:HG13	1:A:76:SER:H	7	2.17
(2,879)	1:A:234:ILE:HD11	1:A:200:LEU:HB2	16	2.17
(2,879)	1:A:234:ILE:HD12	1:A:200:LEU:HB2	16	2.17
(2,879)	1:A:234:ILE:HD13	1:A:200:LEU:HB2	16	2.17
(2,836)	1:A:120:ILE:HD13	1:A:200:LEU:HD21	19	2.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,727)	1:A:211:VAL:HG11	1:A:226:LEU:HD21	6	2.17
(2,598)	1:A:235:GLN:H	1:A:238:TYR:HE1	4	2.17
(2,598)	1:A:235:GLN:H	1:A:238:TYR:HE2	4	2.17
(2,531)	1:A:205:SER:H	1:A:204:HIS:HE1	18	2.17
(2,598)	1:A:235:GLN:H	1:A:238:TYR:HE1	10	2.16
(2,598)	1:A:235:GLN:H	1:A:238:TYR:HE2	10	2.16
(2,836)	1:A:120:ILE:HD13	1:A:200:LEU:HD21	3	2.15
(2,732)	1:A:211:VAL:HG13	1:A:226:LEU:HD22	7	2.15
(2,732)	1:A:211:VAL:HG13	1:A:226:LEU:HD23	7	2.15
(2,510)	1:A:200:LEU:HD21	1:A:199:SER:H	3	2.15
(3,21)	1:A:77:LEU:H	4:A:305:PX4:C35	3	2.13
(3,21)	1:A:77:LEU:H	4:A:307:PX4:C35	3	2.13
(3,21)	1:A:77:LEU:H	4:A:309:PX4:C35	3	2.13
(3,21)	1:A:77:LEU:H	4:A:311:PX4:C35	3	2.13
(3,21)	1:A:77:LEU:H	4:A:313:PX4:C35	3	2.13
(3,21)	1:A:77:LEU:H	4:A:315:PX4:C35	3	2.13
(3,21)	1:A:77:LEU:H	4:A:317:PX4:C35	3	2.13
(3,21)	1:A:77:LEU:H	4:A:319:PX4:C35	3	2.13
(3,21)	1:A:77:LEU:H	4:A:321:PX4:C35	3	2.13
(3,21)	1:A:77:LEU:H	4:A:323:PX4:C35	3	2.13
(3,21)	1:A:77:LEU:H	4:A:325:PX4:C35	3	2.13
(3,21)	1:A:77:LEU:H	4:A:327:PX4:C35	3	2.13
(3,21)	1:A:77:LEU:H	4:A:329:PX4:C35	3	2.13
(3,21)	1:A:77:LEU:H	4:A:331:PX4:C35	3	2.13
(3,21)	1:A:77:LEU:H	4:A:333:PX4:C35	3	2.13
(3,21)	1:A:77:LEU:H	4:A:335:PX4:C35	3	2.13
(3,21)	1:A:77:LEU:H	4:A:337:PX4:C35	3	2.13
(3,21)	1:A:77:LEU:H	4:A:339:PX4:C35	3	2.13
(3,21)	1:A:77:LEU:H	4:A:341:PX4:C35	3	2.13
(3,21)	1:A:77:LEU:H	4:A:343:PX4:C35	3	2.13
(3,21)	1:A:77:LEU:H	4:A:345:PX4:C35	3	2.13
(3,21)	1:A:77:LEU:H	4:A:347:PX4:C35	3	2.13
(3,21)	1:A:77:LEU:H	4:A:349:PX4:C35	3	2.13
(3,21)	1:A:77:LEU:H	4:A:351:PX4:C35	3	2.13
(3,21)	1:A:77:LEU:H	4:A:353:PX4:C35	3	2.13
(3,21)	1:A:77:LEU:H	4:A:355:PX4:C35	3	2.13
(3,21)	1:A:77:LEU:H	4:A:357:PX4:C35	3	2.13
(3,21)	1:A:77:LEU:H	4:A:359:PX4:C35	3	2.13
(3,21)	1:A:77:LEU:H	4:A:361:PX4:C35	3	2.13
(3,21)	1:A:77:LEU:H	4:A:363:PX4:C35	3	2.13
(3,21)	1:A:77:LEU:H	4:A:402:PX4:C35	3	2.13
(3,21)	1:A:77:LEU:H	4:A:404:PX4:C35	3	2.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,21)	1:A:77:LEU:H	4:A:406:PX4:C35	3	2.13
(3,21)	1:A:77:LEU:H	4:A:408:PX4:C35	3	2.13
(3,21)	1:A:77:LEU:H	4:A:410:PX4:C35	3	2.13
(3,21)	1:A:77:LEU:H	4:A:412:PX4:C35	3	2.13
(3,21)	1:A:77:LEU:H	4:A:414:PX4:C35	3	2.13
(3,21)	1:A:77:LEU:H	4:A:416:PX4:C35	3	2.13
(3,21)	1:A:77:LEU:H	4:A:418:PX4:C35	3	2.13
(3,21)	1:A:77:LEU:H	4:A:420:PX4:C35	3	2.13
(3,21)	1:A:77:LEU:H	4:A:422:PX4:C35	3	2.13
(3,21)	1:A:77:LEU:H	4:A:424:PX4:C35	3	2.13
(3,21)	1:A:77:LEU:H	4:A:426:PX4:C35	3	2.13
(3,21)	1:A:77:LEU:H	4:A:428:PX4:C35	3	2.13
(3,21)	1:A:77:LEU:H	4:A:430:PX4:C35	3	2.13
(2,975)	1:A:78:PHE:H	1:A:77:LEU:HD22	18	2.13
(2,975)	1:A:78:PHE:H	1:A:77:LEU:HD23	18	2.13
(2,879)	1:A:234:ILE:HD11	1:A:200:LEU:HB2	7	2.13
(2,879)	1:A:234:ILE:HD12	1:A:200:LEU:HB2	7	2.13
(2,879)	1:A:234:ILE:HD13	1:A:200:LEU:HB2	7	2.13
(2,321)	1:A:128:VAL:HG11	1:A:126:LYS:H	18	2.13
(2,321)	1:A:128:VAL:HG12	1:A:126:LYS:H	18	2.13
(2,321)	1:A:128:VAL:HG13	1:A:126:LYS:H	18	2.13
(2,982)	1:A:78:PHE:HD1	1:A:80:ASN:H	20	2.12
(2,836)	1:A:120:ILE:HD13	1:A:200:LEU:HD21	13	2.12
(2,833)	1:A:120:ILE:HD11	1:A:200:LEU:HD22	12	2.12
(2,833)	1:A:120:ILE:HD11	1:A:200:LEU:HD23	12	2.12
(2,321)	1:A:128:VAL:HG11	1:A:126:LYS:H	15	2.12
(2,321)	1:A:128:VAL:HG12	1:A:126:LYS:H	15	2.12
(2,321)	1:A:128:VAL:HG13	1:A:126:LYS:H	15	2.12
(2,879)	1:A:234:ILE:HD11	1:A:200:LEU:HB2	6	2.11
(2,879)	1:A:234:ILE:HD12	1:A:200:LEU:HB2	6	2.11
(2,879)	1:A:234:ILE:HD13	1:A:200:LEU:HB2	6	2.11
(2,844)	1:A:200:LEU:HD22	1:A:122:LEU:HD21	9	2.11
(2,765)	1:A:22:PHE:H	1:A:19:LEU:HD21	8	2.11
(2,730)	1:A:211:VAL:HG12	1:A:226:LEU:HD22	17	2.11
(2,730)	1:A:211:VAL:HG12	1:A:226:LEU:HD23	17	2.11
(3,6)	1:A:78:PHE:H	4:A:305:PX4:C27	7	2.1
(3,6)	1:A:78:PHE:H	4:A:307:PX4:C27	7	2.1
(3,6)	1:A:78:PHE:H	4:A:309:PX4:C27	7	2.1
(3,6)	1:A:78:PHE:H	4:A:311:PX4:C27	7	2.1
(3,6)	1:A:78:PHE:H	4:A:313:PX4:C27	7	2.1
(3,6)	1:A:78:PHE:H	4:A:315:PX4:C27	7	2.1
(3,6)	1:A:78:PHE:H	4:A:317:PX4:C27	7	2.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,6)	1:A:78:PHE:H	4:A:319:PX4:C27	7	2.1
(3,6)	1:A:78:PHE:H	4:A:321:PX4:C27	7	2.1
(3,6)	1:A:78:PHE:H	4:A:323:PX4:C27	7	2.1
(3,6)	1:A:78:PHE:H	4:A:325:PX4:C27	7	2.1
(3,6)	1:A:78:PHE:H	4:A:327:PX4:C27	7	2.1
(3,6)	1:A:78:PHE:H	4:A:329:PX4:C27	7	2.1
(3,6)	1:A:78:PHE:H	4:A:331:PX4:C27	7	2.1
(3,6)	1:A:78:PHE:H	4:A:333:PX4:C27	7	2.1
(3,6)	1:A:78:PHE:H	4:A:335:PX4:C27	7	2.1
(3,6)	1:A:78:PHE:H	4:A:337:PX4:C27	7	2.1
(3,6)	1:A:78:PHE:H	4:A:339:PX4:C27	7	2.1
(3,6)	1:A:78:PHE:H	4:A:341:PX4:C27	7	2.1
(3,6)	1:A:78:PHE:H	4:A:343:PX4:C27	7	2.1
(3,6)	1:A:78:PHE:H	4:A:345:PX4:C27	7	2.1
(3,6)	1:A:78:PHE:H	4:A:347:PX4:C27	7	2.1
(3,6)	1:A:78:PHE:H	4:A:349:PX4:C27	7	2.1
(3,6)	1:A:78:PHE:H	4:A:351:PX4:C27	7	2.1
(3,6)	1:A:78:PHE:H	4:A:353:PX4:C27	7	2.1
(3,6)	1:A:78:PHE:H	4:A:355:PX4:C27	7	2.1
(3,6)	1:A:78:PHE:H	4:A:357:PX4:C27	7	2.1
(3,6)	1:A:78:PHE:H	4:A:359:PX4:C27	7	2.1
(3,6)	1:A:78:PHE:H	4:A:361:PX4:C27	7	2.1
(3,6)	1:A:78:PHE:H	4:A:363:PX4:C27	7	2.1
(3,6)	1:A:78:PHE:H	4:A:402:PX4:C27	7	2.1
(3,6)	1:A:78:PHE:H	4:A:404:PX4:C27	7	2.1
(3,6)	1:A:78:PHE:H	4:A:406:PX4:C27	7	2.1
(3,6)	1:A:78:PHE:H	4:A:408:PX4:C27	7	2.1
(3,6)	1:A:78:PHE:H	4:A:410:PX4:C27	7	2.1
(3,6)	1:A:78:PHE:H	4:A:412:PX4:C27	7	2.1
(3,6)	1:A:78:PHE:H	4:A:414:PX4:C27	7	2.1
(3,6)	1:A:78:PHE:H	4:A:416:PX4:C27	7	2.1
(3,6)	1:A:78:PHE:H	4:A:418:PX4:C27	7	2.1
(3,6)	1:A:78:PHE:H	4:A:420:PX4:C27	7	2.1
(3,6)	1:A:78:PHE:H	4:A:422:PX4:C27	7	2.1
(3,6)	1:A:78:PHE:H	4:A:424:PX4:C27	7	2.1
(3,6)	1:A:78:PHE:H	4:A:426:PX4:C27	7	2.1
(3,6)	1:A:78:PHE:H	4:A:428:PX4:C27	7	2.1
(3,6)	1:A:78:PHE:H	4:A:430:PX4:C27	7	2.1
(2,871)	1:A:186:ILE:HD13	1:A:156:LEU:HD21	19	2.1
(2,837)	1:A:120:ILE:HD13	1:A:200:LEU:HD22	4	2.1
(2,837)	1:A:120:ILE:HD13	1:A:200:LEU:HD23	4	2.1
(2,727)	1:A:211:VAL:HG11	1:A:226:LEU:HD21	7	2.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,833)	1:A:120:ILE:HD11	1:A:200:LEU:HD22	2	2.08
(2,833)	1:A:120:ILE:HD11	1:A:200:LEU:HD23	2	2.08
(2,82)	1:A:58:VAL:H	1:A:48:LEU:HD21	16	2.08
(2,765)	1:A:22:PHE:H	1:A:19:LEU:HD21	19	2.08
(2,760)	1:A:54:LEU:HD22	1:A:59:ILE:HD11	7	2.07
(2,760)	1:A:54:LEU:HD22	1:A:59:ILE:HD12	7	2.07
(2,760)	1:A:54:LEU:HD22	1:A:59:ILE:HD13	7	2.07
(2,760)	1:A:54:LEU:HD23	1:A:59:ILE:HD11	7	2.07
(2,760)	1:A:54:LEU:HD23	1:A:59:ILE:HD12	7	2.07
(2,760)	1:A:54:LEU:HD23	1:A:59:ILE:HD13	7	2.07
(2,728)	1:A:211:VAL:HG11	1:A:226:LEU:HD22	7	2.07
(2,728)	1:A:211:VAL:HG11	1:A:226:LEU:HD23	7	2.07
(2,510)	1:A:200:LEU:HD21	1:A:199:SER:H	13	2.07
(2,932)	1:A:72:VAL:HG11	1:A:76:SER:H	2	2.06
(2,932)	1:A:72:VAL:HG12	1:A:76:SER:H	2	2.06
(2,932)	1:A:72:VAL:HG13	1:A:76:SER:H	2	2.06
(2,837)	1:A:120:ILE:HD13	1:A:200:LEU:HD22	5	2.06
(2,837)	1:A:120:ILE:HD13	1:A:200:LEU:HD23	5	2.06
(2,832)	1:A:120:ILE:HD11	1:A:200:LEU:HD21	3	2.06
(2,759)	1:A:54:LEU:HD21	1:A:59:ILE:HD11	5	2.06
(2,759)	1:A:54:LEU:HD21	1:A:59:ILE:HD12	5	2.06
(2,759)	1:A:54:LEU:HD21	1:A:59:ILE:HD13	5	2.06
(2,757)	1:A:54:LEU:HD21	1:A:39:LEU:HD11	6	2.06
(2,757)	1:A:54:LEU:HD21	1:A:39:LEU:HD12	6	2.06
(2,757)	1:A:54:LEU:HD21	1:A:39:LEU:HD13	6	2.06
(3,36)	1:A:129:TRP:HE1	4:A:305:PX4:N1	19	2.04
(3,36)	1:A:129:TRP:HE1	4:A:307:PX4:N1	19	2.04
(3,36)	1:A:129:TRP:HE1	4:A:309:PX4:N1	19	2.04
(3,36)	1:A:129:TRP:HE1	4:A:311:PX4:N1	19	2.04
(3,36)	1:A:129:TRP:HE1	4:A:313:PX4:N1	19	2.04
(3,36)	1:A:129:TRP:HE1	4:A:315:PX4:N1	19	2.04
(3,36)	1:A:129:TRP:HE1	4:A:317:PX4:N1	19	2.04
(3,36)	1:A:129:TRP:HE1	4:A:319:PX4:N1	19	2.04
(3,36)	1:A:129:TRP:HE1	4:A:321:PX4:N1	19	2.04
(3,36)	1:A:129:TRP:HE1	4:A:323:PX4:N1	19	2.04
(3,36)	1:A:129:TRP:HE1	4:A:325:PX4:N1	19	2.04
(3,36)	1:A:129:TRP:HE1	4:A:327:PX4:N1	19	2.04
(3,36)	1:A:129:TRP:HE1	4:A:329:PX4:N1	19	2.04
(3,36)	1:A:129:TRP:HE1	4:A:331:PX4:N1	19	2.04
(3,36)	1:A:129:TRP:HE1	4:A:333:PX4:N1	19	2.04
(3,36)	1:A:129:TRP:HE1	4:A:335:PX4:N1	19	2.04
(3,36)	1:A:129:TRP:HE1	4:A:337:PX4:N1	19	2.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,36)	1:A:129:TRP:HE1	4:A:339:PX4:N1	19	2.04
(3,36)	1:A:129:TRP:HE1	4:A:341:PX4:N1	19	2.04
(3,36)	1:A:129:TRP:HE1	4:A:343:PX4:N1	19	2.04
(3,36)	1:A:129:TRP:HE1	4:A:345:PX4:N1	19	2.04
(3,36)	1:A:129:TRP:HE1	4:A:347:PX4:N1	19	2.04
(3,36)	1:A:129:TRP:HE1	4:A:349:PX4:N1	19	2.04
(3,36)	1:A:129:TRP:HE1	4:A:351:PX4:N1	19	2.04
(3,36)	1:A:129:TRP:HE1	4:A:353:PX4:N1	19	2.04
(3,36)	1:A:129:TRP:HE1	4:A:355:PX4:N1	19	2.04
(3,36)	1:A:129:TRP:HE1	4:A:357:PX4:N1	19	2.04
(3,36)	1:A:129:TRP:HE1	4:A:359:PX4:N1	19	2.04
(3,36)	1:A:129:TRP:HE1	4:A:361:PX4:N1	19	2.04
(3,36)	1:A:129:TRP:HE1	4:A:363:PX4:N1	19	2.04
(3,36)	1:A:129:TRP:HE1	4:A:402:PX4:N1	19	2.04
(3,36)	1:A:129:TRP:HE1	4:A:404:PX4:N1	19	2.04
(3,36)	1:A:129:TRP:HE1	4:A:406:PX4:N1	19	2.04
(3,36)	1:A:129:TRP:HE1	4:A:408:PX4:N1	19	2.04
(3,36)	1:A:129:TRP:HE1	4:A:410:PX4:N1	19	2.04
(3,36)	1:A:129:TRP:HE1	4:A:412:PX4:N1	19	2.04
(3,36)	1:A:129:TRP:HE1	4:A:414:PX4:N1	19	2.04
(3,36)	1:A:129:TRP:HE1	4:A:416:PX4:N1	19	2.04
(3,36)	1:A:129:TRP:HE1	4:A:418:PX4:N1	19	2.04
(3,36)	1:A:129:TRP:HE1	4:A:420:PX4:N1	19	2.04
(3,36)	1:A:129:TRP:HE1	4:A:422:PX4:N1	19	2.04
(3,36)	1:A:129:TRP:HE1	4:A:424:PX4:N1	19	2.04
(3,36)	1:A:129:TRP:HE1	4:A:426:PX4:N1	19	2.04
(3,36)	1:A:129:TRP:HE1	4:A:428:PX4:N1	19	2.04
(3,36)	1:A:129:TRP:HE1	4:A:430:PX4:N1	19	2.04
(2,982)	1:A:78:PHE:HD1	1:A:80:ASN:H	2	2.03
(2,857)	1:A:186:ILE:HD11	1:A:156:LEU:HD21	1	2.03
(2,837)	1:A:120:ILE:HD13	1:A:200:LEU:HD22	17	2.03
(2,837)	1:A:120:ILE:HD13	1:A:200:LEU:HD23	17	2.03
(2,834)	1:A:120:ILE:HD12	1:A:200:LEU:HD21	15	2.03
(2,832)	1:A:120:ILE:HD11	1:A:200:LEU:HD21	7	2.03
(2,879)	1:A:234:ILE:HD11	1:A:200:LEU:HB2	15	2.02
(2,879)	1:A:234:ILE:HD12	1:A:200:LEU:HB2	15	2.02
(2,879)	1:A:234:ILE:HD13	1:A:200:LEU:HB2	15	2.02
(2,472)	1:A:186:ILE:H	1:A:156:LEU:HD21	3	2.02
(2,773)	1:A:61:ILE:HD11	1:A:48:LEU:HD21	9	2.01
(2,746)	1:A:89:VAL:HG11	1:A:122:LEU:HD21	4	2.01
(2,656)	1:A:39:LEU:H	1:A:19:LEU:HD21	7	2.01
(2,775)	1:A:61:ILE:HD12	1:A:48:LEU:HD21	11	1.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,657)	1:A:39:LEU:H	1:A:19:LEU:HD22	10	1.99
(2,657)	1:A:39:LEU:H	1:A:19:LEU:HD23	10	1.99
(2,932)	1:A:72:VAL:HG11	1:A:76:SER:H	19	1.98
(2,932)	1:A:72:VAL:HG12	1:A:76:SER:H	19	1.98
(2,932)	1:A:72:VAL:HG13	1:A:76:SER:H	19	1.98
(2,871)	1:A:186:ILE:HD13	1:A:156:LEU:HD21	1	1.98
(2,598)	1:A:235:GLN:H	1:A:238:TYR:HE1	8	1.98
(2,598)	1:A:235:GLN:H	1:A:238:TYR:HE2	8	1.98
(2,879)	1:A:234:ILE:HD11	1:A:200:LEU:HB2	9	1.97
(2,879)	1:A:234:ILE:HD12	1:A:200:LEU:HB2	9	1.97
(2,879)	1:A:234:ILE:HD13	1:A:200:LEU:HB2	9	1.97
(2,472)	1:A:186:ILE:H	1:A:156:LEU:HD21	13	1.97
(2,471)	1:A:186:ILE:H	1:A:156:LEU:HD11	18	1.97
(2,471)	1:A:186:ILE:H	1:A:156:LEU:HD12	18	1.97
(2,471)	1:A:186:ILE:H	1:A:156:LEU:HD13	18	1.97
(2,379)	1:A:10:LEU:H	1:A:10:LEU:HD21	20	1.97
(3,6)	1:A:78:PHE:H	4:A:305:PX4:C27	13	1.96
(3,6)	1:A:78:PHE:H	4:A:307:PX4:C27	13	1.96
(3,6)	1:A:78:PHE:H	4:A:309:PX4:C27	13	1.96
(3,6)	1:A:78:PHE:H	4:A:311:PX4:C27	13	1.96
(3,6)	1:A:78:PHE:H	4:A:313:PX4:C27	13	1.96
(3,6)	1:A:78:PHE:H	4:A:315:PX4:C27	13	1.96
(3,6)	1:A:78:PHE:H	4:A:317:PX4:C27	13	1.96
(3,6)	1:A:78:PHE:H	4:A:319:PX4:C27	13	1.96
(3,6)	1:A:78:PHE:H	4:A:321:PX4:C27	13	1.96
(3,6)	1:A:78:PHE:H	4:A:323:PX4:C27	13	1.96
(3,6)	1:A:78:PHE:H	4:A:325:PX4:C27	13	1.96
(3,6)	1:A:78:PHE:H	4:A:327:PX4:C27	13	1.96
(3,6)	1:A:78:PHE:H	4:A:329:PX4:C27	13	1.96
(3,6)	1:A:78:PHE:H	4:A:331:PX4:C27	13	1.96
(3,6)	1:A:78:PHE:H	4:A:333:PX4:C27	13	1.96
(3,6)	1:A:78:PHE:H	4:A:335:PX4:C27	13	1.96
(3,6)	1:A:78:PHE:H	4:A:337:PX4:C27	13	1.96
(3,6)	1:A:78:PHE:H	4:A:339:PX4:C27	13	1.96
(3,6)	1:A:78:PHE:H	4:A:341:PX4:C27	13	1.96
(3,6)	1:A:78:PHE:H	4:A:343:PX4:C27	13	1.96
(3,6)	1:A:78:PHE:H	4:A:345:PX4:C27	13	1.96
(3,6)	1:A:78:PHE:H	4:A:347:PX4:C27	13	1.96
(3,6)	1:A:78:PHE:H	4:A:349:PX4:C27	13	1.96
(3,6)	1:A:78:PHE:H	4:A:351:PX4:C27	13	1.96
(3,6)	1:A:78:PHE:H	4:A:353:PX4:C27	13	1.96
(3,6)	1:A:78:PHE:H	4:A:355:PX4:C27	13	1.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,6)	1:A:78:PHE:H	4:A:357:PX4:C27	13	1.96
(3,6)	1:A:78:PHE:H	4:A:359:PX4:C27	13	1.96
(3,6)	1:A:78:PHE:H	4:A:361:PX4:C27	13	1.96
(3,6)	1:A:78:PHE:H	4:A:363:PX4:C27	13	1.96
(3,6)	1:A:78:PHE:H	4:A:402:PX4:C27	13	1.96
(3,6)	1:A:78:PHE:H	4:A:404:PX4:C27	13	1.96
(3,6)	1:A:78:PHE:H	4:A:406:PX4:C27	13	1.96
(3,6)	1:A:78:PHE:H	4:A:408:PX4:C27	13	1.96
(3,6)	1:A:78:PHE:H	4:A:410:PX4:C27	13	1.96
(3,6)	1:A:78:PHE:H	4:A:412:PX4:C27	13	1.96
(3,6)	1:A:78:PHE:H	4:A:414:PX4:C27	13	1.96
(3,6)	1:A:78:PHE:H	4:A:416:PX4:C27	13	1.96
(3,6)	1:A:78:PHE:H	4:A:418:PX4:C27	13	1.96
(3,6)	1:A:78:PHE:H	4:A:420:PX4:C27	13	1.96
(3,6)	1:A:78:PHE:H	4:A:422:PX4:C27	13	1.96
(3,6)	1:A:78:PHE:H	4:A:424:PX4:C27	13	1.96
(3,6)	1:A:78:PHE:H	4:A:426:PX4:C27	13	1.96
(3,6)	1:A:78:PHE:H	4:A:428:PX4:C27	13	1.96
(3,6)	1:A:78:PHE:H	4:A:430:PX4:C27	13	1.96
(2,982)	1:A:78:PHE:HD1	1:A:80:ASN:H	13	1.96
(2,833)	1:A:120:ILE:HD11	1:A:200:LEU:HD22	5	1.96
(2,833)	1:A:120:ILE:HD11	1:A:200:LEU:HD23	5	1.96
(2,757)	1:A:54:LEU:HD21	1:A:39:LEU:HD11	12	1.96
(2,757)	1:A:54:LEU:HD21	1:A:39:LEU:HD12	12	1.96
(2,757)	1:A:54:LEU:HD21	1:A:39:LEU:HD13	12	1.96
(2,727)	1:A:211:VAL:HG11	1:A:226:LEU:HD21	5	1.96
(3,36)	1:A:129:TRP:HE1	4:A:305:PX4:N1	9	1.95
(3,36)	1:A:129:TRP:HE1	4:A:307:PX4:N1	9	1.95
(3,36)	1:A:129:TRP:HE1	4:A:309:PX4:N1	9	1.95
(3,36)	1:A:129:TRP:HE1	4:A:311:PX4:N1	9	1.95
(3,36)	1:A:129:TRP:HE1	4:A:313:PX4:N1	9	1.95
(3,36)	1:A:129:TRP:HE1	4:A:315:PX4:N1	9	1.95
(3,36)	1:A:129:TRP:HE1	4:A:317:PX4:N1	9	1.95
(3,36)	1:A:129:TRP:HE1	4:A:319:PX4:N1	9	1.95
(3,36)	1:A:129:TRP:HE1	4:A:321:PX4:N1	9	1.95
(3,36)	1:A:129:TRP:HE1	4:A:323:PX4:N1	9	1.95
(3,36)	1:A:129:TRP:HE1	4:A:325:PX4:N1	9	1.95
(3,36)	1:A:129:TRP:HE1	4:A:327:PX4:N1	9	1.95
(3,36)	1:A:129:TRP:HE1	4:A:329:PX4:N1	9	1.95
(3,36)	1:A:129:TRP:HE1	4:A:331:PX4:N1	9	1.95
(3,36)	1:A:129:TRP:HE1	4:A:333:PX4:N1	9	1.95
(3,36)	1:A:129:TRP:HE1	4:A:335:PX4:N1	9	1.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,36)	1:A:129:TRP:HE1	4:A:337:PX4:N1	9	1.95
(3,36)	1:A:129:TRP:HE1	4:A:339:PX4:N1	9	1.95
(3,36)	1:A:129:TRP:HE1	4:A:341:PX4:N1	9	1.95
(3,36)	1:A:129:TRP:HE1	4:A:343:PX4:N1	9	1.95
(3,36)	1:A:129:TRP:HE1	4:A:345:PX4:N1	9	1.95
(3,36)	1:A:129:TRP:HE1	4:A:347:PX4:N1	9	1.95
(3,36)	1:A:129:TRP:HE1	4:A:349:PX4:N1	9	1.95
(3,36)	1:A:129:TRP:HE1	4:A:351:PX4:N1	9	1.95
(3,36)	1:A:129:TRP:HE1	4:A:353:PX4:N1	9	1.95
(3,36)	1:A:129:TRP:HE1	4:A:355:PX4:N1	9	1.95
(3,36)	1:A:129:TRP:HE1	4:A:357:PX4:N1	9	1.95
(3,36)	1:A:129:TRP:HE1	4:A:359:PX4:N1	9	1.95
(3,36)	1:A:129:TRP:HE1	4:A:361:PX4:N1	9	1.95
(3,36)	1:A:129:TRP:HE1	4:A:363:PX4:N1	9	1.95
(3,36)	1:A:129:TRP:HE1	4:A:402:PX4:N1	9	1.95
(3,36)	1:A:129:TRP:HE1	4:A:404:PX4:N1	9	1.95
(3,36)	1:A:129:TRP:HE1	4:A:406:PX4:N1	9	1.95
(3,36)	1:A:129:TRP:HE1	4:A:408:PX4:N1	9	1.95
(3,36)	1:A:129:TRP:HE1	4:A:410:PX4:N1	9	1.95
(3,36)	1:A:129:TRP:HE1	4:A:412:PX4:N1	9	1.95
(3,36)	1:A:129:TRP:HE1	4:A:414:PX4:N1	9	1.95
(3,36)	1:A:129:TRP:HE1	4:A:416:PX4:N1	9	1.95
(3,36)	1:A:129:TRP:HE1	4:A:418:PX4:N1	9	1.95
(3,36)	1:A:129:TRP:HE1	4:A:420:PX4:N1	9	1.95
(3,36)	1:A:129:TRP:HE1	4:A:422:PX4:N1	9	1.95
(3,36)	1:A:129:TRP:HE1	4:A:424:PX4:N1	9	1.95
(3,36)	1:A:129:TRP:HE1	4:A:426:PX4:N1	9	1.95
(3,36)	1:A:129:TRP:HE1	4:A:428:PX4:N1	9	1.95
(3,36)	1:A:129:TRP:HE1	4:A:430:PX4:N1	9	1.95
(2,858)	1:A:186:ILE:HD11	1:A:156:LEU:HD22	1	1.95
(2,858)	1:A:186:ILE:HD11	1:A:156:LEU:HD23	1	1.95
(2,982)	1:A:78:PHE:HD1	1:A:80:ASN:H	19	1.94
(2,932)	1:A:72:VAL:HG11	1:A:76:SER:H	10	1.94
(2,932)	1:A:72:VAL:HG12	1:A:76:SER:H	10	1.94
(2,932)	1:A:72:VAL:HG13	1:A:76:SER:H	10	1.94
(2,757)	1:A:54:LEU:HD21	1:A:39:LEU:HD11	8	1.94
(2,757)	1:A:54:LEU:HD21	1:A:39:LEU:HD12	8	1.94
(2,757)	1:A:54:LEU:HD21	1:A:39:LEU:HD13	8	1.94
(2,517)	1:A:200:LEU:H	1:A:196:LEU:HD21	9	1.94
(2,517)	1:A:200:LEU:H	1:A:196:LEU:HD21	17	1.94
(2,932)	1:A:72:VAL:HG11	1:A:76:SER:H	13	1.93
(2,932)	1:A:72:VAL:HG12	1:A:76:SER:H	13	1.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,932)	1:A:72:VAL:HG13	1:A:76:SER:H	13	1.93
(2,517)	1:A:200:LEU:H	1:A:196:LEU:HD21	6	1.93
(2,472)	1:A:186:ILE:H	1:A:156:LEU:HD21	5	1.93
(2,984)	1:A:78:PHE:HD1	1:A:80:ASN:HD21	5	1.92
(2,984)	1:A:78:PHE:HD1	1:A:80:ASN:HD22	5	1.92
(2,984)	1:A:78:PHE:HD1	1:A:80:ASN:HD21	5	1.92
(2,984)	1:A:78:PHE:HD1	1:A:80:ASN:HD22	5	1.92
(2,748)	1:A:89:VAL:HG12	1:A:122:LEU:HD21	4	1.92
(2,598)	1:A:235:GLN:H	1:A:238:TYR:HE1	12	1.92
(2,598)	1:A:235:GLN:H	1:A:238:TYR:HE2	12	1.92
(2,517)	1:A:200:LEU:H	1:A:196:LEU:HD21	13	1.92
(2,872)	1:A:186:ILE:HD13	1:A:156:LEU:HD22	12	1.91
(2,872)	1:A:186:ILE:HD13	1:A:156:LEU:HD23	12	1.91
(2,967)	1:A:77:LEU:H	1:A:77:LEU:HG	11	1.9
(2,932)	1:A:72:VAL:HG11	1:A:76:SER:H	1	1.9
(2,932)	1:A:72:VAL:HG12	1:A:76:SER:H	1	1.9
(2,932)	1:A:72:VAL:HG13	1:A:76:SER:H	1	1.9
(2,531)	1:A:205:SER:H	1:A:204:HIS:HE1	9	1.9
(2,832)	1:A:120:ILE:HD11	1:A:200:LEU:HD21	9	1.89
(2,729)	1:A:211:VAL:HG12	1:A:226:LEU:HD21	6	1.89
(2,321)	1:A:128:VAL:HG11	1:A:126:LYS:H	14	1.89
(2,321)	1:A:128:VAL:HG12	1:A:126:LYS:H	14	1.89
(2,321)	1:A:128:VAL:HG13	1:A:126:LYS:H	14	1.89
(2,967)	1:A:77:LEU:H	1:A:77:LEU:HG	4	1.88
(2,758)	1:A:54:LEU:HD22	1:A:39:LEU:HD11	15	1.88
(2,758)	1:A:54:LEU:HD22	1:A:39:LEU:HD12	15	1.88
(2,758)	1:A:54:LEU:HD22	1:A:39:LEU:HD13	15	1.88
(2,758)	1:A:54:LEU:HD23	1:A:39:LEU:HD11	15	1.88
(2,758)	1:A:54:LEU:HD23	1:A:39:LEU:HD12	15	1.88
(2,758)	1:A:54:LEU:HD23	1:A:39:LEU:HD13	15	1.88
(2,472)	1:A:186:ILE:H	1:A:156:LEU:HD21	4	1.88
(3,21)	1:A:77:LEU:H	4:A:305:PX4:C35	19	1.87
(3,21)	1:A:77:LEU:H	4:A:307:PX4:C35	19	1.87
(3,21)	1:A:77:LEU:H	4:A:309:PX4:C35	19	1.87
(3,21)	1:A:77:LEU:H	4:A:311:PX4:C35	19	1.87
(3,21)	1:A:77:LEU:H	4:A:313:PX4:C35	19	1.87
(3,21)	1:A:77:LEU:H	4:A:315:PX4:C35	19	1.87
(3,21)	1:A:77:LEU:H	4:A:317:PX4:C35	19	1.87
(3,21)	1:A:77:LEU:H	4:A:319:PX4:C35	19	1.87
(3,21)	1:A:77:LEU:H	4:A:321:PX4:C35	19	1.87
(3,21)	1:A:77:LEU:H	4:A:323:PX4:C35	19	1.87
(3,21)	1:A:77:LEU:H	4:A:325:PX4:C35	19	1.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,21)	1:A:77:LEU:H	4:A:327:PX4:C35	19	1.87
(3,21)	1:A:77:LEU:H	4:A:329:PX4:C35	19	1.87
(3,21)	1:A:77:LEU:H	4:A:331:PX4:C35	19	1.87
(3,21)	1:A:77:LEU:H	4:A:333:PX4:C35	19	1.87
(3,21)	1:A:77:LEU:H	4:A:335:PX4:C35	19	1.87
(3,21)	1:A:77:LEU:H	4:A:337:PX4:C35	19	1.87
(3,21)	1:A:77:LEU:H	4:A:339:PX4:C35	19	1.87
(3,21)	1:A:77:LEU:H	4:A:341:PX4:C35	19	1.87
(3,21)	1:A:77:LEU:H	4:A:343:PX4:C35	19	1.87
(3,21)	1:A:77:LEU:H	4:A:345:PX4:C35	19	1.87
(3,21)	1:A:77:LEU:H	4:A:347:PX4:C35	19	1.87
(3,21)	1:A:77:LEU:H	4:A:349:PX4:C35	19	1.87
(3,21)	1:A:77:LEU:H	4:A:351:PX4:C35	19	1.87
(3,21)	1:A:77:LEU:H	4:A:353:PX4:C35	19	1.87
(3,21)	1:A:77:LEU:H	4:A:355:PX4:C35	19	1.87
(3,21)	1:A:77:LEU:H	4:A:357:PX4:C35	19	1.87
(3,21)	1:A:77:LEU:H	4:A:359:PX4:C35	19	1.87
(3,21)	1:A:77:LEU:H	4:A:361:PX4:C35	19	1.87
(3,21)	1:A:77:LEU:H	4:A:363:PX4:C35	19	1.87
(3,21)	1:A:77:LEU:H	4:A:402:PX4:C35	19	1.87
(3,21)	1:A:77:LEU:H	4:A:404:PX4:C35	19	1.87
(3,21)	1:A:77:LEU:H	4:A:406:PX4:C35	19	1.87
(3,21)	1:A:77:LEU:H	4:A:408:PX4:C35	19	1.87
(3,21)	1:A:77:LEU:H	4:A:410:PX4:C35	19	1.87
(3,21)	1:A:77:LEU:H	4:A:412:PX4:C35	19	1.87
(3,21)	1:A:77:LEU:H	4:A:414:PX4:C35	19	1.87
(3,21)	1:A:77:LEU:H	4:A:416:PX4:C35	19	1.87
(3,21)	1:A:77:LEU:H	4:A:418:PX4:C35	19	1.87
(3,21)	1:A:77:LEU:H	4:A:420:PX4:C35	19	1.87
(3,21)	1:A:77:LEU:H	4:A:422:PX4:C35	19	1.87
(3,21)	1:A:77:LEU:H	4:A:424:PX4:C35	19	1.87
(3,21)	1:A:77:LEU:H	4:A:426:PX4:C35	19	1.87
(3,21)	1:A:77:LEU:H	4:A:428:PX4:C35	19	1.87
(3,21)	1:A:77:LEU:H	4:A:430:PX4:C35	19	1.87
(2,879)	1:A:234:ILE:HD11	1:A:200:LEU:HB2	14	1.87
(2,879)	1:A:234:ILE:HD12	1:A:200:LEU:HB2	14	1.87
(2,879)	1:A:234:ILE:HD13	1:A:200:LEU:HB2	14	1.87
(2,837)	1:A:120:ILE:HD13	1:A:200:LEU:HD22	12	1.87
(2,837)	1:A:120:ILE:HD13	1:A:200:LEU:HD23	12	1.87
(2,392)	1:A:157:ALA:H	1:A:68:GLY:H	16	1.87
(2,264)	1:A:113:LEU:H	1:A:196:LEU:HD21	10	1.87
(2,932)	1:A:72:VAL:HG11	1:A:76:SER:H	3	1.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,932)	1:A:72:VAL:HG12	1:A:76:SER:H	3	1.86
(2,932)	1:A:72:VAL:HG13	1:A:76:SER:H	3	1.86
(2,598)	1:A:235:GLN:H	1:A:238:TYR:HE1	5	1.86
(2,598)	1:A:235:GLN:H	1:A:238:TYR:HE2	5	1.86
(2,471)	1:A:186:ILE:H	1:A:156:LEU:HD11	7	1.86
(2,471)	1:A:186:ILE:H	1:A:156:LEU:HD12	7	1.86
(2,471)	1:A:186:ILE:H	1:A:156:LEU:HD13	7	1.86
(2,932)	1:A:72:VAL:HG11	1:A:76:SER:H	6	1.85
(2,932)	1:A:72:VAL:HG12	1:A:76:SER:H	6	1.85
(2,932)	1:A:72:VAL:HG13	1:A:76:SER:H	6	1.85
(2,178)	1:A:171:HIS:H	1:A:69:VAL:HG11	15	1.85
(2,178)	1:A:171:HIS:H	1:A:69:VAL:HG12	15	1.85
(2,178)	1:A:171:HIS:H	1:A:69:VAL:HG13	15	1.85
(2,967)	1:A:77:LEU:H	1:A:77:LEU:HG	3	1.84
(2,861)	1:A:186:ILE:HD13	1:A:156:LEU:HD21	12	1.84
(2,510)	1:A:200:LEU:HD21	1:A:199:SER:H	12	1.84
(2,765)	1:A:22:PHE:H	1:A:19:LEU:HD21	14	1.83
(2,657)	1:A:39:LEU:H	1:A:19:LEU:HD22	7	1.83
(2,657)	1:A:39:LEU:H	1:A:19:LEU:HD23	7	1.83
(2,932)	1:A:72:VAL:HG11	1:A:76:SER:H	11	1.82
(2,932)	1:A:72:VAL:HG12	1:A:76:SER:H	11	1.82
(2,932)	1:A:72:VAL:HG13	1:A:76:SER:H	11	1.82
(2,729)	1:A:211:VAL:HG12	1:A:226:LEU:HD21	1	1.82
(2,833)	1:A:120:ILE:HD11	1:A:200:LEU:HD22	20	1.81
(2,833)	1:A:120:ILE:HD11	1:A:200:LEU:HD23	20	1.81
(3,6)	1:A:78:PHE:H	4:A:305:PX4:C27	1	1.8
(3,6)	1:A:78:PHE:H	4:A:307:PX4:C27	1	1.8
(3,6)	1:A:78:PHE:H	4:A:309:PX4:C27	1	1.8
(3,6)	1:A:78:PHE:H	4:A:311:PX4:C27	1	1.8
(3,6)	1:A:78:PHE:H	4:A:313:PX4:C27	1	1.8
(3,6)	1:A:78:PHE:H	4:A:315:PX4:C27	1	1.8
(3,6)	1:A:78:PHE:H	4:A:317:PX4:C27	1	1.8
(3,6)	1:A:78:PHE:H	4:A:319:PX4:C27	1	1.8
(3,6)	1:A:78:PHE:H	4:A:321:PX4:C27	1	1.8
(3,6)	1:A:78:PHE:H	4:A:323:PX4:C27	1	1.8
(3,6)	1:A:78:PHE:H	4:A:325:PX4:C27	1	1.8
(3,6)	1:A:78:PHE:H	4:A:327:PX4:C27	1	1.8
(3,6)	1:A:78:PHE:H	4:A:329:PX4:C27	1	1.8
(3,6)	1:A:78:PHE:H	4:A:331:PX4:C27	1	1.8
(3,6)	1:A:78:PHE:H	4:A:333:PX4:C27	1	1.8
(3,6)	1:A:78:PHE:H	4:A:335:PX4:C27	1	1.8
(3,6)	1:A:78:PHE:H	4:A:337:PX4:C27	1	1.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,6)	1:A:78:PHE:H	4:A:339:PX4:C27	1	1.8
(3,6)	1:A:78:PHE:H	4:A:341:PX4:C27	1	1.8
(3,6)	1:A:78:PHE:H	4:A:343:PX4:C27	1	1.8
(3,6)	1:A:78:PHE:H	4:A:345:PX4:C27	1	1.8
(3,6)	1:A:78:PHE:H	4:A:347:PX4:C27	1	1.8
(3,6)	1:A:78:PHE:H	4:A:349:PX4:C27	1	1.8
(3,6)	1:A:78:PHE:H	4:A:351:PX4:C27	1	1.8
(3,6)	1:A:78:PHE:H	4:A:353:PX4:C27	1	1.8
(3,6)	1:A:78:PHE:H	4:A:355:PX4:C27	1	1.8
(3,6)	1:A:78:PHE:H	4:A:357:PX4:C27	1	1.8
(3,6)	1:A:78:PHE:H	4:A:359:PX4:C27	1	1.8
(3,6)	1:A:78:PHE:H	4:A:361:PX4:C27	1	1.8
(3,6)	1:A:78:PHE:H	4:A:363:PX4:C27	1	1.8
(3,6)	1:A:78:PHE:H	4:A:402:PX4:C27	1	1.8
(3,6)	1:A:78:PHE:H	4:A:404:PX4:C27	1	1.8
(3,6)	1:A:78:PHE:H	4:A:406:PX4:C27	1	1.8
(3,6)	1:A:78:PHE:H	4:A:408:PX4:C27	1	1.8
(3,6)	1:A:78:PHE:H	4:A:410:PX4:C27	1	1.8
(3,6)	1:A:78:PHE:H	4:A:412:PX4:C27	1	1.8
(3,6)	1:A:78:PHE:H	4:A:414:PX4:C27	1	1.8
(3,6)	1:A:78:PHE:H	4:A:416:PX4:C27	1	1.8
(3,6)	1:A:78:PHE:H	4:A:418:PX4:C27	1	1.8
(3,6)	1:A:78:PHE:H	4:A:420:PX4:C27	1	1.8
(3,6)	1:A:78:PHE:H	4:A:422:PX4:C27	1	1.8
(3,6)	1:A:78:PHE:H	4:A:424:PX4:C27	1	1.8
(3,6)	1:A:78:PHE:H	4:A:426:PX4:C27	1	1.8
(3,6)	1:A:78:PHE:H	4:A:428:PX4:C27	1	1.8
(3,6)	1:A:78:PHE:H	4:A:430:PX4:C27	1	1.8
(3,21)	1:A:77:LEU:H	4:A:305:PX4:C35	6	1.8
(3,21)	1:A:77:LEU:H	4:A:307:PX4:C35	6	1.8
(3,21)	1:A:77:LEU:H	4:A:309:PX4:C35	6	1.8
(3,21)	1:A:77:LEU:H	4:A:311:PX4:C35	6	1.8
(3,21)	1:A:77:LEU:H	4:A:313:PX4:C35	6	1.8
(3,21)	1:A:77:LEU:H	4:A:315:PX4:C35	6	1.8
(3,21)	1:A:77:LEU:H	4:A:317:PX4:C35	6	1.8
(3,21)	1:A:77:LEU:H	4:A:319:PX4:C35	6	1.8
(3,21)	1:A:77:LEU:H	4:A:321:PX4:C35	6	1.8
(3,21)	1:A:77:LEU:H	4:A:323:PX4:C35	6	1.8
(3,21)	1:A:77:LEU:H	4:A:325:PX4:C35	6	1.8
(3,21)	1:A:77:LEU:H	4:A:327:PX4:C35	6	1.8
(3,21)	1:A:77:LEU:H	4:A:329:PX4:C35	6	1.8
(3,21)	1:A:77:LEU:H	4:A:331:PX4:C35	6	1.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,21)	1:A:77:LEU:H	4:A:333:PX4:C35	6	1.8
(3,21)	1:A:77:LEU:H	4:A:335:PX4:C35	6	1.8
(3,21)	1:A:77:LEU:H	4:A:337:PX4:C35	6	1.8
(3,21)	1:A:77:LEU:H	4:A:339:PX4:C35	6	1.8
(3,21)	1:A:77:LEU:H	4:A:341:PX4:C35	6	1.8
(3,21)	1:A:77:LEU:H	4:A:343:PX4:C35	6	1.8
(3,21)	1:A:77:LEU:H	4:A:345:PX4:C35	6	1.8
(3,21)	1:A:77:LEU:H	4:A:347:PX4:C35	6	1.8
(3,21)	1:A:77:LEU:H	4:A:349:PX4:C35	6	1.8
(3,21)	1:A:77:LEU:H	4:A:351:PX4:C35	6	1.8
(3,21)	1:A:77:LEU:H	4:A:353:PX4:C35	6	1.8
(3,21)	1:A:77:LEU:H	4:A:355:PX4:C35	6	1.8
(3,21)	1:A:77:LEU:H	4:A:357:PX4:C35	6	1.8
(3,21)	1:A:77:LEU:H	4:A:359:PX4:C35	6	1.8
(3,21)	1:A:77:LEU:H	4:A:361:PX4:C35	6	1.8
(3,21)	1:A:77:LEU:H	4:A:363:PX4:C35	6	1.8
(3,21)	1:A:77:LEU:H	4:A:402:PX4:C35	6	1.8
(3,21)	1:A:77:LEU:H	4:A:404:PX4:C35	6	1.8
(3,21)	1:A:77:LEU:H	4:A:406:PX4:C35	6	1.8
(3,21)	1:A:77:LEU:H	4:A:408:PX4:C35	6	1.8
(3,21)	1:A:77:LEU:H	4:A:410:PX4:C35	6	1.8
(3,21)	1:A:77:LEU:H	4:A:412:PX4:C35	6	1.8
(3,21)	1:A:77:LEU:H	4:A:414:PX4:C35	6	1.8
(3,21)	1:A:77:LEU:H	4:A:416:PX4:C35	6	1.8
(3,21)	1:A:77:LEU:H	4:A:418:PX4:C35	6	1.8
(3,21)	1:A:77:LEU:H	4:A:420:PX4:C35	6	1.8
(3,21)	1:A:77:LEU:H	4:A:422:PX4:C35	6	1.8
(3,21)	1:A:77:LEU:H	4:A:424:PX4:C35	6	1.8
(3,21)	1:A:77:LEU:H	4:A:426:PX4:C35	6	1.8
(3,21)	1:A:77:LEU:H	4:A:428:PX4:C35	6	1.8
(3,21)	1:A:77:LEU:H	4:A:430:PX4:C35	6	1.8
(2,657)	1:A:39:LEU:H	1:A:19:LEU:HD22	1	1.8
(2,657)	1:A:39:LEU:H	1:A:19:LEU:HD23	1	1.8
(2,472)	1:A:186:ILE:H	1:A:156:LEU:HD21	18	1.8
(2,984)	1:A:78:PHE:HD1	1:A:80:ASN:HD21	7	1.79
(2,984)	1:A:78:PHE:HD1	1:A:80:ASN:HD22	7	1.79
(2,984)	1:A:78:PHE:HD1	1:A:80:ASN:HD21	7	1.79
(2,984)	1:A:78:PHE:HD1	1:A:80:ASN:HD22	7	1.79
(2,879)	1:A:234:ILE:HD11	1:A:200:LEU:HB2	12	1.79
(2,879)	1:A:234:ILE:HD12	1:A:200:LEU:HB2	12	1.79
(2,879)	1:A:234:ILE:HD13	1:A:200:LEU:HB2	12	1.79
(2,833)	1:A:120:ILE:HD11	1:A:200:LEU:HD22	8	1.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,833)	1:A:120:ILE:HD11	1:A:200:LEU:HD23	8	1.79
(2,517)	1:A:200:LEU:H	1:A:196:LEU:HD21	11	1.79
(2,835)	1:A:120:ILE:HD12	1:A:200:LEU:HD22	13	1.78
(2,835)	1:A:120:ILE:HD12	1:A:200:LEU:HD23	13	1.78
(2,760)	1:A:54:LEU:HD22	1:A:59:ILE:HD11	1	1.78
(2,760)	1:A:54:LEU:HD22	1:A:59:ILE:HD12	1	1.78
(2,760)	1:A:54:LEU:HD22	1:A:59:ILE:HD13	1	1.78
(2,760)	1:A:54:LEU:HD23	1:A:59:ILE:HD11	1	1.78
(2,760)	1:A:54:LEU:HD23	1:A:59:ILE:HD12	1	1.78
(2,760)	1:A:54:LEU:HD23	1:A:59:ILE:HD13	1	1.78
(3,6)	1:A:78:PHE:H	4:A:305:PX4:C27	8	1.76
(3,6)	1:A:78:PHE:H	4:A:307:PX4:C27	8	1.76
(3,6)	1:A:78:PHE:H	4:A:309:PX4:C27	8	1.76
(3,6)	1:A:78:PHE:H	4:A:311:PX4:C27	8	1.76
(3,6)	1:A:78:PHE:H	4:A:313:PX4:C27	8	1.76
(3,6)	1:A:78:PHE:H	4:A:315:PX4:C27	8	1.76
(3,6)	1:A:78:PHE:H	4:A:317:PX4:C27	8	1.76
(3,6)	1:A:78:PHE:H	4:A:319:PX4:C27	8	1.76
(3,6)	1:A:78:PHE:H	4:A:321:PX4:C27	8	1.76
(3,6)	1:A:78:PHE:H	4:A:323:PX4:C27	8	1.76
(3,6)	1:A:78:PHE:H	4:A:325:PX4:C27	8	1.76
(3,6)	1:A:78:PHE:H	4:A:327:PX4:C27	8	1.76
(3,6)	1:A:78:PHE:H	4:A:329:PX4:C27	8	1.76
(3,6)	1:A:78:PHE:H	4:A:331:PX4:C27	8	1.76
(3,6)	1:A:78:PHE:H	4:A:333:PX4:C27	8	1.76
(3,6)	1:A:78:PHE:H	4:A:335:PX4:C27	8	1.76
(3,6)	1:A:78:PHE:H	4:A:337:PX4:C27	8	1.76
(3,6)	1:A:78:PHE:H	4:A:339:PX4:C27	8	1.76
(3,6)	1:A:78:PHE:H	4:A:341:PX4:C27	8	1.76
(3,6)	1:A:78:PHE:H	4:A:343:PX4:C27	8	1.76
(3,6)	1:A:78:PHE:H	4:A:345:PX4:C27	8	1.76
(3,6)	1:A:78:PHE:H	4:A:347:PX4:C27	8	1.76
(3,6)	1:A:78:PHE:H	4:A:349:PX4:C27	8	1.76
(3,6)	1:A:78:PHE:H	4:A:351:PX4:C27	8	1.76
(3,6)	1:A:78:PHE:H	4:A:353:PX4:C27	8	1.76
(3,6)	1:A:78:PHE:H	4:A:355:PX4:C27	8	1.76
(3,6)	1:A:78:PHE:H	4:A:357:PX4:C27	8	1.76
(3,6)	1:A:78:PHE:H	4:A:359:PX4:C27	8	1.76
(3,6)	1:A:78:PHE:H	4:A:361:PX4:C27	8	1.76
(3,6)	1:A:78:PHE:H	4:A:363:PX4:C27	8	1.76
(3,6)	1:A:78:PHE:H	4:A:402:PX4:C27	8	1.76
(3,6)	1:A:78:PHE:H	4:A:404:PX4:C27	8	1.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,6)	1:A:78:PHE:H	4:A:406:PX4:C27	8	1.76
(3,6)	1:A:78:PHE:H	4:A:408:PX4:C27	8	1.76
(3,6)	1:A:78:PHE:H	4:A:410:PX4:C27	8	1.76
(3,6)	1:A:78:PHE:H	4:A:412:PX4:C27	8	1.76
(3,6)	1:A:78:PHE:H	4:A:414:PX4:C27	8	1.76
(3,6)	1:A:78:PHE:H	4:A:416:PX4:C27	8	1.76
(3,6)	1:A:78:PHE:H	4:A:418:PX4:C27	8	1.76
(3,6)	1:A:78:PHE:H	4:A:420:PX4:C27	8	1.76
(3,6)	1:A:78:PHE:H	4:A:422:PX4:C27	8	1.76
(3,6)	1:A:78:PHE:H	4:A:424:PX4:C27	8	1.76
(3,6)	1:A:78:PHE:H	4:A:426:PX4:C27	8	1.76
(3,6)	1:A:78:PHE:H	4:A:428:PX4:C27	8	1.76
(3,6)	1:A:78:PHE:H	4:A:430:PX4:C27	8	1.76
(3,21)	1:A:77:LEU:H	4:A:305:PX4:C35	10	1.76
(3,21)	1:A:77:LEU:H	4:A:307:PX4:C35	10	1.76
(3,21)	1:A:77:LEU:H	4:A:309:PX4:C35	10	1.76
(3,21)	1:A:77:LEU:H	4:A:311:PX4:C35	10	1.76
(3,21)	1:A:77:LEU:H	4:A:313:PX4:C35	10	1.76
(3,21)	1:A:77:LEU:H	4:A:315:PX4:C35	10	1.76
(3,21)	1:A:77:LEU:H	4:A:317:PX4:C35	10	1.76
(3,21)	1:A:77:LEU:H	4:A:319:PX4:C35	10	1.76
(3,21)	1:A:77:LEU:H	4:A:321:PX4:C35	10	1.76
(3,21)	1:A:77:LEU:H	4:A:323:PX4:C35	10	1.76
(3,21)	1:A:77:LEU:H	4:A:325:PX4:C35	10	1.76
(3,21)	1:A:77:LEU:H	4:A:327:PX4:C35	10	1.76
(3,21)	1:A:77:LEU:H	4:A:329:PX4:C35	10	1.76
(3,21)	1:A:77:LEU:H	4:A:331:PX4:C35	10	1.76
(3,21)	1:A:77:LEU:H	4:A:333:PX4:C35	10	1.76
(3,21)	1:A:77:LEU:H	4:A:335:PX4:C35	10	1.76
(3,21)	1:A:77:LEU:H	4:A:337:PX4:C35	10	1.76
(3,21)	1:A:77:LEU:H	4:A:339:PX4:C35	10	1.76
(3,21)	1:A:77:LEU:H	4:A:341:PX4:C35	10	1.76
(3,21)	1:A:77:LEU:H	4:A:343:PX4:C35	10	1.76
(3,21)	1:A:77:LEU:H	4:A:345:PX4:C35	10	1.76
(3,21)	1:A:77:LEU:H	4:A:347:PX4:C35	10	1.76
(3,21)	1:A:77:LEU:H	4:A:349:PX4:C35	10	1.76
(3,21)	1:A:77:LEU:H	4:A:351:PX4:C35	10	1.76
(3,21)	1:A:77:LEU:H	4:A:353:PX4:C35	10	1.76
(3,21)	1:A:77:LEU:H	4:A:355:PX4:C35	10	1.76
(3,21)	1:A:77:LEU:H	4:A:357:PX4:C35	10	1.76
(3,21)	1:A:77:LEU:H	4:A:359:PX4:C35	10	1.76
(3,21)	1:A:77:LEU:H	4:A:361:PX4:C35	10	1.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,21)	1:A:77:LEU:H	4:A:363:PX4:C35	10	1.76
(3,21)	1:A:77:LEU:H	4:A:402:PX4:C35	10	1.76
(3,21)	1:A:77:LEU:H	4:A:404:PX4:C35	10	1.76
(3,21)	1:A:77:LEU:H	4:A:406:PX4:C35	10	1.76
(3,21)	1:A:77:LEU:H	4:A:408:PX4:C35	10	1.76
(3,21)	1:A:77:LEU:H	4:A:410:PX4:C35	10	1.76
(3,21)	1:A:77:LEU:H	4:A:412:PX4:C35	10	1.76
(3,21)	1:A:77:LEU:H	4:A:414:PX4:C35	10	1.76
(3,21)	1:A:77:LEU:H	4:A:416:PX4:C35	10	1.76
(3,21)	1:A:77:LEU:H	4:A:418:PX4:C35	10	1.76
(3,21)	1:A:77:LEU:H	4:A:420:PX4:C35	10	1.76
(3,21)	1:A:77:LEU:H	4:A:422:PX4:C35	10	1.76
(3,21)	1:A:77:LEU:H	4:A:424:PX4:C35	10	1.76
(3,21)	1:A:77:LEU:H	4:A:426:PX4:C35	10	1.76
(3,21)	1:A:77:LEU:H	4:A:428:PX4:C35	10	1.76
(3,21)	1:A:77:LEU:H	4:A:430:PX4:C35	10	1.76
(2,835)	1:A:120:ILE:HD12	1:A:200:LEU:HD22	19	1.76
(2,835)	1:A:120:ILE:HD12	1:A:200:LEU:HD23	19	1.76
(2,757)	1:A:54:LEU:HD21	1:A:39:LEU:HD11	2	1.76
(2,757)	1:A:54:LEU:HD21	1:A:39:LEU:HD12	2	1.76
(2,757)	1:A:54:LEU:HD21	1:A:39:LEU:HD13	2	1.76
(2,598)	1:A:235:GLN:H	1:A:238:TYR:HE1	13	1.75
(2,598)	1:A:235:GLN:H	1:A:238:TYR:HE2	13	1.75
(2,967)	1:A:77:LEU:H	1:A:77:LEU:HG	16	1.74
(2,765)	1:A:22:PHE:H	1:A:19:LEU:HD21	7	1.74
(2,542)	1:A:210:ALA:H	1:A:209:ASN:HD22	9	1.74
(2,264)	1:A:113:LEU:H	1:A:196:LEU:HD21	2	1.74
(2,988)	1:A:129:TRP:HE1	4:A:305:PX4:C2	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:307:PX4:C2	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:309:PX4:C2	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:311:PX4:C2	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:313:PX4:C2	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:315:PX4:C2	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:317:PX4:C2	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:319:PX4:C2	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:321:PX4:C2	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:323:PX4:C2	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:325:PX4:C2	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:327:PX4:C2	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:329:PX4:C2	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:331:PX4:C2	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:333:PX4:C2	1	1.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,988)	1:A:129:TRP:HE1	4:A:335:PX4:C2	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:337:PX4:C2	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:339:PX4:C2	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:341:PX4:C2	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:343:PX4:C2	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:345:PX4:C2	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:347:PX4:C2	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:349:PX4:C2	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:351:PX4:C2	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:353:PX4:C2	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:355:PX4:C2	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:357:PX4:C2	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:359:PX4:C2	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:361:PX4:C2	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:363:PX4:C2	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:402:PX4:C2	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:404:PX4:C2	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:406:PX4:C2	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:408:PX4:C2	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:410:PX4:C2	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:412:PX4:C2	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:414:PX4:C2	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:416:PX4:C2	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:418:PX4:C2	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:420:PX4:C2	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:422:PX4:C2	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:424:PX4:C2	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:426:PX4:C2	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:428:PX4:C2	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:430:PX4:C2	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:305:PX4:C1	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:307:PX4:C1	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:309:PX4:C1	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:311:PX4:C1	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:313:PX4:C1	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:315:PX4:C1	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:317:PX4:C1	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:319:PX4:C1	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:321:PX4:C1	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:323:PX4:C1	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:325:PX4:C1	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:327:PX4:C1	1	1.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,988)	1:A:129:TRP:HE1	4:A:329:PX4:C1	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:331:PX4:C1	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:333:PX4:C1	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:335:PX4:C1	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:337:PX4:C1	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:339:PX4:C1	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:341:PX4:C1	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:343:PX4:C1	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:345:PX4:C1	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:347:PX4:C1	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:349:PX4:C1	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:351:PX4:C1	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:353:PX4:C1	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:355:PX4:C1	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:357:PX4:C1	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:359:PX4:C1	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:361:PX4:C1	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:363:PX4:C1	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:402:PX4:C1	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:404:PX4:C1	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:406:PX4:C1	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:408:PX4:C1	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:410:PX4:C1	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:412:PX4:C1	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:414:PX4:C1	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:416:PX4:C1	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:418:PX4:C1	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:420:PX4:C1	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:422:PX4:C1	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:424:PX4:C1	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:426:PX4:C1	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:428:PX4:C1	1	1.73
(2,988)	1:A:129:TRP:HE1	4:A:430:PX4:C1	1	1.73
(2,967)	1:A:77:LEU:H	1:A:77:LEU:HG	10	1.73
(2,837)	1:A:120:ILE:HD13	1:A:200:LEU:HD22	1	1.73
(2,837)	1:A:120:ILE:HD13	1:A:200:LEU:HD23	1	1.73
(2,83)	1:A:58:VAL:H	1:A:48:LEU:HD22	9	1.73
(2,83)	1:A:58:VAL:H	1:A:48:LEU:HD23	9	1.73
(2,598)	1:A:235:GLN:H	1:A:238:TYR:HE1	3	1.73
(2,598)	1:A:235:GLN:H	1:A:238:TYR:HE2	3	1.73
(2,932)	1:A:72:VAL:HG11	1:A:76:SER:H	5	1.72
(2,932)	1:A:72:VAL:HG12	1:A:76:SER:H	5	1.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,932)	1:A:72:VAL:HG13	1:A:76:SER:H	5	1.72
(2,879)	1:A:234:ILE:HD11	1:A:200:LEU:HB2	2	1.71
(2,879)	1:A:234:ILE:HD12	1:A:200:LEU:HB2	2	1.71
(2,879)	1:A:234:ILE:HD13	1:A:200:LEU:HB2	2	1.71
(2,765)	1:A:22:PHE:H	1:A:19:LEU:HD21	4	1.71
(2,765)	1:A:22:PHE:H	1:A:19:LEU:HD21	6	1.71
(2,728)	1:A:211:VAL:HG11	1:A:226:LEU:HD22	17	1.71
(2,728)	1:A:211:VAL:HG11	1:A:226:LEU:HD23	17	1.71
(2,517)	1:A:200:LEU:H	1:A:196:LEU:HD21	15	1.71
(2,967)	1:A:77:LEU:H	1:A:77:LEU:HG	5	1.7
(2,967)	1:A:77:LEU:H	1:A:77:LEU:HG	20	1.7
(2,510)	1:A:200:LEU:HD21	1:A:199:SER:H	1	1.7
(2,777)	1:A:61:ILE:HD13	1:A:48:LEU:HD21	18	1.69
(2,598)	1:A:235:GLN:H	1:A:238:TYR:HE1	6	1.69
(2,598)	1:A:235:GLN:H	1:A:238:TYR:HE2	6	1.69
(2,967)	1:A:77:LEU:H	1:A:77:LEU:HG	19	1.68
(2,392)	1:A:157:ALA:H	1:A:68:GLY:H	9	1.68
(2,264)	1:A:113:LEU:H	1:A:196:LEU:HD21	7	1.68
(2,836)	1:A:120:ILE:HD13	1:A:200:LEU:HD21	7	1.67
(2,760)	1:A:54:LEU:HD22	1:A:59:ILE:HD11	13	1.67
(2,760)	1:A:54:LEU:HD22	1:A:59:ILE:HD12	13	1.67
(2,760)	1:A:54:LEU:HD22	1:A:59:ILE:HD13	13	1.67
(2,760)	1:A:54:LEU:HD23	1:A:59:ILE:HD11	13	1.67
(2,760)	1:A:54:LEU:HD23	1:A:59:ILE:HD12	13	1.67
(2,760)	1:A:54:LEU:HD23	1:A:59:ILE:HD13	13	1.67
(2,473)	1:A:186:ILE:H	1:A:156:LEU:HD22	4	1.67
(2,473)	1:A:186:ILE:H	1:A:156:LEU:HD23	4	1.67
(2,967)	1:A:77:LEU:H	1:A:77:LEU:HG	17	1.66
(2,928)	1:A:72:VAL:H	1:A:73:ALA:HB1	20	1.66
(2,833)	1:A:120:ILE:HD11	1:A:200:LEU:HD22	1	1.66
(2,833)	1:A:120:ILE:HD11	1:A:200:LEU:HD23	1	1.66
(2,967)	1:A:77:LEU:H	1:A:77:LEU:HG	12	1.65
(2,967)	1:A:77:LEU:H	1:A:77:LEU:HG	13	1.65
(2,517)	1:A:200:LEU:H	1:A:196:LEU:HD21	19	1.65
(2,879)	1:A:234:ILE:HD11	1:A:200:LEU:HB2	1	1.64
(2,879)	1:A:234:ILE:HD12	1:A:200:LEU:HB2	1	1.64
(2,879)	1:A:234:ILE:HD13	1:A:200:LEU:HB2	1	1.64
(2,867)	1:A:186:ILE:HD11	1:A:156:LEU:HD21	16	1.63
(2,775)	1:A:61:ILE:HD12	1:A:48:LEU:HD21	13	1.63
(2,760)	1:A:54:LEU:HD22	1:A:59:ILE:HD11	2	1.63
(2,760)	1:A:54:LEU:HD22	1:A:59:ILE:HD12	2	1.63
(2,760)	1:A:54:LEU:HD22	1:A:59:ILE:HD13	2	1.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,760)	1:A:54:LEU:HD23	1:A:59:ILE:HD11	2	1.63
(2,760)	1:A:54:LEU:HD23	1:A:59:ILE:HD12	2	1.63
(2,760)	1:A:54:LEU:HD23	1:A:59:ILE:HD13	2	1.63
(2,757)	1:A:54:LEU:HD21	1:A:39:LEU:HD11	11	1.63
(2,757)	1:A:54:LEU:HD21	1:A:39:LEU:HD12	11	1.63
(2,757)	1:A:54:LEU:HD21	1:A:39:LEU:HD13	11	1.63
(2,516)	1:A:200:LEU:H	1:A:196:LEU:HD11	16	1.63
(2,516)	1:A:200:LEU:H	1:A:196:LEU:HD12	16	1.63
(2,516)	1:A:200:LEU:H	1:A:196:LEU:HD13	16	1.63
(2,178)	1:A:171:HIS:H	1:A:69:VAL:HG11	17	1.63
(2,178)	1:A:171:HIS:H	1:A:69:VAL:HG12	17	1.63
(2,178)	1:A:171:HIS:H	1:A:69:VAL:HG13	17	1.63
(3,21)	1:A:77:LEU:H	4:A:305:PX4:C35	12	1.61
(3,21)	1:A:77:LEU:H	4:A:307:PX4:C35	12	1.61
(3,21)	1:A:77:LEU:H	4:A:309:PX4:C35	12	1.61
(3,21)	1:A:77:LEU:H	4:A:311:PX4:C35	12	1.61
(3,21)	1:A:77:LEU:H	4:A:313:PX4:C35	12	1.61
(3,21)	1:A:77:LEU:H	4:A:315:PX4:C35	12	1.61
(3,21)	1:A:77:LEU:H	4:A:317:PX4:C35	12	1.61
(3,21)	1:A:77:LEU:H	4:A:319:PX4:C35	12	1.61
(3,21)	1:A:77:LEU:H	4:A:321:PX4:C35	12	1.61
(3,21)	1:A:77:LEU:H	4:A:323:PX4:C35	12	1.61
(3,21)	1:A:77:LEU:H	4:A:325:PX4:C35	12	1.61
(3,21)	1:A:77:LEU:H	4:A:327:PX4:C35	12	1.61
(3,21)	1:A:77:LEU:H	4:A:329:PX4:C35	12	1.61
(3,21)	1:A:77:LEU:H	4:A:331:PX4:C35	12	1.61
(3,21)	1:A:77:LEU:H	4:A:333:PX4:C35	12	1.61
(3,21)	1:A:77:LEU:H	4:A:335:PX4:C35	12	1.61
(3,21)	1:A:77:LEU:H	4:A:337:PX4:C35	12	1.61
(3,21)	1:A:77:LEU:H	4:A:339:PX4:C35	12	1.61
(3,21)	1:A:77:LEU:H	4:A:341:PX4:C35	12	1.61
(3,21)	1:A:77:LEU:H	4:A:343:PX4:C35	12	1.61
(3,21)	1:A:77:LEU:H	4:A:345:PX4:C35	12	1.61
(3,21)	1:A:77:LEU:H	4:A:347:PX4:C35	12	1.61
(3,21)	1:A:77:LEU:H	4:A:349:PX4:C35	12	1.61
(3,21)	1:A:77:LEU:H	4:A:351:PX4:C35	12	1.61
(3,21)	1:A:77:LEU:H	4:A:353:PX4:C35	12	1.61
(3,21)	1:A:77:LEU:H	4:A:355:PX4:C35	12	1.61
(3,21)	1:A:77:LEU:H	4:A:357:PX4:C35	12	1.61
(3,21)	1:A:77:LEU:H	4:A:359:PX4:C35	12	1.61
(3,21)	1:A:77:LEU:H	4:A:361:PX4:C35	12	1.61
(3,21)	1:A:77:LEU:H	4:A:363:PX4:C35	12	1.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,21)	1:A:77:LEU:H	4:A:402:PX4:C35	12	1.61
(3,21)	1:A:77:LEU:H	4:A:404:PX4:C35	12	1.61
(3,21)	1:A:77:LEU:H	4:A:406:PX4:C35	12	1.61
(3,21)	1:A:77:LEU:H	4:A:408:PX4:C35	12	1.61
(3,21)	1:A:77:LEU:H	4:A:410:PX4:C35	12	1.61
(3,21)	1:A:77:LEU:H	4:A:412:PX4:C35	12	1.61
(3,21)	1:A:77:LEU:H	4:A:414:PX4:C35	12	1.61
(3,21)	1:A:77:LEU:H	4:A:416:PX4:C35	12	1.61
(3,21)	1:A:77:LEU:H	4:A:418:PX4:C35	12	1.61
(3,21)	1:A:77:LEU:H	4:A:420:PX4:C35	12	1.61
(3,21)	1:A:77:LEU:H	4:A:422:PX4:C35	12	1.61
(3,21)	1:A:77:LEU:H	4:A:424:PX4:C35	12	1.61
(3,21)	1:A:77:LEU:H	4:A:426:PX4:C35	12	1.61
(3,21)	1:A:77:LEU:H	4:A:428:PX4:C35	12	1.61
(3,21)	1:A:77:LEU:H	4:A:430:PX4:C35	12	1.61
(2,760)	1:A:54:LEU:HD22	1:A:59:ILE:HD11	12	1.61
(2,760)	1:A:54:LEU:HD22	1:A:59:ILE:HD12	12	1.61
(2,760)	1:A:54:LEU:HD22	1:A:59:ILE:HD13	12	1.61
(2,760)	1:A:54:LEU:HD23	1:A:59:ILE:HD11	12	1.61
(2,760)	1:A:54:LEU:HD23	1:A:59:ILE:HD12	12	1.61
(2,760)	1:A:54:LEU:HD23	1:A:59:ILE:HD13	12	1.61
(2,657)	1:A:39:LEU:H	1:A:19:LEU:HD22	6	1.61
(2,657)	1:A:39:LEU:H	1:A:19:LEU:HD23	6	1.61
(2,518)	1:A:200:LEU:H	1:A:196:LEU:HD22	16	1.61
(2,518)	1:A:200:LEU:H	1:A:196:LEU:HD23	16	1.61
(2,879)	1:A:234:ILE:HD11	1:A:200:LEU:HB2	3	1.6
(2,879)	1:A:234:ILE:HD12	1:A:200:LEU:HB2	3	1.6
(2,879)	1:A:234:ILE:HD13	1:A:200:LEU:HB2	3	1.6
(2,967)	1:A:77:LEU:H	1:A:77:LEU:HG	2	1.59
(2,967)	1:A:77:LEU:H	1:A:77:LEU:HG	6	1.59
(2,940)	1:A:73:ALA:HB1	1:A:75:TYR:H	5	1.59
(2,940)	1:A:73:ALA:HB2	1:A:75:TYR:H	5	1.59
(2,940)	1:A:73:ALA:HB3	1:A:75:TYR:H	5	1.59
(2,932)	1:A:72:VAL:HG11	1:A:76:SER:H	20	1.59
(2,932)	1:A:72:VAL:HG12	1:A:76:SER:H	20	1.59
(2,932)	1:A:72:VAL:HG13	1:A:76:SER:H	20	1.59
(2,902)	1:A:66:ARG:HA	1:A:68:GLY:H	8	1.59
(2,932)	1:A:72:VAL:HG11	1:A:76:SER:H	16	1.58
(2,932)	1:A:72:VAL:HG12	1:A:76:SER:H	16	1.58
(2,932)	1:A:72:VAL:HG13	1:A:76:SER:H	16	1.58
(2,902)	1:A:66:ARG:HA	1:A:68:GLY:H	1	1.58
(2,598)	1:A:235:GLN:H	1:A:238:TYR:HE1	14	1.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,598)	1:A:235:GLN:H	1:A:238:TYR:HE2	14	1.58
(2,257)	1:A:112:ALA:H	1:A:189:LEU:HD21	5	1.58
(3,33)	1:A:155:THR:H	4:A:305:PX4:C35	7	1.57
(3,33)	1:A:155:THR:H	4:A:307:PX4:C35	7	1.57
(3,33)	1:A:155:THR:H	4:A:309:PX4:C35	7	1.57
(3,33)	1:A:155:THR:H	4:A:311:PX4:C35	7	1.57
(3,33)	1:A:155:THR:H	4:A:313:PX4:C35	7	1.57
(3,33)	1:A:155:THR:H	4:A:315:PX4:C35	7	1.57
(3,33)	1:A:155:THR:H	4:A:317:PX4:C35	7	1.57
(3,33)	1:A:155:THR:H	4:A:319:PX4:C35	7	1.57
(3,33)	1:A:155:THR:H	4:A:321:PX4:C35	7	1.57
(3,33)	1:A:155:THR:H	4:A:323:PX4:C35	7	1.57
(3,33)	1:A:155:THR:H	4:A:325:PX4:C35	7	1.57
(3,33)	1:A:155:THR:H	4:A:327:PX4:C35	7	1.57
(3,33)	1:A:155:THR:H	4:A:329:PX4:C35	7	1.57
(3,33)	1:A:155:THR:H	4:A:331:PX4:C35	7	1.57
(3,33)	1:A:155:THR:H	4:A:333:PX4:C35	7	1.57
(3,33)	1:A:155:THR:H	4:A:335:PX4:C35	7	1.57
(3,33)	1:A:155:THR:H	4:A:337:PX4:C35	7	1.57
(3,33)	1:A:155:THR:H	4:A:339:PX4:C35	7	1.57
(3,33)	1:A:155:THR:H	4:A:341:PX4:C35	7	1.57
(3,33)	1:A:155:THR:H	4:A:343:PX4:C35	7	1.57
(3,33)	1:A:155:THR:H	4:A:345:PX4:C35	7	1.57
(3,33)	1:A:155:THR:H	4:A:347:PX4:C35	7	1.57
(3,33)	1:A:155:THR:H	4:A:349:PX4:C35	7	1.57
(3,33)	1:A:155:THR:H	4:A:351:PX4:C35	7	1.57
(3,33)	1:A:155:THR:H	4:A:353:PX4:C35	7	1.57
(3,33)	1:A:155:THR:H	4:A:355:PX4:C35	7	1.57
(3,33)	1:A:155:THR:H	4:A:357:PX4:C35	7	1.57
(3,33)	1:A:155:THR:H	4:A:359:PX4:C35	7	1.57
(3,33)	1:A:155:THR:H	4:A:361:PX4:C35	7	1.57
(3,33)	1:A:155:THR:H	4:A:363:PX4:C35	7	1.57
(3,33)	1:A:155:THR:H	4:A:402:PX4:C35	7	1.57
(3,33)	1:A:155:THR:H	4:A:404:PX4:C35	7	1.57
(3,33)	1:A:155:THR:H	4:A:406:PX4:C35	7	1.57
(3,33)	1:A:155:THR:H	4:A:408:PX4:C35	7	1.57
(3,33)	1:A:155:THR:H	4:A:410:PX4:C35	7	1.57
(3,33)	1:A:155:THR:H	4:A:412:PX4:C35	7	1.57
(3,33)	1:A:155:THR:H	4:A:414:PX4:C35	7	1.57
(3,33)	1:A:155:THR:H	4:A:416:PX4:C35	7	1.57
(3,33)	1:A:155:THR:H	4:A:418:PX4:C35	7	1.57
(3,33)	1:A:155:THR:H	4:A:420:PX4:C35	7	1.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,33)	1:A:155:THR:H	4:A:422:PX4:C35	7	1.57
(3,33)	1:A:155:THR:H	4:A:424:PX4:C35	7	1.57
(3,33)	1:A:155:THR:H	4:A:426:PX4:C35	7	1.57
(3,33)	1:A:155:THR:H	4:A:428:PX4:C35	7	1.57
(3,33)	1:A:155:THR:H	4:A:430:PX4:C35	7	1.57
(2,967)	1:A:77:LEU:H	1:A:77:LEU:HG	1	1.57
(2,967)	1:A:77:LEU:H	1:A:77:LEU:HG	7	1.57
(2,833)	1:A:120:ILE:HD11	1:A:200:LEU:HD22	4	1.57
(2,833)	1:A:120:ILE:HD11	1:A:200:LEU:HD23	4	1.57
(2,777)	1:A:61:ILE:HD13	1:A:48:LEU:HD21	16	1.57
(2,542)	1:A:210:ALA:H	1:A:209:ASN:HD22	8	1.57
(2,517)	1:A:200:LEU:H	1:A:196:LEU:HD21	16	1.57
(2,472)	1:A:186:ILE:H	1:A:156:LEU:HD21	2	1.57
(2,967)	1:A:77:LEU:H	1:A:77:LEU:HG	14	1.56
(2,75)	1:A:55:ASN:H	1:A:59:ILE:H	5	1.56
(2,948)	1:A:74:GLU:HG3	1:A:75:TYR:H	9	1.55
(2,948)	1:A:74:GLU:HG3	1:A:75:TYR:H	9	1.55
(2,902)	1:A:66:ARG:HA	1:A:68:GLY:H	3	1.55
(2,899)	1:A:66:ARG:H	1:A:64:LYS:H	17	1.55
(2,879)	1:A:234:ILE:HD11	1:A:200:LEU:HB2	10	1.55
(2,879)	1:A:234:ILE:HD12	1:A:200:LEU:HB2	10	1.55
(2,879)	1:A:234:ILE:HD13	1:A:200:LEU:HB2	10	1.55
(2,832)	1:A:120:ILE:HD11	1:A:200:LEU:HD21	12	1.55
(2,902)	1:A:66:ARG:HA	1:A:68:GLY:H	12	1.54
(2,727)	1:A:211:VAL:HG11	1:A:226:LEU:HD21	10	1.54
(3,33)	1:A:155:THR:H	4:A:305:PX4:C35	13	1.53
(3,33)	1:A:155:THR:H	4:A:307:PX4:C35	13	1.53
(3,33)	1:A:155:THR:H	4:A:309:PX4:C35	13	1.53
(3,33)	1:A:155:THR:H	4:A:311:PX4:C35	13	1.53
(3,33)	1:A:155:THR:H	4:A:313:PX4:C35	13	1.53
(3,33)	1:A:155:THR:H	4:A:315:PX4:C35	13	1.53
(3,33)	1:A:155:THR:H	4:A:317:PX4:C35	13	1.53
(3,33)	1:A:155:THR:H	4:A:319:PX4:C35	13	1.53
(3,33)	1:A:155:THR:H	4:A:321:PX4:C35	13	1.53
(3,33)	1:A:155:THR:H	4:A:323:PX4:C35	13	1.53
(3,33)	1:A:155:THR:H	4:A:325:PX4:C35	13	1.53
(3,33)	1:A:155:THR:H	4:A:327:PX4:C35	13	1.53
(3,33)	1:A:155:THR:H	4:A:329:PX4:C35	13	1.53
(3,33)	1:A:155:THR:H	4:A:331:PX4:C35	13	1.53
(3,33)	1:A:155:THR:H	4:A:333:PX4:C35	13	1.53
(3,33)	1:A:155:THR:H	4:A:335:PX4:C35	13	1.53
(3,33)	1:A:155:THR:H	4:A:337:PX4:C35	13	1.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,33)	1:A:155:THR:H	4:A:339:PX4:C35	13	1.53
(3,33)	1:A:155:THR:H	4:A:341:PX4:C35	13	1.53
(3,33)	1:A:155:THR:H	4:A:343:PX4:C35	13	1.53
(3,33)	1:A:155:THR:H	4:A:345:PX4:C35	13	1.53
(3,33)	1:A:155:THR:H	4:A:347:PX4:C35	13	1.53
(3,33)	1:A:155:THR:H	4:A:349:PX4:C35	13	1.53
(3,33)	1:A:155:THR:H	4:A:351:PX4:C35	13	1.53
(3,33)	1:A:155:THR:H	4:A:353:PX4:C35	13	1.53
(3,33)	1:A:155:THR:H	4:A:355:PX4:C35	13	1.53
(3,33)	1:A:155:THR:H	4:A:357:PX4:C35	13	1.53
(3,33)	1:A:155:THR:H	4:A:359:PX4:C35	13	1.53
(3,33)	1:A:155:THR:H	4:A:361:PX4:C35	13	1.53
(3,33)	1:A:155:THR:H	4:A:363:PX4:C35	13	1.53
(3,33)	1:A:155:THR:H	4:A:402:PX4:C35	13	1.53
(3,33)	1:A:155:THR:H	4:A:404:PX4:C35	13	1.53
(3,33)	1:A:155:THR:H	4:A:406:PX4:C35	13	1.53
(3,33)	1:A:155:THR:H	4:A:408:PX4:C35	13	1.53
(3,33)	1:A:155:THR:H	4:A:410:PX4:C35	13	1.53
(3,33)	1:A:155:THR:H	4:A:412:PX4:C35	13	1.53
(3,33)	1:A:155:THR:H	4:A:414:PX4:C35	13	1.53
(3,33)	1:A:155:THR:H	4:A:416:PX4:C35	13	1.53
(3,33)	1:A:155:THR:H	4:A:418:PX4:C35	13	1.53
(3,33)	1:A:155:THR:H	4:A:420:PX4:C35	13	1.53
(3,33)	1:A:155:THR:H	4:A:422:PX4:C35	13	1.53
(3,33)	1:A:155:THR:H	4:A:424:PX4:C35	13	1.53
(3,33)	1:A:155:THR:H	4:A:426:PX4:C35	13	1.53
(3,33)	1:A:155:THR:H	4:A:428:PX4:C35	13	1.53
(3,33)	1:A:155:THR:H	4:A:430:PX4:C35	13	1.53
(2,940)	1:A:73:ALA:HB1	1:A:75:TYR:H	12	1.53
(2,940)	1:A:73:ALA:HB2	1:A:75:TYR:H	12	1.53
(2,940)	1:A:73:ALA:HB3	1:A:75:TYR:H	12	1.53
(2,902)	1:A:66:ARG:HA	1:A:68:GLY:H	4	1.53
(2,869)	1:A:186:ILE:HD12	1:A:156:LEU:HD21	12	1.53
(2,765)	1:A:22:PHE:H	1:A:19:LEU:HD21	13	1.53
(3,33)	1:A:155:THR:H	4:A:305:PX4:C35	17	1.52
(3,33)	1:A:155:THR:H	4:A:307:PX4:C35	17	1.52
(3,33)	1:A:155:THR:H	4:A:309:PX4:C35	17	1.52
(3,33)	1:A:155:THR:H	4:A:311:PX4:C35	17	1.52
(3,33)	1:A:155:THR:H	4:A:313:PX4:C35	17	1.52
(3,33)	1:A:155:THR:H	4:A:315:PX4:C35	17	1.52
(3,33)	1:A:155:THR:H	4:A:317:PX4:C35	17	1.52
(3,33)	1:A:155:THR:H	4:A:319:PX4:C35	17	1.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,33)	1:A:155:THR:H	4:A:321:PX4:C35	17	1.52
(3,33)	1:A:155:THR:H	4:A:323:PX4:C35	17	1.52
(3,33)	1:A:155:THR:H	4:A:325:PX4:C35	17	1.52
(3,33)	1:A:155:THR:H	4:A:327:PX4:C35	17	1.52
(3,33)	1:A:155:THR:H	4:A:329:PX4:C35	17	1.52
(3,33)	1:A:155:THR:H	4:A:331:PX4:C35	17	1.52
(3,33)	1:A:155:THR:H	4:A:333:PX4:C35	17	1.52
(3,33)	1:A:155:THR:H	4:A:335:PX4:C35	17	1.52
(3,33)	1:A:155:THR:H	4:A:337:PX4:C35	17	1.52
(3,33)	1:A:155:THR:H	4:A:339:PX4:C35	17	1.52
(3,33)	1:A:155:THR:H	4:A:341:PX4:C35	17	1.52
(3,33)	1:A:155:THR:H	4:A:343:PX4:C35	17	1.52
(3,33)	1:A:155:THR:H	4:A:345:PX4:C35	17	1.52
(3,33)	1:A:155:THR:H	4:A:347:PX4:C35	17	1.52
(3,33)	1:A:155:THR:H	4:A:349:PX4:C35	17	1.52
(3,33)	1:A:155:THR:H	4:A:351:PX4:C35	17	1.52
(3,33)	1:A:155:THR:H	4:A:353:PX4:C35	17	1.52
(3,33)	1:A:155:THR:H	4:A:355:PX4:C35	17	1.52
(3,33)	1:A:155:THR:H	4:A:357:PX4:C35	17	1.52
(3,33)	1:A:155:THR:H	4:A:359:PX4:C35	17	1.52
(3,33)	1:A:155:THR:H	4:A:361:PX4:C35	17	1.52
(3,33)	1:A:155:THR:H	4:A:363:PX4:C35	17	1.52
(3,33)	1:A:155:THR:H	4:A:402:PX4:C35	17	1.52
(3,33)	1:A:155:THR:H	4:A:404:PX4:C35	17	1.52
(3,33)	1:A:155:THR:H	4:A:406:PX4:C35	17	1.52
(3,33)	1:A:155:THR:H	4:A:408:PX4:C35	17	1.52
(3,33)	1:A:155:THR:H	4:A:410:PX4:C35	17	1.52
(3,33)	1:A:155:THR:H	4:A:412:PX4:C35	17	1.52
(3,33)	1:A:155:THR:H	4:A:414:PX4:C35	17	1.52
(3,33)	1:A:155:THR:H	4:A:416:PX4:C35	17	1.52
(3,33)	1:A:155:THR:H	4:A:418:PX4:C35	17	1.52
(3,33)	1:A:155:THR:H	4:A:420:PX4:C35	17	1.52
(3,33)	1:A:155:THR:H	4:A:422:PX4:C35	17	1.52
(3,33)	1:A:155:THR:H	4:A:424:PX4:C35	17	1.52
(3,33)	1:A:155:THR:H	4:A:426:PX4:C35	17	1.52
(3,33)	1:A:155:THR:H	4:A:428:PX4:C35	17	1.52
(3,33)	1:A:155:THR:H	4:A:430:PX4:C35	17	1.52
(2,932)	1:A:72:VAL:HG11	1:A:76:SER:H	8	1.52
(2,932)	1:A:72:VAL:HG12	1:A:76:SER:H	8	1.52
(2,932)	1:A:72:VAL:HG13	1:A:76:SER:H	8	1.52
(2,902)	1:A:66:ARG:HA	1:A:68:GLY:H	17	1.52
(2,871)	1:A:186:ILE:HD13	1:A:156:LEU:HD21	16	1.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,870)	1:A:186:ILE:HD12	1:A:156:LEU:HD22	1	1.52
(2,870)	1:A:186:ILE:HD12	1:A:156:LEU:HD23	1	1.52
(2,760)	1:A:54:LEU:HD22	1:A:59:ILE:HD11	19	1.52
(2,760)	1:A:54:LEU:HD22	1:A:59:ILE:HD12	19	1.52
(2,760)	1:A:54:LEU:HD22	1:A:59:ILE:HD13	19	1.52
(2,760)	1:A:54:LEU:HD23	1:A:59:ILE:HD11	19	1.52
(2,760)	1:A:54:LEU:HD23	1:A:59:ILE:HD12	19	1.52
(2,760)	1:A:54:LEU:HD23	1:A:59:ILE:HD13	19	1.52
(2,598)	1:A:235:GLN:H	1:A:238:TYR:HE1	19	1.52
(2,598)	1:A:235:GLN:H	1:A:238:TYR:HE2	19	1.52
(2,542)	1:A:210:ALA:H	1:A:209:ASN:HD22	11	1.52
(2,516)	1:A:200:LEU:H	1:A:196:LEU:HD11	19	1.52
(2,516)	1:A:200:LEU:H	1:A:196:LEU:HD12	19	1.52
(2,516)	1:A:200:LEU:H	1:A:196:LEU:HD13	19	1.52
(2,473)	1:A:186:ILE:H	1:A:156:LEU:HD22	2	1.52
(2,473)	1:A:186:ILE:H	1:A:156:LEU:HD23	2	1.52
(2,178)	1:A:171:HIS:H	1:A:69:VAL:HG11	16	1.52
(2,178)	1:A:171:HIS:H	1:A:69:VAL:HG12	16	1.52
(2,178)	1:A:171:HIS:H	1:A:69:VAL:HG13	16	1.52
(2,940)	1:A:73:ALA:HB1	1:A:75:TYR:H	10	1.51
(2,940)	1:A:73:ALA:HB2	1:A:75:TYR:H	10	1.51
(2,940)	1:A:73:ALA:HB3	1:A:75:TYR:H	10	1.51
(2,765)	1:A:22:PHE:H	1:A:19:LEU:HD21	12	1.51
(2,598)	1:A:235:GLN:H	1:A:238:TYR:HE1	1	1.51
(2,598)	1:A:235:GLN:H	1:A:238:TYR:HE2	1	1.51
(2,940)	1:A:73:ALA:HB1	1:A:75:TYR:H	15	1.5
(2,940)	1:A:73:ALA:HB2	1:A:75:TYR:H	15	1.5
(2,940)	1:A:73:ALA:HB3	1:A:75:TYR:H	15	1.5
(2,902)	1:A:66:ARG:HA	1:A:68:GLY:H	15	1.5
(2,981)	1:A:78:PHE:H	1:A:79:PRO:HG3	20	1.49
(2,981)	1:A:78:PHE:H	1:A:79:PRO:HG3	20	1.49
(2,178)	1:A:171:HIS:H	1:A:69:VAL:HG11	18	1.49
(2,178)	1:A:171:HIS:H	1:A:69:VAL:HG12	18	1.49
(2,178)	1:A:171:HIS:H	1:A:69:VAL:HG13	18	1.49
(3,36)	1:A:129:TRP:HE1	4:A:305:PX4:N1	15	1.48
(3,36)	1:A:129:TRP:HE1	4:A:307:PX4:N1	15	1.48
(3,36)	1:A:129:TRP:HE1	4:A:309:PX4:N1	15	1.48
(3,36)	1:A:129:TRP:HE1	4:A:311:PX4:N1	15	1.48
(3,36)	1:A:129:TRP:HE1	4:A:313:PX4:N1	15	1.48
(3,36)	1:A:129:TRP:HE1	4:A:315:PX4:N1	15	1.48
(3,36)	1:A:129:TRP:HE1	4:A:317:PX4:N1	15	1.48
(3,36)	1:A:129:TRP:HE1	4:A:319:PX4:N1	15	1.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,36)	1:A:129:TRP:HE1	4:A:321:PX4:N1	15	1.48
(3,36)	1:A:129:TRP:HE1	4:A:323:PX4:N1	15	1.48
(3,36)	1:A:129:TRP:HE1	4:A:325:PX4:N1	15	1.48
(3,36)	1:A:129:TRP:HE1	4:A:327:PX4:N1	15	1.48
(3,36)	1:A:129:TRP:HE1	4:A:329:PX4:N1	15	1.48
(3,36)	1:A:129:TRP:HE1	4:A:331:PX4:N1	15	1.48
(3,36)	1:A:129:TRP:HE1	4:A:333:PX4:N1	15	1.48
(3,36)	1:A:129:TRP:HE1	4:A:335:PX4:N1	15	1.48
(3,36)	1:A:129:TRP:HE1	4:A:337:PX4:N1	15	1.48
(3,36)	1:A:129:TRP:HE1	4:A:339:PX4:N1	15	1.48
(3,36)	1:A:129:TRP:HE1	4:A:341:PX4:N1	15	1.48
(3,36)	1:A:129:TRP:HE1	4:A:343:PX4:N1	15	1.48
(3,36)	1:A:129:TRP:HE1	4:A:345:PX4:N1	15	1.48
(3,36)	1:A:129:TRP:HE1	4:A:347:PX4:N1	15	1.48
(3,36)	1:A:129:TRP:HE1	4:A:349:PX4:N1	15	1.48
(3,36)	1:A:129:TRP:HE1	4:A:351:PX4:N1	15	1.48
(3,36)	1:A:129:TRP:HE1	4:A:353:PX4:N1	15	1.48
(3,36)	1:A:129:TRP:HE1	4:A:355:PX4:N1	15	1.48
(3,36)	1:A:129:TRP:HE1	4:A:357:PX4:N1	15	1.48
(3,36)	1:A:129:TRP:HE1	4:A:359:PX4:N1	15	1.48
(3,36)	1:A:129:TRP:HE1	4:A:361:PX4:N1	15	1.48
(3,36)	1:A:129:TRP:HE1	4:A:363:PX4:N1	15	1.48
(3,36)	1:A:129:TRP:HE1	4:A:402:PX4:N1	15	1.48
(3,36)	1:A:129:TRP:HE1	4:A:404:PX4:N1	15	1.48
(3,36)	1:A:129:TRP:HE1	4:A:406:PX4:N1	15	1.48
(3,36)	1:A:129:TRP:HE1	4:A:408:PX4:N1	15	1.48
(3,36)	1:A:129:TRP:HE1	4:A:410:PX4:N1	15	1.48
(3,36)	1:A:129:TRP:HE1	4:A:412:PX4:N1	15	1.48
(3,36)	1:A:129:TRP:HE1	4:A:414:PX4:N1	15	1.48
(3,36)	1:A:129:TRP:HE1	4:A:416:PX4:N1	15	1.48
(3,36)	1:A:129:TRP:HE1	4:A:418:PX4:N1	15	1.48
(3,36)	1:A:129:TRP:HE1	4:A:420:PX4:N1	15	1.48
(3,36)	1:A:129:TRP:HE1	4:A:422:PX4:N1	15	1.48
(3,36)	1:A:129:TRP:HE1	4:A:424:PX4:N1	15	1.48
(3,36)	1:A:129:TRP:HE1	4:A:426:PX4:N1	15	1.48
(3,36)	1:A:129:TRP:HE1	4:A:428:PX4:N1	15	1.48
(3,36)	1:A:129:TRP:HE1	4:A:430:PX4:N1	15	1.48
(2,981)	1:A:78:PHE:H	1:A:79:PRO:HG3	13	1.48
(2,981)	1:A:78:PHE:H	1:A:79:PRO:HG3	13	1.48
(2,902)	1:A:66:ARG:HA	1:A:68:GLY:H	5	1.48
(2,804)	1:A:93:ILE:HD11	1:A:105:VAL:HG21	17	1.48
(2,804)	1:A:93:ILE:HD11	1:A:105:VAL:HG22	17	1.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,804)	1:A:93:ILE:HD11	1:A:105:VAL:HG23	17	1.48
(2,804)	1:A:93:ILE:HD12	1:A:105:VAL:HG21	17	1.48
(2,804)	1:A:93:ILE:HD12	1:A:105:VAL:HG22	17	1.48
(2,804)	1:A:93:ILE:HD12	1:A:105:VAL:HG23	17	1.48
(2,804)	1:A:93:ILE:HD13	1:A:105:VAL:HG21	17	1.48
(2,804)	1:A:93:ILE:HD13	1:A:105:VAL:HG22	17	1.48
(2,804)	1:A:93:ILE:HD13	1:A:105:VAL:HG23	17	1.48
(2,516)	1:A:200:LEU:H	1:A:196:LEU:HD11	20	1.48
(2,516)	1:A:200:LEU:H	1:A:196:LEU:HD12	20	1.48
(2,516)	1:A:200:LEU:H	1:A:196:LEU:HD13	20	1.48
(2,178)	1:A:171:HIS:H	1:A:69:VAL:HG11	20	1.48
(2,178)	1:A:171:HIS:H	1:A:69:VAL:HG12	20	1.48
(2,178)	1:A:171:HIS:H	1:A:69:VAL:HG13	20	1.48
(3,6)	1:A:78:PHE:H	4:A:305:PX4:C27	14	1.47
(3,6)	1:A:78:PHE:H	4:A:307:PX4:C27	14	1.47
(3,6)	1:A:78:PHE:H	4:A:309:PX4:C27	14	1.47
(3,6)	1:A:78:PHE:H	4:A:311:PX4:C27	14	1.47
(3,6)	1:A:78:PHE:H	4:A:313:PX4:C27	14	1.47
(3,6)	1:A:78:PHE:H	4:A:315:PX4:C27	14	1.47
(3,6)	1:A:78:PHE:H	4:A:317:PX4:C27	14	1.47
(3,6)	1:A:78:PHE:H	4:A:319:PX4:C27	14	1.47
(3,6)	1:A:78:PHE:H	4:A:321:PX4:C27	14	1.47
(3,6)	1:A:78:PHE:H	4:A:323:PX4:C27	14	1.47
(3,6)	1:A:78:PHE:H	4:A:325:PX4:C27	14	1.47
(3,6)	1:A:78:PHE:H	4:A:327:PX4:C27	14	1.47
(3,6)	1:A:78:PHE:H	4:A:329:PX4:C27	14	1.47
(3,6)	1:A:78:PHE:H	4:A:331:PX4:C27	14	1.47
(3,6)	1:A:78:PHE:H	4:A:333:PX4:C27	14	1.47
(3,6)	1:A:78:PHE:H	4:A:335:PX4:C27	14	1.47
(3,6)	1:A:78:PHE:H	4:A:337:PX4:C27	14	1.47
(3,6)	1:A:78:PHE:H	4:A:339:PX4:C27	14	1.47
(3,6)	1:A:78:PHE:H	4:A:341:PX4:C27	14	1.47
(3,6)	1:A:78:PHE:H	4:A:343:PX4:C27	14	1.47
(3,6)	1:A:78:PHE:H	4:A:345:PX4:C27	14	1.47
(3,6)	1:A:78:PHE:H	4:A:347:PX4:C27	14	1.47
(3,6)	1:A:78:PHE:H	4:A:349:PX4:C27	14	1.47
(3,6)	1:A:78:PHE:H	4:A:351:PX4:C27	14	1.47
(3,6)	1:A:78:PHE:H	4:A:353:PX4:C27	14	1.47
(3,6)	1:A:78:PHE:H	4:A:355:PX4:C27	14	1.47
(3,6)	1:A:78:PHE:H	4:A:357:PX4:C27	14	1.47
(3,6)	1:A:78:PHE:H	4:A:359:PX4:C27	14	1.47
(3,6)	1:A:78:PHE:H	4:A:361:PX4:C27	14	1.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,6)	1:A:78:PHE:H	4:A:363:PX4:C27	14	1.47
(3,6)	1:A:78:PHE:H	4:A:402:PX4:C27	14	1.47
(3,6)	1:A:78:PHE:H	4:A:404:PX4:C27	14	1.47
(3,6)	1:A:78:PHE:H	4:A:406:PX4:C27	14	1.47
(3,6)	1:A:78:PHE:H	4:A:408:PX4:C27	14	1.47
(3,6)	1:A:78:PHE:H	4:A:410:PX4:C27	14	1.47
(3,6)	1:A:78:PHE:H	4:A:412:PX4:C27	14	1.47
(3,6)	1:A:78:PHE:H	4:A:414:PX4:C27	14	1.47
(3,6)	1:A:78:PHE:H	4:A:416:PX4:C27	14	1.47
(3,6)	1:A:78:PHE:H	4:A:418:PX4:C27	14	1.47
(3,6)	1:A:78:PHE:H	4:A:420:PX4:C27	14	1.47
(3,6)	1:A:78:PHE:H	4:A:422:PX4:C27	14	1.47
(3,6)	1:A:78:PHE:H	4:A:424:PX4:C27	14	1.47
(3,6)	1:A:78:PHE:H	4:A:426:PX4:C27	14	1.47
(3,6)	1:A:78:PHE:H	4:A:428:PX4:C27	14	1.47
(3,6)	1:A:78:PHE:H	4:A:430:PX4:C27	14	1.47
(2,982)	1:A:78:PHE:HD1	1:A:80:ASN:H	7	1.47
(2,967)	1:A:77:LEU:H	1:A:77:LEU:HG	15	1.47
(2,954)	1:A:74:GLU:HB3	1:A:77:LEU:H	20	1.47
(2,954)	1:A:74:GLU:HB3	1:A:77:LEU:H	20	1.47
(2,928)	1:A:72:VAL:H	1:A:73:ALA:HB1	10	1.47
(2,899)	1:A:66:ARG:H	1:A:64:LYS:H	3	1.47
(2,836)	1:A:120:ILE:HD13	1:A:200:LEU:HD21	4	1.47
(2,835)	1:A:120:ILE:HD12	1:A:200:LEU:HD22	17	1.47
(2,835)	1:A:120:ILE:HD12	1:A:200:LEU:HD23	17	1.47
(2,729)	1:A:211:VAL:HG12	1:A:226:LEU:HD21	10	1.47
(2,257)	1:A:112:ALA:H	1:A:189:LEU:HD21	17	1.47
(2,110)	1:A:11:GLN:H	1:A:14:GLN:H	7	1.47
(3,36)	1:A:129:TRP:HE1	4:A:305:PX4:N1	1	1.46
(3,36)	1:A:129:TRP:HE1	4:A:307:PX4:N1	1	1.46
(3,36)	1:A:129:TRP:HE1	4:A:309:PX4:N1	1	1.46
(3,36)	1:A:129:TRP:HE1	4:A:311:PX4:N1	1	1.46
(3,36)	1:A:129:TRP:HE1	4:A:313:PX4:N1	1	1.46
(3,36)	1:A:129:TRP:HE1	4:A:315:PX4:N1	1	1.46
(3,36)	1:A:129:TRP:HE1	4:A:317:PX4:N1	1	1.46
(3,36)	1:A:129:TRP:HE1	4:A:319:PX4:N1	1	1.46
(3,36)	1:A:129:TRP:HE1	4:A:321:PX4:N1	1	1.46
(3,36)	1:A:129:TRP:HE1	4:A:323:PX4:N1	1	1.46
(3,36)	1:A:129:TRP:HE1	4:A:325:PX4:N1	1	1.46
(3,36)	1:A:129:TRP:HE1	4:A:327:PX4:N1	1	1.46
(3,36)	1:A:129:TRP:HE1	4:A:329:PX4:N1	1	1.46
(3,36)	1:A:129:TRP:HE1	4:A:331:PX4:N1	1	1.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,36)	1:A:129:TRP:HE1	4:A:333:PX4:N1	1	1.46
(3,36)	1:A:129:TRP:HE1	4:A:335:PX4:N1	1	1.46
(3,36)	1:A:129:TRP:HE1	4:A:337:PX4:N1	1	1.46
(3,36)	1:A:129:TRP:HE1	4:A:339:PX4:N1	1	1.46
(3,36)	1:A:129:TRP:HE1	4:A:341:PX4:N1	1	1.46
(3,36)	1:A:129:TRP:HE1	4:A:343:PX4:N1	1	1.46
(3,36)	1:A:129:TRP:HE1	4:A:345:PX4:N1	1	1.46
(3,36)	1:A:129:TRP:HE1	4:A:347:PX4:N1	1	1.46
(3,36)	1:A:129:TRP:HE1	4:A:349:PX4:N1	1	1.46
(3,36)	1:A:129:TRP:HE1	4:A:351:PX4:N1	1	1.46
(3,36)	1:A:129:TRP:HE1	4:A:353:PX4:N1	1	1.46
(3,36)	1:A:129:TRP:HE1	4:A:355:PX4:N1	1	1.46
(3,36)	1:A:129:TRP:HE1	4:A:357:PX4:N1	1	1.46
(3,36)	1:A:129:TRP:HE1	4:A:359:PX4:N1	1	1.46
(3,36)	1:A:129:TRP:HE1	4:A:361:PX4:N1	1	1.46
(3,36)	1:A:129:TRP:HE1	4:A:363:PX4:N1	1	1.46
(3,36)	1:A:129:TRP:HE1	4:A:402:PX4:N1	1	1.46
(3,36)	1:A:129:TRP:HE1	4:A:404:PX4:N1	1	1.46
(3,36)	1:A:129:TRP:HE1	4:A:406:PX4:N1	1	1.46
(3,36)	1:A:129:TRP:HE1	4:A:408:PX4:N1	1	1.46
(3,36)	1:A:129:TRP:HE1	4:A:410:PX4:N1	1	1.46
(3,36)	1:A:129:TRP:HE1	4:A:412:PX4:N1	1	1.46
(3,36)	1:A:129:TRP:HE1	4:A:414:PX4:N1	1	1.46
(3,36)	1:A:129:TRP:HE1	4:A:416:PX4:N1	1	1.46
(3,36)	1:A:129:TRP:HE1	4:A:418:PX4:N1	1	1.46
(3,36)	1:A:129:TRP:HE1	4:A:420:PX4:N1	1	1.46
(3,36)	1:A:129:TRP:HE1	4:A:422:PX4:N1	1	1.46
(3,36)	1:A:129:TRP:HE1	4:A:424:PX4:N1	1	1.46
(3,36)	1:A:129:TRP:HE1	4:A:426:PX4:N1	1	1.46
(3,36)	1:A:129:TRP:HE1	4:A:428:PX4:N1	1	1.46
(3,36)	1:A:129:TRP:HE1	4:A:430:PX4:N1	1	1.46
(2,981)	1:A:78:PHE:H	1:A:79:PRO:HG3	8	1.46
(2,981)	1:A:78:PHE:H	1:A:79:PRO:HG3	8	1.46
(2,940)	1:A:73:ALA:HB1	1:A:75:TYR:H	6	1.46
(2,940)	1:A:73:ALA:HB2	1:A:75:TYR:H	6	1.46
(2,940)	1:A:73:ALA:HB3	1:A:75:TYR:H	6	1.46
(2,542)	1:A:210:ALA:H	1:A:209:ASN:HD22	3	1.46
(2,948)	1:A:74:GLU:HG3	1:A:75:TYR:H	2	1.45
(2,948)	1:A:74:GLU:HG3	1:A:75:TYR:H	2	1.45
(2,940)	1:A:73:ALA:HB1	1:A:75:TYR:H	3	1.45
(2,940)	1:A:73:ALA:HB2	1:A:75:TYR:H	3	1.45
(2,940)	1:A:73:ALA:HB3	1:A:75:TYR:H	3	1.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,542)	1:A:210:ALA:H	1:A:209:ASN:HD22	15	1.45
(2,517)	1:A:200:LEU:H	1:A:196:LEU:HD21	3	1.45
(3,21)	1:A:77:LEU:H	4:A:305:PX4:C35	4	1.44
(3,21)	1:A:77:LEU:H	4:A:307:PX4:C35	4	1.44
(3,21)	1:A:77:LEU:H	4:A:309:PX4:C35	4	1.44
(3,21)	1:A:77:LEU:H	4:A:311:PX4:C35	4	1.44
(3,21)	1:A:77:LEU:H	4:A:313:PX4:C35	4	1.44
(3,21)	1:A:77:LEU:H	4:A:315:PX4:C35	4	1.44
(3,21)	1:A:77:LEU:H	4:A:317:PX4:C35	4	1.44
(3,21)	1:A:77:LEU:H	4:A:319:PX4:C35	4	1.44
(3,21)	1:A:77:LEU:H	4:A:321:PX4:C35	4	1.44
(3,21)	1:A:77:LEU:H	4:A:323:PX4:C35	4	1.44
(3,21)	1:A:77:LEU:H	4:A:325:PX4:C35	4	1.44
(3,21)	1:A:77:LEU:H	4:A:327:PX4:C35	4	1.44
(3,21)	1:A:77:LEU:H	4:A:329:PX4:C35	4	1.44
(3,21)	1:A:77:LEU:H	4:A:331:PX4:C35	4	1.44
(3,21)	1:A:77:LEU:H	4:A:333:PX4:C35	4	1.44
(3,21)	1:A:77:LEU:H	4:A:335:PX4:C35	4	1.44
(3,21)	1:A:77:LEU:H	4:A:337:PX4:C35	4	1.44
(3,21)	1:A:77:LEU:H	4:A:339:PX4:C35	4	1.44
(3,21)	1:A:77:LEU:H	4:A:341:PX4:C35	4	1.44
(3,21)	1:A:77:LEU:H	4:A:343:PX4:C35	4	1.44
(3,21)	1:A:77:LEU:H	4:A:345:PX4:C35	4	1.44
(3,21)	1:A:77:LEU:H	4:A:347:PX4:C35	4	1.44
(3,21)	1:A:77:LEU:H	4:A:349:PX4:C35	4	1.44
(3,21)	1:A:77:LEU:H	4:A:351:PX4:C35	4	1.44
(3,21)	1:A:77:LEU:H	4:A:353:PX4:C35	4	1.44
(3,21)	1:A:77:LEU:H	4:A:355:PX4:C35	4	1.44
(3,21)	1:A:77:LEU:H	4:A:357:PX4:C35	4	1.44
(3,21)	1:A:77:LEU:H	4:A:359:PX4:C35	4	1.44
(3,21)	1:A:77:LEU:H	4:A:361:PX4:C35	4	1.44
(3,21)	1:A:77:LEU:H	4:A:363:PX4:C35	4	1.44
(3,21)	1:A:77:LEU:H	4:A:402:PX4:C35	4	1.44
(3,21)	1:A:77:LEU:H	4:A:404:PX4:C35	4	1.44
(3,21)	1:A:77:LEU:H	4:A:406:PX4:C35	4	1.44
(3,21)	1:A:77:LEU:H	4:A:408:PX4:C35	4	1.44
(3,21)	1:A:77:LEU:H	4:A:410:PX4:C35	4	1.44
(3,21)	1:A:77:LEU:H	4:A:412:PX4:C35	4	1.44
(3,21)	1:A:77:LEU:H	4:A:414:PX4:C35	4	1.44
(3,21)	1:A:77:LEU:H	4:A:416:PX4:C35	4	1.44
(3,21)	1:A:77:LEU:H	4:A:418:PX4:C35	4	1.44
(3,21)	1:A:77:LEU:H	4:A:420:PX4:C35	4	1.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,21)	1:A:77:LEU:H	4:A:422:PX4:C35	4	1.44
(3,21)	1:A:77:LEU:H	4:A:424:PX4:C35	4	1.44
(3,21)	1:A:77:LEU:H	4:A:426:PX4:C35	4	1.44
(3,21)	1:A:77:LEU:H	4:A:428:PX4:C35	4	1.44
(3,21)	1:A:77:LEU:H	4:A:430:PX4:C35	4	1.44
(2,974)	1:A:78:PHE:H	1:A:77:LEU:HD21	8	1.44
(2,899)	1:A:66:ARG:H	1:A:64:LYS:H	5	1.44
(2,510)	1:A:200:LEU:HD21	1:A:199:SER:H	4	1.44
(2,981)	1:A:78:PHE:H	1:A:79:PRO:HG3	19	1.43
(2,981)	1:A:78:PHE:H	1:A:79:PRO:HG3	19	1.43
(2,940)	1:A:73:ALA:HB1	1:A:75:TYR:H	1	1.43
(2,940)	1:A:73:ALA:HB2	1:A:75:TYR:H	1	1.43
(2,940)	1:A:73:ALA:HB3	1:A:75:TYR:H	1	1.43
(2,775)	1:A:61:ILE:HD12	1:A:48:LEU:HD21	18	1.43
(2,760)	1:A:54:LEU:HD22	1:A:59:ILE:HD11	8	1.43
(2,760)	1:A:54:LEU:HD22	1:A:59:ILE:HD12	8	1.43
(2,760)	1:A:54:LEU:HD22	1:A:59:ILE:HD13	8	1.43
(2,760)	1:A:54:LEU:HD23	1:A:59:ILE:HD11	8	1.43
(2,760)	1:A:54:LEU:HD23	1:A:59:ILE:HD12	8	1.43
(2,760)	1:A:54:LEU:HD23	1:A:59:ILE:HD13	8	1.43
(3,33)	1:A:155:THR:H	4:A:305:PX4:C35	15	1.42
(3,33)	1:A:155:THR:H	4:A:307:PX4:C35	15	1.42
(3,33)	1:A:155:THR:H	4:A:309:PX4:C35	15	1.42
(3,33)	1:A:155:THR:H	4:A:311:PX4:C35	15	1.42
(3,33)	1:A:155:THR:H	4:A:313:PX4:C35	15	1.42
(3,33)	1:A:155:THR:H	4:A:315:PX4:C35	15	1.42
(3,33)	1:A:155:THR:H	4:A:317:PX4:C35	15	1.42
(3,33)	1:A:155:THR:H	4:A:319:PX4:C35	15	1.42
(3,33)	1:A:155:THR:H	4:A:321:PX4:C35	15	1.42
(3,33)	1:A:155:THR:H	4:A:323:PX4:C35	15	1.42
(3,33)	1:A:155:THR:H	4:A:325:PX4:C35	15	1.42
(3,33)	1:A:155:THR:H	4:A:327:PX4:C35	15	1.42
(3,33)	1:A:155:THR:H	4:A:329:PX4:C35	15	1.42
(3,33)	1:A:155:THR:H	4:A:331:PX4:C35	15	1.42
(3,33)	1:A:155:THR:H	4:A:333:PX4:C35	15	1.42
(3,33)	1:A:155:THR:H	4:A:335:PX4:C35	15	1.42
(3,33)	1:A:155:THR:H	4:A:337:PX4:C35	15	1.42
(3,33)	1:A:155:THR:H	4:A:339:PX4:C35	15	1.42
(3,33)	1:A:155:THR:H	4:A:341:PX4:C35	15	1.42
(3,33)	1:A:155:THR:H	4:A:343:PX4:C35	15	1.42
(3,33)	1:A:155:THR:H	4:A:345:PX4:C35	15	1.42
(3,33)	1:A:155:THR:H	4:A:347:PX4:C35	15	1.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,33)	1:A:155:THR:H	4:A:349:PX4:C35	15	1.42
(3,33)	1:A:155:THR:H	4:A:351:PX4:C35	15	1.42
(3,33)	1:A:155:THR:H	4:A:353:PX4:C35	15	1.42
(3,33)	1:A:155:THR:H	4:A:355:PX4:C35	15	1.42
(3,33)	1:A:155:THR:H	4:A:357:PX4:C35	15	1.42
(3,33)	1:A:155:THR:H	4:A:359:PX4:C35	15	1.42
(3,33)	1:A:155:THR:H	4:A:361:PX4:C35	15	1.42
(3,33)	1:A:155:THR:H	4:A:363:PX4:C35	15	1.42
(3,33)	1:A:155:THR:H	4:A:402:PX4:C35	15	1.42
(3,33)	1:A:155:THR:H	4:A:404:PX4:C35	15	1.42
(3,33)	1:A:155:THR:H	4:A:406:PX4:C35	15	1.42
(3,33)	1:A:155:THR:H	4:A:408:PX4:C35	15	1.42
(3,33)	1:A:155:THR:H	4:A:410:PX4:C35	15	1.42
(3,33)	1:A:155:THR:H	4:A:412:PX4:C35	15	1.42
(3,33)	1:A:155:THR:H	4:A:414:PX4:C35	15	1.42
(3,33)	1:A:155:THR:H	4:A:416:PX4:C35	15	1.42
(3,33)	1:A:155:THR:H	4:A:418:PX4:C35	15	1.42
(3,33)	1:A:155:THR:H	4:A:420:PX4:C35	15	1.42
(3,33)	1:A:155:THR:H	4:A:422:PX4:C35	15	1.42
(3,33)	1:A:155:THR:H	4:A:424:PX4:C35	15	1.42
(3,33)	1:A:155:THR:H	4:A:426:PX4:C35	15	1.42
(3,33)	1:A:155:THR:H	4:A:428:PX4:C35	15	1.42
(3,33)	1:A:155:THR:H	4:A:430:PX4:C35	15	1.42
(2,981)	1:A:78:PHE:H	1:A:79:PRO:HG3	11	1.42
(2,981)	1:A:78:PHE:H	1:A:79:PRO:HG3	11	1.42
(2,948)	1:A:74:GLU:HG3	1:A:75:TYR:H	12	1.42
(2,948)	1:A:74:GLU:HG3	1:A:75:TYR:H	12	1.42
(2,836)	1:A:120:ILE:HD13	1:A:200:LEU:HD21	12	1.42
(2,264)	1:A:113:LEU:H	1:A:196:LEU:HD21	12	1.42
(2,988)	1:A:129:TRP:HE1	4:A:305:PX4:C2	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:307:PX4:C2	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:309:PX4:C2	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:311:PX4:C2	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:313:PX4:C2	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:315:PX4:C2	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:317:PX4:C2	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:319:PX4:C2	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:321:PX4:C2	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:323:PX4:C2	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:325:PX4:C2	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:327:PX4:C2	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:329:PX4:C2	14	1.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,988)	1:A:129:TRP:HE1	4:A:331:PX4:C2	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:333:PX4:C2	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:335:PX4:C2	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:337:PX4:C2	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:339:PX4:C2	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:341:PX4:C2	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:343:PX4:C2	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:345:PX4:C2	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:347:PX4:C2	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:349:PX4:C2	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:351:PX4:C2	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:353:PX4:C2	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:355:PX4:C2	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:357:PX4:C2	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:359:PX4:C2	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:361:PX4:C2	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:363:PX4:C2	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:402:PX4:C2	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:404:PX4:C2	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:406:PX4:C2	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:408:PX4:C2	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:410:PX4:C2	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:412:PX4:C2	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:414:PX4:C2	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:416:PX4:C2	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:418:PX4:C2	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:420:PX4:C2	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:422:PX4:C2	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:424:PX4:C2	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:426:PX4:C2	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:428:PX4:C2	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:430:PX4:C2	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:305:PX4:C1	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:307:PX4:C1	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:309:PX4:C1	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:311:PX4:C1	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:313:PX4:C1	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:315:PX4:C1	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:317:PX4:C1	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:319:PX4:C1	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:321:PX4:C1	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:323:PX4:C1	14	1.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,988)	1:A:129:TRP:HE1	4:A:325:PX4:C1	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:327:PX4:C1	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:329:PX4:C1	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:331:PX4:C1	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:333:PX4:C1	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:335:PX4:C1	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:337:PX4:C1	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:339:PX4:C1	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:341:PX4:C1	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:343:PX4:C1	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:345:PX4:C1	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:347:PX4:C1	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:349:PX4:C1	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:351:PX4:C1	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:353:PX4:C1	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:355:PX4:C1	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:357:PX4:C1	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:359:PX4:C1	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:361:PX4:C1	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:363:PX4:C1	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:402:PX4:C1	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:404:PX4:C1	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:406:PX4:C1	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:408:PX4:C1	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:410:PX4:C1	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:412:PX4:C1	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:414:PX4:C1	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:416:PX4:C1	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:418:PX4:C1	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:420:PX4:C1	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:422:PX4:C1	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:424:PX4:C1	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:426:PX4:C1	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:428:PX4:C1	14	1.41
(2,988)	1:A:129:TRP:HE1	4:A:430:PX4:C1	14	1.41
(2,981)	1:A:78:PHE:H	1:A:79:PRO:HG3	10	1.41
(2,981)	1:A:78:PHE:H	1:A:79:PRO:HG3	10	1.41
(2,940)	1:A:73:ALA:HB1	1:A:75:TYR:H	4	1.41
(2,940)	1:A:73:ALA:HB2	1:A:75:TYR:H	4	1.41
(2,940)	1:A:73:ALA:HB3	1:A:75:TYR:H	4	1.41
(2,932)	1:A:72:VAL:HG11	1:A:76:SER:H	17	1.41
(2,932)	1:A:72:VAL:HG12	1:A:76:SER:H	17	1.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,932)	1:A:72:VAL:HG13	1:A:76:SER:H	17	1.41
(2,928)	1:A:72:VAL:H	1:A:73:ALA:HB1	18	1.41
(2,899)	1:A:66:ARG:H	1:A:64:LYS:H	4	1.41
(2,869)	1:A:186:ILE:HD12	1:A:156:LEU:HD21	1	1.41
(2,510)	1:A:200:LEU:HD21	1:A:199:SER:H	7	1.41
(2,981)	1:A:78:PHE:H	1:A:79:PRO:HG3	15	1.4
(2,981)	1:A:78:PHE:H	1:A:79:PRO:HG3	15	1.4
(2,948)	1:A:74:GLU:HG3	1:A:75:TYR:H	15	1.4
(2,948)	1:A:74:GLU:HG3	1:A:75:TYR:H	15	1.4
(2,940)	1:A:73:ALA:HB1	1:A:75:TYR:H	8	1.4
(2,940)	1:A:73:ALA:HB2	1:A:75:TYR:H	8	1.4
(2,940)	1:A:73:ALA:HB3	1:A:75:TYR:H	8	1.4
(2,940)	1:A:73:ALA:HB1	1:A:75:TYR:H	9	1.4
(2,940)	1:A:73:ALA:HB2	1:A:75:TYR:H	9	1.4
(2,940)	1:A:73:ALA:HB3	1:A:75:TYR:H	9	1.4
(2,940)	1:A:73:ALA:HB1	1:A:75:TYR:H	18	1.4
(2,940)	1:A:73:ALA:HB2	1:A:75:TYR:H	18	1.4
(2,940)	1:A:73:ALA:HB3	1:A:75:TYR:H	18	1.4
(2,867)	1:A:186:ILE:HD11	1:A:156:LEU:HD21	14	1.4
(2,835)	1:A:120:ILE:HD12	1:A:200:LEU:HD22	6	1.4
(2,835)	1:A:120:ILE:HD12	1:A:200:LEU:HD23	6	1.4
(2,765)	1:A:22:PHE:H	1:A:19:LEU:HD21	3	1.4
(2,748)	1:A:89:VAL:HG12	1:A:122:LEU:HD21	9	1.4
(2,657)	1:A:39:LEU:H	1:A:19:LEU:HD22	17	1.4
(2,657)	1:A:39:LEU:H	1:A:19:LEU:HD23	17	1.4
(2,83)	1:A:58:VAL:H	1:A:48:LEU:HD22	16	1.39
(2,83)	1:A:58:VAL:H	1:A:48:LEU:HD23	16	1.39
(2,516)	1:A:200:LEU:H	1:A:196:LEU:HD11	15	1.39
(2,516)	1:A:200:LEU:H	1:A:196:LEU:HD12	15	1.39
(2,516)	1:A:200:LEU:H	1:A:196:LEU:HD13	15	1.39
(3,6)	1:A:78:PHE:H	4:A:305:PX4:C27	12	1.38
(3,6)	1:A:78:PHE:H	4:A:307:PX4:C27	12	1.38
(3,6)	1:A:78:PHE:H	4:A:309:PX4:C27	12	1.38
(3,6)	1:A:78:PHE:H	4:A:311:PX4:C27	12	1.38
(3,6)	1:A:78:PHE:H	4:A:313:PX4:C27	12	1.38
(3,6)	1:A:78:PHE:H	4:A:315:PX4:C27	12	1.38
(3,6)	1:A:78:PHE:H	4:A:317:PX4:C27	12	1.38
(3,6)	1:A:78:PHE:H	4:A:319:PX4:C27	12	1.38
(3,6)	1:A:78:PHE:H	4:A:321:PX4:C27	12	1.38
(3,6)	1:A:78:PHE:H	4:A:323:PX4:C27	12	1.38
(3,6)	1:A:78:PHE:H	4:A:325:PX4:C27	12	1.38
(3,6)	1:A:78:PHE:H	4:A:327:PX4:C27	12	1.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,6)	1:A:78:PHE:H	4:A:329:PX4:C27	12	1.38
(3,6)	1:A:78:PHE:H	4:A:331:PX4:C27	12	1.38
(3,6)	1:A:78:PHE:H	4:A:333:PX4:C27	12	1.38
(3,6)	1:A:78:PHE:H	4:A:335:PX4:C27	12	1.38
(3,6)	1:A:78:PHE:H	4:A:337:PX4:C27	12	1.38
(3,6)	1:A:78:PHE:H	4:A:339:PX4:C27	12	1.38
(3,6)	1:A:78:PHE:H	4:A:341:PX4:C27	12	1.38
(3,6)	1:A:78:PHE:H	4:A:343:PX4:C27	12	1.38
(3,6)	1:A:78:PHE:H	4:A:345:PX4:C27	12	1.38
(3,6)	1:A:78:PHE:H	4:A:347:PX4:C27	12	1.38
(3,6)	1:A:78:PHE:H	4:A:349:PX4:C27	12	1.38
(3,6)	1:A:78:PHE:H	4:A:351:PX4:C27	12	1.38
(3,6)	1:A:78:PHE:H	4:A:353:PX4:C27	12	1.38
(3,6)	1:A:78:PHE:H	4:A:355:PX4:C27	12	1.38
(3,6)	1:A:78:PHE:H	4:A:357:PX4:C27	12	1.38
(3,6)	1:A:78:PHE:H	4:A:359:PX4:C27	12	1.38
(3,6)	1:A:78:PHE:H	4:A:361:PX4:C27	12	1.38
(3,6)	1:A:78:PHE:H	4:A:363:PX4:C27	12	1.38
(3,6)	1:A:78:PHE:H	4:A:402:PX4:C27	12	1.38
(3,6)	1:A:78:PHE:H	4:A:404:PX4:C27	12	1.38
(3,6)	1:A:78:PHE:H	4:A:406:PX4:C27	12	1.38
(3,6)	1:A:78:PHE:H	4:A:408:PX4:C27	12	1.38
(3,6)	1:A:78:PHE:H	4:A:410:PX4:C27	12	1.38
(3,6)	1:A:78:PHE:H	4:A:412:PX4:C27	12	1.38
(3,6)	1:A:78:PHE:H	4:A:414:PX4:C27	12	1.38
(3,6)	1:A:78:PHE:H	4:A:416:PX4:C27	12	1.38
(3,6)	1:A:78:PHE:H	4:A:418:PX4:C27	12	1.38
(3,6)	1:A:78:PHE:H	4:A:420:PX4:C27	12	1.38
(3,6)	1:A:78:PHE:H	4:A:422:PX4:C27	12	1.38
(3,6)	1:A:78:PHE:H	4:A:424:PX4:C27	12	1.38
(3,6)	1:A:78:PHE:H	4:A:426:PX4:C27	12	1.38
(3,6)	1:A:78:PHE:H	4:A:428:PX4:C27	12	1.38
(3,6)	1:A:78:PHE:H	4:A:430:PX4:C27	12	1.38
(3,33)	1:A:155:THR:H	4:A:305:PX4:C35	10	1.38
(3,33)	1:A:155:THR:H	4:A:307:PX4:C35	10	1.38
(3,33)	1:A:155:THR:H	4:A:309:PX4:C35	10	1.38
(3,33)	1:A:155:THR:H	4:A:311:PX4:C35	10	1.38
(3,33)	1:A:155:THR:H	4:A:313:PX4:C35	10	1.38
(3,33)	1:A:155:THR:H	4:A:315:PX4:C35	10	1.38
(3,33)	1:A:155:THR:H	4:A:317:PX4:C35	10	1.38
(3,33)	1:A:155:THR:H	4:A:319:PX4:C35	10	1.38
(3,33)	1:A:155:THR:H	4:A:321:PX4:C35	10	1.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,33)	1:A:155:THR:H	4:A:323:PX4:C35	10	1.38
(3,33)	1:A:155:THR:H	4:A:325:PX4:C35	10	1.38
(3,33)	1:A:155:THR:H	4:A:327:PX4:C35	10	1.38
(3,33)	1:A:155:THR:H	4:A:329:PX4:C35	10	1.38
(3,33)	1:A:155:THR:H	4:A:331:PX4:C35	10	1.38
(3,33)	1:A:155:THR:H	4:A:333:PX4:C35	10	1.38
(3,33)	1:A:155:THR:H	4:A:335:PX4:C35	10	1.38
(3,33)	1:A:155:THR:H	4:A:337:PX4:C35	10	1.38
(3,33)	1:A:155:THR:H	4:A:339:PX4:C35	10	1.38
(3,33)	1:A:155:THR:H	4:A:341:PX4:C35	10	1.38
(3,33)	1:A:155:THR:H	4:A:343:PX4:C35	10	1.38
(3,33)	1:A:155:THR:H	4:A:345:PX4:C35	10	1.38
(3,33)	1:A:155:THR:H	4:A:347:PX4:C35	10	1.38
(3,33)	1:A:155:THR:H	4:A:349:PX4:C35	10	1.38
(3,33)	1:A:155:THR:H	4:A:351:PX4:C35	10	1.38
(3,33)	1:A:155:THR:H	4:A:353:PX4:C35	10	1.38
(3,33)	1:A:155:THR:H	4:A:355:PX4:C35	10	1.38
(3,33)	1:A:155:THR:H	4:A:357:PX4:C35	10	1.38
(3,33)	1:A:155:THR:H	4:A:359:PX4:C35	10	1.38
(3,33)	1:A:155:THR:H	4:A:361:PX4:C35	10	1.38
(3,33)	1:A:155:THR:H	4:A:363:PX4:C35	10	1.38
(3,33)	1:A:155:THR:H	4:A:402:PX4:C35	10	1.38
(3,33)	1:A:155:THR:H	4:A:404:PX4:C35	10	1.38
(3,33)	1:A:155:THR:H	4:A:406:PX4:C35	10	1.38
(3,33)	1:A:155:THR:H	4:A:408:PX4:C35	10	1.38
(3,33)	1:A:155:THR:H	4:A:410:PX4:C35	10	1.38
(3,33)	1:A:155:THR:H	4:A:412:PX4:C35	10	1.38
(3,33)	1:A:155:THR:H	4:A:414:PX4:C35	10	1.38
(3,33)	1:A:155:THR:H	4:A:416:PX4:C35	10	1.38
(3,33)	1:A:155:THR:H	4:A:418:PX4:C35	10	1.38
(3,33)	1:A:155:THR:H	4:A:420:PX4:C35	10	1.38
(3,33)	1:A:155:THR:H	4:A:422:PX4:C35	10	1.38
(3,33)	1:A:155:THR:H	4:A:424:PX4:C35	10	1.38
(3,33)	1:A:155:THR:H	4:A:426:PX4:C35	10	1.38
(3,33)	1:A:155:THR:H	4:A:428:PX4:C35	10	1.38
(3,33)	1:A:155:THR:H	4:A:430:PX4:C35	10	1.38
(2,940)	1:A:73:ALA:HB1	1:A:75:TYR:H	13	1.38
(2,940)	1:A:73:ALA:HB2	1:A:75:TYR:H	13	1.38
(2,940)	1:A:73:ALA:HB3	1:A:75:TYR:H	13	1.38
(2,932)	1:A:72:VAL:HG11	1:A:76:SER:H	12	1.38
(2,932)	1:A:72:VAL:HG12	1:A:76:SER:H	12	1.38
(2,932)	1:A:72:VAL:HG13	1:A:76:SER:H	12	1.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,928)	1:A:72:VAL:H	1:A:73:ALA:HB1	5	1.38
(2,729)	1:A:211:VAL:HG12	1:A:226:LEU:HD21	5	1.38
(2,542)	1:A:210:ALA:H	1:A:209:ASN:HD22	16	1.38
(2,473)	1:A:186:ILE:H	1:A:156:LEU:HD22	11	1.38
(2,473)	1:A:186:ILE:H	1:A:156:LEU:HD23	11	1.38
(3,33)	1:A:155:THR:H	4:A:305:PX4:C35	1	1.37
(3,33)	1:A:155:THR:H	4:A:307:PX4:C35	1	1.37
(3,33)	1:A:155:THR:H	4:A:309:PX4:C35	1	1.37
(3,33)	1:A:155:THR:H	4:A:311:PX4:C35	1	1.37
(3,33)	1:A:155:THR:H	4:A:313:PX4:C35	1	1.37
(3,33)	1:A:155:THR:H	4:A:315:PX4:C35	1	1.37
(3,33)	1:A:155:THR:H	4:A:317:PX4:C35	1	1.37
(3,33)	1:A:155:THR:H	4:A:319:PX4:C35	1	1.37
(3,33)	1:A:155:THR:H	4:A:321:PX4:C35	1	1.37
(3,33)	1:A:155:THR:H	4:A:323:PX4:C35	1	1.37
(3,33)	1:A:155:THR:H	4:A:325:PX4:C35	1	1.37
(3,33)	1:A:155:THR:H	4:A:327:PX4:C35	1	1.37
(3,33)	1:A:155:THR:H	4:A:329:PX4:C35	1	1.37
(3,33)	1:A:155:THR:H	4:A:331:PX4:C35	1	1.37
(3,33)	1:A:155:THR:H	4:A:333:PX4:C35	1	1.37
(3,33)	1:A:155:THR:H	4:A:335:PX4:C35	1	1.37
(3,33)	1:A:155:THR:H	4:A:337:PX4:C35	1	1.37
(3,33)	1:A:155:THR:H	4:A:339:PX4:C35	1	1.37
(3,33)	1:A:155:THR:H	4:A:341:PX4:C35	1	1.37
(3,33)	1:A:155:THR:H	4:A:343:PX4:C35	1	1.37
(3,33)	1:A:155:THR:H	4:A:345:PX4:C35	1	1.37
(3,33)	1:A:155:THR:H	4:A:347:PX4:C35	1	1.37
(3,33)	1:A:155:THR:H	4:A:349:PX4:C35	1	1.37
(3,33)	1:A:155:THR:H	4:A:351:PX4:C35	1	1.37
(3,33)	1:A:155:THR:H	4:A:353:PX4:C35	1	1.37
(3,33)	1:A:155:THR:H	4:A:355:PX4:C35	1	1.37
(3,33)	1:A:155:THR:H	4:A:357:PX4:C35	1	1.37
(3,33)	1:A:155:THR:H	4:A:359:PX4:C35	1	1.37
(3,33)	1:A:155:THR:H	4:A:361:PX4:C35	1	1.37
(3,33)	1:A:155:THR:H	4:A:363:PX4:C35	1	1.37
(3,33)	1:A:155:THR:H	4:A:402:PX4:C35	1	1.37
(3,33)	1:A:155:THR:H	4:A:404:PX4:C35	1	1.37
(3,33)	1:A:155:THR:H	4:A:406:PX4:C35	1	1.37
(3,33)	1:A:155:THR:H	4:A:408:PX4:C35	1	1.37
(3,33)	1:A:155:THR:H	4:A:410:PX4:C35	1	1.37
(3,33)	1:A:155:THR:H	4:A:412:PX4:C35	1	1.37
(3,33)	1:A:155:THR:H	4:A:414:PX4:C35	1	1.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,33)	1:A:155:THR:H	4:A:416:PX4:C35	1	1.37
(3,33)	1:A:155:THR:H	4:A:418:PX4:C35	1	1.37
(3,33)	1:A:155:THR:H	4:A:420:PX4:C35	1	1.37
(3,33)	1:A:155:THR:H	4:A:422:PX4:C35	1	1.37
(3,33)	1:A:155:THR:H	4:A:424:PX4:C35	1	1.37
(3,33)	1:A:155:THR:H	4:A:426:PX4:C35	1	1.37
(3,33)	1:A:155:THR:H	4:A:428:PX4:C35	1	1.37
(3,33)	1:A:155:THR:H	4:A:430:PX4:C35	1	1.37
(2,948)	1:A:74:GLU:HG3	1:A:75:TYR:H	1	1.37
(2,948)	1:A:74:GLU:HG3	1:A:75:TYR:H	1	1.37
(2,861)	1:A:186:ILE:HD13	1:A:156:LEU:HD21	8	1.37
(2,732)	1:A:211:VAL:HG13	1:A:226:LEU:HD22	5	1.37
(2,732)	1:A:211:VAL:HG13	1:A:226:LEU:HD23	5	1.37
(2,542)	1:A:210:ALA:H	1:A:209:ASN:HD22	12	1.37
(3,33)	1:A:155:THR:H	4:A:305:PX4:C35	20	1.36
(3,33)	1:A:155:THR:H	4:A:307:PX4:C35	20	1.36
(3,33)	1:A:155:THR:H	4:A:309:PX4:C35	20	1.36
(3,33)	1:A:155:THR:H	4:A:311:PX4:C35	20	1.36
(3,33)	1:A:155:THR:H	4:A:313:PX4:C35	20	1.36
(3,33)	1:A:155:THR:H	4:A:315:PX4:C35	20	1.36
(3,33)	1:A:155:THR:H	4:A:317:PX4:C35	20	1.36
(3,33)	1:A:155:THR:H	4:A:319:PX4:C35	20	1.36
(3,33)	1:A:155:THR:H	4:A:321:PX4:C35	20	1.36
(3,33)	1:A:155:THR:H	4:A:323:PX4:C35	20	1.36
(3,33)	1:A:155:THR:H	4:A:325:PX4:C35	20	1.36
(3,33)	1:A:155:THR:H	4:A:327:PX4:C35	20	1.36
(3,33)	1:A:155:THR:H	4:A:329:PX4:C35	20	1.36
(3,33)	1:A:155:THR:H	4:A:331:PX4:C35	20	1.36
(3,33)	1:A:155:THR:H	4:A:333:PX4:C35	20	1.36
(3,33)	1:A:155:THR:H	4:A:335:PX4:C35	20	1.36
(3,33)	1:A:155:THR:H	4:A:337:PX4:C35	20	1.36
(3,33)	1:A:155:THR:H	4:A:339:PX4:C35	20	1.36
(3,33)	1:A:155:THR:H	4:A:341:PX4:C35	20	1.36
(3,33)	1:A:155:THR:H	4:A:343:PX4:C35	20	1.36
(3,33)	1:A:155:THR:H	4:A:345:PX4:C35	20	1.36
(3,33)	1:A:155:THR:H	4:A:347:PX4:C35	20	1.36
(3,33)	1:A:155:THR:H	4:A:349:PX4:C35	20	1.36
(3,33)	1:A:155:THR:H	4:A:351:PX4:C35	20	1.36
(3,33)	1:A:155:THR:H	4:A:353:PX4:C35	20	1.36
(3,33)	1:A:155:THR:H	4:A:355:PX4:C35	20	1.36
(3,33)	1:A:155:THR:H	4:A:357:PX4:C35	20	1.36
(3,33)	1:A:155:THR:H	4:A:359:PX4:C35	20	1.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,33)	1:A:155:THR:H	4:A:361:PX4:C35	20	1.36
(3,33)	1:A:155:THR:H	4:A:363:PX4:C35	20	1.36
(3,33)	1:A:155:THR:H	4:A:402:PX4:C35	20	1.36
(3,33)	1:A:155:THR:H	4:A:404:PX4:C35	20	1.36
(3,33)	1:A:155:THR:H	4:A:406:PX4:C35	20	1.36
(3,33)	1:A:155:THR:H	4:A:408:PX4:C35	20	1.36
(3,33)	1:A:155:THR:H	4:A:410:PX4:C35	20	1.36
(3,33)	1:A:155:THR:H	4:A:412:PX4:C35	20	1.36
(3,33)	1:A:155:THR:H	4:A:414:PX4:C35	20	1.36
(3,33)	1:A:155:THR:H	4:A:416:PX4:C35	20	1.36
(3,33)	1:A:155:THR:H	4:A:418:PX4:C35	20	1.36
(3,33)	1:A:155:THR:H	4:A:420:PX4:C35	20	1.36
(3,33)	1:A:155:THR:H	4:A:422:PX4:C35	20	1.36
(3,33)	1:A:155:THR:H	4:A:424:PX4:C35	20	1.36
(3,33)	1:A:155:THR:H	4:A:426:PX4:C35	20	1.36
(3,33)	1:A:155:THR:H	4:A:428:PX4:C35	20	1.36
(3,33)	1:A:155:THR:H	4:A:430:PX4:C35	20	1.36
(2,981)	1:A:78:PHE:H	1:A:79:PRO:HG3	1	1.36
(2,981)	1:A:78:PHE:H	1:A:79:PRO:HG3	1	1.36
(2,948)	1:A:74:GLU:HG3	1:A:75:TYR:H	3	1.36
(2,948)	1:A:74:GLU:HG3	1:A:75:TYR:H	3	1.36
(2,948)	1:A:74:GLU:HG3	1:A:75:TYR:H	14	1.36
(2,948)	1:A:74:GLU:HG3	1:A:75:TYR:H	14	1.36
(2,902)	1:A:66:ARG:HA	1:A:68:GLY:H	13	1.36
(2,727)	1:A:211:VAL:HG11	1:A:226:LEU:HD21	4	1.36
(2,516)	1:A:200:LEU:H	1:A:196:LEU:HD11	9	1.36
(2,516)	1:A:200:LEU:H	1:A:196:LEU:HD12	9	1.36
(2,516)	1:A:200:LEU:H	1:A:196:LEU:HD13	9	1.36
(2,981)	1:A:78:PHE:H	1:A:79:PRO:HG3	5	1.35
(2,981)	1:A:78:PHE:H	1:A:79:PRO:HG3	5	1.35
(2,981)	1:A:78:PHE:H	1:A:79:PRO:HG3	14	1.35
(2,981)	1:A:78:PHE:H	1:A:79:PRO:HG3	14	1.35
(2,974)	1:A:78:PHE:H	1:A:77:LEU:HD21	3	1.35
(2,954)	1:A:74:GLU:HB3	1:A:77:LEU:H	13	1.35
(2,954)	1:A:74:GLU:HB3	1:A:77:LEU:H	13	1.35
(2,940)	1:A:73:ALA:HB1	1:A:75:TYR:H	20	1.35
(2,940)	1:A:73:ALA:HB2	1:A:75:TYR:H	20	1.35
(2,940)	1:A:73:ALA:HB3	1:A:75:TYR:H	20	1.35
(2,759)	1:A:54:LEU:HD21	1:A:59:ILE:HD11	2	1.35
(2,759)	1:A:54:LEU:HD21	1:A:59:ILE:HD12	2	1.35
(2,759)	1:A:54:LEU:HD21	1:A:59:ILE:HD13	2	1.35
(2,178)	1:A:171:HIS:H	1:A:69:VAL:HG11	3	1.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,178)	1:A:171:HIS:H	1:A:69:VAL:HG12	3	1.35
(2,178)	1:A:171:HIS:H	1:A:69:VAL:HG13	3	1.35
(3,21)	1:A:77:LEU:H	4:A:305:PX4:C35	5	1.34
(3,21)	1:A:77:LEU:H	4:A:307:PX4:C35	5	1.34
(3,21)	1:A:77:LEU:H	4:A:309:PX4:C35	5	1.34
(3,21)	1:A:77:LEU:H	4:A:311:PX4:C35	5	1.34
(3,21)	1:A:77:LEU:H	4:A:313:PX4:C35	5	1.34
(3,21)	1:A:77:LEU:H	4:A:315:PX4:C35	5	1.34
(3,21)	1:A:77:LEU:H	4:A:317:PX4:C35	5	1.34
(3,21)	1:A:77:LEU:H	4:A:319:PX4:C35	5	1.34
(3,21)	1:A:77:LEU:H	4:A:321:PX4:C35	5	1.34
(3,21)	1:A:77:LEU:H	4:A:323:PX4:C35	5	1.34
(3,21)	1:A:77:LEU:H	4:A:325:PX4:C35	5	1.34
(3,21)	1:A:77:LEU:H	4:A:327:PX4:C35	5	1.34
(3,21)	1:A:77:LEU:H	4:A:329:PX4:C35	5	1.34
(3,21)	1:A:77:LEU:H	4:A:331:PX4:C35	5	1.34
(3,21)	1:A:77:LEU:H	4:A:333:PX4:C35	5	1.34
(3,21)	1:A:77:LEU:H	4:A:335:PX4:C35	5	1.34
(3,21)	1:A:77:LEU:H	4:A:337:PX4:C35	5	1.34
(3,21)	1:A:77:LEU:H	4:A:339:PX4:C35	5	1.34
(3,21)	1:A:77:LEU:H	4:A:341:PX4:C35	5	1.34
(3,21)	1:A:77:LEU:H	4:A:343:PX4:C35	5	1.34
(3,21)	1:A:77:LEU:H	4:A:345:PX4:C35	5	1.34
(3,21)	1:A:77:LEU:H	4:A:347:PX4:C35	5	1.34
(3,21)	1:A:77:LEU:H	4:A:349:PX4:C35	5	1.34
(3,21)	1:A:77:LEU:H	4:A:351:PX4:C35	5	1.34
(3,21)	1:A:77:LEU:H	4:A:353:PX4:C35	5	1.34
(3,21)	1:A:77:LEU:H	4:A:355:PX4:C35	5	1.34
(3,21)	1:A:77:LEU:H	4:A:357:PX4:C35	5	1.34
(3,21)	1:A:77:LEU:H	4:A:359:PX4:C35	5	1.34
(3,21)	1:A:77:LEU:H	4:A:361:PX4:C35	5	1.34
(3,21)	1:A:77:LEU:H	4:A:363:PX4:C35	5	1.34
(3,21)	1:A:77:LEU:H	4:A:402:PX4:C35	5	1.34
(3,21)	1:A:77:LEU:H	4:A:404:PX4:C35	5	1.34
(3,21)	1:A:77:LEU:H	4:A:406:PX4:C35	5	1.34
(3,21)	1:A:77:LEU:H	4:A:408:PX4:C35	5	1.34
(3,21)	1:A:77:LEU:H	4:A:410:PX4:C35	5	1.34
(3,21)	1:A:77:LEU:H	4:A:412:PX4:C35	5	1.34
(3,21)	1:A:77:LEU:H	4:A:414:PX4:C35	5	1.34
(3,21)	1:A:77:LEU:H	4:A:416:PX4:C35	5	1.34
(3,21)	1:A:77:LEU:H	4:A:418:PX4:C35	5	1.34
(3,21)	1:A:77:LEU:H	4:A:420:PX4:C35	5	1.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,21)	1:A:77:LEU:H	4:A:422:PX4:C35	5	1.34
(3,21)	1:A:77:LEU:H	4:A:424:PX4:C35	5	1.34
(3,21)	1:A:77:LEU:H	4:A:426:PX4:C35	5	1.34
(3,21)	1:A:77:LEU:H	4:A:428:PX4:C35	5	1.34
(3,21)	1:A:77:LEU:H	4:A:430:PX4:C35	5	1.34
(2,974)	1:A:78:PHE:H	1:A:77:LEU:HD21	11	1.34
(2,940)	1:A:73:ALA:HB1	1:A:75:TYR:H	2	1.34
(2,940)	1:A:73:ALA:HB2	1:A:75:TYR:H	2	1.34
(2,940)	1:A:73:ALA:HB3	1:A:75:TYR:H	2	1.34
(2,940)	1:A:73:ALA:HB1	1:A:75:TYR:H	14	1.34
(2,940)	1:A:73:ALA:HB2	1:A:75:TYR:H	14	1.34
(2,940)	1:A:73:ALA:HB3	1:A:75:TYR:H	14	1.34
(2,932)	1:A:72:VAL:HG11	1:A:76:SER:H	18	1.34
(2,932)	1:A:72:VAL:HG12	1:A:76:SER:H	18	1.34
(2,932)	1:A:72:VAL:HG13	1:A:76:SER:H	18	1.34
(2,902)	1:A:66:ARG:HA	1:A:68:GLY:H	10	1.34
(2,766)	1:A:22:PHE:H	1:A:19:LEU:HD22	4	1.34
(2,766)	1:A:22:PHE:H	1:A:19:LEU:HD23	4	1.34
(2,656)	1:A:39:LEU:H	1:A:19:LEU:HD21	2	1.34
(2,542)	1:A:210:ALA:H	1:A:209:ASN:HD22	14	1.34
(2,466)	1:A:84:TRP:H	1:A:200:LEU:HD21	20	1.34
(3,6)	1:A:78:PHE:H	4:A:305:PX4:C27	10	1.33
(3,6)	1:A:78:PHE:H	4:A:307:PX4:C27	10	1.33
(3,6)	1:A:78:PHE:H	4:A:309:PX4:C27	10	1.33
(3,6)	1:A:78:PHE:H	4:A:311:PX4:C27	10	1.33
(3,6)	1:A:78:PHE:H	4:A:313:PX4:C27	10	1.33
(3,6)	1:A:78:PHE:H	4:A:315:PX4:C27	10	1.33
(3,6)	1:A:78:PHE:H	4:A:317:PX4:C27	10	1.33
(3,6)	1:A:78:PHE:H	4:A:319:PX4:C27	10	1.33
(3,6)	1:A:78:PHE:H	4:A:321:PX4:C27	10	1.33
(3,6)	1:A:78:PHE:H	4:A:323:PX4:C27	10	1.33
(3,6)	1:A:78:PHE:H	4:A:325:PX4:C27	10	1.33
(3,6)	1:A:78:PHE:H	4:A:327:PX4:C27	10	1.33
(3,6)	1:A:78:PHE:H	4:A:329:PX4:C27	10	1.33
(3,6)	1:A:78:PHE:H	4:A:331:PX4:C27	10	1.33
(3,6)	1:A:78:PHE:H	4:A:333:PX4:C27	10	1.33
(3,6)	1:A:78:PHE:H	4:A:335:PX4:C27	10	1.33
(3,6)	1:A:78:PHE:H	4:A:337:PX4:C27	10	1.33
(3,6)	1:A:78:PHE:H	4:A:339:PX4:C27	10	1.33
(3,6)	1:A:78:PHE:H	4:A:341:PX4:C27	10	1.33
(3,6)	1:A:78:PHE:H	4:A:343:PX4:C27	10	1.33
(3,6)	1:A:78:PHE:H	4:A:345:PX4:C27	10	1.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,6)	1:A:78:PHE:H	4:A:347:PX4:C27	10	1.33
(3,6)	1:A:78:PHE:H	4:A:349:PX4:C27	10	1.33
(3,6)	1:A:78:PHE:H	4:A:351:PX4:C27	10	1.33
(3,6)	1:A:78:PHE:H	4:A:353:PX4:C27	10	1.33
(3,6)	1:A:78:PHE:H	4:A:355:PX4:C27	10	1.33
(3,6)	1:A:78:PHE:H	4:A:357:PX4:C27	10	1.33
(3,6)	1:A:78:PHE:H	4:A:359:PX4:C27	10	1.33
(3,6)	1:A:78:PHE:H	4:A:361:PX4:C27	10	1.33
(3,6)	1:A:78:PHE:H	4:A:363:PX4:C27	10	1.33
(3,6)	1:A:78:PHE:H	4:A:402:PX4:C27	10	1.33
(3,6)	1:A:78:PHE:H	4:A:404:PX4:C27	10	1.33
(3,6)	1:A:78:PHE:H	4:A:406:PX4:C27	10	1.33
(3,6)	1:A:78:PHE:H	4:A:408:PX4:C27	10	1.33
(3,6)	1:A:78:PHE:H	4:A:410:PX4:C27	10	1.33
(3,6)	1:A:78:PHE:H	4:A:412:PX4:C27	10	1.33
(3,6)	1:A:78:PHE:H	4:A:414:PX4:C27	10	1.33
(3,6)	1:A:78:PHE:H	4:A:416:PX4:C27	10	1.33
(3,6)	1:A:78:PHE:H	4:A:418:PX4:C27	10	1.33
(3,6)	1:A:78:PHE:H	4:A:420:PX4:C27	10	1.33
(3,6)	1:A:78:PHE:H	4:A:422:PX4:C27	10	1.33
(3,6)	1:A:78:PHE:H	4:A:424:PX4:C27	10	1.33
(3,6)	1:A:78:PHE:H	4:A:426:PX4:C27	10	1.33
(3,6)	1:A:78:PHE:H	4:A:428:PX4:C27	10	1.33
(3,6)	1:A:78:PHE:H	4:A:430:PX4:C27	10	1.33
(2,981)	1:A:78:PHE:H	1:A:79:PRO:HG3	4	1.33
(2,981)	1:A:78:PHE:H	1:A:79:PRO:HG3	4	1.33
(2,948)	1:A:74:GLU:HG3	1:A:75:TYR:H	8	1.33
(2,948)	1:A:74:GLU:HG3	1:A:75:TYR:H	8	1.33
(2,773)	1:A:61:ILE:HD11	1:A:48:LEU:HD21	13	1.33
(2,510)	1:A:200:LEU:HD21	1:A:199:SER:H	16	1.33
(2,954)	1:A:74:GLU:HB3	1:A:77:LEU:H	10	1.32
(2,954)	1:A:74:GLU:HB3	1:A:77:LEU:H	10	1.32
(2,940)	1:A:73:ALA:HB1	1:A:75:TYR:H	19	1.32
(2,940)	1:A:73:ALA:HB2	1:A:75:TYR:H	19	1.32
(2,940)	1:A:73:ALA:HB3	1:A:75:TYR:H	19	1.32
(2,879)	1:A:234:ILE:HD11	1:A:200:LEU:HB2	4	1.32
(2,879)	1:A:234:ILE:HD12	1:A:200:LEU:HB2	4	1.32
(2,879)	1:A:234:ILE:HD13	1:A:200:LEU:HB2	4	1.32
(2,834)	1:A:120:ILE:HD12	1:A:200:LEU:HD21	19	1.32
(2,758)	1:A:54:LEU:HD22	1:A:39:LEU:HD11	13	1.32
(2,758)	1:A:54:LEU:HD22	1:A:39:LEU:HD12	13	1.32
(2,758)	1:A:54:LEU:HD22	1:A:39:LEU:HD13	13	1.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,758)	1:A:54:LEU:HD23	1:A:39:LEU:HD11	13	1.32
(2,758)	1:A:54:LEU:HD23	1:A:39:LEU:HD12	13	1.32
(2,758)	1:A:54:LEU:HD23	1:A:39:LEU:HD13	13	1.32
(2,727)	1:A:211:VAL:HG11	1:A:226:LEU:HD21	12	1.32
(2,392)	1:A:157:ALA:H	1:A:68:GLY:H	18	1.32
(3,36)	1:A:129:TRP:HE1	4:A:305:PX4:N1	10	1.31
(3,36)	1:A:129:TRP:HE1	4:A:307:PX4:N1	10	1.31
(3,36)	1:A:129:TRP:HE1	4:A:309:PX4:N1	10	1.31
(3,36)	1:A:129:TRP:HE1	4:A:311:PX4:N1	10	1.31
(3,36)	1:A:129:TRP:HE1	4:A:313:PX4:N1	10	1.31
(3,36)	1:A:129:TRP:HE1	4:A:315:PX4:N1	10	1.31
(3,36)	1:A:129:TRP:HE1	4:A:317:PX4:N1	10	1.31
(3,36)	1:A:129:TRP:HE1	4:A:319:PX4:N1	10	1.31
(3,36)	1:A:129:TRP:HE1	4:A:321:PX4:N1	10	1.31
(3,36)	1:A:129:TRP:HE1	4:A:323:PX4:N1	10	1.31
(3,36)	1:A:129:TRP:HE1	4:A:325:PX4:N1	10	1.31
(3,36)	1:A:129:TRP:HE1	4:A:327:PX4:N1	10	1.31
(3,36)	1:A:129:TRP:HE1	4:A:329:PX4:N1	10	1.31
(3,36)	1:A:129:TRP:HE1	4:A:331:PX4:N1	10	1.31
(3,36)	1:A:129:TRP:HE1	4:A:333:PX4:N1	10	1.31
(3,36)	1:A:129:TRP:HE1	4:A:335:PX4:N1	10	1.31
(3,36)	1:A:129:TRP:HE1	4:A:337:PX4:N1	10	1.31
(3,36)	1:A:129:TRP:HE1	4:A:339:PX4:N1	10	1.31
(3,36)	1:A:129:TRP:HE1	4:A:341:PX4:N1	10	1.31
(3,36)	1:A:129:TRP:HE1	4:A:343:PX4:N1	10	1.31
(3,36)	1:A:129:TRP:HE1	4:A:345:PX4:N1	10	1.31
(3,36)	1:A:129:TRP:HE1	4:A:347:PX4:N1	10	1.31
(3,36)	1:A:129:TRP:HE1	4:A:349:PX4:N1	10	1.31
(3,36)	1:A:129:TRP:HE1	4:A:351:PX4:N1	10	1.31
(3,36)	1:A:129:TRP:HE1	4:A:353:PX4:N1	10	1.31
(3,36)	1:A:129:TRP:HE1	4:A:355:PX4:N1	10	1.31
(3,36)	1:A:129:TRP:HE1	4:A:357:PX4:N1	10	1.31
(3,36)	1:A:129:TRP:HE1	4:A:359:PX4:N1	10	1.31
(3,36)	1:A:129:TRP:HE1	4:A:361:PX4:N1	10	1.31
(3,36)	1:A:129:TRP:HE1	4:A:363:PX4:N1	10	1.31
(3,36)	1:A:129:TRP:HE1	4:A:402:PX4:N1	10	1.31
(3,36)	1:A:129:TRP:HE1	4:A:404:PX4:N1	10	1.31
(3,36)	1:A:129:TRP:HE1	4:A:406:PX4:N1	10	1.31
(3,36)	1:A:129:TRP:HE1	4:A:408:PX4:N1	10	1.31
(3,36)	1:A:129:TRP:HE1	4:A:410:PX4:N1	10	1.31
(3,36)	1:A:129:TRP:HE1	4:A:412:PX4:N1	10	1.31
(3,36)	1:A:129:TRP:HE1	4:A:414:PX4:N1	10	1.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,36)	1:A:129:TRP:HE1	4:A:416:PX4:N1	10	1.31
(3,36)	1:A:129:TRP:HE1	4:A:418:PX4:N1	10	1.31
(3,36)	1:A:129:TRP:HE1	4:A:420:PX4:N1	10	1.31
(3,36)	1:A:129:TRP:HE1	4:A:422:PX4:N1	10	1.31
(3,36)	1:A:129:TRP:HE1	4:A:424:PX4:N1	10	1.31
(3,36)	1:A:129:TRP:HE1	4:A:426:PX4:N1	10	1.31
(3,36)	1:A:129:TRP:HE1	4:A:428:PX4:N1	10	1.31
(3,36)	1:A:129:TRP:HE1	4:A:430:PX4:N1	10	1.31
(3,33)	1:A:155:THR:H	4:A:305:PX4:C35	5	1.31
(3,33)	1:A:155:THR:H	4:A:307:PX4:C35	5	1.31
(3,33)	1:A:155:THR:H	4:A:309:PX4:C35	5	1.31
(3,33)	1:A:155:THR:H	4:A:311:PX4:C35	5	1.31
(3,33)	1:A:155:THR:H	4:A:313:PX4:C35	5	1.31
(3,33)	1:A:155:THR:H	4:A:315:PX4:C35	5	1.31
(3,33)	1:A:155:THR:H	4:A:317:PX4:C35	5	1.31
(3,33)	1:A:155:THR:H	4:A:319:PX4:C35	5	1.31
(3,33)	1:A:155:THR:H	4:A:321:PX4:C35	5	1.31
(3,33)	1:A:155:THR:H	4:A:323:PX4:C35	5	1.31
(3,33)	1:A:155:THR:H	4:A:325:PX4:C35	5	1.31
(3,33)	1:A:155:THR:H	4:A:327:PX4:C35	5	1.31
(3,33)	1:A:155:THR:H	4:A:329:PX4:C35	5	1.31
(3,33)	1:A:155:THR:H	4:A:331:PX4:C35	5	1.31
(3,33)	1:A:155:THR:H	4:A:333:PX4:C35	5	1.31
(3,33)	1:A:155:THR:H	4:A:335:PX4:C35	5	1.31
(3,33)	1:A:155:THR:H	4:A:337:PX4:C35	5	1.31
(3,33)	1:A:155:THR:H	4:A:339:PX4:C35	5	1.31
(3,33)	1:A:155:THR:H	4:A:341:PX4:C35	5	1.31
(3,33)	1:A:155:THR:H	4:A:343:PX4:C35	5	1.31
(3,33)	1:A:155:THR:H	4:A:345:PX4:C35	5	1.31
(3,33)	1:A:155:THR:H	4:A:347:PX4:C35	5	1.31
(3,33)	1:A:155:THR:H	4:A:349:PX4:C35	5	1.31
(3,33)	1:A:155:THR:H	4:A:351:PX4:C35	5	1.31
(3,33)	1:A:155:THR:H	4:A:353:PX4:C35	5	1.31
(3,33)	1:A:155:THR:H	4:A:355:PX4:C35	5	1.31
(3,33)	1:A:155:THR:H	4:A:357:PX4:C35	5	1.31
(3,33)	1:A:155:THR:H	4:A:359:PX4:C35	5	1.31
(3,33)	1:A:155:THR:H	4:A:361:PX4:C35	5	1.31
(3,33)	1:A:155:THR:H	4:A:363:PX4:C35	5	1.31
(3,33)	1:A:155:THR:H	4:A:402:PX4:C35	5	1.31
(3,33)	1:A:155:THR:H	4:A:404:PX4:C35	5	1.31
(3,33)	1:A:155:THR:H	4:A:406:PX4:C35	5	1.31
(3,33)	1:A:155:THR:H	4:A:408:PX4:C35	5	1.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,33)	1:A:155:THR:H	4:A:410:PX4:C35	5	1.31
(3,33)	1:A:155:THR:H	4:A:412:PX4:C35	5	1.31
(3,33)	1:A:155:THR:H	4:A:414:PX4:C35	5	1.31
(3,33)	1:A:155:THR:H	4:A:416:PX4:C35	5	1.31
(3,33)	1:A:155:THR:H	4:A:418:PX4:C35	5	1.31
(3,33)	1:A:155:THR:H	4:A:420:PX4:C35	5	1.31
(3,33)	1:A:155:THR:H	4:A:422:PX4:C35	5	1.31
(3,33)	1:A:155:THR:H	4:A:424:PX4:C35	5	1.31
(3,33)	1:A:155:THR:H	4:A:426:PX4:C35	5	1.31
(3,33)	1:A:155:THR:H	4:A:428:PX4:C35	5	1.31
(3,33)	1:A:155:THR:H	4:A:430:PX4:C35	5	1.31
(2,879)	1:A:234:ILE:HD11	1:A:200:LEU:HB2	5	1.31
(2,879)	1:A:234:ILE:HD12	1:A:200:LEU:HB2	5	1.31
(2,879)	1:A:234:ILE:HD13	1:A:200:LEU:HB2	5	1.31
(2,835)	1:A:120:ILE:HD12	1:A:200:LEU:HD22	10	1.31
(2,835)	1:A:120:ILE:HD12	1:A:200:LEU:HD23	10	1.31
(2,750)	1:A:89:VAL:HG13	1:A:122:LEU:HD21	12	1.31
(2,264)	1:A:113:LEU:H	1:A:196:LEU:HD21	14	1.31
(2,229)	1:A:106:ASP:H	1:A:109:VAL:H	11	1.31
(2,954)	1:A:74:GLU:HB3	1:A:77:LEU:H	15	1.3
(2,954)	1:A:74:GLU:HB3	1:A:77:LEU:H	15	1.3
(2,940)	1:A:73:ALA:HB1	1:A:75:TYR:H	7	1.3
(2,940)	1:A:73:ALA:HB2	1:A:75:TYR:H	7	1.3
(2,940)	1:A:73:ALA:HB3	1:A:75:TYR:H	7	1.3
(2,728)	1:A:211:VAL:HG11	1:A:226:LEU:HD22	6	1.3
(2,728)	1:A:211:VAL:HG11	1:A:226:LEU:HD23	6	1.3
(2,598)	1:A:235:GLN:H	1:A:238:TYR:HE1	2	1.3
(2,598)	1:A:235:GLN:H	1:A:238:TYR:HE2	2	1.3
(2,981)	1:A:78:PHE:H	1:A:79:PRO:HG3	16	1.29
(2,981)	1:A:78:PHE:H	1:A:79:PRO:HG3	16	1.29
(2,970)	1:A:77:LEU:HG	1:A:78:PHE:H	2	1.29
(2,940)	1:A:73:ALA:HB1	1:A:75:TYR:H	11	1.29
(2,940)	1:A:73:ALA:HB2	1:A:75:TYR:H	11	1.29
(2,940)	1:A:73:ALA:HB3	1:A:75:TYR:H	11	1.29
(2,902)	1:A:66:ARG:HA	1:A:68:GLY:H	19	1.29
(2,837)	1:A:120:ILE:HD13	1:A:200:LEU:HD22	15	1.29
(2,837)	1:A:120:ILE:HD13	1:A:200:LEU:HD23	15	1.29
(2,774)	1:A:61:ILE:HD11	1:A:48:LEU:HD22	16	1.29
(2,774)	1:A:61:ILE:HD11	1:A:48:LEU:HD23	16	1.29
(2,773)	1:A:61:ILE:HD11	1:A:48:LEU:HD21	4	1.29
(2,598)	1:A:235:GLN:H	1:A:238:TYR:HE1	17	1.29
(2,598)	1:A:235:GLN:H	1:A:238:TYR:HE2	17	1.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,472)	1:A:186:ILE:H	1:A:156:LEU:HD21	16	1.29
(2,466)	1:A:84:TRP:H	1:A:200:LEU:HD21	4	1.29
(2,982)	1:A:78:PHE:HD1	1:A:80:ASN:H	1	1.28
(2,948)	1:A:74:GLU:HG3	1:A:75:TYR:H	4	1.28
(2,948)	1:A:74:GLU:HG3	1:A:75:TYR:H	4	1.28
(2,948)	1:A:74:GLU:HG3	1:A:75:TYR:H	13	1.28
(2,948)	1:A:74:GLU:HG3	1:A:75:TYR:H	13	1.28
(2,902)	1:A:66:ARG:HA	1:A:68:GLY:H	2	1.28
(2,867)	1:A:186:ILE:HD11	1:A:156:LEU:HD21	8	1.28
(2,473)	1:A:186:ILE:H	1:A:156:LEU:HD22	9	1.28
(2,473)	1:A:186:ILE:H	1:A:156:LEU:HD23	9	1.28
(2,928)	1:A:72:VAL:H	1:A:73:ALA:HB1	11	1.27
(2,879)	1:A:234:ILE:HD11	1:A:200:LEU:HB2	20	1.27
(2,879)	1:A:234:ILE:HD12	1:A:200:LEU:HB2	20	1.27
(2,879)	1:A:234:ILE:HD13	1:A:200:LEU:HB2	20	1.27
(2,424)	1:A:169:ASP:H	1:A:166:LEU:HB3	18	1.27
(2,988)	1:A:129:TRP:HE1	4:A:305:PX4:C2	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:307:PX4:C2	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:309:PX4:C2	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:311:PX4:C2	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:313:PX4:C2	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:315:PX4:C2	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:317:PX4:C2	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:319:PX4:C2	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:321:PX4:C2	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:323:PX4:C2	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:325:PX4:C2	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:327:PX4:C2	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:329:PX4:C2	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:331:PX4:C2	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:333:PX4:C2	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:335:PX4:C2	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:337:PX4:C2	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:339:PX4:C2	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:341:PX4:C2	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:343:PX4:C2	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:345:PX4:C2	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:347:PX4:C2	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:349:PX4:C2	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:351:PX4:C2	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:353:PX4:C2	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:355:PX4:C2	19	1.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,988)	1:A:129:TRP:HE1	4:A:357:PX4:C2	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:359:PX4:C2	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:361:PX4:C2	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:363:PX4:C2	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:402:PX4:C2	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:404:PX4:C2	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:406:PX4:C2	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:408:PX4:C2	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:410:PX4:C2	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:412:PX4:C2	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:414:PX4:C2	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:416:PX4:C2	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:418:PX4:C2	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:420:PX4:C2	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:422:PX4:C2	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:424:PX4:C2	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:426:PX4:C2	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:428:PX4:C2	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:430:PX4:C2	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:305:PX4:C1	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:307:PX4:C1	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:309:PX4:C1	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:311:PX4:C1	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:313:PX4:C1	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:315:PX4:C1	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:317:PX4:C1	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:319:PX4:C1	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:321:PX4:C1	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:323:PX4:C1	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:325:PX4:C1	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:327:PX4:C1	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:329:PX4:C1	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:331:PX4:C1	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:333:PX4:C1	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:335:PX4:C1	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:337:PX4:C1	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:339:PX4:C1	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:341:PX4:C1	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:343:PX4:C1	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:345:PX4:C1	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:347:PX4:C1	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:349:PX4:C1	19	1.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,988)	1:A:129:TRP:HE1	4:A:351:PX4:C1	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:353:PX4:C1	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:355:PX4:C1	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:357:PX4:C1	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:359:PX4:C1	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:361:PX4:C1	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:363:PX4:C1	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:402:PX4:C1	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:404:PX4:C1	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:406:PX4:C1	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:408:PX4:C1	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:410:PX4:C1	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:412:PX4:C1	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:414:PX4:C1	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:416:PX4:C1	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:418:PX4:C1	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:420:PX4:C1	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:422:PX4:C1	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:424:PX4:C1	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:426:PX4:C1	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:428:PX4:C1	19	1.26
(2,988)	1:A:129:TRP:HE1	4:A:430:PX4:C1	19	1.26
(2,981)	1:A:78:PHE:H	1:A:79:PRO:HG3	6	1.26
(2,981)	1:A:78:PHE:H	1:A:79:PRO:HG3	6	1.26
(2,928)	1:A:72:VAL:H	1:A:73:ALA:HB1	9	1.26
(2,837)	1:A:120:ILE:HD13	1:A:200:LEU:HD22	3	1.26
(2,837)	1:A:120:ILE:HD13	1:A:200:LEU:HD23	3	1.26
(2,766)	1:A:22:PHE:H	1:A:19:LEU:HD22	11	1.26
(2,766)	1:A:22:PHE:H	1:A:19:LEU:HD23	11	1.26
(2,760)	1:A:54:LEU:HD22	1:A:59:ILE:HD11	18	1.26
(2,760)	1:A:54:LEU:HD22	1:A:59:ILE:HD12	18	1.26
(2,760)	1:A:54:LEU:HD22	1:A:59:ILE:HD13	18	1.26
(2,760)	1:A:54:LEU:HD23	1:A:59:ILE:HD11	18	1.26
(2,760)	1:A:54:LEU:HD23	1:A:59:ILE:HD12	18	1.26
(2,760)	1:A:54:LEU:HD23	1:A:59:ILE:HD13	18	1.26
(2,758)	1:A:54:LEU:HD22	1:A:39:LEU:HD11	11	1.26
(2,758)	1:A:54:LEU:HD22	1:A:39:LEU:HD12	11	1.26
(2,758)	1:A:54:LEU:HD22	1:A:39:LEU:HD13	11	1.26
(2,758)	1:A:54:LEU:HD23	1:A:39:LEU:HD11	11	1.26
(2,758)	1:A:54:LEU:HD23	1:A:39:LEU:HD12	11	1.26
(2,758)	1:A:54:LEU:HD23	1:A:39:LEU:HD13	11	1.26
(2,472)	1:A:186:ILE:H	1:A:156:LEU:HD21	15	1.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,835)	1:A:120:ILE:HD12	1:A:200:LEU:HD22	11	1.25
(2,835)	1:A:120:ILE:HD12	1:A:200:LEU:HD23	11	1.25
(2,732)	1:A:211:VAL:HG13	1:A:226:LEU:HD22	9	1.25
(2,732)	1:A:211:VAL:HG13	1:A:226:LEU:HD23	9	1.25
(2,516)	1:A:200:LEU:H	1:A:196:LEU:HD11	18	1.25
(2,516)	1:A:200:LEU:H	1:A:196:LEU:HD12	18	1.25
(2,516)	1:A:200:LEU:H	1:A:196:LEU:HD13	18	1.25
(2,466)	1:A:84:TRP:H	1:A:200:LEU:HD21	19	1.25
(3,36)	1:A:129:TRP:HE1	4:A:305:PX4:N1	13	1.24
(3,36)	1:A:129:TRP:HE1	4:A:307:PX4:N1	13	1.24
(3,36)	1:A:129:TRP:HE1	4:A:309:PX4:N1	13	1.24
(3,36)	1:A:129:TRP:HE1	4:A:311:PX4:N1	13	1.24
(3,36)	1:A:129:TRP:HE1	4:A:313:PX4:N1	13	1.24
(3,36)	1:A:129:TRP:HE1	4:A:315:PX4:N1	13	1.24
(3,36)	1:A:129:TRP:HE1	4:A:317:PX4:N1	13	1.24
(3,36)	1:A:129:TRP:HE1	4:A:319:PX4:N1	13	1.24
(3,36)	1:A:129:TRP:HE1	4:A:321:PX4:N1	13	1.24
(3,36)	1:A:129:TRP:HE1	4:A:323:PX4:N1	13	1.24
(3,36)	1:A:129:TRP:HE1	4:A:325:PX4:N1	13	1.24
(3,36)	1:A:129:TRP:HE1	4:A:327:PX4:N1	13	1.24
(3,36)	1:A:129:TRP:HE1	4:A:329:PX4:N1	13	1.24
(3,36)	1:A:129:TRP:HE1	4:A:331:PX4:N1	13	1.24
(3,36)	1:A:129:TRP:HE1	4:A:333:PX4:N1	13	1.24
(3,36)	1:A:129:TRP:HE1	4:A:335:PX4:N1	13	1.24
(3,36)	1:A:129:TRP:HE1	4:A:337:PX4:N1	13	1.24
(3,36)	1:A:129:TRP:HE1	4:A:339:PX4:N1	13	1.24
(3,36)	1:A:129:TRP:HE1	4:A:341:PX4:N1	13	1.24
(3,36)	1:A:129:TRP:HE1	4:A:343:PX4:N1	13	1.24
(3,36)	1:A:129:TRP:HE1	4:A:345:PX4:N1	13	1.24
(3,36)	1:A:129:TRP:HE1	4:A:347:PX4:N1	13	1.24
(3,36)	1:A:129:TRP:HE1	4:A:349:PX4:N1	13	1.24
(3,36)	1:A:129:TRP:HE1	4:A:351:PX4:N1	13	1.24
(3,36)	1:A:129:TRP:HE1	4:A:353:PX4:N1	13	1.24
(3,36)	1:A:129:TRP:HE1	4:A:355:PX4:N1	13	1.24
(3,36)	1:A:129:TRP:HE1	4:A:357:PX4:N1	13	1.24
(3,36)	1:A:129:TRP:HE1	4:A:359:PX4:N1	13	1.24
(3,36)	1:A:129:TRP:HE1	4:A:361:PX4:N1	13	1.24
(3,36)	1:A:129:TRP:HE1	4:A:363:PX4:N1	13	1.24
(3,36)	1:A:129:TRP:HE1	4:A:402:PX4:N1	13	1.24
(3,36)	1:A:129:TRP:HE1	4:A:404:PX4:N1	13	1.24
(3,36)	1:A:129:TRP:HE1	4:A:406:PX4:N1	13	1.24
(3,36)	1:A:129:TRP:HE1	4:A:408:PX4:N1	13	1.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,36)	1:A:129:TRP:HE1	4:A:410:PX4:N1	13	1.24
(3,36)	1:A:129:TRP:HE1	4:A:412:PX4:N1	13	1.24
(3,36)	1:A:129:TRP:HE1	4:A:414:PX4:N1	13	1.24
(3,36)	1:A:129:TRP:HE1	4:A:416:PX4:N1	13	1.24
(3,36)	1:A:129:TRP:HE1	4:A:418:PX4:N1	13	1.24
(3,36)	1:A:129:TRP:HE1	4:A:420:PX4:N1	13	1.24
(3,36)	1:A:129:TRP:HE1	4:A:422:PX4:N1	13	1.24
(3,36)	1:A:129:TRP:HE1	4:A:424:PX4:N1	13	1.24
(3,36)	1:A:129:TRP:HE1	4:A:426:PX4:N1	13	1.24
(3,36)	1:A:129:TRP:HE1	4:A:428:PX4:N1	13	1.24
(3,36)	1:A:129:TRP:HE1	4:A:430:PX4:N1	13	1.24
(2,981)	1:A:78:PHE:H	1:A:79:PRO:HG3	3	1.24
(2,981)	1:A:78:PHE:H	1:A:79:PRO:HG3	3	1.24
(2,974)	1:A:78:PHE:H	1:A:77:LEU:HD21	14	1.24
(2,954)	1:A:74:GLU:HB3	1:A:77:LEU:H	1	1.24
(2,954)	1:A:74:GLU:HB3	1:A:77:LEU:H	1	1.24
(2,948)	1:A:74:GLU:HG3	1:A:75:TYR:H	10	1.24
(2,948)	1:A:74:GLU:HG3	1:A:75:TYR:H	10	1.24
(2,928)	1:A:72:VAL:H	1:A:73:ALA:HB1	14	1.24
(2,902)	1:A:66:ARG:HA	1:A:68:GLY:H	18	1.24
(2,867)	1:A:186:ILE:HD11	1:A:156:LEU:HD21	12	1.24
(2,110)	1:A:11:GLN:H	1:A:14:GLN:H	14	1.24
(2,899)	1:A:66:ARG:H	1:A:64:LYS:H	16	1.23
(2,765)	1:A:22:PHE:H	1:A:19:LEU:HD21	18	1.23
(2,424)	1:A:169:ASP:H	1:A:166:LEU:HB3	3	1.23
(3,33)	1:A:155:THR:H	4:A:305:PX4:C35	16	1.22
(3,33)	1:A:155:THR:H	4:A:307:PX4:C35	16	1.22
(3,33)	1:A:155:THR:H	4:A:309:PX4:C35	16	1.22
(3,33)	1:A:155:THR:H	4:A:311:PX4:C35	16	1.22
(3,33)	1:A:155:THR:H	4:A:313:PX4:C35	16	1.22
(3,33)	1:A:155:THR:H	4:A:315:PX4:C35	16	1.22
(3,33)	1:A:155:THR:H	4:A:317:PX4:C35	16	1.22
(3,33)	1:A:155:THR:H	4:A:319:PX4:C35	16	1.22
(3,33)	1:A:155:THR:H	4:A:321:PX4:C35	16	1.22
(3,33)	1:A:155:THR:H	4:A:323:PX4:C35	16	1.22
(3,33)	1:A:155:THR:H	4:A:325:PX4:C35	16	1.22
(3,33)	1:A:155:THR:H	4:A:327:PX4:C35	16	1.22
(3,33)	1:A:155:THR:H	4:A:329:PX4:C35	16	1.22
(3,33)	1:A:155:THR:H	4:A:331:PX4:C35	16	1.22
(3,33)	1:A:155:THR:H	4:A:333:PX4:C35	16	1.22
(3,33)	1:A:155:THR:H	4:A:335:PX4:C35	16	1.22
(3,33)	1:A:155:THR:H	4:A:337:PX4:C35	16	1.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,33)	1:A:155:THR:H	4:A:339:PX4:C35	16	1.22
(3,33)	1:A:155:THR:H	4:A:341:PX4:C35	16	1.22
(3,33)	1:A:155:THR:H	4:A:343:PX4:C35	16	1.22
(3,33)	1:A:155:THR:H	4:A:345:PX4:C35	16	1.22
(3,33)	1:A:155:THR:H	4:A:347:PX4:C35	16	1.22
(3,33)	1:A:155:THR:H	4:A:349:PX4:C35	16	1.22
(3,33)	1:A:155:THR:H	4:A:351:PX4:C35	16	1.22
(3,33)	1:A:155:THR:H	4:A:353:PX4:C35	16	1.22
(3,33)	1:A:155:THR:H	4:A:355:PX4:C35	16	1.22
(3,33)	1:A:155:THR:H	4:A:357:PX4:C35	16	1.22
(3,33)	1:A:155:THR:H	4:A:359:PX4:C35	16	1.22
(3,33)	1:A:155:THR:H	4:A:361:PX4:C35	16	1.22
(3,33)	1:A:155:THR:H	4:A:363:PX4:C35	16	1.22
(3,33)	1:A:155:THR:H	4:A:402:PX4:C35	16	1.22
(3,33)	1:A:155:THR:H	4:A:404:PX4:C35	16	1.22
(3,33)	1:A:155:THR:H	4:A:406:PX4:C35	16	1.22
(3,33)	1:A:155:THR:H	4:A:408:PX4:C35	16	1.22
(3,33)	1:A:155:THR:H	4:A:410:PX4:C35	16	1.22
(3,33)	1:A:155:THR:H	4:A:412:PX4:C35	16	1.22
(3,33)	1:A:155:THR:H	4:A:414:PX4:C35	16	1.22
(3,33)	1:A:155:THR:H	4:A:416:PX4:C35	16	1.22
(3,33)	1:A:155:THR:H	4:A:418:PX4:C35	16	1.22
(3,33)	1:A:155:THR:H	4:A:420:PX4:C35	16	1.22
(3,33)	1:A:155:THR:H	4:A:422:PX4:C35	16	1.22
(3,33)	1:A:155:THR:H	4:A:424:PX4:C35	16	1.22
(3,33)	1:A:155:THR:H	4:A:426:PX4:C35	16	1.22
(3,33)	1:A:155:THR:H	4:A:428:PX4:C35	16	1.22
(3,33)	1:A:155:THR:H	4:A:430:PX4:C35	16	1.22
(2,981)	1:A:78:PHE:H	1:A:79:PRO:HG3	17	1.22
(2,981)	1:A:78:PHE:H	1:A:79:PRO:HG3	17	1.22
(2,940)	1:A:73:ALA:HB1	1:A:75:TYR:H	17	1.22
(2,940)	1:A:73:ALA:HB2	1:A:75:TYR:H	17	1.22
(2,940)	1:A:73:ALA:HB3	1:A:75:TYR:H	17	1.22
(2,928)	1:A:72:VAL:H	1:A:73:ALA:HB1	19	1.22
(2,902)	1:A:66:ARG:HA	1:A:68:GLY:H	11	1.22
(2,542)	1:A:210:ALA:H	1:A:209:ASN:HD22	6	1.22
(2,392)	1:A:157:ALA:H	1:A:68:GLY:H	20	1.22
(2,264)	1:A:113:LEU:H	1:A:196:LEU:HD21	6	1.22
(3,6)	1:A:78:PHE:H	4:A:305:PX4:C27	9	1.21
(3,6)	1:A:78:PHE:H	4:A:307:PX4:C27	9	1.21
(3,6)	1:A:78:PHE:H	4:A:309:PX4:C27	9	1.21
(3,6)	1:A:78:PHE:H	4:A:311:PX4:C27	9	1.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,6)	1:A:78:PHE:H	4:A:313:PX4:C27	9	1.21
(3,6)	1:A:78:PHE:H	4:A:315:PX4:C27	9	1.21
(3,6)	1:A:78:PHE:H	4:A:317:PX4:C27	9	1.21
(3,6)	1:A:78:PHE:H	4:A:319:PX4:C27	9	1.21
(3,6)	1:A:78:PHE:H	4:A:321:PX4:C27	9	1.21
(3,6)	1:A:78:PHE:H	4:A:323:PX4:C27	9	1.21
(3,6)	1:A:78:PHE:H	4:A:325:PX4:C27	9	1.21
(3,6)	1:A:78:PHE:H	4:A:327:PX4:C27	9	1.21
(3,6)	1:A:78:PHE:H	4:A:329:PX4:C27	9	1.21
(3,6)	1:A:78:PHE:H	4:A:331:PX4:C27	9	1.21
(3,6)	1:A:78:PHE:H	4:A:333:PX4:C27	9	1.21
(3,6)	1:A:78:PHE:H	4:A:335:PX4:C27	9	1.21
(3,6)	1:A:78:PHE:H	4:A:337:PX4:C27	9	1.21
(3,6)	1:A:78:PHE:H	4:A:339:PX4:C27	9	1.21
(3,6)	1:A:78:PHE:H	4:A:341:PX4:C27	9	1.21
(3,6)	1:A:78:PHE:H	4:A:343:PX4:C27	9	1.21
(3,6)	1:A:78:PHE:H	4:A:345:PX4:C27	9	1.21
(3,6)	1:A:78:PHE:H	4:A:347:PX4:C27	9	1.21
(3,6)	1:A:78:PHE:H	4:A:349:PX4:C27	9	1.21
(3,6)	1:A:78:PHE:H	4:A:351:PX4:C27	9	1.21
(3,6)	1:A:78:PHE:H	4:A:353:PX4:C27	9	1.21
(3,6)	1:A:78:PHE:H	4:A:355:PX4:C27	9	1.21
(3,6)	1:A:78:PHE:H	4:A:357:PX4:C27	9	1.21
(3,6)	1:A:78:PHE:H	4:A:359:PX4:C27	9	1.21
(3,6)	1:A:78:PHE:H	4:A:361:PX4:C27	9	1.21
(3,6)	1:A:78:PHE:H	4:A:363:PX4:C27	9	1.21
(3,6)	1:A:78:PHE:H	4:A:402:PX4:C27	9	1.21
(3,6)	1:A:78:PHE:H	4:A:404:PX4:C27	9	1.21
(3,6)	1:A:78:PHE:H	4:A:406:PX4:C27	9	1.21
(3,6)	1:A:78:PHE:H	4:A:408:PX4:C27	9	1.21
(3,6)	1:A:78:PHE:H	4:A:410:PX4:C27	9	1.21
(3,6)	1:A:78:PHE:H	4:A:412:PX4:C27	9	1.21
(3,6)	1:A:78:PHE:H	4:A:414:PX4:C27	9	1.21
(3,6)	1:A:78:PHE:H	4:A:416:PX4:C27	9	1.21
(3,6)	1:A:78:PHE:H	4:A:418:PX4:C27	9	1.21
(3,6)	1:A:78:PHE:H	4:A:420:PX4:C27	9	1.21
(3,6)	1:A:78:PHE:H	4:A:422:PX4:C27	9	1.21
(3,6)	1:A:78:PHE:H	4:A:424:PX4:C27	9	1.21
(3,6)	1:A:78:PHE:H	4:A:426:PX4:C27	9	1.21
(3,6)	1:A:78:PHE:H	4:A:428:PX4:C27	9	1.21
(3,6)	1:A:78:PHE:H	4:A:430:PX4:C27	9	1.21
(2,979)	1:A:78:PHE:H	1:A:78:PHE:HD1	1	1.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,979)	1:A:78:PHE:H	1:A:78:PHE:HD1	13	1.21
(2,976)	1:A:78:PHE:H	1:A:78:PHE:HD1	1	1.21
(2,976)	1:A:78:PHE:H	1:A:78:PHE:HD2	1	1.21
(2,976)	1:A:78:PHE:H	1:A:78:PHE:HD1	13	1.21
(2,976)	1:A:78:PHE:H	1:A:78:PHE:HD2	13	1.21
(2,940)	1:A:73:ALA:HB1	1:A:75:TYR:H	16	1.21
(2,940)	1:A:73:ALA:HB2	1:A:75:TYR:H	16	1.21
(2,940)	1:A:73:ALA:HB3	1:A:75:TYR:H	16	1.21
(2,925)	1:A:72:VAL:HG21	1:A:73:ALA:H	20	1.21
(2,925)	1:A:72:VAL:HG22	1:A:73:ALA:H	20	1.21
(2,925)	1:A:72:VAL:HG23	1:A:73:ALA:H	20	1.21
(2,925)	1:A:72:VAL:HG11	1:A:73:ALA:H	20	1.21
(2,925)	1:A:72:VAL:HG12	1:A:73:ALA:H	20	1.21
(2,925)	1:A:72:VAL:HG13	1:A:73:ALA:H	20	1.21
(2,869)	1:A:186:ILE:HD12	1:A:156:LEU:HD21	14	1.21
(2,837)	1:A:120:ILE:HD13	1:A:200:LEU:HD22	20	1.21
(2,837)	1:A:120:ILE:HD13	1:A:200:LEU:HD23	20	1.21
(2,835)	1:A:120:ILE:HD12	1:A:200:LEU:HD22	14	1.21
(2,835)	1:A:120:ILE:HD12	1:A:200:LEU:HD23	14	1.21
(2,731)	1:A:211:VAL:HG13	1:A:226:LEU:HD21	4	1.21
(2,542)	1:A:210:ALA:H	1:A:209:ASN:HD22	1	1.21
(2,517)	1:A:200:LEU:H	1:A:196:LEU:HD21	5	1.21
(2,264)	1:A:113:LEU:H	1:A:196:LEU:HD21	16	1.21
(2,178)	1:A:171:HIS:H	1:A:69:VAL:HG11	14	1.21
(2,178)	1:A:171:HIS:H	1:A:69:VAL:HG12	14	1.21
(2,178)	1:A:171:HIS:H	1:A:69:VAL:HG13	14	1.21
(2,110)	1:A:11:GLN:H	1:A:14:GLN:H	3	1.21
(3,21)	1:A:77:LEU:H	4:A:305:PX4:C35	17	1.2
(3,21)	1:A:77:LEU:H	4:A:307:PX4:C35	17	1.2
(3,21)	1:A:77:LEU:H	4:A:309:PX4:C35	17	1.2
(3,21)	1:A:77:LEU:H	4:A:311:PX4:C35	17	1.2
(3,21)	1:A:77:LEU:H	4:A:313:PX4:C35	17	1.2
(3,21)	1:A:77:LEU:H	4:A:315:PX4:C35	17	1.2
(3,21)	1:A:77:LEU:H	4:A:317:PX4:C35	17	1.2
(3,21)	1:A:77:LEU:H	4:A:319:PX4:C35	17	1.2
(3,21)	1:A:77:LEU:H	4:A:321:PX4:C35	17	1.2
(3,21)	1:A:77:LEU:H	4:A:323:PX4:C35	17	1.2
(3,21)	1:A:77:LEU:H	4:A:325:PX4:C35	17	1.2
(3,21)	1:A:77:LEU:H	4:A:327:PX4:C35	17	1.2
(3,21)	1:A:77:LEU:H	4:A:329:PX4:C35	17	1.2
(3,21)	1:A:77:LEU:H	4:A:331:PX4:C35	17	1.2
(3,21)	1:A:77:LEU:H	4:A:333:PX4:C35	17	1.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,21)	1:A:77:LEU:H	4:A:335:PX4:C35	17	1.2
(3,21)	1:A:77:LEU:H	4:A:337:PX4:C35	17	1.2
(3,21)	1:A:77:LEU:H	4:A:339:PX4:C35	17	1.2
(3,21)	1:A:77:LEU:H	4:A:341:PX4:C35	17	1.2
(3,21)	1:A:77:LEU:H	4:A:343:PX4:C35	17	1.2
(3,21)	1:A:77:LEU:H	4:A:345:PX4:C35	17	1.2
(3,21)	1:A:77:LEU:H	4:A:347:PX4:C35	17	1.2
(3,21)	1:A:77:LEU:H	4:A:349:PX4:C35	17	1.2
(3,21)	1:A:77:LEU:H	4:A:351:PX4:C35	17	1.2
(3,21)	1:A:77:LEU:H	4:A:353:PX4:C35	17	1.2
(3,21)	1:A:77:LEU:H	4:A:355:PX4:C35	17	1.2
(3,21)	1:A:77:LEU:H	4:A:357:PX4:C35	17	1.2
(3,21)	1:A:77:LEU:H	4:A:359:PX4:C35	17	1.2
(3,21)	1:A:77:LEU:H	4:A:361:PX4:C35	17	1.2
(3,21)	1:A:77:LEU:H	4:A:363:PX4:C35	17	1.2
(3,21)	1:A:77:LEU:H	4:A:402:PX4:C35	17	1.2
(3,21)	1:A:77:LEU:H	4:A:404:PX4:C35	17	1.2
(3,21)	1:A:77:LEU:H	4:A:406:PX4:C35	17	1.2
(3,21)	1:A:77:LEU:H	4:A:408:PX4:C35	17	1.2
(3,21)	1:A:77:LEU:H	4:A:410:PX4:C35	17	1.2
(3,21)	1:A:77:LEU:H	4:A:412:PX4:C35	17	1.2
(3,21)	1:A:77:LEU:H	4:A:414:PX4:C35	17	1.2
(3,21)	1:A:77:LEU:H	4:A:416:PX4:C35	17	1.2
(3,21)	1:A:77:LEU:H	4:A:418:PX4:C35	17	1.2
(3,21)	1:A:77:LEU:H	4:A:420:PX4:C35	17	1.2
(3,21)	1:A:77:LEU:H	4:A:422:PX4:C35	17	1.2
(3,21)	1:A:77:LEU:H	4:A:424:PX4:C35	17	1.2
(3,21)	1:A:77:LEU:H	4:A:426:PX4:C35	17	1.2
(3,21)	1:A:77:LEU:H	4:A:428:PX4:C35	17	1.2
(3,21)	1:A:77:LEU:H	4:A:430:PX4:C35	17	1.2
(2,981)	1:A:78:PHE:H	1:A:79:PRO:HG3	7	1.2
(2,981)	1:A:78:PHE:H	1:A:79:PRO:HG3	7	1.2
(2,954)	1:A:74:GLU:HB3	1:A:77:LEU:H	7	1.2
(2,954)	1:A:74:GLU:HB3	1:A:77:LEU:H	7	1.2
(2,948)	1:A:74:GLU:HG3	1:A:75:TYR:H	5	1.2
(2,948)	1:A:74:GLU:HG3	1:A:75:TYR:H	5	1.2
(2,861)	1:A:186:ILE:HD13	1:A:156:LEU:HD21	6	1.2
(2,758)	1:A:54:LEU:HD22	1:A:39:LEU:HD11	19	1.2
(2,758)	1:A:54:LEU:HD22	1:A:39:LEU:HD12	19	1.2
(2,758)	1:A:54:LEU:HD22	1:A:39:LEU:HD13	19	1.2
(2,758)	1:A:54:LEU:HD23	1:A:39:LEU:HD11	19	1.2
(2,758)	1:A:54:LEU:HD23	1:A:39:LEU:HD12	19	1.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,758)	1:A:54:LEU:HD23	1:A:39:LEU:HD13	19	1.2
(2,733)	1:A:196:LEU:HD21	1:A:113:LEU:HD21	13	1.2
(2,185)	1:A:94:VAL:H	1:A:92:ARG:H	20	1.2
(2,981)	1:A:78:PHE:H	1:A:79:PRO:HG3	2	1.19
(2,981)	1:A:78:PHE:H	1:A:79:PRO:HG3	2	1.19
(2,967)	1:A:77:LEU:H	1:A:77:LEU:HG	8	1.19
(2,954)	1:A:74:GLU:HB3	1:A:77:LEU:H	19	1.19
(2,954)	1:A:74:GLU:HB3	1:A:77:LEU:H	19	1.19
(2,931)	1:A:72:VAL:H	1:A:75:TYR:HB3	16	1.19
(2,931)	1:A:72:VAL:H	1:A:75:TYR:HB3	16	1.19
(2,912)	1:A:70:PRO:HB3	1:A:76:SER:H	15	1.19
(2,912)	1:A:70:PRO:HB2	1:A:76:SER:H	15	1.19
(2,902)	1:A:66:ARG:HA	1:A:68:GLY:H	7	1.19
(2,869)	1:A:186:ILE:HD12	1:A:156:LEU:HD21	6	1.19
(2,842)	1:A:200:LEU:HD21	1:A:122:LEU:HD21	18	1.19
(2,657)	1:A:39:LEU:H	1:A:19:LEU:HD22	15	1.19
(2,657)	1:A:39:LEU:H	1:A:19:LEU:HD23	15	1.19
(2,542)	1:A:210:ALA:H	1:A:209:ASN:HD22	10	1.19
(2,507)	1:A:199:SER:H	1:A:202:MET:H	13	1.19
(2,264)	1:A:113:LEU:H	1:A:196:LEU:HD21	18	1.19
(2,229)	1:A:106:ASP:H	1:A:109:VAL:H	12	1.19
(3,21)	1:A:77:LEU:H	4:A:305:PX4:C35	16	1.18
(3,21)	1:A:77:LEU:H	4:A:307:PX4:C35	16	1.18
(3,21)	1:A:77:LEU:H	4:A:309:PX4:C35	16	1.18
(3,21)	1:A:77:LEU:H	4:A:311:PX4:C35	16	1.18
(3,21)	1:A:77:LEU:H	4:A:313:PX4:C35	16	1.18
(3,21)	1:A:77:LEU:H	4:A:315:PX4:C35	16	1.18
(3,21)	1:A:77:LEU:H	4:A:317:PX4:C35	16	1.18
(3,21)	1:A:77:LEU:H	4:A:319:PX4:C35	16	1.18
(3,21)	1:A:77:LEU:H	4:A:321:PX4:C35	16	1.18
(3,21)	1:A:77:LEU:H	4:A:323:PX4:C35	16	1.18
(3,21)	1:A:77:LEU:H	4:A:325:PX4:C35	16	1.18
(3,21)	1:A:77:LEU:H	4:A:327:PX4:C35	16	1.18
(3,21)	1:A:77:LEU:H	4:A:329:PX4:C35	16	1.18
(3,21)	1:A:77:LEU:H	4:A:331:PX4:C35	16	1.18
(3,21)	1:A:77:LEU:H	4:A:333:PX4:C35	16	1.18
(3,21)	1:A:77:LEU:H	4:A:335:PX4:C35	16	1.18
(3,21)	1:A:77:LEU:H	4:A:337:PX4:C35	16	1.18
(3,21)	1:A:77:LEU:H	4:A:339:PX4:C35	16	1.18
(3,21)	1:A:77:LEU:H	4:A:341:PX4:C35	16	1.18
(3,21)	1:A:77:LEU:H	4:A:343:PX4:C35	16	1.18
(3,21)	1:A:77:LEU:H	4:A:345:PX4:C35	16	1.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,21)	1:A:77:LEU:H	4:A:347:PX4:C35	16	1.18
(3,21)	1:A:77:LEU:H	4:A:349:PX4:C35	16	1.18
(3,21)	1:A:77:LEU:H	4:A:351:PX4:C35	16	1.18
(3,21)	1:A:77:LEU:H	4:A:353:PX4:C35	16	1.18
(3,21)	1:A:77:LEU:H	4:A:355:PX4:C35	16	1.18
(3,21)	1:A:77:LEU:H	4:A:357:PX4:C35	16	1.18
(3,21)	1:A:77:LEU:H	4:A:359:PX4:C35	16	1.18
(3,21)	1:A:77:LEU:H	4:A:361:PX4:C35	16	1.18
(3,21)	1:A:77:LEU:H	4:A:363:PX4:C35	16	1.18
(3,21)	1:A:77:LEU:H	4:A:402:PX4:C35	16	1.18
(3,21)	1:A:77:LEU:H	4:A:404:PX4:C35	16	1.18
(3,21)	1:A:77:LEU:H	4:A:406:PX4:C35	16	1.18
(3,21)	1:A:77:LEU:H	4:A:408:PX4:C35	16	1.18
(3,21)	1:A:77:LEU:H	4:A:410:PX4:C35	16	1.18
(3,21)	1:A:77:LEU:H	4:A:412:PX4:C35	16	1.18
(3,21)	1:A:77:LEU:H	4:A:414:PX4:C35	16	1.18
(3,21)	1:A:77:LEU:H	4:A:416:PX4:C35	16	1.18
(3,21)	1:A:77:LEU:H	4:A:418:PX4:C35	16	1.18
(3,21)	1:A:77:LEU:H	4:A:420:PX4:C35	16	1.18
(3,21)	1:A:77:LEU:H	4:A:422:PX4:C35	16	1.18
(3,21)	1:A:77:LEU:H	4:A:424:PX4:C35	16	1.18
(3,21)	1:A:77:LEU:H	4:A:426:PX4:C35	16	1.18
(3,21)	1:A:77:LEU:H	4:A:428:PX4:C35	16	1.18
(3,21)	1:A:77:LEU:H	4:A:430:PX4:C35	16	1.18
(2,948)	1:A:74:GLU:HG3	1:A:75:TYR:H	20	1.18
(2,948)	1:A:74:GLU:HG3	1:A:75:TYR:H	20	1.18
(2,931)	1:A:72:VAL:H	1:A:75:TYR:HB3	9	1.18
(2,931)	1:A:72:VAL:H	1:A:75:TYR:HB3	9	1.18
(2,902)	1:A:66:ARG:HA	1:A:68:GLY:H	6	1.18
(2,835)	1:A:120:ILE:HD12	1:A:200:LEU:HD22	7	1.18
(2,835)	1:A:120:ILE:HD12	1:A:200:LEU:HD23	7	1.18
(2,671)	1:A:66:ARG:H	1:A:156:LEU:HD21	7	1.18
(2,542)	1:A:210:ALA:H	1:A:209:ASN:HD22	4	1.18
(2,516)	1:A:200:LEU:H	1:A:196:LEU:HD11	7	1.18
(2,516)	1:A:200:LEU:H	1:A:196:LEU:HD12	7	1.18
(2,516)	1:A:200:LEU:H	1:A:196:LEU:HD13	7	1.18
(2,257)	1:A:112:ALA:H	1:A:189:LEU:HD21	20	1.18
(2,110)	1:A:11:GLN:H	1:A:14:GLN:H	12	1.18
(3,33)	1:A:155:THR:H	4:A:305:PX4:C35	3	1.17
(3,33)	1:A:155:THR:H	4:A:307:PX4:C35	3	1.17
(3,33)	1:A:155:THR:H	4:A:309:PX4:C35	3	1.17
(3,33)	1:A:155:THR:H	4:A:311:PX4:C35	3	1.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,33)	1:A:155:THR:H	4:A:313:PX4:C35	3	1.17
(3,33)	1:A:155:THR:H	4:A:315:PX4:C35	3	1.17
(3,33)	1:A:155:THR:H	4:A:317:PX4:C35	3	1.17
(3,33)	1:A:155:THR:H	4:A:319:PX4:C35	3	1.17
(3,33)	1:A:155:THR:H	4:A:321:PX4:C35	3	1.17
(3,33)	1:A:155:THR:H	4:A:323:PX4:C35	3	1.17
(3,33)	1:A:155:THR:H	4:A:325:PX4:C35	3	1.17
(3,33)	1:A:155:THR:H	4:A:327:PX4:C35	3	1.17
(3,33)	1:A:155:THR:H	4:A:329:PX4:C35	3	1.17
(3,33)	1:A:155:THR:H	4:A:331:PX4:C35	3	1.17
(3,33)	1:A:155:THR:H	4:A:333:PX4:C35	3	1.17
(3,33)	1:A:155:THR:H	4:A:335:PX4:C35	3	1.17
(3,33)	1:A:155:THR:H	4:A:337:PX4:C35	3	1.17
(3,33)	1:A:155:THR:H	4:A:339:PX4:C35	3	1.17
(3,33)	1:A:155:THR:H	4:A:341:PX4:C35	3	1.17
(3,33)	1:A:155:THR:H	4:A:343:PX4:C35	3	1.17
(3,33)	1:A:155:THR:H	4:A:345:PX4:C35	3	1.17
(3,33)	1:A:155:THR:H	4:A:347:PX4:C35	3	1.17
(3,33)	1:A:155:THR:H	4:A:349:PX4:C35	3	1.17
(3,33)	1:A:155:THR:H	4:A:351:PX4:C35	3	1.17
(3,33)	1:A:155:THR:H	4:A:353:PX4:C35	3	1.17
(3,33)	1:A:155:THR:H	4:A:355:PX4:C35	3	1.17
(3,33)	1:A:155:THR:H	4:A:357:PX4:C35	3	1.17
(3,33)	1:A:155:THR:H	4:A:359:PX4:C35	3	1.17
(3,33)	1:A:155:THR:H	4:A:361:PX4:C35	3	1.17
(3,33)	1:A:155:THR:H	4:A:363:PX4:C35	3	1.17
(3,33)	1:A:155:THR:H	4:A:402:PX4:C35	3	1.17
(3,33)	1:A:155:THR:H	4:A:404:PX4:C35	3	1.17
(3,33)	1:A:155:THR:H	4:A:406:PX4:C35	3	1.17
(3,33)	1:A:155:THR:H	4:A:408:PX4:C35	3	1.17
(3,33)	1:A:155:THR:H	4:A:410:PX4:C35	3	1.17
(3,33)	1:A:155:THR:H	4:A:412:PX4:C35	3	1.17
(3,33)	1:A:155:THR:H	4:A:414:PX4:C35	3	1.17
(3,33)	1:A:155:THR:H	4:A:416:PX4:C35	3	1.17
(3,33)	1:A:155:THR:H	4:A:418:PX4:C35	3	1.17
(3,33)	1:A:155:THR:H	4:A:420:PX4:C35	3	1.17
(3,33)	1:A:155:THR:H	4:A:422:PX4:C35	3	1.17
(3,33)	1:A:155:THR:H	4:A:424:PX4:C35	3	1.17
(3,33)	1:A:155:THR:H	4:A:426:PX4:C35	3	1.17
(3,33)	1:A:155:THR:H	4:A:428:PX4:C35	3	1.17
(3,33)	1:A:155:THR:H	4:A:430:PX4:C35	3	1.17
(2,928)	1:A:72:VAL:H	1:A:73:ALA:HB1	13	1.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,879)	1:A:234:ILE:HD11	1:A:200:LEU:HB2	17	1.17
(2,879)	1:A:234:ILE:HD12	1:A:200:LEU:HB2	17	1.17
(2,879)	1:A:234:ILE:HD13	1:A:200:LEU:HB2	17	1.17
(2,656)	1:A:39:LEU:H	1:A:19:LEU:HD21	4	1.17
(2,598)	1:A:235:GLN:H	1:A:238:TYR:HE1	11	1.17
(2,598)	1:A:235:GLN:H	1:A:238:TYR:HE2	11	1.17
(2,975)	1:A:78:PHE:H	1:A:77:LEU:HD22	13	1.16
(2,975)	1:A:78:PHE:H	1:A:77:LEU:HD23	13	1.16
(2,661)	1:A:4:ALA:H	1:A:59:ILE:HG21	17	1.16
(2,661)	1:A:4:ALA:H	1:A:59:ILE:HG22	17	1.16
(2,661)	1:A:4:ALA:H	1:A:59:ILE:HG23	17	1.16
(2,178)	1:A:171:HIS:H	1:A:69:VAL:HG11	9	1.16
(2,178)	1:A:171:HIS:H	1:A:69:VAL:HG12	9	1.16
(2,178)	1:A:171:HIS:H	1:A:69:VAL:HG13	9	1.16
(2,970)	1:A:77:LEU:HG	1:A:78:PHE:H	18	1.15
(2,928)	1:A:72:VAL:H	1:A:73:ALA:HB1	2	1.15
(2,899)	1:A:66:ARG:H	1:A:64:LYS:H	9	1.15
(2,731)	1:A:211:VAL:HG13	1:A:226:LEU:HD21	17	1.15
(2,516)	1:A:200:LEU:H	1:A:196:LEU:HD11	4	1.15
(2,516)	1:A:200:LEU:H	1:A:196:LEU:HD12	4	1.15
(2,516)	1:A:200:LEU:H	1:A:196:LEU:HD13	4	1.15
(2,229)	1:A:106:ASP:H	1:A:109:VAL:H	2	1.15
(2,229)	1:A:106:ASP:H	1:A:109:VAL:H	18	1.15
(2,110)	1:A:11:GLN:H	1:A:14:GLN:H	15	1.15
(3,33)	1:A:155:THR:H	4:A:305:PX4:C35	2	1.14
(3,33)	1:A:155:THR:H	4:A:307:PX4:C35	2	1.14
(3,33)	1:A:155:THR:H	4:A:309:PX4:C35	2	1.14
(3,33)	1:A:155:THR:H	4:A:311:PX4:C35	2	1.14
(3,33)	1:A:155:THR:H	4:A:313:PX4:C35	2	1.14
(3,33)	1:A:155:THR:H	4:A:315:PX4:C35	2	1.14
(3,33)	1:A:155:THR:H	4:A:317:PX4:C35	2	1.14
(3,33)	1:A:155:THR:H	4:A:319:PX4:C35	2	1.14
(3,33)	1:A:155:THR:H	4:A:321:PX4:C35	2	1.14
(3,33)	1:A:155:THR:H	4:A:323:PX4:C35	2	1.14
(3,33)	1:A:155:THR:H	4:A:325:PX4:C35	2	1.14
(3,33)	1:A:155:THR:H	4:A:327:PX4:C35	2	1.14
(3,33)	1:A:155:THR:H	4:A:329:PX4:C35	2	1.14
(3,33)	1:A:155:THR:H	4:A:331:PX4:C35	2	1.14
(3,33)	1:A:155:THR:H	4:A:333:PX4:C35	2	1.14
(3,33)	1:A:155:THR:H	4:A:335:PX4:C35	2	1.14
(3,33)	1:A:155:THR:H	4:A:337:PX4:C35	2	1.14
(3,33)	1:A:155:THR:H	4:A:339:PX4:C35	2	1.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,33)	1:A:155:THR:H	4:A:341:PX4:C35	2	1.14
(3,33)	1:A:155:THR:H	4:A:343:PX4:C35	2	1.14
(3,33)	1:A:155:THR:H	4:A:345:PX4:C35	2	1.14
(3,33)	1:A:155:THR:H	4:A:347:PX4:C35	2	1.14
(3,33)	1:A:155:THR:H	4:A:349:PX4:C35	2	1.14
(3,33)	1:A:155:THR:H	4:A:351:PX4:C35	2	1.14
(3,33)	1:A:155:THR:H	4:A:353:PX4:C35	2	1.14
(3,33)	1:A:155:THR:H	4:A:355:PX4:C35	2	1.14
(3,33)	1:A:155:THR:H	4:A:357:PX4:C35	2	1.14
(3,33)	1:A:155:THR:H	4:A:359:PX4:C35	2	1.14
(3,33)	1:A:155:THR:H	4:A:361:PX4:C35	2	1.14
(3,33)	1:A:155:THR:H	4:A:363:PX4:C35	2	1.14
(3,33)	1:A:155:THR:H	4:A:402:PX4:C35	2	1.14
(3,33)	1:A:155:THR:H	4:A:404:PX4:C35	2	1.14
(3,33)	1:A:155:THR:H	4:A:406:PX4:C35	2	1.14
(3,33)	1:A:155:THR:H	4:A:408:PX4:C35	2	1.14
(3,33)	1:A:155:THR:H	4:A:410:PX4:C35	2	1.14
(3,33)	1:A:155:THR:H	4:A:412:PX4:C35	2	1.14
(3,33)	1:A:155:THR:H	4:A:414:PX4:C35	2	1.14
(3,33)	1:A:155:THR:H	4:A:416:PX4:C35	2	1.14
(3,33)	1:A:155:THR:H	4:A:418:PX4:C35	2	1.14
(3,33)	1:A:155:THR:H	4:A:420:PX4:C35	2	1.14
(3,33)	1:A:155:THR:H	4:A:422:PX4:C35	2	1.14
(3,33)	1:A:155:THR:H	4:A:424:PX4:C35	2	1.14
(3,33)	1:A:155:THR:H	4:A:426:PX4:C35	2	1.14
(3,33)	1:A:155:THR:H	4:A:428:PX4:C35	2	1.14
(3,33)	1:A:155:THR:H	4:A:430:PX4:C35	2	1.14
(2,932)	1:A:72:VAL:HG11	1:A:76:SER:H	14	1.14
(2,932)	1:A:72:VAL:HG12	1:A:76:SER:H	14	1.14
(2,932)	1:A:72:VAL:HG13	1:A:76:SER:H	14	1.14
(2,507)	1:A:199:SER:H	1:A:202:MET:H	1	1.14
(2,110)	1:A:11:GLN:H	1:A:14:GLN:H	5	1.14
(2,971)	1:A:77:LEU:HB3	1:A:78:PHE:H	12	1.13
(2,971)	1:A:77:LEU:HB3	1:A:78:PHE:H	12	1.13
(2,970)	1:A:77:LEU:HG	1:A:78:PHE:H	9	1.13
(2,954)	1:A:74:GLU:HB3	1:A:77:LEU:H	2	1.13
(2,954)	1:A:74:GLU:HB3	1:A:77:LEU:H	2	1.13
(2,948)	1:A:74:GLU:HG3	1:A:75:TYR:H	18	1.13
(2,948)	1:A:74:GLU:HG3	1:A:75:TYR:H	18	1.13
(2,902)	1:A:66:ARG:HA	1:A:68:GLY:H	14	1.13
(2,846)	1:A:200:LEU:HD23	1:A:122:LEU:HD21	18	1.13
(2,756)	1:A:54:LEU:HD22	1:A:58:VAL:HG11	12	1.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,756)	1:A:54:LEU:HD22	1:A:58:VAL:HG12	12	1.13
(2,756)	1:A:54:LEU:HD22	1:A:58:VAL:HG13	12	1.13
(2,756)	1:A:54:LEU:HD23	1:A:58:VAL:HG11	12	1.13
(2,756)	1:A:54:LEU:HD23	1:A:58:VAL:HG12	12	1.13
(2,756)	1:A:54:LEU:HD23	1:A:58:VAL:HG13	12	1.13
(2,598)	1:A:235:GLN:H	1:A:238:TYR:HE1	20	1.13
(2,598)	1:A:235:GLN:H	1:A:238:TYR:HE2	20	1.13
(2,379)	1:A:10:LEU:H	1:A:10:LEU:HD21	19	1.13
(2,178)	1:A:171:HIS:H	1:A:69:VAL:HG11	10	1.13
(2,178)	1:A:171:HIS:H	1:A:69:VAL:HG12	10	1.13
(2,178)	1:A:171:HIS:H	1:A:69:VAL:HG13	10	1.13
(2,954)	1:A:74:GLU:HB3	1:A:77:LEU:H	3	1.12
(2,954)	1:A:74:GLU:HB3	1:A:77:LEU:H	3	1.12
(2,928)	1:A:72:VAL:H	1:A:73:ALA:HB1	3	1.12
(2,773)	1:A:61:ILE:HD11	1:A:48:LEU:HD21	11	1.12
(2,730)	1:A:211:VAL:HG12	1:A:226:LEU:HD22	6	1.12
(2,730)	1:A:211:VAL:HG12	1:A:226:LEU:HD23	6	1.12
(2,725)	1:A:113:LEU:HD13	1:A:196:LEU:HD21	7	1.12
(2,723)	1:A:113:LEU:HD12	1:A:196:LEU:HD21	7	1.12
(2,510)	1:A:200:LEU:HD21	1:A:199:SER:H	15	1.12
(2,473)	1:A:186:ILE:H	1:A:156:LEU:HD22	15	1.12
(2,473)	1:A:186:ILE:H	1:A:156:LEU:HD23	15	1.12
(2,466)	1:A:84:TRP:H	1:A:200:LEU:HD21	6	1.12
(2,257)	1:A:112:ALA:H	1:A:189:LEU:HD21	13	1.12
(2,212)	1:A:120:ILE:HD11	1:A:237:LEU:H	8	1.12
(2,212)	1:A:120:ILE:HD12	1:A:237:LEU:H	8	1.12
(2,212)	1:A:120:ILE:HD13	1:A:237:LEU:H	8	1.12
(2,979)	1:A:78:PHE:H	1:A:78:PHE:HD1	19	1.11
(2,976)	1:A:78:PHE:H	1:A:78:PHE:HD1	19	1.11
(2,976)	1:A:78:PHE:H	1:A:78:PHE:HD2	19	1.11
(2,948)	1:A:74:GLU:HG3	1:A:75:TYR:H	19	1.11
(2,948)	1:A:74:GLU:HG3	1:A:75:TYR:H	19	1.11
(2,925)	1:A:72:VAL:HG21	1:A:73:ALA:H	13	1.11
(2,925)	1:A:72:VAL:HG22	1:A:73:ALA:H	13	1.11
(2,925)	1:A:72:VAL:HG23	1:A:73:ALA:H	13	1.11
(2,925)	1:A:72:VAL:HG11	1:A:73:ALA:H	13	1.11
(2,925)	1:A:72:VAL:HG12	1:A:73:ALA:H	13	1.11
(2,925)	1:A:72:VAL:HG13	1:A:73:ALA:H	13	1.11
(2,911)	1:A:69:VAL:HG21	1:A:69:VAL:H	3	1.11
(2,911)	1:A:69:VAL:HG22	1:A:69:VAL:H	3	1.11
(2,911)	1:A:69:VAL:HG23	1:A:69:VAL:H	3	1.11
(2,911)	1:A:69:VAL:HG11	1:A:69:VAL:H	3	1.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,911)	1:A:69:VAL:HG12	1:A:69:VAL:H	3	1.11
(2,911)	1:A:69:VAL:HG13	1:A:69:VAL:H	3	1.11
(2,867)	1:A:186:ILE:HD11	1:A:156:LEU:HD21	19	1.11
(2,846)	1:A:200:LEU:HD23	1:A:122:LEU:HD21	9	1.11
(2,379)	1:A:10:LEU:H	1:A:10:LEU:HD21	1	1.11
(2,902)	1:A:66:ARG:HA	1:A:68:GLY:H	9	1.1
(2,861)	1:A:186:ILE:HD13	1:A:156:LEU:HD21	19	1.1
(2,212)	1:A:120:ILE:HD11	1:A:237:LEU:H	10	1.1
(2,212)	1:A:120:ILE:HD12	1:A:237:LEU:H	10	1.1
(2,212)	1:A:120:ILE:HD13	1:A:237:LEU:H	10	1.1
(2,974)	1:A:78:PHE:H	1:A:77:LEU:HD21	15	1.09
(2,891)	1:A:63:GLN:H	1:A:63:GLN:HB3	4	1.09
(2,891)	1:A:63:GLN:H	1:A:63:GLN:HB2	4	1.09
(2,891)	1:A:63:GLN:H	1:A:63:GLN:HB3	4	1.09
(2,891)	1:A:63:GLN:H	1:A:63:GLN:HB2	4	1.09
(2,869)	1:A:186:ILE:HD12	1:A:156:LEU:HD21	19	1.09
(2,804)	1:A:93:ILE:HD11	1:A:105:VAL:HG21	19	1.09
(2,804)	1:A:93:ILE:HD11	1:A:105:VAL:HG22	19	1.09
(2,804)	1:A:93:ILE:HD11	1:A:105:VAL:HG23	19	1.09
(2,804)	1:A:93:ILE:HD12	1:A:105:VAL:HG21	19	1.09
(2,804)	1:A:93:ILE:HD12	1:A:105:VAL:HG22	19	1.09
(2,804)	1:A:93:ILE:HD12	1:A:105:VAL:HG23	19	1.09
(2,804)	1:A:93:ILE:HD13	1:A:105:VAL:HG21	19	1.09
(2,804)	1:A:93:ILE:HD13	1:A:105:VAL:HG22	19	1.09
(2,804)	1:A:93:ILE:HD13	1:A:105:VAL:HG23	19	1.09
(2,777)	1:A:61:ILE:HD13	1:A:48:LEU:HD21	10	1.09
(2,758)	1:A:54:LEU:HD22	1:A:39:LEU:HD11	3	1.09
(2,758)	1:A:54:LEU:HD22	1:A:39:LEU:HD12	3	1.09
(2,758)	1:A:54:LEU:HD22	1:A:39:LEU:HD13	3	1.09
(2,758)	1:A:54:LEU:HD23	1:A:39:LEU:HD11	3	1.09
(2,758)	1:A:54:LEU:HD23	1:A:39:LEU:HD12	3	1.09
(2,758)	1:A:54:LEU:HD23	1:A:39:LEU:HD13	3	1.09
(2,608)	1:A:238:TYR:H	1:A:120:ILE:HD11	14	1.09
(2,608)	1:A:238:TYR:H	1:A:120:ILE:HD12	14	1.09
(2,608)	1:A:238:TYR:H	1:A:120:ILE:HD13	14	1.09
(2,542)	1:A:210:ALA:H	1:A:209:ASN:HD22	13	1.09
(2,185)	1:A:94:VAL:H	1:A:92:ARG:H	19	1.09
(2,110)	1:A:11:GLN:H	1:A:14:GLN:H	6	1.09
(3,33)	1:A:155:THR:H	4:A:305:PX4:C35	18	1.08
(3,33)	1:A:155:THR:H	4:A:307:PX4:C35	18	1.08
(3,33)	1:A:155:THR:H	4:A:309:PX4:C35	18	1.08
(3,33)	1:A:155:THR:H	4:A:311:PX4:C35	18	1.08

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,33)	1:A:155:THR:H	4:A:313:PX4:C35	18	1.08
(3,33)	1:A:155:THR:H	4:A:315:PX4:C35	18	1.08
(3,33)	1:A:155:THR:H	4:A:317:PX4:C35	18	1.08
(3,33)	1:A:155:THR:H	4:A:319:PX4:C35	18	1.08
(3,33)	1:A:155:THR:H	4:A:321:PX4:C35	18	1.08
(3,33)	1:A:155:THR:H	4:A:323:PX4:C35	18	1.08
(3,33)	1:A:155:THR:H	4:A:325:PX4:C35	18	1.08
(3,33)	1:A:155:THR:H	4:A:327:PX4:C35	18	1.08
(3,33)	1:A:155:THR:H	4:A:329:PX4:C35	18	1.08
(3,33)	1:A:155:THR:H	4:A:331:PX4:C35	18	1.08
(3,33)	1:A:155:THR:H	4:A:333:PX4:C35	18	1.08
(3,33)	1:A:155:THR:H	4:A:335:PX4:C35	18	1.08
(3,33)	1:A:155:THR:H	4:A:337:PX4:C35	18	1.08
(3,33)	1:A:155:THR:H	4:A:339:PX4:C35	18	1.08
(3,33)	1:A:155:THR:H	4:A:341:PX4:C35	18	1.08
(3,33)	1:A:155:THR:H	4:A:343:PX4:C35	18	1.08
(3,33)	1:A:155:THR:H	4:A:345:PX4:C35	18	1.08
(3,33)	1:A:155:THR:H	4:A:347:PX4:C35	18	1.08
(3,33)	1:A:155:THR:H	4:A:349:PX4:C35	18	1.08
(3,33)	1:A:155:THR:H	4:A:351:PX4:C35	18	1.08
(3,33)	1:A:155:THR:H	4:A:353:PX4:C35	18	1.08
(3,33)	1:A:155:THR:H	4:A:355:PX4:C35	18	1.08
(3,33)	1:A:155:THR:H	4:A:357:PX4:C35	18	1.08
(3,33)	1:A:155:THR:H	4:A:359:PX4:C35	18	1.08
(3,33)	1:A:155:THR:H	4:A:361:PX4:C35	18	1.08
(3,33)	1:A:155:THR:H	4:A:363:PX4:C35	18	1.08
(3,33)	1:A:155:THR:H	4:A:402:PX4:C35	18	1.08
(3,33)	1:A:155:THR:H	4:A:404:PX4:C35	18	1.08
(3,33)	1:A:155:THR:H	4:A:406:PX4:C35	18	1.08
(3,33)	1:A:155:THR:H	4:A:408:PX4:C35	18	1.08
(3,33)	1:A:155:THR:H	4:A:410:PX4:C35	18	1.08
(3,33)	1:A:155:THR:H	4:A:412:PX4:C35	18	1.08
(3,33)	1:A:155:THR:H	4:A:414:PX4:C35	18	1.08
(3,33)	1:A:155:THR:H	4:A:416:PX4:C35	18	1.08
(3,33)	1:A:155:THR:H	4:A:418:PX4:C35	18	1.08
(3,33)	1:A:155:THR:H	4:A:420:PX4:C35	18	1.08
(3,33)	1:A:155:THR:H	4:A:422:PX4:C35	18	1.08
(3,33)	1:A:155:THR:H	4:A:424:PX4:C35	18	1.08
(3,33)	1:A:155:THR:H	4:A:426:PX4:C35	18	1.08
(3,33)	1:A:155:THR:H	4:A:428:PX4:C35	18	1.08
(3,33)	1:A:155:THR:H	4:A:430:PX4:C35	18	1.08
(2,928)	1:A:72:VAL:H	1:A:73:ALA:HB1	6	1.08

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,899)	1:A:66:ARG:H	1:A:64:LYS:H	20	1.08
(2,774)	1:A:61:ILE:HD11	1:A:48:LEU:HD22	18	1.08
(2,774)	1:A:61:ILE:HD11	1:A:48:LEU:HD23	18	1.08
(2,766)	1:A:22:PHE:H	1:A:19:LEU:HD22	8	1.08
(2,766)	1:A:22:PHE:H	1:A:19:LEU:HD23	8	1.08
(2,755)	1:A:54:LEU:HD21	1:A:58:VAL:HG11	3	1.08
(2,755)	1:A:54:LEU:HD21	1:A:58:VAL:HG12	3	1.08
(2,755)	1:A:54:LEU:HD21	1:A:58:VAL:HG13	3	1.08
(2,730)	1:A:211:VAL:HG12	1:A:226:LEU:HD22	7	1.08
(2,730)	1:A:211:VAL:HG12	1:A:226:LEU:HD23	7	1.08
(2,414)	1:A:167:GLY:H	1:A:166:LEU:HD21	3	1.08
(2,983)	1:A:79:PRO:HD3	1:A:80:ASN:H	9	1.07
(2,983)	1:A:79:PRO:HD3	1:A:80:ASN:H	9	1.07
(2,932)	1:A:72:VAL:HG11	1:A:76:SER:H	4	1.07
(2,932)	1:A:72:VAL:HG12	1:A:76:SER:H	4	1.07
(2,932)	1:A:72:VAL:HG13	1:A:76:SER:H	4	1.07
(2,891)	1:A:63:GLN:H	1:A:63:GLN:HB3	9	1.07
(2,891)	1:A:63:GLN:H	1:A:63:GLN:HB2	9	1.07
(2,891)	1:A:63:GLN:H	1:A:63:GLN:HB3	9	1.07
(2,891)	1:A:63:GLN:H	1:A:63:GLN:HB2	9	1.07
(2,834)	1:A:120:ILE:HD12	1:A:200:LEU:HD21	13	1.07
(2,758)	1:A:54:LEU:HD22	1:A:39:LEU:HD11	2	1.07
(2,758)	1:A:54:LEU:HD22	1:A:39:LEU:HD12	2	1.07
(2,758)	1:A:54:LEU:HD22	1:A:39:LEU:HD13	2	1.07
(2,758)	1:A:54:LEU:HD23	1:A:39:LEU:HD11	2	1.07
(2,758)	1:A:54:LEU:HD23	1:A:39:LEU:HD12	2	1.07
(2,758)	1:A:54:LEU:HD23	1:A:39:LEU:HD13	2	1.07
(2,758)	1:A:54:LEU:HD22	1:A:39:LEU:HD11	7	1.07
(2,758)	1:A:54:LEU:HD22	1:A:39:LEU:HD12	7	1.07
(2,758)	1:A:54:LEU:HD22	1:A:39:LEU:HD13	7	1.07
(2,758)	1:A:54:LEU:HD23	1:A:39:LEU:HD11	7	1.07
(2,758)	1:A:54:LEU:HD23	1:A:39:LEU:HD12	7	1.07
(2,758)	1:A:54:LEU:HD23	1:A:39:LEU:HD13	7	1.07
(2,510)	1:A:200:LEU:HD21	1:A:199:SER:H	19	1.07
(2,257)	1:A:112:ALA:H	1:A:189:LEU:HD21	15	1.07
(2,229)	1:A:106:ASP:H	1:A:109:VAL:H	8	1.07
(2,229)	1:A:106:ASP:H	1:A:109:VAL:H	10	1.07
(2,110)	1:A:11:GLN:H	1:A:14:GLN:H	8	1.07
(2,981)	1:A:78:PHE:H	1:A:79:PRO:HG3	18	1.06
(2,981)	1:A:78:PHE:H	1:A:79:PRO:HG3	18	1.06
(2,750)	1:A:89:VAL:HG13	1:A:122:LEU:HD21	18	1.06
(2,735)	1:A:196:LEU:HD22	1:A:113:LEU:HD21	18	1.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,516)	1:A:200:LEU:H	1:A:196:LEU:HD11	8	1.06
(2,516)	1:A:200:LEU:H	1:A:196:LEU:HD12	8	1.06
(2,516)	1:A:200:LEU:H	1:A:196:LEU:HD13	8	1.06
(2,510)	1:A:200:LEU:HD21	1:A:199:SER:H	14	1.06
(2,212)	1:A:120:ILE:HD11	1:A:237:LEU:H	1	1.06
(2,212)	1:A:120:ILE:HD12	1:A:237:LEU:H	1	1.06
(2,212)	1:A:120:ILE:HD13	1:A:237:LEU:H	1	1.06
(2,212)	1:A:120:ILE:HD11	1:A:237:LEU:H	16	1.06
(2,212)	1:A:120:ILE:HD12	1:A:237:LEU:H	16	1.06
(2,212)	1:A:120:ILE:HD13	1:A:237:LEU:H	16	1.06
(2,110)	1:A:11:GLN:H	1:A:14:GLN:H	1	1.06
(2,911)	1:A:69:VAL:HG21	1:A:69:VAL:H	2	1.05
(2,911)	1:A:69:VAL:HG22	1:A:69:VAL:H	2	1.05
(2,911)	1:A:69:VAL:HG23	1:A:69:VAL:H	2	1.05
(2,911)	1:A:69:VAL:HG11	1:A:69:VAL:H	2	1.05
(2,911)	1:A:69:VAL:HG12	1:A:69:VAL:H	2	1.05
(2,911)	1:A:69:VAL:HG13	1:A:69:VAL:H	2	1.05
(2,905)	1:A:67:CYS:HA	1:A:68:GLY:H	20	1.05
(2,804)	1:A:93:ILE:HD11	1:A:105:VAL:HG21	12	1.05
(2,804)	1:A:93:ILE:HD11	1:A:105:VAL:HG22	12	1.05
(2,804)	1:A:93:ILE:HD11	1:A:105:VAL:HG23	12	1.05
(2,804)	1:A:93:ILE:HD12	1:A:105:VAL:HG21	12	1.05
(2,804)	1:A:93:ILE:HD12	1:A:105:VAL:HG22	12	1.05
(2,804)	1:A:93:ILE:HD12	1:A:105:VAL:HG23	12	1.05
(2,804)	1:A:93:ILE:HD13	1:A:105:VAL:HG21	12	1.05
(2,804)	1:A:93:ILE:HD13	1:A:105:VAL:HG22	12	1.05
(2,804)	1:A:93:ILE:HD13	1:A:105:VAL:HG23	12	1.05
(2,765)	1:A:22:PHE:H	1:A:19:LEU:HD21	9	1.05
(2,229)	1:A:106:ASP:H	1:A:109:VAL:H	3	1.05
(3,33)	1:A:155:THR:H	4:A:305:PX4:C35	12	1.04
(3,33)	1:A:155:THR:H	4:A:307:PX4:C35	12	1.04
(3,33)	1:A:155:THR:H	4:A:309:PX4:C35	12	1.04
(3,33)	1:A:155:THR:H	4:A:311:PX4:C35	12	1.04
(3,33)	1:A:155:THR:H	4:A:313:PX4:C35	12	1.04
(3,33)	1:A:155:THR:H	4:A:315:PX4:C35	12	1.04
(3,33)	1:A:155:THR:H	4:A:317:PX4:C35	12	1.04
(3,33)	1:A:155:THR:H	4:A:319:PX4:C35	12	1.04
(3,33)	1:A:155:THR:H	4:A:321:PX4:C35	12	1.04
(3,33)	1:A:155:THR:H	4:A:323:PX4:C35	12	1.04
(3,33)	1:A:155:THR:H	4:A:325:PX4:C35	12	1.04
(3,33)	1:A:155:THR:H	4:A:327:PX4:C35	12	1.04
(3,33)	1:A:155:THR:H	4:A:329:PX4:C35	12	1.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,33)	1:A:155:THR:H	4:A:331:PX4:C35	12	1.04
(3,33)	1:A:155:THR:H	4:A:333:PX4:C35	12	1.04
(3,33)	1:A:155:THR:H	4:A:335:PX4:C35	12	1.04
(3,33)	1:A:155:THR:H	4:A:337:PX4:C35	12	1.04
(3,33)	1:A:155:THR:H	4:A:339:PX4:C35	12	1.04
(3,33)	1:A:155:THR:H	4:A:341:PX4:C35	12	1.04
(3,33)	1:A:155:THR:H	4:A:343:PX4:C35	12	1.04
(3,33)	1:A:155:THR:H	4:A:345:PX4:C35	12	1.04
(3,33)	1:A:155:THR:H	4:A:347:PX4:C35	12	1.04
(3,33)	1:A:155:THR:H	4:A:349:PX4:C35	12	1.04
(3,33)	1:A:155:THR:H	4:A:351:PX4:C35	12	1.04
(3,33)	1:A:155:THR:H	4:A:353:PX4:C35	12	1.04
(3,33)	1:A:155:THR:H	4:A:355:PX4:C35	12	1.04
(3,33)	1:A:155:THR:H	4:A:357:PX4:C35	12	1.04
(3,33)	1:A:155:THR:H	4:A:359:PX4:C35	12	1.04
(3,33)	1:A:155:THR:H	4:A:361:PX4:C35	12	1.04
(3,33)	1:A:155:THR:H	4:A:363:PX4:C35	12	1.04
(3,33)	1:A:155:THR:H	4:A:402:PX4:C35	12	1.04
(3,33)	1:A:155:THR:H	4:A:404:PX4:C35	12	1.04
(3,33)	1:A:155:THR:H	4:A:406:PX4:C35	12	1.04
(3,33)	1:A:155:THR:H	4:A:408:PX4:C35	12	1.04
(3,33)	1:A:155:THR:H	4:A:410:PX4:C35	12	1.04
(3,33)	1:A:155:THR:H	4:A:412:PX4:C35	12	1.04
(3,33)	1:A:155:THR:H	4:A:414:PX4:C35	12	1.04
(3,33)	1:A:155:THR:H	4:A:416:PX4:C35	12	1.04
(3,33)	1:A:155:THR:H	4:A:418:PX4:C35	12	1.04
(3,33)	1:A:155:THR:H	4:A:420:PX4:C35	12	1.04
(3,33)	1:A:155:THR:H	4:A:422:PX4:C35	12	1.04
(3,33)	1:A:155:THR:H	4:A:424:PX4:C35	12	1.04
(3,33)	1:A:155:THR:H	4:A:426:PX4:C35	12	1.04
(3,33)	1:A:155:THR:H	4:A:428:PX4:C35	12	1.04
(3,33)	1:A:155:THR:H	4:A:430:PX4:C35	12	1.04
(2,954)	1:A:74:GLU:HB3	1:A:77:LEU:H	16	1.04
(2,954)	1:A:74:GLU:HB3	1:A:77:LEU:H	16	1.04
(2,948)	1:A:74:GLU:HG3	1:A:75:TYR:H	16	1.04
(2,948)	1:A:74:GLU:HG3	1:A:75:TYR:H	16	1.04
(2,920)	1:A:72:VAL:H	1:A:71:ASP:H	5	1.04
(2,920)	1:A:72:VAL:H	1:A:71:ASP:H	5	1.04
(2,899)	1:A:66:ARG:H	1:A:64:LYS:H	11	1.04
(2,804)	1:A:93:ILE:HD11	1:A:105:VAL:HG21	3	1.04
(2,804)	1:A:93:ILE:HD11	1:A:105:VAL:HG22	3	1.04
(2,804)	1:A:93:ILE:HD11	1:A:105:VAL:HG23	3	1.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,804)	1:A:93:ILE:HD12	1:A:105:VAL:HG21	3	1.04
(2,804)	1:A:93:ILE:HD12	1:A:105:VAL:HG22	3	1.04
(2,804)	1:A:93:ILE:HD12	1:A:105:VAL:HG23	3	1.04
(2,804)	1:A:93:ILE:HD13	1:A:105:VAL:HG21	3	1.04
(2,804)	1:A:93:ILE:HD13	1:A:105:VAL:HG22	3	1.04
(2,804)	1:A:93:ILE:HD13	1:A:105:VAL:HG23	3	1.04
(2,804)	1:A:93:ILE:HD11	1:A:105:VAL:HG21	11	1.04
(2,804)	1:A:93:ILE:HD11	1:A:105:VAL:HG22	11	1.04
(2,804)	1:A:93:ILE:HD11	1:A:105:VAL:HG23	11	1.04
(2,804)	1:A:93:ILE:HD12	1:A:105:VAL:HG21	11	1.04
(2,804)	1:A:93:ILE:HD12	1:A:105:VAL:HG22	11	1.04
(2,804)	1:A:93:ILE:HD12	1:A:105:VAL:HG23	11	1.04
(2,804)	1:A:93:ILE:HD13	1:A:105:VAL:HG21	11	1.04
(2,804)	1:A:93:ILE:HD13	1:A:105:VAL:HG22	11	1.04
(2,804)	1:A:93:ILE:HD13	1:A:105:VAL:HG23	11	1.04
(2,728)	1:A:211:VAL:HG11	1:A:226:LEU:HD22	9	1.04
(2,728)	1:A:211:VAL:HG11	1:A:226:LEU:HD23	9	1.04
(2,517)	1:A:200:LEU:H	1:A:196:LEU:HD21	10	1.04
(2,974)	1:A:78:PHE:H	1:A:77:LEU:HD21	13	1.03
(2,954)	1:A:74:GLU:HB3	1:A:77:LEU:H	11	1.03
(2,954)	1:A:74:GLU:HB3	1:A:77:LEU:H	11	1.03
(2,928)	1:A:72:VAL:H	1:A:73:ALA:HB1	16	1.03
(2,891)	1:A:63:GLN:H	1:A:63:GLN:HB3	1	1.03
(2,891)	1:A:63:GLN:H	1:A:63:GLN:HB2	1	1.03
(2,891)	1:A:63:GLN:H	1:A:63:GLN:HB3	1	1.03
(2,891)	1:A:63:GLN:H	1:A:63:GLN:HB2	1	1.03
(2,804)	1:A:93:ILE:HD11	1:A:105:VAL:HG21	10	1.03
(2,804)	1:A:93:ILE:HD11	1:A:105:VAL:HG22	10	1.03
(2,804)	1:A:93:ILE:HD11	1:A:105:VAL:HG23	10	1.03
(2,804)	1:A:93:ILE:HD12	1:A:105:VAL:HG21	10	1.03
(2,804)	1:A:93:ILE:HD12	1:A:105:VAL:HG22	10	1.03
(2,804)	1:A:93:ILE:HD12	1:A:105:VAL:HG23	10	1.03
(2,804)	1:A:93:ILE:HD13	1:A:105:VAL:HG21	10	1.03
(2,804)	1:A:93:ILE:HD13	1:A:105:VAL:HG22	10	1.03
(2,804)	1:A:93:ILE:HD13	1:A:105:VAL:HG23	10	1.03
(2,777)	1:A:61:ILE:HD13	1:A:48:LEU:HD21	9	1.03
(2,773)	1:A:61:ILE:HD11	1:A:48:LEU:HD21	10	1.03
(2,755)	1:A:54:LEU:HD21	1:A:58:VAL:HG11	19	1.03
(2,755)	1:A:54:LEU:HD21	1:A:58:VAL:HG12	19	1.03
(2,755)	1:A:54:LEU:HD21	1:A:58:VAL:HG13	19	1.03
(2,746)	1:A:89:VAL:HG11	1:A:122:LEU:HD21	15	1.03
(2,732)	1:A:211:VAL:HG13	1:A:226:LEU:HD22	1	1.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,732)	1:A:211:VAL:HG13	1:A:226:LEU:HD23	1	1.03
(2,542)	1:A:210:ALA:H	1:A:209:ASN:HD22	7	1.03
(2,229)	1:A:106:ASP:H	1:A:109:VAL:H	13	1.03
(2,229)	1:A:106:ASP:H	1:A:109:VAL:H	19	1.03
(2,178)	1:A:171:HIS:H	1:A:69:VAL:HG11	5	1.03
(2,178)	1:A:171:HIS:H	1:A:69:VAL:HG12	5	1.03
(2,178)	1:A:171:HIS:H	1:A:69:VAL:HG13	5	1.03
(3,6)	1:A:78:PHE:H	4:A:305:PX4:C27	3	1.02
(3,6)	1:A:78:PHE:H	4:A:307:PX4:C27	3	1.02
(3,6)	1:A:78:PHE:H	4:A:309:PX4:C27	3	1.02
(3,6)	1:A:78:PHE:H	4:A:311:PX4:C27	3	1.02
(3,6)	1:A:78:PHE:H	4:A:313:PX4:C27	3	1.02
(3,6)	1:A:78:PHE:H	4:A:315:PX4:C27	3	1.02
(3,6)	1:A:78:PHE:H	4:A:317:PX4:C27	3	1.02
(3,6)	1:A:78:PHE:H	4:A:319:PX4:C27	3	1.02
(3,6)	1:A:78:PHE:H	4:A:321:PX4:C27	3	1.02
(3,6)	1:A:78:PHE:H	4:A:323:PX4:C27	3	1.02
(3,6)	1:A:78:PHE:H	4:A:325:PX4:C27	3	1.02
(3,6)	1:A:78:PHE:H	4:A:327:PX4:C27	3	1.02
(3,6)	1:A:78:PHE:H	4:A:329:PX4:C27	3	1.02
(3,6)	1:A:78:PHE:H	4:A:331:PX4:C27	3	1.02
(3,6)	1:A:78:PHE:H	4:A:333:PX4:C27	3	1.02
(3,6)	1:A:78:PHE:H	4:A:335:PX4:C27	3	1.02
(3,6)	1:A:78:PHE:H	4:A:337:PX4:C27	3	1.02
(3,6)	1:A:78:PHE:H	4:A:339:PX4:C27	3	1.02
(3,6)	1:A:78:PHE:H	4:A:341:PX4:C27	3	1.02
(3,6)	1:A:78:PHE:H	4:A:343:PX4:C27	3	1.02
(3,6)	1:A:78:PHE:H	4:A:345:PX4:C27	3	1.02
(3,6)	1:A:78:PHE:H	4:A:347:PX4:C27	3	1.02
(3,6)	1:A:78:PHE:H	4:A:349:PX4:C27	3	1.02
(3,6)	1:A:78:PHE:H	4:A:351:PX4:C27	3	1.02
(3,6)	1:A:78:PHE:H	4:A:353:PX4:C27	3	1.02
(3,6)	1:A:78:PHE:H	4:A:355:PX4:C27	3	1.02
(3,6)	1:A:78:PHE:H	4:A:357:PX4:C27	3	1.02
(3,6)	1:A:78:PHE:H	4:A:359:PX4:C27	3	1.02
(3,6)	1:A:78:PHE:H	4:A:361:PX4:C27	3	1.02
(3,6)	1:A:78:PHE:H	4:A:363:PX4:C27	3	1.02
(3,6)	1:A:78:PHE:H	4:A:402:PX4:C27	3	1.02
(3,6)	1:A:78:PHE:H	4:A:404:PX4:C27	3	1.02
(3,6)	1:A:78:PHE:H	4:A:406:PX4:C27	3	1.02
(3,6)	1:A:78:PHE:H	4:A:408:PX4:C27	3	1.02
(3,6)	1:A:78:PHE:H	4:A:410:PX4:C27	3	1.02

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,6)	1:A:78:PHE:H	4:A:412:PX4:C27	3	1.02
(3,6)	1:A:78:PHE:H	4:A:414:PX4:C27	3	1.02
(3,6)	1:A:78:PHE:H	4:A:416:PX4:C27	3	1.02
(3,6)	1:A:78:PHE:H	4:A:418:PX4:C27	3	1.02
(3,6)	1:A:78:PHE:H	4:A:420:PX4:C27	3	1.02
(3,6)	1:A:78:PHE:H	4:A:422:PX4:C27	3	1.02
(3,6)	1:A:78:PHE:H	4:A:424:PX4:C27	3	1.02
(3,6)	1:A:78:PHE:H	4:A:426:PX4:C27	3	1.02
(3,6)	1:A:78:PHE:H	4:A:428:PX4:C27	3	1.02
(3,6)	1:A:78:PHE:H	4:A:430:PX4:C27	3	1.02
(2,930)	1:A:72:VAL:HG11	1:A:75:TYR:H	15	1.02
(2,930)	1:A:72:VAL:HG12	1:A:75:TYR:H	15	1.02
(2,930)	1:A:72:VAL:HG13	1:A:75:TYR:H	15	1.02
(2,928)	1:A:72:VAL:H	1:A:73:ALA:HB1	15	1.02
(2,766)	1:A:22:PHE:H	1:A:19:LEU:HD22	5	1.02
(2,766)	1:A:22:PHE:H	1:A:19:LEU:HD23	5	1.02
(2,729)	1:A:211:VAL:HG12	1:A:226:LEU:HD21	7	1.02
(2,542)	1:A:210:ALA:H	1:A:209:ASN:HD22	17	1.02
(2,466)	1:A:84:TRP:H	1:A:200:LEU:HD21	14	1.02
(2,424)	1:A:169:ASP:H	1:A:166:LEU:HB3	14	1.02
(2,936)	1:A:73:ALA:HB1	1:A:73:ALA:H	6	1.01
(2,936)	1:A:73:ALA:HB2	1:A:73:ALA:H	6	1.01
(2,936)	1:A:73:ALA:HB3	1:A:73:ALA:H	6	1.01
(2,928)	1:A:72:VAL:H	1:A:73:ALA:HB1	17	1.01
(2,774)	1:A:61:ILE:HD11	1:A:48:LEU:HD22	9	1.01
(2,774)	1:A:61:ILE:HD11	1:A:48:LEU:HD23	9	1.01
(2,766)	1:A:22:PHE:H	1:A:19:LEU:HD22	13	1.01
(2,766)	1:A:22:PHE:H	1:A:19:LEU:HD23	13	1.01
(2,731)	1:A:211:VAL:HG13	1:A:226:LEU:HD21	3	1.01
(2,466)	1:A:84:TRP:H	1:A:200:LEU:HD21	7	1.01
(2,229)	1:A:106:ASP:H	1:A:109:VAL:H	16	1.01
(2,229)	1:A:106:ASP:H	1:A:109:VAL:H	17	1.01
(2,984)	1:A:78:PHE:HD1	1:A:80:ASN:HD21	6	1.0
(2,984)	1:A:78:PHE:HD1	1:A:80:ASN:HD22	6	1.0
(2,984)	1:A:78:PHE:HD1	1:A:80:ASN:HD21	6	1.0
(2,984)	1:A:78:PHE:HD1	1:A:80:ASN:HD22	6	1.0
(2,516)	1:A:200:LEU:H	1:A:196:LEU:HD11	2	1.0
(2,516)	1:A:200:LEU:H	1:A:196:LEU:HD12	2	1.0
(2,516)	1:A:200:LEU:H	1:A:196:LEU:HD13	2	1.0
(2,212)	1:A:120:ILE:HD11	1:A:237:LEU:H	14	1.0
(2,212)	1:A:120:ILE:HD12	1:A:237:LEU:H	14	1.0
(2,212)	1:A:120:ILE:HD13	1:A:237:LEU:H	14	1.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,110)	1:A:11:GLN:H	1:A:14:GLN:H	9	1.0
(2,110)	1:A:11:GLN:H	1:A:14:GLN:H	11	1.0
(2,951)	1:A:74:GLU:H	1:A:76:SER:H	2	0.99
(2,930)	1:A:72:VAL:HG11	1:A:75:TYR:H	6	0.99
(2,930)	1:A:72:VAL:HG12	1:A:75:TYR:H	6	0.99
(2,930)	1:A:72:VAL:HG13	1:A:75:TYR:H	6	0.99
(2,899)	1:A:66:ARG:H	1:A:64:LYS:H	18	0.99
(2,869)	1:A:186:ILE:HD12	1:A:156:LEU:HD21	8	0.99
(2,835)	1:A:120:ILE:HD12	1:A:200:LEU:HD22	12	0.99
(2,835)	1:A:120:ILE:HD12	1:A:200:LEU:HD23	12	0.99
(2,746)	1:A:89:VAL:HG11	1:A:122:LEU:HD21	6	0.99
(2,543)	1:A:210:ALA:H	1:A:213:TYR:H	13	0.99
(2,542)	1:A:210:ALA:H	1:A:209:ASN:HD22	18	0.99
(2,414)	1:A:167:GLY:H	1:A:166:LEU:HD21	19	0.99
(2,229)	1:A:106:ASP:H	1:A:109:VAL:H	15	0.99
(2,983)	1:A:79:PRO:HD3	1:A:80:ASN:H	8	0.98
(2,983)	1:A:79:PRO:HD3	1:A:80:ASN:H	8	0.98
(2,973)	1:A:78:PHE:H	1:A:77:LEU:HD11	17	0.98
(2,973)	1:A:78:PHE:H	1:A:77:LEU:HD12	17	0.98
(2,973)	1:A:78:PHE:H	1:A:77:LEU:HD13	17	0.98
(2,954)	1:A:74:GLU:HB3	1:A:77:LEU:H	12	0.98
(2,954)	1:A:74:GLU:HB3	1:A:77:LEU:H	12	0.98
(2,891)	1:A:63:GLN:H	1:A:63:GLN:HB3	6	0.98
(2,891)	1:A:63:GLN:H	1:A:63:GLN:HB2	6	0.98
(2,891)	1:A:63:GLN:H	1:A:63:GLN:HB3	6	0.98
(2,891)	1:A:63:GLN:H	1:A:63:GLN:HB2	6	0.98
(2,861)	1:A:186:ILE:HD13	1:A:156:LEU:HD21	1	0.98
(2,708)	1:A:226:LEU:HD11	1:A:231:ILE:HG13	19	0.98
(2,708)	1:A:226:LEU:HD12	1:A:231:ILE:HG13	19	0.98
(2,708)	1:A:226:LEU:HD13	1:A:231:ILE:HG13	19	0.98
(2,708)	1:A:226:LEU:HD11	1:A:231:ILE:HG12	19	0.98
(2,708)	1:A:226:LEU:HD12	1:A:231:ILE:HG12	19	0.98
(2,708)	1:A:226:LEU:HD13	1:A:231:ILE:HG12	19	0.98
(2,110)	1:A:11:GLN:H	1:A:14:GLN:H	13	0.98
(2,928)	1:A:72:VAL:H	1:A:73:ALA:HB1	1	0.97
(2,912)	1:A:70:PRO:HB3	1:A:76:SER:H	10	0.97
(2,912)	1:A:70:PRO:HB2	1:A:76:SER:H	10	0.97
(2,905)	1:A:67:CYS:HA	1:A:68:GLY:H	7	0.97
(2,902)	1:A:66:ARG:HA	1:A:68:GLY:H	16	0.97
(2,899)	1:A:66:ARG:H	1:A:64:LYS:H	1	0.97
(2,836)	1:A:120:ILE:HD13	1:A:200:LEU:HD21	1	0.97
(2,775)	1:A:61:ILE:HD12	1:A:48:LEU:HD21	16	0.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,755)	1:A:54:LEU:HD21	1:A:58:VAL:HG11	2	0.97
(2,755)	1:A:54:LEU:HD21	1:A:58:VAL:HG12	2	0.97
(2,755)	1:A:54:LEU:HD21	1:A:58:VAL:HG13	2	0.97
(2,542)	1:A:210:ALA:H	1:A:209:ASN:HD22	5	0.97
(2,467)	1:A:84:TRP:H	1:A:200:LEU:HD22	19	0.97
(2,467)	1:A:84:TRP:H	1:A:200:LEU:HD23	19	0.97
(2,424)	1:A:169:ASP:H	1:A:166:LEU:HB3	17	0.97
(2,264)	1:A:113:LEU:H	1:A:196:LEU:HD21	11	0.97
(2,905)	1:A:67:CYS:HA	1:A:68:GLY:H	19	0.96
(2,899)	1:A:66:ARG:H	1:A:64:LYS:H	2	0.96
(2,891)	1:A:63:GLN:H	1:A:63:GLN:HB3	14	0.96
(2,891)	1:A:63:GLN:H	1:A:63:GLN:HB2	14	0.96
(2,891)	1:A:63:GLN:H	1:A:63:GLN:HB3	14	0.96
(2,891)	1:A:63:GLN:H	1:A:63:GLN:HB2	14	0.96
(2,891)	1:A:63:GLN:H	1:A:63:GLN:HB3	17	0.96
(2,891)	1:A:63:GLN:H	1:A:63:GLN:HB2	17	0.96
(2,891)	1:A:63:GLN:H	1:A:63:GLN:HB3	17	0.96
(2,891)	1:A:63:GLN:H	1:A:63:GLN:HB2	17	0.96
(2,804)	1:A:93:ILE:HD11	1:A:105:VAL:HG21	8	0.96
(2,804)	1:A:93:ILE:HD11	1:A:105:VAL:HG22	8	0.96
(2,804)	1:A:93:ILE:HD11	1:A:105:VAL:HG23	8	0.96
(2,804)	1:A:93:ILE:HD12	1:A:105:VAL:HG21	8	0.96
(2,804)	1:A:93:ILE:HD12	1:A:105:VAL:HG22	8	0.96
(2,804)	1:A:93:ILE:HD12	1:A:105:VAL:HG23	8	0.96
(2,804)	1:A:93:ILE:HD13	1:A:105:VAL:HG21	8	0.96
(2,804)	1:A:93:ILE:HD13	1:A:105:VAL:HG22	8	0.96
(2,804)	1:A:93:ILE:HD13	1:A:105:VAL:HG23	8	0.96
(2,732)	1:A:211:VAL:HG13	1:A:226:LEU:HD22	17	0.96
(2,732)	1:A:211:VAL:HG13	1:A:226:LEU:HD23	17	0.96
(2,229)	1:A:106:ASP:H	1:A:109:VAL:H	5	0.96
(2,229)	1:A:106:ASP:H	1:A:109:VAL:H	9	0.96
(2,229)	1:A:106:ASP:H	1:A:109:VAL:H	14	0.96
(2,178)	1:A:171:HIS:H	1:A:69:VAL:HG11	11	0.96
(2,178)	1:A:171:HIS:H	1:A:69:VAL:HG12	11	0.96
(2,178)	1:A:171:HIS:H	1:A:69:VAL:HG13	11	0.96
(2,10)	1:A:92:ARG:H	1:A:93:ILE:HG13	17	0.96
(2,10)	1:A:92:ARG:H	1:A:93:ILE:HG12	17	0.96
(3,33)	1:A:155:THR:H	4:A:305:PX4:C35	19	0.95
(3,33)	1:A:155:THR:H	4:A:307:PX4:C35	19	0.95
(3,33)	1:A:155:THR:H	4:A:309:PX4:C35	19	0.95
(3,33)	1:A:155:THR:H	4:A:311:PX4:C35	19	0.95
(3,33)	1:A:155:THR:H	4:A:313:PX4:C35	19	0.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,33)	1:A:155:THR:H	4:A:315:PX4:C35	19	0.95
(3,33)	1:A:155:THR:H	4:A:317:PX4:C35	19	0.95
(3,33)	1:A:155:THR:H	4:A:319:PX4:C35	19	0.95
(3,33)	1:A:155:THR:H	4:A:321:PX4:C35	19	0.95
(3,33)	1:A:155:THR:H	4:A:323:PX4:C35	19	0.95
(3,33)	1:A:155:THR:H	4:A:325:PX4:C35	19	0.95
(3,33)	1:A:155:THR:H	4:A:327:PX4:C35	19	0.95
(3,33)	1:A:155:THR:H	4:A:329:PX4:C35	19	0.95
(3,33)	1:A:155:THR:H	4:A:331:PX4:C35	19	0.95
(3,33)	1:A:155:THR:H	4:A:333:PX4:C35	19	0.95
(3,33)	1:A:155:THR:H	4:A:335:PX4:C35	19	0.95
(3,33)	1:A:155:THR:H	4:A:337:PX4:C35	19	0.95
(3,33)	1:A:155:THR:H	4:A:339:PX4:C35	19	0.95
(3,33)	1:A:155:THR:H	4:A:341:PX4:C35	19	0.95
(3,33)	1:A:155:THR:H	4:A:343:PX4:C35	19	0.95
(3,33)	1:A:155:THR:H	4:A:345:PX4:C35	19	0.95
(3,33)	1:A:155:THR:H	4:A:347:PX4:C35	19	0.95
(3,33)	1:A:155:THR:H	4:A:349:PX4:C35	19	0.95
(3,33)	1:A:155:THR:H	4:A:351:PX4:C35	19	0.95
(3,33)	1:A:155:THR:H	4:A:353:PX4:C35	19	0.95
(3,33)	1:A:155:THR:H	4:A:355:PX4:C35	19	0.95
(3,33)	1:A:155:THR:H	4:A:357:PX4:C35	19	0.95
(3,33)	1:A:155:THR:H	4:A:359:PX4:C35	19	0.95
(3,33)	1:A:155:THR:H	4:A:361:PX4:C35	19	0.95
(3,33)	1:A:155:THR:H	4:A:363:PX4:C35	19	0.95
(3,33)	1:A:155:THR:H	4:A:402:PX4:C35	19	0.95
(3,33)	1:A:155:THR:H	4:A:404:PX4:C35	19	0.95
(3,33)	1:A:155:THR:H	4:A:406:PX4:C35	19	0.95
(3,33)	1:A:155:THR:H	4:A:408:PX4:C35	19	0.95
(3,33)	1:A:155:THR:H	4:A:410:PX4:C35	19	0.95
(3,33)	1:A:155:THR:H	4:A:412:PX4:C35	19	0.95
(3,33)	1:A:155:THR:H	4:A:414:PX4:C35	19	0.95
(3,33)	1:A:155:THR:H	4:A:416:PX4:C35	19	0.95
(3,33)	1:A:155:THR:H	4:A:418:PX4:C35	19	0.95
(3,33)	1:A:155:THR:H	4:A:420:PX4:C35	19	0.95
(3,33)	1:A:155:THR:H	4:A:422:PX4:C35	19	0.95
(3,33)	1:A:155:THR:H	4:A:424:PX4:C35	19	0.95
(3,33)	1:A:155:THR:H	4:A:426:PX4:C35	19	0.95
(3,33)	1:A:155:THR:H	4:A:428:PX4:C35	19	0.95
(3,33)	1:A:155:THR:H	4:A:430:PX4:C35	19	0.95
(3,21)	1:A:77:LEU:H	4:A:305:PX4:C35	11	0.95
(3,21)	1:A:77:LEU:H	4:A:307:PX4:C35	11	0.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,21)	1:A:77:LEU:H	4:A:309:PX4:C35	11	0.95
(3,21)	1:A:77:LEU:H	4:A:311:PX4:C35	11	0.95
(3,21)	1:A:77:LEU:H	4:A:313:PX4:C35	11	0.95
(3,21)	1:A:77:LEU:H	4:A:315:PX4:C35	11	0.95
(3,21)	1:A:77:LEU:H	4:A:317:PX4:C35	11	0.95
(3,21)	1:A:77:LEU:H	4:A:319:PX4:C35	11	0.95
(3,21)	1:A:77:LEU:H	4:A:321:PX4:C35	11	0.95
(3,21)	1:A:77:LEU:H	4:A:323:PX4:C35	11	0.95
(3,21)	1:A:77:LEU:H	4:A:325:PX4:C35	11	0.95
(3,21)	1:A:77:LEU:H	4:A:327:PX4:C35	11	0.95
(3,21)	1:A:77:LEU:H	4:A:329:PX4:C35	11	0.95
(3,21)	1:A:77:LEU:H	4:A:331:PX4:C35	11	0.95
(3,21)	1:A:77:LEU:H	4:A:333:PX4:C35	11	0.95
(3,21)	1:A:77:LEU:H	4:A:335:PX4:C35	11	0.95
(3,21)	1:A:77:LEU:H	4:A:337:PX4:C35	11	0.95
(3,21)	1:A:77:LEU:H	4:A:339:PX4:C35	11	0.95
(3,21)	1:A:77:LEU:H	4:A:341:PX4:C35	11	0.95
(3,21)	1:A:77:LEU:H	4:A:343:PX4:C35	11	0.95
(3,21)	1:A:77:LEU:H	4:A:345:PX4:C35	11	0.95
(3,21)	1:A:77:LEU:H	4:A:347:PX4:C35	11	0.95
(3,21)	1:A:77:LEU:H	4:A:349:PX4:C35	11	0.95
(3,21)	1:A:77:LEU:H	4:A:351:PX4:C35	11	0.95
(3,21)	1:A:77:LEU:H	4:A:353:PX4:C35	11	0.95
(3,21)	1:A:77:LEU:H	4:A:355:PX4:C35	11	0.95
(3,21)	1:A:77:LEU:H	4:A:357:PX4:C35	11	0.95
(3,21)	1:A:77:LEU:H	4:A:359:PX4:C35	11	0.95
(3,21)	1:A:77:LEU:H	4:A:361:PX4:C35	11	0.95
(3,21)	1:A:77:LEU:H	4:A:363:PX4:C35	11	0.95
(3,21)	1:A:77:LEU:H	4:A:402:PX4:C35	11	0.95
(3,21)	1:A:77:LEU:H	4:A:404:PX4:C35	11	0.95
(3,21)	1:A:77:LEU:H	4:A:406:PX4:C35	11	0.95
(3,21)	1:A:77:LEU:H	4:A:408:PX4:C35	11	0.95
(3,21)	1:A:77:LEU:H	4:A:410:PX4:C35	11	0.95
(3,21)	1:A:77:LEU:H	4:A:412:PX4:C35	11	0.95
(3,21)	1:A:77:LEU:H	4:A:414:PX4:C35	11	0.95
(3,21)	1:A:77:LEU:H	4:A:416:PX4:C35	11	0.95
(3,21)	1:A:77:LEU:H	4:A:418:PX4:C35	11	0.95
(3,21)	1:A:77:LEU:H	4:A:420:PX4:C35	11	0.95
(3,21)	1:A:77:LEU:H	4:A:422:PX4:C35	11	0.95
(3,21)	1:A:77:LEU:H	4:A:424:PX4:C35	11	0.95
(3,21)	1:A:77:LEU:H	4:A:426:PX4:C35	11	0.95
(3,21)	1:A:77:LEU:H	4:A:428:PX4:C35	11	0.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,21)	1:A:77:LEU:H	4:A:430:PX4:C35	11	0.95
(2,975)	1:A:78:PHE:H	1:A:77:LEU:HD22	10	0.95
(2,975)	1:A:78:PHE:H	1:A:77:LEU:HD23	10	0.95
(2,948)	1:A:74:GLU:HG3	1:A:75:TYR:H	11	0.95
(2,948)	1:A:74:GLU:HG3	1:A:75:TYR:H	11	0.95
(2,930)	1:A:72:VAL:HG11	1:A:75:TYR:H	3	0.95
(2,930)	1:A:72:VAL:HG12	1:A:75:TYR:H	3	0.95
(2,930)	1:A:72:VAL:HG13	1:A:75:TYR:H	3	0.95
(2,928)	1:A:72:VAL:H	1:A:73:ALA:HB1	4	0.95
(2,928)	1:A:72:VAL:H	1:A:73:ALA:HB1	8	0.95
(2,898)	1:A:66:ARG:H	1:A:63:GLN:HB3	20	0.95
(2,898)	1:A:66:ARG:H	1:A:63:GLN:HB2	20	0.95
(2,891)	1:A:63:GLN:H	1:A:63:GLN:HB3	2	0.95
(2,891)	1:A:63:GLN:H	1:A:63:GLN:HB2	2	0.95
(2,891)	1:A:63:GLN:H	1:A:63:GLN:HB3	2	0.95
(2,891)	1:A:63:GLN:H	1:A:63:GLN:HB2	2	0.95
(2,766)	1:A:22:PHE:H	1:A:19:LEU:HD22	12	0.95
(2,766)	1:A:22:PHE:H	1:A:19:LEU:HD23	12	0.95
(2,766)	1:A:22:PHE:H	1:A:19:LEU:HD22	19	0.95
(2,766)	1:A:22:PHE:H	1:A:19:LEU:HD23	19	0.95
(2,760)	1:A:54:LEU:HD22	1:A:59:ILE:HD11	5	0.95
(2,760)	1:A:54:LEU:HD22	1:A:59:ILE:HD12	5	0.95
(2,760)	1:A:54:LEU:HD22	1:A:59:ILE:HD13	5	0.95
(2,760)	1:A:54:LEU:HD23	1:A:59:ILE:HD11	5	0.95
(2,760)	1:A:54:LEU:HD23	1:A:59:ILE:HD12	5	0.95
(2,760)	1:A:54:LEU:HD23	1:A:59:ILE:HD13	5	0.95
(2,760)	1:A:54:LEU:HD22	1:A:59:ILE:HD11	10	0.95
(2,760)	1:A:54:LEU:HD22	1:A:59:ILE:HD12	10	0.95
(2,760)	1:A:54:LEU:HD22	1:A:59:ILE:HD13	10	0.95
(2,760)	1:A:54:LEU:HD23	1:A:59:ILE:HD11	10	0.95
(2,760)	1:A:54:LEU:HD23	1:A:59:ILE:HD12	10	0.95
(2,760)	1:A:54:LEU:HD23	1:A:59:ILE:HD13	10	0.95
(2,627)	1:A:13:GLU:H	1:A:10:LEU:H	7	0.95
(2,516)	1:A:200:LEU:H	1:A:196:LEU:HD11	3	0.95
(2,516)	1:A:200:LEU:H	1:A:196:LEU:HD12	3	0.95
(2,516)	1:A:200:LEU:H	1:A:196:LEU:HD13	3	0.95
(2,110)	1:A:11:GLN:H	1:A:14:GLN:H	17	0.95
(2,983)	1:A:79:PRO:HD3	1:A:80:ASN:H	18	0.94
(2,983)	1:A:79:PRO:HD3	1:A:80:ASN:H	18	0.94
(2,899)	1:A:66:ARG:H	1:A:64:LYS:H	19	0.94
(2,759)	1:A:54:LEU:HD21	1:A:59:ILE:HD11	3	0.94
(2,759)	1:A:54:LEU:HD21	1:A:59:ILE:HD12	3	0.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,759)	1:A:54:LEU:HD21	1:A:59:ILE:HD13	3	0.94
(2,758)	1:A:54:LEU:HD22	1:A:39:LEU:HD11	8	0.94
(2,758)	1:A:54:LEU:HD22	1:A:39:LEU:HD12	8	0.94
(2,758)	1:A:54:LEU:HD22	1:A:39:LEU:HD13	8	0.94
(2,758)	1:A:54:LEU:HD23	1:A:39:LEU:HD11	8	0.94
(2,758)	1:A:54:LEU:HD23	1:A:39:LEU:HD12	8	0.94
(2,758)	1:A:54:LEU:HD23	1:A:39:LEU:HD13	8	0.94
(2,75)	1:A:55:ASN:H	1:A:59:ILE:H	10	0.94
(2,510)	1:A:200:LEU:HD21	1:A:199:SER:H	6	0.94
(2,212)	1:A:120:ILE:HD11	1:A:237:LEU:H	4	0.94
(2,212)	1:A:120:ILE:HD12	1:A:237:LEU:H	4	0.94
(2,212)	1:A:120:ILE:HD13	1:A:237:LEU:H	4	0.94
(3,33)	1:A:155:THR:H	4:A:305:PX4:C35	6	0.93
(3,33)	1:A:155:THR:H	4:A:307:PX4:C35	6	0.93
(3,33)	1:A:155:THR:H	4:A:309:PX4:C35	6	0.93
(3,33)	1:A:155:THR:H	4:A:311:PX4:C35	6	0.93
(3,33)	1:A:155:THR:H	4:A:313:PX4:C35	6	0.93
(3,33)	1:A:155:THR:H	4:A:315:PX4:C35	6	0.93
(3,33)	1:A:155:THR:H	4:A:317:PX4:C35	6	0.93
(3,33)	1:A:155:THR:H	4:A:319:PX4:C35	6	0.93
(3,33)	1:A:155:THR:H	4:A:321:PX4:C35	6	0.93
(3,33)	1:A:155:THR:H	4:A:323:PX4:C35	6	0.93
(3,33)	1:A:155:THR:H	4:A:325:PX4:C35	6	0.93
(3,33)	1:A:155:THR:H	4:A:327:PX4:C35	6	0.93
(3,33)	1:A:155:THR:H	4:A:329:PX4:C35	6	0.93
(3,33)	1:A:155:THR:H	4:A:331:PX4:C35	6	0.93
(3,33)	1:A:155:THR:H	4:A:333:PX4:C35	6	0.93
(3,33)	1:A:155:THR:H	4:A:335:PX4:C35	6	0.93
(3,33)	1:A:155:THR:H	4:A:337:PX4:C35	6	0.93
(3,33)	1:A:155:THR:H	4:A:339:PX4:C35	6	0.93
(3,33)	1:A:155:THR:H	4:A:341:PX4:C35	6	0.93
(3,33)	1:A:155:THR:H	4:A:343:PX4:C35	6	0.93
(3,33)	1:A:155:THR:H	4:A:345:PX4:C35	6	0.93
(3,33)	1:A:155:THR:H	4:A:347:PX4:C35	6	0.93
(3,33)	1:A:155:THR:H	4:A:349:PX4:C35	6	0.93
(3,33)	1:A:155:THR:H	4:A:351:PX4:C35	6	0.93
(3,33)	1:A:155:THR:H	4:A:353:PX4:C35	6	0.93
(3,33)	1:A:155:THR:H	4:A:355:PX4:C35	6	0.93
(3,33)	1:A:155:THR:H	4:A:357:PX4:C35	6	0.93
(3,33)	1:A:155:THR:H	4:A:359:PX4:C35	6	0.93
(3,33)	1:A:155:THR:H	4:A:361:PX4:C35	6	0.93
(3,33)	1:A:155:THR:H	4:A:363:PX4:C35	6	0.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,33)	1:A:155:THR:H	4:A:402:PX4:C35	6	0.93
(3,33)	1:A:155:THR:H	4:A:404:PX4:C35	6	0.93
(3,33)	1:A:155:THR:H	4:A:406:PX4:C35	6	0.93
(3,33)	1:A:155:THR:H	4:A:408:PX4:C35	6	0.93
(3,33)	1:A:155:THR:H	4:A:410:PX4:C35	6	0.93
(3,33)	1:A:155:THR:H	4:A:412:PX4:C35	6	0.93
(3,33)	1:A:155:THR:H	4:A:414:PX4:C35	6	0.93
(3,33)	1:A:155:THR:H	4:A:416:PX4:C35	6	0.93
(3,33)	1:A:155:THR:H	4:A:418:PX4:C35	6	0.93
(3,33)	1:A:155:THR:H	4:A:420:PX4:C35	6	0.93
(3,33)	1:A:155:THR:H	4:A:422:PX4:C35	6	0.93
(3,33)	1:A:155:THR:H	4:A:424:PX4:C35	6	0.93
(3,33)	1:A:155:THR:H	4:A:426:PX4:C35	6	0.93
(3,33)	1:A:155:THR:H	4:A:428:PX4:C35	6	0.93
(3,33)	1:A:155:THR:H	4:A:430:PX4:C35	6	0.93
(2,974)	1:A:78:PHE:H	1:A:77:LEU:HD21	6	0.93
(2,970)	1:A:77:LEU:HG	1:A:78:PHE:H	19	0.93
(2,954)	1:A:74:GLU:HB3	1:A:77:LEU:H	6	0.93
(2,954)	1:A:74:GLU:HB3	1:A:77:LEU:H	6	0.93
(2,936)	1:A:73:ALA:HB1	1:A:73:ALA:H	5	0.93
(2,936)	1:A:73:ALA:HB2	1:A:73:ALA:H	5	0.93
(2,936)	1:A:73:ALA:HB3	1:A:73:ALA:H	5	0.93
(2,936)	1:A:73:ALA:HB1	1:A:73:ALA:H	12	0.93
(2,936)	1:A:73:ALA:HB2	1:A:73:ALA:H	12	0.93
(2,936)	1:A:73:ALA:HB3	1:A:73:ALA:H	12	0.93
(2,932)	1:A:72:VAL:HG11	1:A:76:SER:H	9	0.93
(2,932)	1:A:72:VAL:HG12	1:A:76:SER:H	9	0.93
(2,932)	1:A:72:VAL:HG13	1:A:76:SER:H	9	0.93
(2,925)	1:A:72:VAL:HG21	1:A:73:ALA:H	9	0.93
(2,925)	1:A:72:VAL:HG22	1:A:73:ALA:H	9	0.93
(2,925)	1:A:72:VAL:HG23	1:A:73:ALA:H	9	0.93
(2,925)	1:A:72:VAL:HG11	1:A:73:ALA:H	9	0.93
(2,925)	1:A:72:VAL:HG12	1:A:73:ALA:H	9	0.93
(2,925)	1:A:72:VAL:HG13	1:A:73:ALA:H	9	0.93
(2,804)	1:A:93:ILE:HD11	1:A:105:VAL:HG21	14	0.93
(2,804)	1:A:93:ILE:HD11	1:A:105:VAL:HG22	14	0.93
(2,804)	1:A:93:ILE:HD11	1:A:105:VAL:HG23	14	0.93
(2,804)	1:A:93:ILE:HD12	1:A:105:VAL:HG21	14	0.93
(2,804)	1:A:93:ILE:HD12	1:A:105:VAL:HG22	14	0.93
(2,804)	1:A:93:ILE:HD12	1:A:105:VAL:HG23	14	0.93
(2,804)	1:A:93:ILE:HD13	1:A:105:VAL:HG21	14	0.93
(2,804)	1:A:93:ILE:HD13	1:A:105:VAL:HG22	14	0.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,804)	1:A:93:ILE:HD13	1:A:105:VAL:HG23	14	0.93
(2,758)	1:A:54:LEU:HD22	1:A:39:LEU:HD11	1	0.93
(2,758)	1:A:54:LEU:HD22	1:A:39:LEU:HD12	1	0.93
(2,758)	1:A:54:LEU:HD22	1:A:39:LEU:HD13	1	0.93
(2,758)	1:A:54:LEU:HD23	1:A:39:LEU:HD11	1	0.93
(2,758)	1:A:54:LEU:HD23	1:A:39:LEU:HD12	1	0.93
(2,758)	1:A:54:LEU:HD23	1:A:39:LEU:HD13	1	0.93
(2,414)	1:A:167:GLY:H	1:A:166:LEU:HD21	10	0.93
(2,264)	1:A:113:LEU:H	1:A:196:LEU:HD21	4	0.93
(2,110)	1:A:11:GLN:H	1:A:14:GLN:H	19	0.93
(2,985)	1:A:80:ASN:H	1:A:78:PHE:HD1	15	0.92
(2,983)	1:A:79:PRO:HD3	1:A:80:ASN:H	12	0.92
(2,983)	1:A:79:PRO:HD3	1:A:80:ASN:H	12	0.92
(2,981)	1:A:78:PHE:H	1:A:79:PRO:HG3	9	0.92
(2,981)	1:A:78:PHE:H	1:A:79:PRO:HG3	9	0.92
(2,930)	1:A:72:VAL:HG11	1:A:75:TYR:H	13	0.92
(2,930)	1:A:72:VAL:HG12	1:A:75:TYR:H	13	0.92
(2,930)	1:A:72:VAL:HG13	1:A:75:TYR:H	13	0.92
(2,902)	1:A:66:ARG:HA	1:A:68:GLY:H	20	0.92
(2,899)	1:A:66:ARG:H	1:A:64:LYS:H	15	0.92
(2,718)	1:A:54:LEU:HD11	1:A:59:ILE:HD11	2	0.92
(2,718)	1:A:54:LEU:HD11	1:A:59:ILE:HD12	2	0.92
(2,718)	1:A:54:LEU:HD11	1:A:59:ILE:HD13	2	0.92
(2,718)	1:A:54:LEU:HD12	1:A:59:ILE:HD11	2	0.92
(2,718)	1:A:54:LEU:HD12	1:A:59:ILE:HD12	2	0.92
(2,718)	1:A:54:LEU:HD12	1:A:59:ILE:HD13	2	0.92
(2,718)	1:A:54:LEU:HD13	1:A:59:ILE:HD11	2	0.92
(2,718)	1:A:54:LEU:HD13	1:A:59:ILE:HD12	2	0.92
(2,718)	1:A:54:LEU:HD13	1:A:59:ILE:HD13	2	0.92
(2,542)	1:A:210:ALA:H	1:A:209:ASN:HD22	2	0.92
(2,542)	1:A:210:ALA:H	1:A:209:ASN:HD22	19	0.92
(2,517)	1:A:200:LEU:H	1:A:196:LEU:HD21	7	0.92
(2,516)	1:A:200:LEU:H	1:A:196:LEU:HD11	10	0.92
(2,516)	1:A:200:LEU:H	1:A:196:LEU:HD12	10	0.92
(2,516)	1:A:200:LEU:H	1:A:196:LEU:HD13	10	0.92
(2,466)	1:A:84:TRP:H	1:A:200:LEU:HD21	12	0.92
(2,424)	1:A:169:ASP:H	1:A:166:LEU:HB3	16	0.92
(2,392)	1:A:157:ALA:H	1:A:68:GLY:H	15	0.92
(2,229)	1:A:106:ASP:H	1:A:109:VAL:H	6	0.92
(2,178)	1:A:171:HIS:H	1:A:69:VAL:HG11	8	0.92
(2,178)	1:A:171:HIS:H	1:A:69:VAL:HG12	8	0.92
(2,178)	1:A:171:HIS:H	1:A:69:VAL:HG13	8	0.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,110)	1:A:11:GLN:H	1:A:14:GLN:H	4	0.92
(3,6)	1:A:78:PHE:H	4:A:305:PX4:C27	6	0.91
(3,6)	1:A:78:PHE:H	4:A:307:PX4:C27	6	0.91
(3,6)	1:A:78:PHE:H	4:A:309:PX4:C27	6	0.91
(3,6)	1:A:78:PHE:H	4:A:311:PX4:C27	6	0.91
(3,6)	1:A:78:PHE:H	4:A:313:PX4:C27	6	0.91
(3,6)	1:A:78:PHE:H	4:A:315:PX4:C27	6	0.91
(3,6)	1:A:78:PHE:H	4:A:317:PX4:C27	6	0.91
(3,6)	1:A:78:PHE:H	4:A:319:PX4:C27	6	0.91
(3,6)	1:A:78:PHE:H	4:A:321:PX4:C27	6	0.91
(3,6)	1:A:78:PHE:H	4:A:323:PX4:C27	6	0.91
(3,6)	1:A:78:PHE:H	4:A:325:PX4:C27	6	0.91
(3,6)	1:A:78:PHE:H	4:A:327:PX4:C27	6	0.91
(3,6)	1:A:78:PHE:H	4:A:329:PX4:C27	6	0.91
(3,6)	1:A:78:PHE:H	4:A:331:PX4:C27	6	0.91
(3,6)	1:A:78:PHE:H	4:A:333:PX4:C27	6	0.91
(3,6)	1:A:78:PHE:H	4:A:335:PX4:C27	6	0.91
(3,6)	1:A:78:PHE:H	4:A:337:PX4:C27	6	0.91
(3,6)	1:A:78:PHE:H	4:A:339:PX4:C27	6	0.91
(3,6)	1:A:78:PHE:H	4:A:341:PX4:C27	6	0.91
(3,6)	1:A:78:PHE:H	4:A:343:PX4:C27	6	0.91
(3,6)	1:A:78:PHE:H	4:A:345:PX4:C27	6	0.91
(3,6)	1:A:78:PHE:H	4:A:347:PX4:C27	6	0.91
(3,6)	1:A:78:PHE:H	4:A:349:PX4:C27	6	0.91
(3,6)	1:A:78:PHE:H	4:A:351:PX4:C27	6	0.91
(3,6)	1:A:78:PHE:H	4:A:353:PX4:C27	6	0.91
(3,6)	1:A:78:PHE:H	4:A:355:PX4:C27	6	0.91
(3,6)	1:A:78:PHE:H	4:A:357:PX4:C27	6	0.91
(3,6)	1:A:78:PHE:H	4:A:359:PX4:C27	6	0.91
(3,6)	1:A:78:PHE:H	4:A:361:PX4:C27	6	0.91
(3,6)	1:A:78:PHE:H	4:A:363:PX4:C27	6	0.91
(3,6)	1:A:78:PHE:H	4:A:402:PX4:C27	6	0.91
(3,6)	1:A:78:PHE:H	4:A:404:PX4:C27	6	0.91
(3,6)	1:A:78:PHE:H	4:A:406:PX4:C27	6	0.91
(3,6)	1:A:78:PHE:H	4:A:408:PX4:C27	6	0.91
(3,6)	1:A:78:PHE:H	4:A:410:PX4:C27	6	0.91
(3,6)	1:A:78:PHE:H	4:A:412:PX4:C27	6	0.91
(3,6)	1:A:78:PHE:H	4:A:414:PX4:C27	6	0.91
(3,6)	1:A:78:PHE:H	4:A:416:PX4:C27	6	0.91
(3,6)	1:A:78:PHE:H	4:A:418:PX4:C27	6	0.91
(3,6)	1:A:78:PHE:H	4:A:420:PX4:C27	6	0.91
(3,6)	1:A:78:PHE:H	4:A:422:PX4:C27	6	0.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,6)	1:A:78:PHE:H	4:A:424:PX4:C27	6	0.91
(3,6)	1:A:78:PHE:H	4:A:426:PX4:C27	6	0.91
(3,6)	1:A:78:PHE:H	4:A:428:PX4:C27	6	0.91
(3,6)	1:A:78:PHE:H	4:A:430:PX4:C27	6	0.91
(2,913)	1:A:71:ASP:H	1:A:70:PRO:HB3	2	0.91
(2,913)	1:A:71:ASP:H	1:A:70:PRO:HB2	2	0.91
(2,899)	1:A:66:ARG:H	1:A:64:LYS:H	7	0.91
(2,891)	1:A:63:GLN:H	1:A:63:GLN:HB3	16	0.91
(2,891)	1:A:63:GLN:H	1:A:63:GLN:HB2	16	0.91
(2,891)	1:A:63:GLN:H	1:A:63:GLN:HB3	16	0.91
(2,891)	1:A:63:GLN:H	1:A:63:GLN:HB2	16	0.91
(2,866)	1:A:186:ILE:HD11	1:A:156:LEU:HD11	16	0.91
(2,866)	1:A:186:ILE:HD11	1:A:156:LEU:HD12	16	0.91
(2,866)	1:A:186:ILE:HD11	1:A:156:LEU:HD13	16	0.91
(2,866)	1:A:186:ILE:HD12	1:A:156:LEU:HD11	16	0.91
(2,866)	1:A:186:ILE:HD12	1:A:156:LEU:HD12	16	0.91
(2,866)	1:A:186:ILE:HD12	1:A:156:LEU:HD13	16	0.91
(2,866)	1:A:186:ILE:HD13	1:A:156:LEU:HD11	16	0.91
(2,866)	1:A:186:ILE:HD13	1:A:156:LEU:HD12	16	0.91
(2,866)	1:A:186:ILE:HD13	1:A:156:LEU:HD13	16	0.91
(2,835)	1:A:120:ILE:HD12	1:A:200:LEU:HD22	2	0.91
(2,835)	1:A:120:ILE:HD12	1:A:200:LEU:HD23	2	0.91
(2,835)	1:A:120:ILE:HD12	1:A:200:LEU:HD22	8	0.91
(2,835)	1:A:120:ILE:HD12	1:A:200:LEU:HD23	8	0.91
(2,746)	1:A:89:VAL:HG11	1:A:122:LEU:HD21	13	0.91
(2,516)	1:A:200:LEU:H	1:A:196:LEU:HD11	11	0.91
(2,516)	1:A:200:LEU:H	1:A:196:LEU:HD12	11	0.91
(2,516)	1:A:200:LEU:H	1:A:196:LEU:HD13	11	0.91
(2,473)	1:A:186:ILE:H	1:A:156:LEU:HD22	17	0.91
(2,473)	1:A:186:ILE:H	1:A:156:LEU:HD23	17	0.91
(2,264)	1:A:113:LEU:H	1:A:196:LEU:HD21	17	0.91
(3,33)	1:A:155:THR:H	4:A:305:PX4:C35	4	0.9
(3,33)	1:A:155:THR:H	4:A:307:PX4:C35	4	0.9
(3,33)	1:A:155:THR:H	4:A:309:PX4:C35	4	0.9
(3,33)	1:A:155:THR:H	4:A:311:PX4:C35	4	0.9
(3,33)	1:A:155:THR:H	4:A:313:PX4:C35	4	0.9
(3,33)	1:A:155:THR:H	4:A:315:PX4:C35	4	0.9
(3,33)	1:A:155:THR:H	4:A:317:PX4:C35	4	0.9
(3,33)	1:A:155:THR:H	4:A:319:PX4:C35	4	0.9
(3,33)	1:A:155:THR:H	4:A:321:PX4:C35	4	0.9
(3,33)	1:A:155:THR:H	4:A:323:PX4:C35	4	0.9
(3,33)	1:A:155:THR:H	4:A:325:PX4:C35	4	0.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,33)	1:A:155:THR:H	4:A:327:PX4:C35	4	0.9
(3,33)	1:A:155:THR:H	4:A:329:PX4:C35	4	0.9
(3,33)	1:A:155:THR:H	4:A:331:PX4:C35	4	0.9
(3,33)	1:A:155:THR:H	4:A:333:PX4:C35	4	0.9
(3,33)	1:A:155:THR:H	4:A:335:PX4:C35	4	0.9
(3,33)	1:A:155:THR:H	4:A:337:PX4:C35	4	0.9
(3,33)	1:A:155:THR:H	4:A:339:PX4:C35	4	0.9
(3,33)	1:A:155:THR:H	4:A:341:PX4:C35	4	0.9
(3,33)	1:A:155:THR:H	4:A:343:PX4:C35	4	0.9
(3,33)	1:A:155:THR:H	4:A:345:PX4:C35	4	0.9
(3,33)	1:A:155:THR:H	4:A:347:PX4:C35	4	0.9
(3,33)	1:A:155:THR:H	4:A:349:PX4:C35	4	0.9
(3,33)	1:A:155:THR:H	4:A:351:PX4:C35	4	0.9
(3,33)	1:A:155:THR:H	4:A:353:PX4:C35	4	0.9
(3,33)	1:A:155:THR:H	4:A:355:PX4:C35	4	0.9
(3,33)	1:A:155:THR:H	4:A:357:PX4:C35	4	0.9
(3,33)	1:A:155:THR:H	4:A:359:PX4:C35	4	0.9
(3,33)	1:A:155:THR:H	4:A:361:PX4:C35	4	0.9
(3,33)	1:A:155:THR:H	4:A:363:PX4:C35	4	0.9
(3,33)	1:A:155:THR:H	4:A:402:PX4:C35	4	0.9
(3,33)	1:A:155:THR:H	4:A:404:PX4:C35	4	0.9
(3,33)	1:A:155:THR:H	4:A:406:PX4:C35	4	0.9
(3,33)	1:A:155:THR:H	4:A:408:PX4:C35	4	0.9
(3,33)	1:A:155:THR:H	4:A:410:PX4:C35	4	0.9
(3,33)	1:A:155:THR:H	4:A:412:PX4:C35	4	0.9
(3,33)	1:A:155:THR:H	4:A:414:PX4:C35	4	0.9
(3,33)	1:A:155:THR:H	4:A:416:PX4:C35	4	0.9
(3,33)	1:A:155:THR:H	4:A:418:PX4:C35	4	0.9
(3,33)	1:A:155:THR:H	4:A:420:PX4:C35	4	0.9
(3,33)	1:A:155:THR:H	4:A:422:PX4:C35	4	0.9
(3,33)	1:A:155:THR:H	4:A:424:PX4:C35	4	0.9
(3,33)	1:A:155:THR:H	4:A:426:PX4:C35	4	0.9
(3,33)	1:A:155:THR:H	4:A:428:PX4:C35	4	0.9
(3,33)	1:A:155:THR:H	4:A:430:PX4:C35	4	0.9
(2,974)	1:A:78:PHE:H	1:A:77:LEU:HD21	17	0.9
(2,905)	1:A:67:CYS:HA	1:A:68:GLY:H	5	0.9
(2,898)	1:A:66:ARG:H	1:A:63:GLN:HB3	18	0.9
(2,898)	1:A:66:ARG:H	1:A:63:GLN:HB2	18	0.9
(2,872)	1:A:186:ILE:HD13	1:A:156:LEU:HD22	6	0.9
(2,872)	1:A:186:ILE:HD13	1:A:156:LEU:HD23	6	0.9
(2,832)	1:A:120:ILE:HD11	1:A:200:LEU:HD21	1	0.9
(2,516)	1:A:200:LEU:H	1:A:196:LEU:HD11	6	0.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,516)	1:A:200:LEU:H	1:A:196:LEU:HD12	6	0.9
(2,516)	1:A:200:LEU:H	1:A:196:LEU:HD13	6	0.9
(2,507)	1:A:199:SER:H	1:A:202:MET:H	10	0.9
(2,424)	1:A:169:ASP:H	1:A:166:LEU:HB3	11	0.9
(2,369)	1:A:143:HIS:H	1:A:145:ASP:H	1	0.9
(2,316)	1:A:125:ARG:H	1:A:89:VAL:H	11	0.9
(2,162)	1:A:125:ARG:H	1:A:89:VAL:H	11	0.9
(2,110)	1:A:11:GLN:H	1:A:14:GLN:H	20	0.9
(2,974)	1:A:78:PHE:H	1:A:77:LEU:HD21	20	0.89
(2,948)	1:A:74:GLU:HG3	1:A:75:TYR:H	7	0.89
(2,948)	1:A:74:GLU:HG3	1:A:75:TYR:H	7	0.89
(2,928)	1:A:72:VAL:H	1:A:73:ALA:HB1	7	0.89
(2,898)	1:A:66:ARG:H	1:A:63:GLN:HB3	16	0.89
(2,898)	1:A:66:ARG:H	1:A:63:GLN:HB2	16	0.89
(2,835)	1:A:120:ILE:HD12	1:A:200:LEU:HD22	5	0.89
(2,835)	1:A:120:ILE:HD12	1:A:200:LEU:HD23	5	0.89
(2,750)	1:A:89:VAL:HG13	1:A:122:LEU:HD21	4	0.89
(2,178)	1:A:171:HIS:H	1:A:69:VAL:HG11	13	0.89
(2,178)	1:A:171:HIS:H	1:A:69:VAL:HG12	13	0.89
(2,178)	1:A:171:HIS:H	1:A:69:VAL:HG13	13	0.89
(2,110)	1:A:11:GLN:H	1:A:14:GLN:H	2	0.89
(2,983)	1:A:79:PRO:HD3	1:A:80:ASN:H	17	0.88
(2,983)	1:A:79:PRO:HD3	1:A:80:ASN:H	17	0.88
(2,975)	1:A:78:PHE:H	1:A:77:LEU:HD22	8	0.88
(2,975)	1:A:78:PHE:H	1:A:77:LEU:HD23	8	0.88
(2,954)	1:A:74:GLU:HB3	1:A:77:LEU:H	5	0.88
(2,954)	1:A:74:GLU:HB3	1:A:77:LEU:H	5	0.88
(2,954)	1:A:74:GLU:HB3	1:A:77:LEU:H	14	0.88
(2,954)	1:A:74:GLU:HB3	1:A:77:LEU:H	14	0.88
(2,936)	1:A:73:ALA:HB1	1:A:73:ALA:H	14	0.88
(2,936)	1:A:73:ALA:HB2	1:A:73:ALA:H	14	0.88
(2,936)	1:A:73:ALA:HB3	1:A:73:ALA:H	14	0.88
(2,930)	1:A:72:VAL:HG11	1:A:75:TYR:H	5	0.88
(2,930)	1:A:72:VAL:HG12	1:A:75:TYR:H	5	0.88
(2,930)	1:A:72:VAL:HG13	1:A:75:TYR:H	5	0.88
(2,833)	1:A:120:ILE:HD11	1:A:200:LEU:HD22	15	0.88
(2,833)	1:A:120:ILE:HD11	1:A:200:LEU:HD23	15	0.88
(2,766)	1:A:22:PHE:H	1:A:19:LEU:HD22	14	0.88
(2,766)	1:A:22:PHE:H	1:A:19:LEU:HD23	14	0.88
(2,229)	1:A:106:ASP:H	1:A:109:VAL:H	4	0.88
(2,985)	1:A:80:ASN:H	1:A:78:PHE:HD1	12	0.87
(2,983)	1:A:79:PRO:HD3	1:A:80:ASN:H	15	0.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,983)	1:A:79:PRO:HD3	1:A:80:ASN:H	15	0.87
(2,951)	1:A:74:GLU:H	1:A:76:SER:H	7	0.87
(2,925)	1:A:72:VAL:HG21	1:A:73:ALA:H	14	0.87
(2,925)	1:A:72:VAL:HG22	1:A:73:ALA:H	14	0.87
(2,925)	1:A:72:VAL:HG23	1:A:73:ALA:H	14	0.87
(2,925)	1:A:72:VAL:HG11	1:A:73:ALA:H	14	0.87
(2,925)	1:A:72:VAL:HG12	1:A:73:ALA:H	14	0.87
(2,925)	1:A:72:VAL:HG13	1:A:73:ALA:H	14	0.87
(2,925)	1:A:72:VAL:HG21	1:A:73:ALA:H	17	0.87
(2,925)	1:A:72:VAL:HG22	1:A:73:ALA:H	17	0.87
(2,925)	1:A:72:VAL:HG23	1:A:73:ALA:H	17	0.87
(2,925)	1:A:72:VAL:HG11	1:A:73:ALA:H	17	0.87
(2,925)	1:A:72:VAL:HG12	1:A:73:ALA:H	17	0.87
(2,925)	1:A:72:VAL:HG13	1:A:73:ALA:H	17	0.87
(2,911)	1:A:69:VAL:HG21	1:A:69:VAL:H	12	0.87
(2,911)	1:A:69:VAL:HG22	1:A:69:VAL:H	12	0.87
(2,911)	1:A:69:VAL:HG23	1:A:69:VAL:H	12	0.87
(2,911)	1:A:69:VAL:HG11	1:A:69:VAL:H	12	0.87
(2,911)	1:A:69:VAL:HG12	1:A:69:VAL:H	12	0.87
(2,911)	1:A:69:VAL:HG13	1:A:69:VAL:H	12	0.87
(2,905)	1:A:67:CYS:HA	1:A:68:GLY:H	6	0.87
(2,905)	1:A:67:CYS:HA	1:A:68:GLY:H	18	0.87
(2,899)	1:A:66:ARG:H	1:A:64:LYS:H	13	0.87
(2,896)	1:A:64:LYS:H	1:A:64:LYS:HE3	12	0.87
(2,896)	1:A:64:LYS:H	1:A:64:LYS:HE3	12	0.87
(2,891)	1:A:63:GLN:H	1:A:63:GLN:HB3	19	0.87
(2,891)	1:A:63:GLN:H	1:A:63:GLN:HB2	19	0.87
(2,891)	1:A:63:GLN:H	1:A:63:GLN:HB3	19	0.87
(2,891)	1:A:63:GLN:H	1:A:63:GLN:HB2	19	0.87
(2,872)	1:A:186:ILE:HD13	1:A:156:LEU:HD22	8	0.87
(2,872)	1:A:186:ILE:HD13	1:A:156:LEU:HD23	8	0.87
(2,835)	1:A:120:ILE:HD12	1:A:200:LEU:HD22	4	0.87
(2,835)	1:A:120:ILE:HD12	1:A:200:LEU:HD23	4	0.87
(2,833)	1:A:120:ILE:HD11	1:A:200:LEU:HD22	3	0.87
(2,833)	1:A:120:ILE:HD11	1:A:200:LEU:HD23	3	0.87
(2,717)	1:A:54:LEU:HD11	1:A:39:LEU:HD11	3	0.87
(2,717)	1:A:54:LEU:HD11	1:A:39:LEU:HD12	3	0.87
(2,717)	1:A:54:LEU:HD11	1:A:39:LEU:HD13	3	0.87
(2,717)	1:A:54:LEU:HD12	1:A:39:LEU:HD11	3	0.87
(2,717)	1:A:54:LEU:HD12	1:A:39:LEU:HD12	3	0.87
(2,717)	1:A:54:LEU:HD12	1:A:39:LEU:HD13	3	0.87
(2,717)	1:A:54:LEU:HD13	1:A:39:LEU:HD11	3	0.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,717)	1:A:54:LEU:HD13	1:A:39:LEU:HD12	3	0.87
(2,717)	1:A:54:LEU:HD13	1:A:39:LEU:HD13	3	0.87
(2,627)	1:A:13:GLU:H	1:A:10:LEU:H	1	0.87
(2,507)	1:A:199:SER:H	1:A:202:MET:H	7	0.87
(2,185)	1:A:94:VAL:H	1:A:92:ARG:H	17	0.87
(2,125)	1:A:157:ALA:H	1:A:68:GLY:H	16	0.87
(2,983)	1:A:79:PRO:HD3	1:A:80:ASN:H	2	0.86
(2,983)	1:A:79:PRO:HD3	1:A:80:ASN:H	2	0.86
(2,964)	1:A:75:TYR:H	1:A:76:SER:H	4	0.86
(2,959)	1:A:75:TYR:H	1:A:76:SER:H	4	0.86
(2,936)	1:A:73:ALA:HB1	1:A:73:ALA:H	9	0.86
(2,936)	1:A:73:ALA:HB2	1:A:73:ALA:H	9	0.86
(2,936)	1:A:73:ALA:HB3	1:A:73:ALA:H	9	0.86
(2,936)	1:A:73:ALA:HB1	1:A:73:ALA:H	18	0.86
(2,936)	1:A:73:ALA:HB2	1:A:73:ALA:H	18	0.86
(2,936)	1:A:73:ALA:HB3	1:A:73:ALA:H	18	0.86
(2,936)	1:A:73:ALA:HB1	1:A:73:ALA:H	19	0.86
(2,936)	1:A:73:ALA:HB2	1:A:73:ALA:H	19	0.86
(2,936)	1:A:73:ALA:HB3	1:A:73:ALA:H	19	0.86
(2,891)	1:A:63:GLN:H	1:A:63:GLN:HB3	3	0.86
(2,891)	1:A:63:GLN:H	1:A:63:GLN:HB2	3	0.86
(2,891)	1:A:63:GLN:H	1:A:63:GLN:HB3	3	0.86
(2,891)	1:A:63:GLN:H	1:A:63:GLN:HB2	3	0.86
(2,870)	1:A:186:ILE:HD12	1:A:156:LEU:HD22	12	0.86
(2,870)	1:A:186:ILE:HD12	1:A:156:LEU:HD23	12	0.86
(2,759)	1:A:54:LEU:HD21	1:A:59:ILE:HD11	4	0.86
(2,759)	1:A:54:LEU:HD21	1:A:59:ILE:HD12	4	0.86
(2,759)	1:A:54:LEU:HD21	1:A:59:ILE:HD13	4	0.86
(2,755)	1:A:54:LEU:HD21	1:A:58:VAL:HG11	1	0.86
(2,755)	1:A:54:LEU:HD21	1:A:58:VAL:HG12	1	0.86
(2,755)	1:A:54:LEU:HD21	1:A:58:VAL:HG13	1	0.86
(2,737)	1:A:196:LEU:HD23	1:A:113:LEU:HD21	5	0.86
(2,737)	1:A:196:LEU:HD23	1:A:113:LEU:HD21	13	0.86
(2,518)	1:A:200:LEU:H	1:A:196:LEU:HD22	4	0.86
(2,518)	1:A:200:LEU:H	1:A:196:LEU:HD23	4	0.86
(2,516)	1:A:200:LEU:H	1:A:196:LEU:HD11	17	0.86
(2,516)	1:A:200:LEU:H	1:A:196:LEU:HD12	17	0.86
(2,516)	1:A:200:LEU:H	1:A:196:LEU:HD13	17	0.86
(2,466)	1:A:84:TRP:H	1:A:200:LEU:HD21	16	0.86
(2,229)	1:A:106:ASP:H	1:A:109:VAL:H	7	0.86
(2,212)	1:A:120:ILE:HD11	1:A:237:LEU:H	12	0.86
(2,212)	1:A:120:ILE:HD12	1:A:237:LEU:H	12	0.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,212)	1:A:120:ILE:HD13	1:A:237:LEU:H	12	0.86
(2,185)	1:A:94:VAL:H	1:A:92:ARG:H	12	0.86
(2,178)	1:A:171:HIS:H	1:A:69:VAL:HG11	12	0.86
(2,178)	1:A:171:HIS:H	1:A:69:VAL:HG12	12	0.86
(2,178)	1:A:171:HIS:H	1:A:69:VAL:HG13	12	0.86
(2,974)	1:A:78:PHE:H	1:A:77:LEU:HD21	4	0.85
(2,936)	1:A:73:ALA:HB1	1:A:73:ALA:H	1	0.85
(2,936)	1:A:73:ALA:HB2	1:A:73:ALA:H	1	0.85
(2,936)	1:A:73:ALA:HB3	1:A:73:ALA:H	1	0.85
(2,936)	1:A:73:ALA:HB1	1:A:73:ALA:H	3	0.85
(2,936)	1:A:73:ALA:HB2	1:A:73:ALA:H	3	0.85
(2,936)	1:A:73:ALA:HB3	1:A:73:ALA:H	3	0.85
(2,936)	1:A:73:ALA:HB1	1:A:73:ALA:H	13	0.85
(2,936)	1:A:73:ALA:HB2	1:A:73:ALA:H	13	0.85
(2,936)	1:A:73:ALA:HB3	1:A:73:ALA:H	13	0.85
(2,930)	1:A:72:VAL:HG11	1:A:75:TYR:H	7	0.85
(2,930)	1:A:72:VAL:HG12	1:A:75:TYR:H	7	0.85
(2,930)	1:A:72:VAL:HG13	1:A:75:TYR:H	7	0.85
(2,913)	1:A:71:ASP:H	1:A:70:PRO:HB3	20	0.85
(2,913)	1:A:71:ASP:H	1:A:70:PRO:HB2	20	0.85
(2,891)	1:A:63:GLN:H	1:A:63:GLN:HB3	5	0.85
(2,891)	1:A:63:GLN:H	1:A:63:GLN:HB2	5	0.85
(2,891)	1:A:63:GLN:H	1:A:63:GLN:HB3	5	0.85
(2,891)	1:A:63:GLN:H	1:A:63:GLN:HB2	5	0.85
(2,759)	1:A:54:LEU:HD21	1:A:59:ILE:HD11	18	0.85
(2,759)	1:A:54:LEU:HD21	1:A:59:ILE:HD12	18	0.85
(2,759)	1:A:54:LEU:HD21	1:A:59:ILE:HD13	18	0.85
(2,717)	1:A:54:LEU:HD11	1:A:39:LEU:HD11	15	0.85
(2,717)	1:A:54:LEU:HD11	1:A:39:LEU:HD12	15	0.85
(2,717)	1:A:54:LEU:HD11	1:A:39:LEU:HD13	15	0.85
(2,717)	1:A:54:LEU:HD12	1:A:39:LEU:HD11	15	0.85
(2,717)	1:A:54:LEU:HD12	1:A:39:LEU:HD12	15	0.85
(2,717)	1:A:54:LEU:HD12	1:A:39:LEU:HD13	15	0.85
(2,717)	1:A:54:LEU:HD13	1:A:39:LEU:HD11	15	0.85
(2,717)	1:A:54:LEU:HD13	1:A:39:LEU:HD12	15	0.85
(2,717)	1:A:54:LEU:HD13	1:A:39:LEU:HD13	15	0.85
(2,518)	1:A:200:LEU:H	1:A:196:LEU:HD22	18	0.85
(2,518)	1:A:200:LEU:H	1:A:196:LEU:HD23	18	0.85
(2,516)	1:A:200:LEU:H	1:A:196:LEU:HD11	5	0.85
(2,516)	1:A:200:LEU:H	1:A:196:LEU:HD12	5	0.85
(2,516)	1:A:200:LEU:H	1:A:196:LEU:HD13	5	0.85
(2,185)	1:A:94:VAL:H	1:A:92:ARG:H	13	0.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,178)	1:A:171:HIS:H	1:A:69:VAL:HG11	1	0.85
(2,178)	1:A:171:HIS:H	1:A:69:VAL:HG12	1	0.85
(2,178)	1:A:171:HIS:H	1:A:69:VAL:HG13	1	0.85
(2,110)	1:A:11:GLN:H	1:A:14:GLN:H	10	0.85
(2,976)	1:A:78:PHE:H	1:A:78:PHE:HD1	16	0.84
(2,976)	1:A:78:PHE:H	1:A:78:PHE:HD2	16	0.84
(2,964)	1:A:75:TYR:H	1:A:76:SER:H	18	0.84
(2,959)	1:A:75:TYR:H	1:A:76:SER:H	18	0.84
(2,891)	1:A:63:GLN:H	1:A:63:GLN:HB3	8	0.84
(2,891)	1:A:63:GLN:H	1:A:63:GLN:HB2	8	0.84
(2,891)	1:A:63:GLN:H	1:A:63:GLN:HB3	8	0.84
(2,891)	1:A:63:GLN:H	1:A:63:GLN:HB2	8	0.84
(2,891)	1:A:63:GLN:H	1:A:63:GLN:HB3	13	0.84
(2,891)	1:A:63:GLN:H	1:A:63:GLN:HB2	13	0.84
(2,891)	1:A:63:GLN:H	1:A:63:GLN:HB3	13	0.84
(2,891)	1:A:63:GLN:H	1:A:63:GLN:HB2	13	0.84
(2,834)	1:A:120:ILE:HD12	1:A:200:LEU:HD21	9	0.84
(2,717)	1:A:54:LEU:HD11	1:A:39:LEU:HD11	6	0.84
(2,717)	1:A:54:LEU:HD11	1:A:39:LEU:HD12	6	0.84
(2,717)	1:A:54:LEU:HD11	1:A:39:LEU:HD13	6	0.84
(2,717)	1:A:54:LEU:HD12	1:A:39:LEU:HD11	6	0.84
(2,717)	1:A:54:LEU:HD12	1:A:39:LEU:HD12	6	0.84
(2,717)	1:A:54:LEU:HD12	1:A:39:LEU:HD13	6	0.84
(2,717)	1:A:54:LEU:HD13	1:A:39:LEU:HD11	6	0.84
(2,717)	1:A:54:LEU:HD13	1:A:39:LEU:HD12	6	0.84
(2,717)	1:A:54:LEU:HD13	1:A:39:LEU:HD13	6	0.84
(2,516)	1:A:200:LEU:H	1:A:196:LEU:HD11	12	0.84
(2,516)	1:A:200:LEU:H	1:A:196:LEU:HD12	12	0.84
(2,516)	1:A:200:LEU:H	1:A:196:LEU:HD13	12	0.84
(2,511)	1:A:200:LEU:HD22	1:A:199:SER:H	3	0.84
(2,511)	1:A:200:LEU:HD23	1:A:199:SER:H	3	0.84
(2,510)	1:A:200:LEU:HD21	1:A:199:SER:H	2	0.84
(2,426)	1:A:170:ALA:H	1:A:136:ILE:HD11	8	0.84
(2,426)	1:A:170:ALA:H	1:A:136:ILE:HD12	8	0.84
(2,426)	1:A:170:ALA:H	1:A:136:ILE:HD13	8	0.84
(2,379)	1:A:10:LEU:H	1:A:10:LEU:HD21	2	0.84
(2,985)	1:A:80:ASN:H	1:A:78:PHE:HD1	11	0.83
(2,954)	1:A:74:GLU:HB3	1:A:77:LEU:H	17	0.83
(2,954)	1:A:74:GLU:HB3	1:A:77:LEU:H	17	0.83
(2,930)	1:A:72:VAL:HG11	1:A:75:TYR:H	11	0.83
(2,930)	1:A:72:VAL:HG12	1:A:75:TYR:H	11	0.83
(2,930)	1:A:72:VAL:HG13	1:A:75:TYR:H	11	0.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,891)	1:A:63:GLN:H	1:A:63:GLN:HB3	18	0.83
(2,891)	1:A:63:GLN:H	1:A:63:GLN:HB2	18	0.83
(2,891)	1:A:63:GLN:H	1:A:63:GLN:HB3	18	0.83
(2,891)	1:A:63:GLN:H	1:A:63:GLN:HB2	18	0.83
(2,788)	1:A:58:VAL:HG11	1:A:39:LEU:HD21	20	0.83
(2,731)	1:A:211:VAL:HG13	1:A:226:LEU:HD21	6	0.83
(2,424)	1:A:169:ASP:H	1:A:166:LEU:HB3	15	0.83
(2,973)	1:A:78:PHE:H	1:A:77:LEU:HD11	8	0.82
(2,973)	1:A:78:PHE:H	1:A:77:LEU:HD12	8	0.82
(2,973)	1:A:78:PHE:H	1:A:77:LEU:HD13	8	0.82
(2,936)	1:A:73:ALA:HB1	1:A:73:ALA:H	7	0.82
(2,936)	1:A:73:ALA:HB2	1:A:73:ALA:H	7	0.82
(2,936)	1:A:73:ALA:HB3	1:A:73:ALA:H	7	0.82
(2,925)	1:A:72:VAL:HG21	1:A:73:ALA:H	4	0.82
(2,925)	1:A:72:VAL:HG22	1:A:73:ALA:H	4	0.82
(2,925)	1:A:72:VAL:HG23	1:A:73:ALA:H	4	0.82
(2,925)	1:A:72:VAL:HG11	1:A:73:ALA:H	4	0.82
(2,925)	1:A:72:VAL:HG12	1:A:73:ALA:H	4	0.82
(2,925)	1:A:72:VAL:HG13	1:A:73:ALA:H	4	0.82
(2,905)	1:A:67:CYS:HA	1:A:68:GLY:H	9	0.82
(2,894)	1:A:64:LYS:H	1:A:64:LYS:HG3	18	0.82
(2,894)	1:A:64:LYS:H	1:A:64:LYS:HG3	18	0.82
(2,891)	1:A:63:GLN:H	1:A:63:GLN:HB3	15	0.82
(2,891)	1:A:63:GLN:H	1:A:63:GLN:HB2	15	0.82
(2,891)	1:A:63:GLN:H	1:A:63:GLN:HB3	15	0.82
(2,891)	1:A:63:GLN:H	1:A:63:GLN:HB2	15	0.82
(2,867)	1:A:186:ILE:HD11	1:A:156:LEU:HD21	6	0.82
(2,765)	1:A:22:PHE:H	1:A:19:LEU:HD21	17	0.82
(2,735)	1:A:196:LEU:HD22	1:A:113:LEU:HD21	5	0.82
(2,424)	1:A:169:ASP:H	1:A:166:LEU:HB3	5	0.82
(2,379)	1:A:10:LEU:H	1:A:10:LEU:HD21	13	0.82
(3,33)	1:A:155:THR:H	4:A:305:PX4:C35	8	0.81
(3,33)	1:A:155:THR:H	4:A:307:PX4:C35	8	0.81
(3,33)	1:A:155:THR:H	4:A:309:PX4:C35	8	0.81
(3,33)	1:A:155:THR:H	4:A:311:PX4:C35	8	0.81
(3,33)	1:A:155:THR:H	4:A:313:PX4:C35	8	0.81
(3,33)	1:A:155:THR:H	4:A:315:PX4:C35	8	0.81
(3,33)	1:A:155:THR:H	4:A:317:PX4:C35	8	0.81
(3,33)	1:A:155:THR:H	4:A:319:PX4:C35	8	0.81
(3,33)	1:A:155:THR:H	4:A:321:PX4:C35	8	0.81
(3,33)	1:A:155:THR:H	4:A:323:PX4:C35	8	0.81
(3,33)	1:A:155:THR:H	4:A:325:PX4:C35	8	0.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,33)	1:A:155:THR:H	4:A:327:PX4:C35	8	0.81
(3,33)	1:A:155:THR:H	4:A:329:PX4:C35	8	0.81
(3,33)	1:A:155:THR:H	4:A:331:PX4:C35	8	0.81
(3,33)	1:A:155:THR:H	4:A:333:PX4:C35	8	0.81
(3,33)	1:A:155:THR:H	4:A:335:PX4:C35	8	0.81
(3,33)	1:A:155:THR:H	4:A:337:PX4:C35	8	0.81
(3,33)	1:A:155:THR:H	4:A:339:PX4:C35	8	0.81
(3,33)	1:A:155:THR:H	4:A:341:PX4:C35	8	0.81
(3,33)	1:A:155:THR:H	4:A:343:PX4:C35	8	0.81
(3,33)	1:A:155:THR:H	4:A:345:PX4:C35	8	0.81
(3,33)	1:A:155:THR:H	4:A:347:PX4:C35	8	0.81
(3,33)	1:A:155:THR:H	4:A:349:PX4:C35	8	0.81
(3,33)	1:A:155:THR:H	4:A:351:PX4:C35	8	0.81
(3,33)	1:A:155:THR:H	4:A:353:PX4:C35	8	0.81
(3,33)	1:A:155:THR:H	4:A:355:PX4:C35	8	0.81
(3,33)	1:A:155:THR:H	4:A:357:PX4:C35	8	0.81
(3,33)	1:A:155:THR:H	4:A:359:PX4:C35	8	0.81
(3,33)	1:A:155:THR:H	4:A:361:PX4:C35	8	0.81
(3,33)	1:A:155:THR:H	4:A:363:PX4:C35	8	0.81
(3,33)	1:A:155:THR:H	4:A:402:PX4:C35	8	0.81
(3,33)	1:A:155:THR:H	4:A:404:PX4:C35	8	0.81
(3,33)	1:A:155:THR:H	4:A:406:PX4:C35	8	0.81
(3,33)	1:A:155:THR:H	4:A:408:PX4:C35	8	0.81
(3,33)	1:A:155:THR:H	4:A:410:PX4:C35	8	0.81
(3,33)	1:A:155:THR:H	4:A:412:PX4:C35	8	0.81
(3,33)	1:A:155:THR:H	4:A:414:PX4:C35	8	0.81
(3,33)	1:A:155:THR:H	4:A:416:PX4:C35	8	0.81
(3,33)	1:A:155:THR:H	4:A:418:PX4:C35	8	0.81
(3,33)	1:A:155:THR:H	4:A:420:PX4:C35	8	0.81
(3,33)	1:A:155:THR:H	4:A:422:PX4:C35	8	0.81
(3,33)	1:A:155:THR:H	4:A:424:PX4:C35	8	0.81
(3,33)	1:A:155:THR:H	4:A:426:PX4:C35	8	0.81
(3,33)	1:A:155:THR:H	4:A:428:PX4:C35	8	0.81
(3,33)	1:A:155:THR:H	4:A:430:PX4:C35	8	0.81
(2,983)	1:A:79:PRO:HD3	1:A:80:ASN:H	19	0.81
(2,983)	1:A:79:PRO:HD3	1:A:80:ASN:H	19	0.81
(2,975)	1:A:78:PHE:H	1:A:77:LEU:HD22	20	0.81
(2,975)	1:A:78:PHE:H	1:A:77:LEU:HD23	20	0.81
(2,974)	1:A:78:PHE:H	1:A:77:LEU:HD21	10	0.81
(2,936)	1:A:73:ALA:HB1	1:A:73:ALA:H	2	0.81
(2,936)	1:A:73:ALA:HB2	1:A:73:ALA:H	2	0.81
(2,936)	1:A:73:ALA:HB3	1:A:73:ALA:H	2	0.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,925)	1:A:72:VAL:HG21	1:A:73:ALA:H	19	0.81
(2,925)	1:A:72:VAL:HG22	1:A:73:ALA:H	19	0.81
(2,925)	1:A:72:VAL:HG23	1:A:73:ALA:H	19	0.81
(2,925)	1:A:72:VAL:HG11	1:A:73:ALA:H	19	0.81
(2,925)	1:A:72:VAL:HG12	1:A:73:ALA:H	19	0.81
(2,925)	1:A:72:VAL:HG13	1:A:73:ALA:H	19	0.81
(2,913)	1:A:71:ASP:H	1:A:70:PRO:HB3	11	0.81
(2,913)	1:A:71:ASP:H	1:A:70:PRO:HB2	11	0.81
(2,907)	1:A:68:GLY:H	1:A:69:VAL:H	3	0.81
(2,842)	1:A:200:LEU:HD21	1:A:122:LEU:HD21	20	0.81
(2,834)	1:A:120:ILE:HD12	1:A:200:LEU:HD21	3	0.81
(2,809)	1:A:136:ILE:H	1:A:94:VAL:HG11	19	0.81
(2,809)	1:A:136:ILE:H	1:A:94:VAL:HG12	19	0.81
(2,809)	1:A:136:ILE:H	1:A:94:VAL:HG13	19	0.81
(2,467)	1:A:84:TRP:H	1:A:200:LEU:HD22	20	0.81
(2,467)	1:A:84:TRP:H	1:A:200:LEU:HD23	20	0.81
(2,424)	1:A:169:ASP:H	1:A:166:LEU:HB3	2	0.81
(2,414)	1:A:167:GLY:H	1:A:166:LEU:HD21	6	0.81
(3,6)	1:A:78:PHE:H	4:A:305:PX4:C27	5	0.8
(3,6)	1:A:78:PHE:H	4:A:307:PX4:C27	5	0.8
(3,6)	1:A:78:PHE:H	4:A:309:PX4:C27	5	0.8
(3,6)	1:A:78:PHE:H	4:A:311:PX4:C27	5	0.8
(3,6)	1:A:78:PHE:H	4:A:313:PX4:C27	5	0.8
(3,6)	1:A:78:PHE:H	4:A:315:PX4:C27	5	0.8
(3,6)	1:A:78:PHE:H	4:A:317:PX4:C27	5	0.8
(3,6)	1:A:78:PHE:H	4:A:319:PX4:C27	5	0.8
(3,6)	1:A:78:PHE:H	4:A:321:PX4:C27	5	0.8
(3,6)	1:A:78:PHE:H	4:A:323:PX4:C27	5	0.8
(3,6)	1:A:78:PHE:H	4:A:325:PX4:C27	5	0.8
(3,6)	1:A:78:PHE:H	4:A:327:PX4:C27	5	0.8
(3,6)	1:A:78:PHE:H	4:A:329:PX4:C27	5	0.8
(3,6)	1:A:78:PHE:H	4:A:331:PX4:C27	5	0.8
(3,6)	1:A:78:PHE:H	4:A:333:PX4:C27	5	0.8
(3,6)	1:A:78:PHE:H	4:A:335:PX4:C27	5	0.8
(3,6)	1:A:78:PHE:H	4:A:337:PX4:C27	5	0.8
(3,6)	1:A:78:PHE:H	4:A:339:PX4:C27	5	0.8
(3,6)	1:A:78:PHE:H	4:A:341:PX4:C27	5	0.8
(3,6)	1:A:78:PHE:H	4:A:343:PX4:C27	5	0.8
(3,6)	1:A:78:PHE:H	4:A:345:PX4:C27	5	0.8
(3,6)	1:A:78:PHE:H	4:A:347:PX4:C27	5	0.8
(3,6)	1:A:78:PHE:H	4:A:349:PX4:C27	5	0.8
(3,6)	1:A:78:PHE:H	4:A:351:PX4:C27	5	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,6)	1:A:78:PHE:H	4:A:353:PX4:C27	5	0.8
(3,6)	1:A:78:PHE:H	4:A:355:PX4:C27	5	0.8
(3,6)	1:A:78:PHE:H	4:A:357:PX4:C27	5	0.8
(3,6)	1:A:78:PHE:H	4:A:359:PX4:C27	5	0.8
(3,6)	1:A:78:PHE:H	4:A:361:PX4:C27	5	0.8
(3,6)	1:A:78:PHE:H	4:A:363:PX4:C27	5	0.8
(3,6)	1:A:78:PHE:H	4:A:402:PX4:C27	5	0.8
(3,6)	1:A:78:PHE:H	4:A:404:PX4:C27	5	0.8
(3,6)	1:A:78:PHE:H	4:A:406:PX4:C27	5	0.8
(3,6)	1:A:78:PHE:H	4:A:408:PX4:C27	5	0.8
(3,6)	1:A:78:PHE:H	4:A:410:PX4:C27	5	0.8
(3,6)	1:A:78:PHE:H	4:A:412:PX4:C27	5	0.8
(3,6)	1:A:78:PHE:H	4:A:414:PX4:C27	5	0.8
(3,6)	1:A:78:PHE:H	4:A:416:PX4:C27	5	0.8
(3,6)	1:A:78:PHE:H	4:A:418:PX4:C27	5	0.8
(3,6)	1:A:78:PHE:H	4:A:420:PX4:C27	5	0.8
(3,6)	1:A:78:PHE:H	4:A:422:PX4:C27	5	0.8
(3,6)	1:A:78:PHE:H	4:A:424:PX4:C27	5	0.8
(3,6)	1:A:78:PHE:H	4:A:426:PX4:C27	5	0.8
(3,6)	1:A:78:PHE:H	4:A:428:PX4:C27	5	0.8
(3,6)	1:A:78:PHE:H	4:A:430:PX4:C27	5	0.8
(2,983)	1:A:79:PRO:HD3	1:A:80:ASN:H	6	0.8
(2,983)	1:A:79:PRO:HD3	1:A:80:ASN:H	6	0.8
(2,983)	1:A:79:PRO:HD3	1:A:80:ASN:H	11	0.8
(2,983)	1:A:79:PRO:HD3	1:A:80:ASN:H	11	0.8
(2,936)	1:A:73:ALA:HB1	1:A:73:ALA:H	15	0.8
(2,936)	1:A:73:ALA:HB2	1:A:73:ALA:H	15	0.8
(2,936)	1:A:73:ALA:HB3	1:A:73:ALA:H	15	0.8
(2,913)	1:A:71:ASP:H	1:A:70:PRO:HB3	10	0.8
(2,913)	1:A:71:ASP:H	1:A:70:PRO:HB2	10	0.8
(2,911)	1:A:69:VAL:HG21	1:A:69:VAL:H	13	0.8
(2,911)	1:A:69:VAL:HG22	1:A:69:VAL:H	13	0.8
(2,911)	1:A:69:VAL:HG23	1:A:69:VAL:H	13	0.8
(2,911)	1:A:69:VAL:HG11	1:A:69:VAL:H	13	0.8
(2,911)	1:A:69:VAL:HG12	1:A:69:VAL:H	13	0.8
(2,911)	1:A:69:VAL:HG13	1:A:69:VAL:H	13	0.8
(2,911)	1:A:69:VAL:HG21	1:A:69:VAL:H	20	0.8
(2,911)	1:A:69:VAL:HG22	1:A:69:VAL:H	20	0.8
(2,911)	1:A:69:VAL:HG23	1:A:69:VAL:H	20	0.8
(2,911)	1:A:69:VAL:HG11	1:A:69:VAL:H	20	0.8
(2,911)	1:A:69:VAL:HG12	1:A:69:VAL:H	20	0.8
(2,911)	1:A:69:VAL:HG13	1:A:69:VAL:H	20	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,905)	1:A:67:CYS:HA	1:A:68:GLY:H	14	0.8
(2,777)	1:A:61:ILE:HD13	1:A:48:LEU:HD21	4	0.8
(2,755)	1:A:54:LEU:HD21	1:A:58:VAL:HG11	5	0.8
(2,755)	1:A:54:LEU:HD21	1:A:58:VAL:HG12	5	0.8
(2,755)	1:A:54:LEU:HD21	1:A:58:VAL:HG13	5	0.8
(2,755)	1:A:54:LEU:HD21	1:A:58:VAL:HG11	11	0.8
(2,755)	1:A:54:LEU:HD21	1:A:58:VAL:HG12	11	0.8
(2,755)	1:A:54:LEU:HD21	1:A:58:VAL:HG13	11	0.8
(2,661)	1:A:4:ALA:H	1:A:59:ILE:HG21	10	0.8
(2,661)	1:A:4:ALA:H	1:A:59:ILE:HG22	10	0.8
(2,661)	1:A:4:ALA:H	1:A:59:ILE:HG23	10	0.8
(2,661)	1:A:4:ALA:H	1:A:59:ILE:HG21	19	0.8
(2,661)	1:A:4:ALA:H	1:A:59:ILE:HG22	19	0.8
(2,661)	1:A:4:ALA:H	1:A:59:ILE:HG23	19	0.8
(2,517)	1:A:200:LEU:H	1:A:196:LEU:HD21	8	0.8
(2,516)	1:A:200:LEU:H	1:A:196:LEU:HD11	13	0.8
(2,516)	1:A:200:LEU:H	1:A:196:LEU:HD12	13	0.8
(2,516)	1:A:200:LEU:H	1:A:196:LEU:HD13	13	0.8
(2,473)	1:A:186:ILE:H	1:A:156:LEU:HD22	5	0.8
(2,473)	1:A:186:ILE:H	1:A:156:LEU:HD23	5	0.8
(2,473)	1:A:186:ILE:H	1:A:156:LEU:HD22	20	0.8
(2,473)	1:A:186:ILE:H	1:A:156:LEU:HD23	20	0.8
(3,21)	1:A:77:LEU:H	4:A:305:PX4:C35	2	0.79
(3,21)	1:A:77:LEU:H	4:A:307:PX4:C35	2	0.79
(3,21)	1:A:77:LEU:H	4:A:309:PX4:C35	2	0.79
(3,21)	1:A:77:LEU:H	4:A:311:PX4:C35	2	0.79
(3,21)	1:A:77:LEU:H	4:A:313:PX4:C35	2	0.79
(3,21)	1:A:77:LEU:H	4:A:315:PX4:C35	2	0.79
(3,21)	1:A:77:LEU:H	4:A:317:PX4:C35	2	0.79
(3,21)	1:A:77:LEU:H	4:A:319:PX4:C35	2	0.79
(3,21)	1:A:77:LEU:H	4:A:321:PX4:C35	2	0.79
(3,21)	1:A:77:LEU:H	4:A:323:PX4:C35	2	0.79
(3,21)	1:A:77:LEU:H	4:A:325:PX4:C35	2	0.79
(3,21)	1:A:77:LEU:H	4:A:327:PX4:C35	2	0.79
(3,21)	1:A:77:LEU:H	4:A:329:PX4:C35	2	0.79
(3,21)	1:A:77:LEU:H	4:A:331:PX4:C35	2	0.79
(3,21)	1:A:77:LEU:H	4:A:333:PX4:C35	2	0.79
(3,21)	1:A:77:LEU:H	4:A:335:PX4:C35	2	0.79
(3,21)	1:A:77:LEU:H	4:A:337:PX4:C35	2	0.79
(3,21)	1:A:77:LEU:H	4:A:339:PX4:C35	2	0.79
(3,21)	1:A:77:LEU:H	4:A:341:PX4:C35	2	0.79
(3,21)	1:A:77:LEU:H	4:A:343:PX4:C35	2	0.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,21)	1:A:77:LEU:H	4:A:345:PX4:C35	2	0.79
(3,21)	1:A:77:LEU:H	4:A:347:PX4:C35	2	0.79
(3,21)	1:A:77:LEU:H	4:A:349:PX4:C35	2	0.79
(3,21)	1:A:77:LEU:H	4:A:351:PX4:C35	2	0.79
(3,21)	1:A:77:LEU:H	4:A:353:PX4:C35	2	0.79
(3,21)	1:A:77:LEU:H	4:A:355:PX4:C35	2	0.79
(3,21)	1:A:77:LEU:H	4:A:357:PX4:C35	2	0.79
(3,21)	1:A:77:LEU:H	4:A:359:PX4:C35	2	0.79
(3,21)	1:A:77:LEU:H	4:A:361:PX4:C35	2	0.79
(3,21)	1:A:77:LEU:H	4:A:363:PX4:C35	2	0.79
(3,21)	1:A:77:LEU:H	4:A:402:PX4:C35	2	0.79
(3,21)	1:A:77:LEU:H	4:A:404:PX4:C35	2	0.79
(3,21)	1:A:77:LEU:H	4:A:406:PX4:C35	2	0.79
(3,21)	1:A:77:LEU:H	4:A:408:PX4:C35	2	0.79
(3,21)	1:A:77:LEU:H	4:A:410:PX4:C35	2	0.79
(3,21)	1:A:77:LEU:H	4:A:412:PX4:C35	2	0.79
(3,21)	1:A:77:LEU:H	4:A:414:PX4:C35	2	0.79
(3,21)	1:A:77:LEU:H	4:A:416:PX4:C35	2	0.79
(3,21)	1:A:77:LEU:H	4:A:418:PX4:C35	2	0.79
(3,21)	1:A:77:LEU:H	4:A:420:PX4:C35	2	0.79
(3,21)	1:A:77:LEU:H	4:A:422:PX4:C35	2	0.79
(3,21)	1:A:77:LEU:H	4:A:424:PX4:C35	2	0.79
(3,21)	1:A:77:LEU:H	4:A:426:PX4:C35	2	0.79
(3,21)	1:A:77:LEU:H	4:A:428:PX4:C35	2	0.79
(3,21)	1:A:77:LEU:H	4:A:430:PX4:C35	2	0.79
(2,976)	1:A:78:PHE:H	1:A:78:PHE:HD1	6	0.79
(2,976)	1:A:78:PHE:H	1:A:78:PHE:HD2	6	0.79
(2,948)	1:A:74:GLU:HG3	1:A:75:TYR:H	17	0.79
(2,948)	1:A:74:GLU:HG3	1:A:75:TYR:H	17	0.79
(2,936)	1:A:73:ALA:HB1	1:A:73:ALA:H	8	0.79
(2,936)	1:A:73:ALA:HB2	1:A:73:ALA:H	8	0.79
(2,936)	1:A:73:ALA:HB3	1:A:73:ALA:H	8	0.79
(2,911)	1:A:69:VAL:HG21	1:A:69:VAL:H	11	0.79
(2,911)	1:A:69:VAL:HG22	1:A:69:VAL:H	11	0.79
(2,911)	1:A:69:VAL:HG23	1:A:69:VAL:H	11	0.79
(2,911)	1:A:69:VAL:HG11	1:A:69:VAL:H	11	0.79
(2,911)	1:A:69:VAL:HG12	1:A:69:VAL:H	11	0.79
(2,911)	1:A:69:VAL:HG13	1:A:69:VAL:H	11	0.79
(2,896)	1:A:64:LYS:H	1:A:64:LYS:HE3	15	0.79
(2,896)	1:A:64:LYS:H	1:A:64:LYS:HE3	15	0.79
(2,891)	1:A:63:GLN:H	1:A:63:GLN:HB3	20	0.79
(2,891)	1:A:63:GLN:H	1:A:63:GLN:HB2	20	0.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,891)	1:A:63:GLN:H	1:A:63:GLN:HB3	20	0.79
(2,891)	1:A:63:GLN:H	1:A:63:GLN:HB2	20	0.79
(2,83)	1:A:58:VAL:H	1:A:48:LEU:HD22	18	0.79
(2,83)	1:A:58:VAL:H	1:A:48:LEU:HD23	18	0.79
(2,786)	1:A:24:LEU:H	1:A:24:LEU:HD21	15	0.79
(2,786)	1:A:24:LEU:H	1:A:24:LEU:HD21	16	0.79
(2,424)	1:A:169:ASP:H	1:A:166:LEU:HB3	19	0.79
(2,264)	1:A:113:LEU:H	1:A:196:LEU:HD21	20	0.79
(2,258)	1:A:112:ALA:H	1:A:189:LEU:HD22	19	0.79
(2,258)	1:A:112:ALA:H	1:A:189:LEU:HD23	19	0.79
(2,212)	1:A:120:ILE:HD11	1:A:237:LEU:H	15	0.79
(2,212)	1:A:120:ILE:HD12	1:A:237:LEU:H	15	0.79
(2,212)	1:A:120:ILE:HD13	1:A:237:LEU:H	15	0.79
(2,178)	1:A:171:HIS:H	1:A:69:VAL:HG11	2	0.79
(2,178)	1:A:171:HIS:H	1:A:69:VAL:HG12	2	0.79
(2,178)	1:A:171:HIS:H	1:A:69:VAL:HG13	2	0.79
(2,984)	1:A:78:PHE:HD1	1:A:80:ASN:HD21	2	0.78
(2,984)	1:A:78:PHE:HD1	1:A:80:ASN:HD22	2	0.78
(2,984)	1:A:78:PHE:HD1	1:A:80:ASN:HD21	2	0.78
(2,984)	1:A:78:PHE:HD1	1:A:80:ASN:HD22	2	0.78
(2,979)	1:A:78:PHE:H	1:A:78:PHE:HD1	6	0.78
(2,979)	1:A:78:PHE:H	1:A:78:PHE:HD1	7	0.78
(2,976)	1:A:78:PHE:H	1:A:78:PHE:HD1	7	0.78
(2,976)	1:A:78:PHE:H	1:A:78:PHE:HD2	7	0.78
(2,925)	1:A:72:VAL:HG21	1:A:73:ALA:H	2	0.78
(2,925)	1:A:72:VAL:HG22	1:A:73:ALA:H	2	0.78
(2,925)	1:A:72:VAL:HG23	1:A:73:ALA:H	2	0.78
(2,925)	1:A:72:VAL:HG11	1:A:73:ALA:H	2	0.78
(2,925)	1:A:72:VAL:HG12	1:A:73:ALA:H	2	0.78
(2,925)	1:A:72:VAL:HG13	1:A:73:ALA:H	2	0.78
(2,925)	1:A:72:VAL:HG21	1:A:73:ALA:H	3	0.78
(2,925)	1:A:72:VAL:HG22	1:A:73:ALA:H	3	0.78
(2,925)	1:A:72:VAL:HG23	1:A:73:ALA:H	3	0.78
(2,925)	1:A:72:VAL:HG11	1:A:73:ALA:H	3	0.78
(2,925)	1:A:72:VAL:HG12	1:A:73:ALA:H	3	0.78
(2,925)	1:A:72:VAL:HG13	1:A:73:ALA:H	3	0.78
(2,905)	1:A:67:CYS:HA	1:A:68:GLY:H	11	0.78
(2,867)	1:A:186:ILE:HD11	1:A:156:LEU:HD21	4	0.78
(2,775)	1:A:61:ILE:HD12	1:A:48:LEU:HD21	9	0.78
(2,756)	1:A:54:LEU:HD22	1:A:58:VAL:HG11	2	0.78
(2,756)	1:A:54:LEU:HD22	1:A:58:VAL:HG12	2	0.78
(2,756)	1:A:54:LEU:HD22	1:A:58:VAL:HG13	2	0.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,756)	1:A:54:LEU:HD23	1:A:58:VAL:HG11	2	0.78
(2,756)	1:A:54:LEU:HD23	1:A:58:VAL:HG12	2	0.78
(2,756)	1:A:54:LEU:HD23	1:A:58:VAL:HG13	2	0.78
(2,755)	1:A:54:LEU:HD21	1:A:58:VAL:HG11	13	0.78
(2,755)	1:A:54:LEU:HD21	1:A:58:VAL:HG12	13	0.78
(2,755)	1:A:54:LEU:HD21	1:A:58:VAL:HG13	13	0.78
(2,75)	1:A:55:ASN:H	1:A:59:ILE:H	19	0.78
(2,731)	1:A:211:VAL:HG13	1:A:226:LEU:HD21	9	0.78
(2,659)	1:A:42:MET:H	1:A:19:LEU:HD11	10	0.78
(2,659)	1:A:42:MET:H	1:A:19:LEU:HD12	10	0.78
(2,659)	1:A:42:MET:H	1:A:19:LEU:HD13	10	0.78
(2,626)	1:A:12:TRP:H	1:A:10:LEU:H	17	0.78
(2,518)	1:A:200:LEU:H	1:A:196:LEU:HD22	19	0.78
(2,518)	1:A:200:LEU:H	1:A:196:LEU:HD23	19	0.78
(2,516)	1:A:200:LEU:H	1:A:196:LEU:HD11	14	0.78
(2,516)	1:A:200:LEU:H	1:A:196:LEU:HD12	14	0.78
(2,516)	1:A:200:LEU:H	1:A:196:LEU:HD13	14	0.78
(2,424)	1:A:169:ASP:H	1:A:166:LEU:HB3	1	0.78
(2,379)	1:A:10:LEU:H	1:A:10:LEU:HD21	5	0.78
(2,229)	1:A:106:ASP:H	1:A:109:VAL:H	1	0.78
(2,229)	1:A:106:ASP:H	1:A:109:VAL:H	20	0.78
(2,226)	1:A:104:THR:H	1:A:106:ASP:H	20	0.78
(2,185)	1:A:94:VAL:H	1:A:92:ARG:H	4	0.78
(2,185)	1:A:94:VAL:H	1:A:92:ARG:H	11	0.78
(2,983)	1:A:79:PRO:HD3	1:A:80:ASN:H	5	0.77
(2,983)	1:A:79:PRO:HD3	1:A:80:ASN:H	5	0.77
(2,970)	1:A:77:LEU:HG	1:A:78:PHE:H	5	0.77
(2,961)	1:A:75:TYR:HD1	1:A:76:SER:H	3	0.77
(2,961)	1:A:75:TYR:HD2	1:A:76:SER:H	3	0.77
(2,925)	1:A:72:VAL:HG21	1:A:73:ALA:H	7	0.77
(2,925)	1:A:72:VAL:HG22	1:A:73:ALA:H	7	0.77
(2,925)	1:A:72:VAL:HG23	1:A:73:ALA:H	7	0.77
(2,925)	1:A:72:VAL:HG11	1:A:73:ALA:H	7	0.77
(2,925)	1:A:72:VAL:HG12	1:A:73:ALA:H	7	0.77
(2,925)	1:A:72:VAL:HG13	1:A:73:ALA:H	7	0.77
(2,912)	1:A:70:PRO:HB3	1:A:76:SER:H	19	0.77
(2,912)	1:A:70:PRO:HB2	1:A:76:SER:H	19	0.77
(2,891)	1:A:63:GLN:H	1:A:63:GLN:HB3	11	0.77
(2,891)	1:A:63:GLN:H	1:A:63:GLN:HB2	11	0.77
(2,891)	1:A:63:GLN:H	1:A:63:GLN:HB3	11	0.77
(2,891)	1:A:63:GLN:H	1:A:63:GLN:HB2	11	0.77
(2,832)	1:A:120:ILE:HD11	1:A:200:LEU:HD21	4	0.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,804)	1:A:93:ILE:HD11	1:A:105:VAL:HG21	2	0.77
(2,804)	1:A:93:ILE:HD11	1:A:105:VAL:HG22	2	0.77
(2,804)	1:A:93:ILE:HD11	1:A:105:VAL:HG23	2	0.77
(2,804)	1:A:93:ILE:HD12	1:A:105:VAL:HG21	2	0.77
(2,804)	1:A:93:ILE:HD12	1:A:105:VAL:HG22	2	0.77
(2,804)	1:A:93:ILE:HD12	1:A:105:VAL:HG23	2	0.77
(2,804)	1:A:93:ILE:HD13	1:A:105:VAL:HG21	2	0.77
(2,804)	1:A:93:ILE:HD13	1:A:105:VAL:HG22	2	0.77
(2,804)	1:A:93:ILE:HD13	1:A:105:VAL:HG23	2	0.77
(2,804)	1:A:93:ILE:HD11	1:A:105:VAL:HG21	13	0.77
(2,804)	1:A:93:ILE:HD11	1:A:105:VAL:HG22	13	0.77
(2,804)	1:A:93:ILE:HD11	1:A:105:VAL:HG23	13	0.77
(2,804)	1:A:93:ILE:HD12	1:A:105:VAL:HG21	13	0.77
(2,804)	1:A:93:ILE:HD12	1:A:105:VAL:HG22	13	0.77
(2,804)	1:A:93:ILE:HD12	1:A:105:VAL:HG23	13	0.77
(2,804)	1:A:93:ILE:HD13	1:A:105:VAL:HG21	13	0.77
(2,804)	1:A:93:ILE:HD13	1:A:105:VAL:HG22	13	0.77
(2,804)	1:A:93:ILE:HD13	1:A:105:VAL:HG23	13	0.77
(2,634)	1:A:54:LEU:HD11	1:A:12:TRP:HE1	3	0.77
(2,634)	1:A:54:LEU:HD12	1:A:12:TRP:HE1	3	0.77
(2,634)	1:A:54:LEU:HD13	1:A:12:TRP:HE1	3	0.77
(2,504)	1:A:198:HIS:H	1:A:202:MET:H	13	0.77
(2,379)	1:A:10:LEU:H	1:A:10:LEU:HD21	9	0.77
(2,369)	1:A:143:HIS:H	1:A:145:ASP:H	20	0.77
(2,985)	1:A:80:ASN:H	1:A:78:PHE:HD1	16	0.76
(2,976)	1:A:78:PHE:H	1:A:78:PHE:HD1	11	0.76
(2,976)	1:A:78:PHE:H	1:A:78:PHE:HD2	11	0.76
(2,973)	1:A:78:PHE:H	1:A:77:LEU:HD11	15	0.76
(2,973)	1:A:78:PHE:H	1:A:77:LEU:HD12	15	0.76
(2,973)	1:A:78:PHE:H	1:A:77:LEU:HD13	15	0.76
(2,961)	1:A:75:TYR:HD1	1:A:76:SER:H	20	0.76
(2,961)	1:A:75:TYR:HD2	1:A:76:SER:H	20	0.76
(2,936)	1:A:73:ALA:HB1	1:A:73:ALA:H	16	0.76
(2,936)	1:A:73:ALA:HB2	1:A:73:ALA:H	16	0.76
(2,936)	1:A:73:ALA:HB3	1:A:73:ALA:H	16	0.76
(2,899)	1:A:66:ARG:H	1:A:64:LYS:H	8	0.76
(2,898)	1:A:66:ARG:H	1:A:63:GLN:HB3	9	0.76
(2,898)	1:A:66:ARG:H	1:A:63:GLN:HB2	9	0.76
(2,891)	1:A:63:GLN:H	1:A:63:GLN:HB3	10	0.76
(2,891)	1:A:63:GLN:H	1:A:63:GLN:HB2	10	0.76
(2,891)	1:A:63:GLN:H	1:A:63:GLN:HB3	10	0.76
(2,891)	1:A:63:GLN:H	1:A:63:GLN:HB2	10	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,890)	1:A:63:GLN:H	1:A:63:GLN:HG3	8	0.76
(2,890)	1:A:63:GLN:H	1:A:63:GLN:HG3	8	0.76
(2,890)	1:A:63:GLN:H	1:A:63:GLN:HG3	19	0.76
(2,890)	1:A:63:GLN:H	1:A:63:GLN:HG3	19	0.76
(2,627)	1:A:13:GLU:H	1:A:10:LEU:H	3	0.76
(2,598)	1:A:235:GLN:H	1:A:238:TYR:HE1	18	0.76
(2,598)	1:A:235:GLN:H	1:A:238:TYR:HE2	18	0.76
(2,507)	1:A:199:SER:H	1:A:202:MET:H	15	0.76
(2,424)	1:A:169:ASP:H	1:A:166:LEU:HB3	9	0.76
(2,988)	1:A:129:TRP:HE1	4:A:305:PX4:C2	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:307:PX4:C2	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:309:PX4:C2	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:311:PX4:C2	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:313:PX4:C2	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:315:PX4:C2	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:317:PX4:C2	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:319:PX4:C2	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:321:PX4:C2	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:323:PX4:C2	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:325:PX4:C2	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:327:PX4:C2	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:329:PX4:C2	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:331:PX4:C2	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:333:PX4:C2	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:335:PX4:C2	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:337:PX4:C2	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:339:PX4:C2	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:341:PX4:C2	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:343:PX4:C2	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:345:PX4:C2	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:347:PX4:C2	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:349:PX4:C2	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:351:PX4:C2	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:353:PX4:C2	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:355:PX4:C2	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:357:PX4:C2	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:359:PX4:C2	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:361:PX4:C2	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:363:PX4:C2	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:402:PX4:C2	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:404:PX4:C2	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:406:PX4:C2	15	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,988)	1:A:129:TRP:HE1	4:A:408:PX4:C2	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:410:PX4:C2	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:412:PX4:C2	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:414:PX4:C2	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:416:PX4:C2	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:418:PX4:C2	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:420:PX4:C2	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:422:PX4:C2	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:424:PX4:C2	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:426:PX4:C2	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:428:PX4:C2	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:430:PX4:C2	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:305:PX4:C1	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:307:PX4:C1	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:309:PX4:C1	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:311:PX4:C1	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:313:PX4:C1	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:315:PX4:C1	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:317:PX4:C1	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:319:PX4:C1	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:321:PX4:C1	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:323:PX4:C1	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:325:PX4:C1	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:327:PX4:C1	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:329:PX4:C1	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:331:PX4:C1	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:333:PX4:C1	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:335:PX4:C1	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:337:PX4:C1	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:339:PX4:C1	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:341:PX4:C1	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:343:PX4:C1	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:345:PX4:C1	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:347:PX4:C1	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:349:PX4:C1	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:351:PX4:C1	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:353:PX4:C1	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:355:PX4:C1	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:357:PX4:C1	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:359:PX4:C1	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:361:PX4:C1	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:363:PX4:C1	15	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,988)	1:A:129:TRP:HE1	4:A:402:PX4:C1	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:404:PX4:C1	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:406:PX4:C1	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:408:PX4:C1	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:410:PX4:C1	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:412:PX4:C1	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:414:PX4:C1	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:416:PX4:C1	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:418:PX4:C1	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:420:PX4:C1	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:422:PX4:C1	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:424:PX4:C1	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:426:PX4:C1	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:428:PX4:C1	15	0.75
(2,988)	1:A:129:TRP:HE1	4:A:430:PX4:C1	15	0.75
(2,983)	1:A:79:PRO:HD3	1:A:80:ASN:H	4	0.75
(2,983)	1:A:79:PRO:HD3	1:A:80:ASN:H	4	0.75
(2,975)	1:A:78:PHE:H	1:A:77:LEU:HD22	12	0.75
(2,975)	1:A:78:PHE:H	1:A:77:LEU:HD23	12	0.75
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG21	11	0.75
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG22	11	0.75
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG23	11	0.75
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG11	11	0.75
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG12	11	0.75
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG13	11	0.75
(2,919)	1:A:72:VAL:H	1:A:71:ASP:HA	4	0.75
(2,913)	1:A:71:ASP:H	1:A:70:PRO:HB3	7	0.75
(2,913)	1:A:71:ASP:H	1:A:70:PRO:HB2	7	0.75
(2,913)	1:A:71:ASP:H	1:A:70:PRO:HB3	9	0.75
(2,913)	1:A:71:ASP:H	1:A:70:PRO:HB2	9	0.75
(2,912)	1:A:70:PRO:HB3	1:A:76:SER:H	3	0.75
(2,912)	1:A:70:PRO:HB2	1:A:76:SER:H	3	0.75
(2,905)	1:A:67:CYS:HA	1:A:68:GLY:H	2	0.75
(2,804)	1:A:93:ILE:HD11	1:A:105:VAL:HG21	18	0.75
(2,804)	1:A:93:ILE:HD11	1:A:105:VAL:HG22	18	0.75
(2,804)	1:A:93:ILE:HD11	1:A:105:VAL:HG23	18	0.75
(2,804)	1:A:93:ILE:HD12	1:A:105:VAL:HG21	18	0.75
(2,804)	1:A:93:ILE:HD12	1:A:105:VAL:HG22	18	0.75
(2,804)	1:A:93:ILE:HD12	1:A:105:VAL:HG23	18	0.75
(2,804)	1:A:93:ILE:HD13	1:A:105:VAL:HG21	18	0.75
(2,804)	1:A:93:ILE:HD13	1:A:105:VAL:HG22	18	0.75
(2,804)	1:A:93:ILE:HD13	1:A:105:VAL:HG23	18	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,746)	1:A:89:VAL:HG11	1:A:122:LEU:HD21	12	0.75
(2,598)	1:A:235:GLN:H	1:A:238:TYR:HE1	16	0.75
(2,598)	1:A:235:GLN:H	1:A:238:TYR:HE2	16	0.75
(2,392)	1:A:157:ALA:H	1:A:68:GLY:H	1	0.75
(2,212)	1:A:120:ILE:HD11	1:A:237:LEU:H	5	0.75
(2,212)	1:A:120:ILE:HD12	1:A:237:LEU:H	5	0.75
(2,212)	1:A:120:ILE:HD13	1:A:237:LEU:H	5	0.75
(2,976)	1:A:78:PHE:H	1:A:78:PHE:HD1	20	0.74
(2,976)	1:A:78:PHE:H	1:A:78:PHE:HD2	20	0.74
(2,970)	1:A:77:LEU:HG	1:A:78:PHE:H	4	0.74
(2,964)	1:A:75:TYR:H	1:A:76:SER:H	5	0.74
(2,959)	1:A:75:TYR:H	1:A:76:SER:H	5	0.74
(2,928)	1:A:72:VAL:H	1:A:73:ALA:HB1	12	0.74
(2,925)	1:A:72:VAL:HG21	1:A:73:ALA:H	11	0.74
(2,925)	1:A:72:VAL:HG22	1:A:73:ALA:H	11	0.74
(2,925)	1:A:72:VAL:HG23	1:A:73:ALA:H	11	0.74
(2,925)	1:A:72:VAL:HG11	1:A:73:ALA:H	11	0.74
(2,925)	1:A:72:VAL:HG12	1:A:73:ALA:H	11	0.74
(2,925)	1:A:72:VAL:HG13	1:A:73:ALA:H	11	0.74
(2,905)	1:A:67:CYS:HA	1:A:68:GLY:H	3	0.74
(2,869)	1:A:186:ILE:HD12	1:A:156:LEU:HD21	16	0.74
(2,809)	1:A:136:ILE:H	1:A:94:VAL:HG11	15	0.74
(2,809)	1:A:136:ILE:H	1:A:94:VAL:HG12	15	0.74
(2,809)	1:A:136:ILE:H	1:A:94:VAL:HG13	15	0.74
(2,756)	1:A:54:LEU:HD22	1:A:58:VAL:HG11	11	0.74
(2,756)	1:A:54:LEU:HD22	1:A:58:VAL:HG12	11	0.74
(2,756)	1:A:54:LEU:HD22	1:A:58:VAL:HG13	11	0.74
(2,756)	1:A:54:LEU:HD23	1:A:58:VAL:HG11	11	0.74
(2,756)	1:A:54:LEU:HD23	1:A:58:VAL:HG12	11	0.74
(2,756)	1:A:54:LEU:HD23	1:A:58:VAL:HG13	11	0.74
(2,414)	1:A:167:GLY:H	1:A:166:LEU:HD21	17	0.74
(2,983)	1:A:79:PRO:HD3	1:A:80:ASN:H	13	0.73
(2,983)	1:A:79:PRO:HD3	1:A:80:ASN:H	13	0.73
(2,979)	1:A:78:PHE:H	1:A:78:PHE:HD1	20	0.73
(2,964)	1:A:75:TYR:H	1:A:76:SER:H	14	0.73
(2,959)	1:A:75:TYR:H	1:A:76:SER:H	14	0.73
(2,936)	1:A:73:ALA:HB1	1:A:73:ALA:H	4	0.73
(2,936)	1:A:73:ALA:HB2	1:A:73:ALA:H	4	0.73
(2,936)	1:A:73:ALA:HB3	1:A:73:ALA:H	4	0.73
(2,930)	1:A:72:VAL:HG11	1:A:75:TYR:H	16	0.73
(2,930)	1:A:72:VAL:HG12	1:A:75:TYR:H	16	0.73
(2,930)	1:A:72:VAL:HG13	1:A:75:TYR:H	16	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,930)	1:A:72:VAL:HG11	1:A:75:TYR:H	18	0.73
(2,930)	1:A:72:VAL:HG12	1:A:75:TYR:H	18	0.73
(2,930)	1:A:72:VAL:HG13	1:A:75:TYR:H	18	0.73
(2,930)	1:A:72:VAL:HG11	1:A:75:TYR:H	20	0.73
(2,930)	1:A:72:VAL:HG12	1:A:75:TYR:H	20	0.73
(2,930)	1:A:72:VAL:HG13	1:A:75:TYR:H	20	0.73
(2,925)	1:A:72:VAL:HG21	1:A:73:ALA:H	16	0.73
(2,925)	1:A:72:VAL:HG22	1:A:73:ALA:H	16	0.73
(2,925)	1:A:72:VAL:HG23	1:A:73:ALA:H	16	0.73
(2,925)	1:A:72:VAL:HG11	1:A:73:ALA:H	16	0.73
(2,925)	1:A:72:VAL:HG12	1:A:73:ALA:H	16	0.73
(2,925)	1:A:72:VAL:HG13	1:A:73:ALA:H	16	0.73
(2,925)	1:A:72:VAL:HG21	1:A:73:ALA:H	18	0.73
(2,925)	1:A:72:VAL:HG22	1:A:73:ALA:H	18	0.73
(2,925)	1:A:72:VAL:HG23	1:A:73:ALA:H	18	0.73
(2,925)	1:A:72:VAL:HG11	1:A:73:ALA:H	18	0.73
(2,925)	1:A:72:VAL:HG12	1:A:73:ALA:H	18	0.73
(2,925)	1:A:72:VAL:HG13	1:A:73:ALA:H	18	0.73
(2,913)	1:A:71:ASP:H	1:A:70:PRO:HB3	5	0.73
(2,913)	1:A:71:ASP:H	1:A:70:PRO:HB2	5	0.73
(2,911)	1:A:69:VAL:HG21	1:A:69:VAL:H	18	0.73
(2,911)	1:A:69:VAL:HG22	1:A:69:VAL:H	18	0.73
(2,911)	1:A:69:VAL:HG23	1:A:69:VAL:H	18	0.73
(2,911)	1:A:69:VAL:HG11	1:A:69:VAL:H	18	0.73
(2,911)	1:A:69:VAL:HG12	1:A:69:VAL:H	18	0.73
(2,911)	1:A:69:VAL:HG13	1:A:69:VAL:H	18	0.73
(2,891)	1:A:63:GLN:H	1:A:63:GLN:HB3	7	0.73
(2,891)	1:A:63:GLN:H	1:A:63:GLN:HB2	7	0.73
(2,891)	1:A:63:GLN:H	1:A:63:GLN:HB3	7	0.73
(2,891)	1:A:63:GLN:H	1:A:63:GLN:HB2	7	0.73
(2,790)	1:A:58:VAL:HG12	1:A:39:LEU:HD21	20	0.73
(2,786)	1:A:24:LEU:H	1:A:24:LEU:HD21	1	0.73
(2,728)	1:A:211:VAL:HG11	1:A:226:LEU:HD22	1	0.73
(2,728)	1:A:211:VAL:HG11	1:A:226:LEU:HD23	1	0.73
(2,518)	1:A:200:LEU:H	1:A:196:LEU:HD22	5	0.73
(2,518)	1:A:200:LEU:H	1:A:196:LEU:HD23	5	0.73
(2,473)	1:A:186:ILE:H	1:A:156:LEU:HD22	10	0.73
(2,473)	1:A:186:ILE:H	1:A:156:LEU:HD23	10	0.73
(2,426)	1:A:170:ALA:H	1:A:136:ILE:HD11	15	0.73
(2,426)	1:A:170:ALA:H	1:A:136:ILE:HD12	15	0.73
(2,426)	1:A:170:ALA:H	1:A:136:ILE:HD13	15	0.73
(2,414)	1:A:167:GLY:H	1:A:166:LEU:HD21	12	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,185)	1:A:94:VAL:H	1:A:92:ARG:H	16	0.73
(2,974)	1:A:78:PHE:H	1:A:77:LEU:HD21	1	0.72
(2,936)	1:A:73:ALA:HB1	1:A:73:ALA:H	11	0.72
(2,936)	1:A:73:ALA:HB2	1:A:73:ALA:H	11	0.72
(2,936)	1:A:73:ALA:HB3	1:A:73:ALA:H	11	0.72
(2,919)	1:A:72:VAL:H	1:A:71:ASP:HA	9	0.72
(2,917)	1:A:71:ASP:H	1:A:72:VAL:HB	18	0.72
(2,913)	1:A:71:ASP:H	1:A:70:PRO:HB3	13	0.72
(2,913)	1:A:71:ASP:H	1:A:70:PRO:HB2	13	0.72
(2,913)	1:A:71:ASP:H	1:A:70:PRO:HB3	17	0.72
(2,913)	1:A:71:ASP:H	1:A:70:PRO:HB2	17	0.72
(2,899)	1:A:66:ARG:H	1:A:64:LYS:H	6	0.72
(2,844)	1:A:200:LEU:HD22	1:A:122:LEU:HD21	20	0.72
(2,75)	1:A:55:ASN:H	1:A:59:ILE:H	2	0.72
(2,659)	1:A:42:MET:H	1:A:19:LEU:HD11	17	0.72
(2,659)	1:A:42:MET:H	1:A:19:LEU:HD12	17	0.72
(2,659)	1:A:42:MET:H	1:A:19:LEU:HD13	17	0.72
(2,608)	1:A:238:TYR:H	1:A:120:ILE:HD11	10	0.72
(2,608)	1:A:238:TYR:H	1:A:120:ILE:HD12	10	0.72
(2,608)	1:A:238:TYR:H	1:A:120:ILE:HD13	10	0.72
(2,543)	1:A:210:ALA:H	1:A:213:TYR:H	5	0.72
(2,110)	1:A:11:GLN:H	1:A:14:GLN:H	18	0.72
(2,964)	1:A:75:TYR:H	1:A:76:SER:H	16	0.71
(2,961)	1:A:75:TYR:HD1	1:A:76:SER:H	18	0.71
(2,961)	1:A:75:TYR:HD2	1:A:76:SER:H	18	0.71
(2,959)	1:A:75:TYR:H	1:A:76:SER:H	16	0.71
(2,951)	1:A:74:GLU:H	1:A:76:SER:H	5	0.71
(2,936)	1:A:73:ALA:HB1	1:A:73:ALA:H	10	0.71
(2,936)	1:A:73:ALA:HB2	1:A:73:ALA:H	10	0.71
(2,936)	1:A:73:ALA:HB3	1:A:73:ALA:H	10	0.71
(2,919)	1:A:72:VAL:H	1:A:71:ASP:HA	17	0.71
(2,905)	1:A:67:CYS:HA	1:A:68:GLY:H	16	0.71
(2,786)	1:A:24:LEU:H	1:A:24:LEU:HD21	8	0.71
(2,570)	1:A:226:LEU:H	1:A:226:LEU:HD21	6	0.71
(2,425)	1:A:170:ALA:H	1:A:169:ASP:H	7	0.71
(2,392)	1:A:157:ALA:H	1:A:68:GLY:H	12	0.71
(2,264)	1:A:113:LEU:H	1:A:196:LEU:HD21	5	0.71
(2,178)	1:A:171:HIS:H	1:A:69:VAL:HG11	19	0.71
(2,178)	1:A:171:HIS:H	1:A:69:VAL:HG12	19	0.71
(2,178)	1:A:171:HIS:H	1:A:69:VAL:HG13	19	0.71
(3,6)	1:A:78:PHE:H	4:A:305:PX4:C27	19	0.7
(3,6)	1:A:78:PHE:H	4:A:307:PX4:C27	19	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,6)	1:A:78:PHE:H	4:A:309:PX4:C27	19	0.7
(3,6)	1:A:78:PHE:H	4:A:311:PX4:C27	19	0.7
(3,6)	1:A:78:PHE:H	4:A:313:PX4:C27	19	0.7
(3,6)	1:A:78:PHE:H	4:A:315:PX4:C27	19	0.7
(3,6)	1:A:78:PHE:H	4:A:317:PX4:C27	19	0.7
(3,6)	1:A:78:PHE:H	4:A:319:PX4:C27	19	0.7
(3,6)	1:A:78:PHE:H	4:A:321:PX4:C27	19	0.7
(3,6)	1:A:78:PHE:H	4:A:323:PX4:C27	19	0.7
(3,6)	1:A:78:PHE:H	4:A:325:PX4:C27	19	0.7
(3,6)	1:A:78:PHE:H	4:A:327:PX4:C27	19	0.7
(3,6)	1:A:78:PHE:H	4:A:329:PX4:C27	19	0.7
(3,6)	1:A:78:PHE:H	4:A:331:PX4:C27	19	0.7
(3,6)	1:A:78:PHE:H	4:A:333:PX4:C27	19	0.7
(3,6)	1:A:78:PHE:H	4:A:335:PX4:C27	19	0.7
(3,6)	1:A:78:PHE:H	4:A:337:PX4:C27	19	0.7
(3,6)	1:A:78:PHE:H	4:A:339:PX4:C27	19	0.7
(3,6)	1:A:78:PHE:H	4:A:341:PX4:C27	19	0.7
(3,6)	1:A:78:PHE:H	4:A:343:PX4:C27	19	0.7
(3,6)	1:A:78:PHE:H	4:A:345:PX4:C27	19	0.7
(3,6)	1:A:78:PHE:H	4:A:347:PX4:C27	19	0.7
(3,6)	1:A:78:PHE:H	4:A:349:PX4:C27	19	0.7
(3,6)	1:A:78:PHE:H	4:A:351:PX4:C27	19	0.7
(3,6)	1:A:78:PHE:H	4:A:353:PX4:C27	19	0.7
(3,6)	1:A:78:PHE:H	4:A:355:PX4:C27	19	0.7
(3,6)	1:A:78:PHE:H	4:A:357:PX4:C27	19	0.7
(3,6)	1:A:78:PHE:H	4:A:359:PX4:C27	19	0.7
(3,6)	1:A:78:PHE:H	4:A:361:PX4:C27	19	0.7
(3,6)	1:A:78:PHE:H	4:A:363:PX4:C27	19	0.7
(3,6)	1:A:78:PHE:H	4:A:402:PX4:C27	19	0.7
(3,6)	1:A:78:PHE:H	4:A:404:PX4:C27	19	0.7
(3,6)	1:A:78:PHE:H	4:A:406:PX4:C27	19	0.7
(3,6)	1:A:78:PHE:H	4:A:408:PX4:C27	19	0.7
(3,6)	1:A:78:PHE:H	4:A:410:PX4:C27	19	0.7
(3,6)	1:A:78:PHE:H	4:A:412:PX4:C27	19	0.7
(3,6)	1:A:78:PHE:H	4:A:414:PX4:C27	19	0.7
(3,6)	1:A:78:PHE:H	4:A:416:PX4:C27	19	0.7
(3,6)	1:A:78:PHE:H	4:A:418:PX4:C27	19	0.7
(3,6)	1:A:78:PHE:H	4:A:420:PX4:C27	19	0.7
(3,6)	1:A:78:PHE:H	4:A:422:PX4:C27	19	0.7
(3,6)	1:A:78:PHE:H	4:A:424:PX4:C27	19	0.7
(3,6)	1:A:78:PHE:H	4:A:426:PX4:C27	19	0.7
(3,6)	1:A:78:PHE:H	4:A:428:PX4:C27	19	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,6)	1:A:78:PHE:H	4:A:430:PX4:C27	19	0.7
(2,973)	1:A:78:PHE:H	1:A:77:LEU:HD11	6	0.7
(2,973)	1:A:78:PHE:H	1:A:77:LEU:HD12	6	0.7
(2,973)	1:A:78:PHE:H	1:A:77:LEU:HD13	6	0.7
(2,913)	1:A:71:ASP:H	1:A:70:PRO:HB3	3	0.7
(2,913)	1:A:71:ASP:H	1:A:70:PRO:HB2	3	0.7
(2,912)	1:A:70:PRO:HB3	1:A:76:SER:H	2	0.7
(2,912)	1:A:70:PRO:HB2	1:A:76:SER:H	2	0.7
(2,903)	1:A:67:CYS:H	1:A:66:ARG:HA	9	0.7
(2,786)	1:A:24:LEU:H	1:A:24:LEU:HD21	5	0.7
(2,786)	1:A:24:LEU:H	1:A:24:LEU:HD21	7	0.7
(2,621)	1:A:200:LEU:HD21	1:A:201:GLY:H	3	0.7
(2,598)	1:A:235:GLN:H	1:A:238:TYR:HE1	9	0.7
(2,598)	1:A:235:GLN:H	1:A:238:TYR:HE2	9	0.7
(2,424)	1:A:169:ASP:H	1:A:166:LEU:HB3	4	0.7
(2,379)	1:A:10:LEU:H	1:A:10:LEU:HD21	6	0.7
(2,305)	1:A:123:HIS:H	1:A:122:LEU:HD21	4	0.7
(2,983)	1:A:79:PRO:HD3	1:A:80:ASN:H	3	0.69
(2,983)	1:A:79:PRO:HD3	1:A:80:ASN:H	3	0.69
(2,983)	1:A:79:PRO:HD3	1:A:80:ASN:H	10	0.69
(2,983)	1:A:79:PRO:HD3	1:A:80:ASN:H	10	0.69
(2,974)	1:A:78:PHE:H	1:A:77:LEU:HD21	7	0.69
(2,970)	1:A:77:LEU:HG	1:A:78:PHE:H	17	0.69
(2,936)	1:A:73:ALA:HB1	1:A:73:ALA:H	17	0.69
(2,936)	1:A:73:ALA:HB2	1:A:73:ALA:H	17	0.69
(2,936)	1:A:73:ALA:HB3	1:A:73:ALA:H	17	0.69
(2,903)	1:A:67:CYS:H	1:A:66:ARG:HA	17	0.69
(2,755)	1:A:54:LEU:HD21	1:A:58:VAL:HG11	15	0.69
(2,755)	1:A:54:LEU:HD21	1:A:58:VAL:HG12	15	0.69
(2,755)	1:A:54:LEU:HD21	1:A:58:VAL:HG13	15	0.69
(2,627)	1:A:13:GLU:H	1:A:10:LEU:H	6	0.69
(2,626)	1:A:12:TRP:H	1:A:10:LEU:H	2	0.69
(2,264)	1:A:113:LEU:H	1:A:196:LEU:HD21	13	0.69
(2,983)	1:A:79:PRO:HD3	1:A:80:ASN:H	16	0.68
(2,983)	1:A:79:PRO:HD3	1:A:80:ASN:H	16	0.68
(2,964)	1:A:75:TYR:H	1:A:76:SER:H	8	0.68
(2,961)	1:A:75:TYR:HD1	1:A:76:SER:H	4	0.68
(2,961)	1:A:75:TYR:HD2	1:A:76:SER:H	4	0.68
(2,959)	1:A:75:TYR:H	1:A:76:SER:H	8	0.68
(2,917)	1:A:71:ASP:H	1:A:72:VAL:HB	4	0.68
(2,905)	1:A:67:CYS:HA	1:A:68:GLY:H	17	0.68
(2,903)	1:A:67:CYS:H	1:A:66:ARG:HA	18	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,898)	1:A:66:ARG:H	1:A:63:GLN:HB3	3	0.68
(2,898)	1:A:66:ARG:H	1:A:63:GLN:HB2	3	0.68
(2,829)	1:A:120:ILE:HD11	1:A:234:ILE:HG12	16	0.68
(2,829)	1:A:120:ILE:HD12	1:A:234:ILE:HG12	16	0.68
(2,829)	1:A:120:ILE:HD13	1:A:234:ILE:HG12	16	0.68
(2,718)	1:A:54:LEU:HD11	1:A:59:ILE:HD11	4	0.68
(2,718)	1:A:54:LEU:HD11	1:A:59:ILE:HD12	4	0.68
(2,718)	1:A:54:LEU:HD11	1:A:59:ILE:HD13	4	0.68
(2,718)	1:A:54:LEU:HD12	1:A:59:ILE:HD11	4	0.68
(2,718)	1:A:54:LEU:HD12	1:A:59:ILE:HD12	4	0.68
(2,718)	1:A:54:LEU:HD12	1:A:59:ILE:HD13	4	0.68
(2,718)	1:A:54:LEU:HD13	1:A:59:ILE:HD11	4	0.68
(2,718)	1:A:54:LEU:HD13	1:A:59:ILE:HD12	4	0.68
(2,718)	1:A:54:LEU:HD13	1:A:59:ILE:HD13	4	0.68
(2,627)	1:A:13:GLU:H	1:A:10:LEU:H	19	0.68
(2,608)	1:A:238:TYR:H	1:A:120:ILE:HD11	5	0.68
(2,608)	1:A:238:TYR:H	1:A:120:ILE:HD12	5	0.68
(2,608)	1:A:238:TYR:H	1:A:120:ILE:HD13	5	0.68
(2,543)	1:A:210:ALA:H	1:A:213:TYR:H	20	0.68
(2,516)	1:A:200:LEU:H	1:A:196:LEU:HD11	1	0.68
(2,516)	1:A:200:LEU:H	1:A:196:LEU:HD12	1	0.68
(2,516)	1:A:200:LEU:H	1:A:196:LEU:HD13	1	0.68
(2,392)	1:A:157:ALA:H	1:A:68:GLY:H	5	0.68
(2,379)	1:A:10:LEU:H	1:A:10:LEU:HD21	12	0.68
(2,212)	1:A:120:ILE:HD11	1:A:237:LEU:H	17	0.68
(2,212)	1:A:120:ILE:HD12	1:A:237:LEU:H	17	0.68
(2,212)	1:A:120:ILE:HD13	1:A:237:LEU:H	17	0.68
(2,178)	1:A:171:HIS:H	1:A:69:VAL:HG11	7	0.68
(2,178)	1:A:171:HIS:H	1:A:69:VAL:HG12	7	0.68
(2,178)	1:A:171:HIS:H	1:A:69:VAL:HG13	7	0.68
(2,125)	1:A:157:ALA:H	1:A:68:GLY:H	9	0.68
(2,979)	1:A:78:PHE:H	1:A:78:PHE:HD1	11	0.67
(2,964)	1:A:75:TYR:H	1:A:76:SER:H	9	0.67
(2,959)	1:A:75:TYR:H	1:A:76:SER:H	9	0.67
(2,948)	1:A:74:GLU:HG3	1:A:75:TYR:H	6	0.67
(2,948)	1:A:74:GLU:HG3	1:A:75:TYR:H	6	0.67
(2,936)	1:A:73:ALA:HB1	1:A:73:ALA:H	20	0.67
(2,936)	1:A:73:ALA:HB2	1:A:73:ALA:H	20	0.67
(2,936)	1:A:73:ALA:HB3	1:A:73:ALA:H	20	0.67
(2,930)	1:A:72:VAL:HG11	1:A:75:TYR:H	19	0.67
(2,930)	1:A:72:VAL:HG12	1:A:75:TYR:H	19	0.67
(2,930)	1:A:72:VAL:HG13	1:A:75:TYR:H	19	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,925)	1:A:72:VAL:HG21	1:A:73:ALA:H	10	0.67
(2,925)	1:A:72:VAL:HG22	1:A:73:ALA:H	10	0.67
(2,925)	1:A:72:VAL:HG23	1:A:73:ALA:H	10	0.67
(2,925)	1:A:72:VAL:HG11	1:A:73:ALA:H	10	0.67
(2,925)	1:A:72:VAL:HG12	1:A:73:ALA:H	10	0.67
(2,925)	1:A:72:VAL:HG13	1:A:73:ALA:H	10	0.67
(2,913)	1:A:71:ASP:H	1:A:70:PRO:HB3	8	0.67
(2,913)	1:A:71:ASP:H	1:A:70:PRO:HB2	8	0.67
(2,913)	1:A:71:ASP:H	1:A:70:PRO:HB3	15	0.67
(2,913)	1:A:71:ASP:H	1:A:70:PRO:HB2	15	0.67
(2,912)	1:A:70:PRO:HB3	1:A:76:SER:H	16	0.67
(2,912)	1:A:70:PRO:HB2	1:A:76:SER:H	16	0.67
(2,905)	1:A:67:CYS:HA	1:A:68:GLY:H	15	0.67
(2,898)	1:A:66:ARG:H	1:A:63:GLN:HB3	5	0.67
(2,898)	1:A:66:ARG:H	1:A:63:GLN:HB2	5	0.67
(2,809)	1:A:136:ILE:H	1:A:94:VAL:HG11	11	0.67
(2,809)	1:A:136:ILE:H	1:A:94:VAL:HG12	11	0.67
(2,809)	1:A:136:ILE:H	1:A:94:VAL:HG13	11	0.67
(2,786)	1:A:24:LEU:H	1:A:24:LEU:HD21	11	0.67
(2,775)	1:A:61:ILE:HD12	1:A:48:LEU:HD21	19	0.67
(2,732)	1:A:211:VAL:HG13	1:A:226:LEU:HD22	18	0.67
(2,732)	1:A:211:VAL:HG13	1:A:226:LEU:HD23	18	0.67
(2,627)	1:A:13:GLU:H	1:A:10:LEU:H	17	0.67
(2,507)	1:A:199:SER:H	1:A:202:MET:H	19	0.67
(2,423)	1:A:169:ASP:H	1:A:134:ILE:HD11	8	0.67
(2,423)	1:A:169:ASP:H	1:A:134:ILE:HD12	8	0.67
(2,423)	1:A:169:ASP:H	1:A:134:ILE:HD13	8	0.67
(2,185)	1:A:94:VAL:H	1:A:92:ARG:H	3	0.67
(2,983)	1:A:79:PRO:HD3	1:A:80:ASN:H	7	0.66
(2,983)	1:A:79:PRO:HD3	1:A:80:ASN:H	7	0.66
(2,981)	1:A:78:PHE:H	1:A:79:PRO:HG3	12	0.66
(2,981)	1:A:78:PHE:H	1:A:79:PRO:HG3	12	0.66
(2,930)	1:A:72:VAL:HG11	1:A:75:TYR:H	10	0.66
(2,930)	1:A:72:VAL:HG12	1:A:75:TYR:H	10	0.66
(2,930)	1:A:72:VAL:HG13	1:A:75:TYR:H	10	0.66
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG21	1	0.66
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG22	1	0.66
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG23	1	0.66
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG11	1	0.66
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG12	1	0.66
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG13	1	0.66
(2,911)	1:A:69:VAL:HG21	1:A:69:VAL:H	1	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,911)	1:A:69:VAL:HG22	1:A:69:VAL:H	1	0.66
(2,911)	1:A:69:VAL:HG23	1:A:69:VAL:H	1	0.66
(2,911)	1:A:69:VAL:HG11	1:A:69:VAL:H	1	0.66
(2,911)	1:A:69:VAL:HG12	1:A:69:VAL:H	1	0.66
(2,911)	1:A:69:VAL:HG13	1:A:69:VAL:H	1	0.66
(2,627)	1:A:13:GLU:H	1:A:10:LEU:H	12	0.66
(2,626)	1:A:12:TRP:H	1:A:10:LEU:H	4	0.66
(2,626)	1:A:12:TRP:H	1:A:10:LEU:H	5	0.66
(2,426)	1:A:170:ALA:H	1:A:136:ILE:HD11	5	0.66
(2,426)	1:A:170:ALA:H	1:A:136:ILE:HD12	5	0.66
(2,426)	1:A:170:ALA:H	1:A:136:ILE:HD13	5	0.66
(2,425)	1:A:170:ALA:H	1:A:169:ASP:H	4	0.66
(2,976)	1:A:78:PHE:H	1:A:78:PHE:HD1	3	0.65
(2,976)	1:A:78:PHE:H	1:A:78:PHE:HD2	3	0.65
(2,964)	1:A:75:TYR:H	1:A:76:SER:H	17	0.65
(2,959)	1:A:75:TYR:H	1:A:76:SER:H	17	0.65
(2,925)	1:A:72:VAL:HG21	1:A:73:ALA:H	12	0.65
(2,925)	1:A:72:VAL:HG22	1:A:73:ALA:H	12	0.65
(2,925)	1:A:72:VAL:HG23	1:A:73:ALA:H	12	0.65
(2,925)	1:A:72:VAL:HG11	1:A:73:ALA:H	12	0.65
(2,925)	1:A:72:VAL:HG12	1:A:73:ALA:H	12	0.65
(2,925)	1:A:72:VAL:HG13	1:A:73:ALA:H	12	0.65
(2,919)	1:A:72:VAL:H	1:A:71:ASP:HA	18	0.65
(2,915)	1:A:71:ASP:H	1:A:72:VAL:HG21	1	0.65
(2,915)	1:A:71:ASP:H	1:A:72:VAL:HG22	1	0.65
(2,915)	1:A:71:ASP:H	1:A:72:VAL:HG23	1	0.65
(2,896)	1:A:64:LYS:H	1:A:64:LYS:HE3	18	0.65
(2,896)	1:A:64:LYS:H	1:A:64:LYS:HE3	18	0.65
(2,890)	1:A:63:GLN:H	1:A:63:GLN:HG3	17	0.65
(2,890)	1:A:63:GLN:H	1:A:63:GLN:HG3	17	0.65
(2,872)	1:A:186:ILE:HD13	1:A:156:LEU:HD22	19	0.65
(2,872)	1:A:186:ILE:HD13	1:A:156:LEU:HD23	19	0.65
(2,846)	1:A:200:LEU:HD23	1:A:122:LEU:HD21	19	0.65
(2,835)	1:A:120:ILE:HD12	1:A:200:LEU:HD22	1	0.65
(2,835)	1:A:120:ILE:HD12	1:A:200:LEU:HD23	1	0.65
(2,804)	1:A:93:ILE:HD11	1:A:105:VAL:HG21	4	0.65
(2,804)	1:A:93:ILE:HD11	1:A:105:VAL:HG22	4	0.65
(2,804)	1:A:93:ILE:HD11	1:A:105:VAL:HG23	4	0.65
(2,804)	1:A:93:ILE:HD12	1:A:105:VAL:HG21	4	0.65
(2,804)	1:A:93:ILE:HD12	1:A:105:VAL:HG22	4	0.65
(2,804)	1:A:93:ILE:HD12	1:A:105:VAL:HG23	4	0.65
(2,804)	1:A:93:ILE:HD13	1:A:105:VAL:HG21	4	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,804)	1:A:93:ILE:HD13	1:A:105:VAL:HG22	4	0.65
(2,804)	1:A:93:ILE:HD13	1:A:105:VAL:HG23	4	0.65
(2,757)	1:A:54:LEU:HD21	1:A:39:LEU:HD11	10	0.65
(2,757)	1:A:54:LEU:HD21	1:A:39:LEU:HD12	10	0.65
(2,757)	1:A:54:LEU:HD21	1:A:39:LEU:HD13	10	0.65
(2,727)	1:A:211:VAL:HG11	1:A:226:LEU:HD21	20	0.65
(2,627)	1:A:13:GLU:H	1:A:10:LEU:H	5	0.65
(2,425)	1:A:170:ALA:H	1:A:169:ASP:H	12	0.65
(2,423)	1:A:169:ASP:H	1:A:134:ILE:HD11	3	0.65
(2,423)	1:A:169:ASP:H	1:A:134:ILE:HD12	3	0.65
(2,423)	1:A:169:ASP:H	1:A:134:ILE:HD13	3	0.65
(2,392)	1:A:157:ALA:H	1:A:68:GLY:H	7	0.65
(2,379)	1:A:10:LEU:H	1:A:10:LEU:HD21	18	0.65
(2,110)	1:A:11:GLN:H	1:A:14:GLN:H	16	0.65
(3,6)	1:A:78:PHE:H	4:A:305:PX4:C27	11	0.64
(3,6)	1:A:78:PHE:H	4:A:307:PX4:C27	11	0.64
(3,6)	1:A:78:PHE:H	4:A:309:PX4:C27	11	0.64
(3,6)	1:A:78:PHE:H	4:A:311:PX4:C27	11	0.64
(3,6)	1:A:78:PHE:H	4:A:313:PX4:C27	11	0.64
(3,6)	1:A:78:PHE:H	4:A:315:PX4:C27	11	0.64
(3,6)	1:A:78:PHE:H	4:A:317:PX4:C27	11	0.64
(3,6)	1:A:78:PHE:H	4:A:319:PX4:C27	11	0.64
(3,6)	1:A:78:PHE:H	4:A:321:PX4:C27	11	0.64
(3,6)	1:A:78:PHE:H	4:A:323:PX4:C27	11	0.64
(3,6)	1:A:78:PHE:H	4:A:325:PX4:C27	11	0.64
(3,6)	1:A:78:PHE:H	4:A:327:PX4:C27	11	0.64
(3,6)	1:A:78:PHE:H	4:A:329:PX4:C27	11	0.64
(3,6)	1:A:78:PHE:H	4:A:331:PX4:C27	11	0.64
(3,6)	1:A:78:PHE:H	4:A:333:PX4:C27	11	0.64
(3,6)	1:A:78:PHE:H	4:A:335:PX4:C27	11	0.64
(3,6)	1:A:78:PHE:H	4:A:337:PX4:C27	11	0.64
(3,6)	1:A:78:PHE:H	4:A:339:PX4:C27	11	0.64
(3,6)	1:A:78:PHE:H	4:A:341:PX4:C27	11	0.64
(3,6)	1:A:78:PHE:H	4:A:343:PX4:C27	11	0.64
(3,6)	1:A:78:PHE:H	4:A:345:PX4:C27	11	0.64
(3,6)	1:A:78:PHE:H	4:A:347:PX4:C27	11	0.64
(3,6)	1:A:78:PHE:H	4:A:349:PX4:C27	11	0.64
(3,6)	1:A:78:PHE:H	4:A:351:PX4:C27	11	0.64
(3,6)	1:A:78:PHE:H	4:A:353:PX4:C27	11	0.64
(3,6)	1:A:78:PHE:H	4:A:355:PX4:C27	11	0.64
(3,6)	1:A:78:PHE:H	4:A:357:PX4:C27	11	0.64
(3,6)	1:A:78:PHE:H	4:A:359:PX4:C27	11	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,6)	1:A:78:PHE:H	4:A:361:PX4:C27	11	0.64
(3,6)	1:A:78:PHE:H	4:A:363:PX4:C27	11	0.64
(3,6)	1:A:78:PHE:H	4:A:402:PX4:C27	11	0.64
(3,6)	1:A:78:PHE:H	4:A:404:PX4:C27	11	0.64
(3,6)	1:A:78:PHE:H	4:A:406:PX4:C27	11	0.64
(3,6)	1:A:78:PHE:H	4:A:408:PX4:C27	11	0.64
(3,6)	1:A:78:PHE:H	4:A:410:PX4:C27	11	0.64
(3,6)	1:A:78:PHE:H	4:A:412:PX4:C27	11	0.64
(3,6)	1:A:78:PHE:H	4:A:414:PX4:C27	11	0.64
(3,6)	1:A:78:PHE:H	4:A:416:PX4:C27	11	0.64
(3,6)	1:A:78:PHE:H	4:A:418:PX4:C27	11	0.64
(3,6)	1:A:78:PHE:H	4:A:420:PX4:C27	11	0.64
(3,6)	1:A:78:PHE:H	4:A:422:PX4:C27	11	0.64
(3,6)	1:A:78:PHE:H	4:A:424:PX4:C27	11	0.64
(3,6)	1:A:78:PHE:H	4:A:426:PX4:C27	11	0.64
(3,6)	1:A:78:PHE:H	4:A:428:PX4:C27	11	0.64
(3,6)	1:A:78:PHE:H	4:A:430:PX4:C27	11	0.64
(2,976)	1:A:78:PHE:H	1:A:78:PHE:HD1	8	0.64
(2,976)	1:A:78:PHE:H	1:A:78:PHE:HD2	8	0.64
(2,964)	1:A:75:TYR:H	1:A:76:SER:H	6	0.64
(2,961)	1:A:75:TYR:HD1	1:A:76:SER:H	12	0.64
(2,961)	1:A:75:TYR:HD2	1:A:76:SER:H	12	0.64
(2,959)	1:A:75:TYR:H	1:A:76:SER:H	6	0.64
(2,951)	1:A:74:GLU:H	1:A:76:SER:H	10	0.64
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG21	5	0.64
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG22	5	0.64
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG23	5	0.64
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG11	5	0.64
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG12	5	0.64
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG13	5	0.64
(2,911)	1:A:69:VAL:HG21	1:A:69:VAL:H	19	0.64
(2,911)	1:A:69:VAL:HG22	1:A:69:VAL:H	19	0.64
(2,911)	1:A:69:VAL:HG23	1:A:69:VAL:H	19	0.64
(2,911)	1:A:69:VAL:HG11	1:A:69:VAL:H	19	0.64
(2,911)	1:A:69:VAL:HG12	1:A:69:VAL:H	19	0.64
(2,911)	1:A:69:VAL:HG13	1:A:69:VAL:H	19	0.64
(2,896)	1:A:64:LYS:H	1:A:64:LYS:HE3	11	0.64
(2,896)	1:A:64:LYS:H	1:A:64:LYS:HE3	11	0.64
(2,896)	1:A:64:LYS:H	1:A:64:LYS:HE3	19	0.64
(2,896)	1:A:64:LYS:H	1:A:64:LYS:HE3	19	0.64
(2,896)	1:A:64:LYS:H	1:A:64:LYS:HE3	20	0.64
(2,896)	1:A:64:LYS:H	1:A:64:LYS:HE3	20	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,890)	1:A:63:GLN:H	1:A:63:GLN:HG3	1	0.64
(2,890)	1:A:63:GLN:H	1:A:63:GLN:HG3	1	0.64
(2,890)	1:A:63:GLN:H	1:A:63:GLN:HG3	13	0.64
(2,890)	1:A:63:GLN:H	1:A:63:GLN:HG3	13	0.64
(2,890)	1:A:63:GLN:H	1:A:63:GLN:HG3	16	0.64
(2,890)	1:A:63:GLN:H	1:A:63:GLN:HG3	16	0.64
(2,839)	1:A:123:HIS:H	1:A:122:LEU:HD11	19	0.64
(2,839)	1:A:123:HIS:H	1:A:122:LEU:HD12	19	0.64
(2,839)	1:A:123:HIS:H	1:A:122:LEU:HD13	19	0.64
(2,729)	1:A:211:VAL:HG12	1:A:226:LEU:HD21	14	0.64
(2,570)	1:A:226:LEU:H	1:A:226:LEU:HD21	19	0.64
(2,466)	1:A:84:TRP:H	1:A:200:LEU:HD21	11	0.64
(2,425)	1:A:170:ALA:H	1:A:169:ASP:H	10	0.64
(2,304)	1:A:123:HIS:H	1:A:122:LEU:HD11	19	0.64
(2,304)	1:A:123:HIS:H	1:A:122:LEU:HD12	19	0.64
(2,304)	1:A:123:HIS:H	1:A:122:LEU:HD13	19	0.64
(2,185)	1:A:94:VAL:H	1:A:92:ARG:H	6	0.64
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG21	15	0.63
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG22	15	0.63
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG23	15	0.63
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG11	15	0.63
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG12	15	0.63
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG13	15	0.63
(2,913)	1:A:71:ASP:H	1:A:70:PRO:HB3	6	0.63
(2,913)	1:A:71:ASP:H	1:A:70:PRO:HB2	6	0.63
(2,913)	1:A:71:ASP:H	1:A:70:PRO:HB3	12	0.63
(2,913)	1:A:71:ASP:H	1:A:70:PRO:HB2	12	0.63
(2,911)	1:A:69:VAL:HG21	1:A:69:VAL:H	17	0.63
(2,911)	1:A:69:VAL:HG22	1:A:69:VAL:H	17	0.63
(2,911)	1:A:69:VAL:HG23	1:A:69:VAL:H	17	0.63
(2,911)	1:A:69:VAL:HG11	1:A:69:VAL:H	17	0.63
(2,911)	1:A:69:VAL:HG12	1:A:69:VAL:H	17	0.63
(2,911)	1:A:69:VAL:HG13	1:A:69:VAL:H	17	0.63
(2,905)	1:A:67:CYS:HA	1:A:68:GLY:H	12	0.63
(2,899)	1:A:66:ARG:H	1:A:64:LYS:H	12	0.63
(2,896)	1:A:64:LYS:H	1:A:64:LYS:HE3	8	0.63
(2,896)	1:A:64:LYS:H	1:A:64:LYS:HE3	8	0.63
(2,896)	1:A:64:LYS:H	1:A:64:LYS:HE3	9	0.63
(2,896)	1:A:64:LYS:H	1:A:64:LYS:HE3	9	0.63
(2,857)	1:A:186:ILE:HD11	1:A:156:LEU:HD21	16	0.63
(2,842)	1:A:200:LEU:HD21	1:A:122:LEU:HD21	17	0.63
(2,760)	1:A:54:LEU:HD22	1:A:59:ILE:HD11	17	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,760)	1:A:54:LEU:HD22	1:A:59:ILE:HD12	17	0.63
(2,760)	1:A:54:LEU:HD22	1:A:59:ILE:HD13	17	0.63
(2,760)	1:A:54:LEU:HD23	1:A:59:ILE:HD11	17	0.63
(2,760)	1:A:54:LEU:HD23	1:A:59:ILE:HD12	17	0.63
(2,760)	1:A:54:LEU:HD23	1:A:59:ILE:HD13	17	0.63
(2,425)	1:A:170:ALA:H	1:A:169:ASP:H	16	0.63
(2,425)	1:A:170:ALA:H	1:A:169:ASP:H	17	0.63
(2,278)	1:A:116:TRP:HE1	1:A:211:VAL:HG11	2	0.63
(2,278)	1:A:116:TRP:HE1	1:A:211:VAL:HG12	2	0.63
(2,278)	1:A:116:TRP:HE1	1:A:211:VAL:HG13	2	0.63
(2,185)	1:A:94:VAL:H	1:A:92:ARG:H	8	0.63
(2,961)	1:A:75:TYR:HD1	1:A:76:SER:H	6	0.62
(2,961)	1:A:75:TYR:HD2	1:A:76:SER:H	6	0.62
(2,961)	1:A:75:TYR:HD1	1:A:76:SER:H	15	0.62
(2,961)	1:A:75:TYR:HD2	1:A:76:SER:H	15	0.62
(2,931)	1:A:72:VAL:H	1:A:75:TYR:HB3	4	0.62
(2,931)	1:A:72:VAL:H	1:A:75:TYR:HB3	4	0.62
(2,759)	1:A:54:LEU:HD21	1:A:59:ILE:HD11	10	0.62
(2,759)	1:A:54:LEU:HD21	1:A:59:ILE:HD12	10	0.62
(2,759)	1:A:54:LEU:HD21	1:A:59:ILE:HD13	10	0.62
(2,75)	1:A:55:ASN:H	1:A:59:ILE:H	4	0.62
(2,507)	1:A:199:SER:H	1:A:202:MET:H	2	0.62
(2,473)	1:A:186:ILE:H	1:A:156:LEU:HD22	16	0.62
(2,473)	1:A:186:ILE:H	1:A:156:LEU:HD23	16	0.62
(2,466)	1:A:84:TRP:H	1:A:200:LEU:HD21	10	0.62
(2,317)	1:A:125:ARG:H	1:A:91:TYR:H	2	0.62
(2,976)	1:A:78:PHE:H	1:A:78:PHE:HD1	5	0.61
(2,976)	1:A:78:PHE:H	1:A:78:PHE:HD2	5	0.61
(2,976)	1:A:78:PHE:H	1:A:78:PHE:HD1	10	0.61
(2,976)	1:A:78:PHE:H	1:A:78:PHE:HD2	10	0.61
(2,973)	1:A:78:PHE:H	1:A:77:LEU:HD11	16	0.61
(2,973)	1:A:78:PHE:H	1:A:77:LEU:HD12	16	0.61
(2,973)	1:A:78:PHE:H	1:A:77:LEU:HD13	16	0.61
(2,973)	1:A:78:PHE:H	1:A:77:LEU:HD11	19	0.61
(2,973)	1:A:78:PHE:H	1:A:77:LEU:HD12	19	0.61
(2,973)	1:A:78:PHE:H	1:A:77:LEU:HD13	19	0.61
(2,951)	1:A:74:GLU:H	1:A:76:SER:H	1	0.61
(2,925)	1:A:72:VAL:HG21	1:A:73:ALA:H	1	0.61
(2,925)	1:A:72:VAL:HG22	1:A:73:ALA:H	1	0.61
(2,925)	1:A:72:VAL:HG23	1:A:73:ALA:H	1	0.61
(2,925)	1:A:72:VAL:HG11	1:A:73:ALA:H	1	0.61
(2,925)	1:A:72:VAL:HG12	1:A:73:ALA:H	1	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,925)	1:A:72:VAL:HG13	1:A:73:ALA:H	1	0.61
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG21	8	0.61
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG22	8	0.61
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG23	8	0.61
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG11	8	0.61
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG12	8	0.61
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG13	8	0.61
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG21	13	0.61
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG22	13	0.61
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG23	13	0.61
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG11	13	0.61
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG12	13	0.61
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG13	13	0.61
(2,905)	1:A:67:CYS:HA	1:A:68:GLY:H	13	0.61
(2,903)	1:A:67:CYS:H	1:A:66:ARG:HA	14	0.61
(2,903)	1:A:67:CYS:H	1:A:66:ARG:HA	20	0.61
(2,890)	1:A:63:GLN:H	1:A:63:GLN:HG3	20	0.61
(2,890)	1:A:63:GLN:H	1:A:63:GLN:HG3	20	0.61
(2,804)	1:A:93:ILE:HD11	1:A:105:VAL:HG21	9	0.61
(2,804)	1:A:93:ILE:HD11	1:A:105:VAL:HG22	9	0.61
(2,804)	1:A:93:ILE:HD11	1:A:105:VAL:HG23	9	0.61
(2,804)	1:A:93:ILE:HD12	1:A:105:VAL:HG21	9	0.61
(2,804)	1:A:93:ILE:HD12	1:A:105:VAL:HG22	9	0.61
(2,804)	1:A:93:ILE:HD12	1:A:105:VAL:HG23	9	0.61
(2,804)	1:A:93:ILE:HD13	1:A:105:VAL:HG21	9	0.61
(2,804)	1:A:93:ILE:HD13	1:A:105:VAL:HG22	9	0.61
(2,804)	1:A:93:ILE:HD13	1:A:105:VAL:HG23	9	0.61
(2,789)	1:A:58:VAL:HG11	1:A:39:LEU:HD22	20	0.61
(2,789)	1:A:58:VAL:HG11	1:A:39:LEU:HD23	20	0.61
(2,659)	1:A:42:MET:H	1:A:19:LEU:HD11	18	0.61
(2,659)	1:A:42:MET:H	1:A:19:LEU:HD12	18	0.61
(2,659)	1:A:42:MET:H	1:A:19:LEU:HD13	18	0.61
(2,621)	1:A:200:LEU:HD21	1:A:201:GLY:H	6	0.61
(2,369)	1:A:143:HIS:H	1:A:145:ASP:H	14	0.61
(2,10)	1:A:92:ARG:H	1:A:93:ILE:HG13	10	0.61
(2,10)	1:A:92:ARG:H	1:A:93:ILE:HG12	10	0.61
(2,979)	1:A:78:PHE:H	1:A:78:PHE:HD1	5	0.6
(2,976)	1:A:78:PHE:H	1:A:78:PHE:HD1	4	0.6
(2,976)	1:A:78:PHE:H	1:A:78:PHE:HD2	4	0.6
(2,930)	1:A:72:VAL:HG11	1:A:75:TYR:H	8	0.6
(2,930)	1:A:72:VAL:HG12	1:A:75:TYR:H	8	0.6
(2,930)	1:A:72:VAL:HG13	1:A:75:TYR:H	8	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,913)	1:A:71:ASP:H	1:A:70:PRO:HB3	14	0.6
(2,913)	1:A:71:ASP:H	1:A:70:PRO:HB2	14	0.6
(2,911)	1:A:69:VAL:HG21	1:A:69:VAL:H	14	0.6
(2,911)	1:A:69:VAL:HG22	1:A:69:VAL:H	14	0.6
(2,911)	1:A:69:VAL:HG23	1:A:69:VAL:H	14	0.6
(2,911)	1:A:69:VAL:HG11	1:A:69:VAL:H	14	0.6
(2,911)	1:A:69:VAL:HG12	1:A:69:VAL:H	14	0.6
(2,911)	1:A:69:VAL:HG13	1:A:69:VAL:H	14	0.6
(2,890)	1:A:63:GLN:H	1:A:63:GLN:HG3	3	0.6
(2,890)	1:A:63:GLN:H	1:A:63:GLN:HG3	3	0.6
(2,804)	1:A:93:ILE:HD11	1:A:105:VAL:HG21	20	0.6
(2,804)	1:A:93:ILE:HD11	1:A:105:VAL:HG22	20	0.6
(2,804)	1:A:93:ILE:HD11	1:A:105:VAL:HG23	20	0.6
(2,804)	1:A:93:ILE:HD12	1:A:105:VAL:HG21	20	0.6
(2,804)	1:A:93:ILE:HD12	1:A:105:VAL:HG22	20	0.6
(2,804)	1:A:93:ILE:HD12	1:A:105:VAL:HG23	20	0.6
(2,804)	1:A:93:ILE:HD13	1:A:105:VAL:HG21	20	0.6
(2,804)	1:A:93:ILE:HD13	1:A:105:VAL:HG22	20	0.6
(2,804)	1:A:93:ILE:HD13	1:A:105:VAL:HG23	20	0.6
(2,727)	1:A:211:VAL:HG11	1:A:226:LEU:HD21	9	0.6
(2,507)	1:A:199:SER:H	1:A:202:MET:H	3	0.6
(2,504)	1:A:198:HIS:H	1:A:202:MET:H	7	0.6
(2,473)	1:A:186:ILE:H	1:A:156:LEU:HD22	3	0.6
(2,473)	1:A:186:ILE:H	1:A:156:LEU:HD23	3	0.6
(2,471)	1:A:186:ILE:H	1:A:156:LEU:HD11	1	0.6
(2,471)	1:A:186:ILE:H	1:A:156:LEU:HD12	1	0.6
(2,471)	1:A:186:ILE:H	1:A:156:LEU:HD13	1	0.6
(2,425)	1:A:170:ALA:H	1:A:169:ASP:H	5	0.6
(2,425)	1:A:170:ALA:H	1:A:169:ASP:H	14	0.6
(2,212)	1:A:120:ILE:HD11	1:A:237:LEU:H	11	0.6
(2,212)	1:A:120:ILE:HD12	1:A:237:LEU:H	11	0.6
(2,212)	1:A:120:ILE:HD13	1:A:237:LEU:H	11	0.6
(2,985)	1:A:80:ASN:H	1:A:78:PHE:HD1	4	0.59
(2,975)	1:A:78:PHE:H	1:A:77:LEU:HD22	3	0.59
(2,975)	1:A:78:PHE:H	1:A:77:LEU:HD23	3	0.59
(2,970)	1:A:77:LEU:HG	1:A:78:PHE:H	1	0.59
(2,930)	1:A:72:VAL:HG11	1:A:75:TYR:H	1	0.59
(2,930)	1:A:72:VAL:HG12	1:A:75:TYR:H	1	0.59
(2,930)	1:A:72:VAL:HG13	1:A:75:TYR:H	1	0.59
(2,917)	1:A:71:ASP:H	1:A:72:VAL:HB	11	0.59
(2,913)	1:A:71:ASP:H	1:A:70:PRO:HB3	4	0.59
(2,913)	1:A:71:ASP:H	1:A:70:PRO:HB2	4	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,912)	1:A:70:PRO:HB3	1:A:76:SER:H	7	0.59
(2,912)	1:A:70:PRO:HB2	1:A:76:SER:H	7	0.59
(2,905)	1:A:67:CYS:HA	1:A:68:GLY:H	10	0.59
(2,896)	1:A:64:LYS:H	1:A:64:LYS:HE3	6	0.59
(2,896)	1:A:64:LYS:H	1:A:64:LYS:HE3	6	0.59
(2,879)	1:A:234:ILE:HD11	1:A:200:LEU:HB2	8	0.59
(2,879)	1:A:234:ILE:HD12	1:A:200:LEU:HB2	8	0.59
(2,879)	1:A:234:ILE:HD13	1:A:200:LEU:HB2	8	0.59
(2,786)	1:A:24:LEU:H	1:A:24:LEU:HD21	9	0.59
(2,775)	1:A:61:ILE:HD12	1:A:48:LEU:HD21	6	0.59
(2,757)	1:A:54:LEU:HD21	1:A:39:LEU:HD11	5	0.59
(2,757)	1:A:54:LEU:HD21	1:A:39:LEU:HD12	5	0.59
(2,757)	1:A:54:LEU:HD21	1:A:39:LEU:HD13	5	0.59
(2,757)	1:A:54:LEU:HD21	1:A:39:LEU:HD11	14	0.59
(2,757)	1:A:54:LEU:HD21	1:A:39:LEU:HD12	14	0.59
(2,757)	1:A:54:LEU:HD21	1:A:39:LEU:HD13	14	0.59
(2,659)	1:A:42:MET:H	1:A:19:LEU:HD11	13	0.59
(2,659)	1:A:42:MET:H	1:A:19:LEU:HD12	13	0.59
(2,659)	1:A:42:MET:H	1:A:19:LEU:HD13	13	0.59
(2,471)	1:A:186:ILE:H	1:A:156:LEU:HD11	6	0.59
(2,471)	1:A:186:ILE:H	1:A:156:LEU:HD12	6	0.59
(2,471)	1:A:186:ILE:H	1:A:156:LEU:HD13	6	0.59
(2,316)	1:A:125:ARG:H	1:A:89:VAL:H	14	0.59
(2,315)	1:A:125:ARG:H	1:A:126:LYS:H	9	0.59
(2,228)	1:A:106:ASP:H	1:A:108:LEU:H	20	0.59
(2,226)	1:A:104:THR:H	1:A:106:ASP:H	8	0.59
(2,178)	1:A:171:HIS:H	1:A:69:VAL:HG11	4	0.59
(2,178)	1:A:171:HIS:H	1:A:69:VAL:HG12	4	0.59
(2,178)	1:A:171:HIS:H	1:A:69:VAL:HG13	4	0.59
(2,162)	1:A:125:ARG:H	1:A:89:VAL:H	14	0.59
(2,976)	1:A:78:PHE:H	1:A:78:PHE:HD1	2	0.58
(2,976)	1:A:78:PHE:H	1:A:78:PHE:HD2	2	0.58
(2,975)	1:A:78:PHE:H	1:A:77:LEU:HD22	1	0.58
(2,975)	1:A:78:PHE:H	1:A:77:LEU:HD23	1	0.58
(2,947)	1:A:74:GLU:HB3	1:A:75:TYR:H	2	0.58
(2,947)	1:A:74:GLU:HB3	1:A:75:TYR:H	2	0.58
(2,75)	1:A:55:ASN:H	1:A:59:ILE:H	11	0.58
(2,748)	1:A:89:VAL:HG12	1:A:122:LEU:HD21	10	0.58
(2,626)	1:A:12:TRP:H	1:A:10:LEU:H	11	0.58
(2,425)	1:A:170:ALA:H	1:A:169:ASP:H	1	0.58
(2,425)	1:A:170:ALA:H	1:A:169:ASP:H	8	0.58
(2,392)	1:A:157:ALA:H	1:A:68:GLY:H	8	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,13)	1:A:135:MET:H	1:A:170:ALA:H	20	0.58
(3,6)	1:A:78:PHE:H	4:A:305:PX4:C27	4	0.57
(3,6)	1:A:78:PHE:H	4:A:307:PX4:C27	4	0.57
(3,6)	1:A:78:PHE:H	4:A:309:PX4:C27	4	0.57
(3,6)	1:A:78:PHE:H	4:A:311:PX4:C27	4	0.57
(3,6)	1:A:78:PHE:H	4:A:313:PX4:C27	4	0.57
(3,6)	1:A:78:PHE:H	4:A:315:PX4:C27	4	0.57
(3,6)	1:A:78:PHE:H	4:A:317:PX4:C27	4	0.57
(3,6)	1:A:78:PHE:H	4:A:319:PX4:C27	4	0.57
(3,6)	1:A:78:PHE:H	4:A:321:PX4:C27	4	0.57
(3,6)	1:A:78:PHE:H	4:A:323:PX4:C27	4	0.57
(3,6)	1:A:78:PHE:H	4:A:325:PX4:C27	4	0.57
(3,6)	1:A:78:PHE:H	4:A:327:PX4:C27	4	0.57
(3,6)	1:A:78:PHE:H	4:A:329:PX4:C27	4	0.57
(3,6)	1:A:78:PHE:H	4:A:331:PX4:C27	4	0.57
(3,6)	1:A:78:PHE:H	4:A:333:PX4:C27	4	0.57
(3,6)	1:A:78:PHE:H	4:A:335:PX4:C27	4	0.57
(3,6)	1:A:78:PHE:H	4:A:337:PX4:C27	4	0.57
(3,6)	1:A:78:PHE:H	4:A:339:PX4:C27	4	0.57
(3,6)	1:A:78:PHE:H	4:A:341:PX4:C27	4	0.57
(3,6)	1:A:78:PHE:H	4:A:343:PX4:C27	4	0.57
(3,6)	1:A:78:PHE:H	4:A:345:PX4:C27	4	0.57
(3,6)	1:A:78:PHE:H	4:A:347:PX4:C27	4	0.57
(3,6)	1:A:78:PHE:H	4:A:349:PX4:C27	4	0.57
(3,6)	1:A:78:PHE:H	4:A:351:PX4:C27	4	0.57
(3,6)	1:A:78:PHE:H	4:A:353:PX4:C27	4	0.57
(3,6)	1:A:78:PHE:H	4:A:355:PX4:C27	4	0.57
(3,6)	1:A:78:PHE:H	4:A:357:PX4:C27	4	0.57
(3,6)	1:A:78:PHE:H	4:A:359:PX4:C27	4	0.57
(3,6)	1:A:78:PHE:H	4:A:361:PX4:C27	4	0.57
(3,6)	1:A:78:PHE:H	4:A:363:PX4:C27	4	0.57
(3,6)	1:A:78:PHE:H	4:A:402:PX4:C27	4	0.57
(3,6)	1:A:78:PHE:H	4:A:404:PX4:C27	4	0.57
(3,6)	1:A:78:PHE:H	4:A:406:PX4:C27	4	0.57
(3,6)	1:A:78:PHE:H	4:A:408:PX4:C27	4	0.57
(3,6)	1:A:78:PHE:H	4:A:410:PX4:C27	4	0.57
(3,6)	1:A:78:PHE:H	4:A:412:PX4:C27	4	0.57
(3,6)	1:A:78:PHE:H	4:A:414:PX4:C27	4	0.57
(3,6)	1:A:78:PHE:H	4:A:416:PX4:C27	4	0.57
(3,6)	1:A:78:PHE:H	4:A:418:PX4:C27	4	0.57
(3,6)	1:A:78:PHE:H	4:A:420:PX4:C27	4	0.57
(3,6)	1:A:78:PHE:H	4:A:422:PX4:C27	4	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,6)	1:A:78:PHE:H	4:A:424:PX4:C27	4	0.57
(3,6)	1:A:78:PHE:H	4:A:426:PX4:C27	4	0.57
(3,6)	1:A:78:PHE:H	4:A:428:PX4:C27	4	0.57
(3,6)	1:A:78:PHE:H	4:A:430:PX4:C27	4	0.57
(2,983)	1:A:79:PRO:HD3	1:A:80:ASN:H	14	0.57
(2,983)	1:A:79:PRO:HD3	1:A:80:ASN:H	14	0.57
(2,983)	1:A:79:PRO:HD3	1:A:80:ASN:H	20	0.57
(2,983)	1:A:79:PRO:HD3	1:A:80:ASN:H	20	0.57
(2,979)	1:A:78:PHE:H	1:A:78:PHE:HD1	2	0.57
(2,964)	1:A:75:TYR:H	1:A:76:SER:H	12	0.57
(2,959)	1:A:75:TYR:H	1:A:76:SER:H	12	0.57
(2,925)	1:A:72:VAL:HG21	1:A:73:ALA:H	15	0.57
(2,925)	1:A:72:VAL:HG22	1:A:73:ALA:H	15	0.57
(2,925)	1:A:72:VAL:HG23	1:A:73:ALA:H	15	0.57
(2,925)	1:A:72:VAL:HG11	1:A:73:ALA:H	15	0.57
(2,925)	1:A:72:VAL:HG12	1:A:73:ALA:H	15	0.57
(2,925)	1:A:72:VAL:HG13	1:A:73:ALA:H	15	0.57
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG21	19	0.57
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG22	19	0.57
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG23	19	0.57
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG11	19	0.57
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG12	19	0.57
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG13	19	0.57
(2,891)	1:A:63:GLN:H	1:A:63:GLN:HB3	12	0.57
(2,891)	1:A:63:GLN:H	1:A:63:GLN:HB2	12	0.57
(2,891)	1:A:63:GLN:H	1:A:63:GLN:HB3	12	0.57
(2,891)	1:A:63:GLN:H	1:A:63:GLN:HB2	12	0.57
(2,836)	1:A:120:ILE:HD13	1:A:200:LEU:HD21	9	0.57
(2,804)	1:A:93:ILE:HD11	1:A:105:VAL:HG21	5	0.57
(2,804)	1:A:93:ILE:HD11	1:A:105:VAL:HG22	5	0.57
(2,804)	1:A:93:ILE:HD11	1:A:105:VAL:HG23	5	0.57
(2,804)	1:A:93:ILE:HD12	1:A:105:VAL:HG21	5	0.57
(2,804)	1:A:93:ILE:HD12	1:A:105:VAL:HG22	5	0.57
(2,804)	1:A:93:ILE:HD12	1:A:105:VAL:HG23	5	0.57
(2,804)	1:A:93:ILE:HD13	1:A:105:VAL:HG21	5	0.57
(2,804)	1:A:93:ILE:HD13	1:A:105:VAL:HG22	5	0.57
(2,804)	1:A:93:ILE:HD13	1:A:105:VAL:HG23	5	0.57
(2,74)	1:A:55:ASN:H	1:A:55:ASN:HD21	8	0.57
(2,74)	1:A:55:ASN:H	1:A:55:ASN:HD21	19	0.57
(2,621)	1:A:200:LEU:HD21	1:A:201:GLY:H	16	0.57
(2,425)	1:A:170:ALA:H	1:A:169:ASP:H	6	0.57
(2,392)	1:A:157:ALA:H	1:A:68:GLY:H	13	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,379)	1:A:10:LEU:H	1:A:10:LEU:HD21	11	0.57
(2,185)	1:A:94:VAL:H	1:A:92:ARG:H	10	0.57
(2,985)	1:A:80:ASN:H	1:A:78:PHE:HD1	17	0.56
(2,970)	1:A:77:LEU:HG	1:A:78:PHE:H	14	0.56
(2,930)	1:A:72:VAL:HG11	1:A:75:TYR:H	12	0.56
(2,930)	1:A:72:VAL:HG12	1:A:75:TYR:H	12	0.56
(2,930)	1:A:72:VAL:HG13	1:A:75:TYR:H	12	0.56
(2,925)	1:A:72:VAL:HG21	1:A:73:ALA:H	8	0.56
(2,925)	1:A:72:VAL:HG22	1:A:73:ALA:H	8	0.56
(2,925)	1:A:72:VAL:HG23	1:A:73:ALA:H	8	0.56
(2,925)	1:A:72:VAL:HG11	1:A:73:ALA:H	8	0.56
(2,925)	1:A:72:VAL:HG12	1:A:73:ALA:H	8	0.56
(2,925)	1:A:72:VAL:HG13	1:A:73:ALA:H	8	0.56
(2,917)	1:A:71:ASP:H	1:A:72:VAL:HB	8	0.56
(2,911)	1:A:69:VAL:HG21	1:A:69:VAL:H	5	0.56
(2,911)	1:A:69:VAL:HG22	1:A:69:VAL:H	5	0.56
(2,911)	1:A:69:VAL:HG23	1:A:69:VAL:H	5	0.56
(2,911)	1:A:69:VAL:HG11	1:A:69:VAL:H	5	0.56
(2,911)	1:A:69:VAL:HG12	1:A:69:VAL:H	5	0.56
(2,911)	1:A:69:VAL:HG13	1:A:69:VAL:H	5	0.56
(2,911)	1:A:69:VAL:HG21	1:A:69:VAL:H	15	0.56
(2,911)	1:A:69:VAL:HG22	1:A:69:VAL:H	15	0.56
(2,911)	1:A:69:VAL:HG23	1:A:69:VAL:H	15	0.56
(2,911)	1:A:69:VAL:HG11	1:A:69:VAL:H	15	0.56
(2,911)	1:A:69:VAL:HG12	1:A:69:VAL:H	15	0.56
(2,911)	1:A:69:VAL:HG13	1:A:69:VAL:H	15	0.56
(2,903)	1:A:67:CYS:H	1:A:66:ARG:HA	11	0.56
(2,871)	1:A:186:ILE:HD13	1:A:156:LEU:HD21	17	0.56
(2,71)	1:A:55:ASN:H	1:A:54:LEU:HD21	5	0.56
(2,621)	1:A:200:LEU:HD21	1:A:201:GLY:H	14	0.56
(2,557)	1:A:21:ARG:H	1:A:23:TYR:H	6	0.56
(2,471)	1:A:186:ILE:H	1:A:156:LEU:HD11	12	0.56
(2,471)	1:A:186:ILE:H	1:A:156:LEU:HD12	12	0.56
(2,471)	1:A:186:ILE:H	1:A:156:LEU:HD13	12	0.56
(2,423)	1:A:169:ASP:H	1:A:134:ILE:HD11	18	0.56
(2,423)	1:A:169:ASP:H	1:A:134:ILE:HD12	18	0.56
(2,423)	1:A:169:ASP:H	1:A:134:ILE:HD13	18	0.56
(2,392)	1:A:157:ALA:H	1:A:68:GLY:H	14	0.56
(2,212)	1:A:120:ILE:HD11	1:A:237:LEU:H	7	0.56
(2,212)	1:A:120:ILE:HD12	1:A:237:LEU:H	7	0.56
(2,212)	1:A:120:ILE:HD13	1:A:237:LEU:H	7	0.56
(2,185)	1:A:94:VAL:H	1:A:92:ARG:H	7	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,980)	1:A:78:PHE:H	1:A:79:PRO:HD3	1	0.55
(2,980)	1:A:78:PHE:H	1:A:79:PRO:HD3	1	0.55
(2,979)	1:A:78:PHE:H	1:A:78:PHE:HD1	16	0.55
(2,945)	1:A:74:GLU:H	1:A:74:GLU:HG3	7	0.55
(2,945)	1:A:74:GLU:H	1:A:74:GLU:HG3	7	0.55
(2,919)	1:A:72:VAL:H	1:A:71:ASP:HA	10	0.55
(2,919)	1:A:72:VAL:H	1:A:71:ASP:HA	14	0.55
(2,911)	1:A:69:VAL:HG21	1:A:69:VAL:H	16	0.55
(2,911)	1:A:69:VAL:HG22	1:A:69:VAL:H	16	0.55
(2,911)	1:A:69:VAL:HG23	1:A:69:VAL:H	16	0.55
(2,911)	1:A:69:VAL:HG11	1:A:69:VAL:H	16	0.55
(2,911)	1:A:69:VAL:HG12	1:A:69:VAL:H	16	0.55
(2,911)	1:A:69:VAL:HG13	1:A:69:VAL:H	16	0.55
(2,871)	1:A:186:ILE:HD13	1:A:156:LEU:HD21	4	0.55
(2,838)	1:A:120:ILE:HD11	1:A:234:ILE:HD11	16	0.55
(2,838)	1:A:120:ILE:HD11	1:A:234:ILE:HD12	16	0.55
(2,838)	1:A:120:ILE:HD11	1:A:234:ILE:HD13	16	0.55
(2,838)	1:A:120:ILE:HD12	1:A:234:ILE:HD11	16	0.55
(2,838)	1:A:120:ILE:HD12	1:A:234:ILE:HD12	16	0.55
(2,838)	1:A:120:ILE:HD12	1:A:234:ILE:HD13	16	0.55
(2,838)	1:A:120:ILE:HD13	1:A:234:ILE:HD11	16	0.55
(2,838)	1:A:120:ILE:HD13	1:A:234:ILE:HD12	16	0.55
(2,838)	1:A:120:ILE:HD13	1:A:234:ILE:HD13	16	0.55
(2,804)	1:A:93:ILE:HD11	1:A:105:VAL:HG21	6	0.55
(2,804)	1:A:93:ILE:HD11	1:A:105:VAL:HG22	6	0.55
(2,804)	1:A:93:ILE:HD11	1:A:105:VAL:HG23	6	0.55
(2,804)	1:A:93:ILE:HD12	1:A:105:VAL:HG21	6	0.55
(2,804)	1:A:93:ILE:HD12	1:A:105:VAL:HG22	6	0.55
(2,804)	1:A:93:ILE:HD12	1:A:105:VAL:HG23	6	0.55
(2,804)	1:A:93:ILE:HD13	1:A:105:VAL:HG21	6	0.55
(2,804)	1:A:93:ILE:HD13	1:A:105:VAL:HG22	6	0.55
(2,804)	1:A:93:ILE:HD13	1:A:105:VAL:HG23	6	0.55
(2,804)	1:A:93:ILE:HD11	1:A:105:VAL:HG21	15	0.55
(2,804)	1:A:93:ILE:HD11	1:A:105:VAL:HG22	15	0.55
(2,804)	1:A:93:ILE:HD11	1:A:105:VAL:HG23	15	0.55
(2,804)	1:A:93:ILE:HD12	1:A:105:VAL:HG21	15	0.55
(2,804)	1:A:93:ILE:HD12	1:A:105:VAL:HG22	15	0.55
(2,804)	1:A:93:ILE:HD12	1:A:105:VAL:HG23	15	0.55
(2,804)	1:A:93:ILE:HD13	1:A:105:VAL:HG21	15	0.55
(2,804)	1:A:93:ILE:HD13	1:A:105:VAL:HG22	15	0.55
(2,804)	1:A:93:ILE:HD13	1:A:105:VAL:HG23	15	0.55
(2,750)	1:A:89:VAL:HG13	1:A:122:LEU:HD21	9	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,693)	1:A:11:GLN:H	1:A:8:SER:H	20	0.55
(2,671)	1:A:66:ARG:H	1:A:156:LEU:HD21	20	0.55
(2,624)	1:A:11:GLN:H	1:A:8:SER:H	20	0.55
(2,543)	1:A:210:ALA:H	1:A:213:TYR:H	14	0.55
(2,517)	1:A:200:LEU:H	1:A:196:LEU:HD21	4	0.55
(2,507)	1:A:199:SER:H	1:A:202:MET:H	14	0.55
(2,426)	1:A:170:ALA:H	1:A:136:ILE:HD11	13	0.55
(2,426)	1:A:170:ALA:H	1:A:136:ILE:HD12	13	0.55
(2,426)	1:A:170:ALA:H	1:A:136:ILE:HD13	13	0.55
(2,185)	1:A:94:VAL:H	1:A:92:ARG:H	15	0.55
(2,980)	1:A:78:PHE:H	1:A:79:PRO:HD3	15	0.54
(2,980)	1:A:78:PHE:H	1:A:79:PRO:HD3	15	0.54
(2,970)	1:A:77:LEU:HG	1:A:78:PHE:H	7	0.54
(2,930)	1:A:72:VAL:HG11	1:A:75:TYR:H	4	0.54
(2,930)	1:A:72:VAL:HG12	1:A:75:TYR:H	4	0.54
(2,930)	1:A:72:VAL:HG13	1:A:75:TYR:H	4	0.54
(2,919)	1:A:72:VAL:H	1:A:71:ASP:HA	11	0.54
(2,913)	1:A:71:ASP:H	1:A:70:PRO:HB3	16	0.54
(2,913)	1:A:71:ASP:H	1:A:70:PRO:HB2	16	0.54
(2,911)	1:A:69:VAL:HG21	1:A:69:VAL:H	4	0.54
(2,911)	1:A:69:VAL:HG22	1:A:69:VAL:H	4	0.54
(2,911)	1:A:69:VAL:HG23	1:A:69:VAL:H	4	0.54
(2,911)	1:A:69:VAL:HG11	1:A:69:VAL:H	4	0.54
(2,911)	1:A:69:VAL:HG12	1:A:69:VAL:H	4	0.54
(2,911)	1:A:69:VAL:HG13	1:A:69:VAL:H	4	0.54
(2,905)	1:A:67:CYS:HA	1:A:68:GLY:H	8	0.54
(2,867)	1:A:186:ILE:HD11	1:A:156:LEU:HD21	7	0.54
(2,765)	1:A:22:PHE:H	1:A:19:LEU:HD21	1	0.54
(2,729)	1:A:211:VAL:HG12	1:A:226:LEU:HD21	13	0.54
(2,517)	1:A:200:LEU:H	1:A:196:LEU:HD21	18	0.54
(2,511)	1:A:200:LEU:HD22	1:A:199:SER:H	15	0.54
(2,511)	1:A:200:LEU:HD23	1:A:199:SER:H	15	0.54
(2,456)	1:A:178:TRP:HE1	1:A:176:GLU:H	13	0.54
(2,445)	1:A:178:TRP:HE1	1:A:176:GLU:H	13	0.54
(2,425)	1:A:170:ALA:H	1:A:169:ASP:H	18	0.54
(2,425)	1:A:170:ALA:H	1:A:169:ASP:H	20	0.54
(2,178)	1:A:171:HIS:H	1:A:69:VAL:HG11	6	0.54
(2,178)	1:A:171:HIS:H	1:A:69:VAL:HG12	6	0.54
(2,178)	1:A:171:HIS:H	1:A:69:VAL:HG13	6	0.54
(3,32)	1:A:154:ASN:ND2	4:A:305:PX4:C35	7	0.53
(3,32)	1:A:154:ASN:ND2	4:A:307:PX4:C35	7	0.53
(3,32)	1:A:154:ASN:ND2	4:A:309:PX4:C35	7	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,32)	1:A:154:ASN:ND2	4:A:311:PX4:C35	7	0.53
(3,32)	1:A:154:ASN:ND2	4:A:313:PX4:C35	7	0.53
(3,32)	1:A:154:ASN:ND2	4:A:315:PX4:C35	7	0.53
(3,32)	1:A:154:ASN:ND2	4:A:317:PX4:C35	7	0.53
(3,32)	1:A:154:ASN:ND2	4:A:319:PX4:C35	7	0.53
(3,32)	1:A:154:ASN:ND2	4:A:321:PX4:C35	7	0.53
(3,32)	1:A:154:ASN:ND2	4:A:323:PX4:C35	7	0.53
(3,32)	1:A:154:ASN:ND2	4:A:325:PX4:C35	7	0.53
(3,32)	1:A:154:ASN:ND2	4:A:327:PX4:C35	7	0.53
(3,32)	1:A:154:ASN:ND2	4:A:329:PX4:C35	7	0.53
(3,32)	1:A:154:ASN:ND2	4:A:331:PX4:C35	7	0.53
(3,32)	1:A:154:ASN:ND2	4:A:333:PX4:C35	7	0.53
(3,32)	1:A:154:ASN:ND2	4:A:335:PX4:C35	7	0.53
(3,32)	1:A:154:ASN:ND2	4:A:337:PX4:C35	7	0.53
(3,32)	1:A:154:ASN:ND2	4:A:339:PX4:C35	7	0.53
(3,32)	1:A:154:ASN:ND2	4:A:341:PX4:C35	7	0.53
(3,32)	1:A:154:ASN:ND2	4:A:343:PX4:C35	7	0.53
(3,32)	1:A:154:ASN:ND2	4:A:345:PX4:C35	7	0.53
(3,32)	1:A:154:ASN:ND2	4:A:347:PX4:C35	7	0.53
(3,32)	1:A:154:ASN:ND2	4:A:349:PX4:C35	7	0.53
(3,32)	1:A:154:ASN:ND2	4:A:351:PX4:C35	7	0.53
(3,32)	1:A:154:ASN:ND2	4:A:353:PX4:C35	7	0.53
(3,32)	1:A:154:ASN:ND2	4:A:355:PX4:C35	7	0.53
(3,32)	1:A:154:ASN:ND2	4:A:357:PX4:C35	7	0.53
(3,32)	1:A:154:ASN:ND2	4:A:359:PX4:C35	7	0.53
(3,32)	1:A:154:ASN:ND2	4:A:361:PX4:C35	7	0.53
(3,32)	1:A:154:ASN:ND2	4:A:363:PX4:C35	7	0.53
(3,32)	1:A:154:ASN:ND2	4:A:402:PX4:C35	7	0.53
(3,32)	1:A:154:ASN:ND2	4:A:404:PX4:C35	7	0.53
(3,32)	1:A:154:ASN:ND2	4:A:406:PX4:C35	7	0.53
(3,32)	1:A:154:ASN:ND2	4:A:408:PX4:C35	7	0.53
(3,32)	1:A:154:ASN:ND2	4:A:410:PX4:C35	7	0.53
(3,32)	1:A:154:ASN:ND2	4:A:412:PX4:C35	7	0.53
(3,32)	1:A:154:ASN:ND2	4:A:414:PX4:C35	7	0.53
(3,32)	1:A:154:ASN:ND2	4:A:416:PX4:C35	7	0.53
(3,32)	1:A:154:ASN:ND2	4:A:418:PX4:C35	7	0.53
(3,32)	1:A:154:ASN:ND2	4:A:420:PX4:C35	7	0.53
(3,32)	1:A:154:ASN:ND2	4:A:422:PX4:C35	7	0.53
(3,32)	1:A:154:ASN:ND2	4:A:424:PX4:C35	7	0.53
(3,32)	1:A:154:ASN:ND2	4:A:426:PX4:C35	7	0.53
(3,32)	1:A:154:ASN:ND2	4:A:428:PX4:C35	7	0.53
(3,32)	1:A:154:ASN:ND2	4:A:430:PX4:C35	7	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,988)	1:A:129:TRP:HE1	4:A:305:PX4:C2	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:307:PX4:C2	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:309:PX4:C2	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:311:PX4:C2	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:313:PX4:C2	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:315:PX4:C2	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:317:PX4:C2	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:319:PX4:C2	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:321:PX4:C2	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:323:PX4:C2	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:325:PX4:C2	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:327:PX4:C2	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:329:PX4:C2	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:331:PX4:C2	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:333:PX4:C2	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:335:PX4:C2	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:337:PX4:C2	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:339:PX4:C2	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:341:PX4:C2	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:343:PX4:C2	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:345:PX4:C2	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:347:PX4:C2	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:349:PX4:C2	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:351:PX4:C2	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:353:PX4:C2	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:355:PX4:C2	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:357:PX4:C2	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:359:PX4:C2	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:361:PX4:C2	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:363:PX4:C2	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:402:PX4:C2	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:404:PX4:C2	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:406:PX4:C2	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:408:PX4:C2	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:410:PX4:C2	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:412:PX4:C2	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:414:PX4:C2	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:416:PX4:C2	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:418:PX4:C2	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:420:PX4:C2	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:422:PX4:C2	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:424:PX4:C2	9	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,988)	1:A:129:TRP:HE1	4:A:426:PX4:C2	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:428:PX4:C2	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:430:PX4:C2	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:305:PX4:C1	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:307:PX4:C1	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:309:PX4:C1	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:311:PX4:C1	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:313:PX4:C1	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:315:PX4:C1	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:317:PX4:C1	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:319:PX4:C1	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:321:PX4:C1	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:323:PX4:C1	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:325:PX4:C1	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:327:PX4:C1	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:329:PX4:C1	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:331:PX4:C1	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:333:PX4:C1	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:335:PX4:C1	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:337:PX4:C1	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:339:PX4:C1	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:341:PX4:C1	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:343:PX4:C1	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:345:PX4:C1	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:347:PX4:C1	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:349:PX4:C1	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:351:PX4:C1	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:353:PX4:C1	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:355:PX4:C1	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:357:PX4:C1	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:359:PX4:C1	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:361:PX4:C1	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:363:PX4:C1	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:402:PX4:C1	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:404:PX4:C1	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:406:PX4:C1	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:408:PX4:C1	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:410:PX4:C1	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:412:PX4:C1	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:414:PX4:C1	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:416:PX4:C1	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:418:PX4:C1	9	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,988)	1:A:129:TRP:HE1	4:A:420:PX4:C1	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:422:PX4:C1	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:424:PX4:C1	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:426:PX4:C1	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:428:PX4:C1	9	0.53
(2,988)	1:A:129:TRP:HE1	4:A:430:PX4:C1	9	0.53
(2,980)	1:A:78:PHE:H	1:A:79:PRO:HD3	20	0.53
(2,980)	1:A:78:PHE:H	1:A:79:PRO:HD3	20	0.53
(2,970)	1:A:77:LEU:HG	1:A:78:PHE:H	11	0.53
(2,951)	1:A:74:GLU:H	1:A:76:SER:H	16	0.53
(2,951)	1:A:74:GLU:H	1:A:76:SER:H	17	0.53
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG21	7	0.53
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG22	7	0.53
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG23	7	0.53
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG11	7	0.53
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG12	7	0.53
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG13	7	0.53
(2,913)	1:A:71:ASP:H	1:A:70:PRO:HB3	19	0.53
(2,913)	1:A:71:ASP:H	1:A:70:PRO:HB2	19	0.53
(2,903)	1:A:67:CYS:H	1:A:66:ARG:HA	6	0.53
(2,898)	1:A:66:ARG:H	1:A:63:GLN:HB3	11	0.53
(2,898)	1:A:66:ARG:H	1:A:63:GLN:HB2	11	0.53
(2,898)	1:A:66:ARG:H	1:A:63:GLN:HB3	17	0.53
(2,898)	1:A:66:ARG:H	1:A:63:GLN:HB2	17	0.53
(2,896)	1:A:64:LYS:H	1:A:64:LYS:HE3	4	0.53
(2,896)	1:A:64:LYS:H	1:A:64:LYS:HE3	4	0.53
(2,859)	1:A:186:ILE:HD12	1:A:156:LEU:HD21	12	0.53
(2,75)	1:A:55:ASN:H	1:A:59:ILE:H	8	0.53
(2,75)	1:A:55:ASN:H	1:A:59:ILE:H	20	0.53
(2,63)	1:A:52:GLY:H	1:A:51:THR:H	20	0.53
(2,557)	1:A:21:ARG:H	1:A:23:TYR:H	12	0.53
(2,557)	1:A:21:ARG:H	1:A:23:TYR:H	18	0.53
(2,540)	1:A:209:ASN:HD21	1:A:209:ASN:HD22	16	0.53
(2,540)	1:A:209:ASN:HD21	1:A:209:ASN:HD22	16	0.53
(2,538)	1:A:205:SER:H	1:A:213:TYR:H	18	0.53
(2,425)	1:A:170:ALA:H	1:A:169:ASP:H	19	0.53
(2,424)	1:A:169:ASP:H	1:A:166:LEU:HB3	7	0.53
(2,414)	1:A:167:GLY:H	1:A:166:LEU:HD21	11	0.53
(2,212)	1:A:120:ILE:HD11	1:A:237:LEU:H	6	0.53
(2,212)	1:A:120:ILE:HD12	1:A:237:LEU:H	6	0.53
(2,212)	1:A:120:ILE:HD13	1:A:237:LEU:H	6	0.53
(2,10)	1:A:92:ARG:H	1:A:93:ILE:HG13	5	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,10)	1:A:92:ARG:H	1:A:93:ILE:HG12	5	0.53
(2,983)	1:A:79:PRO:HD3	1:A:80:ASN:H	1	0.52
(2,983)	1:A:79:PRO:HD3	1:A:80:ASN:H	1	0.52
(2,970)	1:A:77:LEU:HG	1:A:78:PHE:H	6	0.52
(2,964)	1:A:75:TYR:H	1:A:76:SER:H	11	0.52
(2,961)	1:A:75:TYR:HD1	1:A:76:SER:H	13	0.52
(2,961)	1:A:75:TYR:HD2	1:A:76:SER:H	13	0.52
(2,959)	1:A:75:TYR:H	1:A:76:SER:H	11	0.52
(2,919)	1:A:72:VAL:H	1:A:71:ASP:HA	13	0.52
(2,911)	1:A:69:VAL:HG21	1:A:69:VAL:H	8	0.52
(2,911)	1:A:69:VAL:HG22	1:A:69:VAL:H	8	0.52
(2,911)	1:A:69:VAL:HG23	1:A:69:VAL:H	8	0.52
(2,911)	1:A:69:VAL:HG11	1:A:69:VAL:H	8	0.52
(2,911)	1:A:69:VAL:HG12	1:A:69:VAL:H	8	0.52
(2,911)	1:A:69:VAL:HG13	1:A:69:VAL:H	8	0.52
(2,861)	1:A:186:ILE:HD13	1:A:156:LEU:HD21	16	0.52
(2,860)	1:A:186:ILE:HD12	1:A:156:LEU:HD22	1	0.52
(2,860)	1:A:186:ILE:HD12	1:A:156:LEU:HD23	1	0.52
(2,777)	1:A:61:ILE:HD13	1:A:48:LEU:HD21	11	0.52
(2,728)	1:A:211:VAL:HG11	1:A:226:LEU:HD22	5	0.52
(2,728)	1:A:211:VAL:HG11	1:A:226:LEU:HD23	5	0.52
(2,718)	1:A:54:LEU:HD11	1:A:59:ILE:HD11	18	0.52
(2,718)	1:A:54:LEU:HD11	1:A:59:ILE:HD12	18	0.52
(2,718)	1:A:54:LEU:HD11	1:A:59:ILE:HD13	18	0.52
(2,718)	1:A:54:LEU:HD12	1:A:59:ILE:HD11	18	0.52
(2,718)	1:A:54:LEU:HD12	1:A:59:ILE:HD12	18	0.52
(2,718)	1:A:54:LEU:HD12	1:A:59:ILE:HD13	18	0.52
(2,718)	1:A:54:LEU:HD13	1:A:59:ILE:HD11	18	0.52
(2,718)	1:A:54:LEU:HD13	1:A:59:ILE:HD12	18	0.52
(2,718)	1:A:54:LEU:HD13	1:A:59:ILE:HD13	18	0.52
(2,626)	1:A:12:TRP:H	1:A:10:LEU:H	6	0.52
(2,540)	1:A:209:ASN:HD21	1:A:209:ASN:HD22	2	0.52
(2,540)	1:A:209:ASN:HD21	1:A:209:ASN:HD22	2	0.52
(2,540)	1:A:209:ASN:HD21	1:A:209:ASN:HD22	8	0.52
(2,540)	1:A:209:ASN:HD21	1:A:209:ASN:HD22	8	0.52
(2,511)	1:A:200:LEU:HD22	1:A:199:SER:H	2	0.52
(2,511)	1:A:200:LEU:HD23	1:A:199:SER:H	2	0.52
(2,384)	1:A:154:ASN:HD22	1:A:154:ASN:HD21	11	0.52
(2,384)	1:A:154:ASN:HD22	1:A:154:ASN:HD21	11	0.52
(2,357)	1:A:136:ILE:HD11	1:A:137:GLY:H	8	0.52
(2,357)	1:A:136:ILE:HD12	1:A:137:GLY:H	8	0.52
(2,357)	1:A:136:ILE:HD13	1:A:137:GLY:H	8	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,265)	1:A:113:LEU:H	1:A:196:LEU:HD22	5	0.52
(2,265)	1:A:113:LEU:H	1:A:196:LEU:HD23	5	0.52
(2,212)	1:A:120:ILE:HD11	1:A:237:LEU:H	2	0.52
(2,212)	1:A:120:ILE:HD12	1:A:237:LEU:H	2	0.52
(2,212)	1:A:120:ILE:HD13	1:A:237:LEU:H	2	0.52
(2,10)	1:A:92:ARG:H	1:A:93:ILE:HG13	18	0.52
(2,10)	1:A:92:ARG:H	1:A:93:ILE:HG12	18	0.52
(2,961)	1:A:75:TYR:HD1	1:A:76:SER:H	19	0.51
(2,961)	1:A:75:TYR:HD2	1:A:76:SER:H	19	0.51
(2,947)	1:A:74:GLU:HB3	1:A:75:TYR:H	14	0.51
(2,947)	1:A:74:GLU:HB3	1:A:75:TYR:H	14	0.51
(2,913)	1:A:71:ASP:H	1:A:70:PRO:HB3	18	0.51
(2,913)	1:A:71:ASP:H	1:A:70:PRO:HB2	18	0.51
(2,905)	1:A:67:CYS:HA	1:A:68:GLY:H	4	0.51
(2,890)	1:A:63:GLN:H	1:A:63:GLN:HG3	11	0.51
(2,890)	1:A:63:GLN:H	1:A:63:GLN:HG3	11	0.51
(2,871)	1:A:186:ILE:HD13	1:A:156:LEU:HD21	2	0.51
(2,741)	1:A:114:ASN:H	1:A:113:LEU:HD21	2	0.51
(2,661)	1:A:4:ALA:H	1:A:59:ILE:HG21	4	0.51
(2,661)	1:A:4:ALA:H	1:A:59:ILE:HG22	4	0.51
(2,661)	1:A:4:ALA:H	1:A:59:ILE:HG23	4	0.51
(2,626)	1:A:12:TRP:H	1:A:10:LEU:H	1	0.51
(2,543)	1:A:210:ALA:H	1:A:213:TYR:H	1	0.51
(2,426)	1:A:170:ALA:H	1:A:136:ILE:HD11	10	0.51
(2,426)	1:A:170:ALA:H	1:A:136:ILE:HD12	10	0.51
(2,426)	1:A:170:ALA:H	1:A:136:ILE:HD13	10	0.51
(2,425)	1:A:170:ALA:H	1:A:169:ASP:H	11	0.51
(2,414)	1:A:167:GLY:H	1:A:166:LEU:HD21	20	0.51
(2,369)	1:A:143:HIS:H	1:A:145:ASP:H	19	0.51
(2,10)	1:A:92:ARG:H	1:A:93:ILE:HG13	14	0.51
(2,10)	1:A:92:ARG:H	1:A:93:ILE:HG12	14	0.51
(3,6)	1:A:78:PHE:H	4:A:305:PX4:C27	18	0.5
(3,6)	1:A:78:PHE:H	4:A:307:PX4:C27	18	0.5
(3,6)	1:A:78:PHE:H	4:A:309:PX4:C27	18	0.5
(3,6)	1:A:78:PHE:H	4:A:311:PX4:C27	18	0.5
(3,6)	1:A:78:PHE:H	4:A:313:PX4:C27	18	0.5
(3,6)	1:A:78:PHE:H	4:A:315:PX4:C27	18	0.5
(3,6)	1:A:78:PHE:H	4:A:317:PX4:C27	18	0.5
(3,6)	1:A:78:PHE:H	4:A:319:PX4:C27	18	0.5
(3,6)	1:A:78:PHE:H	4:A:321:PX4:C27	18	0.5
(3,6)	1:A:78:PHE:H	4:A:323:PX4:C27	18	0.5
(3,6)	1:A:78:PHE:H	4:A:325:PX4:C27	18	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,6)	1:A:78:PHE:H	4:A:327:PX4:C27	18	0.5
(3,6)	1:A:78:PHE:H	4:A:329:PX4:C27	18	0.5
(3,6)	1:A:78:PHE:H	4:A:331:PX4:C27	18	0.5
(3,6)	1:A:78:PHE:H	4:A:333:PX4:C27	18	0.5
(3,6)	1:A:78:PHE:H	4:A:335:PX4:C27	18	0.5
(3,6)	1:A:78:PHE:H	4:A:337:PX4:C27	18	0.5
(3,6)	1:A:78:PHE:H	4:A:339:PX4:C27	18	0.5
(3,6)	1:A:78:PHE:H	4:A:341:PX4:C27	18	0.5
(3,6)	1:A:78:PHE:H	4:A:343:PX4:C27	18	0.5
(3,6)	1:A:78:PHE:H	4:A:345:PX4:C27	18	0.5
(3,6)	1:A:78:PHE:H	4:A:347:PX4:C27	18	0.5
(3,6)	1:A:78:PHE:H	4:A:349:PX4:C27	18	0.5
(3,6)	1:A:78:PHE:H	4:A:351:PX4:C27	18	0.5
(3,6)	1:A:78:PHE:H	4:A:353:PX4:C27	18	0.5
(3,6)	1:A:78:PHE:H	4:A:355:PX4:C27	18	0.5
(3,6)	1:A:78:PHE:H	4:A:357:PX4:C27	18	0.5
(3,6)	1:A:78:PHE:H	4:A:359:PX4:C27	18	0.5
(3,6)	1:A:78:PHE:H	4:A:361:PX4:C27	18	0.5
(3,6)	1:A:78:PHE:H	4:A:363:PX4:C27	18	0.5
(3,6)	1:A:78:PHE:H	4:A:402:PX4:C27	18	0.5
(3,6)	1:A:78:PHE:H	4:A:404:PX4:C27	18	0.5
(3,6)	1:A:78:PHE:H	4:A:406:PX4:C27	18	0.5
(3,6)	1:A:78:PHE:H	4:A:408:PX4:C27	18	0.5
(3,6)	1:A:78:PHE:H	4:A:410:PX4:C27	18	0.5
(3,6)	1:A:78:PHE:H	4:A:412:PX4:C27	18	0.5
(3,6)	1:A:78:PHE:H	4:A:414:PX4:C27	18	0.5
(3,6)	1:A:78:PHE:H	4:A:416:PX4:C27	18	0.5
(3,6)	1:A:78:PHE:H	4:A:418:PX4:C27	18	0.5
(3,6)	1:A:78:PHE:H	4:A:420:PX4:C27	18	0.5
(3,6)	1:A:78:PHE:H	4:A:422:PX4:C27	18	0.5
(3,6)	1:A:78:PHE:H	4:A:424:PX4:C27	18	0.5
(3,6)	1:A:78:PHE:H	4:A:426:PX4:C27	18	0.5
(3,6)	1:A:78:PHE:H	4:A:428:PX4:C27	18	0.5
(3,6)	1:A:78:PHE:H	4:A:430:PX4:C27	18	0.5
(2,964)	1:A:75:TYR:H	1:A:76:SER:H	20	0.5
(2,961)	1:A:75:TYR:HD1	1:A:76:SER:H	5	0.5
(2,961)	1:A:75:TYR:HD2	1:A:76:SER:H	5	0.5
(2,959)	1:A:75:TYR:H	1:A:76:SER:H	20	0.5
(2,915)	1:A:71:ASP:H	1:A:72:VAL:HG21	13	0.5
(2,915)	1:A:71:ASP:H	1:A:72:VAL:HG22	13	0.5
(2,915)	1:A:71:ASP:H	1:A:72:VAL:HG23	13	0.5
(2,912)	1:A:70:PRO:HB3	1:A:76:SER:H	6	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,912)	1:A:70:PRO:HB2	1:A:76:SER:H	6	0.5
(2,912)	1:A:70:PRO:HB3	1:A:76:SER:H	11	0.5
(2,912)	1:A:70:PRO:HB2	1:A:76:SER:H	11	0.5
(2,890)	1:A:63:GLN:H	1:A:63:GLN:HG3	18	0.5
(2,890)	1:A:63:GLN:H	1:A:63:GLN:HG3	18	0.5
(2,804)	1:A:93:ILE:HD11	1:A:105:VAL:HG21	1	0.5
(2,804)	1:A:93:ILE:HD11	1:A:105:VAL:HG22	1	0.5
(2,804)	1:A:93:ILE:HD11	1:A:105:VAL:HG23	1	0.5
(2,804)	1:A:93:ILE:HD12	1:A:105:VAL:HG21	1	0.5
(2,804)	1:A:93:ILE:HD12	1:A:105:VAL:HG22	1	0.5
(2,804)	1:A:93:ILE:HD12	1:A:105:VAL:HG23	1	0.5
(2,804)	1:A:93:ILE:HD13	1:A:105:VAL:HG21	1	0.5
(2,804)	1:A:93:ILE:HD13	1:A:105:VAL:HG22	1	0.5
(2,804)	1:A:93:ILE:HD13	1:A:105:VAL:HG23	1	0.5
(2,627)	1:A:13:GLU:H	1:A:10:LEU:H	11	0.5
(2,627)	1:A:13:GLU:H	1:A:10:LEU:H	13	0.5
(2,621)	1:A:200:LEU:HD21	1:A:201:GLY:H	17	0.5
(2,542)	1:A:210:ALA:H	1:A:209:ASN:HD22	20	0.5
(2,518)	1:A:200:LEU:H	1:A:196:LEU:HD22	14	0.5
(2,518)	1:A:200:LEU:H	1:A:196:LEU:HD23	14	0.5
(2,511)	1:A:200:LEU:HD22	1:A:199:SER:H	10	0.5
(2,511)	1:A:200:LEU:HD23	1:A:199:SER:H	10	0.5
(2,507)	1:A:199:SER:H	1:A:202:MET:H	8	0.5
(2,392)	1:A:157:ALA:H	1:A:68:GLY:H	17	0.5
(2,264)	1:A:113:LEU:H	1:A:196:LEU:HD21	3	0.5
(2,239)	1:A:108:LEU:H	1:A:108:LEU:HD21	17	0.5
(3,33)	1:A:155:THR:H	4:A:305:PX4:C35	9	0.49
(3,33)	1:A:155:THR:H	4:A:307:PX4:C35	9	0.49
(3,33)	1:A:155:THR:H	4:A:309:PX4:C35	9	0.49
(3,33)	1:A:155:THR:H	4:A:311:PX4:C35	9	0.49
(3,33)	1:A:155:THR:H	4:A:313:PX4:C35	9	0.49
(3,33)	1:A:155:THR:H	4:A:315:PX4:C35	9	0.49
(3,33)	1:A:155:THR:H	4:A:317:PX4:C35	9	0.49
(3,33)	1:A:155:THR:H	4:A:319:PX4:C35	9	0.49
(3,33)	1:A:155:THR:H	4:A:321:PX4:C35	9	0.49
(3,33)	1:A:155:THR:H	4:A:323:PX4:C35	9	0.49
(3,33)	1:A:155:THR:H	4:A:325:PX4:C35	9	0.49
(3,33)	1:A:155:THR:H	4:A:327:PX4:C35	9	0.49
(3,33)	1:A:155:THR:H	4:A:329:PX4:C35	9	0.49
(3,33)	1:A:155:THR:H	4:A:331:PX4:C35	9	0.49
(3,33)	1:A:155:THR:H	4:A:333:PX4:C35	9	0.49
(3,33)	1:A:155:THR:H	4:A:335:PX4:C35	9	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,33)	1:A:155:THR:H	4:A:337:PX4:C35	9	0.49
(3,33)	1:A:155:THR:H	4:A:339:PX4:C35	9	0.49
(3,33)	1:A:155:THR:H	4:A:341:PX4:C35	9	0.49
(3,33)	1:A:155:THR:H	4:A:343:PX4:C35	9	0.49
(3,33)	1:A:155:THR:H	4:A:345:PX4:C35	9	0.49
(3,33)	1:A:155:THR:H	4:A:347:PX4:C35	9	0.49
(3,33)	1:A:155:THR:H	4:A:349:PX4:C35	9	0.49
(3,33)	1:A:155:THR:H	4:A:351:PX4:C35	9	0.49
(3,33)	1:A:155:THR:H	4:A:353:PX4:C35	9	0.49
(3,33)	1:A:155:THR:H	4:A:355:PX4:C35	9	0.49
(3,33)	1:A:155:THR:H	4:A:357:PX4:C35	9	0.49
(3,33)	1:A:155:THR:H	4:A:359:PX4:C35	9	0.49
(3,33)	1:A:155:THR:H	4:A:361:PX4:C35	9	0.49
(3,33)	1:A:155:THR:H	4:A:363:PX4:C35	9	0.49
(3,33)	1:A:155:THR:H	4:A:402:PX4:C35	9	0.49
(3,33)	1:A:155:THR:H	4:A:404:PX4:C35	9	0.49
(3,33)	1:A:155:THR:H	4:A:406:PX4:C35	9	0.49
(3,33)	1:A:155:THR:H	4:A:408:PX4:C35	9	0.49
(3,33)	1:A:155:THR:H	4:A:410:PX4:C35	9	0.49
(3,33)	1:A:155:THR:H	4:A:412:PX4:C35	9	0.49
(3,33)	1:A:155:THR:H	4:A:414:PX4:C35	9	0.49
(3,33)	1:A:155:THR:H	4:A:416:PX4:C35	9	0.49
(3,33)	1:A:155:THR:H	4:A:418:PX4:C35	9	0.49
(3,33)	1:A:155:THR:H	4:A:420:PX4:C35	9	0.49
(3,33)	1:A:155:THR:H	4:A:422:PX4:C35	9	0.49
(3,33)	1:A:155:THR:H	4:A:424:PX4:C35	9	0.49
(3,33)	1:A:155:THR:H	4:A:426:PX4:C35	9	0.49
(3,33)	1:A:155:THR:H	4:A:428:PX4:C35	9	0.49
(3,33)	1:A:155:THR:H	4:A:430:PX4:C35	9	0.49
(2,980)	1:A:78:PHE:H	1:A:79:PRO:HD3	8	0.49
(2,980)	1:A:78:PHE:H	1:A:79:PRO:HD3	8	0.49
(2,976)	1:A:78:PHE:H	1:A:78:PHE:HD1	14	0.49
(2,976)	1:A:78:PHE:H	1:A:78:PHE:HD2	14	0.49
(2,951)	1:A:74:GLU:H	1:A:76:SER:H	19	0.49
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG21	18	0.49
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG22	18	0.49
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG23	18	0.49
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG11	18	0.49
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG12	18	0.49
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG13	18	0.49
(2,907)	1:A:68:GLY:H	1:A:69:VAL:H	12	0.49
(2,890)	1:A:63:GLN:H	1:A:63:GLN:HG3	6	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,890)	1:A:63:GLN:H	1:A:63:GLN:HG3	6	0.49
(2,868)	1:A:186:ILE:HD11	1:A:156:LEU:HD22	12	0.49
(2,868)	1:A:186:ILE:HD11	1:A:156:LEU:HD23	12	0.49
(2,835)	1:A:120:ILE:HD12	1:A:200:LEU:HD22	20	0.49
(2,835)	1:A:120:ILE:HD12	1:A:200:LEU:HD23	20	0.49
(2,809)	1:A:136:ILE:H	1:A:94:VAL:HG11	4	0.49
(2,809)	1:A:136:ILE:H	1:A:94:VAL:HG12	4	0.49
(2,809)	1:A:136:ILE:H	1:A:94:VAL:HG13	4	0.49
(2,735)	1:A:196:LEU:HD22	1:A:113:LEU:HD21	14	0.49
(2,656)	1:A:39:LEU:H	1:A:19:LEU:HD21	14	0.49
(2,608)	1:A:238:TYR:H	1:A:120:ILE:HD11	11	0.49
(2,608)	1:A:238:TYR:H	1:A:120:ILE:HD12	11	0.49
(2,608)	1:A:238:TYR:H	1:A:120:ILE:HD13	11	0.49
(2,570)	1:A:226:LEU:H	1:A:226:LEU:HD21	17	0.49
(2,471)	1:A:186:ILE:H	1:A:156:LEU:HD11	19	0.49
(2,471)	1:A:186:ILE:H	1:A:156:LEU:HD12	19	0.49
(2,471)	1:A:186:ILE:H	1:A:156:LEU:HD13	19	0.49
(2,424)	1:A:169:ASP:H	1:A:166:LEU:HB3	6	0.49
(2,392)	1:A:157:ALA:H	1:A:68:GLY:H	19	0.49
(2,212)	1:A:120:ILE:HD11	1:A:237:LEU:H	18	0.49
(2,212)	1:A:120:ILE:HD12	1:A:237:LEU:H	18	0.49
(2,212)	1:A:120:ILE:HD13	1:A:237:LEU:H	18	0.49
(2,185)	1:A:94:VAL:H	1:A:92:ARG:H	5	0.49
(2,961)	1:A:75:TYR:HD1	1:A:76:SER:H	9	0.48
(2,961)	1:A:75:TYR:HD2	1:A:76:SER:H	9	0.48
(2,951)	1:A:74:GLU:H	1:A:76:SER:H	6	0.48
(2,951)	1:A:74:GLU:H	1:A:76:SER:H	15	0.48
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG21	2	0.48
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG22	2	0.48
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG23	2	0.48
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG11	2	0.48
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG12	2	0.48
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG13	2	0.48
(2,911)	1:A:69:VAL:HG21	1:A:69:VAL:H	6	0.48
(2,911)	1:A:69:VAL:HG22	1:A:69:VAL:H	6	0.48
(2,911)	1:A:69:VAL:HG23	1:A:69:VAL:H	6	0.48
(2,911)	1:A:69:VAL:HG11	1:A:69:VAL:H	6	0.48
(2,911)	1:A:69:VAL:HG12	1:A:69:VAL:H	6	0.48
(2,911)	1:A:69:VAL:HG13	1:A:69:VAL:H	6	0.48
(2,899)	1:A:66:ARG:H	1:A:64:LYS:H	14	0.48
(2,895)	1:A:64:LYS:H	1:A:64:LYS:HA	19	0.48
(2,834)	1:A:120:ILE:HD12	1:A:200:LEU:HD21	7	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,748)	1:A:89:VAL:HG12	1:A:122:LEU:HD21	17	0.48
(2,557)	1:A:21:ARG:H	1:A:23:TYR:H	3	0.48
(2,543)	1:A:210:ALA:H	1:A:213:TYR:H	19	0.48
(2,540)	1:A:209:ASN:HD21	1:A:209:ASN:HD22	11	0.48
(2,540)	1:A:209:ASN:HD21	1:A:209:ASN:HD22	11	0.48
(2,425)	1:A:170:ALA:H	1:A:169:ASP:H	13	0.48
(2,424)	1:A:169:ASP:H	1:A:166:LEU:HB3	10	0.48
(2,392)	1:A:157:ALA:H	1:A:68:GLY:H	3	0.48
(2,384)	1:A:154:ASN:HD22	1:A:154:ASN:HD21	10	0.48
(2,384)	1:A:154:ASN:HD22	1:A:154:ASN:HD21	10	0.48
(2,315)	1:A:125:ARG:H	1:A:126:LYS:H	8	0.48
(2,207)	1:A:98:ARG:H	1:A:100:LEU:H	11	0.48
(2,207)	1:A:98:ARG:H	1:A:100:LEU:H	13	0.48
(2,984)	1:A:78:PHE:HD1	1:A:80:ASN:HD21	20	0.47
(2,984)	1:A:78:PHE:HD1	1:A:80:ASN:HD22	20	0.47
(2,984)	1:A:78:PHE:HD1	1:A:80:ASN:HD21	20	0.47
(2,984)	1:A:78:PHE:HD1	1:A:80:ASN:HD22	20	0.47
(2,980)	1:A:78:PHE:H	1:A:79:PRO:HD3	11	0.47
(2,980)	1:A:78:PHE:H	1:A:79:PRO:HD3	11	0.47
(2,975)	1:A:78:PHE:H	1:A:77:LEU:HD22	7	0.47
(2,975)	1:A:78:PHE:H	1:A:77:LEU:HD23	7	0.47
(2,974)	1:A:78:PHE:H	1:A:77:LEU:HD21	5	0.47
(2,945)	1:A:74:GLU:H	1:A:74:GLU:HG3	17	0.47
(2,945)	1:A:74:GLU:H	1:A:74:GLU:HG3	17	0.47
(2,930)	1:A:72:VAL:HG11	1:A:75:TYR:H	2	0.47
(2,930)	1:A:72:VAL:HG12	1:A:75:TYR:H	2	0.47
(2,930)	1:A:72:VAL:HG13	1:A:75:TYR:H	2	0.47
(2,930)	1:A:72:VAL:HG11	1:A:75:TYR:H	17	0.47
(2,930)	1:A:72:VAL:HG12	1:A:75:TYR:H	17	0.47
(2,930)	1:A:72:VAL:HG13	1:A:75:TYR:H	17	0.47
(2,903)	1:A:67:CYS:H	1:A:66:ARG:HA	13	0.47
(2,903)	1:A:67:CYS:H	1:A:66:ARG:HA	16	0.47
(2,661)	1:A:4:ALA:H	1:A:59:ILE:HG21	5	0.47
(2,661)	1:A:4:ALA:H	1:A:59:ILE:HG22	5	0.47
(2,661)	1:A:4:ALA:H	1:A:59:ILE:HG23	5	0.47
(2,659)	1:A:42:MET:H	1:A:19:LEU:HD11	5	0.47
(2,659)	1:A:42:MET:H	1:A:19:LEU:HD12	5	0.47
(2,659)	1:A:42:MET:H	1:A:19:LEU:HD13	5	0.47
(2,659)	1:A:42:MET:H	1:A:19:LEU:HD11	19	0.47
(2,659)	1:A:42:MET:H	1:A:19:LEU:HD12	19	0.47
(2,659)	1:A:42:MET:H	1:A:19:LEU:HD13	19	0.47
(2,557)	1:A:21:ARG:H	1:A:23:TYR:H	7	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,540)	1:A:209:ASN:HD21	1:A:209:ASN:HD22	5	0.47
(2,540)	1:A:209:ASN:HD21	1:A:209:ASN:HD22	5	0.47
(2,540)	1:A:209:ASN:HD21	1:A:209:ASN:HD22	15	0.47
(2,540)	1:A:209:ASN:HD21	1:A:209:ASN:HD22	15	0.47
(2,540)	1:A:209:ASN:HD21	1:A:209:ASN:HD22	20	0.47
(2,540)	1:A:209:ASN:HD21	1:A:209:ASN:HD22	20	0.47
(2,507)	1:A:199:SER:H	1:A:202:MET:H	18	0.47
(2,453)	1:A:178:TRP:HE1	1:A:175:ASP:H	15	0.47
(2,442)	1:A:175:ASP:H	1:A:178:TRP:HE1	15	0.47
(2,424)	1:A:169:ASP:H	1:A:166:LEU:HB3	12	0.47
(2,384)	1:A:154:ASN:HD22	1:A:154:ASN:HD21	5	0.47
(2,384)	1:A:154:ASN:HD22	1:A:154:ASN:HD21	5	0.47
(2,384)	1:A:154:ASN:HD22	1:A:154:ASN:HD21	6	0.47
(2,384)	1:A:154:ASN:HD22	1:A:154:ASN:HD21	6	0.47
(2,384)	1:A:154:ASN:HD22	1:A:154:ASN:HD21	12	0.47
(2,384)	1:A:154:ASN:HD22	1:A:154:ASN:HD21	12	0.47
(2,384)	1:A:154:ASN:HD22	1:A:154:ASN:HD21	18	0.47
(2,384)	1:A:154:ASN:HD22	1:A:154:ASN:HD21	18	0.47
(2,384)	1:A:154:ASN:HD22	1:A:154:ASN:HD21	20	0.47
(2,384)	1:A:154:ASN:HD22	1:A:154:ASN:HD21	20	0.47
(2,315)	1:A:125:ARG:H	1:A:126:LYS:H	1	0.47
(2,228)	1:A:106:ASP:H	1:A:108:LEU:H	8	0.47
(2,228)	1:A:106:ASP:H	1:A:108:LEU:H	19	0.47
(2,207)	1:A:98:ARG:H	1:A:100:LEU:H	6	0.47
(2,207)	1:A:98:ARG:H	1:A:100:LEU:H	10	0.47
(2,207)	1:A:98:ARG:H	1:A:100:LEU:H	12	0.47
(2,980)	1:A:78:PHE:H	1:A:79:PRO:HD3	13	0.46
(2,980)	1:A:78:PHE:H	1:A:79:PRO:HD3	13	0.46
(2,980)	1:A:78:PHE:H	1:A:79:PRO:HD3	19	0.46
(2,980)	1:A:78:PHE:H	1:A:79:PRO:HD3	19	0.46
(2,973)	1:A:78:PHE:H	1:A:77:LEU:HD11	1	0.46
(2,973)	1:A:78:PHE:H	1:A:77:LEU:HD12	1	0.46
(2,973)	1:A:78:PHE:H	1:A:77:LEU:HD13	1	0.46
(2,969)	1:A:77:LEU:H	1:A:78:PHE:H	4	0.46
(2,964)	1:A:75:TYR:H	1:A:76:SER:H	13	0.46
(2,959)	1:A:75:TYR:H	1:A:76:SER:H	13	0.46
(2,947)	1:A:74:GLU:HB3	1:A:75:TYR:H	4	0.46
(2,947)	1:A:74:GLU:HB3	1:A:75:TYR:H	4	0.46
(2,945)	1:A:74:GLU:H	1:A:74:GLU:HG3	4	0.46
(2,945)	1:A:74:GLU:H	1:A:74:GLU:HG3	4	0.46
(2,917)	1:A:71:ASP:H	1:A:72:VAL:HB	17	0.46
(2,908)	1:A:68:GLY:HA3	1:A:69:VAL:H	3	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,908)	1:A:68:GLY:HA3	1:A:69:VAL:H	3	0.46
(2,903)	1:A:67:CYS:H	1:A:66:ARG:HA	2	0.46
(2,693)	1:A:11:GLN:H	1:A:8:SER:H	9	0.46
(2,673)	1:A:77:LEU:H	1:A:78:PHE:H	4	0.46
(2,627)	1:A:13:GLU:H	1:A:10:LEU:H	8	0.46
(2,624)	1:A:11:GLN:H	1:A:8:SER:H	9	0.46
(2,557)	1:A:21:ARG:H	1:A:23:TYR:H	14	0.46
(2,540)	1:A:209:ASN:HD21	1:A:209:ASN:HD22	7	0.46
(2,540)	1:A:209:ASN:HD21	1:A:209:ASN:HD22	7	0.46
(2,517)	1:A:200:LEU:H	1:A:196:LEU:HD21	2	0.46
(2,471)	1:A:186:ILE:H	1:A:156:LEU:HD11	8	0.46
(2,471)	1:A:186:ILE:H	1:A:156:LEU:HD12	8	0.46
(2,471)	1:A:186:ILE:H	1:A:156:LEU:HD13	8	0.46
(2,466)	1:A:84:TRP:H	1:A:200:LEU:HD21	1	0.46
(2,426)	1:A:170:ALA:H	1:A:136:ILE:HD11	2	0.46
(2,426)	1:A:170:ALA:H	1:A:136:ILE:HD12	2	0.46
(2,426)	1:A:170:ALA:H	1:A:136:ILE:HD13	2	0.46
(2,425)	1:A:170:ALA:H	1:A:169:ASP:H	2	0.46
(2,384)	1:A:154:ASN:HD22	1:A:154:ASN:HD21	4	0.46
(2,384)	1:A:154:ASN:HD22	1:A:154:ASN:HD21	4	0.46
(2,384)	1:A:154:ASN:HD22	1:A:154:ASN:HD21	16	0.46
(2,384)	1:A:154:ASN:HD22	1:A:154:ASN:HD21	16	0.46
(2,315)	1:A:125:ARG:H	1:A:126:LYS:H	10	0.46
(2,303)	1:A:122:LEU:H	1:A:120:ILE:HG13	13	0.46
(2,303)	1:A:122:LEU:H	1:A:120:ILE:HG12	13	0.46
(2,185)	1:A:94:VAL:H	1:A:92:ARG:H	2	0.46
(3,21)	1:A:77:LEU:H	4:A:305:PX4:C35	15	0.45
(3,21)	1:A:77:LEU:H	4:A:307:PX4:C35	15	0.45
(3,21)	1:A:77:LEU:H	4:A:309:PX4:C35	15	0.45
(3,21)	1:A:77:LEU:H	4:A:311:PX4:C35	15	0.45
(3,21)	1:A:77:LEU:H	4:A:313:PX4:C35	15	0.45
(3,21)	1:A:77:LEU:H	4:A:315:PX4:C35	15	0.45
(3,21)	1:A:77:LEU:H	4:A:317:PX4:C35	15	0.45
(3,21)	1:A:77:LEU:H	4:A:319:PX4:C35	15	0.45
(3,21)	1:A:77:LEU:H	4:A:321:PX4:C35	15	0.45
(3,21)	1:A:77:LEU:H	4:A:323:PX4:C35	15	0.45
(3,21)	1:A:77:LEU:H	4:A:325:PX4:C35	15	0.45
(3,21)	1:A:77:LEU:H	4:A:327:PX4:C35	15	0.45
(3,21)	1:A:77:LEU:H	4:A:329:PX4:C35	15	0.45
(3,21)	1:A:77:LEU:H	4:A:331:PX4:C35	15	0.45
(3,21)	1:A:77:LEU:H	4:A:333:PX4:C35	15	0.45
(3,21)	1:A:77:LEU:H	4:A:335:PX4:C35	15	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,21)	1:A:77:LEU:H	4:A:337:PX4:C35	15	0.45
(3,21)	1:A:77:LEU:H	4:A:339:PX4:C35	15	0.45
(3,21)	1:A:77:LEU:H	4:A:341:PX4:C35	15	0.45
(3,21)	1:A:77:LEU:H	4:A:343:PX4:C35	15	0.45
(3,21)	1:A:77:LEU:H	4:A:345:PX4:C35	15	0.45
(3,21)	1:A:77:LEU:H	4:A:347:PX4:C35	15	0.45
(3,21)	1:A:77:LEU:H	4:A:349:PX4:C35	15	0.45
(3,21)	1:A:77:LEU:H	4:A:351:PX4:C35	15	0.45
(3,21)	1:A:77:LEU:H	4:A:353:PX4:C35	15	0.45
(3,21)	1:A:77:LEU:H	4:A:355:PX4:C35	15	0.45
(3,21)	1:A:77:LEU:H	4:A:357:PX4:C35	15	0.45
(3,21)	1:A:77:LEU:H	4:A:359:PX4:C35	15	0.45
(3,21)	1:A:77:LEU:H	4:A:361:PX4:C35	15	0.45
(3,21)	1:A:77:LEU:H	4:A:363:PX4:C35	15	0.45
(3,21)	1:A:77:LEU:H	4:A:402:PX4:C35	15	0.45
(3,21)	1:A:77:LEU:H	4:A:404:PX4:C35	15	0.45
(3,21)	1:A:77:LEU:H	4:A:406:PX4:C35	15	0.45
(3,21)	1:A:77:LEU:H	4:A:408:PX4:C35	15	0.45
(3,21)	1:A:77:LEU:H	4:A:410:PX4:C35	15	0.45
(3,21)	1:A:77:LEU:H	4:A:412:PX4:C35	15	0.45
(3,21)	1:A:77:LEU:H	4:A:414:PX4:C35	15	0.45
(3,21)	1:A:77:LEU:H	4:A:416:PX4:C35	15	0.45
(3,21)	1:A:77:LEU:H	4:A:418:PX4:C35	15	0.45
(3,21)	1:A:77:LEU:H	4:A:420:PX4:C35	15	0.45
(3,21)	1:A:77:LEU:H	4:A:422:PX4:C35	15	0.45
(3,21)	1:A:77:LEU:H	4:A:424:PX4:C35	15	0.45
(3,21)	1:A:77:LEU:H	4:A:426:PX4:C35	15	0.45
(3,21)	1:A:77:LEU:H	4:A:428:PX4:C35	15	0.45
(3,21)	1:A:77:LEU:H	4:A:430:PX4:C35	15	0.45
(2,980)	1:A:78:PHE:H	1:A:79:PRO:HD3	5	0.45
(2,980)	1:A:78:PHE:H	1:A:79:PRO:HD3	5	0.45
(2,954)	1:A:74:GLU:HB3	1:A:77:LEU:H	4	0.45
(2,954)	1:A:74:GLU:HB3	1:A:77:LEU:H	4	0.45
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG21	10	0.45
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG22	10	0.45
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG23	10	0.45
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG11	10	0.45
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG12	10	0.45
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG13	10	0.45
(2,912)	1:A:70:PRO:HB3	1:A:76:SER:H	20	0.45
(2,912)	1:A:70:PRO:HB2	1:A:76:SER:H	20	0.45
(2,899)	1:A:66:ARG:H	1:A:64:LYS:H	10	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,896)	1:A:64:LYS:H	1:A:64:LYS:HE3	3	0.45
(2,896)	1:A:64:LYS:H	1:A:64:LYS:HE3	3	0.45
(2,895)	1:A:64:LYS:H	1:A:64:LYS:HA	4	0.45
(2,843)	1:A:200:LEU:HD21	1:A:122:LEU:HD22	9	0.45
(2,843)	1:A:200:LEU:HD21	1:A:122:LEU:HD23	9	0.45
(2,758)	1:A:54:LEU:HD22	1:A:39:LEU:HD11	10	0.45
(2,758)	1:A:54:LEU:HD22	1:A:39:LEU:HD12	10	0.45
(2,758)	1:A:54:LEU:HD22	1:A:39:LEU:HD13	10	0.45
(2,758)	1:A:54:LEU:HD23	1:A:39:LEU:HD11	10	0.45
(2,758)	1:A:54:LEU:HD23	1:A:39:LEU:HD12	10	0.45
(2,758)	1:A:54:LEU:HD23	1:A:39:LEU:HD13	10	0.45
(2,741)	1:A:114:ASN:H	1:A:113:LEU:HD21	4	0.45
(2,717)	1:A:54:LEU:HD11	1:A:39:LEU:HD11	10	0.45
(2,717)	1:A:54:LEU:HD11	1:A:39:LEU:HD12	10	0.45
(2,717)	1:A:54:LEU:HD11	1:A:39:LEU:HD13	10	0.45
(2,717)	1:A:54:LEU:HD12	1:A:39:LEU:HD11	10	0.45
(2,717)	1:A:54:LEU:HD12	1:A:39:LEU:HD12	10	0.45
(2,717)	1:A:54:LEU:HD12	1:A:39:LEU:HD13	10	0.45
(2,717)	1:A:54:LEU:HD13	1:A:39:LEU:HD11	10	0.45
(2,717)	1:A:54:LEU:HD13	1:A:39:LEU:HD12	10	0.45
(2,717)	1:A:54:LEU:HD13	1:A:39:LEU:HD13	10	0.45
(2,659)	1:A:42:MET:H	1:A:19:LEU:HD11	8	0.45
(2,659)	1:A:42:MET:H	1:A:19:LEU:HD12	8	0.45
(2,659)	1:A:42:MET:H	1:A:19:LEU:HD13	8	0.45
(2,634)	1:A:54:LEU:HD11	1:A:12:TRP:HE1	6	0.45
(2,634)	1:A:54:LEU:HD12	1:A:12:TRP:HE1	6	0.45
(2,634)	1:A:54:LEU:HD13	1:A:12:TRP:HE1	6	0.45
(2,634)	1:A:54:LEU:HD11	1:A:12:TRP:HE1	15	0.45
(2,634)	1:A:54:LEU:HD12	1:A:12:TRP:HE1	15	0.45
(2,634)	1:A:54:LEU:HD13	1:A:12:TRP:HE1	15	0.45
(2,63)	1:A:52:GLY:H	1:A:51:THR:H	5	0.45
(2,608)	1:A:238:TYR:H	1:A:120:ILE:HD11	8	0.45
(2,608)	1:A:238:TYR:H	1:A:120:ILE:HD12	8	0.45
(2,608)	1:A:238:TYR:H	1:A:120:ILE:HD13	8	0.45
(2,60)	1:A:50:ILE:H	1:A:50:ILE:HD11	12	0.45
(2,60)	1:A:50:ILE:H	1:A:50:ILE:HD12	12	0.45
(2,60)	1:A:50:ILE:H	1:A:50:ILE:HD13	12	0.45
(2,540)	1:A:209:ASN:HD21	1:A:209:ASN:HD22	13	0.45
(2,540)	1:A:209:ASN:HD21	1:A:209:ASN:HD22	13	0.45
(2,518)	1:A:200:LEU:H	1:A:196:LEU:HD22	10	0.45
(2,518)	1:A:200:LEU:H	1:A:196:LEU:HD23	10	0.45
(2,388)	1:A:66:ARG:H	1:A:156:LEU:H	10	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,388)	1:A:66:ARG:H	1:A:156:LEU:H	16	0.45
(2,384)	1:A:154:ASN:HD22	1:A:154:ASN:HD21	2	0.45
(2,384)	1:A:154:ASN:HD22	1:A:154:ASN:HD21	2	0.45
(2,384)	1:A:154:ASN:HD22	1:A:154:ASN:HD21	7	0.45
(2,384)	1:A:154:ASN:HD22	1:A:154:ASN:HD21	7	0.45
(2,384)	1:A:154:ASN:HD22	1:A:154:ASN:HD21	8	0.45
(2,384)	1:A:154:ASN:HD22	1:A:154:ASN:HD21	8	0.45
(2,316)	1:A:125:ARG:H	1:A:89:VAL:H	5	0.45
(2,316)	1:A:125:ARG:H	1:A:89:VAL:H	12	0.45
(2,315)	1:A:125:ARG:H	1:A:126:LYS:H	18	0.45
(2,265)	1:A:113:LEU:H	1:A:196:LEU:HD22	6	0.45
(2,265)	1:A:113:LEU:H	1:A:196:LEU:HD23	6	0.45
(2,226)	1:A:104:THR:H	1:A:106:ASP:H	1	0.45
(2,162)	1:A:125:ARG:H	1:A:89:VAL:H	5	0.45
(2,162)	1:A:125:ARG:H	1:A:89:VAL:H	12	0.45
(2,120)	1:A:66:ARG:H	1:A:156:LEU:H	10	0.45
(2,120)	1:A:66:ARG:H	1:A:156:LEU:H	16	0.45
(3,6)	1:A:78:PHE:H	4:A:305:PX4:C27	17	0.44
(3,6)	1:A:78:PHE:H	4:A:307:PX4:C27	17	0.44
(3,6)	1:A:78:PHE:H	4:A:309:PX4:C27	17	0.44
(3,6)	1:A:78:PHE:H	4:A:311:PX4:C27	17	0.44
(3,6)	1:A:78:PHE:H	4:A:313:PX4:C27	17	0.44
(3,6)	1:A:78:PHE:H	4:A:315:PX4:C27	17	0.44
(3,6)	1:A:78:PHE:H	4:A:317:PX4:C27	17	0.44
(3,6)	1:A:78:PHE:H	4:A:319:PX4:C27	17	0.44
(3,6)	1:A:78:PHE:H	4:A:321:PX4:C27	17	0.44
(3,6)	1:A:78:PHE:H	4:A:323:PX4:C27	17	0.44
(3,6)	1:A:78:PHE:H	4:A:325:PX4:C27	17	0.44
(3,6)	1:A:78:PHE:H	4:A:327:PX4:C27	17	0.44
(3,6)	1:A:78:PHE:H	4:A:329:PX4:C27	17	0.44
(3,6)	1:A:78:PHE:H	4:A:331:PX4:C27	17	0.44
(3,6)	1:A:78:PHE:H	4:A:333:PX4:C27	17	0.44
(3,6)	1:A:78:PHE:H	4:A:335:PX4:C27	17	0.44
(3,6)	1:A:78:PHE:H	4:A:337:PX4:C27	17	0.44
(3,6)	1:A:78:PHE:H	4:A:339:PX4:C27	17	0.44
(3,6)	1:A:78:PHE:H	4:A:341:PX4:C27	17	0.44
(3,6)	1:A:78:PHE:H	4:A:343:PX4:C27	17	0.44
(3,6)	1:A:78:PHE:H	4:A:345:PX4:C27	17	0.44
(3,6)	1:A:78:PHE:H	4:A:347:PX4:C27	17	0.44
(3,6)	1:A:78:PHE:H	4:A:349:PX4:C27	17	0.44
(3,6)	1:A:78:PHE:H	4:A:351:PX4:C27	17	0.44
(3,6)	1:A:78:PHE:H	4:A:353:PX4:C27	17	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,6)	1:A:78:PHE:H	4:A:355:PX4:C27	17	0.44
(3,6)	1:A:78:PHE:H	4:A:357:PX4:C27	17	0.44
(3,6)	1:A:78:PHE:H	4:A:359:PX4:C27	17	0.44
(3,6)	1:A:78:PHE:H	4:A:361:PX4:C27	17	0.44
(3,6)	1:A:78:PHE:H	4:A:363:PX4:C27	17	0.44
(3,6)	1:A:78:PHE:H	4:A:402:PX4:C27	17	0.44
(3,6)	1:A:78:PHE:H	4:A:404:PX4:C27	17	0.44
(3,6)	1:A:78:PHE:H	4:A:406:PX4:C27	17	0.44
(3,6)	1:A:78:PHE:H	4:A:408:PX4:C27	17	0.44
(3,6)	1:A:78:PHE:H	4:A:410:PX4:C27	17	0.44
(3,6)	1:A:78:PHE:H	4:A:412:PX4:C27	17	0.44
(3,6)	1:A:78:PHE:H	4:A:414:PX4:C27	17	0.44
(3,6)	1:A:78:PHE:H	4:A:416:PX4:C27	17	0.44
(3,6)	1:A:78:PHE:H	4:A:418:PX4:C27	17	0.44
(3,6)	1:A:78:PHE:H	4:A:420:PX4:C27	17	0.44
(3,6)	1:A:78:PHE:H	4:A:422:PX4:C27	17	0.44
(3,6)	1:A:78:PHE:H	4:A:424:PX4:C27	17	0.44
(3,6)	1:A:78:PHE:H	4:A:426:PX4:C27	17	0.44
(3,6)	1:A:78:PHE:H	4:A:428:PX4:C27	17	0.44
(3,6)	1:A:78:PHE:H	4:A:430:PX4:C27	17	0.44
(2,980)	1:A:78:PHE:H	1:A:79:PRO:HD3	10	0.44
(2,980)	1:A:78:PHE:H	1:A:79:PRO:HD3	10	0.44
(2,945)	1:A:74:GLU:H	1:A:74:GLU:HG3	1	0.44
(2,945)	1:A:74:GLU:H	1:A:74:GLU:HG3	1	0.44
(2,927)	1:A:72:VAL:H	1:A:73:ALA:H	3	0.44
(2,927)	1:A:72:VAL:H	1:A:73:ALA:H	3	0.44
(2,925)	1:A:72:VAL:HG21	1:A:73:ALA:H	6	0.44
(2,925)	1:A:72:VAL:HG22	1:A:73:ALA:H	6	0.44
(2,925)	1:A:72:VAL:HG23	1:A:73:ALA:H	6	0.44
(2,925)	1:A:72:VAL:HG11	1:A:73:ALA:H	6	0.44
(2,925)	1:A:72:VAL:HG12	1:A:73:ALA:H	6	0.44
(2,925)	1:A:72:VAL:HG13	1:A:73:ALA:H	6	0.44
(2,919)	1:A:72:VAL:H	1:A:71:ASP:HA	2	0.44
(2,917)	1:A:71:ASP:H	1:A:72:VAL:HB	14	0.44
(2,896)	1:A:64:LYS:H	1:A:64:LYS:HE3	14	0.44
(2,896)	1:A:64:LYS:H	1:A:64:LYS:HE3	14	0.44
(2,890)	1:A:63:GLN:H	1:A:63:GLN:HG3	15	0.44
(2,890)	1:A:63:GLN:H	1:A:63:GLN:HG3	15	0.44
(2,766)	1:A:22:PHE:H	1:A:19:LEU:HD22	15	0.44
(2,766)	1:A:22:PHE:H	1:A:19:LEU:HD23	15	0.44
(2,765)	1:A:22:PHE:H	1:A:19:LEU:HD21	20	0.44
(2,75)	1:A:55:ASN:H	1:A:59:ILE:H	9	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,746)	1:A:89:VAL:HG11	1:A:122:LEU:HD21	9	0.44
(2,659)	1:A:42:MET:H	1:A:19:LEU:HD11	16	0.44
(2,659)	1:A:42:MET:H	1:A:19:LEU:HD12	16	0.44
(2,659)	1:A:42:MET:H	1:A:19:LEU:HD13	16	0.44
(2,627)	1:A:13:GLU:H	1:A:10:LEU:H	15	0.44
(2,626)	1:A:12:TRP:H	1:A:10:LEU:H	19	0.44
(2,608)	1:A:238:TYR:H	1:A:120:ILE:HD11	1	0.44
(2,608)	1:A:238:TYR:H	1:A:120:ILE:HD12	1	0.44
(2,608)	1:A:238:TYR:H	1:A:120:ILE:HD13	1	0.44
(2,540)	1:A:209:ASN:HD21	1:A:209:ASN:HD22	14	0.44
(2,540)	1:A:209:ASN:HD21	1:A:209:ASN:HD22	14	0.44
(2,540)	1:A:209:ASN:HD21	1:A:209:ASN:HD22	18	0.44
(2,540)	1:A:209:ASN:HD21	1:A:209:ASN:HD22	18	0.44
(2,538)	1:A:205:SER:H	1:A:213:TYR:H	9	0.44
(2,511)	1:A:200:LEU:HD22	1:A:199:SER:H	1	0.44
(2,511)	1:A:200:LEU:HD23	1:A:199:SER:H	1	0.44
(2,466)	1:A:84:TRP:H	1:A:200:LEU:HD21	5	0.44
(2,425)	1:A:170:ALA:H	1:A:169:ASP:H	9	0.44
(2,414)	1:A:167:GLY:H	1:A:166:LEU:HD21	18	0.44
(2,384)	1:A:154:ASN:HD22	1:A:154:ASN:HD21	1	0.44
(2,384)	1:A:154:ASN:HD22	1:A:154:ASN:HD21	1	0.44
(2,384)	1:A:154:ASN:HD22	1:A:154:ASN:HD21	9	0.44
(2,384)	1:A:154:ASN:HD22	1:A:154:ASN:HD21	9	0.44
(2,384)	1:A:154:ASN:HD22	1:A:154:ASN:HD21	14	0.44
(2,384)	1:A:154:ASN:HD22	1:A:154:ASN:HD21	14	0.44
(2,384)	1:A:154:ASN:HD22	1:A:154:ASN:HD21	15	0.44
(2,384)	1:A:154:ASN:HD22	1:A:154:ASN:HD21	15	0.44
(2,384)	1:A:154:ASN:HD22	1:A:154:ASN:HD21	19	0.44
(2,384)	1:A:154:ASN:HD22	1:A:154:ASN:HD21	19	0.44
(2,258)	1:A:112:ALA:H	1:A:189:LEU:HD22	15	0.44
(2,258)	1:A:112:ALA:H	1:A:189:LEU:HD23	15	0.44
(2,228)	1:A:106:ASP:H	1:A:108:LEU:H	6	0.44
(2,986)	1:A:80:ASN:H	1:A:79:PRO:HB3	15	0.43
(2,986)	1:A:80:ASN:H	1:A:79:PRO:HB2	15	0.43
(2,986)	1:A:80:ASN:H	1:A:79:PRO:HB3	15	0.43
(2,986)	1:A:80:ASN:H	1:A:79:PRO:HB2	15	0.43
(2,980)	1:A:78:PHE:H	1:A:79:PRO:HD3	4	0.43
(2,980)	1:A:78:PHE:H	1:A:79:PRO:HD3	4	0.43
(2,961)	1:A:75:TYR:HD1	1:A:76:SER:H	10	0.43
(2,961)	1:A:75:TYR:HD2	1:A:76:SER:H	10	0.43
(2,947)	1:A:74:GLU:HB3	1:A:75:TYR:H	8	0.43
(2,947)	1:A:74:GLU:HB3	1:A:75:TYR:H	8	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,927)	1:A:72:VAL:H	1:A:73:ALA:H	15	0.43
(2,927)	1:A:72:VAL:H	1:A:73:ALA:H	15	0.43
(2,925)	1:A:72:VAL:HG21	1:A:73:ALA:H	5	0.43
(2,925)	1:A:72:VAL:HG22	1:A:73:ALA:H	5	0.43
(2,925)	1:A:72:VAL:HG23	1:A:73:ALA:H	5	0.43
(2,925)	1:A:72:VAL:HG11	1:A:73:ALA:H	5	0.43
(2,925)	1:A:72:VAL:HG12	1:A:73:ALA:H	5	0.43
(2,925)	1:A:72:VAL:HG13	1:A:73:ALA:H	5	0.43
(2,920)	1:A:72:VAL:H	1:A:71:ASP:H	18	0.43
(2,920)	1:A:72:VAL:H	1:A:71:ASP:H	18	0.43
(2,911)	1:A:69:VAL:HG21	1:A:69:VAL:H	7	0.43
(2,911)	1:A:69:VAL:HG22	1:A:69:VAL:H	7	0.43
(2,911)	1:A:69:VAL:HG23	1:A:69:VAL:H	7	0.43
(2,911)	1:A:69:VAL:HG11	1:A:69:VAL:H	7	0.43
(2,911)	1:A:69:VAL:HG12	1:A:69:VAL:H	7	0.43
(2,911)	1:A:69:VAL:HG13	1:A:69:VAL:H	7	0.43
(2,896)	1:A:64:LYS:H	1:A:64:LYS:HE3	7	0.43
(2,896)	1:A:64:LYS:H	1:A:64:LYS:HE3	7	0.43
(2,895)	1:A:64:LYS:H	1:A:64:LYS:HA	6	0.43
(2,871)	1:A:186:ILE:HD13	1:A:156:LEU:HD21	18	0.43
(2,776)	1:A:61:ILE:HD12	1:A:48:LEU:HD22	1	0.43
(2,776)	1:A:61:ILE:HD12	1:A:48:LEU:HD23	1	0.43
(2,773)	1:A:61:ILE:HD11	1:A:48:LEU:HD21	15	0.43
(2,75)	1:A:55:ASN:H	1:A:59:ILE:H	12	0.43
(2,748)	1:A:89:VAL:HG12	1:A:122:LEU:HD21	20	0.43
(2,731)	1:A:211:VAL:HG13	1:A:226:LEU:HD21	18	0.43
(2,627)	1:A:13:GLU:H	1:A:10:LEU:H	14	0.43
(2,540)	1:A:209:ASN:HD21	1:A:209:ASN:HD22	17	0.43
(2,540)	1:A:209:ASN:HD21	1:A:209:ASN:HD22	17	0.43
(2,511)	1:A:200:LEU:HD22	1:A:199:SER:H	13	0.43
(2,511)	1:A:200:LEU:HD23	1:A:199:SER:H	13	0.43
(2,510)	1:A:200:LEU:HD21	1:A:199:SER:H	5	0.43
(2,503)	1:A:198:HIS:H	1:A:201:GLY:H	8	0.43
(2,426)	1:A:170:ALA:H	1:A:136:ILE:HD11	20	0.43
(2,426)	1:A:170:ALA:H	1:A:136:ILE:HD12	20	0.43
(2,426)	1:A:170:ALA:H	1:A:136:ILE:HD13	20	0.43
(2,410)	1:A:167:GLY:H	1:A:165:GLY:H	2	0.43
(2,384)	1:A:154:ASN:HD22	1:A:154:ASN:HD21	3	0.43
(2,384)	1:A:154:ASN:HD22	1:A:154:ASN:HD21	3	0.43
(2,384)	1:A:154:ASN:HD22	1:A:154:ASN:HD21	17	0.43
(2,384)	1:A:154:ASN:HD22	1:A:154:ASN:HD21	17	0.43
(2,357)	1:A:136:ILE:HD11	1:A:137:GLY:H	17	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,357)	1:A:136:ILE:HD12	1:A:137:GLY:H	17	0.43
(2,357)	1:A:136:ILE:HD13	1:A:137:GLY:H	17	0.43
(2,315)	1:A:125:ARG:H	1:A:126:LYS:H	4	0.43
(2,228)	1:A:106:ASP:H	1:A:108:LEU:H	2	0.43
(2,212)	1:A:120:ILE:HD11	1:A:237:LEU:H	3	0.43
(2,212)	1:A:120:ILE:HD12	1:A:237:LEU:H	3	0.43
(2,212)	1:A:120:ILE:HD13	1:A:237:LEU:H	3	0.43
(2,207)	1:A:98:ARG:H	1:A:100:LEU:H	4	0.43
(2,974)	1:A:78:PHE:H	1:A:77:LEU:HD21	16	0.42
(2,974)	1:A:78:PHE:H	1:A:77:LEU:HD21	19	0.42
(2,966)	1:A:77:LEU:H	1:A:77:LEU:HB3	9	0.42
(2,966)	1:A:77:LEU:H	1:A:77:LEU:HB3	9	0.42
(2,920)	1:A:72:VAL:H	1:A:71:ASP:H	13	0.42
(2,920)	1:A:72:VAL:H	1:A:71:ASP:H	13	0.42
(2,912)	1:A:70:PRO:HB3	1:A:76:SER:H	9	0.42
(2,912)	1:A:70:PRO:HB2	1:A:76:SER:H	9	0.42
(2,907)	1:A:68:GLY:H	1:A:69:VAL:H	1	0.42
(2,810)	1:A:93:ILE:H	1:A:94:VAL:HG11	6	0.42
(2,810)	1:A:93:ILE:H	1:A:94:VAL:HG12	6	0.42
(2,810)	1:A:93:ILE:H	1:A:94:VAL:HG13	6	0.42
(2,810)	1:A:93:ILE:H	1:A:94:VAL:HG11	7	0.42
(2,810)	1:A:93:ILE:H	1:A:94:VAL:HG12	7	0.42
(2,810)	1:A:93:ILE:H	1:A:94:VAL:HG13	7	0.42
(2,773)	1:A:61:ILE:HD11	1:A:48:LEU:HD21	12	0.42
(2,758)	1:A:54:LEU:HD22	1:A:39:LEU:HD11	6	0.42
(2,758)	1:A:54:LEU:HD22	1:A:39:LEU:HD12	6	0.42
(2,758)	1:A:54:LEU:HD22	1:A:39:LEU:HD13	6	0.42
(2,758)	1:A:54:LEU:HD23	1:A:39:LEU:HD11	6	0.42
(2,758)	1:A:54:LEU:HD23	1:A:39:LEU:HD12	6	0.42
(2,758)	1:A:54:LEU:HD23	1:A:39:LEU:HD13	6	0.42
(2,725)	1:A:113:LEU:HD13	1:A:196:LEU:HD21	10	0.42
(2,716)	1:A:54:LEU:HD11	1:A:58:VAL:HG11	4	0.42
(2,716)	1:A:54:LEU:HD11	1:A:58:VAL:HG12	4	0.42
(2,716)	1:A:54:LEU:HD11	1:A:58:VAL:HG13	4	0.42
(2,716)	1:A:54:LEU:HD12	1:A:58:VAL:HG11	4	0.42
(2,716)	1:A:54:LEU:HD12	1:A:58:VAL:HG12	4	0.42
(2,716)	1:A:54:LEU:HD12	1:A:58:VAL:HG13	4	0.42
(2,716)	1:A:54:LEU:HD13	1:A:58:VAL:HG11	4	0.42
(2,716)	1:A:54:LEU:HD13	1:A:58:VAL:HG12	4	0.42
(2,716)	1:A:54:LEU:HD13	1:A:58:VAL:HG13	4	0.42
(2,661)	1:A:4:ALA:H	1:A:59:ILE:HG21	13	0.42
(2,661)	1:A:4:ALA:H	1:A:59:ILE:HG22	13	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,661)	1:A:4:ALA:H	1:A:59:ILE:HG23	13	0.42
(2,659)	1:A:42:MET:H	1:A:19:LEU:HD11	20	0.42
(2,659)	1:A:42:MET:H	1:A:19:LEU:HD12	20	0.42
(2,659)	1:A:42:MET:H	1:A:19:LEU:HD13	20	0.42
(2,626)	1:A:12:TRP:H	1:A:10:LEU:H	7	0.42
(2,608)	1:A:238:TYR:H	1:A:120:ILE:HD11	17	0.42
(2,608)	1:A:238:TYR:H	1:A:120:ILE:HD12	17	0.42
(2,608)	1:A:238:TYR:H	1:A:120:ILE:HD13	17	0.42
(2,570)	1:A:226:LEU:H	1:A:226:LEU:HD21	7	0.42
(2,540)	1:A:209:ASN:HD21	1:A:209:ASN:HD22	19	0.42
(2,540)	1:A:209:ASN:HD21	1:A:209:ASN:HD22	19	0.42
(2,538)	1:A:205:SER:H	1:A:213:TYR:H	6	0.42
(2,507)	1:A:199:SER:H	1:A:202:MET:H	4	0.42
(2,507)	1:A:199:SER:H	1:A:202:MET:H	5	0.42
(2,504)	1:A:198:HIS:H	1:A:202:MET:H	1	0.42
(2,501)	1:A:198:HIS:H	1:A:195:ALA:H	7	0.42
(2,466)	1:A:84:TRP:H	1:A:200:LEU:HD21	9	0.42
(2,357)	1:A:136:ILE:HD11	1:A:137:GLY:H	2	0.42
(2,357)	1:A:136:ILE:HD12	1:A:137:GLY:H	2	0.42
(2,357)	1:A:136:ILE:HD13	1:A:137:GLY:H	2	0.42
(2,228)	1:A:106:ASP:H	1:A:108:LEU:H	18	0.42
(2,113)	1:A:25:TYR:H	1:A:26:ASP:H	17	0.42
(3,33)	1:A:155:THR:H	4:A:305:PX4:C35	11	0.41
(3,33)	1:A:155:THR:H	4:A:307:PX4:C35	11	0.41
(3,33)	1:A:155:THR:H	4:A:309:PX4:C35	11	0.41
(3,33)	1:A:155:THR:H	4:A:311:PX4:C35	11	0.41
(3,33)	1:A:155:THR:H	4:A:313:PX4:C35	11	0.41
(3,33)	1:A:155:THR:H	4:A:315:PX4:C35	11	0.41
(3,33)	1:A:155:THR:H	4:A:317:PX4:C35	11	0.41
(3,33)	1:A:155:THR:H	4:A:319:PX4:C35	11	0.41
(3,33)	1:A:155:THR:H	4:A:321:PX4:C35	11	0.41
(3,33)	1:A:155:THR:H	4:A:323:PX4:C35	11	0.41
(3,33)	1:A:155:THR:H	4:A:325:PX4:C35	11	0.41
(3,33)	1:A:155:THR:H	4:A:327:PX4:C35	11	0.41
(3,33)	1:A:155:THR:H	4:A:329:PX4:C35	11	0.41
(3,33)	1:A:155:THR:H	4:A:331:PX4:C35	11	0.41
(3,33)	1:A:155:THR:H	4:A:333:PX4:C35	11	0.41
(3,33)	1:A:155:THR:H	4:A:335:PX4:C35	11	0.41
(3,33)	1:A:155:THR:H	4:A:337:PX4:C35	11	0.41
(3,33)	1:A:155:THR:H	4:A:339:PX4:C35	11	0.41
(3,33)	1:A:155:THR:H	4:A:341:PX4:C35	11	0.41
(3,33)	1:A:155:THR:H	4:A:343:PX4:C35	11	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,33)	1:A:155:THR:H	4:A:345:PX4:C35	11	0.41
(3,33)	1:A:155:THR:H	4:A:347:PX4:C35	11	0.41
(3,33)	1:A:155:THR:H	4:A:349:PX4:C35	11	0.41
(3,33)	1:A:155:THR:H	4:A:351:PX4:C35	11	0.41
(3,33)	1:A:155:THR:H	4:A:353:PX4:C35	11	0.41
(3,33)	1:A:155:THR:H	4:A:355:PX4:C35	11	0.41
(3,33)	1:A:155:THR:H	4:A:357:PX4:C35	11	0.41
(3,33)	1:A:155:THR:H	4:A:359:PX4:C35	11	0.41
(3,33)	1:A:155:THR:H	4:A:361:PX4:C35	11	0.41
(3,33)	1:A:155:THR:H	4:A:363:PX4:C35	11	0.41
(3,33)	1:A:155:THR:H	4:A:402:PX4:C35	11	0.41
(3,33)	1:A:155:THR:H	4:A:404:PX4:C35	11	0.41
(3,33)	1:A:155:THR:H	4:A:406:PX4:C35	11	0.41
(3,33)	1:A:155:THR:H	4:A:408:PX4:C35	11	0.41
(3,33)	1:A:155:THR:H	4:A:410:PX4:C35	11	0.41
(3,33)	1:A:155:THR:H	4:A:412:PX4:C35	11	0.41
(3,33)	1:A:155:THR:H	4:A:414:PX4:C35	11	0.41
(3,33)	1:A:155:THR:H	4:A:416:PX4:C35	11	0.41
(3,33)	1:A:155:THR:H	4:A:418:PX4:C35	11	0.41
(3,33)	1:A:155:THR:H	4:A:420:PX4:C35	11	0.41
(3,33)	1:A:155:THR:H	4:A:422:PX4:C35	11	0.41
(3,33)	1:A:155:THR:H	4:A:424:PX4:C35	11	0.41
(3,33)	1:A:155:THR:H	4:A:426:PX4:C35	11	0.41
(3,33)	1:A:155:THR:H	4:A:428:PX4:C35	11	0.41
(3,33)	1:A:155:THR:H	4:A:430:PX4:C35	11	0.41
(2,980)	1:A:78:PHE:H	1:A:79:PRO:HD3	17	0.41
(2,980)	1:A:78:PHE:H	1:A:79:PRO:HD3	17	0.41
(2,979)	1:A:78:PHE:H	1:A:78:PHE:HD1	10	0.41
(2,961)	1:A:75:TYR:HD1	1:A:76:SER:H	11	0.41
(2,961)	1:A:75:TYR:HD2	1:A:76:SER:H	11	0.41
(2,947)	1:A:74:GLU:HB3	1:A:75:TYR:H	9	0.41
(2,947)	1:A:74:GLU:HB3	1:A:75:TYR:H	9	0.41
(2,945)	1:A:74:GLU:H	1:A:74:GLU:HG3	14	0.41
(2,945)	1:A:74:GLU:H	1:A:74:GLU:HG3	14	0.41
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG21	3	0.41
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG22	3	0.41
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG23	3	0.41
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG11	3	0.41
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG12	3	0.41
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG13	3	0.41
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG21	9	0.41
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG22	9	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG23	9	0.41
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG11	9	0.41
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG12	9	0.41
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG13	9	0.41
(2,912)	1:A:70:PRO:HB3	1:A:76:SER:H	5	0.41
(2,912)	1:A:70:PRO:HB2	1:A:76:SER:H	5	0.41
(2,903)	1:A:67:CYS:H	1:A:66:ARG:HA	1	0.41
(2,903)	1:A:67:CYS:H	1:A:66:ARG:HA	4	0.41
(2,903)	1:A:67:CYS:H	1:A:66:ARG:HA	19	0.41
(2,896)	1:A:64:LYS:H	1:A:64:LYS:HE3	2	0.41
(2,896)	1:A:64:LYS:H	1:A:64:LYS:HE3	2	0.41
(2,896)	1:A:64:LYS:H	1:A:64:LYS:HE3	13	0.41
(2,896)	1:A:64:LYS:H	1:A:64:LYS:HE3	13	0.41
(2,895)	1:A:64:LYS:H	1:A:64:LYS:HA	2	0.41
(2,859)	1:A:186:ILE:HD12	1:A:156:LEU:HD21	1	0.41
(2,832)	1:A:120:ILE:HD11	1:A:200:LEU:HD21	18	0.41
(2,810)	1:A:93:ILE:H	1:A:94:VAL:HG11	19	0.41
(2,810)	1:A:93:ILE:H	1:A:94:VAL:HG12	19	0.41
(2,810)	1:A:93:ILE:H	1:A:94:VAL:HG13	19	0.41
(2,733)	1:A:196:LEU:HD21	1:A:113:LEU:HD21	20	0.41
(2,693)	1:A:11:GLN:H	1:A:8:SER:H	1	0.41
(2,624)	1:A:11:GLN:H	1:A:8:SER:H	1	0.41
(2,557)	1:A:21:ARG:H	1:A:23:TYR:H	2	0.41
(2,540)	1:A:209:ASN:HD21	1:A:209:ASN:HD22	1	0.41
(2,540)	1:A:209:ASN:HD21	1:A:209:ASN:HD22	1	0.41
(2,540)	1:A:209:ASN:HD21	1:A:209:ASN:HD22	3	0.41
(2,540)	1:A:209:ASN:HD21	1:A:209:ASN:HD22	3	0.41
(2,540)	1:A:209:ASN:HD21	1:A:209:ASN:HD22	12	0.41
(2,540)	1:A:209:ASN:HD21	1:A:209:ASN:HD22	12	0.41
(2,510)	1:A:200:LEU:HD21	1:A:199:SER:H	17	0.41
(2,510)	1:A:200:LEU:HD21	1:A:199:SER:H	18	0.41
(2,453)	1:A:178:TRP:HE1	1:A:175:ASP:H	2	0.41
(2,453)	1:A:178:TRP:HE1	1:A:175:ASP:H	17	0.41
(2,442)	1:A:175:ASP:H	1:A:178:TRP:HE1	2	0.41
(2,442)	1:A:175:ASP:H	1:A:178:TRP:HE1	17	0.41
(2,303)	1:A:122:LEU:H	1:A:120:ILE:HG13	2	0.41
(2,303)	1:A:122:LEU:H	1:A:120:ILE:HG12	2	0.41
(2,228)	1:A:106:ASP:H	1:A:108:LEU:H	13	0.41
(2,228)	1:A:106:ASP:H	1:A:108:LEU:H	16	0.41
(2,113)	1:A:25:TYR:H	1:A:26:ASP:H	2	0.41
(2,975)	1:A:78:PHE:H	1:A:77:LEU:HD22	15	0.4
(2,975)	1:A:78:PHE:H	1:A:77:LEU:HD23	15	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,973)	1:A:78:PHE:H	1:A:77:LEU:HD11	4	0.4
(2,973)	1:A:78:PHE:H	1:A:77:LEU:HD12	4	0.4
(2,973)	1:A:78:PHE:H	1:A:77:LEU:HD13	4	0.4
(2,970)	1:A:77:LEU:HG	1:A:78:PHE:H	20	0.4
(2,961)	1:A:75:TYR:HD1	1:A:76:SER:H	2	0.4
(2,961)	1:A:75:TYR:HD2	1:A:76:SER:H	2	0.4
(2,930)	1:A:72:VAL:HG11	1:A:75:TYR:H	9	0.4
(2,930)	1:A:72:VAL:HG12	1:A:75:TYR:H	9	0.4
(2,930)	1:A:72:VAL:HG13	1:A:75:TYR:H	9	0.4
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG21	16	0.4
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG22	16	0.4
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG23	16	0.4
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG11	16	0.4
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG12	16	0.4
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG13	16	0.4
(2,913)	1:A:71:ASP:H	1:A:70:PRO:HB3	1	0.4
(2,913)	1:A:71:ASP:H	1:A:70:PRO:HB2	1	0.4
(2,895)	1:A:64:LYS:H	1:A:64:LYS:HA	9	0.4
(2,857)	1:A:186:ILE:HD11	1:A:156:LEU:HD21	14	0.4
(2,8)	1:A:135:MET:H	1:A:92:ARG:H	12	0.4
(2,74)	1:A:55:ASN:H	1:A:55:ASN:HD21	7	0.4
(2,730)	1:A:211:VAL:HG12	1:A:226:LEU:HD22	12	0.4
(2,730)	1:A:211:VAL:HG12	1:A:226:LEU:HD23	12	0.4
(2,693)	1:A:11:GLN:H	1:A:8:SER:H	6	0.4
(2,624)	1:A:11:GLN:H	1:A:8:SER:H	6	0.4
(2,621)	1:A:200:LEU:HD21	1:A:201:GLY:H	15	0.4
(2,608)	1:A:238:TYR:H	1:A:120:ILE:HD11	18	0.4
(2,608)	1:A:238:TYR:H	1:A:120:ILE:HD12	18	0.4
(2,608)	1:A:238:TYR:H	1:A:120:ILE:HD13	18	0.4
(2,540)	1:A:209:ASN:HD21	1:A:209:ASN:HD22	4	0.4
(2,540)	1:A:209:ASN:HD21	1:A:209:ASN:HD22	4	0.4
(2,518)	1:A:200:LEU:H	1:A:196:LEU:HD22	7	0.4
(2,518)	1:A:200:LEU:H	1:A:196:LEU:HD23	7	0.4
(2,467)	1:A:84:TRP:H	1:A:200:LEU:HD22	17	0.4
(2,467)	1:A:84:TRP:H	1:A:200:LEU:HD23	17	0.4
(2,414)	1:A:167:GLY:H	1:A:166:LEU:HD21	4	0.4
(2,380)	1:A:10:LEU:H	1:A:10:LEU:HD22	20	0.4
(2,380)	1:A:10:LEU:H	1:A:10:LEU:HD23	20	0.4
(2,207)	1:A:98:ARG:H	1:A:100:LEU:H	3	0.4
(2,979)	1:A:78:PHE:H	1:A:78:PHE:HD1	12	0.39
(2,970)	1:A:77:LEU:HG	1:A:78:PHE:H	15	0.39
(2,920)	1:A:72:VAL:H	1:A:71:ASP:H	11	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,920)	1:A:72:VAL:H	1:A:71:ASP:H	11	0.39
(2,896)	1:A:64:LYS:H	1:A:64:LYS:HE3	1	0.39
(2,896)	1:A:64:LYS:H	1:A:64:LYS:HE3	1	0.39
(2,866)	1:A:186:ILE:HD11	1:A:156:LEU:HD11	4	0.39
(2,866)	1:A:186:ILE:HD11	1:A:156:LEU:HD12	4	0.39
(2,866)	1:A:186:ILE:HD11	1:A:156:LEU:HD13	4	0.39
(2,866)	1:A:186:ILE:HD12	1:A:156:LEU:HD11	4	0.39
(2,866)	1:A:186:ILE:HD12	1:A:156:LEU:HD12	4	0.39
(2,866)	1:A:186:ILE:HD12	1:A:156:LEU:HD13	4	0.39
(2,866)	1:A:186:ILE:HD13	1:A:156:LEU:HD11	4	0.39
(2,866)	1:A:186:ILE:HD13	1:A:156:LEU:HD12	4	0.39
(2,866)	1:A:186:ILE:HD13	1:A:156:LEU:HD13	4	0.39
(2,75)	1:A:55:ASN:H	1:A:59:ILE:H	16	0.39
(2,741)	1:A:114:ASN:H	1:A:113:LEU:HD21	19	0.39
(2,60)	1:A:50:ILE:H	1:A:50:ILE:HD11	20	0.39
(2,60)	1:A:50:ILE:H	1:A:50:ILE:HD12	20	0.39
(2,60)	1:A:50:ILE:H	1:A:50:ILE:HD13	20	0.39
(2,543)	1:A:210:ALA:H	1:A:213:TYR:H	12	0.39
(2,489)	1:A:116:TRP:HE1	1:A:196:LEU:H	8	0.39
(2,450)	1:A:177:ARG:H	1:A:186:ILE:HG13	12	0.39
(2,450)	1:A:177:ARG:H	1:A:186:ILE:HG12	12	0.39
(2,392)	1:A:157:ALA:H	1:A:68:GLY:H	10	0.39
(2,317)	1:A:125:ARG:H	1:A:91:TYR:H	9	0.39
(2,275)	1:A:116:TRP:HE1	1:A:196:LEU:H	8	0.39
(2,969)	1:A:77:LEU:H	1:A:78:PHE:H	18	0.38
(2,964)	1:A:75:TYR:H	1:A:76:SER:H	15	0.38
(2,959)	1:A:75:TYR:H	1:A:76:SER:H	15	0.38
(2,927)	1:A:72:VAL:H	1:A:73:ALA:H	7	0.38
(2,927)	1:A:72:VAL:H	1:A:73:ALA:H	7	0.38
(2,919)	1:A:72:VAL:H	1:A:71:ASP:HA	1	0.38
(2,919)	1:A:72:VAL:H	1:A:71:ASP:HA	20	0.38
(2,903)	1:A:67:CYS:H	1:A:66:ARG:HA	8	0.38
(2,898)	1:A:66:ARG:H	1:A:63:GLN:HB3	7	0.38
(2,898)	1:A:66:ARG:H	1:A:63:GLN:HB2	7	0.38
(2,839)	1:A:123:HIS:H	1:A:122:LEU:HD11	7	0.38
(2,839)	1:A:123:HIS:H	1:A:122:LEU:HD12	7	0.38
(2,839)	1:A:123:HIS:H	1:A:122:LEU:HD13	7	0.38
(2,765)	1:A:22:PHE:H	1:A:19:LEU:HD21	15	0.38
(2,758)	1:A:54:LEU:HD22	1:A:39:LEU:HD11	4	0.38
(2,758)	1:A:54:LEU:HD22	1:A:39:LEU:HD12	4	0.38
(2,758)	1:A:54:LEU:HD22	1:A:39:LEU:HD13	4	0.38
(2,758)	1:A:54:LEU:HD23	1:A:39:LEU:HD11	4	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,758)	1:A:54:LEU:HD23	1:A:39:LEU:HD12	4	0.38
(2,758)	1:A:54:LEU:HD23	1:A:39:LEU:HD13	4	0.38
(2,750)	1:A:89:VAL:HG13	1:A:122:LEU:HD21	19	0.38
(2,746)	1:A:89:VAL:HG11	1:A:122:LEU:HD21	18	0.38
(2,741)	1:A:114:ASN:H	1:A:113:LEU:HD21	8	0.38
(2,693)	1:A:11:GLN:H	1:A:8:SER:H	5	0.38
(2,659)	1:A:42:MET:H	1:A:19:LEU:HD11	4	0.38
(2,659)	1:A:42:MET:H	1:A:19:LEU:HD12	4	0.38
(2,659)	1:A:42:MET:H	1:A:19:LEU:HD13	4	0.38
(2,624)	1:A:11:GLN:H	1:A:8:SER:H	5	0.38
(2,570)	1:A:226:LEU:H	1:A:226:LEU:HD21	4	0.38
(2,570)	1:A:226:LEU:H	1:A:226:LEU:HD21	14	0.38
(2,540)	1:A:209:ASN:HD21	1:A:209:ASN:HD22	9	0.38
(2,540)	1:A:209:ASN:HD21	1:A:209:ASN:HD22	9	0.38
(2,510)	1:A:200:LEU:HD21	1:A:199:SER:H	10	0.38
(2,380)	1:A:10:LEU:H	1:A:10:LEU:HD22	19	0.38
(2,380)	1:A:10:LEU:H	1:A:10:LEU:HD23	19	0.38
(2,379)	1:A:10:LEU:H	1:A:10:LEU:HD21	3	0.38
(2,357)	1:A:136:ILE:HD11	1:A:137:GLY:H	15	0.38
(2,357)	1:A:136:ILE:HD12	1:A:137:GLY:H	15	0.38
(2,357)	1:A:136:ILE:HD13	1:A:137:GLY:H	15	0.38
(2,321)	1:A:128:VAL:HG11	1:A:126:LYS:H	13	0.38
(2,321)	1:A:128:VAL:HG12	1:A:126:LYS:H	13	0.38
(2,321)	1:A:128:VAL:HG13	1:A:126:LYS:H	13	0.38
(2,315)	1:A:125:ARG:H	1:A:126:LYS:H	5	0.38
(2,304)	1:A:123:HIS:H	1:A:122:LEU:HD11	7	0.38
(2,304)	1:A:123:HIS:H	1:A:122:LEU:HD12	7	0.38
(2,304)	1:A:123:HIS:H	1:A:122:LEU:HD13	7	0.38
(2,10)	1:A:92:ARG:H	1:A:93:ILE:HG13	1	0.38
(2,10)	1:A:92:ARG:H	1:A:93:ILE:HG12	1	0.38
(2,980)	1:A:78:PHE:H	1:A:79:PRO:HD3	6	0.37
(2,980)	1:A:78:PHE:H	1:A:79:PRO:HD3	6	0.37
(2,969)	1:A:77:LEU:H	1:A:78:PHE:H	14	0.37
(2,954)	1:A:74:GLU:HB3	1:A:77:LEU:H	8	0.37
(2,954)	1:A:74:GLU:HB3	1:A:77:LEU:H	8	0.37
(2,951)	1:A:74:GLU:H	1:A:76:SER:H	14	0.37
(2,945)	1:A:74:GLU:H	1:A:74:GLU:HG3	13	0.37
(2,945)	1:A:74:GLU:H	1:A:74:GLU:HG3	13	0.37
(2,931)	1:A:72:VAL:H	1:A:75:TYR:HB3	18	0.37
(2,931)	1:A:72:VAL:H	1:A:75:TYR:HB3	18	0.37
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG21	14	0.37
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG22	14	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG23	14	0.37
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG11	14	0.37
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG12	14	0.37
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG13	14	0.37
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG21	17	0.37
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG22	17	0.37
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG23	17	0.37
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG11	17	0.37
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG12	17	0.37
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG13	17	0.37
(2,919)	1:A:72:VAL:H	1:A:71:ASP:HA	8	0.37
(2,911)	1:A:69:VAL:HG21	1:A:69:VAL:H	10	0.37
(2,911)	1:A:69:VAL:HG22	1:A:69:VAL:H	10	0.37
(2,911)	1:A:69:VAL:HG23	1:A:69:VAL:H	10	0.37
(2,911)	1:A:69:VAL:HG11	1:A:69:VAL:H	10	0.37
(2,911)	1:A:69:VAL:HG12	1:A:69:VAL:H	10	0.37
(2,911)	1:A:69:VAL:HG13	1:A:69:VAL:H	10	0.37
(2,905)	1:A:67:CYS:HA	1:A:68:GLY:H	1	0.37
(2,867)	1:A:186:ILE:HD11	1:A:156:LEU:HD21	20	0.37
(2,750)	1:A:89:VAL:HG13	1:A:122:LEU:HD21	20	0.37
(2,680)	1:A:158:HIS:H	1:A:172:PHE:H	3	0.37
(2,673)	1:A:77:LEU:H	1:A:78:PHE:H	14	0.37
(2,661)	1:A:4:ALA:H	1:A:59:ILE:HG21	2	0.37
(2,661)	1:A:4:ALA:H	1:A:59:ILE:HG22	2	0.37
(2,661)	1:A:4:ALA:H	1:A:59:ILE:HG23	2	0.37
(2,627)	1:A:13:GLU:H	1:A:10:LEU:H	10	0.37
(2,626)	1:A:12:TRP:H	1:A:10:LEU:H	9	0.37
(2,621)	1:A:200:LEU:HD21	1:A:201:GLY:H	18	0.37
(2,557)	1:A:21:ARG:H	1:A:23:TYR:H	19	0.37
(2,510)	1:A:200:LEU:HD21	1:A:199:SER:H	8	0.37
(2,507)	1:A:199:SER:H	1:A:202:MET:H	11	0.37
(2,507)	1:A:199:SER:H	1:A:202:MET:H	12	0.37
(2,501)	1:A:198:HIS:H	1:A:195:ALA:H	17	0.37
(2,500)	1:A:116:TRP:HE1	1:A:198:HIS:H	17	0.37
(2,456)	1:A:178:TRP:HE1	1:A:176:GLU:H	16	0.37
(2,445)	1:A:178:TRP:HE1	1:A:176:GLU:H	16	0.37
(2,426)	1:A:170:ALA:H	1:A:136:ILE:HD11	1	0.37
(2,426)	1:A:170:ALA:H	1:A:136:ILE:HD12	1	0.37
(2,426)	1:A:170:ALA:H	1:A:136:ILE:HD13	1	0.37
(2,426)	1:A:170:ALA:H	1:A:136:ILE:HD11	19	0.37
(2,426)	1:A:170:ALA:H	1:A:136:ILE:HD12	19	0.37
(2,426)	1:A:170:ALA:H	1:A:136:ILE:HD13	19	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,392)	1:A:157:ALA:H	1:A:68:GLY:H	4	0.37
(2,317)	1:A:125:ARG:H	1:A:91:TYR:H	18	0.37
(2,315)	1:A:125:ARG:H	1:A:126:LYS:H	11	0.37
(2,303)	1:A:122:LEU:H	1:A:120:ILE:HG13	11	0.37
(2,303)	1:A:122:LEU:H	1:A:120:ILE:HG12	11	0.37
(2,302)	1:A:120:ILE:HG21	1:A:122:LEU:H	18	0.37
(2,302)	1:A:120:ILE:HG22	1:A:122:LEU:H	18	0.37
(2,302)	1:A:120:ILE:HG23	1:A:122:LEU:H	18	0.37
(2,185)	1:A:94:VAL:H	1:A:92:ARG:H	14	0.37
(2,988)	1:A:129:TRP:HE1	4:A:305:PX4:C2	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:307:PX4:C2	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:309:PX4:C2	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:311:PX4:C2	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:313:PX4:C2	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:315:PX4:C2	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:317:PX4:C2	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:319:PX4:C2	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:321:PX4:C2	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:323:PX4:C2	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:325:PX4:C2	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:327:PX4:C2	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:329:PX4:C2	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:331:PX4:C2	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:333:PX4:C2	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:335:PX4:C2	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:337:PX4:C2	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:339:PX4:C2	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:341:PX4:C2	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:343:PX4:C2	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:345:PX4:C2	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:347:PX4:C2	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:349:PX4:C2	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:351:PX4:C2	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:353:PX4:C2	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:355:PX4:C2	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:357:PX4:C2	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:359:PX4:C2	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:361:PX4:C2	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:363:PX4:C2	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:402:PX4:C2	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:404:PX4:C2	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:406:PX4:C2	13	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,988)	1:A:129:TRP:HE1	4:A:408:PX4:C2	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:410:PX4:C2	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:412:PX4:C2	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:414:PX4:C2	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:416:PX4:C2	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:418:PX4:C2	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:420:PX4:C2	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:422:PX4:C2	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:424:PX4:C2	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:426:PX4:C2	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:428:PX4:C2	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:430:PX4:C2	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:305:PX4:C1	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:307:PX4:C1	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:309:PX4:C1	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:311:PX4:C1	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:313:PX4:C1	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:315:PX4:C1	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:317:PX4:C1	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:319:PX4:C1	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:321:PX4:C1	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:323:PX4:C1	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:325:PX4:C1	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:327:PX4:C1	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:329:PX4:C1	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:331:PX4:C1	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:333:PX4:C1	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:335:PX4:C1	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:337:PX4:C1	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:339:PX4:C1	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:341:PX4:C1	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:343:PX4:C1	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:345:PX4:C1	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:347:PX4:C1	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:349:PX4:C1	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:351:PX4:C1	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:353:PX4:C1	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:355:PX4:C1	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:357:PX4:C1	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:359:PX4:C1	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:361:PX4:C1	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:363:PX4:C1	13	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,988)	1:A:129:TRP:HE1	4:A:402:PX4:C1	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:404:PX4:C1	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:406:PX4:C1	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:408:PX4:C1	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:410:PX4:C1	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:412:PX4:C1	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:414:PX4:C1	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:416:PX4:C1	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:418:PX4:C1	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:420:PX4:C1	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:422:PX4:C1	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:424:PX4:C1	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:426:PX4:C1	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:428:PX4:C1	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:430:PX4:C1	13	0.36
(2,988)	1:A:129:TRP:HE1	4:A:305:PX4:C2	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:307:PX4:C2	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:309:PX4:C2	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:311:PX4:C2	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:313:PX4:C2	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:315:PX4:C2	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:317:PX4:C2	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:319:PX4:C2	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:321:PX4:C2	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:323:PX4:C2	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:325:PX4:C2	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:327:PX4:C2	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:329:PX4:C2	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:331:PX4:C2	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:333:PX4:C2	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:335:PX4:C2	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:337:PX4:C2	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:339:PX4:C2	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:341:PX4:C2	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:343:PX4:C2	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:345:PX4:C2	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:347:PX4:C2	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:349:PX4:C2	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:351:PX4:C2	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:353:PX4:C2	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:355:PX4:C2	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:357:PX4:C2	17	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,988)	1:A:129:TRP:HE1	4:A:359:PX4:C2	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:361:PX4:C2	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:363:PX4:C2	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:402:PX4:C2	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:404:PX4:C2	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:406:PX4:C2	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:408:PX4:C2	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:410:PX4:C2	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:412:PX4:C2	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:414:PX4:C2	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:416:PX4:C2	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:418:PX4:C2	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:420:PX4:C2	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:422:PX4:C2	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:424:PX4:C2	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:426:PX4:C2	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:428:PX4:C2	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:430:PX4:C2	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:305:PX4:C1	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:307:PX4:C1	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:309:PX4:C1	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:311:PX4:C1	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:313:PX4:C1	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:315:PX4:C1	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:317:PX4:C1	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:319:PX4:C1	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:321:PX4:C1	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:323:PX4:C1	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:325:PX4:C1	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:327:PX4:C1	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:329:PX4:C1	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:331:PX4:C1	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:333:PX4:C1	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:335:PX4:C1	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:337:PX4:C1	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:339:PX4:C1	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:341:PX4:C1	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:343:PX4:C1	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:345:PX4:C1	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:347:PX4:C1	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:349:PX4:C1	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:351:PX4:C1	17	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,988)	1:A:129:TRP:HE1	4:A:353:PX4:C1	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:355:PX4:C1	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:357:PX4:C1	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:359:PX4:C1	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:361:PX4:C1	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:363:PX4:C1	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:402:PX4:C1	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:404:PX4:C1	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:406:PX4:C1	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:408:PX4:C1	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:410:PX4:C1	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:412:PX4:C1	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:414:PX4:C1	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:416:PX4:C1	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:418:PX4:C1	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:420:PX4:C1	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:422:PX4:C1	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:424:PX4:C1	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:426:PX4:C1	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:428:PX4:C1	17	0.36
(2,988)	1:A:129:TRP:HE1	4:A:430:PX4:C1	17	0.36
(2,986)	1:A:80:ASN:H	1:A:79:PRO:HB3	9	0.36
(2,986)	1:A:80:ASN:H	1:A:79:PRO:HB2	9	0.36
(2,986)	1:A:80:ASN:H	1:A:79:PRO:HB3	9	0.36
(2,986)	1:A:80:ASN:H	1:A:79:PRO:HB2	9	0.36
(2,980)	1:A:78:PHE:H	1:A:79:PRO:HD3	3	0.36
(2,980)	1:A:78:PHE:H	1:A:79:PRO:HD3	3	0.36
(2,977)	1:A:78:PHE:H	1:A:78:PHE:HA	13	0.36
(2,947)	1:A:74:GLU:HB3	1:A:75:TYR:H	1	0.36
(2,947)	1:A:74:GLU:HB3	1:A:75:TYR:H	1	0.36
(2,945)	1:A:74:GLU:H	1:A:74:GLU:HG3	12	0.36
(2,945)	1:A:74:GLU:H	1:A:74:GLU:HG3	12	0.36
(2,931)	1:A:72:VAL:H	1:A:75:TYR:HB3	5	0.36
(2,931)	1:A:72:VAL:H	1:A:75:TYR:HB3	5	0.36
(2,927)	1:A:72:VAL:H	1:A:73:ALA:H	8	0.36
(2,927)	1:A:72:VAL:H	1:A:73:ALA:H	8	0.36
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG21	20	0.36
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG22	20	0.36
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG23	20	0.36
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG11	20	0.36
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG12	20	0.36
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG13	20	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,912)	1:A:70:PRO:HB3	1:A:76:SER:H	18	0.36
(2,912)	1:A:70:PRO:HB2	1:A:76:SER:H	18	0.36
(2,911)	1:A:69:VAL:HG21	1:A:69:VAL:H	9	0.36
(2,911)	1:A:69:VAL:HG22	1:A:69:VAL:H	9	0.36
(2,911)	1:A:69:VAL:HG23	1:A:69:VAL:H	9	0.36
(2,911)	1:A:69:VAL:HG11	1:A:69:VAL:H	9	0.36
(2,911)	1:A:69:VAL:HG12	1:A:69:VAL:H	9	0.36
(2,911)	1:A:69:VAL:HG13	1:A:69:VAL:H	9	0.36
(2,852)	1:A:127:VAL:HG21	1:A:125:ARG:HG2	20	0.36
(2,852)	1:A:127:VAL:HG22	1:A:125:ARG:HG2	20	0.36
(2,852)	1:A:127:VAL:HG23	1:A:125:ARG:HG2	20	0.36
(2,844)	1:A:200:LEU:HD22	1:A:122:LEU:HD21	19	0.36
(2,765)	1:A:22:PHE:H	1:A:19:LEU:HD21	16	0.36
(2,748)	1:A:89:VAL:HG12	1:A:122:LEU:HD21	16	0.36
(2,733)	1:A:196:LEU:HD21	1:A:113:LEU:HD21	18	0.36
(2,693)	1:A:11:GLN:H	1:A:8:SER:H	17	0.36
(2,672)	1:A:66:ARG:H	1:A:156:LEU:HD22	16	0.36
(2,672)	1:A:66:ARG:H	1:A:156:LEU:HD23	16	0.36
(2,626)	1:A:12:TRP:H	1:A:10:LEU:H	10	0.36
(2,624)	1:A:11:GLN:H	1:A:8:SER:H	17	0.36
(2,621)	1:A:200:LEU:HD21	1:A:201:GLY:H	13	0.36
(2,557)	1:A:21:ARG:H	1:A:23:TYR:H	17	0.36
(2,540)	1:A:209:ASN:HD21	1:A:209:ASN:HD22	10	0.36
(2,540)	1:A:209:ASN:HD21	1:A:209:ASN:HD22	10	0.36
(2,518)	1:A:200:LEU:H	1:A:196:LEU:HD22	8	0.36
(2,518)	1:A:200:LEU:H	1:A:196:LEU:HD23	8	0.36
(2,507)	1:A:199:SER:H	1:A:202:MET:H	9	0.36
(2,466)	1:A:84:TRP:H	1:A:200:LEU:HD21	13	0.36
(2,390)	1:A:156:LEU:H	1:A:68:GLY:H	16	0.36
(2,369)	1:A:143:HIS:H	1:A:145:ASP:H	10	0.36
(2,357)	1:A:136:ILE:HD11	1:A:137:GLY:H	9	0.36
(2,357)	1:A:136:ILE:HD12	1:A:137:GLY:H	9	0.36
(2,357)	1:A:136:ILE:HD13	1:A:137:GLY:H	9	0.36
(2,315)	1:A:125:ARG:H	1:A:126:LYS:H	15	0.36
(2,124)	1:A:156:LEU:H	1:A:68:GLY:H	16	0.36
(2,985)	1:A:80:ASN:H	1:A:78:PHE:HD1	9	0.35
(2,961)	1:A:75:TYR:HD1	1:A:76:SER:H	14	0.35
(2,961)	1:A:75:TYR:HD2	1:A:76:SER:H	14	0.35
(2,917)	1:A:71:ASP:H	1:A:72:VAL:HB	10	0.35
(2,912)	1:A:70:PRO:HB3	1:A:76:SER:H	13	0.35
(2,912)	1:A:70:PRO:HB2	1:A:76:SER:H	13	0.35
(2,903)	1:A:67:CYS:H	1:A:66:ARG:HA	10	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,896)	1:A:64:LYS:H	1:A:64:LYS:HE3	17	0.35
(2,896)	1:A:64:LYS:H	1:A:64:LYS:HE3	17	0.35
(2,895)	1:A:64:LYS:H	1:A:64:LYS:HA	8	0.35
(2,895)	1:A:64:LYS:H	1:A:64:LYS:HA	15	0.35
(2,759)	1:A:54:LEU:HD21	1:A:59:ILE:HD11	15	0.35
(2,759)	1:A:54:LEU:HD21	1:A:59:ILE:HD12	15	0.35
(2,759)	1:A:54:LEU:HD21	1:A:59:ILE:HD13	15	0.35
(2,74)	1:A:55:ASN:H	1:A:55:ASN:HD21	17	0.35
(2,671)	1:A:66:ARG:H	1:A:156:LEU:HD21	9	0.35
(2,62)	1:A:50:ILE:HG12	1:A:50:ILE:H	13	0.35
(2,540)	1:A:209:ASN:HD21	1:A:209:ASN:HD22	6	0.35
(2,540)	1:A:209:ASN:HD21	1:A:209:ASN:HD22	6	0.35
(2,504)	1:A:198:HIS:H	1:A:202:MET:H	19	0.35
(2,473)	1:A:186:ILE:H	1:A:156:LEU:HD22	7	0.35
(2,473)	1:A:186:ILE:H	1:A:156:LEU:HD23	7	0.35
(2,472)	1:A:186:ILE:H	1:A:156:LEU:HD21	7	0.35
(2,425)	1:A:170:ALA:H	1:A:169:ASP:H	15	0.35
(2,424)	1:A:169:ASP:H	1:A:166:LEU:HB3	13	0.35
(2,379)	1:A:10:LEU:H	1:A:10:LEU:HD21	8	0.35
(2,357)	1:A:136:ILE:HD11	1:A:137:GLY:H	19	0.35
(2,357)	1:A:136:ILE:HD12	1:A:137:GLY:H	19	0.35
(2,357)	1:A:136:ILE:HD13	1:A:137:GLY:H	19	0.35
(2,257)	1:A:112:ALA:H	1:A:189:LEU:HD21	6	0.35
(2,226)	1:A:104:THR:H	1:A:106:ASP:H	12	0.35
(2,226)	1:A:104:THR:H	1:A:106:ASP:H	13	0.35
(2,212)	1:A:120:ILE:HD11	1:A:237:LEU:H	19	0.35
(2,212)	1:A:120:ILE:HD12	1:A:237:LEU:H	19	0.35
(2,212)	1:A:120:ILE:HD13	1:A:237:LEU:H	19	0.35
(2,113)	1:A:25:TYR:H	1:A:26:ASP:H	11	0.35
(2,980)	1:A:78:PHE:H	1:A:79:PRO:HD3	14	0.34
(2,980)	1:A:78:PHE:H	1:A:79:PRO:HD3	14	0.34
(2,953)	1:A:74:GLU:HB3	1:A:76:SER:H	19	0.34
(2,953)	1:A:74:GLU:HB3	1:A:76:SER:H	19	0.34
(2,945)	1:A:74:GLU:H	1:A:74:GLU:HG3	10	0.34
(2,945)	1:A:74:GLU:H	1:A:74:GLU:HG3	10	0.34
(2,917)	1:A:71:ASP:H	1:A:72:VAL:HB	16	0.34
(2,839)	1:A:123:HIS:H	1:A:122:LEU:HD11	20	0.34
(2,839)	1:A:123:HIS:H	1:A:122:LEU:HD12	20	0.34
(2,839)	1:A:123:HIS:H	1:A:122:LEU:HD13	20	0.34
(2,810)	1:A:93:ILE:H	1:A:94:VAL:HG11	1	0.34
(2,810)	1:A:93:ILE:H	1:A:94:VAL:HG12	1	0.34
(2,810)	1:A:93:ILE:H	1:A:94:VAL:HG13	1	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,741)	1:A:114:ASN:H	1:A:113:LEU:HD21	11	0.34
(2,67)	1:A:53:MET:H	1:A:52:GLY:H	4	0.34
(2,64)	1:A:52:GLY:H	1:A:53:MET:H	4	0.34
(2,608)	1:A:238:TYR:H	1:A:120:ILE:HD11	4	0.34
(2,608)	1:A:238:TYR:H	1:A:120:ILE:HD12	4	0.34
(2,608)	1:A:238:TYR:H	1:A:120:ILE:HD13	4	0.34
(2,557)	1:A:21:ARG:H	1:A:23:TYR:H	20	0.34
(2,518)	1:A:200:LEU:H	1:A:196:LEU:HD22	20	0.34
(2,518)	1:A:200:LEU:H	1:A:196:LEU:HD23	20	0.34
(2,511)	1:A:200:LEU:HD22	1:A:199:SER:H	16	0.34
(2,511)	1:A:200:LEU:HD23	1:A:199:SER:H	16	0.34
(2,507)	1:A:199:SER:H	1:A:202:MET:H	20	0.34
(2,423)	1:A:169:ASP:H	1:A:134:ILE:HD11	16	0.34
(2,423)	1:A:169:ASP:H	1:A:134:ILE:HD12	16	0.34
(2,423)	1:A:169:ASP:H	1:A:134:ILE:HD13	16	0.34
(2,392)	1:A:157:ALA:H	1:A:68:GLY:H	2	0.34
(2,378)	1:A:10:LEU:H	1:A:10:LEU:HD11	6	0.34
(2,378)	1:A:10:LEU:H	1:A:10:LEU:HD12	6	0.34
(2,378)	1:A:10:LEU:H	1:A:10:LEU:HD13	6	0.34
(2,369)	1:A:143:HIS:H	1:A:145:ASP:H	8	0.34
(2,357)	1:A:136:ILE:HD11	1:A:137:GLY:H	1	0.34
(2,357)	1:A:136:ILE:HD12	1:A:137:GLY:H	1	0.34
(2,357)	1:A:136:ILE:HD13	1:A:137:GLY:H	1	0.34
(2,357)	1:A:136:ILE:HD11	1:A:137:GLY:H	14	0.34
(2,357)	1:A:136:ILE:HD12	1:A:137:GLY:H	14	0.34
(2,357)	1:A:136:ILE:HD13	1:A:137:GLY:H	14	0.34
(2,316)	1:A:125:ARG:H	1:A:89:VAL:H	20	0.34
(2,315)	1:A:125:ARG:H	1:A:126:LYS:H	17	0.34
(2,304)	1:A:123:HIS:H	1:A:122:LEU:HD11	20	0.34
(2,304)	1:A:123:HIS:H	1:A:122:LEU:HD12	20	0.34
(2,304)	1:A:123:HIS:H	1:A:122:LEU:HD13	20	0.34
(2,274)	1:A:116:TRP:HE1	1:A:197:GLY:H	10	0.34
(2,228)	1:A:106:ASP:H	1:A:108:LEU:H	7	0.34
(2,207)	1:A:98:ARG:H	1:A:100:LEU:H	17	0.34
(2,162)	1:A:125:ARG:H	1:A:89:VAL:H	20	0.34
(2,10)	1:A:92:ARG:H	1:A:93:ILE:HG13	19	0.34
(2,10)	1:A:92:ARG:H	1:A:93:ILE:HG12	19	0.34
(2,973)	1:A:78:PHE:H	1:A:77:LEU:HD11	14	0.33
(2,973)	1:A:78:PHE:H	1:A:77:LEU:HD12	14	0.33
(2,973)	1:A:78:PHE:H	1:A:77:LEU:HD13	14	0.33
(2,953)	1:A:74:GLU:HB3	1:A:76:SER:H	6	0.33
(2,953)	1:A:74:GLU:HB3	1:A:76:SER:H	6	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,896)	1:A:64:LYS:H	1:A:64:LYS:HE3	10	0.33
(2,896)	1:A:64:LYS:H	1:A:64:LYS:HE3	10	0.33
(2,885)	1:A:134:ILE:HD11	1:A:89:VAL:HG11	6	0.33
(2,885)	1:A:134:ILE:HD11	1:A:89:VAL:HG12	6	0.33
(2,885)	1:A:134:ILE:HD11	1:A:89:VAL:HG13	6	0.33
(2,885)	1:A:134:ILE:HD12	1:A:89:VAL:HG11	6	0.33
(2,885)	1:A:134:ILE:HD12	1:A:89:VAL:HG12	6	0.33
(2,885)	1:A:134:ILE:HD12	1:A:89:VAL:HG13	6	0.33
(2,885)	1:A:134:ILE:HD13	1:A:89:VAL:HG11	6	0.33
(2,885)	1:A:134:ILE:HD13	1:A:89:VAL:HG12	6	0.33
(2,885)	1:A:134:ILE:HD13	1:A:89:VAL:HG13	6	0.33
(2,868)	1:A:186:ILE:HD11	1:A:156:LEU:HD22	14	0.33
(2,868)	1:A:186:ILE:HD11	1:A:156:LEU:HD23	14	0.33
(2,868)	1:A:186:ILE:HD11	1:A:156:LEU:HD22	16	0.33
(2,868)	1:A:186:ILE:HD11	1:A:156:LEU:HD23	16	0.33
(2,839)	1:A:123:HIS:H	1:A:122:LEU:HD11	10	0.33
(2,839)	1:A:123:HIS:H	1:A:122:LEU:HD12	10	0.33
(2,839)	1:A:123:HIS:H	1:A:122:LEU:HD13	10	0.33
(2,8)	1:A:135:MET:H	1:A:92:ARG:H	6	0.33
(2,757)	1:A:54:LEU:HD21	1:A:39:LEU:HD11	4	0.33
(2,757)	1:A:54:LEU:HD21	1:A:39:LEU:HD12	4	0.33
(2,757)	1:A:54:LEU:HD21	1:A:39:LEU:HD13	4	0.33
(2,744)	1:A:134:ILE:HD11	1:A:89:VAL:HG11	6	0.33
(2,744)	1:A:134:ILE:HD11	1:A:89:VAL:HG12	6	0.33
(2,744)	1:A:134:ILE:HD11	1:A:89:VAL:HG13	6	0.33
(2,744)	1:A:134:ILE:HD12	1:A:89:VAL:HG11	6	0.33
(2,744)	1:A:134:ILE:HD12	1:A:89:VAL:HG12	6	0.33
(2,744)	1:A:134:ILE:HD12	1:A:89:VAL:HG13	6	0.33
(2,744)	1:A:134:ILE:HD13	1:A:89:VAL:HG11	6	0.33
(2,744)	1:A:134:ILE:HD13	1:A:89:VAL:HG12	6	0.33
(2,744)	1:A:134:ILE:HD13	1:A:89:VAL:HG13	6	0.33
(2,741)	1:A:114:ASN:H	1:A:113:LEU:HD21	7	0.33
(2,731)	1:A:211:VAL:HG13	1:A:226:LEU:HD21	19	0.33
(2,659)	1:A:42:MET:H	1:A:19:LEU:HD11	15	0.33
(2,659)	1:A:42:MET:H	1:A:19:LEU:HD12	15	0.33
(2,659)	1:A:42:MET:H	1:A:19:LEU:HD13	15	0.33
(2,621)	1:A:200:LEU:HD21	1:A:201:GLY:H	4	0.33
(2,60)	1:A:50:ILE:H	1:A:50:ILE:HD11	8	0.33
(2,60)	1:A:50:ILE:H	1:A:50:ILE:HD12	8	0.33
(2,60)	1:A:50:ILE:H	1:A:50:ILE:HD13	8	0.33
(2,60)	1:A:50:ILE:H	1:A:50:ILE:HD11	19	0.33
(2,60)	1:A:50:ILE:H	1:A:50:ILE:HD12	19	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,60)	1:A:50:ILE:H	1:A:50:ILE:HD13	19	0.33
(2,538)	1:A:205:SER:H	1:A:213:TYR:H	5	0.33
(2,471)	1:A:186:ILE:H	1:A:156:LEU:HD11	14	0.33
(2,471)	1:A:186:ILE:H	1:A:156:LEU:HD12	14	0.33
(2,471)	1:A:186:ILE:H	1:A:156:LEU:HD13	14	0.33
(2,454)	1:A:178:TRP:HE1	1:A:178:TRP:H	15	0.33
(2,384)	1:A:154:ASN:HD22	1:A:154:ASN:HD21	13	0.33
(2,384)	1:A:154:ASN:HD22	1:A:154:ASN:HD21	13	0.33
(2,379)	1:A:10:LEU:H	1:A:10:LEU:HD21	14	0.33
(2,315)	1:A:125:ARG:H	1:A:126:LYS:H	12	0.33
(2,304)	1:A:123:HIS:H	1:A:122:LEU:HD11	10	0.33
(2,304)	1:A:123:HIS:H	1:A:122:LEU:HD12	10	0.33
(2,304)	1:A:123:HIS:H	1:A:122:LEU:HD13	10	0.33
(2,264)	1:A:113:LEU:H	1:A:196:LEU:HD21	9	0.33
(3,33)	1:A:155:THR:H	4:A:305:PX4:C35	14	0.32
(3,33)	1:A:155:THR:H	4:A:307:PX4:C35	14	0.32
(3,33)	1:A:155:THR:H	4:A:309:PX4:C35	14	0.32
(3,33)	1:A:155:THR:H	4:A:311:PX4:C35	14	0.32
(3,33)	1:A:155:THR:H	4:A:313:PX4:C35	14	0.32
(3,33)	1:A:155:THR:H	4:A:315:PX4:C35	14	0.32
(3,33)	1:A:155:THR:H	4:A:317:PX4:C35	14	0.32
(3,33)	1:A:155:THR:H	4:A:319:PX4:C35	14	0.32
(3,33)	1:A:155:THR:H	4:A:321:PX4:C35	14	0.32
(3,33)	1:A:155:THR:H	4:A:323:PX4:C35	14	0.32
(3,33)	1:A:155:THR:H	4:A:325:PX4:C35	14	0.32
(3,33)	1:A:155:THR:H	4:A:327:PX4:C35	14	0.32
(3,33)	1:A:155:THR:H	4:A:329:PX4:C35	14	0.32
(3,33)	1:A:155:THR:H	4:A:331:PX4:C35	14	0.32
(3,33)	1:A:155:THR:H	4:A:333:PX4:C35	14	0.32
(3,33)	1:A:155:THR:H	4:A:335:PX4:C35	14	0.32
(3,33)	1:A:155:THR:H	4:A:337:PX4:C35	14	0.32
(3,33)	1:A:155:THR:H	4:A:339:PX4:C35	14	0.32
(3,33)	1:A:155:THR:H	4:A:341:PX4:C35	14	0.32
(3,33)	1:A:155:THR:H	4:A:343:PX4:C35	14	0.32
(3,33)	1:A:155:THR:H	4:A:345:PX4:C35	14	0.32
(3,33)	1:A:155:THR:H	4:A:347:PX4:C35	14	0.32
(3,33)	1:A:155:THR:H	4:A:349:PX4:C35	14	0.32
(3,33)	1:A:155:THR:H	4:A:351:PX4:C35	14	0.32
(3,33)	1:A:155:THR:H	4:A:353:PX4:C35	14	0.32
(3,33)	1:A:155:THR:H	4:A:355:PX4:C35	14	0.32
(3,33)	1:A:155:THR:H	4:A:357:PX4:C35	14	0.32
(3,33)	1:A:155:THR:H	4:A:359:PX4:C35	14	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,33)	1:A:155:THR:H	4:A:361:PX4:C35	14	0.32
(3,33)	1:A:155:THR:H	4:A:363:PX4:C35	14	0.32
(3,33)	1:A:155:THR:H	4:A:402:PX4:C35	14	0.32
(3,33)	1:A:155:THR:H	4:A:404:PX4:C35	14	0.32
(3,33)	1:A:155:THR:H	4:A:406:PX4:C35	14	0.32
(3,33)	1:A:155:THR:H	4:A:408:PX4:C35	14	0.32
(3,33)	1:A:155:THR:H	4:A:410:PX4:C35	14	0.32
(3,33)	1:A:155:THR:H	4:A:412:PX4:C35	14	0.32
(3,33)	1:A:155:THR:H	4:A:414:PX4:C35	14	0.32
(3,33)	1:A:155:THR:H	4:A:416:PX4:C35	14	0.32
(3,33)	1:A:155:THR:H	4:A:418:PX4:C35	14	0.32
(3,33)	1:A:155:THR:H	4:A:420:PX4:C35	14	0.32
(3,33)	1:A:155:THR:H	4:A:422:PX4:C35	14	0.32
(3,33)	1:A:155:THR:H	4:A:424:PX4:C35	14	0.32
(3,33)	1:A:155:THR:H	4:A:426:PX4:C35	14	0.32
(3,33)	1:A:155:THR:H	4:A:428:PX4:C35	14	0.32
(3,33)	1:A:155:THR:H	4:A:430:PX4:C35	14	0.32
(2,985)	1:A:80:ASN:H	1:A:78:PHE:HD1	8	0.32
(2,975)	1:A:78:PHE:H	1:A:77:LEU:HD22	5	0.32
(2,975)	1:A:78:PHE:H	1:A:77:LEU:HD23	5	0.32
(2,975)	1:A:78:PHE:H	1:A:77:LEU:HD22	14	0.32
(2,975)	1:A:78:PHE:H	1:A:77:LEU:HD23	14	0.32
(2,919)	1:A:72:VAL:H	1:A:71:ASP:HA	12	0.32
(2,915)	1:A:71:ASP:H	1:A:72:VAL:HG21	12	0.32
(2,915)	1:A:71:ASP:H	1:A:72:VAL:HG22	12	0.32
(2,915)	1:A:71:ASP:H	1:A:72:VAL:HG23	12	0.32
(2,898)	1:A:66:ARG:H	1:A:63:GLN:HB3	1	0.32
(2,898)	1:A:66:ARG:H	1:A:63:GLN:HB2	1	0.32
(2,895)	1:A:64:LYS:H	1:A:64:LYS:HA	1	0.32
(2,895)	1:A:64:LYS:H	1:A:64:LYS:HA	11	0.32
(2,809)	1:A:136:ILE:H	1:A:94:VAL:HG11	7	0.32
(2,809)	1:A:136:ILE:H	1:A:94:VAL:HG12	7	0.32
(2,809)	1:A:136:ILE:H	1:A:94:VAL:HG13	7	0.32
(2,778)	1:A:61:ILE:HD13	1:A:48:LEU:HD22	16	0.32
(2,778)	1:A:61:ILE:HD13	1:A:48:LEU:HD23	16	0.32
(2,741)	1:A:114:ASN:H	1:A:113:LEU:HD21	3	0.32
(2,727)	1:A:211:VAL:HG11	1:A:226:LEU:HD21	13	0.32
(2,67)	1:A:53:MET:H	1:A:52:GLY:H	6	0.32
(2,64)	1:A:52:GLY:H	1:A:53:MET:H	6	0.32
(2,62)	1:A:50:ILE:HG12	1:A:50:ILE:H	1	0.32
(2,60)	1:A:50:ILE:H	1:A:50:ILE:HD11	3	0.32
(2,60)	1:A:50:ILE:H	1:A:50:ILE:HD12	3	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,60)	1:A:50:ILE:H	1:A:50:ILE:HD13	3	0.32
(2,543)	1:A:210:ALA:H	1:A:213:TYR:H	17	0.32
(2,517)	1:A:200:LEU:H	1:A:196:LEU:HD21	1	0.32
(2,489)	1:A:116:TRP:HE1	1:A:196:LEU:H	10	0.32
(2,425)	1:A:170:ALA:H	1:A:169:ASP:H	3	0.32
(2,275)	1:A:116:TRP:HE1	1:A:196:LEU:H	10	0.32
(2,239)	1:A:108:LEU:H	1:A:108:LEU:HD21	6	0.32
(2,125)	1:A:157:ALA:H	1:A:68:GLY:H	18	0.32
(2,961)	1:A:75:TYR:HD1	1:A:76:SER:H	1	0.31
(2,961)	1:A:75:TYR:HD2	1:A:76:SER:H	1	0.31
(2,953)	1:A:74:GLU:HB3	1:A:76:SER:H	7	0.31
(2,953)	1:A:74:GLU:HB3	1:A:76:SER:H	7	0.31
(2,951)	1:A:74:GLU:H	1:A:76:SER:H	13	0.31
(2,926)	1:A:72:VAL:HB	1:A:73:ALA:H	12	0.31
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG21	6	0.31
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG22	6	0.31
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG23	6	0.31
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG11	6	0.31
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG12	6	0.31
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG13	6	0.31
(2,920)	1:A:72:VAL:H	1:A:71:ASP:H	20	0.31
(2,920)	1:A:72:VAL:H	1:A:71:ASP:H	20	0.31
(2,917)	1:A:71:ASP:H	1:A:72:VAL:HB	2	0.31
(2,904)	1:A:67:CYS:H	1:A:67:CYS:HA	1	0.31
(2,903)	1:A:67:CYS:H	1:A:66:ARG:HA	7	0.31
(2,867)	1:A:186:ILE:HD11	1:A:156:LEU:HD21	9	0.31
(2,786)	1:A:24:LEU:H	1:A:24:LEU:HD21	20	0.31
(2,746)	1:A:89:VAL:HG11	1:A:122:LEU:HD21	16	0.31
(2,74)	1:A:55:ASN:H	1:A:55:ASN:HD21	2	0.31
(2,732)	1:A:211:VAL:HG13	1:A:226:LEU:HD22	6	0.31
(2,732)	1:A:211:VAL:HG13	1:A:226:LEU:HD23	6	0.31
(2,721)	1:A:113:LEU:HD11	1:A:196:LEU:HD21	2	0.31
(2,655)	1:A:16:GLN:HE21	1:A:16:GLN:HE22	2	0.31
(2,655)	1:A:16:GLN:HE21	1:A:16:GLN:HE22	8	0.31
(2,653)	1:A:11:GLN:HE22	1:A:11:GLN:HE21	4	0.31
(2,653)	1:A:11:GLN:HE22	1:A:11:GLN:HE21	12	0.31
(2,627)	1:A:13:GLU:H	1:A:10:LEU:H	2	0.31
(2,626)	1:A:12:TRP:H	1:A:10:LEU:H	12	0.31
(2,577)	1:A:231:ILE:HD11	1:A:226:LEU:H	19	0.31
(2,577)	1:A:231:ILE:HD12	1:A:226:LEU:H	19	0.31
(2,577)	1:A:231:ILE:HD13	1:A:226:LEU:H	19	0.31
(2,557)	1:A:21:ARG:H	1:A:23:TYR:H	8	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,489)	1:A:116:TRP:HE1	1:A:196:LEU:H	17	0.31
(2,424)	1:A:169:ASP:H	1:A:166:LEU:HB3	8	0.31
(2,423)	1:A:169:ASP:H	1:A:134:ILE:HD11	2	0.31
(2,423)	1:A:169:ASP:H	1:A:134:ILE:HD12	2	0.31
(2,423)	1:A:169:ASP:H	1:A:134:ILE:HD13	2	0.31
(2,423)	1:A:169:ASP:H	1:A:134:ILE:HD11	5	0.31
(2,423)	1:A:169:ASP:H	1:A:134:ILE:HD12	5	0.31
(2,423)	1:A:169:ASP:H	1:A:134:ILE:HD13	5	0.31
(2,414)	1:A:167:GLY:H	1:A:166:LEU:HD21	8	0.31
(2,410)	1:A:167:GLY:H	1:A:165:GLY:H	20	0.31
(2,388)	1:A:66:ARG:H	1:A:156:LEU:H	9	0.31
(2,369)	1:A:143:HIS:H	1:A:145:ASP:H	2	0.31
(2,357)	1:A:136:ILE:HD11	1:A:137:GLY:H	5	0.31
(2,357)	1:A:136:ILE:HD12	1:A:137:GLY:H	5	0.31
(2,357)	1:A:136:ILE:HD13	1:A:137:GLY:H	5	0.31
(2,275)	1:A:116:TRP:HE1	1:A:196:LEU:H	17	0.31
(2,265)	1:A:113:LEU:H	1:A:196:LEU:HD22	8	0.31
(2,265)	1:A:113:LEU:H	1:A:196:LEU:HD23	8	0.31
(2,228)	1:A:106:ASP:H	1:A:108:LEU:H	15	0.31
(2,207)	1:A:98:ARG:H	1:A:100:LEU:H	20	0.31
(2,120)	1:A:66:ARG:H	1:A:156:LEU:H	9	0.31
(2,103)	1:A:39:LEU:H	1:A:37:ALA:H	13	0.31
(2,982)	1:A:78:PHE:HD1	1:A:80:ASN:H	14	0.3
(2,975)	1:A:78:PHE:H	1:A:77:LEU:HD22	6	0.3
(2,975)	1:A:78:PHE:H	1:A:77:LEU:HD23	6	0.3
(2,973)	1:A:78:PHE:H	1:A:77:LEU:HD11	7	0.3
(2,973)	1:A:78:PHE:H	1:A:77:LEU:HD12	7	0.3
(2,973)	1:A:78:PHE:H	1:A:77:LEU:HD13	7	0.3
(2,969)	1:A:77:LEU:H	1:A:78:PHE:H	2	0.3
(2,964)	1:A:75:TYR:H	1:A:76:SER:H	3	0.3
(2,959)	1:A:75:TYR:H	1:A:76:SER:H	3	0.3
(2,951)	1:A:74:GLU:H	1:A:76:SER:H	12	0.3
(2,945)	1:A:74:GLU:H	1:A:74:GLU:HG3	9	0.3
(2,945)	1:A:74:GLU:H	1:A:74:GLU:HG3	9	0.3
(2,927)	1:A:72:VAL:H	1:A:73:ALA:H	1	0.3
(2,927)	1:A:72:VAL:H	1:A:73:ALA:H	1	0.3
(2,927)	1:A:72:VAL:H	1:A:73:ALA:H	19	0.3
(2,927)	1:A:72:VAL:H	1:A:73:ALA:H	19	0.3
(2,921)	1:A:72:VAL:H	1:A:72:VAL:HA	3	0.3
(2,919)	1:A:72:VAL:H	1:A:71:ASP:HA	19	0.3
(2,916)	1:A:71:ASP:H	1:A:72:VAL:HA	19	0.3
(2,912)	1:A:70:PRO:HB3	1:A:76:SER:H	12	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,912)	1:A:70:PRO:HB2	1:A:76:SER:H	12	0.3
(2,903)	1:A:67:CYS:H	1:A:66:ARG:HA	3	0.3
(2,890)	1:A:63:GLN:H	1:A:63:GLN:HG3	7	0.3
(2,890)	1:A:63:GLN:H	1:A:63:GLN:HG3	7	0.3
(2,759)	1:A:54:LEU:HD21	1:A:59:ILE:HD11	17	0.3
(2,759)	1:A:54:LEU:HD21	1:A:59:ILE:HD12	17	0.3
(2,759)	1:A:54:LEU:HD21	1:A:59:ILE:HD13	17	0.3
(2,755)	1:A:54:LEU:HD21	1:A:58:VAL:HG11	18	0.3
(2,755)	1:A:54:LEU:HD21	1:A:58:VAL:HG12	18	0.3
(2,755)	1:A:54:LEU:HD21	1:A:58:VAL:HG13	18	0.3
(2,680)	1:A:158:HIS:H	1:A:172:PHE:H	1	0.3
(2,673)	1:A:77:LEU:H	1:A:78:PHE:H	2	0.3
(2,653)	1:A:11:GLN:HE22	1:A:11:GLN:HE21	6	0.3
(2,626)	1:A:12:TRP:H	1:A:10:LEU:H	8	0.3
(2,608)	1:A:238:TYR:H	1:A:120:ILE:HD11	16	0.3
(2,608)	1:A:238:TYR:H	1:A:120:ILE:HD12	16	0.3
(2,608)	1:A:238:TYR:H	1:A:120:ILE:HD13	16	0.3
(2,587)	1:A:232:LYS:H	1:A:231:ILE:HD11	2	0.3
(2,587)	1:A:232:LYS:H	1:A:231:ILE:HD12	2	0.3
(2,587)	1:A:232:LYS:H	1:A:231:ILE:HD13	2	0.3
(2,504)	1:A:198:HIS:H	1:A:202:MET:H	4	0.3
(2,500)	1:A:116:TRP:HE1	1:A:198:HIS:H	4	0.3
(2,467)	1:A:84:TRP:H	1:A:200:LEU:HD22	18	0.3
(2,467)	1:A:84:TRP:H	1:A:200:LEU:HD23	18	0.3
(2,397)	1:A:169:ASP:H	1:A:160:PHE:H	10	0.3
(2,39)	1:A:43:GLN:HE21	1:A:43:GLN:HE22	4	0.3
(2,380)	1:A:10:LEU:H	1:A:10:LEU:HD22	10	0.3
(2,380)	1:A:10:LEU:H	1:A:10:LEU:HD23	10	0.3
(2,357)	1:A:136:ILE:HD11	1:A:137:GLY:H	6	0.3
(2,357)	1:A:136:ILE:HD12	1:A:137:GLY:H	6	0.3
(2,357)	1:A:136:ILE:HD13	1:A:137:GLY:H	6	0.3
(2,357)	1:A:136:ILE:HD11	1:A:137:GLY:H	12	0.3
(2,357)	1:A:136:ILE:HD12	1:A:137:GLY:H	12	0.3
(2,357)	1:A:136:ILE:HD13	1:A:137:GLY:H	12	0.3
(2,303)	1:A:122:LEU:H	1:A:120:ILE:HG13	8	0.3
(2,303)	1:A:122:LEU:H	1:A:120:ILE:HG12	8	0.3
(2,274)	1:A:116:TRP:HE1	1:A:197:GLY:H	5	0.3
(2,113)	1:A:25:TYR:H	1:A:26:ASP:H	8	0.3
(2,961)	1:A:75:TYR:HD1	1:A:76:SER:H	16	0.29
(2,961)	1:A:75:TYR:HD2	1:A:76:SER:H	16	0.29
(2,947)	1:A:74:GLU:HB3	1:A:75:TYR:H	17	0.29
(2,947)	1:A:74:GLU:HB3	1:A:75:TYR:H	17	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,930)	1:A:72:VAL:HG11	1:A:75:TYR:H	14	0.29
(2,930)	1:A:72:VAL:HG12	1:A:75:TYR:H	14	0.29
(2,930)	1:A:72:VAL:HG13	1:A:75:TYR:H	14	0.29
(2,927)	1:A:72:VAL:H	1:A:73:ALA:H	11	0.29
(2,927)	1:A:72:VAL:H	1:A:73:ALA:H	11	0.29
(2,927)	1:A:72:VAL:H	1:A:73:ALA:H	16	0.29
(2,927)	1:A:72:VAL:H	1:A:73:ALA:H	16	0.29
(2,919)	1:A:72:VAL:H	1:A:71:ASP:HA	6	0.29
(2,919)	1:A:72:VAL:H	1:A:71:ASP:HA	15	0.29
(2,903)	1:A:67:CYS:H	1:A:66:ARG:HA	12	0.29
(2,898)	1:A:66:ARG:H	1:A:63:GLN:HB3	10	0.29
(2,898)	1:A:66:ARG:H	1:A:63:GLN:HB2	10	0.29
(2,896)	1:A:64:LYS:H	1:A:64:LYS:HE3	5	0.29
(2,896)	1:A:64:LYS:H	1:A:64:LYS:HE3	5	0.29
(2,896)	1:A:64:LYS:H	1:A:64:LYS:HE3	16	0.29
(2,896)	1:A:64:LYS:H	1:A:64:LYS:HE3	16	0.29
(2,895)	1:A:64:LYS:H	1:A:64:LYS:HA	3	0.29
(2,895)	1:A:64:LYS:H	1:A:64:LYS:HA	17	0.29
(2,810)	1:A:93:ILE:H	1:A:94:VAL:HG11	3	0.29
(2,810)	1:A:93:ILE:H	1:A:94:VAL:HG12	3	0.29
(2,810)	1:A:93:ILE:H	1:A:94:VAL:HG13	3	0.29
(2,810)	1:A:93:ILE:H	1:A:94:VAL:HG11	12	0.29
(2,810)	1:A:93:ILE:H	1:A:94:VAL:HG12	12	0.29
(2,810)	1:A:93:ILE:H	1:A:94:VAL:HG13	12	0.29
(2,810)	1:A:93:ILE:H	1:A:94:VAL:HG11	15	0.29
(2,810)	1:A:93:ILE:H	1:A:94:VAL:HG12	15	0.29
(2,810)	1:A:93:ILE:H	1:A:94:VAL:HG13	15	0.29
(2,809)	1:A:136:ILE:H	1:A:94:VAL:HG11	3	0.29
(2,809)	1:A:136:ILE:H	1:A:94:VAL:HG12	3	0.29
(2,809)	1:A:136:ILE:H	1:A:94:VAL:HG13	3	0.29
(2,788)	1:A:58:VAL:HG11	1:A:39:LEU:HD21	9	0.29
(2,75)	1:A:55:ASN:H	1:A:59:ILE:H	14	0.29
(2,713)	1:A:105:VAL:HG21	1:A:100:LEU:H	4	0.29
(2,713)	1:A:105:VAL:HG22	1:A:100:LEU:H	4	0.29
(2,713)	1:A:105:VAL:HG23	1:A:100:LEU:H	4	0.29
(2,655)	1:A:16:GLN:HE21	1:A:16:GLN:HE22	5	0.29
(2,655)	1:A:16:GLN:HE21	1:A:16:GLN:HE22	11	0.29
(2,653)	1:A:11:GLN:HE22	1:A:11:GLN:HE21	8	0.29
(2,621)	1:A:200:LEU:HD21	1:A:201:GLY:H	7	0.29
(2,568)	1:A:235:GLN:H	1:A:233:GLY:H	3	0.29
(2,557)	1:A:21:ARG:H	1:A:23:TYR:H	1	0.29
(2,557)	1:A:21:ARG:H	1:A:23:TYR:H	11	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,557)	1:A:21:ARG:H	1:A:23:TYR:H	15	0.29
(2,538)	1:A:205:SER:H	1:A:213:TYR:H	13	0.29
(2,39)	1:A:43:GLN:HE21	1:A:43:GLN:HE22	1	0.29
(2,388)	1:A:66:ARG:H	1:A:156:LEU:H	12	0.29
(2,381)	1:A:151:GLY:H	1:A:150:ASP:H	12	0.29
(2,368)	1:A:151:GLY:H	1:A:150:ASP:H	12	0.29
(2,357)	1:A:136:ILE:HD11	1:A:137:GLY:H	4	0.29
(2,357)	1:A:136:ILE:HD12	1:A:137:GLY:H	4	0.29
(2,357)	1:A:136:ILE:HD13	1:A:137:GLY:H	4	0.29
(2,335)	1:A:133:ASP:H	1:A:127:VAL:HG11	10	0.29
(2,335)	1:A:133:ASP:H	1:A:127:VAL:HG12	10	0.29
(2,335)	1:A:133:ASP:H	1:A:127:VAL:HG13	10	0.29
(2,302)	1:A:120:ILE:HG21	1:A:122:LEU:H	9	0.29
(2,302)	1:A:120:ILE:HG22	1:A:122:LEU:H	9	0.29
(2,302)	1:A:120:ILE:HG23	1:A:122:LEU:H	9	0.29
(2,228)	1:A:106:ASP:H	1:A:108:LEU:H	11	0.29
(2,226)	1:A:104:THR:H	1:A:106:ASP:H	19	0.29
(2,212)	1:A:120:ILE:HD11	1:A:237:LEU:H	20	0.29
(2,212)	1:A:120:ILE:HD12	1:A:237:LEU:H	20	0.29
(2,212)	1:A:120:ILE:HD13	1:A:237:LEU:H	20	0.29
(2,209)	1:A:105:VAL:HG21	1:A:100:LEU:H	4	0.29
(2,209)	1:A:105:VAL:HG22	1:A:100:LEU:H	4	0.29
(2,209)	1:A:105:VAL:HG23	1:A:100:LEU:H	4	0.29
(2,120)	1:A:66:ARG:H	1:A:156:LEU:H	12	0.29
(2,103)	1:A:39:LEU:H	1:A:37:ALA:H	7	0.29
(2,945)	1:A:74:GLU:H	1:A:74:GLU:HG3	5	0.28
(2,945)	1:A:74:GLU:H	1:A:74:GLU:HG3	5	0.28
(2,927)	1:A:72:VAL:H	1:A:73:ALA:H	12	0.28
(2,927)	1:A:72:VAL:H	1:A:73:ALA:H	12	0.28
(2,926)	1:A:72:VAL:HB	1:A:73:ALA:H	3	0.28
(2,919)	1:A:72:VAL:H	1:A:71:ASP:HA	3	0.28
(2,918)	1:A:72:VAL:H	1:A:70:PRO:HB3	5	0.28
(2,918)	1:A:72:VAL:H	1:A:70:PRO:HB2	5	0.28
(2,918)	1:A:72:VAL:H	1:A:70:PRO:HB3	5	0.28
(2,918)	1:A:72:VAL:H	1:A:70:PRO:HB2	5	0.28
(2,915)	1:A:71:ASP:H	1:A:72:VAL:HG21	19	0.28
(2,915)	1:A:71:ASP:H	1:A:72:VAL:HG22	19	0.28
(2,915)	1:A:71:ASP:H	1:A:72:VAL:HG23	19	0.28
(2,895)	1:A:64:LYS:H	1:A:64:LYS:HA	12	0.28
(2,895)	1:A:64:LYS:H	1:A:64:LYS:HA	13	0.28
(2,857)	1:A:186:ILE:HD11	1:A:156:LEU:HD21	8	0.28
(2,845)	1:A:200:LEU:HD22	1:A:122:LEU:HD22	9	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,845)	1:A:200:LEU:HD22	1:A:122:LEU:HD23	9	0.28
(2,791)	1:A:58:VAL:HG12	1:A:39:LEU:HD22	20	0.28
(2,791)	1:A:58:VAL:HG12	1:A:39:LEU:HD23	20	0.28
(2,74)	1:A:55:ASN:H	1:A:55:ASN:HD21	1	0.28
(2,727)	1:A:211:VAL:HG11	1:A:226:LEU:HD21	8	0.28
(2,655)	1:A:16:GLN:HE21	1:A:16:GLN:HE22	15	0.28
(2,653)	1:A:11:GLN:HE22	1:A:11:GLN:HE21	10	0.28
(2,653)	1:A:11:GLN:HE22	1:A:11:GLN:HE21	14	0.28
(2,538)	1:A:205:SER:H	1:A:213:TYR:H	4	0.28
(2,504)	1:A:198:HIS:H	1:A:202:MET:H	10	0.28
(2,426)	1:A:170:ALA:H	1:A:136:ILE:HD11	11	0.28
(2,426)	1:A:170:ALA:H	1:A:136:ILE:HD12	11	0.28
(2,426)	1:A:170:ALA:H	1:A:136:ILE:HD13	11	0.28
(2,423)	1:A:169:ASP:H	1:A:134:ILE:HD11	11	0.28
(2,423)	1:A:169:ASP:H	1:A:134:ILE:HD12	11	0.28
(2,423)	1:A:169:ASP:H	1:A:134:ILE:HD13	11	0.28
(2,39)	1:A:43:GLN:HE21	1:A:43:GLN:HE22	3	0.28
(2,39)	1:A:43:GLN:HE21	1:A:43:GLN:HE22	9	0.28
(2,39)	1:A:43:GLN:HE21	1:A:43:GLN:HE22	20	0.28
(2,381)	1:A:151:GLY:H	1:A:150:ASP:H	17	0.28
(2,368)	1:A:151:GLY:H	1:A:150:ASP:H	17	0.28
(2,357)	1:A:136:ILE:HD11	1:A:137:GLY:H	10	0.28
(2,357)	1:A:136:ILE:HD12	1:A:137:GLY:H	10	0.28
(2,357)	1:A:136:ILE:HD13	1:A:137:GLY:H	10	0.28
(2,305)	1:A:123:HIS:H	1:A:122:LEU:HD21	7	0.28
(2,207)	1:A:98:ARG:H	1:A:100:LEU:H	15	0.28
(2,113)	1:A:25:TYR:H	1:A:26:ASP:H	20	0.28
(2,969)	1:A:77:LEU:H	1:A:78:PHE:H	8	0.27
(2,968)	1:A:77:LEU:H	1:A:77:LEU:HA	1	0.27
(2,968)	1:A:77:LEU:H	1:A:77:LEU:HA	17	0.27
(2,966)	1:A:77:LEU:H	1:A:77:LEU:HB3	18	0.27
(2,966)	1:A:77:LEU:H	1:A:77:LEU:HB3	18	0.27
(2,961)	1:A:75:TYR:HD1	1:A:76:SER:H	8	0.27
(2,961)	1:A:75:TYR:HD2	1:A:76:SER:H	8	0.27
(2,961)	1:A:75:TYR:HD1	1:A:76:SER:H	17	0.27
(2,961)	1:A:75:TYR:HD2	1:A:76:SER:H	17	0.27
(2,953)	1:A:74:GLU:HB3	1:A:76:SER:H	10	0.27
(2,953)	1:A:74:GLU:HB3	1:A:76:SER:H	10	0.27
(2,949)	1:A:74:GLU:H	1:A:75:TYR:H	12	0.27
(2,926)	1:A:72:VAL:HB	1:A:73:ALA:H	4	0.27
(2,919)	1:A:72:VAL:H	1:A:71:ASP:HA	5	0.27
(2,917)	1:A:71:ASP:H	1:A:72:VAL:HB	20	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,885)	1:A:134:ILE:HD11	1:A:89:VAL:HG11	15	0.27
(2,885)	1:A:134:ILE:HD11	1:A:89:VAL:HG12	15	0.27
(2,885)	1:A:134:ILE:HD11	1:A:89:VAL:HG13	15	0.27
(2,885)	1:A:134:ILE:HD12	1:A:89:VAL:HG11	15	0.27
(2,885)	1:A:134:ILE:HD12	1:A:89:VAL:HG12	15	0.27
(2,885)	1:A:134:ILE:HD12	1:A:89:VAL:HG13	15	0.27
(2,885)	1:A:134:ILE:HD13	1:A:89:VAL:HG11	15	0.27
(2,885)	1:A:134:ILE:HD13	1:A:89:VAL:HG12	15	0.27
(2,885)	1:A:134:ILE:HD13	1:A:89:VAL:HG13	15	0.27
(2,809)	1:A:136:ILE:H	1:A:94:VAL:HG11	6	0.27
(2,809)	1:A:136:ILE:H	1:A:94:VAL:HG12	6	0.27
(2,809)	1:A:136:ILE:H	1:A:94:VAL:HG13	6	0.27
(2,809)	1:A:136:ILE:H	1:A:94:VAL:HG11	8	0.27
(2,809)	1:A:136:ILE:H	1:A:94:VAL:HG12	8	0.27
(2,809)	1:A:136:ILE:H	1:A:94:VAL:HG13	8	0.27
(2,755)	1:A:54:LEU:HD21	1:A:58:VAL:HG11	7	0.27
(2,755)	1:A:54:LEU:HD21	1:A:58:VAL:HG12	7	0.27
(2,755)	1:A:54:LEU:HD21	1:A:58:VAL:HG13	7	0.27
(2,744)	1:A:134:ILE:HD11	1:A:89:VAL:HG11	15	0.27
(2,744)	1:A:134:ILE:HD11	1:A:89:VAL:HG12	15	0.27
(2,744)	1:A:134:ILE:HD11	1:A:89:VAL:HG13	15	0.27
(2,744)	1:A:134:ILE:HD12	1:A:89:VAL:HG11	15	0.27
(2,744)	1:A:134:ILE:HD12	1:A:89:VAL:HG12	15	0.27
(2,744)	1:A:134:ILE:HD12	1:A:89:VAL:HG13	15	0.27
(2,744)	1:A:134:ILE:HD13	1:A:89:VAL:HG11	15	0.27
(2,744)	1:A:134:ILE:HD13	1:A:89:VAL:HG12	15	0.27
(2,744)	1:A:134:ILE:HD13	1:A:89:VAL:HG13	15	0.27
(2,74)	1:A:55:ASN:H	1:A:55:ASN:HD21	16	0.27
(2,71)	1:A:55:ASN:H	1:A:54:LEU:HD21	13	0.27
(2,693)	1:A:11:GLN:H	1:A:8:SER:H	19	0.27
(2,680)	1:A:158:HIS:H	1:A:172:PHE:H	18	0.27
(2,673)	1:A:77:LEU:H	1:A:78:PHE:H	8	0.27
(2,655)	1:A:16:GLN:HE21	1:A:16:GLN:HE22	1	0.27
(2,655)	1:A:16:GLN:HE21	1:A:16:GLN:HE22	3	0.27
(2,655)	1:A:16:GLN:HE21	1:A:16:GLN:HE22	6	0.27
(2,655)	1:A:16:GLN:HE21	1:A:16:GLN:HE22	7	0.27
(2,653)	1:A:11:GLN:HE22	1:A:11:GLN:HE21	18	0.27
(2,63)	1:A:52:GLY:H	1:A:51:THR:H	16	0.27
(2,624)	1:A:11:GLN:H	1:A:8:SER:H	19	0.27
(2,547)	1:A:211:VAL:H	1:A:211:VAL:HG11	4	0.27
(2,547)	1:A:211:VAL:H	1:A:211:VAL:HG12	4	0.27
(2,547)	1:A:211:VAL:H	1:A:211:VAL:HG13	4	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,547)	1:A:211:VAL:H	1:A:211:VAL:HG21	4	0.27
(2,547)	1:A:211:VAL:H	1:A:211:VAL:HG22	4	0.27
(2,547)	1:A:211:VAL:H	1:A:211:VAL:HG23	4	0.27
(2,538)	1:A:205:SER:H	1:A:213:TYR:H	1	0.27
(2,511)	1:A:200:LEU:HD22	1:A:199:SER:H	5	0.27
(2,511)	1:A:200:LEU:HD23	1:A:199:SER:H	5	0.27
(2,500)	1:A:116:TRP:HE1	1:A:198:HIS:H	3	0.27
(2,453)	1:A:178:TRP:HE1	1:A:175:ASP:H	14	0.27
(2,442)	1:A:175:ASP:H	1:A:178:TRP:HE1	14	0.27
(2,39)	1:A:43:GLN:HE21	1:A:43:GLN:HE22	7	0.27
(2,39)	1:A:43:GLN:HE21	1:A:43:GLN:HE22	16	0.27
(2,378)	1:A:10:LEU:H	1:A:10:LEU:HD11	20	0.27
(2,378)	1:A:10:LEU:H	1:A:10:LEU:HD12	20	0.27
(2,378)	1:A:10:LEU:H	1:A:10:LEU:HD13	20	0.27
(2,357)	1:A:136:ILE:HD11	1:A:137:GLY:H	7	0.27
(2,357)	1:A:136:ILE:HD12	1:A:137:GLY:H	7	0.27
(2,357)	1:A:136:ILE:HD13	1:A:137:GLY:H	7	0.27
(2,321)	1:A:128:VAL:HG11	1:A:126:LYS:H	3	0.27
(2,321)	1:A:128:VAL:HG12	1:A:126:LYS:H	3	0.27
(2,321)	1:A:128:VAL:HG13	1:A:126:LYS:H	3	0.27
(2,315)	1:A:125:ARG:H	1:A:126:LYS:H	2	0.27
(2,305)	1:A:123:HIS:H	1:A:122:LEU:HD21	15	0.27
(2,228)	1:A:106:ASP:H	1:A:108:LEU:H	14	0.27
(2,207)	1:A:98:ARG:H	1:A:100:LEU:H	14	0.27
(2,185)	1:A:94:VAL:H	1:A:92:ARG:H	9	0.27
(2,103)	1:A:39:LEU:H	1:A:37:ALA:H	2	0.27
(2,103)	1:A:39:LEU:H	1:A:37:ALA:H	15	0.27
(2,980)	1:A:78:PHE:H	1:A:79:PRO:HD3	7	0.26
(2,980)	1:A:78:PHE:H	1:A:79:PRO:HD3	7	0.26
(2,969)	1:A:77:LEU:H	1:A:78:PHE:H	1	0.26
(2,968)	1:A:77:LEU:H	1:A:77:LEU:HA	5	0.26
(2,947)	1:A:74:GLU:HB3	1:A:75:TYR:H	12	0.26
(2,947)	1:A:74:GLU:HB3	1:A:75:TYR:H	12	0.26
(2,926)	1:A:72:VAL:HB	1:A:73:ALA:H	6	0.26
(2,921)	1:A:72:VAL:H	1:A:72:VAL:HA	17	0.26
(2,920)	1:A:72:VAL:H	1:A:71:ASP:H	2	0.26
(2,920)	1:A:72:VAL:H	1:A:71:ASP:H	2	0.26
(2,920)	1:A:72:VAL:H	1:A:71:ASP:H	9	0.26
(2,920)	1:A:72:VAL:H	1:A:71:ASP:H	9	0.26
(2,916)	1:A:71:ASP:H	1:A:72:VAL:HA	1	0.26
(2,898)	1:A:66:ARG:H	1:A:63:GLN:HB3	2	0.26
(2,898)	1:A:66:ARG:H	1:A:63:GLN:HB2	2	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,792)	1:A:58:VAL:HG13	1:A:39:LEU:HD21	6	0.26
(2,764)	1:A:120:ILE:HD11	1:A:122:LEU:H	13	0.26
(2,764)	1:A:120:ILE:HD12	1:A:122:LEU:H	13	0.26
(2,764)	1:A:120:ILE:HD13	1:A:122:LEU:H	13	0.26
(2,764)	1:A:120:ILE:HD11	1:A:122:LEU:H	14	0.26
(2,764)	1:A:120:ILE:HD12	1:A:122:LEU:H	14	0.26
(2,764)	1:A:120:ILE:HD13	1:A:122:LEU:H	14	0.26
(2,758)	1:A:54:LEU:HD22	1:A:39:LEU:HD11	12	0.26
(2,758)	1:A:54:LEU:HD22	1:A:39:LEU:HD12	12	0.26
(2,758)	1:A:54:LEU:HD22	1:A:39:LEU:HD13	12	0.26
(2,758)	1:A:54:LEU:HD23	1:A:39:LEU:HD11	12	0.26
(2,758)	1:A:54:LEU:HD23	1:A:39:LEU:HD12	12	0.26
(2,758)	1:A:54:LEU:HD23	1:A:39:LEU:HD13	12	0.26
(2,74)	1:A:55:ASN:H	1:A:55:ASN:HD21	15	0.26
(2,673)	1:A:77:LEU:H	1:A:78:PHE:H	1	0.26
(2,653)	1:A:11:GLN:HE22	1:A:11:GLN:HE21	1	0.26
(2,626)	1:A:12:TRP:H	1:A:10:LEU:H	3	0.26
(2,626)	1:A:12:TRP:H	1:A:10:LEU:H	13	0.26
(2,626)	1:A:12:TRP:H	1:A:10:LEU:H	14	0.26
(2,62)	1:A:50:ILE:HG12	1:A:50:ILE:H	14	0.26
(2,608)	1:A:238:TYR:H	1:A:120:ILE:HD11	2	0.26
(2,608)	1:A:238:TYR:H	1:A:120:ILE:HD12	2	0.26
(2,608)	1:A:238:TYR:H	1:A:120:ILE:HD13	2	0.26
(2,608)	1:A:238:TYR:H	1:A:120:ILE:HD11	19	0.26
(2,608)	1:A:238:TYR:H	1:A:120:ILE:HD12	19	0.26
(2,608)	1:A:238:TYR:H	1:A:120:ILE:HD13	19	0.26
(2,579)	1:A:227:SER:H	1:A:230:ASP:H	17	0.26
(2,557)	1:A:21:ARG:H	1:A:23:TYR:H	4	0.26
(2,543)	1:A:210:ALA:H	1:A:213:TYR:H	7	0.26
(2,503)	1:A:198:HIS:H	1:A:201:GLY:H	4	0.26
(2,489)	1:A:116:TRP:HE1	1:A:196:LEU:H	5	0.26
(2,467)	1:A:84:TRP:H	1:A:200:LEU:HD22	11	0.26
(2,467)	1:A:84:TRP:H	1:A:200:LEU:HD23	11	0.26
(2,454)	1:A:178:TRP:HE1	1:A:178:TRP:H	2	0.26
(2,39)	1:A:43:GLN:HE21	1:A:43:GLN:HE22	2	0.26
(2,381)	1:A:151:GLY:H	1:A:150:ASP:H	13	0.26
(2,368)	1:A:151:GLY:H	1:A:150:ASP:H	13	0.26
(2,316)	1:A:125:ARG:H	1:A:89:VAL:H	19	0.26
(2,315)	1:A:125:ARG:H	1:A:126:LYS:H	13	0.26
(2,315)	1:A:125:ARG:H	1:A:126:LYS:H	16	0.26
(2,303)	1:A:122:LEU:H	1:A:120:ILE:HG13	19	0.26
(2,303)	1:A:122:LEU:H	1:A:120:ILE:HG12	19	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,301)	1:A:120:ILE:HD11	1:A:122:LEU:H	13	0.26
(2,301)	1:A:120:ILE:HD12	1:A:122:LEU:H	13	0.26
(2,301)	1:A:120:ILE:HD13	1:A:122:LEU:H	13	0.26
(2,301)	1:A:120:ILE:HD11	1:A:122:LEU:H	14	0.26
(2,301)	1:A:120:ILE:HD12	1:A:122:LEU:H	14	0.26
(2,301)	1:A:120:ILE:HD13	1:A:122:LEU:H	14	0.26
(2,275)	1:A:116:TRP:HE1	1:A:196:LEU:H	5	0.26
(2,22)	1:A:227:SER:H	1:A:230:ASP:H	17	0.26
(2,162)	1:A:125:ARG:H	1:A:89:VAL:H	19	0.26
(2,977)	1:A:78:PHE:H	1:A:78:PHE:HA	12	0.25
(2,968)	1:A:77:LEU:H	1:A:77:LEU:HA	19	0.25
(2,947)	1:A:74:GLU:HB3	1:A:75:TYR:H	20	0.25
(2,947)	1:A:74:GLU:HB3	1:A:75:TYR:H	20	0.25
(2,920)	1:A:72:VAL:H	1:A:71:ASP:H	8	0.25
(2,920)	1:A:72:VAL:H	1:A:71:ASP:H	8	0.25
(2,917)	1:A:71:ASP:H	1:A:72:VAL:HB	6	0.25
(2,916)	1:A:71:ASP:H	1:A:72:VAL:HA	12	0.25
(2,834)	1:A:120:ILE:HD12	1:A:200:LEU:HD21	12	0.25
(2,810)	1:A:93:ILE:H	1:A:94:VAL:HG11	9	0.25
(2,810)	1:A:93:ILE:H	1:A:94:VAL:HG12	9	0.25
(2,810)	1:A:93:ILE:H	1:A:94:VAL:HG13	9	0.25
(2,809)	1:A:136:ILE:H	1:A:94:VAL:HG11	5	0.25
(2,809)	1:A:136:ILE:H	1:A:94:VAL:HG12	5	0.25
(2,809)	1:A:136:ILE:H	1:A:94:VAL:HG13	5	0.25
(2,788)	1:A:58:VAL:HG11	1:A:39:LEU:HD21	1	0.25
(2,777)	1:A:61:ILE:HD13	1:A:48:LEU:HD21	14	0.25
(2,759)	1:A:54:LEU:HD21	1:A:59:ILE:HD11	20	0.25
(2,759)	1:A:54:LEU:HD21	1:A:59:ILE:HD12	20	0.25
(2,759)	1:A:54:LEU:HD21	1:A:59:ILE:HD13	20	0.25
(2,733)	1:A:196:LEU:HD21	1:A:113:LEU:HD21	10	0.25
(2,717)	1:A:54:LEU:HD11	1:A:39:LEU:HD11	4	0.25
(2,717)	1:A:54:LEU:HD11	1:A:39:LEU:HD12	4	0.25
(2,717)	1:A:54:LEU:HD11	1:A:39:LEU:HD13	4	0.25
(2,717)	1:A:54:LEU:HD12	1:A:39:LEU:HD11	4	0.25
(2,717)	1:A:54:LEU:HD12	1:A:39:LEU:HD12	4	0.25
(2,717)	1:A:54:LEU:HD12	1:A:39:LEU:HD13	4	0.25
(2,717)	1:A:54:LEU:HD13	1:A:39:LEU:HD11	4	0.25
(2,717)	1:A:54:LEU:HD13	1:A:39:LEU:HD12	4	0.25
(2,717)	1:A:54:LEU:HD13	1:A:39:LEU:HD13	4	0.25
(2,708)	1:A:226:LEU:HD11	1:A:231:ILE:HG13	6	0.25
(2,708)	1:A:226:LEU:HD12	1:A:231:ILE:HG13	6	0.25
(2,708)	1:A:226:LEU:HD13	1:A:231:ILE:HG13	6	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,708)	1:A:226:LEU:HD11	1:A:231:ILE:HG12	6	0.25
(2,708)	1:A:226:LEU:HD12	1:A:231:ILE:HG12	6	0.25
(2,708)	1:A:226:LEU:HD13	1:A:231:ILE:HG12	6	0.25
(2,680)	1:A:158:HIS:H	1:A:172:PHE:H	20	0.25
(2,655)	1:A:16:GLN:HE21	1:A:16:GLN:HE22	16	0.25
(2,653)	1:A:11:GLN:HE22	1:A:11:GLN:HE21	5	0.25
(2,653)	1:A:11:GLN:HE22	1:A:11:GLN:HE21	20	0.25
(2,62)	1:A:50:ILE:HG12	1:A:50:ILE:H	8	0.25
(2,60)	1:A:50:ILE:H	1:A:50:ILE:HD11	15	0.25
(2,60)	1:A:50:ILE:H	1:A:50:ILE:HD12	15	0.25
(2,60)	1:A:50:ILE:H	1:A:50:ILE:HD13	15	0.25
(2,564)	1:A:231:ILE:H	1:A:231:ILE:HG13	16	0.25
(2,564)	1:A:231:ILE:H	1:A:231:ILE:HG12	16	0.25
(2,557)	1:A:21:ARG:H	1:A:23:TYR:H	16	0.25
(2,543)	1:A:210:ALA:H	1:A:213:TYR:H	6	0.25
(2,511)	1:A:200:LEU:HD22	1:A:199:SER:H	8	0.25
(2,511)	1:A:200:LEU:HD23	1:A:199:SER:H	8	0.25
(2,499)	1:A:197:GLY:H	1:A:198:HIS:H	16	0.25
(2,499)	1:A:197:GLY:H	1:A:198:HIS:H	16	0.25
(2,473)	1:A:186:ILE:H	1:A:156:LEU:HD22	18	0.25
(2,473)	1:A:186:ILE:H	1:A:156:LEU:HD23	18	0.25
(2,467)	1:A:84:TRP:H	1:A:200:LEU:HD22	12	0.25
(2,467)	1:A:84:TRP:H	1:A:200:LEU:HD23	12	0.25
(2,462)	1:A:182:SER:H	1:A:181:GLY:H	19	0.25
(2,462)	1:A:182:SER:H	1:A:181:GLY:H	19	0.25
(2,454)	1:A:178:TRP:HE1	1:A:178:TRP:H	3	0.25
(2,423)	1:A:169:ASP:H	1:A:134:ILE:HD11	9	0.25
(2,423)	1:A:169:ASP:H	1:A:134:ILE:HD12	9	0.25
(2,423)	1:A:169:ASP:H	1:A:134:ILE:HD13	9	0.25
(2,39)	1:A:43:GLN:HE21	1:A:43:GLN:HE22	5	0.25
(2,381)	1:A:151:GLY:H	1:A:150:ASP:H	7	0.25
(2,368)	1:A:151:GLY:H	1:A:150:ASP:H	7	0.25
(2,315)	1:A:125:ARG:H	1:A:126:LYS:H	3	0.25
(2,315)	1:A:125:ARG:H	1:A:126:LYS:H	7	0.25
(2,303)	1:A:122:LEU:H	1:A:120:ILE:HG13	7	0.25
(2,303)	1:A:122:LEU:H	1:A:120:ILE:HG12	7	0.25
(2,257)	1:A:112:ALA:H	1:A:189:LEU:HD21	2	0.25
(2,228)	1:A:106:ASP:H	1:A:108:LEU:H	12	0.25
(2,215)	1:A:103:ILE:H	1:A:103:ILE:HG13	7	0.25
(2,215)	1:A:103:ILE:H	1:A:103:ILE:HG12	7	0.25
(2,113)	1:A:25:TYR:H	1:A:26:ASP:H	13	0.25
(2,977)	1:A:78:PHE:H	1:A:78:PHE:HA	16	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,968)	1:A:77:LEU:H	1:A:77:LEU:HA	11	0.24
(2,945)	1:A:74:GLU:H	1:A:74:GLU:HG3	3	0.24
(2,945)	1:A:74:GLU:H	1:A:74:GLU:HG3	3	0.24
(2,927)	1:A:72:VAL:H	1:A:73:ALA:H	2	0.24
(2,927)	1:A:72:VAL:H	1:A:73:ALA:H	2	0.24
(2,927)	1:A:72:VAL:H	1:A:73:ALA:H	10	0.24
(2,927)	1:A:72:VAL:H	1:A:73:ALA:H	10	0.24
(2,926)	1:A:72:VAL:HB	1:A:73:ALA:H	1	0.24
(2,912)	1:A:70:PRO:HB3	1:A:76:SER:H	17	0.24
(2,912)	1:A:70:PRO:HB2	1:A:76:SER:H	17	0.24
(2,909)	1:A:69:VAL:H	1:A:69:VAL:HA	14	0.24
(2,901)	1:A:66:ARG:H	1:A:66:ARG:HB3	8	0.24
(2,901)	1:A:66:ARG:H	1:A:66:ARG:HB3	8	0.24
(2,857)	1:A:186:ILE:HD11	1:A:156:LEU:HD21	12	0.24
(2,755)	1:A:54:LEU:HD21	1:A:58:VAL:HG11	8	0.24
(2,755)	1:A:54:LEU:HD21	1:A:58:VAL:HG12	8	0.24
(2,755)	1:A:54:LEU:HD21	1:A:58:VAL:HG13	8	0.24
(2,683)	1:A:179:THR:HG21	1:A:185:GLY:H	8	0.24
(2,683)	1:A:179:THR:HG22	1:A:185:GLY:H	8	0.24
(2,683)	1:A:179:THR:HG23	1:A:185:GLY:H	8	0.24
(2,680)	1:A:158:HIS:H	1:A:172:PHE:H	9	0.24
(2,671)	1:A:66:ARG:H	1:A:156:LEU:HD21	15	0.24
(2,655)	1:A:16:GLN:HE21	1:A:16:GLN:HE22	4	0.24
(2,655)	1:A:16:GLN:HE21	1:A:16:GLN:HE22	19	0.24
(2,655)	1:A:16:GLN:HE21	1:A:16:GLN:HE22	20	0.24
(2,653)	1:A:11:GLN:HE22	1:A:11:GLN:HE21	7	0.24
(2,653)	1:A:11:GLN:HE22	1:A:11:GLN:HE21	11	0.24
(2,653)	1:A:11:GLN:HE22	1:A:11:GLN:HE21	16	0.24
(2,558)	1:A:23:TYR:H	1:A:24:LEU:H	5	0.24
(2,533)	1:A:23:TYR:H	1:A:24:LEU:H	5	0.24
(2,391)	1:A:157:ALA:H	1:A:156:LEU:H	10	0.24
(2,39)	1:A:43:GLN:HE21	1:A:43:GLN:HE22	8	0.24
(2,385)	1:A:157:ALA:H	1:A:156:LEU:H	10	0.24
(2,357)	1:A:136:ILE:HD11	1:A:137:GLY:H	3	0.24
(2,357)	1:A:136:ILE:HD12	1:A:137:GLY:H	3	0.24
(2,357)	1:A:136:ILE:HD13	1:A:137:GLY:H	3	0.24
(2,357)	1:A:136:ILE:HD11	1:A:137:GLY:H	16	0.24
(2,357)	1:A:136:ILE:HD12	1:A:137:GLY:H	16	0.24
(2,357)	1:A:136:ILE:HD13	1:A:137:GLY:H	16	0.24
(2,317)	1:A:125:ARG:H	1:A:91:TYR:H	1	0.24
(2,228)	1:A:106:ASP:H	1:A:108:LEU:H	5	0.24
(2,14)	1:A:159:ALA:H	1:A:171:HIS:H	1	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,14)	1:A:159:ALA:H	1:A:171:HIS:H	3	0.24
(2,113)	1:A:25:TYR:H	1:A:26:ASP:H	1	0.24
(3,35)	1:A:194:HIS:H	4:A:305:PX4:C35	3	0.23
(3,35)	1:A:194:HIS:H	4:A:307:PX4:C35	3	0.23
(3,35)	1:A:194:HIS:H	4:A:309:PX4:C35	3	0.23
(3,35)	1:A:194:HIS:H	4:A:311:PX4:C35	3	0.23
(3,35)	1:A:194:HIS:H	4:A:313:PX4:C35	3	0.23
(3,35)	1:A:194:HIS:H	4:A:315:PX4:C35	3	0.23
(3,35)	1:A:194:HIS:H	4:A:317:PX4:C35	3	0.23
(3,35)	1:A:194:HIS:H	4:A:319:PX4:C35	3	0.23
(3,35)	1:A:194:HIS:H	4:A:321:PX4:C35	3	0.23
(3,35)	1:A:194:HIS:H	4:A:323:PX4:C35	3	0.23
(3,35)	1:A:194:HIS:H	4:A:325:PX4:C35	3	0.23
(3,35)	1:A:194:HIS:H	4:A:327:PX4:C35	3	0.23
(3,35)	1:A:194:HIS:H	4:A:329:PX4:C35	3	0.23
(3,35)	1:A:194:HIS:H	4:A:331:PX4:C35	3	0.23
(3,35)	1:A:194:HIS:H	4:A:333:PX4:C35	3	0.23
(3,35)	1:A:194:HIS:H	4:A:335:PX4:C35	3	0.23
(3,35)	1:A:194:HIS:H	4:A:337:PX4:C35	3	0.23
(3,35)	1:A:194:HIS:H	4:A:339:PX4:C35	3	0.23
(3,35)	1:A:194:HIS:H	4:A:341:PX4:C35	3	0.23
(3,35)	1:A:194:HIS:H	4:A:343:PX4:C35	3	0.23
(3,35)	1:A:194:HIS:H	4:A:345:PX4:C35	3	0.23
(3,35)	1:A:194:HIS:H	4:A:347:PX4:C35	3	0.23
(3,35)	1:A:194:HIS:H	4:A:349:PX4:C35	3	0.23
(3,35)	1:A:194:HIS:H	4:A:351:PX4:C35	3	0.23
(3,35)	1:A:194:HIS:H	4:A:353:PX4:C35	3	0.23
(3,35)	1:A:194:HIS:H	4:A:355:PX4:C35	3	0.23
(3,35)	1:A:194:HIS:H	4:A:357:PX4:C35	3	0.23
(3,35)	1:A:194:HIS:H	4:A:359:PX4:C35	3	0.23
(3,35)	1:A:194:HIS:H	4:A:361:PX4:C35	3	0.23
(3,35)	1:A:194:HIS:H	4:A:363:PX4:C35	3	0.23
(3,35)	1:A:194:HIS:H	4:A:402:PX4:C35	3	0.23
(3,35)	1:A:194:HIS:H	4:A:404:PX4:C35	3	0.23
(3,35)	1:A:194:HIS:H	4:A:406:PX4:C35	3	0.23
(3,35)	1:A:194:HIS:H	4:A:408:PX4:C35	3	0.23
(3,35)	1:A:194:HIS:H	4:A:410:PX4:C35	3	0.23
(3,35)	1:A:194:HIS:H	4:A:412:PX4:C35	3	0.23
(3,35)	1:A:194:HIS:H	4:A:414:PX4:C35	3	0.23
(3,35)	1:A:194:HIS:H	4:A:416:PX4:C35	3	0.23
(3,35)	1:A:194:HIS:H	4:A:418:PX4:C35	3	0.23
(3,35)	1:A:194:HIS:H	4:A:420:PX4:C35	3	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,35)	1:A:194:HIS:H	4:A:422:PX4:C35	3	0.23
(3,35)	1:A:194:HIS:H	4:A:424:PX4:C35	3	0.23
(3,35)	1:A:194:HIS:H	4:A:426:PX4:C35	3	0.23
(3,35)	1:A:194:HIS:H	4:A:428:PX4:C35	3	0.23
(3,35)	1:A:194:HIS:H	4:A:430:PX4:C35	3	0.23
(2,988)	1:A:129:TRP:HE1	4:A:305:PX4:C2	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:307:PX4:C2	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:309:PX4:C2	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:311:PX4:C2	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:313:PX4:C2	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:315:PX4:C2	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:317:PX4:C2	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:319:PX4:C2	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:321:PX4:C2	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:323:PX4:C2	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:325:PX4:C2	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:327:PX4:C2	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:329:PX4:C2	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:331:PX4:C2	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:333:PX4:C2	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:335:PX4:C2	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:337:PX4:C2	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:339:PX4:C2	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:341:PX4:C2	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:343:PX4:C2	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:345:PX4:C2	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:347:PX4:C2	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:349:PX4:C2	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:351:PX4:C2	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:353:PX4:C2	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:355:PX4:C2	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:357:PX4:C2	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:359:PX4:C2	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:361:PX4:C2	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:363:PX4:C2	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:402:PX4:C2	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:404:PX4:C2	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:406:PX4:C2	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:408:PX4:C2	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:410:PX4:C2	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:412:PX4:C2	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:414:PX4:C2	11	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,988)	1:A:129:TRP:HE1	4:A:416:PX4:C2	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:418:PX4:C2	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:420:PX4:C2	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:422:PX4:C2	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:424:PX4:C2	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:426:PX4:C2	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:428:PX4:C2	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:430:PX4:C2	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:305:PX4:C1	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:307:PX4:C1	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:309:PX4:C1	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:311:PX4:C1	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:313:PX4:C1	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:315:PX4:C1	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:317:PX4:C1	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:319:PX4:C1	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:321:PX4:C1	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:323:PX4:C1	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:325:PX4:C1	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:327:PX4:C1	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:329:PX4:C1	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:331:PX4:C1	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:333:PX4:C1	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:335:PX4:C1	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:337:PX4:C1	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:339:PX4:C1	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:341:PX4:C1	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:343:PX4:C1	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:345:PX4:C1	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:347:PX4:C1	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:349:PX4:C1	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:351:PX4:C1	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:353:PX4:C1	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:355:PX4:C1	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:357:PX4:C1	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:359:PX4:C1	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:361:PX4:C1	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:363:PX4:C1	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:402:PX4:C1	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:404:PX4:C1	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:406:PX4:C1	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:408:PX4:C1	11	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,988)	1:A:129:TRP:HE1	4:A:410:PX4:C1	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:412:PX4:C1	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:414:PX4:C1	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:416:PX4:C1	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:418:PX4:C1	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:420:PX4:C1	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:422:PX4:C1	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:424:PX4:C1	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:426:PX4:C1	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:428:PX4:C1	11	0.23
(2,988)	1:A:129:TRP:HE1	4:A:430:PX4:C1	11	0.23
(2,986)	1:A:80:ASN:H	1:A:79:PRO:HB3	5	0.23
(2,986)	1:A:80:ASN:H	1:A:79:PRO:HB2	5	0.23
(2,986)	1:A:80:ASN:H	1:A:79:PRO:HB3	5	0.23
(2,986)	1:A:80:ASN:H	1:A:79:PRO:HB2	5	0.23
(2,980)	1:A:78:PHE:H	1:A:79:PRO:HD3	2	0.23
(2,980)	1:A:78:PHE:H	1:A:79:PRO:HD3	2	0.23
(2,975)	1:A:78:PHE:H	1:A:77:LEU:HD22	4	0.23
(2,975)	1:A:78:PHE:H	1:A:77:LEU:HD23	4	0.23
(2,968)	1:A:77:LEU:H	1:A:77:LEU:HA	7	0.23
(2,964)	1:A:75:TYR:H	1:A:76:SER:H	7	0.23
(2,959)	1:A:75:TYR:H	1:A:76:SER:H	7	0.23
(2,951)	1:A:74:GLU:H	1:A:76:SER:H	18	0.23
(2,926)	1:A:72:VAL:HB	1:A:73:ALA:H	11	0.23
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG21	12	0.23
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG22	12	0.23
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG23	12	0.23
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG11	12	0.23
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG12	12	0.23
(2,922)	1:A:72:VAL:H	1:A:72:VAL:HG13	12	0.23
(2,921)	1:A:72:VAL:H	1:A:72:VAL:HA	12	0.23
(2,912)	1:A:70:PRO:HB3	1:A:76:SER:H	1	0.23
(2,912)	1:A:70:PRO:HB2	1:A:76:SER:H	1	0.23
(2,895)	1:A:64:LYS:H	1:A:64:LYS:HA	5	0.23
(2,895)	1:A:64:LYS:H	1:A:64:LYS:HA	7	0.23
(2,847)	1:A:200:LEU:HD23	1:A:122:LEU:HD22	18	0.23
(2,847)	1:A:200:LEU:HD23	1:A:122:LEU:HD23	18	0.23
(2,766)	1:A:22:PHE:H	1:A:19:LEU:HD22	2	0.23
(2,766)	1:A:22:PHE:H	1:A:19:LEU:HD23	2	0.23
(2,727)	1:A:211:VAL:HG11	1:A:226:LEU:HD21	11	0.23
(2,677)	1:A:125:ARG:H	1:A:90:THR:H	11	0.23
(2,661)	1:A:4:ALA:H	1:A:59:ILE:HG21	11	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,661)	1:A:4:ALA:H	1:A:59:ILE:HG22	11	0.23
(2,661)	1:A:4:ALA:H	1:A:59:ILE:HG23	11	0.23
(2,655)	1:A:16:GLN:HE21	1:A:16:GLN:HE22	10	0.23
(2,655)	1:A:16:GLN:HE21	1:A:16:GLN:HE22	17	0.23
(2,655)	1:A:16:GLN:HE21	1:A:16:GLN:HE22	18	0.23
(2,653)	1:A:11:GLN:HE22	1:A:11:GLN:HE21	2	0.23
(2,653)	1:A:11:GLN:HE22	1:A:11:GLN:HE21	13	0.23
(2,653)	1:A:11:GLN:HE22	1:A:11:GLN:HE21	19	0.23
(2,608)	1:A:238:TYR:H	1:A:120:ILE:HD11	12	0.23
(2,608)	1:A:238:TYR:H	1:A:120:ILE:HD12	12	0.23
(2,608)	1:A:238:TYR:H	1:A:120:ILE:HD13	12	0.23
(2,570)	1:A:226:LEU:H	1:A:226:LEU:HD21	18	0.23
(2,564)	1:A:231:ILE:H	1:A:231:ILE:HG13	3	0.23
(2,564)	1:A:231:ILE:H	1:A:231:ILE:HG12	3	0.23
(2,503)	1:A:198:HIS:H	1:A:201:GLY:H	13	0.23
(2,454)	1:A:178:TRP:HE1	1:A:178:TRP:H	10	0.23
(2,423)	1:A:169:ASP:H	1:A:134:ILE:HD11	14	0.23
(2,423)	1:A:169:ASP:H	1:A:134:ILE:HD12	14	0.23
(2,423)	1:A:169:ASP:H	1:A:134:ILE:HD13	14	0.23
(2,39)	1:A:43:GLN:HE21	1:A:43:GLN:HE22	6	0.23
(2,39)	1:A:43:GLN:HE21	1:A:43:GLN:HE22	10	0.23
(2,39)	1:A:43:GLN:HE21	1:A:43:GLN:HE22	12	0.23
(2,39)	1:A:43:GLN:HE21	1:A:43:GLN:HE22	14	0.23
(2,39)	1:A:43:GLN:HE21	1:A:43:GLN:HE22	17	0.23
(2,369)	1:A:143:HIS:H	1:A:145:ASP:H	7	0.23
(2,316)	1:A:125:ARG:H	1:A:89:VAL:H	15	0.23
(2,264)	1:A:113:LEU:H	1:A:196:LEU:HD21	8	0.23
(2,228)	1:A:106:ASP:H	1:A:108:LEU:H	3	0.23
(2,226)	1:A:104:THR:H	1:A:106:ASP:H	3	0.23
(2,162)	1:A:125:ARG:H	1:A:89:VAL:H	15	0.23
(2,103)	1:A:39:LEU:H	1:A:37:ALA:H	20	0.23
(2,979)	1:A:78:PHE:H	1:A:78:PHE:HD1	18	0.22
(2,977)	1:A:78:PHE:H	1:A:78:PHE:HA	1	0.22
(2,977)	1:A:78:PHE:H	1:A:78:PHE:HA	6	0.22
(2,970)	1:A:77:LEU:HG	1:A:78:PHE:H	3	0.22
(2,964)	1:A:75:TYR:H	1:A:76:SER:H	19	0.22
(2,959)	1:A:75:TYR:H	1:A:76:SER:H	19	0.22
(2,945)	1:A:74:GLU:H	1:A:74:GLU:HG3	20	0.22
(2,945)	1:A:74:GLU:H	1:A:74:GLU:HG3	20	0.22
(2,926)	1:A:72:VAL:HB	1:A:73:ALA:H	5	0.22
(2,921)	1:A:72:VAL:H	1:A:72:VAL:HA	4	0.22
(2,921)	1:A:72:VAL:H	1:A:72:VAL:HA	10	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,909)	1:A:69:VAL:H	1:A:69:VAL:HA	10	0.22
(2,904)	1:A:67:CYS:H	1:A:67:CYS:HA	10	0.22
(2,895)	1:A:64:LYS:H	1:A:64:LYS:HA	14	0.22
(2,865)	1:A:186:ILE:HD11	1:A:186:ILE:HG13	8	0.22
(2,865)	1:A:186:ILE:HD12	1:A:186:ILE:HG13	8	0.22
(2,865)	1:A:186:ILE:HD13	1:A:186:ILE:HG13	8	0.22
(2,865)	1:A:186:ILE:HD11	1:A:186:ILE:HG12	8	0.22
(2,865)	1:A:186:ILE:HD12	1:A:186:ILE:HG12	8	0.22
(2,865)	1:A:186:ILE:HD13	1:A:186:ILE:HG12	8	0.22
(2,810)	1:A:93:ILE:H	1:A:94:VAL:HG11	2	0.22
(2,810)	1:A:93:ILE:H	1:A:94:VAL:HG12	2	0.22
(2,810)	1:A:93:ILE:H	1:A:94:VAL:HG13	2	0.22
(2,785)	1:A:19:LEU:HD11	1:A:39:LEU:HD11	20	0.22
(2,785)	1:A:19:LEU:HD11	1:A:39:LEU:HD12	20	0.22
(2,785)	1:A:19:LEU:HD11	1:A:39:LEU:HD13	20	0.22
(2,785)	1:A:19:LEU:HD12	1:A:39:LEU:HD11	20	0.22
(2,785)	1:A:19:LEU:HD12	1:A:39:LEU:HD12	20	0.22
(2,785)	1:A:19:LEU:HD12	1:A:39:LEU:HD13	20	0.22
(2,785)	1:A:19:LEU:HD13	1:A:39:LEU:HD11	20	0.22
(2,785)	1:A:19:LEU:HD13	1:A:39:LEU:HD12	20	0.22
(2,785)	1:A:19:LEU:HD13	1:A:39:LEU:HD13	20	0.22
(2,75)	1:A:55:ASN:H	1:A:59:ILE:H	3	0.22
(2,748)	1:A:89:VAL:HG12	1:A:122:LEU:HD21	6	0.22
(2,732)	1:A:211:VAL:HG13	1:A:226:LEU:HD22	19	0.22
(2,732)	1:A:211:VAL:HG13	1:A:226:LEU:HD23	19	0.22
(2,731)	1:A:211:VAL:HG13	1:A:226:LEU:HD21	10	0.22
(2,71)	1:A:55:ASN:H	1:A:54:LEU:HD21	8	0.22
(2,693)	1:A:11:GLN:H	1:A:8:SER:H	13	0.22
(2,680)	1:A:158:HIS:H	1:A:172:PHE:H	12	0.22
(2,655)	1:A:16:GLN:HE21	1:A:16:GLN:HE22	13	0.22
(2,653)	1:A:11:GLN:HE22	1:A:11:GLN:HE21	17	0.22
(2,63)	1:A:52:GLY:H	1:A:51:THR:H	11	0.22
(2,624)	1:A:11:GLN:H	1:A:8:SER:H	13	0.22
(2,62)	1:A:50:ILE:HG12	1:A:50:ILE:H	12	0.22
(2,557)	1:A:21:ARG:H	1:A:23:TYR:H	10	0.22
(2,501)	1:A:198:HIS:H	1:A:195:ALA:H	4	0.22
(2,482)	1:A:189:LEU:HD21	1:A:189:LEU:H	2	0.22
(2,39)	1:A:43:GLN:HE21	1:A:43:GLN:HE22	15	0.22
(2,381)	1:A:151:GLY:H	1:A:150:ASP:H	14	0.22
(2,369)	1:A:143:HIS:H	1:A:145:ASP:H	12	0.22
(2,368)	1:A:151:GLY:H	1:A:150:ASP:H	14	0.22
(2,303)	1:A:122:LEU:H	1:A:120:ILE:HG13	14	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,303)	1:A:122:LEU:H	1:A:120:ILE:HG12	14	0.22
(2,278)	1:A:116:TRP:HE1	1:A:211:VAL:HG11	6	0.22
(2,278)	1:A:116:TRP:HE1	1:A:211:VAL:HG12	6	0.22
(2,278)	1:A:116:TRP:HE1	1:A:211:VAL:HG13	6	0.22
(2,265)	1:A:113:LEU:H	1:A:196:LEU:HD22	2	0.22
(2,265)	1:A:113:LEU:H	1:A:196:LEU:HD23	2	0.22
(2,207)	1:A:98:ARG:H	1:A:100:LEU:H	2	0.22
(2,14)	1:A:159:ALA:H	1:A:171:HIS:H	9	0.22
(2,125)	1:A:157:ALA:H	1:A:68:GLY:H	20	0.22
(2,977)	1:A:78:PHE:H	1:A:78:PHE:HA	7	0.21
(2,977)	1:A:78:PHE:H	1:A:78:PHE:HA	14	0.21
(2,977)	1:A:78:PHE:H	1:A:78:PHE:HA	15	0.21
(2,977)	1:A:78:PHE:H	1:A:78:PHE:HA	18	0.21
(2,969)	1:A:77:LEU:H	1:A:78:PHE:H	3	0.21
(2,968)	1:A:77:LEU:H	1:A:77:LEU:HA	6	0.21
(2,949)	1:A:74:GLU:H	1:A:75:TYR:H	4	0.21
(2,949)	1:A:74:GLU:H	1:A:75:TYR:H	5	0.21
(2,919)	1:A:72:VAL:H	1:A:71:ASP:HA	7	0.21
(2,912)	1:A:70:PRO:HB3	1:A:76:SER:H	8	0.21
(2,912)	1:A:70:PRO:HB2	1:A:76:SER:H	8	0.21
(2,909)	1:A:69:VAL:H	1:A:69:VAL:HA	16	0.21
(2,898)	1:A:66:ARG:H	1:A:63:GLN:HB3	14	0.21
(2,898)	1:A:66:ARG:H	1:A:63:GLN:HB2	14	0.21
(2,895)	1:A:64:LYS:H	1:A:64:LYS:HA	18	0.21
(2,859)	1:A:186:ILE:HD12	1:A:156:LEU:HD21	14	0.21
(2,835)	1:A:120:ILE:HD12	1:A:200:LEU:HD22	15	0.21
(2,835)	1:A:120:ILE:HD12	1:A:200:LEU:HD23	15	0.21
(2,809)	1:A:136:ILE:H	1:A:94:VAL:HG11	9	0.21
(2,809)	1:A:136:ILE:H	1:A:94:VAL:HG12	9	0.21
(2,809)	1:A:136:ILE:H	1:A:94:VAL:HG13	9	0.21
(2,8)	1:A:135:MET:H	1:A:92:ARG:H	9	0.21
(2,75)	1:A:55:ASN:H	1:A:59:ILE:H	18	0.21
(2,741)	1:A:114:ASN:H	1:A:113:LEU:HD21	6	0.21
(2,673)	1:A:77:LEU:H	1:A:78:PHE:H	3	0.21
(2,655)	1:A:16:GLN:HE21	1:A:16:GLN:HE22	12	0.21
(2,626)	1:A:12:TRP:H	1:A:10:LEU:H	15	0.21
(2,602)	1:A:237:LEU:H	1:A:239:GLY:H	7	0.21
(2,538)	1:A:205:SER:H	1:A:213:TYR:H	16	0.21
(2,538)	1:A:205:SER:H	1:A:213:TYR:H	20	0.21
(2,504)	1:A:198:HIS:H	1:A:202:MET:H	14	0.21
(2,501)	1:A:198:HIS:H	1:A:195:ALA:H	20	0.21
(2,454)	1:A:178:TRP:HE1	1:A:178:TRP:H	9	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,454)	1:A:178:TRP:HE1	1:A:178:TRP:H	14	0.21
(2,426)	1:A:170:ALA:H	1:A:136:ILE:HD11	7	0.21
(2,426)	1:A:170:ALA:H	1:A:136:ILE:HD12	7	0.21
(2,426)	1:A:170:ALA:H	1:A:136:ILE:HD13	7	0.21
(2,426)	1:A:170:ALA:H	1:A:136:ILE:HD11	14	0.21
(2,426)	1:A:170:ALA:H	1:A:136:ILE:HD12	14	0.21
(2,426)	1:A:170:ALA:H	1:A:136:ILE:HD13	14	0.21
(2,39)	1:A:43:GLN:HE21	1:A:43:GLN:HE22	18	0.21
(2,39)	1:A:43:GLN:HE21	1:A:43:GLN:HE22	19	0.21
(2,381)	1:A:151:GLY:H	1:A:150:ASP:H	5	0.21
(2,368)	1:A:151:GLY:H	1:A:150:ASP:H	5	0.21
(2,326)	1:A:128:VAL:H	1:A:129:TRP:H	12	0.21
(2,324)	1:A:128:VAL:H	1:A:129:TRP:H	12	0.21
(2,316)	1:A:125:ARG:H	1:A:89:VAL:H	6	0.21
(2,235)	1:A:104:THR:H	1:A:107:ARG:H	5	0.21
(2,181)	1:A:93:ILE:H	1:A:136:ILE:H	12	0.21
(2,162)	1:A:125:ARG:H	1:A:89:VAL:H	6	0.21
(2,137)	1:A:73:ALA:H	1:A:72:VAL:HG11	20	0.21
(2,137)	1:A:73:ALA:H	1:A:72:VAL:HG12	20	0.21
(2,137)	1:A:73:ALA:H	1:A:72:VAL:HG13	20	0.21
(2,137)	1:A:73:ALA:H	1:A:72:VAL:HG21	20	0.21
(2,137)	1:A:73:ALA:H	1:A:72:VAL:HG22	20	0.21
(2,137)	1:A:73:ALA:H	1:A:72:VAL:HG23	20	0.21
(2,113)	1:A:25:TYR:H	1:A:26:ASP:H	5	0.21
(2,113)	1:A:25:TYR:H	1:A:26:ASP:H	14	0.21
(2,103)	1:A:39:LEU:H	1:A:37:ALA:H	3	0.21
(2,103)	1:A:39:LEU:H	1:A:37:ALA:H	17	0.21
(2,968)	1:A:77:LEU:H	1:A:77:LEU:HA	4	0.2
(2,945)	1:A:74:GLU:H	1:A:74:GLU:HG3	2	0.2
(2,945)	1:A:74:GLU:H	1:A:74:GLU:HG3	2	0.2
(2,945)	1:A:74:GLU:H	1:A:74:GLU:HG3	6	0.2
(2,945)	1:A:74:GLU:H	1:A:74:GLU:HG3	6	0.2
(2,927)	1:A:72:VAL:H	1:A:73:ALA:H	20	0.2
(2,927)	1:A:72:VAL:H	1:A:73:ALA:H	20	0.2
(2,926)	1:A:72:VAL:HB	1:A:73:ALA:H	13	0.2
(2,921)	1:A:72:VAL:H	1:A:72:VAL:HA	15	0.2
(2,921)	1:A:72:VAL:H	1:A:72:VAL:HA	16	0.2
(2,917)	1:A:71:ASP:H	1:A:72:VAL:HB	5	0.2
(2,916)	1:A:71:ASP:H	1:A:72:VAL:HA	15	0.2
(2,915)	1:A:71:ASP:H	1:A:72:VAL:HG21	7	0.2
(2,915)	1:A:71:ASP:H	1:A:72:VAL:HG22	7	0.2
(2,915)	1:A:71:ASP:H	1:A:72:VAL:HG23	7	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,904)	1:A:67:CYS:H	1:A:67:CYS:HA	8	0.2
(2,898)	1:A:66:ARG:H	1:A:63:GLN:HB3	12	0.2
(2,898)	1:A:66:ARG:H	1:A:63:GLN:HB2	12	0.2
(2,895)	1:A:64:LYS:H	1:A:64:LYS:HA	20	0.2
(2,889)	1:A:63:GLN:HA	1:A:63:GLN:H	8	0.2
(2,848)	1:A:127:VAL:HG21	1:A:129:TRP:H	1	0.2
(2,848)	1:A:127:VAL:HG22	1:A:129:TRP:H	1	0.2
(2,848)	1:A:127:VAL:HG23	1:A:129:TRP:H	1	0.2
(2,810)	1:A:93:ILE:H	1:A:94:VAL:HG11	8	0.2
(2,810)	1:A:93:ILE:H	1:A:94:VAL:HG12	8	0.2
(2,810)	1:A:93:ILE:H	1:A:94:VAL:HG13	8	0.2
(2,810)	1:A:93:ILE:H	1:A:94:VAL:HG11	18	0.2
(2,810)	1:A:93:ILE:H	1:A:94:VAL:HG12	18	0.2
(2,810)	1:A:93:ILE:H	1:A:94:VAL:HG13	18	0.2
(2,803)	1:A:93:ILE:HD11	1:A:93:ILE:HG13	12	0.2
(2,803)	1:A:93:ILE:HD12	1:A:93:ILE:HG13	12	0.2
(2,803)	1:A:93:ILE:HD13	1:A:93:ILE:HG13	12	0.2
(2,803)	1:A:93:ILE:HD11	1:A:93:ILE:HG12	12	0.2
(2,803)	1:A:93:ILE:HD12	1:A:93:ILE:HG12	12	0.2
(2,803)	1:A:93:ILE:HD13	1:A:93:ILE:HG12	12	0.2
(2,8)	1:A:135:MET:H	1:A:92:ARG:H	10	0.2
(2,8)	1:A:135:MET:H	1:A:92:ARG:H	18	0.2
(2,786)	1:A:24:LEU:H	1:A:24:LEU:HD21	2	0.2
(2,776)	1:A:61:ILE:HD12	1:A:48:LEU:HD22	8	0.2
(2,776)	1:A:61:ILE:HD12	1:A:48:LEU:HD23	8	0.2
(2,748)	1:A:89:VAL:HG12	1:A:122:LEU:HD21	12	0.2
(2,683)	1:A:179:THR:HG21	1:A:185:GLY:H	14	0.2
(2,683)	1:A:179:THR:HG22	1:A:185:GLY:H	14	0.2
(2,683)	1:A:179:THR:HG23	1:A:185:GLY:H	14	0.2
(2,680)	1:A:158:HIS:H	1:A:172:PHE:H	10	0.2
(2,677)	1:A:125:ARG:H	1:A:90:THR:H	12	0.2
(2,670)	1:A:66:ARG:H	1:A:156:LEU:HD11	16	0.2
(2,670)	1:A:66:ARG:H	1:A:156:LEU:HD12	16	0.2
(2,670)	1:A:66:ARG:H	1:A:156:LEU:HD13	16	0.2
(2,655)	1:A:16:GLN:HE21	1:A:16:GLN:HE22	9	0.2
(2,653)	1:A:11:GLN:HE22	1:A:11:GLN:HE21	3	0.2
(2,653)	1:A:11:GLN:HE22	1:A:11:GLN:HE21	9	0.2
(2,632)	1:A:25:TYR:H	1:A:24:LEU:HD21	9	0.2
(2,62)	1:A:50:ILE:HG12	1:A:50:ILE:H	10	0.2
(2,539)	1:A:206:SER:H	1:A:207:ASP:H	19	0.2
(2,539)	1:A:206:SER:H	1:A:207:ASP:H	19	0.2
(2,467)	1:A:84:TRP:H	1:A:200:LEU:HD22	2	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,467)	1:A:84:TRP:H	1:A:200:LEU:HD23	2	0.2
(2,462)	1:A:182:SER:H	1:A:181:GLY:H	18	0.2
(2,462)	1:A:182:SER:H	1:A:181:GLY:H	18	0.2
(2,39)	1:A:43:GLN:HE21	1:A:43:GLN:HE22	11	0.2
(2,357)	1:A:136:ILE:HD11	1:A:137:GLY:H	18	0.2
(2,357)	1:A:136:ILE:HD12	1:A:137:GLY:H	18	0.2
(2,357)	1:A:136:ILE:HD13	1:A:137:GLY:H	18	0.2
(2,327)	1:A:129:TRP:H	1:A:127:VAL:HG21	1	0.2
(2,327)	1:A:129:TRP:H	1:A:127:VAL:HG22	1	0.2
(2,327)	1:A:129:TRP:H	1:A:127:VAL:HG23	1	0.2
(2,326)	1:A:128:VAL:H	1:A:129:TRP:H	7	0.2
(2,326)	1:A:128:VAL:H	1:A:129:TRP:H	9	0.2
(2,324)	1:A:128:VAL:H	1:A:129:TRP:H	7	0.2
(2,324)	1:A:128:VAL:H	1:A:129:TRP:H	9	0.2
(2,316)	1:A:125:ARG:H	1:A:89:VAL:H	2	0.2
(2,315)	1:A:125:ARG:H	1:A:126:LYS:H	6	0.2
(2,303)	1:A:122:LEU:H	1:A:120:ILE:HG13	12	0.2
(2,303)	1:A:122:LEU:H	1:A:120:ILE:HG12	12	0.2
(2,162)	1:A:125:ARG:H	1:A:89:VAL:H	2	0.2
(2,157)	1:A:88:VAL:H	1:A:123:HIS:H	16	0.2
(2,113)	1:A:25:TYR:H	1:A:26:ASP:H	7	0.2
(2,103)	1:A:39:LEU:H	1:A:37:ALA:H	11	0.2
(2,980)	1:A:78:PHE:H	1:A:79:PRO:HD3	9	0.19
(2,980)	1:A:78:PHE:H	1:A:79:PRO:HD3	9	0.19
(2,977)	1:A:78:PHE:H	1:A:78:PHE:HA	9	0.19
(2,969)	1:A:77:LEU:H	1:A:78:PHE:H	10	0.19
(2,968)	1:A:77:LEU:H	1:A:77:LEU:HA	15	0.19
(2,947)	1:A:74:GLU:HB3	1:A:75:TYR:H	15	0.19
(2,947)	1:A:74:GLU:HB3	1:A:75:TYR:H	15	0.19
(2,935)	1:A:73:ALA:H	1:A:73:ALA:HA	13	0.19
(2,927)	1:A:72:VAL:H	1:A:73:ALA:H	4	0.19
(2,927)	1:A:72:VAL:H	1:A:73:ALA:H	4	0.19
(2,921)	1:A:72:VAL:H	1:A:72:VAL:HA	1	0.19
(2,921)	1:A:72:VAL:H	1:A:72:VAL:HA	2	0.19
(2,921)	1:A:72:VAL:H	1:A:72:VAL:HA	7	0.19
(2,916)	1:A:71:ASP:H	1:A:72:VAL:HA	13	0.19
(2,915)	1:A:71:ASP:H	1:A:72:VAL:HG21	6	0.19
(2,915)	1:A:71:ASP:H	1:A:72:VAL:HG22	6	0.19
(2,915)	1:A:71:ASP:H	1:A:72:VAL:HG23	6	0.19
(2,909)	1:A:69:VAL:H	1:A:69:VAL:HA	15	0.19
(2,887)	1:A:134:ILE:HD11	1:A:134:ILE:HG21	3	0.19
(2,887)	1:A:134:ILE:HD11	1:A:134:ILE:HG22	3	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,887)	1:A:134:ILE:HD11	1:A:134:ILE:HG23	3	0.19
(2,887)	1:A:134:ILE:HD12	1:A:134:ILE:HG21	3	0.19
(2,887)	1:A:134:ILE:HD12	1:A:134:ILE:HG22	3	0.19
(2,887)	1:A:134:ILE:HD12	1:A:134:ILE:HG23	3	0.19
(2,887)	1:A:134:ILE:HD13	1:A:134:ILE:HG21	3	0.19
(2,887)	1:A:134:ILE:HD13	1:A:134:ILE:HG22	3	0.19
(2,887)	1:A:134:ILE:HD13	1:A:134:ILE:HG23	3	0.19
(2,885)	1:A:134:ILE:HD11	1:A:89:VAL:HG11	10	0.19
(2,885)	1:A:134:ILE:HD11	1:A:89:VAL:HG12	10	0.19
(2,885)	1:A:134:ILE:HD11	1:A:89:VAL:HG13	10	0.19
(2,885)	1:A:134:ILE:HD12	1:A:89:VAL:HG11	10	0.19
(2,885)	1:A:134:ILE:HD12	1:A:89:VAL:HG12	10	0.19
(2,885)	1:A:134:ILE:HD12	1:A:89:VAL:HG13	10	0.19
(2,885)	1:A:134:ILE:HD13	1:A:89:VAL:HG11	10	0.19
(2,885)	1:A:134:ILE:HD13	1:A:89:VAL:HG12	10	0.19
(2,885)	1:A:134:ILE:HD13	1:A:89:VAL:HG13	10	0.19
(2,866)	1:A:186:ILE:HD11	1:A:156:LEU:HD11	14	0.19
(2,866)	1:A:186:ILE:HD11	1:A:156:LEU:HD12	14	0.19
(2,866)	1:A:186:ILE:HD11	1:A:156:LEU:HD13	14	0.19
(2,866)	1:A:186:ILE:HD12	1:A:156:LEU:HD11	14	0.19
(2,866)	1:A:186:ILE:HD12	1:A:156:LEU:HD12	14	0.19
(2,866)	1:A:186:ILE:HD12	1:A:156:LEU:HD13	14	0.19
(2,866)	1:A:186:ILE:HD13	1:A:156:LEU:HD11	14	0.19
(2,866)	1:A:186:ILE:HD13	1:A:156:LEU:HD12	14	0.19
(2,866)	1:A:186:ILE:HD13	1:A:156:LEU:HD13	14	0.19
(2,862)	1:A:186:ILE:HD13	1:A:156:LEU:HD22	14	0.19
(2,862)	1:A:186:ILE:HD13	1:A:156:LEU:HD23	14	0.19
(2,862)	1:A:186:ILE:HD11	1:A:156:LEU:HD11	14	0.19
(2,862)	1:A:186:ILE:HD11	1:A:156:LEU:HD12	14	0.19
(2,862)	1:A:186:ILE:HD11	1:A:156:LEU:HD13	14	0.19
(2,862)	1:A:186:ILE:HD12	1:A:156:LEU:HD11	14	0.19
(2,862)	1:A:186:ILE:HD12	1:A:156:LEU:HD12	14	0.19
(2,862)	1:A:186:ILE:HD12	1:A:156:LEU:HD13	14	0.19
(2,862)	1:A:186:ILE:HD13	1:A:156:LEU:HD11	14	0.19
(2,862)	1:A:186:ILE:HD13	1:A:156:LEU:HD12	14	0.19
(2,862)	1:A:186:ILE:HD13	1:A:156:LEU:HD13	14	0.19
(2,859)	1:A:186:ILE:HD12	1:A:156:LEU:HD21	6	0.19
(2,839)	1:A:123:HIS:H	1:A:122:LEU:HD11	3	0.19
(2,839)	1:A:123:HIS:H	1:A:122:LEU:HD12	3	0.19
(2,839)	1:A:123:HIS:H	1:A:122:LEU:HD13	3	0.19
(2,831)	1:A:120:ILE:HD11	1:A:120:ILE:HG21	17	0.19
(2,831)	1:A:120:ILE:HD11	1:A:120:ILE:HG22	17	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,831)	1:A:120:ILE:HD11	1:A:120:ILE:HG23	17	0.19
(2,831)	1:A:120:ILE:HD12	1:A:120:ILE:HG21	17	0.19
(2,831)	1:A:120:ILE:HD12	1:A:120:ILE:HG22	17	0.19
(2,831)	1:A:120:ILE:HD12	1:A:120:ILE:HG23	17	0.19
(2,831)	1:A:120:ILE:HD13	1:A:120:ILE:HG21	17	0.19
(2,831)	1:A:120:ILE:HD13	1:A:120:ILE:HG22	17	0.19
(2,831)	1:A:120:ILE:HD13	1:A:120:ILE:HG23	17	0.19
(2,810)	1:A:93:ILE:H	1:A:94:VAL:HG11	11	0.19
(2,810)	1:A:93:ILE:H	1:A:94:VAL:HG12	11	0.19
(2,810)	1:A:93:ILE:H	1:A:94:VAL:HG13	11	0.19
(2,806)	1:A:93:ILE:HD11	1:A:93:ILE:HG21	16	0.19
(2,806)	1:A:93:ILE:HD11	1:A:93:ILE:HG22	16	0.19
(2,806)	1:A:93:ILE:HD11	1:A:93:ILE:HG23	16	0.19
(2,806)	1:A:93:ILE:HD12	1:A:93:ILE:HG21	16	0.19
(2,806)	1:A:93:ILE:HD12	1:A:93:ILE:HG22	16	0.19
(2,806)	1:A:93:ILE:HD12	1:A:93:ILE:HG23	16	0.19
(2,806)	1:A:93:ILE:HD13	1:A:93:ILE:HG21	16	0.19
(2,806)	1:A:93:ILE:HD13	1:A:93:ILE:HG22	16	0.19
(2,806)	1:A:93:ILE:HD13	1:A:93:ILE:HG23	16	0.19
(2,8)	1:A:135:MET:H	1:A:92:ARG:H	14	0.19
(2,786)	1:A:24:LEU:H	1:A:24:LEU:HD21	4	0.19
(2,744)	1:A:134:ILE:HD11	1:A:89:VAL:HG11	10	0.19
(2,744)	1:A:134:ILE:HD11	1:A:89:VAL:HG12	10	0.19
(2,744)	1:A:134:ILE:HD11	1:A:89:VAL:HG13	10	0.19
(2,744)	1:A:134:ILE:HD12	1:A:89:VAL:HG11	10	0.19
(2,744)	1:A:134:ILE:HD12	1:A:89:VAL:HG12	10	0.19
(2,744)	1:A:134:ILE:HD12	1:A:89:VAL:HG13	10	0.19
(2,744)	1:A:134:ILE:HD13	1:A:89:VAL:HG11	10	0.19
(2,744)	1:A:134:ILE:HD13	1:A:89:VAL:HG12	10	0.19
(2,744)	1:A:134:ILE:HD13	1:A:89:VAL:HG13	10	0.19
(2,74)	1:A:55:ASN:H	1:A:55:ASN:HD21	6	0.19
(2,732)	1:A:211:VAL:HG13	1:A:226:LEU:HD22	12	0.19
(2,732)	1:A:211:VAL:HG13	1:A:226:LEU:HD23	12	0.19
(2,693)	1:A:11:GLN:H	1:A:8:SER:H	18	0.19
(2,673)	1:A:77:LEU:H	1:A:78:PHE:H	10	0.19
(2,655)	1:A:16:GLN:HE21	1:A:16:GLN:HE22	14	0.19
(2,626)	1:A:12:TRP:H	1:A:10:LEU:H	20	0.19
(2,624)	1:A:11:GLN:H	1:A:8:SER:H	18	0.19
(2,570)	1:A:226:LEU:H	1:A:226:LEU:HD21	12	0.19
(2,539)	1:A:206:SER:H	1:A:207:ASP:H	10	0.19
(2,539)	1:A:206:SER:H	1:A:207:ASP:H	10	0.19
(2,514)	1:A:200:LEU:H	1:A:202:MET:H	1	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,456)	1:A:178:TRP:HE1	1:A:176:GLU:H	17	0.19
(2,445)	1:A:178:TRP:HE1	1:A:176:GLU:H	17	0.19
(2,423)	1:A:169:ASP:H	1:A:134:ILE:HD11	1	0.19
(2,423)	1:A:169:ASP:H	1:A:134:ILE:HD12	1	0.19
(2,423)	1:A:169:ASP:H	1:A:134:ILE:HD13	1	0.19
(2,391)	1:A:157:ALA:H	1:A:156:LEU:H	8	0.19
(2,391)	1:A:157:ALA:H	1:A:156:LEU:H	12	0.19
(2,385)	1:A:157:ALA:H	1:A:156:LEU:H	8	0.19
(2,385)	1:A:157:ALA:H	1:A:156:LEU:H	12	0.19
(2,36)	1:A:46:PHE:H	1:A:43:GLN:H	18	0.19
(2,315)	1:A:125:ARG:H	1:A:126:LYS:H	19	0.19
(2,304)	1:A:123:HIS:H	1:A:122:LEU:HD11	3	0.19
(2,304)	1:A:123:HIS:H	1:A:122:LEU:HD12	3	0.19
(2,304)	1:A:123:HIS:H	1:A:122:LEU:HD13	3	0.19
(2,274)	1:A:116:TRP:HE1	1:A:197:GLY:H	17	0.19
(2,257)	1:A:112:ALA:H	1:A:189:LEU:HD21	8	0.19
(2,239)	1:A:108:LEU:H	1:A:108:LEU:HD21	5	0.19
(2,228)	1:A:106:ASP:H	1:A:108:LEU:H	9	0.19
(2,226)	1:A:104:THR:H	1:A:106:ASP:H	16	0.19
(2,113)	1:A:25:TYR:H	1:A:26:ASP:H	19	0.19
(2,103)	1:A:39:LEU:H	1:A:37:ALA:H	8	0.19
(2,101)	1:A:37:ALA:H	1:A:36:GLU:H	3	0.19
(3,32)	1:A:154:ASN:ND2	4:A:305:PX4:C35	16	0.18
(3,32)	1:A:154:ASN:ND2	4:A:307:PX4:C35	16	0.18
(3,32)	1:A:154:ASN:ND2	4:A:309:PX4:C35	16	0.18
(3,32)	1:A:154:ASN:ND2	4:A:311:PX4:C35	16	0.18
(3,32)	1:A:154:ASN:ND2	4:A:313:PX4:C35	16	0.18
(3,32)	1:A:154:ASN:ND2	4:A:315:PX4:C35	16	0.18
(3,32)	1:A:154:ASN:ND2	4:A:317:PX4:C35	16	0.18
(3,32)	1:A:154:ASN:ND2	4:A:319:PX4:C35	16	0.18
(3,32)	1:A:154:ASN:ND2	4:A:321:PX4:C35	16	0.18
(3,32)	1:A:154:ASN:ND2	4:A:323:PX4:C35	16	0.18
(3,32)	1:A:154:ASN:ND2	4:A:325:PX4:C35	16	0.18
(3,32)	1:A:154:ASN:ND2	4:A:327:PX4:C35	16	0.18
(3,32)	1:A:154:ASN:ND2	4:A:329:PX4:C35	16	0.18
(3,32)	1:A:154:ASN:ND2	4:A:331:PX4:C35	16	0.18
(3,32)	1:A:154:ASN:ND2	4:A:333:PX4:C35	16	0.18
(3,32)	1:A:154:ASN:ND2	4:A:335:PX4:C35	16	0.18
(3,32)	1:A:154:ASN:ND2	4:A:337:PX4:C35	16	0.18
(3,32)	1:A:154:ASN:ND2	4:A:339:PX4:C35	16	0.18
(3,32)	1:A:154:ASN:ND2	4:A:341:PX4:C35	16	0.18
(3,32)	1:A:154:ASN:ND2	4:A:343:PX4:C35	16	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,32)	1:A:154:ASN:ND2	4:A:345:PX4:C35	16	0.18
(3,32)	1:A:154:ASN:ND2	4:A:347:PX4:C35	16	0.18
(3,32)	1:A:154:ASN:ND2	4:A:349:PX4:C35	16	0.18
(3,32)	1:A:154:ASN:ND2	4:A:351:PX4:C35	16	0.18
(3,32)	1:A:154:ASN:ND2	4:A:353:PX4:C35	16	0.18
(3,32)	1:A:154:ASN:ND2	4:A:355:PX4:C35	16	0.18
(3,32)	1:A:154:ASN:ND2	4:A:357:PX4:C35	16	0.18
(3,32)	1:A:154:ASN:ND2	4:A:359:PX4:C35	16	0.18
(3,32)	1:A:154:ASN:ND2	4:A:361:PX4:C35	16	0.18
(3,32)	1:A:154:ASN:ND2	4:A:363:PX4:C35	16	0.18
(3,32)	1:A:154:ASN:ND2	4:A:402:PX4:C35	16	0.18
(3,32)	1:A:154:ASN:ND2	4:A:404:PX4:C35	16	0.18
(3,32)	1:A:154:ASN:ND2	4:A:406:PX4:C35	16	0.18
(3,32)	1:A:154:ASN:ND2	4:A:408:PX4:C35	16	0.18
(3,32)	1:A:154:ASN:ND2	4:A:410:PX4:C35	16	0.18
(3,32)	1:A:154:ASN:ND2	4:A:412:PX4:C35	16	0.18
(3,32)	1:A:154:ASN:ND2	4:A:414:PX4:C35	16	0.18
(3,32)	1:A:154:ASN:ND2	4:A:416:PX4:C35	16	0.18
(3,32)	1:A:154:ASN:ND2	4:A:418:PX4:C35	16	0.18
(3,32)	1:A:154:ASN:ND2	4:A:420:PX4:C35	16	0.18
(3,32)	1:A:154:ASN:ND2	4:A:422:PX4:C35	16	0.18
(3,32)	1:A:154:ASN:ND2	4:A:424:PX4:C35	16	0.18
(3,32)	1:A:154:ASN:ND2	4:A:426:PX4:C35	16	0.18
(3,32)	1:A:154:ASN:ND2	4:A:428:PX4:C35	16	0.18
(3,32)	1:A:154:ASN:ND2	4:A:430:PX4:C35	16	0.18
(2,980)	1:A:78:PHE:H	1:A:79:PRO:HD3	18	0.18
(2,980)	1:A:78:PHE:H	1:A:79:PRO:HD3	18	0.18
(2,977)	1:A:78:PHE:H	1:A:78:PHE:HA	19	0.18
(2,974)	1:A:78:PHE:H	1:A:77:LEU:HD21	12	0.18
(2,969)	1:A:77:LEU:H	1:A:78:PHE:H	9	0.18
(2,945)	1:A:74:GLU:H	1:A:74:GLU:HG3	15	0.18
(2,945)	1:A:74:GLU:H	1:A:74:GLU:HG3	15	0.18
(2,945)	1:A:74:GLU:H	1:A:74:GLU:HG3	18	0.18
(2,945)	1:A:74:GLU:H	1:A:74:GLU:HG3	18	0.18
(2,935)	1:A:73:ALA:H	1:A:73:ALA:HA	3	0.18
(2,927)	1:A:72:VAL:H	1:A:73:ALA:H	17	0.18
(2,927)	1:A:72:VAL:H	1:A:73:ALA:H	17	0.18
(2,926)	1:A:72:VAL:HB	1:A:73:ALA:H	2	0.18
(2,920)	1:A:72:VAL:H	1:A:71:ASP:H	14	0.18
(2,920)	1:A:72:VAL:H	1:A:71:ASP:H	14	0.18
(2,919)	1:A:72:VAL:H	1:A:71:ASP:HA	16	0.18
(2,917)	1:A:71:ASP:H	1:A:72:VAL:HB	9	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,904)	1:A:67:CYS:H	1:A:67:CYS:HA	11	0.18
(2,903)	1:A:67:CYS:H	1:A:66:ARG:HA	15	0.18
(2,895)	1:A:64:LYS:H	1:A:64:LYS:HA	10	0.18
(2,895)	1:A:64:LYS:H	1:A:64:LYS:HA	16	0.18
(2,830)	1:A:120:ILE:HD11	1:A:120:ILE:HG13	13	0.18
(2,830)	1:A:120:ILE:HD12	1:A:120:ILE:HG13	13	0.18
(2,830)	1:A:120:ILE:HD13	1:A:120:ILE:HG13	13	0.18
(2,830)	1:A:120:ILE:HD11	1:A:120:ILE:HG12	13	0.18
(2,830)	1:A:120:ILE:HD12	1:A:120:ILE:HG12	13	0.18
(2,830)	1:A:120:ILE:HD13	1:A:120:ILE:HG12	13	0.18
(2,801)	1:A:93:ILE:H	1:A:93:ILE:HD11	14	0.18
(2,801)	1:A:93:ILE:H	1:A:93:ILE:HD12	14	0.18
(2,801)	1:A:93:ILE:H	1:A:93:ILE:HD13	14	0.18
(2,8)	1:A:135:MET:H	1:A:92:ARG:H	7	0.18
(2,793)	1:A:58:VAL:HG13	1:A:39:LEU:HD22	9	0.18
(2,793)	1:A:58:VAL:HG13	1:A:39:LEU:HD23	9	0.18
(2,793)	1:A:58:VAL:HG11	1:A:39:LEU:HD11	9	0.18
(2,793)	1:A:58:VAL:HG11	1:A:39:LEU:HD12	9	0.18
(2,793)	1:A:58:VAL:HG11	1:A:39:LEU:HD13	9	0.18
(2,793)	1:A:58:VAL:HG12	1:A:39:LEU:HD11	9	0.18
(2,793)	1:A:58:VAL:HG12	1:A:39:LEU:HD12	9	0.18
(2,793)	1:A:58:VAL:HG12	1:A:39:LEU:HD13	9	0.18
(2,793)	1:A:58:VAL:HG13	1:A:39:LEU:HD11	9	0.18
(2,793)	1:A:58:VAL:HG13	1:A:39:LEU:HD12	9	0.18
(2,793)	1:A:58:VAL:HG13	1:A:39:LEU:HD13	9	0.18
(2,775)	1:A:61:ILE:HD12	1:A:48:LEU:HD21	5	0.18
(2,767)	1:A:61:ILE:HD11	1:A:60:GLU:H	4	0.18
(2,767)	1:A:61:ILE:HD12	1:A:60:GLU:H	4	0.18
(2,767)	1:A:61:ILE:HD13	1:A:60:GLU:H	4	0.18
(2,756)	1:A:54:LEU:HD22	1:A:58:VAL:HG11	18	0.18
(2,756)	1:A:54:LEU:HD22	1:A:58:VAL:HG12	18	0.18
(2,756)	1:A:54:LEU:HD22	1:A:58:VAL:HG13	18	0.18
(2,756)	1:A:54:LEU:HD23	1:A:58:VAL:HG11	18	0.18
(2,756)	1:A:54:LEU:HD23	1:A:58:VAL:HG12	18	0.18
(2,756)	1:A:54:LEU:HD23	1:A:58:VAL:HG13	18	0.18
(2,755)	1:A:54:LEU:HD21	1:A:58:VAL:HG11	6	0.18
(2,755)	1:A:54:LEU:HD21	1:A:58:VAL:HG12	6	0.18
(2,755)	1:A:54:LEU:HD21	1:A:58:VAL:HG13	6	0.18
(2,74)	1:A:55:ASN:H	1:A:55:ASN:HD21	3	0.18
(2,729)	1:A:211:VAL:HG12	1:A:226:LEU:HD21	20	0.18
(2,716)	1:A:54:LEU:HD11	1:A:58:VAL:HG11	20	0.18
(2,716)	1:A:54:LEU:HD11	1:A:58:VAL:HG12	20	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,716)	1:A:54:LEU:HD11	1:A:58:VAL:HG13	20	0.18
(2,716)	1:A:54:LEU:HD12	1:A:58:VAL:HG11	20	0.18
(2,716)	1:A:54:LEU:HD12	1:A:58:VAL:HG12	20	0.18
(2,716)	1:A:54:LEU:HD12	1:A:58:VAL:HG13	20	0.18
(2,716)	1:A:54:LEU:HD13	1:A:58:VAL:HG11	20	0.18
(2,716)	1:A:54:LEU:HD13	1:A:58:VAL:HG12	20	0.18
(2,716)	1:A:54:LEU:HD13	1:A:58:VAL:HG13	20	0.18
(2,70)	1:A:58:VAL:HG21	1:A:55:ASN:H	18	0.18
(2,70)	1:A:58:VAL:HG22	1:A:55:ASN:H	18	0.18
(2,70)	1:A:58:VAL:HG23	1:A:55:ASN:H	18	0.18
(2,699)	1:A:58:VAL:HG21	1:A:55:ASN:H	18	0.18
(2,699)	1:A:58:VAL:HG22	1:A:55:ASN:H	18	0.18
(2,699)	1:A:58:VAL:HG23	1:A:55:ASN:H	18	0.18
(2,683)	1:A:179:THR:HG21	1:A:185:GLY:H	7	0.18
(2,683)	1:A:179:THR:HG22	1:A:185:GLY:H	7	0.18
(2,683)	1:A:179:THR:HG23	1:A:185:GLY:H	7	0.18
(2,672)	1:A:66:ARG:H	1:A:156:LEU:HD22	20	0.18
(2,672)	1:A:66:ARG:H	1:A:156:LEU:HD23	20	0.18
(2,659)	1:A:42:MET:H	1:A:19:LEU:HD11	6	0.18
(2,659)	1:A:42:MET:H	1:A:19:LEU:HD12	6	0.18
(2,659)	1:A:42:MET:H	1:A:19:LEU:HD13	6	0.18
(2,653)	1:A:11:GLN:HE22	1:A:11:GLN:HE21	15	0.18
(2,621)	1:A:200:LEU:HD21	1:A:201:GLY:H	12	0.18
(2,60)	1:A:50:ILE:H	1:A:50:ILE:HD11	2	0.18
(2,60)	1:A:50:ILE:H	1:A:50:ILE:HD12	2	0.18
(2,60)	1:A:50:ILE:H	1:A:50:ILE:HD13	2	0.18
(2,570)	1:A:226:LEU:H	1:A:226:LEU:HD21	9	0.18
(2,511)	1:A:200:LEU:HD22	1:A:199:SER:H	4	0.18
(2,511)	1:A:200:LEU:HD23	1:A:199:SER:H	4	0.18
(2,511)	1:A:200:LEU:HD22	1:A:199:SER:H	12	0.18
(2,511)	1:A:200:LEU:HD23	1:A:199:SER:H	12	0.18
(2,456)	1:A:178:TRP:HE1	1:A:176:GLU:H	19	0.18
(2,445)	1:A:178:TRP:HE1	1:A:176:GLU:H	19	0.18
(2,388)	1:A:66:ARG:H	1:A:156:LEU:H	20	0.18
(2,353)	1:A:136:ILE:H	1:A:136:ILE:HD11	14	0.18
(2,353)	1:A:136:ILE:H	1:A:136:ILE:HD12	14	0.18
(2,353)	1:A:136:ILE:H	1:A:136:ILE:HD13	14	0.18
(2,235)	1:A:104:THR:H	1:A:107:ARG:H	12	0.18
(2,17)	1:A:93:ILE:H	1:A:93:ILE:HD11	14	0.18
(2,17)	1:A:93:ILE:H	1:A:93:ILE:HD12	14	0.18
(2,17)	1:A:93:ILE:H	1:A:93:ILE:HD13	14	0.18
(2,14)	1:A:159:ALA:H	1:A:171:HIS:H	10	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,120)	1:A:66:ARG:H	1:A:156:LEU:H	20	0.18
(2,113)	1:A:25:TYR:H	1:A:26:ASP:H	6	0.18
(2,10)	1:A:92:ARG:H	1:A:93:ILE:HG13	20	0.18
(2,10)	1:A:92:ARG:H	1:A:93:ILE:HG12	20	0.18
(2,977)	1:A:78:PHE:H	1:A:78:PHE:HA	8	0.17
(2,971)	1:A:77:LEU:HB3	1:A:78:PHE:H	9	0.17
(2,971)	1:A:77:LEU:HB3	1:A:78:PHE:H	9	0.17
(2,969)	1:A:77:LEU:H	1:A:78:PHE:H	7	0.17
(2,964)	1:A:75:TYR:H	1:A:76:SER:H	1	0.17
(2,959)	1:A:75:TYR:H	1:A:76:SER:H	1	0.17
(2,947)	1:A:74:GLU:HB3	1:A:75:TYR:H	10	0.17
(2,947)	1:A:74:GLU:HB3	1:A:75:TYR:H	10	0.17
(2,945)	1:A:74:GLU:H	1:A:74:GLU:HG3	16	0.17
(2,945)	1:A:74:GLU:H	1:A:74:GLU:HG3	16	0.17
(2,927)	1:A:72:VAL:H	1:A:73:ALA:H	6	0.17
(2,927)	1:A:72:VAL:H	1:A:73:ALA:H	6	0.17
(2,927)	1:A:72:VAL:H	1:A:73:ALA:H	13	0.17
(2,927)	1:A:72:VAL:H	1:A:73:ALA:H	13	0.17
(2,926)	1:A:72:VAL:HB	1:A:73:ALA:H	10	0.17
(2,921)	1:A:72:VAL:H	1:A:72:VAL:HA	8	0.17
(2,921)	1:A:72:VAL:H	1:A:72:VAL:HA	20	0.17
(2,917)	1:A:71:ASP:H	1:A:72:VAL:HB	3	0.17
(2,870)	1:A:186:ILE:HD12	1:A:156:LEU:HD22	6	0.17
(2,870)	1:A:186:ILE:HD12	1:A:156:LEU:HD23	6	0.17
(2,865)	1:A:186:ILE:HD11	1:A:186:ILE:HG13	13	0.17
(2,865)	1:A:186:ILE:HD12	1:A:186:ILE:HG13	13	0.17
(2,865)	1:A:186:ILE:HD13	1:A:186:ILE:HG13	13	0.17
(2,865)	1:A:186:ILE:HD11	1:A:186:ILE:HG12	13	0.17
(2,865)	1:A:186:ILE:HD12	1:A:186:ILE:HG12	13	0.17
(2,865)	1:A:186:ILE:HD13	1:A:186:ILE:HG12	13	0.17
(2,830)	1:A:120:ILE:HD11	1:A:120:ILE:HG13	10	0.17
(2,830)	1:A:120:ILE:HD12	1:A:120:ILE:HG13	10	0.17
(2,830)	1:A:120:ILE:HD13	1:A:120:ILE:HG13	10	0.17
(2,830)	1:A:120:ILE:HD11	1:A:120:ILE:HG12	10	0.17
(2,830)	1:A:120:ILE:HD12	1:A:120:ILE:HG12	10	0.17
(2,830)	1:A:120:ILE:HD13	1:A:120:ILE:HG12	10	0.17
(2,811)	1:A:103:ILE:HD11	1:A:103:ILE:HG13	10	0.17
(2,811)	1:A:103:ILE:HD12	1:A:103:ILE:HG13	10	0.17
(2,811)	1:A:103:ILE:HD13	1:A:103:ILE:HG13	10	0.17
(2,811)	1:A:103:ILE:HD11	1:A:103:ILE:HG12	10	0.17
(2,811)	1:A:103:ILE:HD12	1:A:103:ILE:HG12	10	0.17
(2,811)	1:A:103:ILE:HD13	1:A:103:ILE:HG12	10	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,809)	1:A:136:ILE:H	1:A:94:VAL:HG11	17	0.17
(2,809)	1:A:136:ILE:H	1:A:94:VAL:HG12	17	0.17
(2,809)	1:A:136:ILE:H	1:A:94:VAL:HG13	17	0.17
(2,804)	1:A:93:ILE:HD11	1:A:105:VAL:HG21	7	0.17
(2,804)	1:A:93:ILE:HD11	1:A:105:VAL:HG22	7	0.17
(2,804)	1:A:93:ILE:HD11	1:A:105:VAL:HG23	7	0.17
(2,804)	1:A:93:ILE:HD12	1:A:105:VAL:HG21	7	0.17
(2,804)	1:A:93:ILE:HD12	1:A:105:VAL:HG22	7	0.17
(2,804)	1:A:93:ILE:HD12	1:A:105:VAL:HG23	7	0.17
(2,804)	1:A:93:ILE:HD13	1:A:105:VAL:HG21	7	0.17
(2,804)	1:A:93:ILE:HD13	1:A:105:VAL:HG22	7	0.17
(2,804)	1:A:93:ILE:HD13	1:A:105:VAL:HG23	7	0.17
(2,803)	1:A:93:ILE:HD11	1:A:93:ILE:HG13	9	0.17
(2,803)	1:A:93:ILE:HD12	1:A:93:ILE:HG13	9	0.17
(2,803)	1:A:93:ILE:HD13	1:A:93:ILE:HG13	9	0.17
(2,803)	1:A:93:ILE:HD11	1:A:93:ILE:HG12	9	0.17
(2,803)	1:A:93:ILE:HD12	1:A:93:ILE:HG12	9	0.17
(2,803)	1:A:93:ILE:HD13	1:A:93:ILE:HG12	9	0.17
(2,803)	1:A:93:ILE:HD11	1:A:93:ILE:HG13	20	0.17
(2,803)	1:A:93:ILE:HD12	1:A:93:ILE:HG13	20	0.17
(2,803)	1:A:93:ILE:HD13	1:A:93:ILE:HG13	20	0.17
(2,803)	1:A:93:ILE:HD11	1:A:93:ILE:HG12	20	0.17
(2,803)	1:A:93:ILE:HD12	1:A:93:ILE:HG12	20	0.17
(2,803)	1:A:93:ILE:HD13	1:A:93:ILE:HG12	20	0.17
(2,75)	1:A:55:ASN:H	1:A:59:ILE:H	15	0.17
(2,737)	1:A:196:LEU:HD23	1:A:113:LEU:HD21	20	0.17
(2,716)	1:A:54:LEU:HD11	1:A:58:VAL:HG11	2	0.17
(2,716)	1:A:54:LEU:HD11	1:A:58:VAL:HG12	2	0.17
(2,716)	1:A:54:LEU:HD11	1:A:58:VAL:HG13	2	0.17
(2,716)	1:A:54:LEU:HD12	1:A:58:VAL:HG11	2	0.17
(2,716)	1:A:54:LEU:HD12	1:A:58:VAL:HG12	2	0.17
(2,716)	1:A:54:LEU:HD12	1:A:58:VAL:HG13	2	0.17
(2,716)	1:A:54:LEU:HD13	1:A:58:VAL:HG11	2	0.17
(2,716)	1:A:54:LEU:HD13	1:A:58:VAL:HG12	2	0.17
(2,716)	1:A:54:LEU:HD13	1:A:58:VAL:HG13	2	0.17
(2,680)	1:A:158:HIS:H	1:A:172:PHE:H	16	0.17
(2,673)	1:A:77:LEU:H	1:A:78:PHE:H	7	0.17
(2,62)	1:A:50:ILE:HG12	1:A:50:ILE:H	4	0.17
(2,500)	1:A:116:TRP:HE1	1:A:198:HIS:H	12	0.17
(2,426)	1:A:170:ALA:H	1:A:136:ILE:HD11	17	0.17
(2,426)	1:A:170:ALA:H	1:A:136:ILE:HD12	17	0.17
(2,426)	1:A:170:ALA:H	1:A:136:ILE:HD13	17	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,423)	1:A:169:ASP:H	1:A:134:ILE:HD11	15	0.17
(2,423)	1:A:169:ASP:H	1:A:134:ILE:HD12	15	0.17
(2,423)	1:A:169:ASP:H	1:A:134:ILE:HD13	15	0.17
(2,391)	1:A:157:ALA:H	1:A:156:LEU:H	18	0.17
(2,39)	1:A:43:GLN:HE21	1:A:43:GLN:HE22	13	0.17
(2,388)	1:A:66:ARG:H	1:A:156:LEU:H	18	0.17
(2,385)	1:A:157:ALA:H	1:A:156:LEU:H	18	0.17
(2,380)	1:A:10:LEU:H	1:A:10:LEU:HD22	6	0.17
(2,380)	1:A:10:LEU:H	1:A:10:LEU:HD23	6	0.17
(2,379)	1:A:10:LEU:H	1:A:10:LEU:HD21	7	0.17
(2,357)	1:A:136:ILE:HD11	1:A:137:GLY:H	13	0.17
(2,357)	1:A:136:ILE:HD12	1:A:137:GLY:H	13	0.17
(2,357)	1:A:136:ILE:HD13	1:A:137:GLY:H	13	0.17
(2,317)	1:A:125:ARG:H	1:A:91:TYR:H	5	0.17
(2,314)	1:A:125:ARG:H	1:A:124:PHE:HA	8	0.17
(2,274)	1:A:116:TRP:HE1	1:A:197:GLY:H	8	0.17
(2,239)	1:A:108:LEU:H	1:A:108:LEU:HD21	18	0.17
(2,228)	1:A:106:ASP:H	1:A:108:LEU:H	10	0.17
(2,226)	1:A:104:THR:H	1:A:106:ASP:H	2	0.17
(2,226)	1:A:104:THR:H	1:A:106:ASP:H	18	0.17
(2,215)	1:A:103:ILE:H	1:A:103:ILE:HG13	9	0.17
(2,215)	1:A:103:ILE:H	1:A:103:ILE:HG12	9	0.17
(2,120)	1:A:66:ARG:H	1:A:156:LEU:H	18	0.17
(2,113)	1:A:25:TYR:H	1:A:26:ASP:H	4	0.17
(2,103)	1:A:39:LEU:H	1:A:37:ALA:H	16	0.17
(3,32)	1:A:154:ASN:ND2	4:A:305:PX4:C35	17	0.16
(3,32)	1:A:154:ASN:ND2	4:A:307:PX4:C35	17	0.16
(3,32)	1:A:154:ASN:ND2	4:A:309:PX4:C35	17	0.16
(3,32)	1:A:154:ASN:ND2	4:A:311:PX4:C35	17	0.16
(3,32)	1:A:154:ASN:ND2	4:A:313:PX4:C35	17	0.16
(3,32)	1:A:154:ASN:ND2	4:A:315:PX4:C35	17	0.16
(3,32)	1:A:154:ASN:ND2	4:A:317:PX4:C35	17	0.16
(3,32)	1:A:154:ASN:ND2	4:A:319:PX4:C35	17	0.16
(3,32)	1:A:154:ASN:ND2	4:A:321:PX4:C35	17	0.16
(3,32)	1:A:154:ASN:ND2	4:A:323:PX4:C35	17	0.16
(3,32)	1:A:154:ASN:ND2	4:A:325:PX4:C35	17	0.16
(3,32)	1:A:154:ASN:ND2	4:A:327:PX4:C35	17	0.16
(3,32)	1:A:154:ASN:ND2	4:A:329:PX4:C35	17	0.16
(3,32)	1:A:154:ASN:ND2	4:A:331:PX4:C35	17	0.16
(3,32)	1:A:154:ASN:ND2	4:A:333:PX4:C35	17	0.16
(3,32)	1:A:154:ASN:ND2	4:A:335:PX4:C35	17	0.16
(3,32)	1:A:154:ASN:ND2	4:A:337:PX4:C35	17	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,32)	1:A:154:ASN:ND2	4:A:339:PX4:C35	17	0.16
(3,32)	1:A:154:ASN:ND2	4:A:341:PX4:C35	17	0.16
(3,32)	1:A:154:ASN:ND2	4:A:343:PX4:C35	17	0.16
(3,32)	1:A:154:ASN:ND2	4:A:345:PX4:C35	17	0.16
(3,32)	1:A:154:ASN:ND2	4:A:347:PX4:C35	17	0.16
(3,32)	1:A:154:ASN:ND2	4:A:349:PX4:C35	17	0.16
(3,32)	1:A:154:ASN:ND2	4:A:351:PX4:C35	17	0.16
(3,32)	1:A:154:ASN:ND2	4:A:353:PX4:C35	17	0.16
(3,32)	1:A:154:ASN:ND2	4:A:355:PX4:C35	17	0.16
(3,32)	1:A:154:ASN:ND2	4:A:357:PX4:C35	17	0.16
(3,32)	1:A:154:ASN:ND2	4:A:359:PX4:C35	17	0.16
(3,32)	1:A:154:ASN:ND2	4:A:361:PX4:C35	17	0.16
(3,32)	1:A:154:ASN:ND2	4:A:363:PX4:C35	17	0.16
(3,32)	1:A:154:ASN:ND2	4:A:402:PX4:C35	17	0.16
(3,32)	1:A:154:ASN:ND2	4:A:404:PX4:C35	17	0.16
(3,32)	1:A:154:ASN:ND2	4:A:406:PX4:C35	17	0.16
(3,32)	1:A:154:ASN:ND2	4:A:408:PX4:C35	17	0.16
(3,32)	1:A:154:ASN:ND2	4:A:410:PX4:C35	17	0.16
(3,32)	1:A:154:ASN:ND2	4:A:412:PX4:C35	17	0.16
(3,32)	1:A:154:ASN:ND2	4:A:414:PX4:C35	17	0.16
(3,32)	1:A:154:ASN:ND2	4:A:416:PX4:C35	17	0.16
(3,32)	1:A:154:ASN:ND2	4:A:418:PX4:C35	17	0.16
(3,32)	1:A:154:ASN:ND2	4:A:420:PX4:C35	17	0.16
(3,32)	1:A:154:ASN:ND2	4:A:422:PX4:C35	17	0.16
(3,32)	1:A:154:ASN:ND2	4:A:424:PX4:C35	17	0.16
(3,32)	1:A:154:ASN:ND2	4:A:426:PX4:C35	17	0.16
(3,32)	1:A:154:ASN:ND2	4:A:428:PX4:C35	17	0.16
(3,32)	1:A:154:ASN:ND2	4:A:430:PX4:C35	17	0.16
(3,32)	1:A:154:ASN:ND2	4:A:305:PX4:C35	19	0.16
(3,32)	1:A:154:ASN:ND2	4:A:307:PX4:C35	19	0.16
(3,32)	1:A:154:ASN:ND2	4:A:309:PX4:C35	19	0.16
(3,32)	1:A:154:ASN:ND2	4:A:311:PX4:C35	19	0.16
(3,32)	1:A:154:ASN:ND2	4:A:313:PX4:C35	19	0.16
(3,32)	1:A:154:ASN:ND2	4:A:315:PX4:C35	19	0.16
(3,32)	1:A:154:ASN:ND2	4:A:317:PX4:C35	19	0.16
(3,32)	1:A:154:ASN:ND2	4:A:319:PX4:C35	19	0.16
(3,32)	1:A:154:ASN:ND2	4:A:321:PX4:C35	19	0.16
(3,32)	1:A:154:ASN:ND2	4:A:323:PX4:C35	19	0.16
(3,32)	1:A:154:ASN:ND2	4:A:325:PX4:C35	19	0.16
(3,32)	1:A:154:ASN:ND2	4:A:327:PX4:C35	19	0.16
(3,32)	1:A:154:ASN:ND2	4:A:329:PX4:C35	19	0.16
(3,32)	1:A:154:ASN:ND2	4:A:331:PX4:C35	19	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,32)	1:A:154:ASN:ND2	4:A:333:PX4:C35	19	0.16
(3,32)	1:A:154:ASN:ND2	4:A:335:PX4:C35	19	0.16
(3,32)	1:A:154:ASN:ND2	4:A:337:PX4:C35	19	0.16
(3,32)	1:A:154:ASN:ND2	4:A:339:PX4:C35	19	0.16
(3,32)	1:A:154:ASN:ND2	4:A:341:PX4:C35	19	0.16
(3,32)	1:A:154:ASN:ND2	4:A:343:PX4:C35	19	0.16
(3,32)	1:A:154:ASN:ND2	4:A:345:PX4:C35	19	0.16
(3,32)	1:A:154:ASN:ND2	4:A:347:PX4:C35	19	0.16
(3,32)	1:A:154:ASN:ND2	4:A:349:PX4:C35	19	0.16
(3,32)	1:A:154:ASN:ND2	4:A:351:PX4:C35	19	0.16
(3,32)	1:A:154:ASN:ND2	4:A:353:PX4:C35	19	0.16
(3,32)	1:A:154:ASN:ND2	4:A:355:PX4:C35	19	0.16
(3,32)	1:A:154:ASN:ND2	4:A:357:PX4:C35	19	0.16
(3,32)	1:A:154:ASN:ND2	4:A:359:PX4:C35	19	0.16
(3,32)	1:A:154:ASN:ND2	4:A:361:PX4:C35	19	0.16
(3,32)	1:A:154:ASN:ND2	4:A:363:PX4:C35	19	0.16
(3,32)	1:A:154:ASN:ND2	4:A:402:PX4:C35	19	0.16
(3,32)	1:A:154:ASN:ND2	4:A:404:PX4:C35	19	0.16
(3,32)	1:A:154:ASN:ND2	4:A:406:PX4:C35	19	0.16
(3,32)	1:A:154:ASN:ND2	4:A:408:PX4:C35	19	0.16
(3,32)	1:A:154:ASN:ND2	4:A:410:PX4:C35	19	0.16
(3,32)	1:A:154:ASN:ND2	4:A:412:PX4:C35	19	0.16
(3,32)	1:A:154:ASN:ND2	4:A:414:PX4:C35	19	0.16
(3,32)	1:A:154:ASN:ND2	4:A:416:PX4:C35	19	0.16
(3,32)	1:A:154:ASN:ND2	4:A:418:PX4:C35	19	0.16
(3,32)	1:A:154:ASN:ND2	4:A:420:PX4:C35	19	0.16
(3,32)	1:A:154:ASN:ND2	4:A:422:PX4:C35	19	0.16
(3,32)	1:A:154:ASN:ND2	4:A:424:PX4:C35	19	0.16
(3,32)	1:A:154:ASN:ND2	4:A:426:PX4:C35	19	0.16
(3,32)	1:A:154:ASN:ND2	4:A:428:PX4:C35	19	0.16
(3,32)	1:A:154:ASN:ND2	4:A:430:PX4:C35	19	0.16
(2,980)	1:A:78:PHE:H	1:A:79:PRO:HD3	16	0.16
(2,980)	1:A:78:PHE:H	1:A:79:PRO:HD3	16	0.16
(2,964)	1:A:75:TYR:H	1:A:76:SER:H	10	0.16
(2,959)	1:A:75:TYR:H	1:A:76:SER:H	10	0.16
(2,949)	1:A:74:GLU:H	1:A:75:TYR:H	3	0.16
(2,938)	1:A:73:ALA:HA	1:A:74:GLU:H	5	0.16
(2,915)	1:A:71:ASP:H	1:A:72:VAL:HG21	15	0.16
(2,915)	1:A:71:ASP:H	1:A:72:VAL:HG22	15	0.16
(2,915)	1:A:71:ASP:H	1:A:72:VAL:HG23	15	0.16
(2,909)	1:A:69:VAL:H	1:A:69:VAL:HA	3	0.16
(2,907)	1:A:68:GLY:H	1:A:69:VAL:H	8	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,907)	1:A:68:GLY:H	1:A:69:VAL:H	15	0.16
(2,904)	1:A:67:CYS:H	1:A:67:CYS:HA	18	0.16
(2,904)	1:A:67:CYS:H	1:A:67:CYS:HA	20	0.16
(2,894)	1:A:64:LYS:H	1:A:64:LYS:HG3	10	0.16
(2,894)	1:A:64:LYS:H	1:A:64:LYS:HG3	10	0.16
(2,889)	1:A:63:GLN:HA	1:A:63:GLN:H	20	0.16
(2,887)	1:A:134:ILE:HD11	1:A:134:ILE:HG21	6	0.16
(2,887)	1:A:134:ILE:HD11	1:A:134:ILE:HG22	6	0.16
(2,887)	1:A:134:ILE:HD11	1:A:134:ILE:HG23	6	0.16
(2,887)	1:A:134:ILE:HD12	1:A:134:ILE:HG21	6	0.16
(2,887)	1:A:134:ILE:HD12	1:A:134:ILE:HG22	6	0.16
(2,887)	1:A:134:ILE:HD12	1:A:134:ILE:HG23	6	0.16
(2,887)	1:A:134:ILE:HD13	1:A:134:ILE:HG21	6	0.16
(2,887)	1:A:134:ILE:HD13	1:A:134:ILE:HG22	6	0.16
(2,887)	1:A:134:ILE:HD13	1:A:134:ILE:HG23	6	0.16
(2,885)	1:A:134:ILE:HD11	1:A:89:VAL:HG11	5	0.16
(2,885)	1:A:134:ILE:HD11	1:A:89:VAL:HG12	5	0.16
(2,885)	1:A:134:ILE:HD11	1:A:89:VAL:HG13	5	0.16
(2,885)	1:A:134:ILE:HD12	1:A:89:VAL:HG11	5	0.16
(2,885)	1:A:134:ILE:HD12	1:A:89:VAL:HG12	5	0.16
(2,885)	1:A:134:ILE:HD12	1:A:89:VAL:HG13	5	0.16
(2,885)	1:A:134:ILE:HD13	1:A:89:VAL:HG11	5	0.16
(2,885)	1:A:134:ILE:HD13	1:A:89:VAL:HG12	5	0.16
(2,885)	1:A:134:ILE:HD13	1:A:89:VAL:HG13	5	0.16
(2,870)	1:A:186:ILE:HD12	1:A:156:LEU:HD22	14	0.16
(2,870)	1:A:186:ILE:HD12	1:A:156:LEU:HD23	14	0.16
(2,865)	1:A:186:ILE:HD11	1:A:186:ILE:HG13	3	0.16
(2,865)	1:A:186:ILE:HD12	1:A:186:ILE:HG13	3	0.16
(2,865)	1:A:186:ILE:HD13	1:A:186:ILE:HG13	3	0.16
(2,865)	1:A:186:ILE:HD11	1:A:186:ILE:HG12	3	0.16
(2,865)	1:A:186:ILE:HD12	1:A:186:ILE:HG12	3	0.16
(2,865)	1:A:186:ILE:HD13	1:A:186:ILE:HG12	3	0.16
(2,865)	1:A:186:ILE:HD11	1:A:186:ILE:HG13	7	0.16
(2,865)	1:A:186:ILE:HD12	1:A:186:ILE:HG13	7	0.16
(2,865)	1:A:186:ILE:HD13	1:A:186:ILE:HG13	7	0.16
(2,865)	1:A:186:ILE:HD11	1:A:186:ILE:HG12	7	0.16
(2,865)	1:A:186:ILE:HD12	1:A:186:ILE:HG12	7	0.16
(2,865)	1:A:186:ILE:HD13	1:A:186:ILE:HG12	7	0.16
(2,839)	1:A:123:HIS:H	1:A:122:LEU:HD11	2	0.16
(2,839)	1:A:123:HIS:H	1:A:122:LEU:HD12	2	0.16
(2,839)	1:A:123:HIS:H	1:A:122:LEU:HD13	2	0.16
(2,830)	1:A:120:ILE:HD11	1:A:120:ILE:HG13	16	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,830)	1:A:120:ILE:HD12	1:A:120:ILE:HG13	16	0.16
(2,830)	1:A:120:ILE:HD13	1:A:120:ILE:HG13	16	0.16
(2,830)	1:A:120:ILE:HD11	1:A:120:ILE:HG12	16	0.16
(2,830)	1:A:120:ILE:HD12	1:A:120:ILE:HG12	16	0.16
(2,830)	1:A:120:ILE:HD13	1:A:120:ILE:HG12	16	0.16
(2,830)	1:A:120:ILE:HD11	1:A:120:ILE:HG13	19	0.16
(2,830)	1:A:120:ILE:HD12	1:A:120:ILE:HG13	19	0.16
(2,830)	1:A:120:ILE:HD13	1:A:120:ILE:HG13	19	0.16
(2,830)	1:A:120:ILE:HD11	1:A:120:ILE:HG12	19	0.16
(2,830)	1:A:120:ILE:HD12	1:A:120:ILE:HG12	19	0.16
(2,830)	1:A:120:ILE:HD13	1:A:120:ILE:HG12	19	0.16
(2,811)	1:A:103:ILE:HD11	1:A:103:ILE:HG13	5	0.16
(2,811)	1:A:103:ILE:HD12	1:A:103:ILE:HG13	5	0.16
(2,811)	1:A:103:ILE:HD13	1:A:103:ILE:HG13	5	0.16
(2,811)	1:A:103:ILE:HD11	1:A:103:ILE:HG12	5	0.16
(2,811)	1:A:103:ILE:HD12	1:A:103:ILE:HG12	5	0.16
(2,811)	1:A:103:ILE:HD13	1:A:103:ILE:HG12	5	0.16
(2,811)	1:A:103:ILE:HD11	1:A:103:ILE:HG13	18	0.16
(2,811)	1:A:103:ILE:HD12	1:A:103:ILE:HG13	18	0.16
(2,811)	1:A:103:ILE:HD13	1:A:103:ILE:HG13	18	0.16
(2,811)	1:A:103:ILE:HD11	1:A:103:ILE:HG12	18	0.16
(2,811)	1:A:103:ILE:HD12	1:A:103:ILE:HG12	18	0.16
(2,811)	1:A:103:ILE:HD13	1:A:103:ILE:HG12	18	0.16
(2,81)	1:A:58:VAL:HG21	1:A:58:VAL:H	6	0.16
(2,81)	1:A:58:VAL:HG22	1:A:58:VAL:H	6	0.16
(2,81)	1:A:58:VAL:HG23	1:A:58:VAL:H	6	0.16
(2,809)	1:A:136:ILE:H	1:A:94:VAL:HG11	13	0.16
(2,809)	1:A:136:ILE:H	1:A:94:VAL:HG12	13	0.16
(2,809)	1:A:136:ILE:H	1:A:94:VAL:HG13	13	0.16
(2,801)	1:A:93:ILE:H	1:A:93:ILE:HD11	12	0.16
(2,801)	1:A:93:ILE:H	1:A:93:ILE:HD12	12	0.16
(2,801)	1:A:93:ILE:H	1:A:93:ILE:HD13	12	0.16
(2,797)	1:A:58:VAL:HG21	1:A:58:VAL:HG11	7	0.16
(2,797)	1:A:58:VAL:HG21	1:A:58:VAL:HG12	7	0.16
(2,797)	1:A:58:VAL:HG21	1:A:58:VAL:HG13	7	0.16
(2,797)	1:A:58:VAL:HG22	1:A:58:VAL:HG11	7	0.16
(2,797)	1:A:58:VAL:HG22	1:A:58:VAL:HG12	7	0.16
(2,797)	1:A:58:VAL:HG22	1:A:58:VAL:HG13	7	0.16
(2,797)	1:A:58:VAL:HG23	1:A:58:VAL:HG11	7	0.16
(2,797)	1:A:58:VAL:HG23	1:A:58:VAL:HG12	7	0.16
(2,797)	1:A:58:VAL:HG23	1:A:58:VAL:HG13	7	0.16
(2,786)	1:A:24:LEU:H	1:A:24:LEU:HD21	13	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,786)	1:A:24:LEU:H	1:A:24:LEU:HD21	19	0.16
(2,773)	1:A:61:ILE:HD11	1:A:48:LEU:HD21	20	0.16
(2,766)	1:A:22:PHE:H	1:A:19:LEU:HD22	1	0.16
(2,766)	1:A:22:PHE:H	1:A:19:LEU:HD23	1	0.16
(2,744)	1:A:134:ILE:HD11	1:A:89:VAL:HG11	5	0.16
(2,744)	1:A:134:ILE:HD11	1:A:89:VAL:HG12	5	0.16
(2,744)	1:A:134:ILE:HD11	1:A:89:VAL:HG13	5	0.16
(2,744)	1:A:134:ILE:HD12	1:A:89:VAL:HG11	5	0.16
(2,744)	1:A:134:ILE:HD12	1:A:89:VAL:HG12	5	0.16
(2,744)	1:A:134:ILE:HD12	1:A:89:VAL:HG13	5	0.16
(2,744)	1:A:134:ILE:HD13	1:A:89:VAL:HG11	5	0.16
(2,744)	1:A:134:ILE:HD13	1:A:89:VAL:HG12	5	0.16
(2,744)	1:A:134:ILE:HD13	1:A:89:VAL:HG13	5	0.16
(2,717)	1:A:54:LEU:HD11	1:A:39:LEU:HD11	14	0.16
(2,717)	1:A:54:LEU:HD11	1:A:39:LEU:HD12	14	0.16
(2,717)	1:A:54:LEU:HD11	1:A:39:LEU:HD13	14	0.16
(2,717)	1:A:54:LEU:HD12	1:A:39:LEU:HD11	14	0.16
(2,717)	1:A:54:LEU:HD12	1:A:39:LEU:HD12	14	0.16
(2,717)	1:A:54:LEU:HD12	1:A:39:LEU:HD13	14	0.16
(2,717)	1:A:54:LEU:HD13	1:A:39:LEU:HD11	14	0.16
(2,717)	1:A:54:LEU:HD13	1:A:39:LEU:HD12	14	0.16
(2,717)	1:A:54:LEU:HD13	1:A:39:LEU:HD13	14	0.16
(2,701)	1:A:58:VAL:HG21	1:A:58:VAL:H	6	0.16
(2,701)	1:A:58:VAL:HG22	1:A:58:VAL:H	6	0.16
(2,701)	1:A:58:VAL:HG23	1:A:58:VAL:H	6	0.16
(2,683)	1:A:179:THR:HG21	1:A:185:GLY:H	9	0.16
(2,683)	1:A:179:THR:HG22	1:A:185:GLY:H	9	0.16
(2,683)	1:A:179:THR:HG23	1:A:185:GLY:H	9	0.16
(2,680)	1:A:158:HIS:H	1:A:172:PHE:H	14	0.16
(2,67)	1:A:53:MET:H	1:A:52:GLY:H	7	0.16
(2,64)	1:A:52:GLY:H	1:A:53:MET:H	7	0.16
(2,626)	1:A:12:TRP:H	1:A:10:LEU:H	18	0.16
(2,558)	1:A:23:TYR:H	1:A:24:LEU:H	2	0.16
(2,558)	1:A:23:TYR:H	1:A:24:LEU:H	19	0.16
(2,557)	1:A:21:ARG:H	1:A:23:TYR:H	13	0.16
(2,533)	1:A:23:TYR:H	1:A:24:LEU:H	2	0.16
(2,533)	1:A:23:TYR:H	1:A:24:LEU:H	19	0.16
(2,511)	1:A:200:LEU:HD22	1:A:199:SER:H	6	0.16
(2,511)	1:A:200:LEU:HD23	1:A:199:SER:H	6	0.16
(2,501)	1:A:198:HIS:H	1:A:195:ALA:H	5	0.16
(2,466)	1:A:84:TRP:H	1:A:200:LEU:HD21	3	0.16
(2,453)	1:A:178:TRP:HE1	1:A:175:ASP:H	3	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,442)	1:A:175:ASP:H	1:A:178:TRP:HE1	3	0.16
(2,397)	1:A:169:ASP:H	1:A:160:PHE:H	13	0.16
(2,326)	1:A:128:VAL:H	1:A:129:TRP:H	6	0.16
(2,326)	1:A:128:VAL:H	1:A:129:TRP:H	13	0.16
(2,324)	1:A:128:VAL:H	1:A:129:TRP:H	6	0.16
(2,324)	1:A:128:VAL:H	1:A:129:TRP:H	13	0.16
(2,304)	1:A:123:HIS:H	1:A:122:LEU:HD11	2	0.16
(2,304)	1:A:123:HIS:H	1:A:122:LEU:HD12	2	0.16
(2,304)	1:A:123:HIS:H	1:A:122:LEU:HD13	2	0.16
(2,258)	1:A:112:ALA:H	1:A:189:LEU:HD22	2	0.16
(2,258)	1:A:112:ALA:H	1:A:189:LEU:HD23	2	0.16
(2,226)	1:A:104:THR:H	1:A:106:ASP:H	5	0.16
(2,17)	1:A:93:ILE:H	1:A:93:ILE:HD11	12	0.16
(2,17)	1:A:93:ILE:H	1:A:93:ILE:HD12	12	0.16
(2,17)	1:A:93:ILE:H	1:A:93:ILE:HD13	12	0.16
(2,13)	1:A:135:MET:H	1:A:170:ALA:H	1	0.16
(2,103)	1:A:39:LEU:H	1:A:37:ALA:H	5	0.16
(2,977)	1:A:78:PHE:H	1:A:78:PHE:HA	5	0.15
(2,977)	1:A:78:PHE:H	1:A:78:PHE:HA	10	0.15
(2,976)	1:A:78:PHE:H	1:A:78:PHE:HD1	17	0.15
(2,976)	1:A:78:PHE:H	1:A:78:PHE:HD2	17	0.15
(2,969)	1:A:77:LEU:H	1:A:78:PHE:H	17	0.15
(2,969)	1:A:77:LEU:H	1:A:78:PHE:H	19	0.15
(2,968)	1:A:77:LEU:H	1:A:77:LEU:HA	18	0.15
(2,953)	1:A:74:GLU:HB3	1:A:76:SER:H	2	0.15
(2,953)	1:A:74:GLU:HB3	1:A:76:SER:H	2	0.15
(2,947)	1:A:74:GLU:HB3	1:A:75:TYR:H	13	0.15
(2,947)	1:A:74:GLU:HB3	1:A:75:TYR:H	13	0.15
(2,945)	1:A:74:GLU:H	1:A:74:GLU:HG3	19	0.15
(2,945)	1:A:74:GLU:H	1:A:74:GLU:HG3	19	0.15
(2,935)	1:A:73:ALA:H	1:A:73:ALA:HA	6	0.15
(2,927)	1:A:72:VAL:H	1:A:73:ALA:H	14	0.15
(2,927)	1:A:72:VAL:H	1:A:73:ALA:H	14	0.15
(2,926)	1:A:72:VAL:HB	1:A:73:ALA:H	19	0.15
(2,921)	1:A:72:VAL:H	1:A:72:VAL:HA	19	0.15
(2,916)	1:A:71:ASP:H	1:A:72:VAL:HA	3	0.15
(2,909)	1:A:69:VAL:H	1:A:69:VAL:HA	17	0.15
(2,892)	1:A:64:LYS:H	1:A:63:GLN:HA	17	0.15
(2,865)	1:A:186:ILE:HD11	1:A:186:ILE:HG13	12	0.15
(2,865)	1:A:186:ILE:HD12	1:A:186:ILE:HG13	12	0.15
(2,865)	1:A:186:ILE:HD13	1:A:186:ILE:HG13	12	0.15
(2,865)	1:A:186:ILE:HD11	1:A:186:ILE:HG12	12	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,865)	1:A:186:ILE:HD12	1:A:186:ILE:HG12	12	0.15
(2,865)	1:A:186:ILE:HD13	1:A:186:ILE:HG12	12	0.15
(2,865)	1:A:186:ILE:HD11	1:A:186:ILE:HG13	16	0.15
(2,865)	1:A:186:ILE:HD12	1:A:186:ILE:HG13	16	0.15
(2,865)	1:A:186:ILE:HD13	1:A:186:ILE:HG13	16	0.15
(2,865)	1:A:186:ILE:HD11	1:A:186:ILE:HG12	16	0.15
(2,865)	1:A:186:ILE:HD12	1:A:186:ILE:HG12	16	0.15
(2,865)	1:A:186:ILE:HD13	1:A:186:ILE:HG12	16	0.15
(2,833)	1:A:120:ILE:HD11	1:A:200:LEU:HD22	9	0.15
(2,833)	1:A:120:ILE:HD11	1:A:200:LEU:HD23	9	0.15
(2,830)	1:A:120:ILE:HD11	1:A:120:ILE:HG13	7	0.15
(2,830)	1:A:120:ILE:HD12	1:A:120:ILE:HG13	7	0.15
(2,830)	1:A:120:ILE:HD13	1:A:120:ILE:HG13	7	0.15
(2,830)	1:A:120:ILE:HD11	1:A:120:ILE:HG12	7	0.15
(2,830)	1:A:120:ILE:HD12	1:A:120:ILE:HG12	7	0.15
(2,830)	1:A:120:ILE:HD13	1:A:120:ILE:HG12	7	0.15
(2,830)	1:A:120:ILE:HD11	1:A:120:ILE:HG13	11	0.15
(2,830)	1:A:120:ILE:HD12	1:A:120:ILE:HG13	11	0.15
(2,830)	1:A:120:ILE:HD13	1:A:120:ILE:HG13	11	0.15
(2,830)	1:A:120:ILE:HD11	1:A:120:ILE:HG12	11	0.15
(2,830)	1:A:120:ILE:HD12	1:A:120:ILE:HG12	11	0.15
(2,830)	1:A:120:ILE:HD13	1:A:120:ILE:HG12	11	0.15
(2,811)	1:A:103:ILE:HD11	1:A:103:ILE:HG13	12	0.15
(2,811)	1:A:103:ILE:HD12	1:A:103:ILE:HG13	12	0.15
(2,811)	1:A:103:ILE:HD13	1:A:103:ILE:HG13	12	0.15
(2,811)	1:A:103:ILE:HD11	1:A:103:ILE:HG12	12	0.15
(2,811)	1:A:103:ILE:HD12	1:A:103:ILE:HG12	12	0.15
(2,811)	1:A:103:ILE:HD13	1:A:103:ILE:HG12	12	0.15
(2,810)	1:A:93:ILE:H	1:A:94:VAL:HG11	5	0.15
(2,810)	1:A:93:ILE:H	1:A:94:VAL:HG12	5	0.15
(2,810)	1:A:93:ILE:H	1:A:94:VAL:HG13	5	0.15
(2,810)	1:A:93:ILE:H	1:A:94:VAL:HG11	14	0.15
(2,810)	1:A:93:ILE:H	1:A:94:VAL:HG12	14	0.15
(2,810)	1:A:93:ILE:H	1:A:94:VAL:HG13	14	0.15
(2,786)	1:A:24:LEU:H	1:A:24:LEU:HD21	17	0.15
(2,764)	1:A:120:ILE:HD11	1:A:122:LEU:H	2	0.15
(2,764)	1:A:120:ILE:HD12	1:A:122:LEU:H	2	0.15
(2,764)	1:A:120:ILE:HD13	1:A:122:LEU:H	2	0.15
(2,74)	1:A:55:ASN:H	1:A:55:ASN:HD21	12	0.15
(2,729)	1:A:211:VAL:HG12	1:A:226:LEU:HD21	4	0.15
(2,729)	1:A:211:VAL:HG12	1:A:226:LEU:HD21	11	0.15
(2,683)	1:A:179:THR:HG21	1:A:185:GLY:H	4	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,683)	1:A:179:THR:HG22	1:A:185:GLY:H	4	0.15
(2,683)	1:A:179:THR:HG23	1:A:185:GLY:H	4	0.15
(2,683)	1:A:179:THR:HG21	1:A:185:GLY:H	10	0.15
(2,683)	1:A:179:THR:HG22	1:A:185:GLY:H	10	0.15
(2,683)	1:A:179:THR:HG23	1:A:185:GLY:H	10	0.15
(2,673)	1:A:77:LEU:H	1:A:78:PHE:H	17	0.15
(2,673)	1:A:77:LEU:H	1:A:78:PHE:H	19	0.15
(2,623)	1:A:6:GLY:H	1:A:7:MET:H	4	0.15
(2,62)	1:A:50:ILE:HG12	1:A:50:ILE:H	16	0.15
(2,62)	1:A:50:ILE:HG12	1:A:50:ILE:H	20	0.15
(2,564)	1:A:231:ILE:H	1:A:231:ILE:HG13	15	0.15
(2,564)	1:A:231:ILE:H	1:A:231:ILE:HG12	15	0.15
(2,557)	1:A:21:ARG:H	1:A:23:TYR:H	9	0.15
(2,547)	1:A:211:VAL:H	1:A:211:VAL:HG11	13	0.15
(2,547)	1:A:211:VAL:H	1:A:211:VAL:HG12	13	0.15
(2,547)	1:A:211:VAL:H	1:A:211:VAL:HG13	13	0.15
(2,547)	1:A:211:VAL:H	1:A:211:VAL:HG21	13	0.15
(2,547)	1:A:211:VAL:H	1:A:211:VAL:HG22	13	0.15
(2,547)	1:A:211:VAL:H	1:A:211:VAL:HG23	13	0.15
(2,547)	1:A:211:VAL:H	1:A:211:VAL:HG11	16	0.15
(2,547)	1:A:211:VAL:H	1:A:211:VAL:HG12	16	0.15
(2,547)	1:A:211:VAL:H	1:A:211:VAL:HG13	16	0.15
(2,547)	1:A:211:VAL:H	1:A:211:VAL:HG21	16	0.15
(2,547)	1:A:211:VAL:H	1:A:211:VAL:HG22	16	0.15
(2,547)	1:A:211:VAL:H	1:A:211:VAL:HG23	16	0.15
(2,547)	1:A:211:VAL:H	1:A:211:VAL:HG11	19	0.15
(2,547)	1:A:211:VAL:H	1:A:211:VAL:HG12	19	0.15
(2,547)	1:A:211:VAL:H	1:A:211:VAL:HG13	19	0.15
(2,547)	1:A:211:VAL:H	1:A:211:VAL:HG21	19	0.15
(2,547)	1:A:211:VAL:H	1:A:211:VAL:HG22	19	0.15
(2,547)	1:A:211:VAL:H	1:A:211:VAL:HG23	19	0.15
(2,538)	1:A:205:SER:H	1:A:213:TYR:H	2	0.15
(2,538)	1:A:205:SER:H	1:A:213:TYR:H	8	0.15
(2,501)	1:A:198:HIS:H	1:A:195:ALA:H	18	0.15
(2,474)	1:A:186:ILE:H	1:A:186:ILE:HG13	15	0.15
(2,474)	1:A:186:ILE:H	1:A:186:ILE:HG12	15	0.15
(2,423)	1:A:169:ASP:H	1:A:134:ILE:HD11	4	0.15
(2,423)	1:A:169:ASP:H	1:A:134:ILE:HD12	4	0.15
(2,423)	1:A:169:ASP:H	1:A:134:ILE:HD13	4	0.15
(2,357)	1:A:136:ILE:HD11	1:A:137:GLY:H	11	0.15
(2,357)	1:A:136:ILE:HD12	1:A:137:GLY:H	11	0.15
(2,357)	1:A:136:ILE:HD13	1:A:137:GLY:H	11	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,357)	1:A:136:ILE:HD11	1:A:137:GLY:H	20	0.15
(2,357)	1:A:136:ILE:HD12	1:A:137:GLY:H	20	0.15
(2,357)	1:A:136:ILE:HD13	1:A:137:GLY:H	20	0.15
(2,353)	1:A:136:ILE:H	1:A:136:ILE:HD11	8	0.15
(2,353)	1:A:136:ILE:H	1:A:136:ILE:HD12	8	0.15
(2,353)	1:A:136:ILE:H	1:A:136:ILE:HD13	8	0.15
(2,326)	1:A:128:VAL:H	1:A:129:TRP:H	14	0.15
(2,324)	1:A:128:VAL:H	1:A:129:TRP:H	14	0.15
(2,317)	1:A:125:ARG:H	1:A:91:TYR:H	8	0.15
(2,301)	1:A:120:ILE:HD11	1:A:122:LEU:H	2	0.15
(2,301)	1:A:120:ILE:HD12	1:A:122:LEU:H	2	0.15
(2,301)	1:A:120:ILE:HD13	1:A:122:LEU:H	2	0.15
(2,226)	1:A:104:THR:H	1:A:106:ASP:H	4	0.15
(2,979)	1:A:78:PHE:H	1:A:78:PHE:HD1	8	0.14
(2,976)	1:A:78:PHE:H	1:A:78:PHE:HD1	15	0.14
(2,976)	1:A:78:PHE:H	1:A:78:PHE:HD2	15	0.14
(2,975)	1:A:78:PHE:H	1:A:77:LEU:HD22	19	0.14
(2,975)	1:A:78:PHE:H	1:A:77:LEU:HD23	19	0.14
(2,974)	1:A:78:PHE:H	1:A:77:LEU:HD21	2	0.14
(2,969)	1:A:77:LEU:H	1:A:78:PHE:H	6	0.14
(2,968)	1:A:77:LEU:H	1:A:77:LEU:HA	2	0.14
(2,935)	1:A:73:ALA:H	1:A:73:ALA:HA	1	0.14
(2,920)	1:A:72:VAL:H	1:A:71:ASP:H	6	0.14
(2,920)	1:A:72:VAL:H	1:A:71:ASP:H	6	0.14
(2,909)	1:A:69:VAL:H	1:A:69:VAL:HA	6	0.14
(2,909)	1:A:69:VAL:H	1:A:69:VAL:HA	9	0.14
(2,904)	1:A:67:CYS:H	1:A:67:CYS:HA	12	0.14
(2,89)	1:A:59:ILE:H	1:A:59:ILE:HG13	18	0.14
(2,89)	1:A:59:ILE:H	1:A:59:ILE:HG12	18	0.14
(2,868)	1:A:186:ILE:HD11	1:A:156:LEU:HD22	4	0.14
(2,868)	1:A:186:ILE:HD11	1:A:156:LEU:HD23	4	0.14
(2,865)	1:A:186:ILE:HD11	1:A:186:ILE:HG13	10	0.14
(2,865)	1:A:186:ILE:HD12	1:A:186:ILE:HG13	10	0.14
(2,865)	1:A:186:ILE:HD13	1:A:186:ILE:HG13	10	0.14
(2,865)	1:A:186:ILE:HD11	1:A:186:ILE:HG12	10	0.14
(2,865)	1:A:186:ILE:HD12	1:A:186:ILE:HG12	10	0.14
(2,865)	1:A:186:ILE:HD13	1:A:186:ILE:HG12	10	0.14
(2,865)	1:A:186:ILE:HD11	1:A:186:ILE:HG13	20	0.14
(2,865)	1:A:186:ILE:HD12	1:A:186:ILE:HG13	20	0.14
(2,865)	1:A:186:ILE:HD13	1:A:186:ILE:HG13	20	0.14
(2,865)	1:A:186:ILE:HD11	1:A:186:ILE:HG12	20	0.14
(2,865)	1:A:186:ILE:HD12	1:A:186:ILE:HG12	20	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,865)	1:A:186:ILE:HD13	1:A:186:ILE:HG12	20	0.14
(2,839)	1:A:123:HIS:H	1:A:122:LEU:HD11	15	0.14
(2,839)	1:A:123:HIS:H	1:A:122:LEU:HD12	15	0.14
(2,839)	1:A:123:HIS:H	1:A:122:LEU:HD13	15	0.14
(2,811)	1:A:103:ILE:HD11	1:A:103:ILE:HG13	9	0.14
(2,811)	1:A:103:ILE:HD12	1:A:103:ILE:HG13	9	0.14
(2,811)	1:A:103:ILE:HD13	1:A:103:ILE:HG13	9	0.14
(2,811)	1:A:103:ILE:HD11	1:A:103:ILE:HG12	9	0.14
(2,811)	1:A:103:ILE:HD12	1:A:103:ILE:HG12	9	0.14
(2,811)	1:A:103:ILE:HD13	1:A:103:ILE:HG12	9	0.14
(2,809)	1:A:136:ILE:H	1:A:94:VAL:HG11	1	0.14
(2,809)	1:A:136:ILE:H	1:A:94:VAL:HG12	1	0.14
(2,809)	1:A:136:ILE:H	1:A:94:VAL:HG13	1	0.14
(2,809)	1:A:136:ILE:H	1:A:94:VAL:HG11	2	0.14
(2,809)	1:A:136:ILE:H	1:A:94:VAL:HG12	2	0.14
(2,809)	1:A:136:ILE:H	1:A:94:VAL:HG13	2	0.14
(2,803)	1:A:93:ILE:HD11	1:A:93:ILE:HG13	13	0.14
(2,803)	1:A:93:ILE:HD12	1:A:93:ILE:HG13	13	0.14
(2,803)	1:A:93:ILE:HD13	1:A:93:ILE:HG13	13	0.14
(2,803)	1:A:93:ILE:HD11	1:A:93:ILE:HG12	13	0.14
(2,803)	1:A:93:ILE:HD12	1:A:93:ILE:HG12	13	0.14
(2,803)	1:A:93:ILE:HD13	1:A:93:ILE:HG12	13	0.14
(2,803)	1:A:93:ILE:HD11	1:A:93:ILE:HG13	15	0.14
(2,803)	1:A:93:ILE:HD12	1:A:93:ILE:HG13	15	0.14
(2,803)	1:A:93:ILE:HD13	1:A:93:ILE:HG13	15	0.14
(2,803)	1:A:93:ILE:HD11	1:A:93:ILE:HG12	15	0.14
(2,803)	1:A:93:ILE:HD12	1:A:93:ILE:HG12	15	0.14
(2,803)	1:A:93:ILE:HD13	1:A:93:ILE:HG12	15	0.14
(2,8)	1:A:135:MET:H	1:A:92:ARG:H	8	0.14
(2,74)	1:A:55:ASN:H	1:A:55:ASN:HD21	14	0.14
(2,731)	1:A:211:VAL:HG13	1:A:226:LEU:HD21	14	0.14
(2,673)	1:A:77:LEU:H	1:A:78:PHE:H	6	0.14
(2,670)	1:A:66:ARG:H	1:A:156:LEU:HD11	9	0.14
(2,670)	1:A:66:ARG:H	1:A:156:LEU:HD12	9	0.14
(2,670)	1:A:66:ARG:H	1:A:156:LEU:HD13	9	0.14
(2,659)	1:A:42:MET:H	1:A:19:LEU:HD11	9	0.14
(2,659)	1:A:42:MET:H	1:A:19:LEU:HD12	9	0.14
(2,659)	1:A:42:MET:H	1:A:19:LEU:HD13	9	0.14
(2,63)	1:A:52:GLY:H	1:A:51:THR:H	4	0.14
(2,63)	1:A:52:GLY:H	1:A:51:THR:H	12	0.14
(2,570)	1:A:226:LEU:H	1:A:226:LEU:HD21	13	0.14
(2,558)	1:A:23:TYR:H	1:A:24:LEU:H	8	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,543)	1:A:210:ALA:H	1:A:213:TYR:H	4	0.14
(2,533)	1:A:23:TYR:H	1:A:24:LEU:H	8	0.14
(2,511)	1:A:200:LEU:HD22	1:A:199:SER:H	9	0.14
(2,511)	1:A:200:LEU:HD23	1:A:199:SER:H	9	0.14
(2,478)	1:A:179:THR:H	1:A:188:PHE:H	7	0.14
(2,457)	1:A:179:THR:H	1:A:188:PHE:H	7	0.14
(2,404)	1:A:161:ALA:H	1:A:161:ALA:HB1	8	0.14
(2,404)	1:A:161:ALA:H	1:A:161:ALA:HB2	8	0.14
(2,404)	1:A:161:ALA:H	1:A:161:ALA:HB3	8	0.14
(2,391)	1:A:157:ALA:H	1:A:156:LEU:H	16	0.14
(2,385)	1:A:157:ALA:H	1:A:156:LEU:H	16	0.14
(2,381)	1:A:151:GLY:H	1:A:150:ASP:H	10	0.14
(2,368)	1:A:151:GLY:H	1:A:150:ASP:H	10	0.14
(2,326)	1:A:128:VAL:H	1:A:129:TRP:H	1	0.14
(2,324)	1:A:128:VAL:H	1:A:129:TRP:H	1	0.14
(2,321)	1:A:128:VAL:HG11	1:A:126:LYS:H	20	0.14
(2,321)	1:A:128:VAL:HG12	1:A:126:LYS:H	20	0.14
(2,321)	1:A:128:VAL:HG13	1:A:126:LYS:H	20	0.14
(2,304)	1:A:123:HIS:H	1:A:122:LEU:HD11	15	0.14
(2,304)	1:A:123:HIS:H	1:A:122:LEU:HD12	15	0.14
(2,304)	1:A:123:HIS:H	1:A:122:LEU:HD13	15	0.14
(2,264)	1:A:113:LEU:H	1:A:196:LEU:HD21	15	0.14
(2,239)	1:A:108:LEU:H	1:A:108:LEU:HD21	4	0.14
(2,226)	1:A:104:THR:H	1:A:106:ASP:H	6	0.14
(2,226)	1:A:104:THR:H	1:A:106:ASP:H	15	0.14
(2,14)	1:A:159:ALA:H	1:A:171:HIS:H	15	0.14
(2,13)	1:A:135:MET:H	1:A:170:ALA:H	14	0.14
(2,968)	1:A:77:LEU:H	1:A:77:LEU:HA	20	0.13
(2,952)	1:A:74:GLU:HA	1:A:76:SER:H	9	0.13
(2,945)	1:A:74:GLU:H	1:A:74:GLU:HG3	11	0.13
(2,945)	1:A:74:GLU:H	1:A:74:GLU:HG3	11	0.13
(2,935)	1:A:73:ALA:H	1:A:73:ALA:HA	4	0.13
(2,935)	1:A:73:ALA:H	1:A:73:ALA:HA	5	0.13
(2,931)	1:A:72:VAL:H	1:A:75:TYR:HB3	1	0.13
(2,931)	1:A:72:VAL:H	1:A:75:TYR:HB3	1	0.13
(2,920)	1:A:72:VAL:H	1:A:71:ASP:H	7	0.13
(2,920)	1:A:72:VAL:H	1:A:71:ASP:H	7	0.13
(2,916)	1:A:71:ASP:H	1:A:72:VAL:HA	6	0.13
(2,916)	1:A:71:ASP:H	1:A:72:VAL:HA	10	0.13
(2,916)	1:A:71:ASP:H	1:A:72:VAL:HA	14	0.13
(2,912)	1:A:70:PRO:HB3	1:A:76:SER:H	14	0.13
(2,912)	1:A:70:PRO:HB2	1:A:76:SER:H	14	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,907)	1:A:68:GLY:H	1:A:69:VAL:H	19	0.13
(2,889)	1:A:63:GLN:HA	1:A:63:GLN:H	17	0.13
(2,885)	1:A:134:ILE:HD11	1:A:89:VAL:HG11	8	0.13
(2,885)	1:A:134:ILE:HD11	1:A:89:VAL:HG12	8	0.13
(2,885)	1:A:134:ILE:HD11	1:A:89:VAL:HG13	8	0.13
(2,885)	1:A:134:ILE:HD12	1:A:89:VAL:HG11	8	0.13
(2,885)	1:A:134:ILE:HD12	1:A:89:VAL:HG12	8	0.13
(2,885)	1:A:134:ILE:HD12	1:A:89:VAL:HG13	8	0.13
(2,885)	1:A:134:ILE:HD13	1:A:89:VAL:HG11	8	0.13
(2,885)	1:A:134:ILE:HD13	1:A:89:VAL:HG12	8	0.13
(2,885)	1:A:134:ILE:HD13	1:A:89:VAL:HG13	8	0.13
(2,866)	1:A:186:ILE:HD11	1:A:156:LEU:HD11	7	0.13
(2,866)	1:A:186:ILE:HD11	1:A:156:LEU:HD12	7	0.13
(2,866)	1:A:186:ILE:HD11	1:A:156:LEU:HD13	7	0.13
(2,866)	1:A:186:ILE:HD12	1:A:156:LEU:HD11	7	0.13
(2,866)	1:A:186:ILE:HD12	1:A:156:LEU:HD12	7	0.13
(2,866)	1:A:186:ILE:HD12	1:A:156:LEU:HD13	7	0.13
(2,866)	1:A:186:ILE:HD13	1:A:156:LEU:HD11	7	0.13
(2,866)	1:A:186:ILE:HD13	1:A:156:LEU:HD12	7	0.13
(2,866)	1:A:186:ILE:HD13	1:A:156:LEU:HD13	7	0.13
(2,865)	1:A:186:ILE:HD11	1:A:186:ILE:HG13	6	0.13
(2,865)	1:A:186:ILE:HD12	1:A:186:ILE:HG13	6	0.13
(2,865)	1:A:186:ILE:HD13	1:A:186:ILE:HG13	6	0.13
(2,865)	1:A:186:ILE:HD11	1:A:186:ILE:HG12	6	0.13
(2,865)	1:A:186:ILE:HD12	1:A:186:ILE:HG12	6	0.13
(2,865)	1:A:186:ILE:HD13	1:A:186:ILE:HG12	6	0.13
(2,865)	1:A:186:ILE:HD11	1:A:186:ILE:HG13	11	0.13
(2,865)	1:A:186:ILE:HD12	1:A:186:ILE:HG13	11	0.13
(2,865)	1:A:186:ILE:HD13	1:A:186:ILE:HG13	11	0.13
(2,865)	1:A:186:ILE:HD11	1:A:186:ILE:HG12	11	0.13
(2,865)	1:A:186:ILE:HD12	1:A:186:ILE:HG12	11	0.13
(2,865)	1:A:186:ILE:HD13	1:A:186:ILE:HG12	11	0.13
(2,843)	1:A:200:LEU:HD21	1:A:122:LEU:HD22	18	0.13
(2,843)	1:A:200:LEU:HD21	1:A:122:LEU:HD23	18	0.13
(2,839)	1:A:123:HIS:H	1:A:122:LEU:HD11	17	0.13
(2,839)	1:A:123:HIS:H	1:A:122:LEU:HD12	17	0.13
(2,839)	1:A:123:HIS:H	1:A:122:LEU:HD13	17	0.13
(2,830)	1:A:120:ILE:HD11	1:A:120:ILE:HG13	1	0.13
(2,830)	1:A:120:ILE:HD12	1:A:120:ILE:HG13	1	0.13
(2,830)	1:A:120:ILE:HD13	1:A:120:ILE:HG13	1	0.13
(2,830)	1:A:120:ILE:HD11	1:A:120:ILE:HG12	1	0.13
(2,830)	1:A:120:ILE:HD12	1:A:120:ILE:HG12	1	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,830)	1:A:120:ILE:HD13	1:A:120:ILE:HG12	1	0.13
(2,830)	1:A:120:ILE:HD11	1:A:120:ILE:HG13	2	0.13
(2,830)	1:A:120:ILE:HD12	1:A:120:ILE:HG13	2	0.13
(2,830)	1:A:120:ILE:HD13	1:A:120:ILE:HG13	2	0.13
(2,830)	1:A:120:ILE:HD11	1:A:120:ILE:HG12	2	0.13
(2,830)	1:A:120:ILE:HD12	1:A:120:ILE:HG12	2	0.13
(2,830)	1:A:120:ILE:HD13	1:A:120:ILE:HG12	2	0.13
(2,830)	1:A:120:ILE:HD11	1:A:120:ILE:HG13	17	0.13
(2,830)	1:A:120:ILE:HD12	1:A:120:ILE:HG13	17	0.13
(2,830)	1:A:120:ILE:HD13	1:A:120:ILE:HG13	17	0.13
(2,830)	1:A:120:ILE:HD11	1:A:120:ILE:HG12	17	0.13
(2,830)	1:A:120:ILE:HD12	1:A:120:ILE:HG12	17	0.13
(2,830)	1:A:120:ILE:HD13	1:A:120:ILE:HG12	17	0.13
(2,811)	1:A:103:ILE:HD11	1:A:103:ILE:HG13	3	0.13
(2,811)	1:A:103:ILE:HD12	1:A:103:ILE:HG13	3	0.13
(2,811)	1:A:103:ILE:HD13	1:A:103:ILE:HG13	3	0.13
(2,811)	1:A:103:ILE:HD11	1:A:103:ILE:HG12	3	0.13
(2,811)	1:A:103:ILE:HD12	1:A:103:ILE:HG12	3	0.13
(2,811)	1:A:103:ILE:HD13	1:A:103:ILE:HG12	3	0.13
(2,811)	1:A:103:ILE:HD11	1:A:103:ILE:HG13	6	0.13
(2,811)	1:A:103:ILE:HD12	1:A:103:ILE:HG13	6	0.13
(2,811)	1:A:103:ILE:HD13	1:A:103:ILE:HG13	6	0.13
(2,811)	1:A:103:ILE:HD11	1:A:103:ILE:HG12	6	0.13
(2,811)	1:A:103:ILE:HD12	1:A:103:ILE:HG12	6	0.13
(2,811)	1:A:103:ILE:HD13	1:A:103:ILE:HG12	6	0.13
(2,811)	1:A:103:ILE:HD11	1:A:103:ILE:HG13	8	0.13
(2,811)	1:A:103:ILE:HD12	1:A:103:ILE:HG13	8	0.13
(2,811)	1:A:103:ILE:HD13	1:A:103:ILE:HG13	8	0.13
(2,811)	1:A:103:ILE:HD11	1:A:103:ILE:HG12	8	0.13
(2,811)	1:A:103:ILE:HD12	1:A:103:ILE:HG12	8	0.13
(2,811)	1:A:103:ILE:HD13	1:A:103:ILE:HG12	8	0.13
(2,811)	1:A:103:ILE:HD11	1:A:103:ILE:HG13	14	0.13
(2,811)	1:A:103:ILE:HD12	1:A:103:ILE:HG13	14	0.13
(2,811)	1:A:103:ILE:HD13	1:A:103:ILE:HG13	14	0.13
(2,811)	1:A:103:ILE:HD11	1:A:103:ILE:HG12	14	0.13
(2,811)	1:A:103:ILE:HD12	1:A:103:ILE:HG12	14	0.13
(2,811)	1:A:103:ILE:HD13	1:A:103:ILE:HG12	14	0.13
(2,811)	1:A:103:ILE:HD11	1:A:103:ILE:HG13	15	0.13
(2,811)	1:A:103:ILE:HD12	1:A:103:ILE:HG13	15	0.13
(2,811)	1:A:103:ILE:HD13	1:A:103:ILE:HG13	15	0.13
(2,811)	1:A:103:ILE:HD11	1:A:103:ILE:HG12	15	0.13
(2,811)	1:A:103:ILE:HD12	1:A:103:ILE:HG12	15	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,811)	1:A:103:ILE:HD13	1:A:103:ILE:HG12	15	0.13
(2,811)	1:A:103:ILE:HD11	1:A:103:ILE:HG13	17	0.13
(2,811)	1:A:103:ILE:HD12	1:A:103:ILE:HG13	17	0.13
(2,811)	1:A:103:ILE:HD13	1:A:103:ILE:HG13	17	0.13
(2,811)	1:A:103:ILE:HD11	1:A:103:ILE:HG12	17	0.13
(2,811)	1:A:103:ILE:HD12	1:A:103:ILE:HG12	17	0.13
(2,811)	1:A:103:ILE:HD13	1:A:103:ILE:HG12	17	0.13
(2,809)	1:A:136:ILE:H	1:A:94:VAL:HG11	12	0.13
(2,809)	1:A:136:ILE:H	1:A:94:VAL:HG12	12	0.13
(2,809)	1:A:136:ILE:H	1:A:94:VAL:HG13	12	0.13
(2,803)	1:A:93:ILE:HD11	1:A:93:ILE:HG13	5	0.13
(2,803)	1:A:93:ILE:HD12	1:A:93:ILE:HG13	5	0.13
(2,803)	1:A:93:ILE:HD13	1:A:93:ILE:HG13	5	0.13
(2,803)	1:A:93:ILE:HD11	1:A:93:ILE:HG12	5	0.13
(2,803)	1:A:93:ILE:HD12	1:A:93:ILE:HG12	5	0.13
(2,803)	1:A:93:ILE:HD13	1:A:93:ILE:HG12	5	0.13
(2,803)	1:A:93:ILE:HD11	1:A:93:ILE:HG13	8	0.13
(2,803)	1:A:93:ILE:HD12	1:A:93:ILE:HG13	8	0.13
(2,803)	1:A:93:ILE:HD13	1:A:93:ILE:HG13	8	0.13
(2,803)	1:A:93:ILE:HD11	1:A:93:ILE:HG12	8	0.13
(2,803)	1:A:93:ILE:HD12	1:A:93:ILE:HG12	8	0.13
(2,803)	1:A:93:ILE:HD13	1:A:93:ILE:HG12	8	0.13
(2,803)	1:A:93:ILE:HD11	1:A:93:ILE:HG13	10	0.13
(2,803)	1:A:93:ILE:HD12	1:A:93:ILE:HG13	10	0.13
(2,803)	1:A:93:ILE:HD13	1:A:93:ILE:HG13	10	0.13
(2,803)	1:A:93:ILE:HD11	1:A:93:ILE:HG12	10	0.13
(2,803)	1:A:93:ILE:HD12	1:A:93:ILE:HG12	10	0.13
(2,803)	1:A:93:ILE:HD13	1:A:93:ILE:HG12	10	0.13
(2,744)	1:A:134:ILE:HD11	1:A:89:VAL:HG11	8	0.13
(2,744)	1:A:134:ILE:HD11	1:A:89:VAL:HG12	8	0.13
(2,744)	1:A:134:ILE:HD11	1:A:89:VAL:HG13	8	0.13
(2,744)	1:A:134:ILE:HD12	1:A:89:VAL:HG11	8	0.13
(2,744)	1:A:134:ILE:HD12	1:A:89:VAL:HG12	8	0.13
(2,744)	1:A:134:ILE:HD12	1:A:89:VAL:HG13	8	0.13
(2,744)	1:A:134:ILE:HD13	1:A:89:VAL:HG11	8	0.13
(2,744)	1:A:134:ILE:HD13	1:A:89:VAL:HG12	8	0.13
(2,744)	1:A:134:ILE:HD13	1:A:89:VAL:HG13	8	0.13
(2,692)	1:A:180:ASP:H	1:A:181:GLY:H	13	0.13
(2,680)	1:A:158:HIS:H	1:A:172:PHE:H	4	0.13
(2,659)	1:A:42:MET:H	1:A:19:LEU:HD11	7	0.13
(2,659)	1:A:42:MET:H	1:A:19:LEU:HD12	7	0.13
(2,659)	1:A:42:MET:H	1:A:19:LEU:HD13	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,632)	1:A:25:TYR:H	1:A:24:LEU:HD21	5	0.13
(2,623)	1:A:6:GLY:H	1:A:7:MET:H	14	0.13
(2,62)	1:A:50:ILE:HG12	1:A:50:ILE:H	3	0.13
(2,62)	1:A:50:ILE:HG12	1:A:50:ILE:H	5	0.13
(2,618)	1:A:13:GLU:H	1:A:12:TRP:H	20	0.13
(2,60)	1:A:50:ILE:H	1:A:50:ILE:HD11	1	0.13
(2,60)	1:A:50:ILE:H	1:A:50:ILE:HD12	1	0.13
(2,60)	1:A:50:ILE:H	1:A:50:ILE:HD13	1	0.13
(2,557)	1:A:21:ARG:H	1:A:23:TYR:H	5	0.13
(2,547)	1:A:211:VAL:H	1:A:211:VAL:HG11	8	0.13
(2,547)	1:A:211:VAL:H	1:A:211:VAL:HG12	8	0.13
(2,547)	1:A:211:VAL:H	1:A:211:VAL:HG13	8	0.13
(2,547)	1:A:211:VAL:H	1:A:211:VAL:HG21	8	0.13
(2,547)	1:A:211:VAL:H	1:A:211:VAL:HG22	8	0.13
(2,547)	1:A:211:VAL:H	1:A:211:VAL:HG23	8	0.13
(2,539)	1:A:206:SER:H	1:A:207:ASP:H	8	0.13
(2,539)	1:A:206:SER:H	1:A:207:ASP:H	8	0.13
(2,504)	1:A:198:HIS:H	1:A:202:MET:H	8	0.13
(2,501)	1:A:198:HIS:H	1:A:195:ALA:H	10	0.13
(2,499)	1:A:197:GLY:H	1:A:198:HIS:H	15	0.13
(2,499)	1:A:197:GLY:H	1:A:198:HIS:H	15	0.13
(2,469)	1:A:177:ARG:H	1:A:186:ILE:H	12	0.13
(2,453)	1:A:178:TRP:HE1	1:A:175:ASP:H	19	0.13
(2,442)	1:A:175:ASP:H	1:A:178:TRP:HE1	19	0.13
(2,414)	1:A:167:GLY:H	1:A:166:LEU:HD21	7	0.13
(2,4)	1:A:13:GLU:H	1:A:12:TRP:H	20	0.13
(2,369)	1:A:143:HIS:H	1:A:145:ASP:H	6	0.13
(2,315)	1:A:125:ARG:H	1:A:126:LYS:H	14	0.13
(2,304)	1:A:123:HIS:H	1:A:122:LEU:HD11	17	0.13
(2,304)	1:A:123:HIS:H	1:A:122:LEU:HD12	17	0.13
(2,304)	1:A:123:HIS:H	1:A:122:LEU:HD13	17	0.13
(2,239)	1:A:108:LEU:H	1:A:108:LEU:HD21	1	0.13
(2,215)	1:A:103:ILE:H	1:A:103:ILE:HG13	20	0.13
(2,215)	1:A:103:ILE:H	1:A:103:ILE:HG12	20	0.13
(2,185)	1:A:94:VAL:H	1:A:92:ARG:H	18	0.13
(2,179)	1:A:92:ARG:H	1:A:134:ILE:HD11	15	0.13
(2,179)	1:A:92:ARG:H	1:A:134:ILE:HD12	15	0.13
(2,179)	1:A:92:ARG:H	1:A:134:ILE:HD13	15	0.13
(2,14)	1:A:159:ALA:H	1:A:171:HIS:H	17	0.13
(2,13)	1:A:135:MET:H	1:A:170:ALA:H	19	0.13
(2,122)	1:A:177:ARG:H	1:A:186:ILE:H	12	0.13
(2,113)	1:A:25:TYR:H	1:A:26:ASP:H	16	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,977)	1:A:78:PHE:H	1:A:78:PHE:HA	11	0.12
(2,969)	1:A:77:LEU:H	1:A:78:PHE:H	15	0.12
(2,968)	1:A:77:LEU:H	1:A:77:LEU:HA	3	0.12
(2,968)	1:A:77:LEU:H	1:A:77:LEU:HA	13	0.12
(2,949)	1:A:74:GLU:H	1:A:75:TYR:H	6	0.12
(2,949)	1:A:74:GLU:H	1:A:75:TYR:H	9	0.12
(2,947)	1:A:74:GLU:HB3	1:A:75:TYR:H	7	0.12
(2,947)	1:A:74:GLU:HB3	1:A:75:TYR:H	7	0.12
(2,935)	1:A:73:ALA:H	1:A:73:ALA:HA	10	0.12
(2,935)	1:A:73:ALA:H	1:A:73:ALA:HA	19	0.12
(2,926)	1:A:72:VAL:HB	1:A:73:ALA:H	14	0.12
(2,920)	1:A:72:VAL:H	1:A:71:ASP:H	4	0.12
(2,920)	1:A:72:VAL:H	1:A:71:ASP:H	4	0.12
(2,916)	1:A:71:ASP:H	1:A:72:VAL:HA	16	0.12
(2,915)	1:A:71:ASP:H	1:A:72:VAL:HG21	3	0.12
(2,915)	1:A:71:ASP:H	1:A:72:VAL:HG22	3	0.12
(2,915)	1:A:71:ASP:H	1:A:72:VAL:HG23	3	0.12
(2,909)	1:A:69:VAL:H	1:A:69:VAL:HA	7	0.12
(2,909)	1:A:69:VAL:H	1:A:69:VAL:HA	11	0.12
(2,909)	1:A:69:VAL:H	1:A:69:VAL:HA	18	0.12
(2,906)	1:A:68:GLY:H	1:A:68:GLY:HA3	10	0.12
(2,906)	1:A:68:GLY:H	1:A:68:GLY:HA3	10	0.12
(2,904)	1:A:67:CYS:H	1:A:67:CYS:HA	16	0.12
(2,901)	1:A:66:ARG:H	1:A:66:ARG:HB3	6	0.12
(2,901)	1:A:66:ARG:H	1:A:66:ARG:HB3	6	0.12
(2,869)	1:A:186:ILE:HD12	1:A:156:LEU:HD21	9	0.12
(2,865)	1:A:186:ILE:HD11	1:A:186:ILE:HG13	2	0.12
(2,865)	1:A:186:ILE:HD12	1:A:186:ILE:HG13	2	0.12
(2,865)	1:A:186:ILE:HD13	1:A:186:ILE:HG13	2	0.12
(2,865)	1:A:186:ILE:HD11	1:A:186:ILE:HG12	2	0.12
(2,865)	1:A:186:ILE:HD12	1:A:186:ILE:HG12	2	0.12
(2,865)	1:A:186:ILE:HD13	1:A:186:ILE:HG12	2	0.12
(2,830)	1:A:120:ILE:HD11	1:A:120:ILE:HG13	5	0.12
(2,830)	1:A:120:ILE:HD12	1:A:120:ILE:HG13	5	0.12
(2,830)	1:A:120:ILE:HD13	1:A:120:ILE:HG13	5	0.12
(2,830)	1:A:120:ILE:HD11	1:A:120:ILE:HG12	5	0.12
(2,830)	1:A:120:ILE:HD12	1:A:120:ILE:HG12	5	0.12
(2,830)	1:A:120:ILE:HD13	1:A:120:ILE:HG12	5	0.12
(2,830)	1:A:120:ILE:HD11	1:A:120:ILE:HG13	12	0.12
(2,830)	1:A:120:ILE:HD12	1:A:120:ILE:HG13	12	0.12
(2,830)	1:A:120:ILE:HD13	1:A:120:ILE:HG13	12	0.12
(2,830)	1:A:120:ILE:HD11	1:A:120:ILE:HG12	12	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,830)	1:A:120:ILE:HD12	1:A:120:ILE:HG12	12	0.12
(2,830)	1:A:120:ILE:HD13	1:A:120:ILE:HG12	12	0.12
(2,811)	1:A:103:ILE:HD11	1:A:103:ILE:HG13	4	0.12
(2,811)	1:A:103:ILE:HD12	1:A:103:ILE:HG13	4	0.12
(2,811)	1:A:103:ILE:HD13	1:A:103:ILE:HG13	4	0.12
(2,811)	1:A:103:ILE:HD11	1:A:103:ILE:HG12	4	0.12
(2,811)	1:A:103:ILE:HD12	1:A:103:ILE:HG12	4	0.12
(2,811)	1:A:103:ILE:HD13	1:A:103:ILE:HG12	4	0.12
(2,803)	1:A:93:ILE:HD11	1:A:93:ILE:HG13	1	0.12
(2,803)	1:A:93:ILE:HD12	1:A:93:ILE:HG13	1	0.12
(2,803)	1:A:93:ILE:HD13	1:A:93:ILE:HG13	1	0.12
(2,803)	1:A:93:ILE:HD11	1:A:93:ILE:HG12	1	0.12
(2,803)	1:A:93:ILE:HD12	1:A:93:ILE:HG12	1	0.12
(2,803)	1:A:93:ILE:HD13	1:A:93:ILE:HG12	1	0.12
(2,803)	1:A:93:ILE:HD11	1:A:93:ILE:HG13	11	0.12
(2,803)	1:A:93:ILE:HD12	1:A:93:ILE:HG13	11	0.12
(2,803)	1:A:93:ILE:HD13	1:A:93:ILE:HG13	11	0.12
(2,803)	1:A:93:ILE:HD11	1:A:93:ILE:HG12	11	0.12
(2,803)	1:A:93:ILE:HD12	1:A:93:ILE:HG12	11	0.12
(2,803)	1:A:93:ILE:HD13	1:A:93:ILE:HG12	11	0.12
(2,8)	1:A:135:MET:H	1:A:92:ARG:H	15	0.12
(2,677)	1:A:125:ARG:H	1:A:90:THR:H	14	0.12
(2,673)	1:A:77:LEU:H	1:A:78:PHE:H	15	0.12
(2,67)	1:A:53:MET:H	1:A:52:GLY:H	10	0.12
(2,659)	1:A:42:MET:H	1:A:19:LEU:HD11	11	0.12
(2,659)	1:A:42:MET:H	1:A:19:LEU:HD12	11	0.12
(2,659)	1:A:42:MET:H	1:A:19:LEU:HD13	11	0.12
(2,64)	1:A:52:GLY:H	1:A:53:MET:H	10	0.12
(2,63)	1:A:52:GLY:H	1:A:51:THR:H	17	0.12
(2,609)	1:A:238:TYR:H	1:A:239:GLY:H	13	0.12
(2,603)	1:A:238:TYR:H	1:A:239:GLY:H	13	0.12
(2,570)	1:A:226:LEU:H	1:A:226:LEU:HD21	15	0.12
(2,547)	1:A:211:VAL:H	1:A:211:VAL:HG11	9	0.12
(2,547)	1:A:211:VAL:H	1:A:211:VAL:HG12	9	0.12
(2,547)	1:A:211:VAL:H	1:A:211:VAL:HG13	9	0.12
(2,547)	1:A:211:VAL:H	1:A:211:VAL:HG21	9	0.12
(2,547)	1:A:211:VAL:H	1:A:211:VAL:HG22	9	0.12
(2,547)	1:A:211:VAL:H	1:A:211:VAL:HG23	9	0.12
(2,547)	1:A:211:VAL:H	1:A:211:VAL:HG11	14	0.12
(2,547)	1:A:211:VAL:H	1:A:211:VAL:HG12	14	0.12
(2,547)	1:A:211:VAL:H	1:A:211:VAL:HG13	14	0.12
(2,547)	1:A:211:VAL:H	1:A:211:VAL:HG21	14	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,547)	1:A:211:VAL:H	1:A:211:VAL:HG22	14	0.12
(2,547)	1:A:211:VAL:H	1:A:211:VAL:HG23	14	0.12
(2,538)	1:A:205:SER:H	1:A:213:TYR:H	10	0.12
(2,518)	1:A:200:LEU:H	1:A:196:LEU:HD22	12	0.12
(2,518)	1:A:200:LEU:H	1:A:196:LEU:HD23	12	0.12
(2,489)	1:A:116:TRP:HE1	1:A:196:LEU:H	14	0.12
(2,462)	1:A:182:SER:H	1:A:181:GLY:H	3	0.12
(2,462)	1:A:182:SER:H	1:A:181:GLY:H	3	0.12
(2,426)	1:A:170:ALA:H	1:A:136:ILE:HD11	6	0.12
(2,426)	1:A:170:ALA:H	1:A:136:ILE:HD12	6	0.12
(2,426)	1:A:170:ALA:H	1:A:136:ILE:HD13	6	0.12
(2,426)	1:A:170:ALA:H	1:A:136:ILE:HD11	9	0.12
(2,426)	1:A:170:ALA:H	1:A:136:ILE:HD12	9	0.12
(2,426)	1:A:170:ALA:H	1:A:136:ILE:HD13	9	0.12
(2,423)	1:A:169:ASP:H	1:A:134:ILE:HD11	6	0.12
(2,423)	1:A:169:ASP:H	1:A:134:ILE:HD12	6	0.12
(2,423)	1:A:169:ASP:H	1:A:134:ILE:HD13	6	0.12
(2,423)	1:A:169:ASP:H	1:A:134:ILE:HD11	10	0.12
(2,423)	1:A:169:ASP:H	1:A:134:ILE:HD12	10	0.12
(2,423)	1:A:169:ASP:H	1:A:134:ILE:HD13	10	0.12
(2,391)	1:A:157:ALA:H	1:A:156:LEU:H	7	0.12
(2,385)	1:A:157:ALA:H	1:A:156:LEU:H	7	0.12
(2,36)	1:A:46:PHE:H	1:A:43:GLN:H	20	0.12
(2,326)	1:A:128:VAL:H	1:A:129:TRP:H	19	0.12
(2,324)	1:A:128:VAL:H	1:A:129:TRP:H	19	0.12
(2,305)	1:A:123:HIS:H	1:A:122:LEU:HD21	13	0.12
(2,275)	1:A:116:TRP:HE1	1:A:196:LEU:H	14	0.12
(2,235)	1:A:104:THR:H	1:A:107:ARG:H	13	0.12
(2,215)	1:A:103:ILE:H	1:A:103:ILE:HG13	18	0.12
(2,215)	1:A:103:ILE:H	1:A:103:ILE:HG12	18	0.12
(2,203)	1:A:99:ASP:H	1:A:98:ARG:H	9	0.12
(2,200)	1:A:99:ASP:H	1:A:98:ARG:H	9	0.12
(2,179)	1:A:92:ARG:H	1:A:134:ILE:HD11	6	0.12
(2,179)	1:A:92:ARG:H	1:A:134:ILE:HD12	6	0.12
(2,179)	1:A:92:ARG:H	1:A:134:ILE:HD13	6	0.12
(2,155)	1:A:88:VAL:H	1:A:87:LYS:H	7	0.12
(2,155)	1:A:88:VAL:H	1:A:87:LYS:H	7	0.12
(2,13)	1:A:135:MET:H	1:A:170:ALA:H	4	0.12
(2,113)	1:A:25:TYR:H	1:A:26:ASP:H	18	0.12
(3,35)	1:A:194:HIS:H	4:A:305:PX4:C35	15	0.11
(3,35)	1:A:194:HIS:H	4:A:307:PX4:C35	15	0.11
(3,35)	1:A:194:HIS:H	4:A:309:PX4:C35	15	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,35)	1:A:194:HIS:H	4:A:311:PX4:C35	15	0.11
(3,35)	1:A:194:HIS:H	4:A:313:PX4:C35	15	0.11
(3,35)	1:A:194:HIS:H	4:A:315:PX4:C35	15	0.11
(3,35)	1:A:194:HIS:H	4:A:317:PX4:C35	15	0.11
(3,35)	1:A:194:HIS:H	4:A:319:PX4:C35	15	0.11
(3,35)	1:A:194:HIS:H	4:A:321:PX4:C35	15	0.11
(3,35)	1:A:194:HIS:H	4:A:323:PX4:C35	15	0.11
(3,35)	1:A:194:HIS:H	4:A:325:PX4:C35	15	0.11
(3,35)	1:A:194:HIS:H	4:A:327:PX4:C35	15	0.11
(3,35)	1:A:194:HIS:H	4:A:329:PX4:C35	15	0.11
(3,35)	1:A:194:HIS:H	4:A:331:PX4:C35	15	0.11
(3,35)	1:A:194:HIS:H	4:A:333:PX4:C35	15	0.11
(3,35)	1:A:194:HIS:H	4:A:335:PX4:C35	15	0.11
(3,35)	1:A:194:HIS:H	4:A:337:PX4:C35	15	0.11
(3,35)	1:A:194:HIS:H	4:A:339:PX4:C35	15	0.11
(3,35)	1:A:194:HIS:H	4:A:341:PX4:C35	15	0.11
(3,35)	1:A:194:HIS:H	4:A:343:PX4:C35	15	0.11
(3,35)	1:A:194:HIS:H	4:A:345:PX4:C35	15	0.11
(3,35)	1:A:194:HIS:H	4:A:347:PX4:C35	15	0.11
(3,35)	1:A:194:HIS:H	4:A:349:PX4:C35	15	0.11
(3,35)	1:A:194:HIS:H	4:A:351:PX4:C35	15	0.11
(3,35)	1:A:194:HIS:H	4:A:353:PX4:C35	15	0.11
(3,35)	1:A:194:HIS:H	4:A:355:PX4:C35	15	0.11
(3,35)	1:A:194:HIS:H	4:A:357:PX4:C35	15	0.11
(3,35)	1:A:194:HIS:H	4:A:359:PX4:C35	15	0.11
(3,35)	1:A:194:HIS:H	4:A:361:PX4:C35	15	0.11
(3,35)	1:A:194:HIS:H	4:A:363:PX4:C35	15	0.11
(3,35)	1:A:194:HIS:H	4:A:402:PX4:C35	15	0.11
(3,35)	1:A:194:HIS:H	4:A:404:PX4:C35	15	0.11
(3,35)	1:A:194:HIS:H	4:A:406:PX4:C35	15	0.11
(3,35)	1:A:194:HIS:H	4:A:408:PX4:C35	15	0.11
(3,35)	1:A:194:HIS:H	4:A:410:PX4:C35	15	0.11
(3,35)	1:A:194:HIS:H	4:A:412:PX4:C35	15	0.11
(3,35)	1:A:194:HIS:H	4:A:414:PX4:C35	15	0.11
(3,35)	1:A:194:HIS:H	4:A:416:PX4:C35	15	0.11
(3,35)	1:A:194:HIS:H	4:A:418:PX4:C35	15	0.11
(3,35)	1:A:194:HIS:H	4:A:420:PX4:C35	15	0.11
(3,35)	1:A:194:HIS:H	4:A:422:PX4:C35	15	0.11
(3,35)	1:A:194:HIS:H	4:A:424:PX4:C35	15	0.11
(3,35)	1:A:194:HIS:H	4:A:426:PX4:C35	15	0.11
(3,35)	1:A:194:HIS:H	4:A:428:PX4:C35	15	0.11
(3,35)	1:A:194:HIS:H	4:A:430:PX4:C35	15	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,977)	1:A:78:PHE:H	1:A:78:PHE:HA	4	0.11
(2,975)	1:A:78:PHE:H	1:A:77:LEU:HD22	11	0.11
(2,975)	1:A:78:PHE:H	1:A:77:LEU:HD23	11	0.11
(2,973)	1:A:78:PHE:H	1:A:77:LEU:HD11	18	0.11
(2,973)	1:A:78:PHE:H	1:A:77:LEU:HD12	18	0.11
(2,973)	1:A:78:PHE:H	1:A:77:LEU:HD13	18	0.11
(2,963)	1:A:75:TYR:HB3	1:A:76:SER:H	12	0.11
(2,963)	1:A:75:TYR:HB3	1:A:76:SER:H	12	0.11
(2,951)	1:A:74:GLU:H	1:A:76:SER:H	8	0.11
(2,945)	1:A:74:GLU:H	1:A:74:GLU:HG3	8	0.11
(2,945)	1:A:74:GLU:H	1:A:74:GLU:HG3	8	0.11
(2,938)	1:A:73:ALA:HA	1:A:74:GLU:H	3	0.11
(2,938)	1:A:73:ALA:HA	1:A:74:GLU:H	7	0.11
(2,935)	1:A:73:ALA:H	1:A:73:ALA:HA	7	0.11
(2,931)	1:A:72:VAL:H	1:A:75:TYR:HB3	14	0.11
(2,931)	1:A:72:VAL:H	1:A:75:TYR:HB3	14	0.11
(2,926)	1:A:72:VAL:HB	1:A:73:ALA:H	8	0.11
(2,921)	1:A:72:VAL:H	1:A:72:VAL:HA	6	0.11
(2,916)	1:A:71:ASP:H	1:A:72:VAL:HA	7	0.11
(2,915)	1:A:71:ASP:H	1:A:72:VAL:HG21	20	0.11
(2,915)	1:A:71:ASP:H	1:A:72:VAL:HG22	20	0.11
(2,915)	1:A:71:ASP:H	1:A:72:VAL:HG23	20	0.11
(2,909)	1:A:69:VAL:H	1:A:69:VAL:HA	8	0.11
(2,909)	1:A:69:VAL:H	1:A:69:VAL:HA	13	0.11
(2,904)	1:A:67:CYS:H	1:A:67:CYS:HA	9	0.11
(2,894)	1:A:64:LYS:H	1:A:64:LYS:HG3	16	0.11
(2,894)	1:A:64:LYS:H	1:A:64:LYS:HG3	16	0.11
(2,871)	1:A:186:ILE:HD13	1:A:156:LEU:HD21	14	0.11
(2,867)	1:A:186:ILE:HD11	1:A:156:LEU:HD21	18	0.11
(2,865)	1:A:186:ILE:HD11	1:A:186:ILE:HG13	14	0.11
(2,865)	1:A:186:ILE:HD12	1:A:186:ILE:HG13	14	0.11
(2,865)	1:A:186:ILE:HD13	1:A:186:ILE:HG13	14	0.11
(2,865)	1:A:186:ILE:HD11	1:A:186:ILE:HG12	14	0.11
(2,865)	1:A:186:ILE:HD12	1:A:186:ILE:HG12	14	0.11
(2,865)	1:A:186:ILE:HD13	1:A:186:ILE:HG12	14	0.11
(2,865)	1:A:186:ILE:HD11	1:A:186:ILE:HG13	15	0.11
(2,865)	1:A:186:ILE:HD12	1:A:186:ILE:HG13	15	0.11
(2,865)	1:A:186:ILE:HD13	1:A:186:ILE:HG13	15	0.11
(2,865)	1:A:186:ILE:HD11	1:A:186:ILE:HG12	15	0.11
(2,865)	1:A:186:ILE:HD12	1:A:186:ILE:HG12	15	0.11
(2,865)	1:A:186:ILE:HD13	1:A:186:ILE:HG12	15	0.11
(2,865)	1:A:186:ILE:HD11	1:A:186:ILE:HG13	17	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,865)	1:A:186:ILE:HD12	1:A:186:ILE:HG13	17	0.11
(2,865)	1:A:186:ILE:HD13	1:A:186:ILE:HG13	17	0.11
(2,865)	1:A:186:ILE:HD11	1:A:186:ILE:HG12	17	0.11
(2,865)	1:A:186:ILE:HD12	1:A:186:ILE:HG12	17	0.11
(2,865)	1:A:186:ILE:HD13	1:A:186:ILE:HG12	17	0.11
(2,857)	1:A:186:ILE:HD11	1:A:156:LEU:HD21	19	0.11
(2,830)	1:A:120:ILE:HD11	1:A:120:ILE:HG13	6	0.11
(2,830)	1:A:120:ILE:HD12	1:A:120:ILE:HG13	6	0.11
(2,830)	1:A:120:ILE:HD13	1:A:120:ILE:HG13	6	0.11
(2,830)	1:A:120:ILE:HD11	1:A:120:ILE:HG12	6	0.11
(2,830)	1:A:120:ILE:HD12	1:A:120:ILE:HG12	6	0.11
(2,830)	1:A:120:ILE:HD13	1:A:120:ILE:HG12	6	0.11
(2,811)	1:A:103:ILE:HD11	1:A:103:ILE:HG13	2	0.11
(2,811)	1:A:103:ILE:HD12	1:A:103:ILE:HG13	2	0.11
(2,811)	1:A:103:ILE:HD13	1:A:103:ILE:HG13	2	0.11
(2,811)	1:A:103:ILE:HD11	1:A:103:ILE:HG12	2	0.11
(2,811)	1:A:103:ILE:HD12	1:A:103:ILE:HG12	2	0.11
(2,811)	1:A:103:ILE:HD13	1:A:103:ILE:HG12	2	0.11
(2,811)	1:A:103:ILE:HD11	1:A:103:ILE:HG13	20	0.11
(2,811)	1:A:103:ILE:HD12	1:A:103:ILE:HG13	20	0.11
(2,811)	1:A:103:ILE:HD13	1:A:103:ILE:HG13	20	0.11
(2,811)	1:A:103:ILE:HD11	1:A:103:ILE:HG12	20	0.11
(2,811)	1:A:103:ILE:HD12	1:A:103:ILE:HG12	20	0.11
(2,811)	1:A:103:ILE:HD13	1:A:103:ILE:HG12	20	0.11
(2,767)	1:A:61:ILE:HD11	1:A:60:GLU:H	19	0.11
(2,767)	1:A:61:ILE:HD12	1:A:60:GLU:H	19	0.11
(2,767)	1:A:61:ILE:HD13	1:A:60:GLU:H	19	0.11
(2,759)	1:A:54:LEU:HD21	1:A:59:ILE:HD11	14	0.11
(2,759)	1:A:54:LEU:HD21	1:A:59:ILE:HD12	14	0.11
(2,759)	1:A:54:LEU:HD21	1:A:59:ILE:HD13	14	0.11
(2,748)	1:A:89:VAL:HG12	1:A:122:LEU:HD21	13	0.11
(2,748)	1:A:89:VAL:HG12	1:A:122:LEU:HD21	15	0.11
(2,63)	1:A:52:GLY:H	1:A:51:THR:H	1	0.11
(2,63)	1:A:52:GLY:H	1:A:51:THR:H	19	0.11
(2,621)	1:A:200:LEU:HD21	1:A:201:GLY:H	1	0.11
(2,602)	1:A:237:LEU:H	1:A:239:GLY:H	20	0.11
(2,587)	1:A:232:LYS:H	1:A:231:ILE:HD11	12	0.11
(2,587)	1:A:232:LYS:H	1:A:231:ILE:HD12	12	0.11
(2,587)	1:A:232:LYS:H	1:A:231:ILE:HD13	12	0.11
(2,584)	1:A:230:ASP:H	1:A:231:ILE:HD11	13	0.11
(2,584)	1:A:230:ASP:H	1:A:231:ILE:HD12	13	0.11
(2,584)	1:A:230:ASP:H	1:A:231:ILE:HD13	13	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,568)	1:A:235:GLN:H	1:A:233:GLY:H	18	0.11
(2,517)	1:A:200:LEU:H	1:A:196:LEU:HD21	14	0.11
(2,454)	1:A:178:TRP:HE1	1:A:178:TRP:H	16	0.11
(2,426)	1:A:170:ALA:H	1:A:136:ILE:HD11	3	0.11
(2,426)	1:A:170:ALA:H	1:A:136:ILE:HD12	3	0.11
(2,426)	1:A:170:ALA:H	1:A:136:ILE:HD13	3	0.11
(2,426)	1:A:170:ALA:H	1:A:136:ILE:HD11	16	0.11
(2,426)	1:A:170:ALA:H	1:A:136:ILE:HD12	16	0.11
(2,426)	1:A:170:ALA:H	1:A:136:ILE:HD13	16	0.11
(2,423)	1:A:169:ASP:H	1:A:134:ILE:HD11	13	0.11
(2,423)	1:A:169:ASP:H	1:A:134:ILE:HD12	13	0.11
(2,423)	1:A:169:ASP:H	1:A:134:ILE:HD13	13	0.11
(2,404)	1:A:161:ALA:H	1:A:161:ALA:HB1	7	0.11
(2,404)	1:A:161:ALA:H	1:A:161:ALA:HB2	7	0.11
(2,404)	1:A:161:ALA:H	1:A:161:ALA:HB3	7	0.11
(2,326)	1:A:128:VAL:H	1:A:129:TRP:H	10	0.11
(2,324)	1:A:128:VAL:H	1:A:129:TRP:H	10	0.11
(2,239)	1:A:108:LEU:H	1:A:108:LEU:HD21	9	0.11
(2,188)	1:A:94:VAL:H	1:A:95:SER:H	19	0.11
(2,183)	1:A:94:VAL:H	1:A:95:SER:H	19	0.11
(2,157)	1:A:88:VAL:H	1:A:123:HIS:H	15	0.11
(2,137)	1:A:73:ALA:H	1:A:72:VAL:HG11	13	0.11
(2,137)	1:A:73:ALA:H	1:A:72:VAL:HG12	13	0.11
(2,137)	1:A:73:ALA:H	1:A:72:VAL:HG13	13	0.11
(2,137)	1:A:73:ALA:H	1:A:72:VAL:HG21	13	0.11
(2,137)	1:A:73:ALA:H	1:A:72:VAL:HG22	13	0.11
(2,137)	1:A:73:ALA:H	1:A:72:VAL:HG23	13	0.11
(2,130)	1:A:69:VAL:H	1:A:69:VAL:HG11	3	0.11
(2,130)	1:A:69:VAL:H	1:A:69:VAL:HG12	3	0.11
(2,130)	1:A:69:VAL:H	1:A:69:VAL:HG13	3	0.11
(2,130)	1:A:69:VAL:H	1:A:69:VAL:HG21	3	0.11
(2,130)	1:A:69:VAL:H	1:A:69:VAL:HG22	3	0.11
(2,130)	1:A:69:VAL:H	1:A:69:VAL:HG23	3	0.11
(2,10)	1:A:92:ARG:H	1:A:93:ILE:HG13	9	0.11
(2,10)	1:A:92:ARG:H	1:A:93:ILE:HG12	9	0.11

10 Dihedral-angle violation analysis (i)

No dihedral-angle restraints found