



Full wwPDB NMR Structure Validation Report ⓘ

Jun 22, 2024 – 05:30 PM EDT

PDB ID : 6CM1
BMRB ID : 30426
Title : MT1-MMP HPX Domain with Blade 2 Loop Bound to Nanodiscs
Authors : Marcink, T.C.; Van Doren, S.R.
Deposited on : 2018-03-02

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

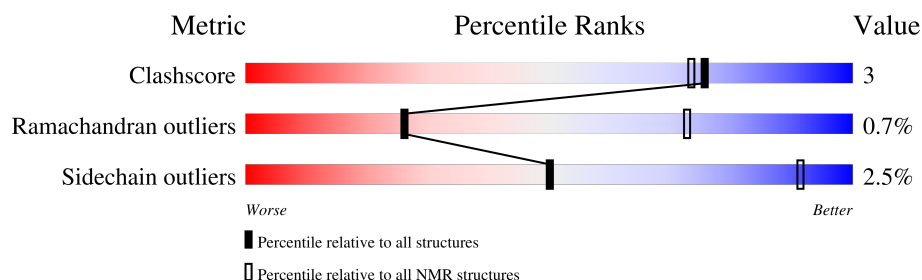
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 4%.

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



| Metric | Whole archive (#Entries) | NMR archive (#Entries) |
|-----------------------|-----------------------------|---------------------------|
| Clashscore | 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 $\leq 5\%$

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | A | 196 | |
| 2 | B | 211 | |
| 2 | C | 211 | |

2 Ensemble composition and analysis

This entry contains 15 models. Model 10 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

| Well-defined (core) protein residues | | | |
|--------------------------------------|--|-------------------|--------------|
| Well-defined core | Residue range (total) | Backbone RMSD (Å) | Medoid model |
| 1 | A:316-A:511, B:55-B:265, C:55-C:262 (615) | 1.54 | 10 |

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

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

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

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

3 Entry composition

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

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

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

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

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

There are 44 discrepancies between the modelled and reference sequences:

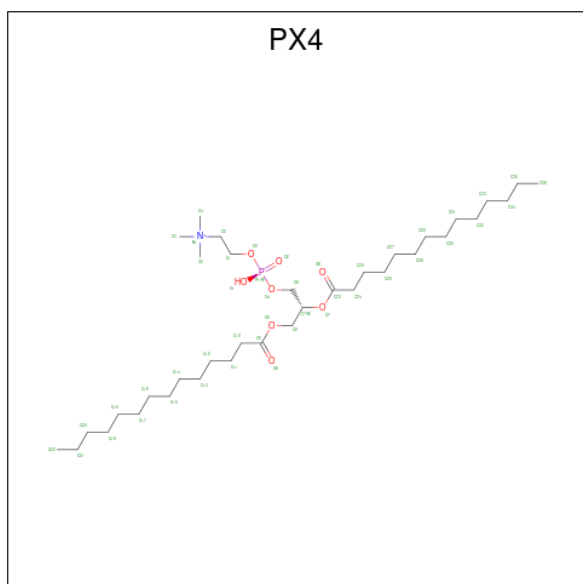
| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-----------|------------|
| B | 99 | PRO | - | insertion | UNP P02647 |
| B | 100 | TYR | - | insertion | UNP P02647 |
| B | 101 | LEU | - | insertion | UNP P02647 |
| B | 102 | ASP | - | insertion |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

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

- Molecule 3 is 1,2-DIMYRISTOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PX4) (formula: C₃₆H₇₃NO₈P).



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

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

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

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

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

| Mol | Chain | Residues | Atoms | |
|-----|-------|----------|-------|----|
| 4 | A | 1 | Total | Na |
| | | | 1 | 1 |

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

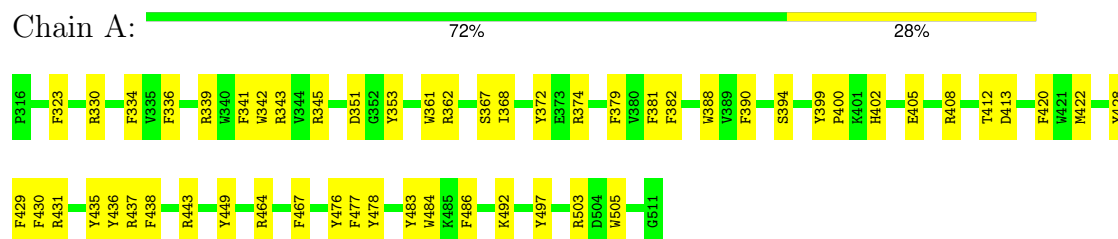
| Mol | Chain | Residues | Atoms | |
|-----|-------|----------|-------|----|
| 5 | A | 1 | Total | Cl |
| | | | 1 | 1 |

4 Residue-property plots

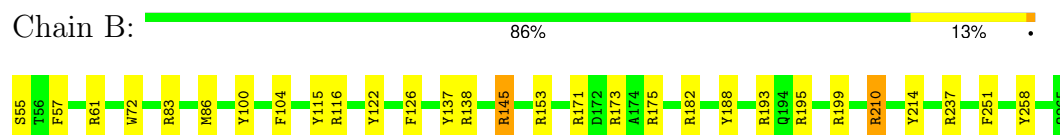
4.1 Average score per residue in the NMR ensemble

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

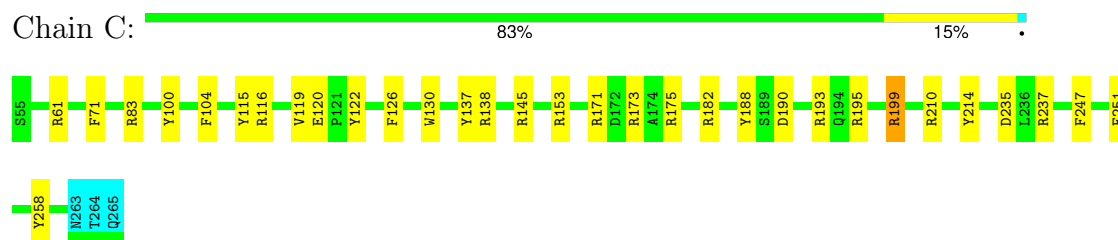
- Molecule 1: Matrix metalloproteinase-14



- Molecule 2: Apolipoprotein A-I



- Molecule 2: Apolipoprotein A-I

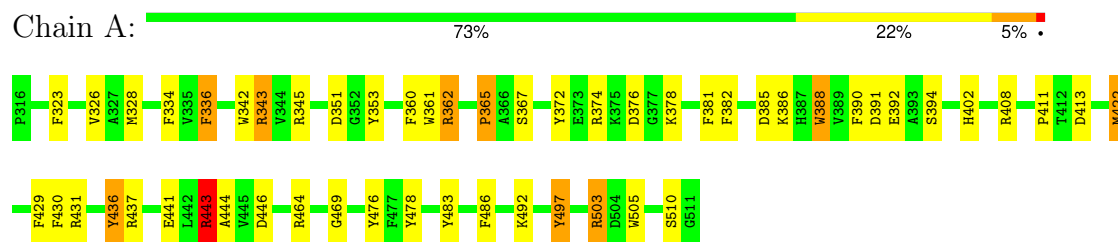


4.2 Scores per residue for each member of the ensemble

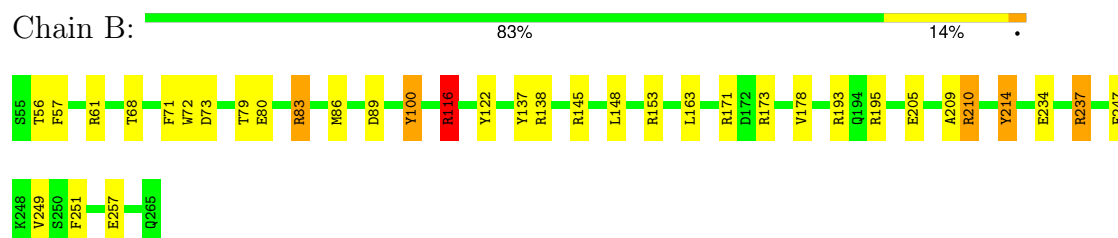
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

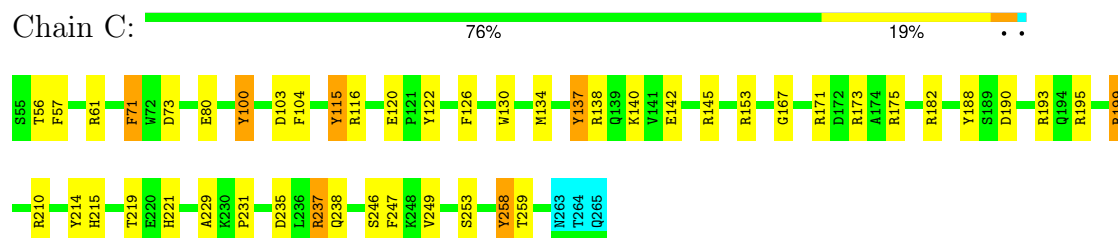
- Molecule 1: Matrix metalloproteinase-14



• Molecule 2: Apolipoprotein A-I

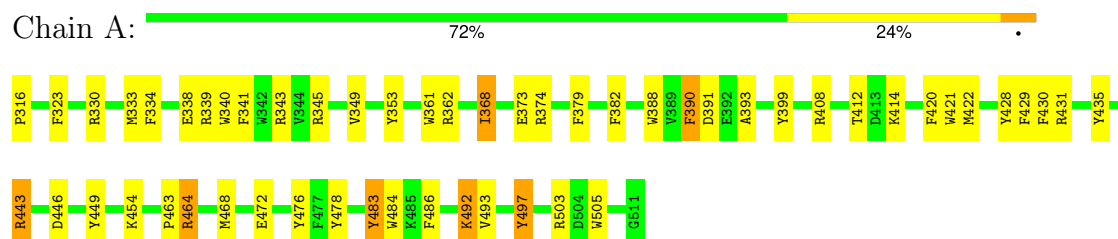


• Molecule 2: Apolipoprotein A-I

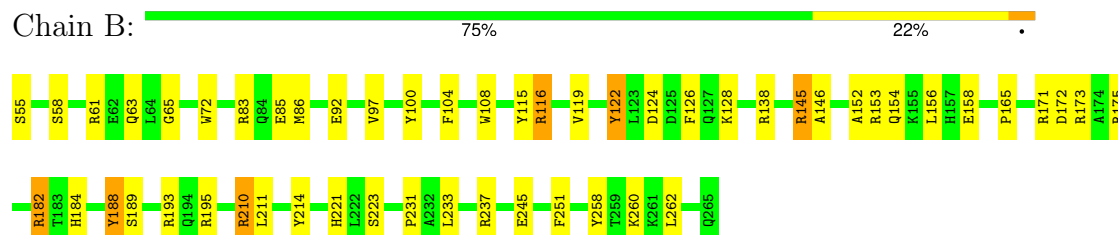


4.2.2 Score per residue for model 2

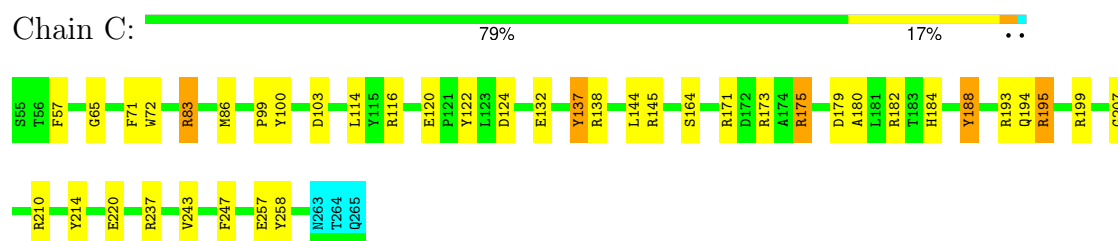
• Molecule 1: Matrix metalloproteinase-14



• Molecule 2: Apolipoprotein A-I

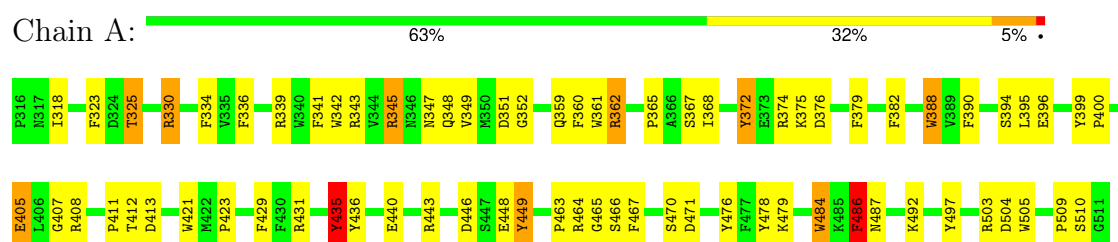


- Molecule 2: Apolipoprotein A-I

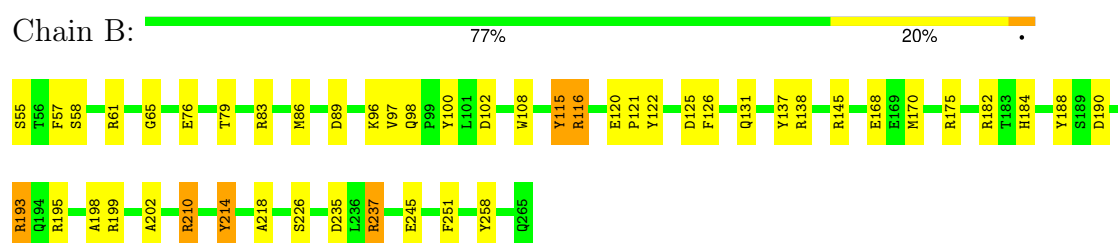


4.2.3 Score per residue for model 3

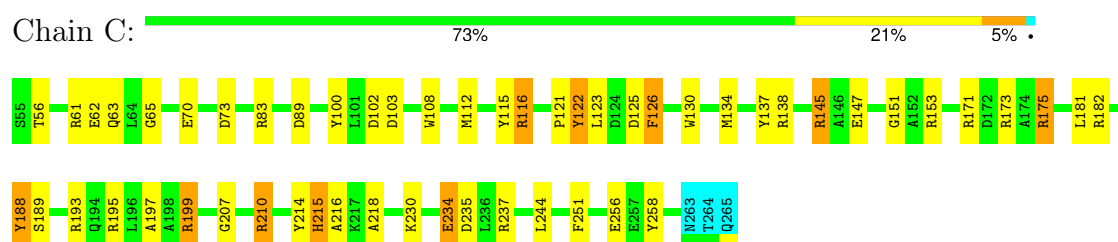
- Molecule 1: Matrix metalloproteinase-14



- Molecule 2: Apolipoprotein A-I



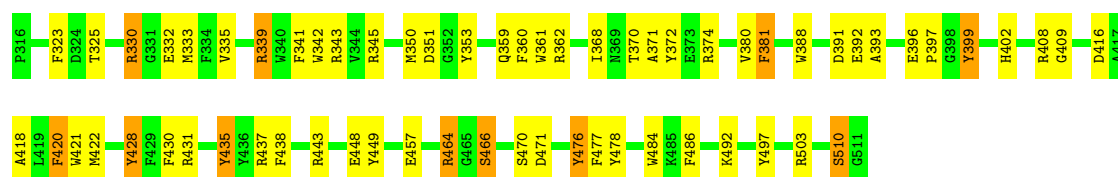
- Molecule 2: Apolipoprotein A-I



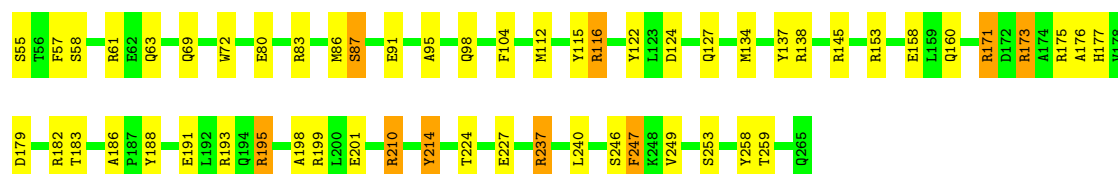
4.2.4 Score per residue for model 4

- Molecule 1: Matrix metalloproteinase-14





• Molecule 2: Apolipoprotein A-I

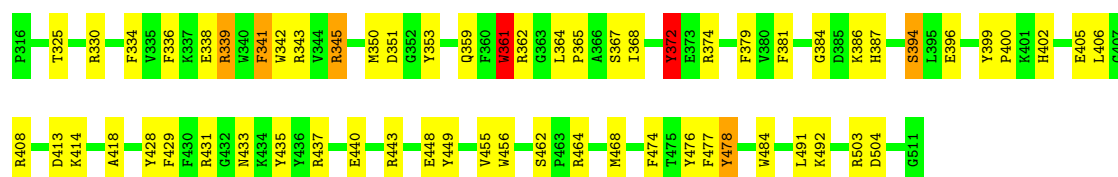


• Molecule 2: Apolipoprotein A-I

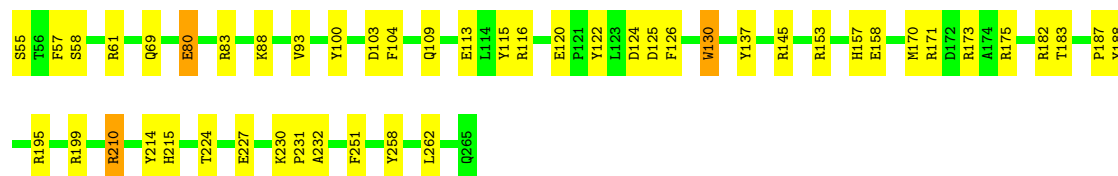
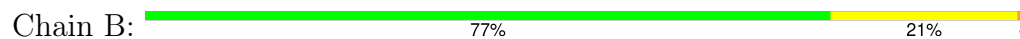


4.2.5 Score per residue for model 5

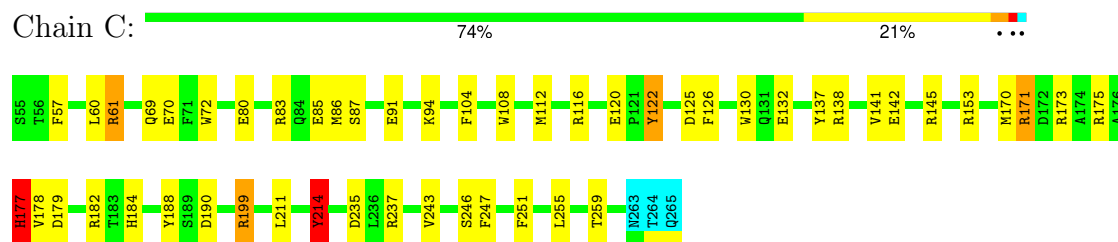
• Molecule 1: Matrix metalloproteinase-14



• Molecule 2: Apolipoprotein A-I

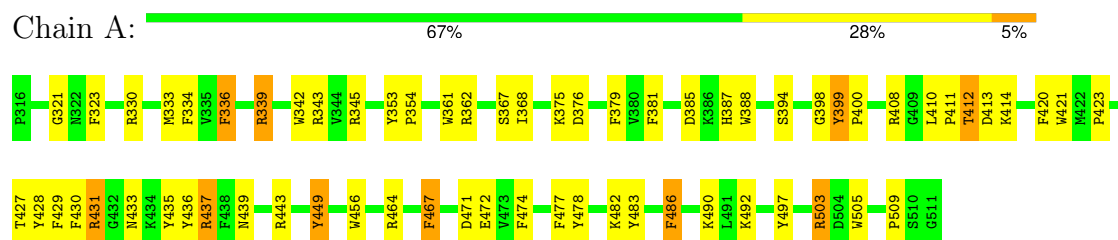


• Molecule 2: Apolipoprotein A-I

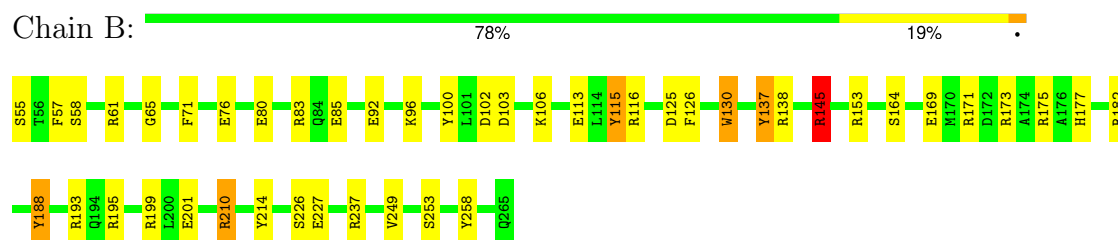


4.2.6 Score per residue for model 6

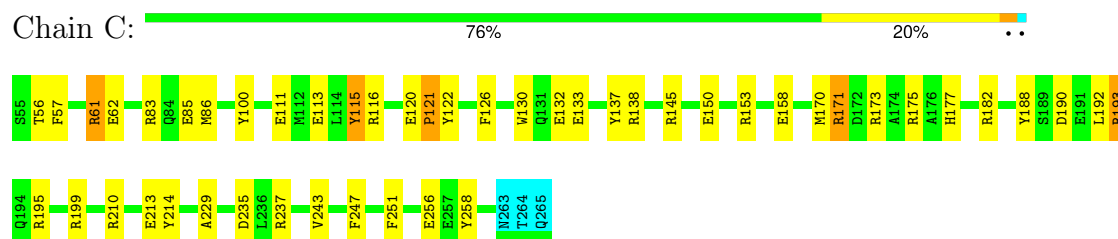
- Molecule 1: Matrix metalloproteinase-14



- Molecule 2: Apolipoprotein A-I

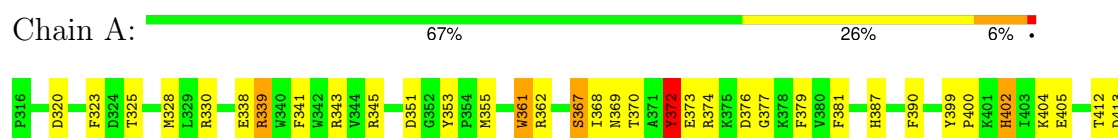


- Molecule 2: Apolipoprotein A-I



4.2.7 Score per residue for model 7

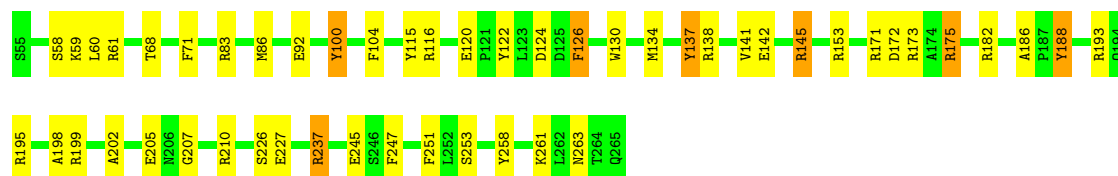
- Molecule 1: Matrix metalloproteinase-14





• Molecule 2: Apolipoprotein A-I

Chain B: 76% 20% •



• Molecule 2: Apolipoprotein A-I

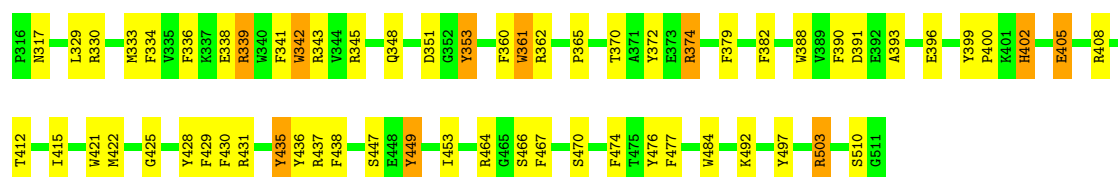
Chain C: 79% 17% ••



4.2.8 Score per residue for model 8

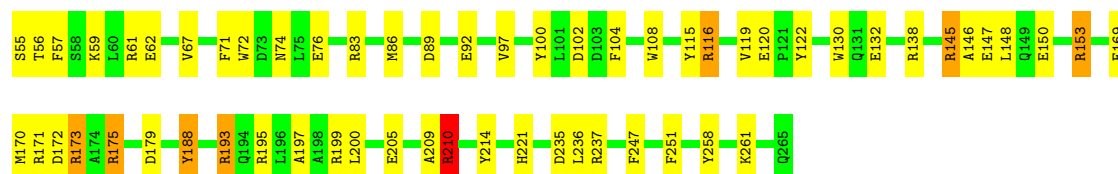
• Molecule 1: Matrix metalloproteinase-14

Chain A: 68% 27% 5%



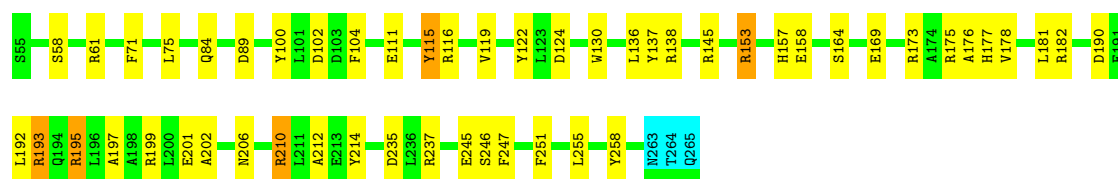
• Molecule 2: Apolipoprotein A-I

Chain B: 72% 24% •



• Molecule 2: Apolipoprotein A-I

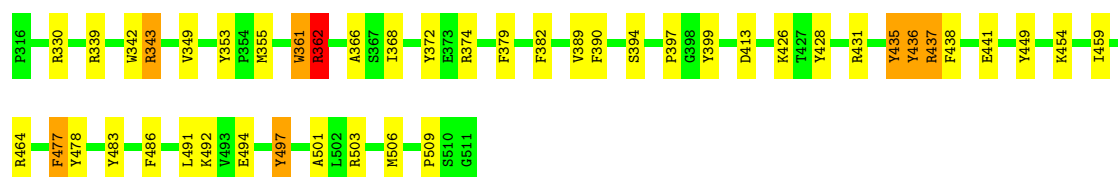
Chain C: 74% 22% ••



4.2.9 Score per residue for model 9

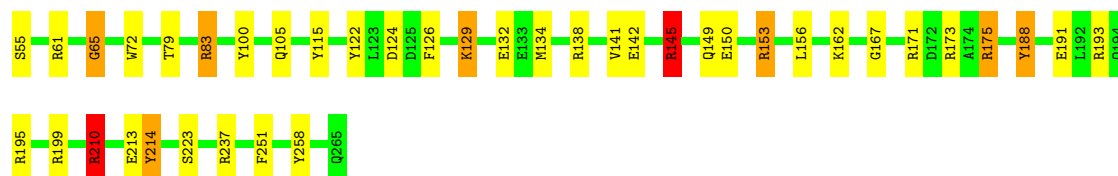
- Molecule 1: Matrix metalloproteinase-14

Chain A: 77% 19%



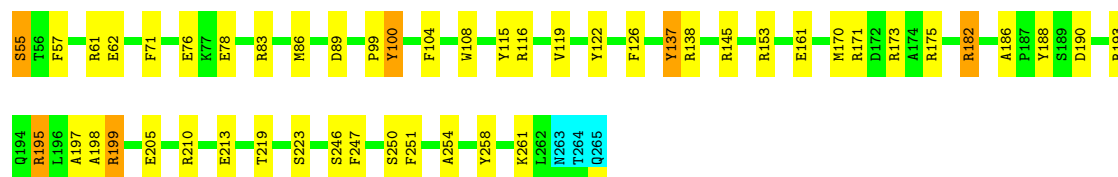
- Molecule 2: Apolipoprotein A-I

Chain B: 81% 15%



- Molecule 2: Apolipoprotein A-I

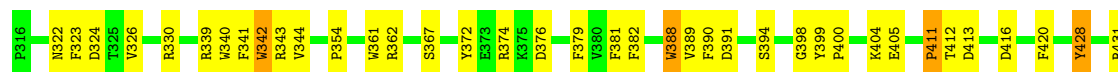
Chain C: 75% 20%



4.2.10 Score per residue for model 10 (medoid)

- Molecule 1: Matrix metalloproteinase-14

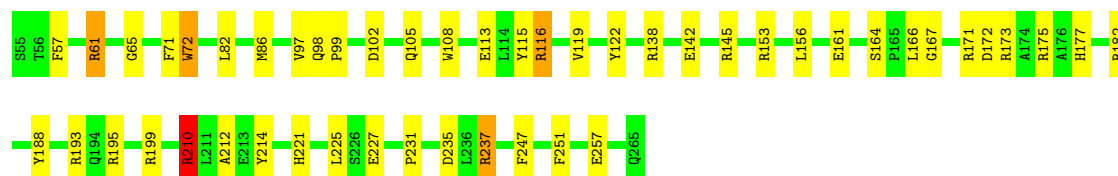
Chain A: 67% 29%





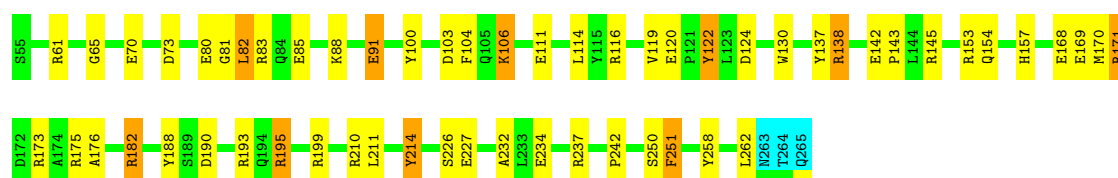
• Molecule 2: Apolipoprotein A-I

Chain B: 77% 21%



• Molecule 2: Apolipoprotein A-I

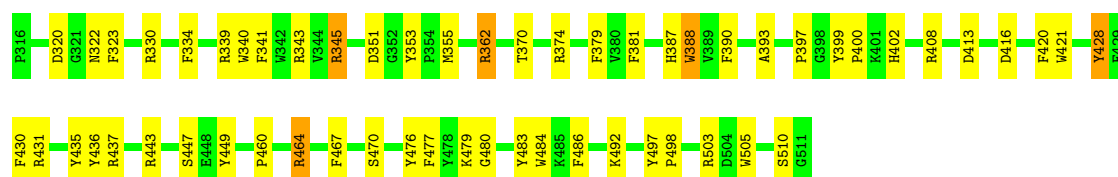
Chain C: 72% 22% 5%



4.2.11 Score per residue for model 11

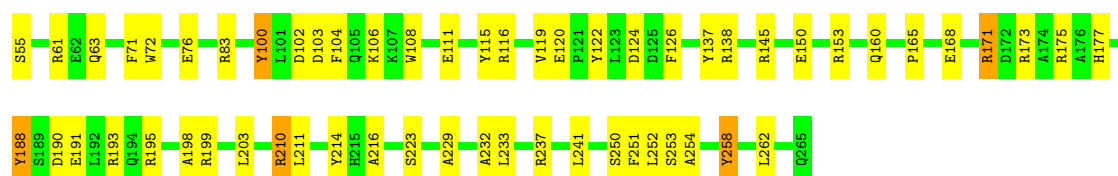
• Molecule 1: Matrix metalloproteinase-14

Chain A: 71% 27%



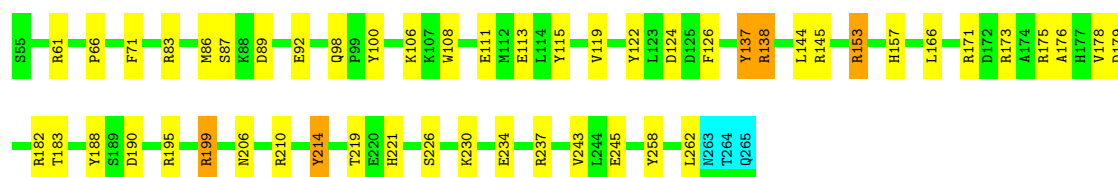
• Molecule 2: Apolipoprotein A-I

Chain B: 73% 25%



• Molecule 2: Apolipoprotein A-I

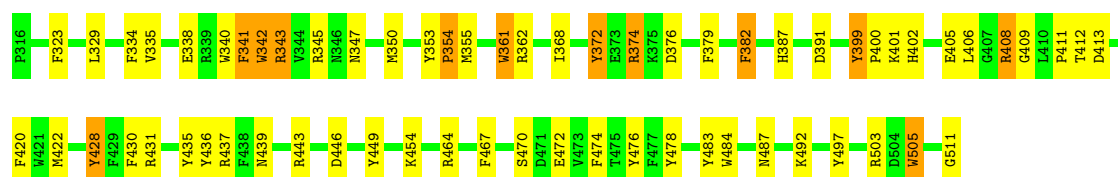
Chain C: 74% 22%



4.2.12 Score per residue for model 12

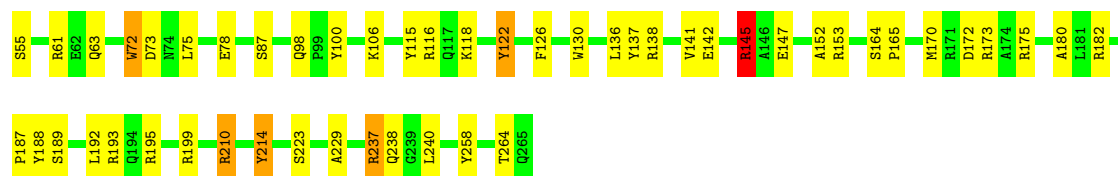
- Molecule 1: Matrix metalloproteinase-14

Chain A: 67% 27% 6%



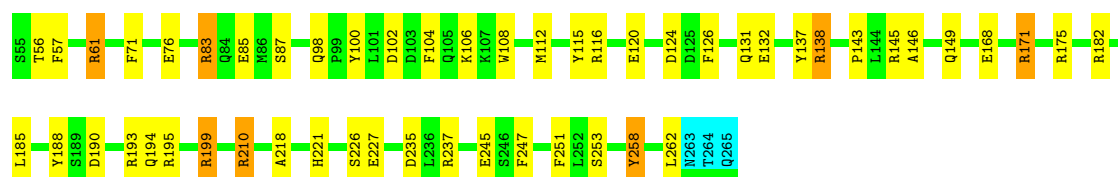
- Molecule 2: Apolipoprotein A-I

Chain B: 76% 21% 3%



- Molecule 2: Apolipoprotein A-I

Chain C: 74% 21% 5%



4.2.13 Score per residue for model 13

- Molecule 1: Matrix metalloproteinase-14

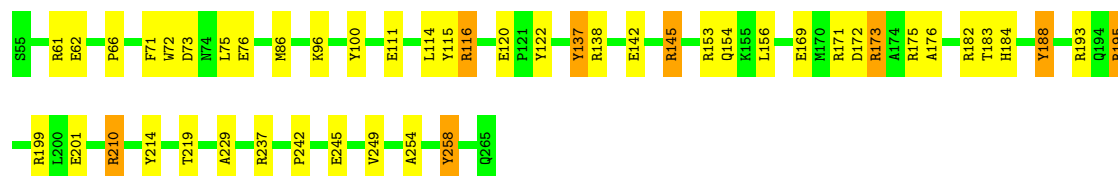
Chain A: 68% 28% 4%





• Molecule 2: Apolipoprotein A-I

Chain B: 77% 19% .



• Molecule 2: Apolipoprotein A-I

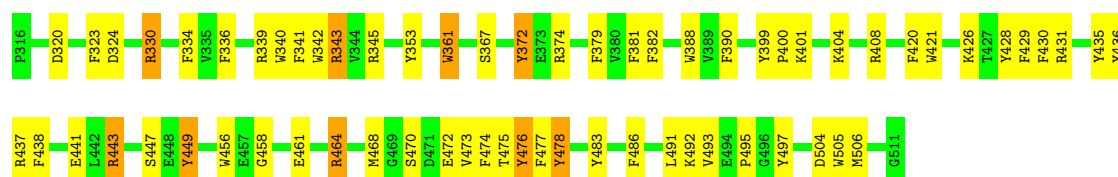
Chain C: 79% 16% . .



4.2.14 Score per residue for model 14

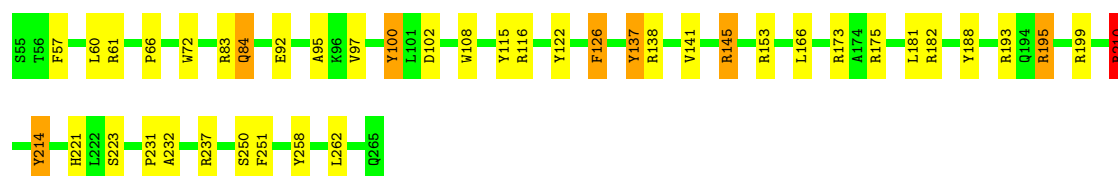
• Molecule 1: Matrix metalloproteinase-14

Chain A: 67% 29% 5%



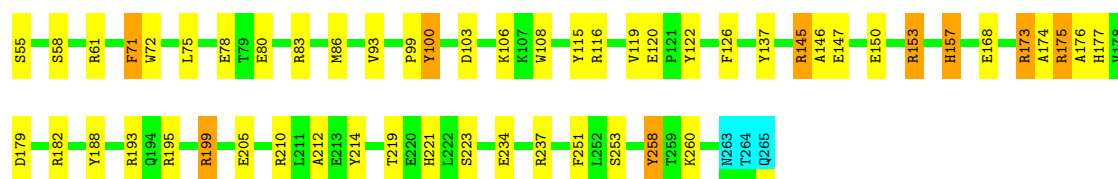
• Molecule 2: Apolipoprotein A-I

Chain B: 80% 16% .



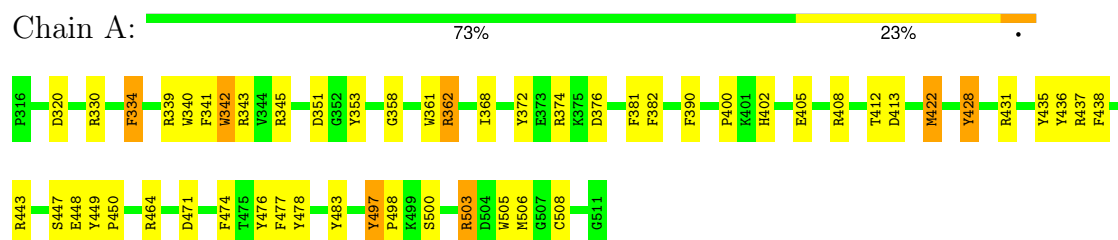
• Molecule 2: Apolipoprotein A-I

Chain C: 73% 21% . .

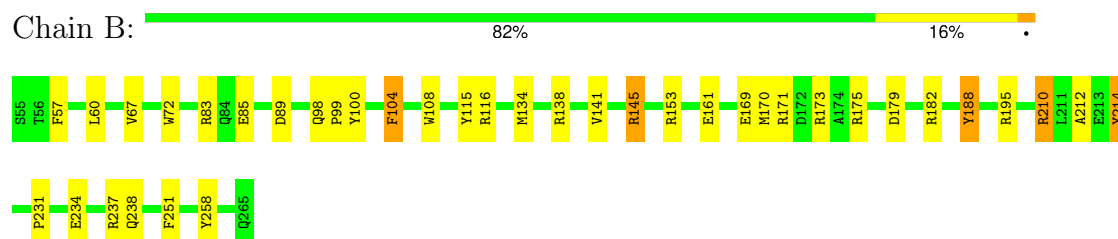


4.2.15 Score per residue for model 15

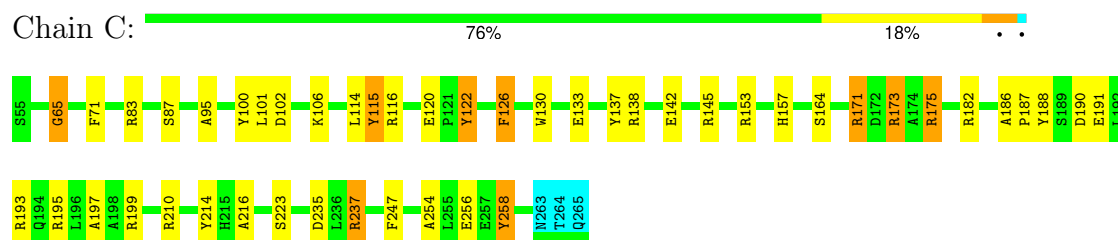
- Molecule 1: Matrix metalloproteinase-14



- Molecule 2: Apolipoprotein A-I



- Molecule 2: Apolipoprotein A-I



5 Refinement protocol and experimental data overview

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

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

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

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

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

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

6 Model quality i

6.1 Standard geometry i

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

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|------------------------|-------------|------------------------|
| | | RMSZ | #Z>5 | RMSZ | #Z>5 |
| 1 | A | 1.70±0.03 | 12±3/1696 (0.7± 0.2%) | 2.16±0.08 | 58±7/2286 (2.6± 0.3%) |
| 2 | B | 1.66±0.03 | 11±3/1784 (0.6± 0.2%) | 2.09±0.06 | 48±9/2394 (2.0± 0.4%) |
| 2 | C | 1.67±0.03 | 12±4/1760 (0.7± 0.2%) | 2.13±0.05 | 53±6/2364 (2.2± 0.3%) |
| All | All | 1.68 | 536/78600 (0.7%) | 2.13 | 2397/105660 (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 | 8.9±2.3 |
| 2 | B | 0.0±0.0 | 5.9±1.6 |
| 2 | C | 0.0±0.0 | 7.5±1.6 |
| All | All | 0 | 335 |

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

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|--------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 2 | C | 110 | GLU | CD-OE1 | 9.32 | 1.35 | 1.25 | 13 | 1 |
| 2 | C | 253 | SER | CA-CB | 9.29 | 1.66 | 1.52 | 14 | 3 |
| 2 | C | 143 | PRO | N-CD | 9.17 | 1.60 | 1.47 | 12 | 1 |
| 2 | C | 251 | PHE | CG-CD2 | 8.85 | 1.52 | 1.38 | 8 | 2 |
| 2 | B | 253 | SER | CB-OG | 8.82 | 1.53 | 1.42 | 6 | 1 |
| 2 | B | 55 | SER | CA-CB | 8.80 | 1.66 | 1.52 | 6 | 3 |
| 2 | C | 111 | GLU | CD-OE2 | 8.58 | 1.35 | 1.25 | 13 | 3 |
| 1 | A | 399 | TYR | CG-CD1 | 8.34 | 1.50 | 1.39 | 4 | 2 |
| 2 | C | 164 | SER | CA-CB | 8.29 | 1.65 | 1.52 | 7 | 3 |
| 1 | A | 353 | TYR | CE1-CZ | 8.22 | 1.49 | 1.38 | 8 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 2 | C | 122 | TYR | CG-CD1 | 8.13 | 1.49 | 1.39 | 3 | 2 |
| 2 | B | 231 | PRO | N-CD | 8.11 | 1.59 | 1.47 | 2 | 2 |
| 1 | A | 353 | TYR | CE2-CZ | 8.01 | 1.49 | 1.38 | 11 | 1 |
| 2 | B | 137 | TYR | CZ-OH | 7.97 | 1.51 | 1.37 | 6 | 3 |
| 2 | C | 122 | TYR | CE2-CZ | 7.87 | 1.48 | 1.38 | 14 | 2 |
| 1 | A | 500 | SER | CA-CB | 7.77 | 1.64 | 1.52 | 13 | 2 |
| 1 | A | 361 | TRP | NE1-CE2 | -7.64 | 1.27 | 1.37 | 12 | 1 |
| 2 | C | 187 | PRO | N-CD | -7.64 | 1.37 | 1.47 | 15 | 1 |
| 1 | A | 484 | TRP | NE1-CE2 | -7.58 | 1.27 | 1.37 | 12 | 3 |
| 2 | B | 188 | TYR | CE1-CZ | 7.55 | 1.48 | 1.38 | 2 | 1 |
| 2 | C | 57 | PHE | CG-CD1 | 7.53 | 1.50 | 1.38 | 1 | 1 |
| 1 | A | 382 | PHE | CG-CD1 | 7.51 | 1.50 | 1.38 | 2 | 1 |
| 1 | A | 497 | TYR | CG-CD1 | 7.47 | 1.48 | 1.39 | 9 | 1 |
| 2 | C | 71 | PHE | CG-CD2 | 7.43 | 1.49 | 1.38 | 4 | 1 |
| 2 | B | 164 | SER | CA-CB | 7.40 | 1.64 | 1.52 | 10 | 1 |
| 2 | C | 100 | TYR | CZ-OH | 7.39 | 1.50 | 1.37 | 2 | 2 |
| 2 | B | 169 | GLU | CD-OE2 | 7.33 | 1.33 | 1.25 | 13 | 1 |
| 2 | B | 147 | GLU | CG-CD | -7.32 | 1.41 | 1.51 | 12 | 1 |
| 2 | B | 57 | PHE | CB-CG | 7.30 | 1.63 | 1.51 | 14 | 1 |
| 2 | C | 138 | ARG | CZ-NH2 | -7.28 | 1.23 | 1.33 | 11 | 1 |
| 2 | B | 226 | SER | CA-CB | 7.28 | 1.63 | 1.52 | 7 | 2 |
| 2 | C | 130 | TRP | NE1-CE2 | -7.28 | 1.28 | 1.37 | 10 | 1 |
| 2 | B | 100 | TYR | CG-CD2 | 7.26 | 1.48 | 1.39 | 14 | 3 |
| 1 | A | 342 | TRP | CD2-CE3 | -7.21 | 1.29 | 1.40 | 9 | 1 |
| 2 | B | 189 | SER | CB-OG | 7.19 | 1.51 | 1.42 | 2 | 1 |
| 2 | C | 246 | SER | CB-OG | 7.16 | 1.51 | 1.42 | 5 | 2 |
| 1 | A | 476 | TYR | CZ-OH | 7.15 | 1.50 | 1.37 | 13 | 2 |
| 2 | C | 122 | TYR | CB-CG | 7.09 | 1.62 | 1.51 | 10 | 1 |
| 2 | C | 223 | SER | CA-CB | 7.08 | 1.63 | 1.52 | 4 | 4 |
| 2 | B | 108 | TRP | NE1-CE2 | -7.07 | 1.28 | 1.37 | 8 | 1 |
| 2 | B | 164 | SER | CB-OG | 6.97 | 1.51 | 1.42 | 6 | 2 |
| 2 | C | 100 | TYR | CE2-CZ | 6.96 | 1.47 | 1.38 | 1 | 4 |
| 2 | C | 251 | PHE | CG-CD1 | 6.96 | 1.49 | 1.38 | 12 | 1 |
| 1 | A | 372 | TYR | CZ-OH | 6.91 | 1.49 | 1.37 | 10 | 2 |
| 2 | C | 71 | PHE | CG-CD1 | 6.91 | 1.49 | 1.38 | 9 | 1 |
| 1 | A | 436 | TYR | CE2-CZ | 6.91 | 1.47 | 1.38 | 15 | 3 |
| 2 | C | 158 | GLU | CD-OE2 | -6.91 | 1.18 | 1.25 | 8 | 1 |
| 2 | B | 152 | ALA | N-CA | -6.88 | 1.32 | 1.46 | 12 | 1 |
| 1 | A | 430 | PHE | CG-CD1 | 6.87 | 1.49 | 1.38 | 6 | 1 |
| 2 | C | 115 | TYR | CG-CD2 | 6.86 | 1.48 | 1.39 | 15 | 2 |
| 2 | C | 65 | GLY | N-CA | 6.83 | 1.56 | 1.46 | 2 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 1 | A | 470 | SER | CB-OG | 6.82 | 1.51 | 1.42 | 14 | 1 |
| 1 | A | 394 | SER | CA-CB | 6.80 | 1.63 | 1.52 | 9 | 4 |
| 1 | A | 372 | TYR | CB-CG | 6.80 | 1.61 | 1.51 | 10 | 2 |
| 2 | C | 201 | GLU | CB-CG | 6.78 | 1.65 | 1.52 | 13 | 1 |
| 1 | A | 379 | PHE | CG-CD2 | 6.73 | 1.48 | 1.38 | 14 | 1 |
| 2 | B | 122 | TYR | CB-CG | -6.70 | 1.41 | 1.51 | 10 | 1 |
| 2 | B | 188 | TYR | CB-CG | -6.68 | 1.41 | 1.51 | 3 | 3 |
| 1 | A | 367 | SER | CB-OG | 6.67 | 1.50 | 1.42 | 10 | 1 |
| 2 | C | 214 | TYR | CE1-CZ | 6.67 | 1.47 | 1.38 | 2 | 1 |
| 1 | A | 372 | TYR | CG-CD2 | 6.65 | 1.47 | 1.39 | 7 | 3 |
| 2 | B | 168 | GLU | CD-OE1 | 6.64 | 1.32 | 1.25 | 11 | 1 |
| 2 | B | 188 | TYR | CZ-OH | 6.64 | 1.49 | 1.37 | 15 | 2 |
| 2 | B | 245 | GLU | CB-CG | 6.64 | 1.64 | 1.52 | 2 | 1 |
| 1 | A | 508 | CYS | CB-SG | 6.62 | 1.93 | 1.82 | 13 | 1 |
| 2 | B | 147 | GLU | CB-CG | 6.62 | 1.64 | 1.52 | 12 | 1 |
| 2 | B | 237 | ARG | CD-NE | 6.58 | 1.57 | 1.46 | 6 | 1 |
| 2 | B | 214 | TYR | CZ-OH | 6.58 | 1.49 | 1.37 | 2 | 3 |
| 1 | A | 352 | GLY | CA-C | -6.57 | 1.41 | 1.51 | 3 | 1 |
| 2 | B | 130 | TRP | CD2-CE2 | 6.54 | 1.49 | 1.41 | 7 | 1 |
| 2 | C | 145 | ARG | CD-NE | 6.51 | 1.57 | 1.46 | 5 | 1 |
| 2 | C | 122 | TYR | CE1-CZ | 6.51 | 1.47 | 1.38 | 13 | 1 |
| 2 | C | 87 | SER | CA-CB | 6.49 | 1.62 | 1.52 | 13 | 3 |
| 2 | C | 158 | GLU | CD-OE1 | 6.49 | 1.32 | 1.25 | 13 | 2 |
| 1 | A | 510 | SER | CA-CB | 6.46 | 1.62 | 1.52 | 3 | 3 |
| 1 | A | 353 | TYR | CZ-OH | 6.45 | 1.48 | 1.37 | 8 | 1 |
| 1 | A | 464 | ARG | CZ-NH2 | -6.44 | 1.24 | 1.33 | 11 | 1 |
| 2 | C | 188 | TYR | CD1-CE1 | 6.44 | 1.49 | 1.39 | 15 | 1 |
| 2 | C | 227 | GLU | CD-OE2 | 6.42 | 1.32 | 1.25 | 12 | 1 |
| 2 | B | 214 | TYR | CG-CD2 | 6.41 | 1.47 | 1.39 | 2 | 3 |
| 1 | A | 483 | TYR | CZ-OH | 6.40 | 1.48 | 1.37 | 11 | 1 |
| 1 | A | 457 | GLU | CB-CG | 6.39 | 1.64 | 1.52 | 4 | 1 |
| 2 | C | 137 | TYR | CG-CD1 | 6.39 | 1.47 | 1.39 | 14 | 2 |
| 1 | A | 447 | SER | CA-CB | 6.37 | 1.62 | 1.52 | 14 | 2 |
| 2 | B | 186 | ALA | C-N | 6.36 | 1.46 | 1.34 | 7 | 1 |
| 2 | B | 214 | TYR | CE2-CZ | 6.36 | 1.46 | 1.38 | 15 | 1 |
| 2 | B | 189 | SER | CA-CB | 6.33 | 1.62 | 1.52 | 12 | 1 |
| 2 | C | 91 | GLU | CD-OE1 | 6.33 | 1.32 | 1.25 | 10 | 1 |
| 2 | C | 167 | GLY | CA-C | 6.32 | 1.61 | 1.51 | 1 | 1 |
| 2 | C | 58 | SER | CA-CB | 6.32 | 1.62 | 1.52 | 8 | 1 |
| 1 | A | 441 | GLU | CB-CG | 6.32 | 1.64 | 1.52 | 9 | 1 |
| 1 | A | 388 | TRP | CE3-CZ3 | 6.32 | 1.49 | 1.38 | 14 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 2 | C | 137 | TYR | CB-CG | -6.32 | 1.42 | 1.51 | 5 | 1 |
| 1 | A | 396 | GLU | CG-CD | -6.31 | 1.42 | 1.51 | 13 | 1 |
| 2 | B | 214 | TYR | CG-CD1 | 6.30 | 1.47 | 1.39 | 10 | 3 |
| 1 | A | 476 | TYR | CE1-CZ | 6.30 | 1.46 | 1.38 | 14 | 1 |
| 2 | B | 223 | SER | CA-CB | 6.29 | 1.62 | 1.52 | 9 | 3 |
| 2 | C | 55 | SER | CA-CB | 6.29 | 1.62 | 1.52 | 9 | 1 |
| 2 | C | 108 | TRP | CD2-CE3 | -6.29 | 1.30 | 1.40 | 9 | 1 |
| 2 | C | 85 | GLU | CB-CG | 6.29 | 1.64 | 1.52 | 6 | 1 |
| 1 | A | 448 | GLU | CG-CD | -6.28 | 1.42 | 1.51 | 13 | 2 |
| 2 | B | 223 | SER | CB-OG | 6.28 | 1.50 | 1.42 | 12 | 1 |
| 2 | B | 111 | GLU | CD-OE2 | -6.28 | 1.18 | 1.25 | 13 | 1 |
| 2 | C | 147 | GLU | CG-CD | -6.26 | 1.42 | 1.51 | 14 | 1 |
| 2 | C | 137 | TYR | CE2-CZ | -6.25 | 1.30 | 1.38 | 10 | 1 |
| 2 | B | 87 | SER | CA-CB | 6.24 | 1.62 | 1.52 | 4 | 1 |
| 2 | B | 122 | TYR | CE1-CZ | 6.23 | 1.46 | 1.38 | 12 | 2 |
| 2 | C | 80 | GLU | CD-OE1 | 6.23 | 1.32 | 1.25 | 1 | 1 |
| 2 | B | 80 | GLU | CG-CD | 6.22 | 1.61 | 1.51 | 4 | 1 |
| 2 | C | 92 | GLU | CG-CD | 6.22 | 1.61 | 1.51 | 11 | 1 |
| 2 | C | 261 | LYS | N-CA | -6.21 | 1.33 | 1.46 | 9 | 1 |
| 2 | B | 100 | TYR | CG-CD1 | 6.21 | 1.47 | 1.39 | 1 | 1 |
| 2 | B | 85 | GLU | CD-OE2 | 6.21 | 1.32 | 1.25 | 6 | 2 |
| 2 | C | 247 | PHE | CB-CG | 6.18 | 1.61 | 1.51 | 15 | 1 |
| 1 | A | 384 | GLY | N-CA | 6.18 | 1.55 | 1.46 | 5 | 1 |
| 2 | C | 227 | GLU | CB-CG | 6.17 | 1.63 | 1.52 | 12 | 2 |
| 2 | C | 227 | GLU | CG-CD | 6.17 | 1.61 | 1.51 | 7 | 2 |
| 2 | B | 148 | LEU | CA-CB | 6.17 | 1.68 | 1.53 | 8 | 1 |
| 2 | C | 137 | TYR | CZ-OH | 6.17 | 1.48 | 1.37 | 8 | 2 |
| 2 | B | 104 | PHE | CG-CD2 | 6.17 | 1.48 | 1.38 | 2 | 2 |
| 1 | A | 367 | SER | CA-CB | 6.16 | 1.62 | 1.52 | 14 | 1 |
| 1 | A | 476 | TYR | CG-CD2 | 6.16 | 1.47 | 1.39 | 11 | 1 |
| 2 | C | 95 | ALA | N-CA | -6.15 | 1.34 | 1.46 | 15 | 1 |
| 1 | A | 469 | GLY | N-CA | 6.14 | 1.55 | 1.46 | 7 | 1 |
| 2 | C | 122 | TYR | CZ-OH | 6.14 | 1.48 | 1.37 | 11 | 1 |
| 2 | C | 214 | TYR | CZ-OH | 6.12 | 1.48 | 1.37 | 11 | 1 |
| 2 | B | 132 | GLU | CD-OE1 | 6.11 | 1.32 | 1.25 | 8 | 1 |
| 1 | A | 494 | GLU | CD-OE1 | 6.11 | 1.32 | 1.25 | 10 | 1 |
| 2 | B | 231 | PRO | CA-C | -6.11 | 1.40 | 1.52 | 14 | 1 |
| 1 | A | 476 | TYR | CG-CD1 | 6.11 | 1.47 | 1.39 | 7 | 2 |
| 1 | A | 429 | PHE | CB-CG | 6.09 | 1.61 | 1.51 | 1 | 1 |
| 1 | A | 420 | PHE | CG-CD2 | 6.09 | 1.47 | 1.38 | 4 | 2 |
| 2 | C | 78 | GLU | CA-CB | 6.08 | 1.67 | 1.53 | 9 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 1 | A | 449 | TYR | CB-CG | -6.08 | 1.42 | 1.51 | 6 | 1 |
| 2 | B | 234 | GLU | CD-OE2 | 6.08 | 1.32 | 1.25 | 1 | 1 |
| 1 | A | 396 | GLU | CD-OE1 | 6.07 | 1.32 | 1.25 | 3 | 1 |
| 1 | A | 497 | TYR | CG-CD2 | 6.06 | 1.47 | 1.39 | 12 | 2 |
| 2 | B | 100 | TYR | CE1-CZ | -6.06 | 1.30 | 1.38 | 15 | 1 |
| 1 | A | 449 | TYR | CE2-CZ | 6.05 | 1.46 | 1.38 | 9 | 3 |
| 2 | C | 207 | GLY | C-N | 6.03 | 1.43 | 1.33 | 2 | 1 |
| 2 | B | 137 | TYR | CG-CD2 | 6.03 | 1.47 | 1.39 | 13 | 1 |
| 1 | A | 399 | TYR | CB-CG | -6.03 | 1.42 | 1.51 | 8 | 1 |
| 2 | B | 182 | ARG | CD-NE | 6.02 | 1.56 | 1.46 | 12 | 1 |
| 2 | B | 76 | GLU | CG-CD | 6.02 | 1.60 | 1.51 | 13 | 1 |
| 2 | C | 85 | GLU | CD-OE1 | 6.01 | 1.32 | 1.25 | 10 | 2 |
| 1 | A | 470 | SER | CA-CB | 6.00 | 1.61 | 1.52 | 11 | 4 |
| 2 | B | 188 | TYR | CG-CD1 | 6.00 | 1.47 | 1.39 | 3 | 1 |
| 1 | A | 477 | PHE | CG-CD2 | 5.99 | 1.47 | 1.38 | 6 | 1 |
| 2 | B | 55 | SER | CB-OG | 5.97 | 1.50 | 1.42 | 8 | 1 |
| 2 | B | 120 | GLU | CB-CG | 5.96 | 1.63 | 1.52 | 13 | 1 |
| 2 | B | 257 | GLU | CB-CG | 5.96 | 1.63 | 1.52 | 1 | 1 |
| 2 | C | 98 | GLN | CG-CD | 5.96 | 1.64 | 1.51 | 7 | 1 |
| 2 | C | 161 | GLU | CD-OE1 | 5.96 | 1.32 | 1.25 | 9 | 1 |
| 2 | C | 80 | GLU | CG-CD | -5.96 | 1.43 | 1.51 | 7 | 1 |
| 2 | B | 199 | ARG | CZ-NH2 | 5.95 | 1.40 | 1.33 | 13 | 3 |
| 2 | C | 151 | GLY | CA-C | -5.93 | 1.42 | 1.51 | 3 | 1 |
| 1 | A | 342 | TRP | CD2-CE2 | -5.93 | 1.34 | 1.41 | 12 | 1 |
| 2 | B | 138 | ARG | CZ-NH1 | -5.92 | 1.25 | 1.33 | 8 | 1 |
| 2 | C | 188 | TYR | CG-CD1 | 5.91 | 1.46 | 1.39 | 5 | 3 |
| 2 | C | 251 | PHE | CE1-CZ | 5.91 | 1.48 | 1.37 | 14 | 1 |
| 1 | A | 483 | TYR | CG-CD2 | 5.91 | 1.46 | 1.39 | 2 | 1 |
| 1 | A | 429 | PHE | CG-CD1 | 5.90 | 1.47 | 1.38 | 8 | 1 |
| 1 | A | 505 | TRP | CD2-CE2 | 5.90 | 1.48 | 1.41 | 11 | 3 |
| 1 | A | 316 | PRO | N-CD | 5.89 | 1.56 | 1.47 | 13 | 1 |
| 1 | A | 483 | TYR | CE2-CZ | 5.89 | 1.46 | 1.38 | 1 | 2 |
| 1 | A | 405 | GLU | CD-OE1 | 5.89 | 1.32 | 1.25 | 3 | 1 |
| 2 | C | 145 | ARG | NE-CZ | 5.88 | 1.40 | 1.33 | 13 | 1 |
| 2 | B | 258 | TYR | CG-CD1 | 5.88 | 1.46 | 1.39 | 6 | 2 |
| 2 | B | 116 | ARG | CD-NE | 5.88 | 1.56 | 1.46 | 8 | 3 |
| 1 | A | 476 | TYR | CB-CG | -5.88 | 1.42 | 1.51 | 12 | 1 |
| 2 | B | 250 | SER | CB-OG | 5.88 | 1.49 | 1.42 | 14 | 2 |
| 1 | A | 431 | ARG | CD-NE | 5.87 | 1.56 | 1.46 | 2 | 1 |
| 1 | A | 420 | PHE | CG-CD1 | 5.87 | 1.47 | 1.38 | 10 | 1 |
| 1 | A | 483 | TYR | CB-CG | 5.87 | 1.60 | 1.51 | 12 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|--------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 2 | B | 84 | GLN | CG-CD | 5.86 | 1.64 | 1.51 | 14 | 1 |
| 1 | A | 405 | GLU | CB-CG | 5.86 | 1.63 | 1.52 | 15 | 1 |
| 2 | B | 115 | TYR | CE1-CZ | 5.85 | 1.46 | 1.38 | 15 | 1 |
| 2 | B | 104 | PHE | CG-CD1 | 5.85 | 1.47 | 1.38 | 5 | 1 |
| 2 | C | 169 | GLU | CG-CD | 5.85 | 1.60 | 1.51 | 10 | 1 |
| 1 | A | 497 | TYR | CZ-OH | 5.83 | 1.47 | 1.37 | 11 | 1 |
| 2 | C | 238 | GLN | CG-CD | 5.81 | 1.64 | 1.51 | 1 | 1 |
| 1 | A | 490 | LYS | CA-CB | 5.81 | 1.66 | 1.53 | 6 | 1 |
| 2 | C | 250 | SER | CA-CB | 5.80 | 1.61 | 1.52 | 10 | 1 |
| 2 | B | 120 | GLU | CD-OE2 | 5.80 | 1.32 | 1.25 | 11 | 1 |
| 2 | C | 115 | TYR | CB-CG | 5.79 | 1.60 | 1.51 | 1 | 1 |
| 2 | B | 258 | TYR | CE2-CZ | 5.79 | 1.46 | 1.38 | 4 | 1 |
| 2 | B | 126 | PHE | CB-CG | 5.77 | 1.61 | 1.51 | 12 | 1 |
| 1 | A | 399 | TYR | CG-CD2 | 5.77 | 1.46 | 1.39 | 10 | 1 |
| 2 | C | 70 | GLU | CG-CD | 5.77 | 1.60 | 1.51 | 5 | 1 |
| 2 | B | 251 | PHE | CB-CG | 5.76 | 1.61 | 1.51 | 1 | 1 |
| 1 | A | 440 | GLU | CD-OE1 | -5.75 | 1.19 | 1.25 | 3 | 1 |
| 2 | C | 115 | TYR | CZ-OH | 5.75 | 1.47 | 1.37 | 12 | 1 |
| 2 | B | 58 | SER | CA-CB | 5.74 | 1.61 | 1.52 | 5 | 1 |
| 2 | C | 226 | SER | CA-CB | 5.73 | 1.61 | 1.52 | 12 | 2 |
| 2 | C | 177 | HIS | CB-CG | 5.72 | 1.60 | 1.50 | 5 | 1 |
| 2 | B | 195 | ARG | CD-NE | 5.72 | 1.56 | 1.46 | 14 | 3 |
| 2 | B | 92 | GLU | CG-CD | 5.71 | 1.60 | 1.51 | 2 | 1 |
| 2 | C | 115 | TYR | CG-CD1 | 5.71 | 1.46 | 1.39 | 4 | 1 |
| 2 | B | 59 | LYS | CA-CB | 5.71 | 1.66 | 1.53 | 8 | 1 |
| 2 | C | 103 | ASP | CA-CB | 5.71 | 1.66 | 1.53 | 4 | 1 |
| 2 | B | 175 | ARG | CZ-NH1 | 5.71 | 1.40 | 1.33 | 9 | 1 |
| 1 | A | 368 | ILE | CA-CB | -5.70 | 1.41 | 1.54 | 9 | 1 |
| 1 | A | 406 | LEU | C-N | 5.68 | 1.43 | 1.33 | 5 | 1 |
| 1 | A | 454 | LYS | CD-CE | 5.68 | 1.65 | 1.51 | 2 | 1 |
| 2 | C | 120 | GLU | CD-OE1 | -5.67 | 1.19 | 1.25 | 15 | 2 |
| 2 | C | 233 | LEU | CA-CB | 5.66 | 1.66 | 1.53 | 4 | 1 |
| 1 | A | 497 | TYR | CE2-CZ | 5.65 | 1.45 | 1.38 | 3 | 1 |
| 2 | C | 168 | GLU | CB-CG | 5.65 | 1.62 | 1.52 | 12 | 1 |
| 1 | A | 360 | PHE | CG-CD1 | 5.65 | 1.47 | 1.38 | 8 | 2 |
| 1 | A | 436 | TYR | CZ-OH | 5.65 | 1.47 | 1.37 | 7 | 3 |
| 1 | A | 323 | PHE | CG-CD2 | 5.64 | 1.47 | 1.38 | 10 | 3 |
| 2 | B | 126 | PHE | CE1-CZ | 5.64 | 1.48 | 1.37 | 2 | 1 |
| 1 | A | 348 | GLN | CA-CB | 5.64 | 1.66 | 1.53 | 3 | 1 |
| 2 | B | 126 | PHE | CG-CD2 | 5.63 | 1.47 | 1.38 | 7 | 2 |
| 2 | C | 245 | GLU | CB-CG | 5.63 | 1.62 | 1.52 | 8 | 2 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 2 | C | 169 | GLU | CD-OE1 | 5.63 | 1.31 | 1.25 | 10 | 1 |
| 2 | C | 195 | ARG | CZ-NH2 | -5.63 | 1.25 | 1.33 | 14 | 1 |
| 2 | C | 147 | GLU | CB-CG | 5.62 | 1.62 | 1.52 | 3 | 1 |
| 2 | B | 115 | TYR | CG-CD1 | 5.62 | 1.46 | 1.39 | 12 | 1 |
| 2 | B | 246 | SER | CA-CB | 5.62 | 1.61 | 1.52 | 4 | 1 |
| 1 | A | 326 | VAL | CB-CG2 | 5.62 | 1.64 | 1.52 | 1 | 1 |
| 2 | C | 189 | SER | CB-OG | 5.61 | 1.49 | 1.42 | 3 | 1 |
| 2 | B | 120 | GLU | CD-OE1 | 5.61 | 1.31 | 1.25 | 7 | 1 |
| 2 | B | 132 | GLU | CB-CG | 5.61 | 1.62 | 1.52 | 8 | 1 |
| 1 | A | 374 | ARG | CD-NE | 5.61 | 1.55 | 1.46 | 9 | 1 |
| 1 | A | 441 | GLU | CG-CD | -5.60 | 1.43 | 1.51 | 10 | 1 |
| 2 | C | 206 | ASN | CB-CG | 5.60 | 1.64 | 1.51 | 11 | 1 |
| 2 | C | 115 | TYR | CE1-CZ | 5.60 | 1.45 | 1.38 | 7 | 1 |
| 2 | B | 97 | VAL | CB-CG2 | 5.59 | 1.64 | 1.52 | 2 | 1 |
| 2 | C | 234 | GLU | CG-CD | 5.59 | 1.60 | 1.51 | 10 | 2 |
| 1 | A | 405 | GLU | CG-CD | -5.59 | 1.43 | 1.51 | 12 | 1 |
| 1 | A | 464 | ARG | NE-CZ | 5.57 | 1.40 | 1.33 | 6 | 1 |
| 1 | A | 428 | TYR | CZ-OH | 5.56 | 1.47 | 1.37 | 5 | 1 |
| 2 | C | 246 | SER | CA-CB | 5.55 | 1.61 | 1.52 | 9 | 1 |
| 1 | A | 497 | TYR | CE1-CZ | 5.54 | 1.45 | 1.38 | 4 | 1 |
| 2 | B | 72 | TRP | CZ2-CH2 | 5.54 | 1.47 | 1.37 | 4 | 1 |
| 1 | A | 435 | TYR | CE2-CZ | 5.54 | 1.45 | 1.38 | 6 | 1 |
| 2 | C | 122 | TYR | CG-CD2 | 5.54 | 1.46 | 1.39 | 8 | 1 |
| 2 | B | 129 | LYS | CE-NZ | -5.53 | 1.35 | 1.49 | 9 | 1 |
| 1 | A | 390 | PHE | CE2-CZ | 5.52 | 1.47 | 1.37 | 14 | 1 |
| 1 | A | 374 | ARG | CZ-NH2 | -5.52 | 1.25 | 1.33 | 8 | 1 |
| 2 | B | 253 | SER | CA-CB | 5.52 | 1.61 | 1.52 | 11 | 1 |
| 2 | C | 221 | HIS | CG-CD2 | 5.52 | 1.45 | 1.35 | 1 | 1 |
| 2 | C | 62 | GLU | CD-OE1 | -5.52 | 1.19 | 1.25 | 6 | 1 |
| 1 | A | 338 | GLU | CB-CG | 5.52 | 1.62 | 1.52 | 12 | 1 |
| 2 | B | 167 | GLY | CA-C | -5.51 | 1.43 | 1.51 | 9 | 1 |
| 1 | A | 486 | PHE | CG-CD2 | 5.51 | 1.47 | 1.38 | 2 | 1 |
| 2 | C | 65 | GLY | CA-C | 5.50 | 1.60 | 1.51 | 15 | 1 |
| 2 | C | 153 | ARG | CD-NE | 5.50 | 1.55 | 1.46 | 8 | 1 |
| 2 | B | 165 | PRO | N-CD | -5.50 | 1.40 | 1.47 | 2 | 1 |
| 1 | A | 321 | GLY | N-CA | -5.49 | 1.37 | 1.46 | 6 | 1 |
| 1 | A | 484 | TRP | CD2-CE2 | 5.49 | 1.48 | 1.41 | 3 | 1 |
| 1 | A | 340 | TRP | CE3-CZ3 | 5.49 | 1.47 | 1.38 | 13 | 1 |
| 1 | A | 355 | MET | N-CA | 5.48 | 1.57 | 1.46 | 7 | 1 |
| 1 | A | 477 | PHE | CG-CD1 | 5.47 | 1.47 | 1.38 | 5 | 1 |
| 2 | B | 158 | GLU | CB-CG | 5.47 | 1.62 | 1.52 | 4 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 1 | A | 373 | GLU | CD-OE1 | -5.47 | 1.19 | 1.25 | 7 | 1 |
| 1 | A | 334 | PHE | CG-CD2 | 5.46 | 1.47 | 1.38 | 1 | 1 |
| 2 | B | 169 | GLU | CB-CG | 5.46 | 1.62 | 1.52 | 15 | 1 |
| 2 | B | 55 | SER | N-CA | 5.46 | 1.57 | 1.46 | 9 | 2 |
| 2 | C | 115 | TYR | CD2-CE2 | 5.46 | 1.47 | 1.39 | 14 | 1 |
| 2 | C | 237 | ARG | CZ-NH2 | -5.45 | 1.25 | 1.33 | 4 | 1 |
| 1 | A | 458 | GLY | CA-C | -5.44 | 1.43 | 1.51 | 14 | 1 |
| 2 | C | 237 | ARG | CZ-NH1 | -5.43 | 1.25 | 1.33 | 14 | 1 |
| 2 | C | 150 | GLU | CD-OE1 | 5.43 | 1.31 | 1.25 | 14 | 1 |
| 1 | A | 462 | SER | CA-CB | 5.42 | 1.61 | 1.52 | 5 | 1 |
| 1 | A | 438 | PHE | CE2-CZ | 5.42 | 1.47 | 1.37 | 9 | 1 |
| 2 | B | 72 | TRP | CB-CG | -5.42 | 1.40 | 1.50 | 4 | 1 |
| 1 | A | 396 | GLU | CD-OE2 | -5.42 | 1.19 | 1.25 | 8 | 1 |
| 2 | C | 175 | ARG | CD-NE | 5.42 | 1.55 | 1.46 | 11 | 1 |
| 1 | A | 449 | TYR | CZ-OH | 5.42 | 1.47 | 1.37 | 12 | 1 |
| 1 | A | 428 | TYR | CG-CD1 | 5.42 | 1.46 | 1.39 | 5 | 2 |
| 2 | B | 65 | GLY | CA-C | -5.42 | 1.43 | 1.51 | 3 | 1 |
| 2 | B | 161 | GLU | CB-CG | 5.41 | 1.62 | 1.52 | 10 | 1 |
| 2 | C | 137 | TYR | CG-CD2 | 5.41 | 1.46 | 1.39 | 6 | 1 |
| 1 | A | 495 | PRO | CA-CB | 5.41 | 1.64 | 1.53 | 14 | 1 |
| 2 | B | 214 | TYR | CD1-CE1 | 5.40 | 1.47 | 1.39 | 5 | 1 |
| 2 | B | 145 | ARG | CD-NE | 5.40 | 1.55 | 1.46 | 12 | 1 |
| 2 | C | 55 | SER | CB-OG | 5.40 | 1.49 | 1.42 | 14 | 1 |
| 2 | B | 121 | PRO | CA-CB | 5.39 | 1.64 | 1.53 | 3 | 1 |
| 2 | B | 227 | GLU | CD-OE2 | 5.39 | 1.31 | 1.25 | 6 | 1 |
| 1 | A | 478 | TYR | CE1-CZ | 5.39 | 1.45 | 1.38 | 14 | 1 |
| 1 | A | 471 | ASP | CA-CB | 5.39 | 1.65 | 1.53 | 10 | 1 |
| 2 | C | 258 | TYR | CG-CD1 | 5.38 | 1.46 | 1.39 | 2 | 1 |
| 2 | C | 201 | GLU | CD-OE1 | 5.38 | 1.31 | 1.25 | 8 | 1 |
| 2 | B | 182 | ARG | NE-CZ | 5.37 | 1.40 | 1.33 | 2 | 1 |
| 1 | A | 334 | PHE | CB-CG | 5.37 | 1.60 | 1.51 | 14 | 1 |
| 2 | B | 258 | TYR | CE1-CZ | 5.37 | 1.45 | 1.38 | 6 | 1 |
| 1 | A | 476 | TYR | CE2-CZ | 5.36 | 1.45 | 1.38 | 15 | 1 |
| 2 | C | 256 | GLU | CD-OE2 | 5.36 | 1.31 | 1.25 | 3 | 1 |
| 1 | A | 449 | TYR | CG-CD2 | 5.36 | 1.46 | 1.39 | 12 | 1 |
| 2 | B | 98 | GLN | C-N | -5.35 | 1.24 | 1.34 | 3 | 1 |
| 2 | C | 173 | ARG | NE-CZ | -5.35 | 1.26 | 1.33 | 15 | 2 |
| 1 | A | 330 | ARG | CZ-NH2 | -5.35 | 1.26 | 1.33 | 2 | 1 |
| 1 | A | 336 | PHE | CG-CD2 | 5.35 | 1.46 | 1.38 | 13 | 1 |
| 2 | B | 168 | GLU | CD-OE2 | 5.35 | 1.31 | 1.25 | 3 | 1 |
| 1 | A | 511 | GLY | N-CA | 5.35 | 1.54 | 1.46 | 12 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 1 | A | 340 | TRP | CG-CD1 | 5.34 | 1.44 | 1.36 | 12 | 1 |
| 2 | C | 157 | HIS | CB-CG | 5.34 | 1.59 | 1.50 | 14 | 1 |
| 2 | C | 105 | GLN | CG-CD | 5.34 | 1.63 | 1.51 | 4 | 1 |
| 1 | A | 437 | ARG | CD-NE | 5.33 | 1.55 | 1.46 | 1 | 2 |
| 1 | A | 379 | PHE | CE2-CZ | 5.33 | 1.47 | 1.37 | 11 | 1 |
| 2 | C | 214 | TYR | CA-CB | 5.32 | 1.65 | 1.53 | 10 | 1 |
| 2 | B | 188 | TYR | CE2-CZ | 5.32 | 1.45 | 1.38 | 13 | 1 |
| 1 | A | 334 | PHE | CA-CB | 5.32 | 1.65 | 1.53 | 2 | 1 |
| 2 | B | 62 | GLU | CG-CD | 5.31 | 1.59 | 1.51 | 13 | 1 |
| 2 | B | 213 | GLU | CD-OE1 | -5.31 | 1.19 | 1.25 | 9 | 1 |
| 2 | C | 258 | TYR | CE2-CZ | 5.31 | 1.45 | 1.38 | 15 | 2 |
| 2 | B | 167 | GLY | N-CA | 5.30 | 1.54 | 1.46 | 10 | 1 |
| 2 | C | 184 | HIS | CA-CB | 5.30 | 1.65 | 1.53 | 5 | 1 |
| 1 | A | 478 | TYR | CG-CD1 | 5.30 | 1.46 | 1.39 | 6 | 1 |
| 1 | A | 464 | ARG | CD-NE | 5.30 | 1.55 | 1.46 | 8 | 1 |
| 2 | C | 78 | GLU | CB-CG | 5.29 | 1.62 | 1.52 | 13 | 1 |
| 2 | C | 191 | GLU | CG-CD | 5.29 | 1.59 | 1.51 | 15 | 1 |
| 1 | A | 408 | ARG | CZ-NH2 | -5.29 | 1.26 | 1.33 | 4 | 1 |
| 1 | A | 476 | TYR | CD1-CE1 | 5.28 | 1.47 | 1.39 | 1 | 1 |
| 2 | C | 80 | GLU | CD-OE2 | 5.28 | 1.31 | 1.25 | 5 | 1 |
| 2 | C | 120 | GLU | CD-OE2 | 5.28 | 1.31 | 1.25 | 5 | 1 |
| 2 | C | 120 | GLU | CG-CD | 5.28 | 1.59 | 1.51 | 4 | 1 |
| 2 | C | 188 | TYR | CG-CD2 | 5.28 | 1.46 | 1.39 | 3 | 2 |
| 2 | C | 104 | PHE | CG-CD1 | 5.28 | 1.46 | 1.38 | 9 | 1 |
| 2 | C | 258 | TYR | CD2-CE2 | 5.27 | 1.47 | 1.39 | 3 | 1 |
| 1 | A | 467 | PHE | CG-CD1 | 5.26 | 1.46 | 1.38 | 7 | 1 |
| 2 | B | 150 | GLU | CD-OE1 | 5.25 | 1.31 | 1.25 | 8 | 1 |
| 1 | A | 323 | PHE | CG-CD1 | 5.25 | 1.46 | 1.38 | 4 | 1 |
| 2 | C | 251 | PHE | CE2-CZ | 5.25 | 1.47 | 1.37 | 5 | 1 |
| 1 | A | 330 | ARG | CD-NE | 5.25 | 1.55 | 1.46 | 5 | 1 |
| 1 | A | 474 | PHE | CG-CD2 | 5.25 | 1.46 | 1.38 | 8 | 1 |
| 2 | B | 187 | PRO | CA-C | 5.24 | 1.63 | 1.52 | 5 | 1 |
| 2 | C | 258 | TYR | CZ-OH | 5.24 | 1.46 | 1.37 | 6 | 1 |
| 2 | B | 173 | ARG | CD-NE | 5.24 | 1.55 | 1.46 | 9 | 1 |
| 2 | B | 205 | GLU | CB-CG | 5.24 | 1.62 | 1.52 | 1 | 1 |
| 1 | A | 436 | TYR | CB-CG | -5.24 | 1.43 | 1.51 | 10 | 1 |
| 2 | B | 142 | GLU | CG-CD | 5.24 | 1.59 | 1.51 | 7 | 1 |
| 2 | B | 72 | TRP | CG-CD1 | 5.24 | 1.44 | 1.36 | 15 | 1 |
| 2 | B | 251 | PHE | CG-CD1 | 5.23 | 1.46 | 1.38 | 9 | 1 |
| 1 | A | 505 | TRP | CE3-CZ3 | 5.23 | 1.47 | 1.38 | 13 | 1 |
| 2 | C | 205 | GLU | CB-CG | 5.23 | 1.62 | 1.52 | 4 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 1 | A | 362 | ARG | C-N | 5.22 | 1.42 | 1.33 | 6 | 1 |
| 2 | B | 229 | ALA | CA-CB | 5.22 | 1.63 | 1.52 | 12 | 1 |
| 2 | B | 232 | ALA | C-N | 5.22 | 1.46 | 1.34 | 5 | 1 |
| 1 | A | 437 | ARG | NE-CZ | -5.22 | 1.26 | 1.33 | 8 | 1 |
| 2 | B | 195 | ARG | NE-CZ | 5.21 | 1.39 | 1.33 | 10 | 1 |
| 1 | A | 405 | GLU | CD-OE2 | -5.21 | 1.20 | 1.25 | 8 | 1 |
| 2 | B | 207 | GLY | CA-C | 5.21 | 1.60 | 1.51 | 7 | 1 |
| 1 | A | 335 | VAL | CB-CG1 | 5.20 | 1.63 | 1.52 | 12 | 1 |
| 1 | A | 418 | ALA | N-CA | -5.20 | 1.35 | 1.46 | 4 | 1 |
| 1 | A | 468 | MET | CG-SD | 5.20 | 1.94 | 1.81 | 5 | 1 |
| 2 | C | 226 | SER | CB-OG | 5.20 | 1.49 | 1.42 | 7 | 1 |
| 1 | A | 386 | LYS | N-CA | -5.20 | 1.35 | 1.46 | 1 | 1 |
| 2 | C | 195 | ARG | NE-CZ | 5.20 | 1.39 | 1.33 | 14 | 1 |
| 2 | C | 104 | PHE | CE2-CZ | 5.20 | 1.47 | 1.37 | 5 | 1 |
| 2 | B | 147 | GLU | CD-OE2 | 5.20 | 1.31 | 1.25 | 8 | 1 |
| 2 | B | 71 | PHE | CG-CD2 | 5.19 | 1.46 | 1.38 | 13 | 1 |
| 2 | C | 142 | GLU | CB-CG | 5.19 | 1.62 | 1.52 | 1 | 1 |
| 1 | A | 396 | GLU | CB-CG | 5.19 | 1.62 | 1.52 | 5 | 1 |
| 2 | B | 150 | GLU | CD-OE2 | 5.18 | 1.31 | 1.25 | 9 | 1 |
| 1 | A | 436 | TYR | C-O | 5.17 | 1.33 | 1.23 | 1 | 1 |
| 1 | A | 361 | TRP | CD2-CE3 | -5.17 | 1.32 | 1.40 | 9 | 1 |
| 2 | B | 104 | PHE | CE2-CZ | 5.17 | 1.47 | 1.37 | 4 | 1 |
| 1 | A | 483 | TYR | CA-CB | 5.17 | 1.65 | 1.53 | 10 | 1 |
| 2 | C | 87 | SER | CB-OG | 5.17 | 1.49 | 1.42 | 11 | 1 |
| 1 | A | 461 | GLU | CD-OE2 | 5.17 | 1.31 | 1.25 | 14 | 1 |
| 2 | C | 92 | GLU | CD-OE2 | -5.17 | 1.20 | 1.25 | 11 | 1 |
| 2 | B | 79 | THR | CA-CB | -5.17 | 1.40 | 1.53 | 1 | 1 |
| 2 | C | 199 | ARG | CD-NE | 5.17 | 1.55 | 1.46 | 9 | 1 |
| 2 | C | 188 | TYR | CE2-CZ | 5.16 | 1.45 | 1.38 | 12 | 1 |
| 2 | C | 247 | PHE | CG-CD2 | 5.16 | 1.46 | 1.38 | 1 | 1 |
| 2 | B | 126 | PHE | CG-CD1 | 5.16 | 1.46 | 1.38 | 11 | 1 |
| 2 | C | 245 | GLU | CD-OE1 | 5.16 | 1.31 | 1.25 | 7 | 1 |
| 2 | B | 247 | PHE | CG-CD1 | 5.16 | 1.46 | 1.38 | 10 | 1 |
| 2 | C | 242 | PRO | N-CD | -5.15 | 1.40 | 1.47 | 10 | 1 |
| 1 | A | 443 | ARG | CZ-NH1 | -5.15 | 1.26 | 1.33 | 6 | 1 |
| 1 | A | 435 | TYR | CE1-CZ | 5.15 | 1.45 | 1.38 | 11 | 1 |
| 2 | B | 72 | TRP | CD2-CE2 | -5.14 | 1.35 | 1.41 | 10 | 2 |
| 2 | C | 257 | GLU | CG-CD | 5.14 | 1.59 | 1.51 | 2 | 1 |
| 2 | B | 227 | GLU | CG-CD | 5.13 | 1.59 | 1.51 | 7 | 1 |
| 1 | A | 420 | PHE | CE1-CZ | 5.13 | 1.47 | 1.37 | 2 | 1 |
| 1 | A | 483 | TYR | CD2-CE2 | -5.12 | 1.31 | 1.39 | 15 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 2 | B | 116 | ARG | CZ-NH1 | -5.12 | 1.26 | 1.33 | 2 | 1 |
| 2 | C | 144 | LEU | CA-CB | -5.12 | 1.42 | 1.53 | 2 | 1 |
| 2 | B | 57 | PHE | CG-CD2 | 5.12 | 1.46 | 1.38 | 4 | 1 |
| 1 | A | 377 | GLY | CA-C | 5.11 | 1.60 | 1.51 | 7 | 1 |
| 2 | B | 61 | ARG | CZ-NH2 | -5.11 | 1.26 | 1.33 | 14 | 1 |
| 2 | C | 130 | TRP | CG-CD1 | -5.11 | 1.29 | 1.36 | 6 | 1 |
| 1 | A | 381 | PHE | CB-CG | 5.11 | 1.60 | 1.51 | 5 | 1 |
| 2 | B | 65 | GLY | N-CA | -5.11 | 1.38 | 1.46 | 10 | 1 |
| 2 | C | 182 | ARG | CD-NE | 5.11 | 1.55 | 1.46 | 10 | 1 |
| 1 | A | 429 | PHE | CE1-CZ | 5.11 | 1.47 | 1.37 | 1 | 1 |
| 1 | A | 466 | SER | CA-CB | 5.11 | 1.60 | 1.52 | 8 | 1 |
| 2 | C | 174 | ALA | CA-CB | 5.10 | 1.63 | 1.52 | 4 | 1 |
| 2 | C | 116 | ARG | CZ-NH2 | -5.10 | 1.26 | 1.33 | 7 | 1 |
| 1 | A | 398 | GLY | CA-C | 5.10 | 1.60 | 1.51 | 10 | 1 |
| 2 | C | 93 | VAL | CB-CG1 | 5.10 | 1.63 | 1.52 | 14 | 1 |
| 2 | C | 258 | TYR | CE1-CZ | 5.10 | 1.45 | 1.38 | 10 | 2 |
| 2 | C | 130 | TRP | CD2-CE3 | -5.09 | 1.32 | 1.40 | 4 | 1 |
| 2 | B | 161 | GLU | CG-CD | 5.09 | 1.59 | 1.51 | 15 | 1 |
| 2 | B | 251 | PHE | CE1-CZ | 5.09 | 1.47 | 1.37 | 8 | 1 |
| 2 | B | 98 | GLN | CB-CG | 5.08 | 1.66 | 1.52 | 12 | 1 |
| 1 | A | 477 | PHE | CA-C | -5.08 | 1.39 | 1.52 | 15 | 1 |
| 1 | A | 394 | SER | N-CA | 5.08 | 1.56 | 1.46 | 5 | 1 |
| 2 | C | 100 | TYR | CB-CG | 5.07 | 1.59 | 1.51 | 8 | 1 |
| 1 | A | 323 | PHE | CE2-CZ | 5.06 | 1.47 | 1.37 | 1 | 1 |
| 1 | A | 361 | TRP | CD2-CE2 | -5.06 | 1.35 | 1.41 | 7 | 1 |
| 2 | C | 106 | LYS | CD-CE | 5.06 | 1.63 | 1.51 | 10 | 1 |
| 2 | B | 168 | GLU | CB-CG | 5.06 | 1.61 | 1.52 | 11 | 1 |
| 2 | B | 150 | GLU | CB-CG | 5.06 | 1.61 | 1.52 | 9 | 1 |
| 2 | B | 58 | SER | CB-OG | 5.05 | 1.48 | 1.42 | 7 | 1 |
| 1 | A | 421 | TRP | NE1-CE2 | -5.05 | 1.30 | 1.37 | 8 | 1 |
| 1 | A | 503 | ARG | CZ-NH1 | -5.05 | 1.26 | 1.33 | 3 | 1 |
| 2 | C | 256 | GLU | CD-OE1 | 5.05 | 1.31 | 1.25 | 15 | 1 |
| 2 | B | 175 | ARG | CZ-NH2 | -5.04 | 1.26 | 1.33 | 13 | 1 |
| 2 | C | 146 | ALA | CA-CB | 5.04 | 1.63 | 1.52 | 14 | 1 |
| 2 | C | 237 | ARG | NE-CZ | 5.04 | 1.39 | 1.33 | 14 | 1 |
| 2 | C | 210 | ARG | CD-NE | 5.04 | 1.55 | 1.46 | 14 | 1 |
| 1 | A | 341 | PHE | CE2-CZ | 5.03 | 1.47 | 1.37 | 2 | 1 |
| 2 | B | 99 | PRO | N-CD | 5.03 | 1.54 | 1.47 | 10 | 1 |
| 2 | B | 63 | GLN | CA-C | -5.03 | 1.39 | 1.52 | 12 | 1 |
| 1 | A | 494 | GLU | CB-CG | 5.03 | 1.61 | 1.52 | 9 | 1 |
| 2 | C | 169 | GLU | CB-CG | 5.03 | 1.61 | 1.52 | 4 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 2 | B | 138 | ARG | CZ-NH2 | -5.03 | 1.26 | 1.33 | 15 | 1 |
| 1 | A | 509 | PRO | N-CA | 5.03 | 1.55 | 1.47 | 3 | 1 |
| 2 | B | 80 | GLU | CD-OE1 | 5.03 | 1.31 | 1.25 | 5 | 1 |
| 2 | C | 234 | GLU | CD-OE1 | 5.02 | 1.31 | 1.25 | 3 | 1 |
| 2 | B | 100 | TYR | CD2-CE2 | 5.02 | 1.46 | 1.39 | 7 | 1 |
| 2 | C | 262 | LEU | CB-CG | 5.02 | 1.67 | 1.52 | 12 | 1 |
| 2 | C | 111 | GLU | CB-CG | 5.02 | 1.61 | 1.52 | 10 | 1 |
| 1 | A | 505 | TRP | CZ2-CH2 | 5.01 | 1.46 | 1.37 | 14 | 1 |
| 2 | C | 235 | ASP | C-N | 5.01 | 1.45 | 1.34 | 5 | 1 |
| 1 | A | 342 | TRP | NE1-CE2 | -5.01 | 1.31 | 1.37 | 14 | 1 |

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

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-----------|--------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 1 | A | 503 | ARG | NE-CZ-NH2 | 28.12 | 134.36 | 120.30 | 6 | 10 |
| 2 | B | 210 | ARG | NE-CZ-NH2 | 25.51 | 133.06 | 120.30 | 11 | 12 |
| 2 | B | 153 | ARG | NE-CZ-NH2 | 25.41 | 133.01 | 120.30 | 1 | 9 |
| 2 | B | 173 | ARG | NE-CZ-NH2 | 25.10 | 132.85 | 120.30 | 12 | 9 |
| 1 | A | 330 | ARG | NE-CZ-NH2 | 24.18 | 132.39 | 120.30 | 10 | 8 |
| 2 | C | 171 | ARG | NE-CZ-NH2 | 24.01 | 132.30 | 120.30 | 15 | 11 |
| 2 | B | 138 | ARG | NE-CZ-NH2 | 23.58 | 132.09 | 120.30 | 2 | 10 |
| 1 | A | 343 | ARG | NE-CZ-NH1 | -22.99 | 108.80 | 120.30 | 11 | 10 |
| 2 | C | 153 | ARG | NE-CZ-NH2 | 22.73 | 131.66 | 120.30 | 10 | 11 |
| 1 | A | 437 | ARG | NE-CZ-NH2 | -22.68 | 108.96 | 120.30 | 4 | 8 |
| 2 | C | 61 | ARG | NE-CZ-NH2 | 22.43 | 131.52 | 120.30 | 4 | 9 |
| 2 | C | 138 | ARG | NE-CZ-NH2 | 21.82 | 131.21 | 120.30 | 2 | 12 |
| 1 | A | 343 | ARG | NE-CZ-NH2 | 21.56 | 131.08 | 120.30 | 2 | 8 |
| 2 | C | 199 | ARG | NE-CZ-NH2 | 21.47 | 131.04 | 120.30 | 12 | 9 |
| 2 | C | 193 | ARG | NE-CZ-NH2 | 21.01 | 130.81 | 120.30 | 8 | 12 |
| 2 | C | 138 | ARG | NE-CZ-NH1 | -20.98 | 109.81 | 120.30 | 2 | 9 |
| 2 | B | 116 | ARG | NE-CZ-NH1 | -20.97 | 109.81 | 120.30 | 1 | 5 |
| 2 | C | 175 | ARG | NE-CZ-NH2 | 20.55 | 130.58 | 120.30 | 2 | 13 |
| 2 | B | 193 | ARG | NE-CZ-NH2 | 20.53 | 130.56 | 120.30 | 1 | 11 |
| 2 | C | 153 | ARG | NE-CZ-NH1 | -20.39 | 110.11 | 120.30 | 6 | 7 |
| 2 | B | 153 | ARG | NE-CZ-NH1 | -20.02 | 110.29 | 120.30 | 5 | 10 |
| 2 | C | 195 | ARG | NE-CZ-NH2 | 19.92 | 130.26 | 120.30 | 8 | 12 |
| 1 | A | 408 | ARG | NE-CZ-NH1 | -19.67 | 110.47 | 120.30 | 4 | 3 |
| 2 | C | 145 | ARG | NE-CZ-NH2 | 19.57 | 130.09 | 120.30 | 4 | 14 |
| 2 | C | 237 | ARG | NE-CZ-NH2 | 19.43 | 130.02 | 120.30 | 11 | 9 |
| 2 | B | 210 | ARG | NE-CZ-NH1 | -19.39 | 110.60 | 120.30 | 13 | 8 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-----------|--------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 2 | B | 195 | ARG | NE-CZ-NH2 | 19.15 | 129.88 | 120.30 | 5 | 13 |
| 1 | A | 345 | ARG | NE-CZ-NH2 | 19.09 | 129.84 | 120.30 | 6 | 10 |
| 2 | B | 195 | ARG | NE-CZ-NH1 | -18.84 | 110.88 | 120.30 | 15 | 11 |
| 1 | A | 464 | ARG | NE-CZ-NH2 | 18.70 | 129.65 | 120.30 | 14 | 9 |
| 2 | C | 173 | ARG | NE-CZ-NH2 | 18.68 | 129.64 | 120.30 | 5 | 11 |
| 2 | C | 173 | ARG | NE-CZ-NH1 | -18.53 | 111.03 | 120.30 | 5 | 9 |
| 2 | C | 116 | ARG | NE-CZ-NH2 | 18.41 | 129.51 | 120.30 | 5 | 9 |
| 2 | C | 83 | ARG | NE-CZ-NH1 | -18.36 | 111.12 | 120.30 | 7 | 6 |
| 1 | A | 443 | ARG | NE-CZ-NH2 | 18.27 | 129.44 | 120.30 | 1 | 10 |
| 2 | B | 61 | ARG | NE-CZ-NH2 | 18.21 | 129.41 | 120.30 | 8 | 9 |
| 2 | B | 193 | ARG | NE-CZ-NH1 | -18.08 | 111.26 | 120.30 | 1 | 10 |
| 2 | C | 210 | ARG | NE-CZ-NH2 | 18.04 | 129.32 | 120.30 | 14 | 12 |
| 2 | C | 199 | ARG | NE-CZ-NH1 | -17.79 | 111.41 | 120.30 | 8 | 9 |
| 1 | A | 408 | ARG | NE-CZ-NH2 | 17.62 | 129.11 | 120.30 | 4 | 11 |
| 2 | C | 171 | ARG | NE-CZ-NH1 | -17.57 | 111.52 | 120.30 | 9 | 11 |
| 2 | B | 61 | ARG | NE-CZ-NH1 | -17.37 | 111.62 | 120.30 | 8 | 7 |
| 1 | A | 437 | ARG | NE-CZ-NH1 | 16.80 | 128.70 | 120.30 | 5 | 12 |
| 1 | A | 339 | ARG | NE-CZ-NH1 | 16.72 | 128.66 | 120.30 | 15 | 7 |
| 1 | A | 443 | ARG | NE-CZ-NH1 | -16.64 | 111.98 | 120.30 | 1 | 8 |
| 2 | C | 182 | ARG | NE-CZ-NH1 | 16.59 | 128.59 | 120.30 | 8 | 12 |
| 2 | B | 138 | ARG | NE-CZ-NH1 | -16.48 | 112.06 | 120.30 | 4 | 6 |
| 2 | B | 145 | ARG | NE-CZ-NH1 | -16.47 | 112.07 | 120.30 | 13 | 5 |
| 2 | B | 175 | ARG | NE-CZ-NH1 | 16.33 | 128.47 | 120.30 | 4 | 8 |
| 2 | B | 173 | ARG | NE-CZ-NH1 | -16.06 | 112.27 | 120.30 | 8 | 11 |
| 2 | C | 182 | ARG | NE-CZ-NH2 | -15.79 | 112.41 | 120.30 | 6 | 11 |
| 2 | B | 182 | ARG | NE-CZ-NH1 | -15.73 | 112.44 | 120.30 | 14 | 4 |
| 2 | B | 199 | ARG | NE-CZ-NH1 | 15.56 | 128.08 | 120.30 | 8 | 6 |
| 2 | C | 210 | ARG | NE-CZ-NH1 | -15.55 | 112.53 | 120.30 | 4 | 7 |
| 2 | C | 83 | ARG | NE-CZ-NH2 | 15.48 | 128.04 | 120.30 | 5 | 8 |
| 2 | B | 126 | PHE | CB-CG-CD1 | 15.35 | 131.54 | 120.80 | 14 | 5 |
| 1 | A | 431 | ARG | NE-CZ-NH2 | 15.24 | 127.92 | 120.30 | 5 | 10 |
| 2 | B | 116 | ARG | NE-CZ-NH2 | 15.18 | 127.89 | 120.30 | 1 | 7 |
| 1 | A | 374 | ARG | NE-CZ-NH2 | 15.18 | 127.89 | 120.30 | 3 | 7 |
| 2 | B | 115 | TYR | CB-CG-CD2 | 15.18 | 130.10 | 121.00 | 9 | 5 |
| 1 | A | 431 | ARG | NE-CZ-NH1 | -14.95 | 112.83 | 120.30 | 12 | 9 |
| 1 | A | 362 | ARG | NE-CZ-NH1 | 14.84 | 127.72 | 120.30 | 5 | 12 |
| 2 | B | 199 | ARG | NE-CZ-NH2 | 14.62 | 127.61 | 120.30 | 5 | 9 |
| 2 | B | 145 | ARG | NE-CZ-NH2 | 14.60 | 127.60 | 120.30 | 13 | 6 |
| 1 | A | 464 | ARG | NE-CZ-NH1 | -14.58 | 113.01 | 120.30 | 11 | 7 |
| 2 | C | 175 | ARG | NE-CZ-NH1 | -14.58 | 113.01 | 120.30 | 2 | 10 |
| 2 | B | 171 | ARG | NE-CZ-NH2 | 14.46 | 127.53 | 120.30 | 2 | 10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-----------|--------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 2 | C | 258 | TYR | CB-CG-CD1 | -14.19 | 112.49 | 121.00 | 15 | 7 |
| 2 | C | 116 | ARG | NE-CZ-NH1 | -14.12 | 113.24 | 120.30 | 5 | 6 |
| 2 | B | 237 | ARG | NE-CZ-NH2 | -14.05 | 113.28 | 120.30 | 2 | 14 |
| 1 | A | 339 | ARG | NE-CZ-NH2 | -14.02 | 113.29 | 120.30 | 6 | 12 |
| 2 | C | 195 | ARG | NE-CZ-NH1 | 13.88 | 127.24 | 120.30 | 11 | 11 |
| 2 | B | 188 | TYR | CB-CG-CD2 | -13.83 | 112.70 | 121.00 | 3 | 9 |
| 1 | A | 374 | ARG | NE-CZ-NH1 | -13.81 | 113.39 | 120.30 | 4 | 8 |
| 2 | B | 237 | ARG | NE-CZ-NH1 | -13.80 | 113.40 | 120.30 | 8 | 10 |
| 2 | B | 175 | ARG | NE-CZ-NH2 | 13.78 | 127.19 | 120.30 | 6 | 11 |
| 2 | C | 100 | TYR | CB-CG-CD2 | -13.72 | 112.77 | 121.00 | 1 | 6 |
| 2 | C | 100 | TYR | CB-CG-CD1 | 13.66 | 129.20 | 121.00 | 1 | 4 |
| 2 | B | 258 | TYR | CB-CG-CD1 | 13.64 | 129.19 | 121.00 | 3 | 5 |
| 2 | C | 61 | ARG | NE-CZ-NH1 | -13.54 | 113.53 | 120.30 | 12 | 9 |
| 2 | B | 83 | ARG | NE-CZ-NH1 | -13.52 | 113.54 | 120.30 | 5 | 8 |
| 2 | B | 57 | PHE | CB-CG-CD2 | 13.52 | 130.26 | 120.80 | 5 | 4 |
| 2 | C | 247 | PHE | CB-CG-CD2 | 13.47 | 130.23 | 120.80 | 2 | 6 |
| 1 | A | 362 | ARG | NE-CZ-NH2 | -13.35 | 113.63 | 120.30 | 3 | 8 |
| 1 | A | 486 | PHE | CB-CG-CD2 | -13.23 | 111.54 | 120.80 | 9 | 6 |
| 2 | B | 83 | ARG | NE-CZ-NH2 | 13.19 | 126.90 | 120.30 | 1 | 7 |
| 2 | B | 137 | TYR | CB-CG-CD2 | -12.83 | 113.30 | 121.00 | 11 | 7 |
| 1 | A | 345 | ARG | NE-CZ-NH1 | -12.79 | 113.91 | 120.30 | 7 | 7 |
| 1 | A | 330 | ARG | NE-CZ-NH1 | -12.72 | 113.94 | 120.30 | 5 | 9 |
| 2 | C | 237 | ARG | NE-CZ-NH1 | -12.65 | 113.97 | 120.30 | 1 | 9 |
| 1 | A | 483 | TYR | CB-CG-CD2 | -12.64 | 113.42 | 121.00 | 1 | 3 |
| 2 | C | 247 | PHE | CB-CG-CD1 | -12.62 | 111.96 | 120.80 | 2 | 6 |
| 2 | B | 126 | PHE | CB-CG-CD2 | -12.29 | 112.19 | 120.80 | 5 | 3 |
| 2 | B | 188 | TYR | CB-CG-CD1 | -12.11 | 113.74 | 121.00 | 11 | 7 |
| 1 | A | 435 | TYR | CB-CG-CD1 | 11.98 | 128.19 | 121.00 | 2 | 5 |
| 2 | B | 137 | TYR | CB-CG-CD1 | -11.95 | 113.83 | 121.00 | 6 | 6 |
| 2 | B | 182 | ARG | NE-CZ-NH2 | 11.75 | 126.17 | 120.30 | 14 | 8 |
| 1 | A | 341 | PHE | CB-CG-CD2 | 11.75 | 129.02 | 120.80 | 5 | 6 |
| 2 | C | 104 | PHE | CB-CG-CD1 | -11.72 | 112.59 | 120.80 | 12 | 3 |
| 2 | C | 258 | TYR | CB-CG-CD2 | 11.71 | 128.03 | 121.00 | 11 | 6 |
| 2 | C | 71 | PHE | CB-CG-CD2 | -11.70 | 112.61 | 120.80 | 9 | 5 |
| 2 | C | 115 | TYR | CB-CG-CD2 | 11.64 | 127.98 | 121.00 | 11 | 7 |
| 2 | B | 122 | TYR | CB-CG-CD1 | -11.56 | 114.07 | 121.00 | 12 | 3 |
| 2 | B | 57 | PHE | CB-CG-CD1 | 11.53 | 128.87 | 120.80 | 3 | 6 |
| 2 | C | 188 | TYR | CB-CG-CD2 | 11.49 | 127.90 | 121.00 | 2 | 2 |
| 2 | B | 258 | TYR | CB-CG-CD2 | -11.47 | 114.12 | 121.00 | 3 | 7 |
| 2 | C | 122 | TYR | CB-CG-CD1 | 11.44 | 127.86 | 121.00 | 5 | 4 |
| 1 | A | 446 | ASP | CB-CG-OD1 | 11.41 | 128.57 | 118.30 | 10 | 4 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|------------|--------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 2 | C | 126 | PHE | CB-CG-CD2 | 11.41 | 128.79 | 120.80 | 15 | 5 |
| 1 | A | 503 | ARG | NH1-CZ-NH2 | -11.40 | 106.86 | 119.40 | 6 | 4 |
| 1 | A | 323 | PHE | CB-CG-CD2 | -11.31 | 112.89 | 120.80 | 1 | 6 |
| 1 | A | 379 | PHE | CB-CG-CD1 | -11.29 | 112.90 | 120.80 | 6 | 3 |
| 2 | B | 171 | ARG | NE-CZ-NH1 | -11.26 | 114.67 | 120.30 | 7 | 7 |
| 1 | A | 449 | TYR | CB-CG-CD2 | 11.03 | 127.62 | 121.00 | 10 | 9 |
| 2 | B | 115 | TYR | CB-CG-CD1 | -10.91 | 114.45 | 121.00 | 11 | 4 |
| 2 | C | 193 | ARG | NE-CZ-NH1 | 10.90 | 125.75 | 120.30 | 14 | 9 |
| 1 | A | 336 | PHE | CB-CG-CD2 | -10.88 | 113.18 | 120.80 | 1 | 4 |
| 1 | A | 438 | PHE | CB-CG-CD1 | -10.85 | 113.21 | 120.80 | 4 | 4 |
| 2 | C | 126 | PHE | CB-CG-CD1 | -10.83 | 113.22 | 120.80 | 14 | 6 |
| 1 | A | 391 | ASP | CB-CG-OD1 | 10.82 | 128.03 | 118.30 | 12 | 4 |
| 2 | C | 188 | TYR | CB-CG-CD1 | -10.61 | 114.63 | 121.00 | 2 | 6 |
| 2 | C | 235 | ASP | CB-CG-OD1 | -10.60 | 108.76 | 118.30 | 15 | 5 |
| 2 | C | 115 | TYR | CB-CG-CD1 | -10.60 | 114.64 | 121.00 | 14 | 6 |
| 1 | A | 483 | TYR | CB-CG-CD1 | 10.58 | 127.35 | 121.00 | 1 | 5 |
| 1 | A | 474 | PHE | CB-CG-CD2 | -10.54 | 113.42 | 120.80 | 6 | 4 |
| 2 | C | 71 | PHE | CB-CG-CD1 | -10.48 | 113.47 | 120.80 | 2 | 4 |
| 1 | A | 353 | TYR | CB-CG-CD1 | -10.46 | 114.72 | 121.00 | 2 | 5 |
| 2 | C | 214 | TYR | CB-CG-CD2 | 10.41 | 127.25 | 121.00 | 6 | 3 |
| 1 | A | 503 | ARG | NE-CZ-NH1 | -10.41 | 115.09 | 120.30 | 15 | 4 |
| 1 | A | 379 | PHE | CB-CG-CD2 | -10.30 | 113.59 | 120.80 | 9 | 11 |
| 2 | C | 122 | TYR | CB-CG-CD2 | 10.29 | 127.17 | 121.00 | 15 | 4 |
| 1 | A | 497 | TYR | CB-CG-CD1 | -10.27 | 114.83 | 121.00 | 12 | 6 |
| 1 | A | 471 | ASP | CB-CG-OD1 | 10.27 | 127.55 | 118.30 | 4 | 2 |
| 2 | B | 251 | PHE | CB-CG-CD2 | -10.19 | 113.66 | 120.80 | 1 | 2 |
| 1 | A | 390 | PHE | CB-CG-CD1 | 10.17 | 127.92 | 120.80 | 1 | 7 |
| 1 | A | 467 | PHE | CB-CG-CD2 | 10.17 | 127.92 | 120.80 | 6 | 4 |
| 2 | B | 172 | ASP | CB-CG-OD1 | -10.17 | 109.15 | 118.30 | 8 | 3 |
| 2 | B | 179 | ASP | CB-CG-OD1 | 10.15 | 127.44 | 118.30 | 4 | 2 |
| 2 | B | 247 | PHE | CB-CG-CD2 | -10.04 | 113.77 | 120.80 | 4 | 4 |
| 1 | A | 474 | PHE | CB-CG-CD1 | -10.04 | 113.77 | 120.80 | 14 | 2 |
| 2 | B | 138 | ARG | NH1-CZ-NH2 | -10.01 | 108.39 | 119.40 | 2 | 2 |
| 1 | A | 467 | PHE | CB-CG-CD1 | -9.97 | 113.82 | 120.80 | 6 | 3 |
| 1 | A | 351 | ASP | CB-CG-OD1 | 9.90 | 127.21 | 118.30 | 3 | 5 |
| 2 | C | 175 | ARG | NH1-CZ-NH2 | -9.89 | 108.52 | 119.40 | 1 | 5 |
| 2 | B | 71 | PHE | CB-CG-CD1 | -9.85 | 113.90 | 120.80 | 10 | 3 |
| 2 | C | 195 | ARG | NH1-CZ-NH2 | -9.82 | 108.59 | 119.40 | 11 | 3 |
| 1 | A | 376 | ASP | CB-CG-OD1 | 9.80 | 127.12 | 118.30 | 7 | 6 |
| 2 | B | 86 | MET | CG-SD-CE | -9.69 | 84.69 | 100.20 | 4 | 4 |
| 2 | B | 125 | ASP | CB-CG-OD1 | -9.69 | 109.58 | 118.30 | 6 | 3 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|------------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 1 | A | 505 | TRP | CE2-CD2-CG | -9.52 | 99.69 | 107.30 | 6 | 2 |
| 2 | B | 170 | MET | CG-SD-CE | -9.49 | 85.02 | 100.20 | 8 | 5 |
| 1 | A | 429 | PHE | CB-CG-CD1 | -9.45 | 114.18 | 120.80 | 5 | 6 |
| 1 | A | 428 | TYR | CB-CG-CD1 | 9.45 | 126.67 | 121.00 | 4 | 7 |
| 2 | C | 103 | ASP | CB-CG-OD1 | 9.38 | 126.74 | 118.30 | 14 | 3 |
| 1 | A | 343 | ARG | NH1-CZ-NH2 | -9.34 | 109.13 | 119.40 | 1 | 4 |
| 2 | B | 172 | ASP | CB-CG-OD2 | 9.33 | 126.70 | 118.30 | 8 | 2 |
| 2 | B | 104 | PHE | CB-CG-CD2 | 9.24 | 127.27 | 120.80 | 15 | 2 |
| 1 | A | 483 | TYR | CG-CD2-CE2 | -9.23 | 113.91 | 121.30 | 2 | 1 |
| 1 | A | 413 | ASP | CB-CG-OD1 | -9.19 | 110.03 | 118.30 | 3 | 6 |
| 1 | A | 430 | PHE | CB-CG-CD1 | 9.18 | 127.23 | 120.80 | 11 | 9 |
| 2 | C | 153 | ARG | NH1-CZ-NH2 | -9.15 | 109.33 | 119.40 | 7 | 5 |
| 1 | A | 464 | ARG | NH1-CZ-NH2 | -9.15 | 109.34 | 119.40 | 5 | 3 |
| 1 | A | 486 | PHE | CB-CG-CD1 | -9.14 | 114.40 | 120.80 | 4 | 5 |
| 2 | C | 57 | PHE | CB-CG-CD2 | -9.07 | 114.45 | 120.80 | 9 | 4 |
| 1 | A | 381 | PHE | CB-CG-CD2 | -9.06 | 114.46 | 120.80 | 6 | 6 |
| 1 | A | 471 | ASP | CB-CG-OD2 | -9.04 | 110.16 | 118.30 | 4 | 2 |
| 2 | C | 137 | TYR | CG-CD1-CE1 | 9.04 | 128.53 | 121.30 | 2 | 1 |
| 1 | A | 353 | TYR | CB-CG-CD2 | 9.00 | 126.40 | 121.00 | 15 | 6 |
| 2 | C | 243 | VAL | CA-CB-CG1 | 9.00 | 124.40 | 110.90 | 5 | 3 |
| 2 | C | 179 | ASP | CB-CG-OD2 | 9.00 | 126.40 | 118.30 | 11 | 2 |
| 2 | B | 89 | ASP | CB-CG-OD2 | 8.99 | 126.39 | 118.30 | 15 | 4 |
| 1 | A | 421 | TRP | CB-CG-CD1 | -8.98 | 115.33 | 127.00 | 3 | 2 |
| 2 | C | 210 | ARG | NH1-CZ-NH2 | -8.95 | 109.55 | 119.40 | 9 | 5 |
| 1 | A | 381 | PHE | CB-CG-CD1 | 8.89 | 127.03 | 120.80 | 4 | 5 |
| 1 | A | 468 | MET | CG-SD-CE | -8.89 | 85.98 | 100.20 | 14 | 2 |
| 2 | B | 115 | TYR | CG-CD2-CE2 | -8.88 | 114.20 | 121.30 | 11 | 2 |
| 1 | A | 428 | TYR | CB-CG-CD2 | -8.87 | 115.68 | 121.00 | 10 | 7 |
| 1 | A | 449 | TYR | CB-CG-CD1 | 8.87 | 126.32 | 121.00 | 6 | 8 |
| 2 | C | 214 | TYR | CB-CG-CD1 | -8.85 | 115.69 | 121.00 | 1 | 5 |
| 2 | B | 100 | TYR | CB-CG-CD1 | -8.85 | 115.69 | 121.00 | 8 | 5 |
| 1 | A | 436 | TYR | CB-CG-CD1 | -8.84 | 115.69 | 121.00 | 9 | 6 |
| 2 | C | 145 | ARG | NE-CZ-NH1 | -8.83 | 115.89 | 120.30 | 12 | 6 |
| 1 | A | 382 | PHE | CB-CG-CD1 | -8.79 | 114.65 | 120.80 | 14 | 4 |
| 1 | A | 372 | TYR | CB-CG-CD2 | 8.79 | 126.27 | 121.00 | 8 | 3 |
| 1 | A | 385 | ASP | CB-CG-OD2 | 8.79 | 126.21 | 118.30 | 6 | 1 |
| 1 | A | 376 | ASP | CB-CG-OD2 | -8.75 | 110.42 | 118.30 | 15 | 2 |
| 1 | A | 374 | ARG | NH1-CZ-NH2 | -8.72 | 109.81 | 119.40 | 3 | 1 |
| 1 | A | 388 | TRP | CB-CG-CD2 | 8.70 | 137.91 | 126.60 | 11 | 7 |
| 2 | B | 173 | ARG | NH1-CZ-NH2 | -8.68 | 109.85 | 119.40 | 7 | 3 |
| 1 | A | 430 | PHE | CB-CG-CD2 | -8.67 | 114.73 | 120.80 | 1 | 6 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|------------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 2 | C | 258 | TYR | CG-CD2-CE2 | -8.63 | 114.39 | 121.30 | 3 | 2 |
| 1 | A | 408 | ARG | NH1-CZ-NH2 | -8.62 | 109.92 | 119.40 | 13 | 1 |
| 2 | B | 100 | TYR | CB-CG-CD2 | 8.57 | 126.14 | 121.00 | 13 | 7 |
| 1 | A | 382 | PHE | CB-CG-CD2 | -8.56 | 114.81 | 120.80 | 10 | 3 |
| 1 | A | 399 | TYR | CB-CG-CD2 | -8.53 | 115.88 | 121.00 | 12 | 7 |
| 2 | B | 158 | GLU | OE1-CD-OE2 | -8.50 | 113.10 | 123.30 | 5 | 2 |
| 2 | C | 89 | ASP | CB-CG-OD1 | 8.49 | 125.94 | 118.30 | 3 | 2 |
| 1 | A | 388 | TRP | CB-CG-CD1 | -8.49 | 115.96 | 127.00 | 11 | 6 |
| 1 | A | 330 | ARG | NH1-CZ-NH2 | -8.48 | 110.07 | 119.40 | 9 | 5 |
| 2 | C | 116 | ARG | NH1-CZ-NH2 | -8.46 | 110.10 | 119.40 | 13 | 3 |
| 1 | A | 438 | PHE | CB-CG-CD2 | 8.45 | 126.71 | 120.80 | 15 | 5 |
| 1 | A | 478 | TYR | CB-CG-CD1 | -8.44 | 115.93 | 121.00 | 5 | 4 |
| 1 | A | 500 | SER | N-CA-CB | 8.44 | 123.16 | 110.50 | 15 | 1 |
| 2 | C | 71 | PHE | CG-CD1-CE1 | 8.44 | 130.08 | 120.80 | 15 | 2 |
| 1 | A | 497 | TYR | CB-CG-CD2 | 8.42 | 126.05 | 121.00 | 14 | 5 |
| 1 | A | 325 | THR | CA-CB-CG2 | 8.41 | 124.18 | 112.40 | 3 | 2 |
| 2 | C | 122 | TYR | CG-CD1-CE1 | -8.40 | 114.58 | 121.30 | 10 | 3 |
| 1 | A | 478 | TYR | CG-CD2-CE2 | -8.38 | 114.60 | 121.30 | 1 | 2 |
| 2 | B | 71 | PHE | CB-CG-CD2 | -8.30 | 114.99 | 120.80 | 8 | 3 |
| 1 | A | 476 | TYR | CB-CG-CD2 | -8.27 | 116.03 | 121.00 | 4 | 1 |
| 1 | A | 422 | MET | CG-SD-CE | -8.27 | 86.97 | 100.20 | 4 | 4 |
| 2 | B | 122 | TYR | CB-CG-CD2 | 8.26 | 125.96 | 121.00 | 3 | 7 |
| 2 | C | 153 | ARG | CD-NE-CZ | 8.25 | 135.15 | 123.60 | 3 | 1 |
| 1 | A | 487 | ASN | CB-CA-C | 8.24 | 126.87 | 110.40 | 3 | 1 |
| 1 | A | 477 | PHE | CB-CG-CD1 | -8.23 | 115.04 | 120.80 | 13 | 3 |
| 1 | A | 404 | LYS | O-C-N | -8.20 | 109.58 | 122.70 | 14 | 1 |
| 2 | C | 137 | TYR | CZ-CE2-CD2 | -8.19 | 112.43 | 119.80 | 1 | 2 |
| 1 | A | 504 | ASP | CB-CG-OD1 | -8.17 | 110.95 | 118.30 | 5 | 1 |
| 1 | A | 505 | TRP | CB-CG-CD2 | -8.17 | 115.98 | 126.60 | 13 | 1 |
| 2 | B | 247 | PHE | CB-CG-CD1 | 8.10 | 126.47 | 120.80 | 4 | 1 |
| 2 | C | 142 | GLU | CA-C-N | 8.10 | 139.78 | 117.10 | 5 | 1 |
| 2 | C | 193 | ARG | NH1-CZ-NH2 | -8.10 | 110.49 | 119.40 | 14 | 4 |
| 1 | A | 390 | PHE | CB-CG-CD2 | 8.09 | 126.46 | 120.80 | 2 | 6 |
| 2 | B | 115 | TYR | CG-CD1-CE1 | -8.05 | 114.86 | 121.30 | 12 | 2 |
| 1 | A | 334 | PHE | CB-CG-CD1 | 8.02 | 126.42 | 120.80 | 12 | 5 |
| 2 | C | 57 | PHE | CB-CG-CD1 | 8.02 | 126.42 | 120.80 | 9 | 3 |
| 1 | A | 413 | ASP | CB-CG-OD2 | 8.02 | 125.52 | 118.30 | 1 | 4 |
| 2 | B | 102 | ASP | CB-CG-OD1 | -8.00 | 111.10 | 118.30 | 11 | 3 |
| 2 | B | 214 | TYR | CB-CG-CD1 | -8.00 | 116.20 | 121.00 | 13 | 5 |
| 2 | C | 235 | ASP | CB-CG-OD2 | 8.00 | 125.50 | 118.30 | 15 | 4 |
| 1 | A | 367 | SER | N-CA-CB | 8.00 | 122.49 | 110.50 | 7 | 2 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 1 | A | 341 | PHE | CB-CG-CD1 | -7.99 | 115.21 | 120.80 | 10 | 6 |
| 1 | A | 416 | ASP | CB-CG-OD1 | 7.97 | 125.47 | 118.30 | 11 | 3 |
| 1 | A | 399 | TYR | CB-CG-CD1 | 7.94 | 125.77 | 121.00 | 8 | 2 |
| 2 | B | 89 | ASP | CB-CG-OD1 | 7.94 | 125.44 | 118.30 | 3 | 3 |
| 1 | A | 466 | SER | N-CA-CB | 7.93 | 122.39 | 110.50 | 4 | 1 |
| 2 | C | 199 | ARG | NH1-CZ-NH2 | -7.92 | 110.68 | 119.40 | 12 | 1 |
| 2 | B | 214 | TYR | CB-CG-CD2 | -7.92 | 116.25 | 121.00 | 12 | 6 |
| 2 | C | 175 | ARG | CD-NE-CZ | 7.92 | 134.69 | 123.60 | 5 | 1 |
| 1 | A | 420 | PHE | CB-CG-CD2 | -7.89 | 115.28 | 120.80 | 11 | 1 |
| 1 | A | 399 | TYR | CG-CD2-CE2 | -7.87 | 115.00 | 121.30 | 6 | 4 |
| 1 | A | 336 | PHE | CB-CG-CD1 | 7.84 | 126.29 | 120.80 | 3 | 3 |
| 1 | A | 435 | TYR | CB-CG-CD2 | 7.82 | 125.69 | 121.00 | 12 | 5 |
| 2 | C | 173 | ARG | NH1-CZ-NH2 | -7.80 | 110.82 | 119.40 | 15 | 2 |
| 2 | B | 100 | TYR | CG-CD2-CE2 | -7.74 | 115.11 | 121.30 | 9 | 1 |
| 1 | A | 478 | TYR | CB-CG-CD2 | 7.72 | 125.63 | 121.00 | 4 | 3 |
| 2 | B | 125 | ASP | CB-CG-OD2 | 7.69 | 125.22 | 118.30 | 3 | 2 |
| 2 | B | 100 | TYR | CD1-CE1-CZ | 7.66 | 126.69 | 119.80 | 15 | 1 |
| 1 | A | 436 | TYR | CB-CG-CD2 | -7.66 | 116.41 | 121.00 | 3 | 3 |
| 2 | C | 103 | ASP | CB-CG-OD2 | 7.63 | 125.17 | 118.30 | 1 | 3 |
| 2 | B | 153 | ARG | NH1-CZ-NH2 | -7.61 | 111.03 | 119.40 | 1 | 4 |
| 1 | A | 446 | ASP | CB-CG-OD2 | -7.61 | 111.45 | 118.30 | 10 | 3 |
| 2 | B | 199 | ARG | NH1-CZ-NH2 | -7.61 | 111.03 | 119.40 | 8 | 3 |
| 2 | B | 136 | LEU | O-C-N | -7.58 | 110.56 | 122.70 | 12 | 1 |
| 1 | A | 351 | ASP | CB-CG-OD2 | 7.57 | 125.11 | 118.30 | 11 | 6 |
| 2 | C | 104 | PHE | CB-CG-CD2 | -7.56 | 115.51 | 120.80 | 4 | 4 |
| 2 | B | 171 | ARG | NH1-CZ-NH2 | -7.55 | 111.10 | 119.40 | 15 | 3 |
| 2 | B | 72 | TRP | CB-CG-CD1 | 7.54 | 136.81 | 127.00 | 8 | 3 |
| 2 | B | 58 | SER | N-CA-CB | 7.53 | 121.80 | 110.50 | 6 | 2 |
| 2 | B | 227 | GLU | OE1-CD-OE2 | -7.53 | 114.27 | 123.30 | 10 | 3 |
| 1 | A | 436 | TYR | CG-CD2-CE2 | -7.52 | 115.28 | 121.30 | 8 | 2 |
| 2 | B | 237 | ARG | NH1-CZ-NH2 | -7.51 | 111.14 | 119.40 | 4 | 2 |
| 1 | A | 372 | TYR | CB-CG-CD1 | -7.49 | 116.50 | 121.00 | 8 | 1 |
| 2 | C | 125 | ASP | CB-CG-OD1 | -7.49 | 111.56 | 118.30 | 13 | 1 |
| 1 | A | 431 | ARG | NH1-CZ-NH2 | -7.48 | 111.17 | 119.40 | 15 | 3 |
| 2 | B | 104 | PHE | CB-CG-CD1 | -7.48 | 115.56 | 120.80 | 11 | 5 |
| 1 | A | 320 | ASP | CB-CG-OD2 | -7.46 | 111.58 | 118.30 | 7 | 3 |
| 1 | A | 361 | TRP | CH2-CZ2-CE2 | 7.46 | 124.86 | 117.40 | 7 | 1 |
| 2 | B | 112 | MET | CG-SD-CE | -7.44 | 88.30 | 100.20 | 4 | 1 |
| 1 | A | 370 | THR | CA-CB-CG2 | 7.42 | 122.79 | 112.40 | 4 | 2 |
| 2 | B | 78 | GLU | OE1-CD-OE2 | -7.41 | 114.41 | 123.30 | 12 | 1 |
| 2 | C | 137 | TYR | CB-CG-CD2 | 7.37 | 125.42 | 121.00 | 5 | 3 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 2 | C | 212 | ALA | CB-CA-C | 7.37 | 121.16 | 110.10 | 8 | 1 |
| 2 | B | 108 | TRP | CD1-CG-CD2 | 7.35 | 112.18 | 106.30 | 11 | 1 |
| 2 | B | 190 | ASP | CB-CG-OD1 | -7.34 | 111.69 | 118.30 | 3 | 2 |
| 2 | B | 195 | ARG | NH1-CZ-NH2 | -7.34 | 111.33 | 119.40 | 11 | 3 |
| 2 | C | 134 | MET | CG-SD-CE | -7.33 | 88.48 | 100.20 | 1 | 2 |
| 2 | C | 125 | ASP | CB-CG-OD2 | 7.32 | 124.89 | 118.30 | 13 | 3 |
| 2 | C | 102 | ASP | CB-CG-OD1 | 7.25 | 124.83 | 118.30 | 3 | 4 |
| 2 | B | 103 | ASP | CB-CG-OD1 | 7.25 | 124.83 | 118.30 | 11 | 2 |
| 2 | B | 116 | ARG | NH1-CZ-NH2 | -7.24 | 111.44 | 119.40 | 11 | 2 |
| 2 | C | 82 | LEU | CB-CG-CD1 | 7.24 | 123.31 | 111.00 | 10 | 1 |
| 1 | A | 421 | TRP | CB-CG-CD2 | 7.24 | 136.00 | 126.60 | 3 | 2 |
| 1 | A | 361 | TRP | CG-CD2-CE3 | -7.22 | 127.40 | 133.90 | 14 | 1 |
| 1 | A | 435 | TYR | CG-CD2-CE2 | 7.21 | 127.07 | 121.30 | 11 | 1 |
| 1 | A | 353 | TYR | CG-CD2-CE2 | 7.21 | 127.07 | 121.30 | 4 | 4 |
| 2 | C | 108 | TRP | CB-CG-CD2 | 7.21 | 135.97 | 126.60 | 14 | 2 |
| 2 | C | 56 | THR | CA-CB-CG2 | -7.21 | 102.31 | 112.40 | 3 | 3 |
| 2 | C | 214 | TYR | CG-CD2-CE2 | -7.19 | 115.55 | 121.30 | 13 | 4 |
| 2 | B | 108 | TRP | CG-CD1-NE1 | -7.19 | 102.91 | 110.10 | 11 | 1 |
| 2 | C | 72 | TRP | CB-CG-CD2 | -7.18 | 117.26 | 126.60 | 5 | 2 |
| 1 | A | 501 | ALA | CB-CA-C | -7.18 | 99.33 | 110.10 | 10 | 2 |
| 2 | B | 130 | TRP | CB-CG-CD2 | 7.17 | 135.92 | 126.60 | 5 | 1 |
| 2 | B | 141 | VAL | CG1-CB-CG2 | -7.15 | 99.46 | 110.90 | 9 | 2 |
| 1 | A | 412 | THR | CA-CB-CG2 | -7.13 | 102.42 | 112.40 | 12 | 3 |
| 2 | C | 61 | ARG | CD-NE-CZ | 7.11 | 133.56 | 123.60 | 3 | 1 |
| 2 | C | 170 | MET | CG-SD-CE | -7.11 | 88.82 | 100.20 | 10 | 4 |
| 1 | A | 334 | PHE | CB-CG-CD2 | -7.11 | 115.83 | 120.80 | 14 | 5 |
| 1 | A | 505 | TRP | CD1-NE1-CE2 | 7.10 | 115.39 | 109.00 | 1 | 1 |
| 1 | A | 497 | TYR | CG-CD2-CE2 | -7.08 | 115.63 | 121.30 | 12 | 2 |
| 1 | A | 426 | LYS | O-C-N | -7.07 | 111.39 | 122.70 | 14 | 1 |
| 2 | C | 78 | GLU | OE1-CD-OE2 | -7.07 | 114.82 | 123.30 | 14 | 1 |
| 2 | C | 137 | TYR | CB-CG-CD1 | 7.06 | 125.23 | 121.00 | 10 | 5 |
| 2 | C | 237 | ARG | NH1-CZ-NH2 | -7.05 | 111.64 | 119.40 | 6 | 3 |
| 1 | A | 484 | TRP | CD1-NE1-CE2 | -7.04 | 102.66 | 109.00 | 5 | 1 |
| 2 | B | 201 | GLU | OE1-CD-OE2 | -7.04 | 114.86 | 123.30 | 4 | 2 |
| 2 | C | 62 | GLU | O-C-N | -7.03 | 111.45 | 122.70 | 3 | 2 |
| 2 | C | 245 | GLU | OE1-CD-OE2 | -7.03 | 114.86 | 123.30 | 8 | 1 |
| 2 | B | 214 | TYR | CZ-CE2-CD2 | -7.02 | 113.48 | 119.80 | 3 | 2 |
| 2 | C | 138 | ARG | NH1-CZ-NH2 | -7.00 | 111.70 | 119.40 | 10 | 3 |
| 2 | C | 214 | TYR | CZ-CE2-CD2 | 6.99 | 126.09 | 119.80 | 8 | 1 |
| 2 | C | 190 | ASP | CB-CG-OD1 | 6.96 | 124.56 | 118.30 | 12 | 5 |
| 1 | A | 428 | TYR | CG-CD2-CE2 | -6.96 | 115.73 | 121.30 | 14 | 3 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 1 | A | 441 | GLU | OE1-CD-OE2 | 6.95 | 131.63 | 123.30 | 13 | 1 |
| 1 | A | 442 | LEU | CB-CG-CD2 | 6.93 | 122.79 | 111.00 | 7 | 1 |
| 2 | B | 100 | TYR | CG-CD1-CE1 | -6.90 | 115.78 | 121.30 | 8 | 3 |
| 2 | B | 116 | ARG | CD-NE-CZ | -6.90 | 113.94 | 123.60 | 13 | 1 |
| 2 | B | 124 | ASP | CB-CG-OD1 | 6.89 | 124.50 | 118.30 | 2 | 3 |
| 1 | A | 365 | PRO | N-CD-CG | 6.89 | 113.54 | 103.20 | 5 | 1 |
| 2 | C | 249 | VAL | CA-CB-CG2 | -6.88 | 100.59 | 110.90 | 1 | 1 |
| 1 | A | 390 | PHE | CG-CD1-CE1 | -6.88 | 113.24 | 120.80 | 8 | 1 |
| 1 | A | 375 | LYS | O-C-N | -6.86 | 111.72 | 122.70 | 3 | 1 |
| 2 | C | 108 | TRP | CB-CG-CD1 | -6.86 | 118.08 | 127.00 | 14 | 2 |
| 1 | A | 391 | ASP | CB-CG-OD2 | -6.85 | 112.13 | 118.30 | 12 | 2 |
| 2 | C | 124 | ASP | CB-CG-OD1 | -6.84 | 112.15 | 118.30 | 2 | 4 |
| 2 | B | 235 | ASP | CB-CG-OD1 | 6.84 | 124.45 | 118.30 | 3 | 2 |
| 1 | A | 340 | TRP | CE2-CD2-CG | -6.84 | 101.83 | 107.30 | 11 | 2 |
| 2 | B | 113 | GLU | OE1-CD-OE2 | -6.82 | 115.12 | 123.30 | 6 | 2 |
| 2 | B | 190 | ASP | CB-CG-OD2 | 6.82 | 124.43 | 118.30 | 3 | 1 |
| 2 | C | 258 | TYR | CG-CD1-CE1 | 6.79 | 126.73 | 121.30 | 11 | 1 |
| 1 | A | 505 | TRP | CH2-CZ2-CE2 | 6.79 | 124.19 | 117.40 | 13 | 1 |
| 1 | A | 362 | ARG | NH1-CZ-NH2 | -6.77 | 111.95 | 119.40 | 5 | 4 |
| 2 | C | 210 | ARG | CD-NE-CZ | 6.75 | 133.04 | 123.60 | 11 | 3 |
| 2 | C | 145 | ARG | NH1-CZ-NH2 | -6.74 | 111.98 | 119.40 | 14 | 5 |
| 1 | A | 338 | GLU | OE1-CD-OE2 | -6.74 | 115.21 | 123.30 | 2 | 1 |
| 2 | C | 197 | ALA | N-CA-CB | -6.74 | 100.66 | 110.10 | 3 | 4 |
| 2 | B | 124 | ASP | CB-CG-OD2 | -6.74 | 112.24 | 118.30 | 7 | 4 |
| 2 | C | 80 | GLU | O-C-N | -6.74 | 111.75 | 123.20 | 10 | 1 |
| 2 | B | 252 | LEU | CB-CG-CD2 | 6.74 | 122.45 | 111.00 | 11 | 1 |
| 2 | B | 254 | ALA | N-CA-CB | -6.72 | 100.69 | 110.10 | 13 | 1 |
| 2 | C | 86 | MET | CG-SD-CE | -6.71 | 89.47 | 100.20 | 2 | 4 |
| 1 | A | 476 | TYR | CA-CB-CG | -6.70 | 100.67 | 113.40 | 10 | 2 |
| 1 | A | 486 | PHE | N-CA-CB | -6.70 | 98.54 | 110.60 | 13 | 1 |
| 1 | A | 332 | GLU | OE1-CD-OE2 | -6.68 | 115.29 | 123.30 | 4 | 1 |
| 2 | B | 108 | TRP | CB-CA-C | 6.68 | 123.75 | 110.40 | 11 | 1 |
| 1 | A | 429 | PHE | CB-CG-CD2 | 6.66 | 125.47 | 120.80 | 3 | 2 |
| 1 | A | 396 | GLU | OE1-CD-OE2 | -6.65 | 115.32 | 123.30 | 4 | 1 |
| 1 | A | 420 | PHE | CB-CG-CD1 | -6.65 | 116.14 | 120.80 | 12 | 1 |
| 1 | A | 350 | MET | CG-SD-CE | 6.65 | 110.83 | 100.20 | 4 | 1 |
| 1 | A | 435 | TYR | CZ-CE2-CD2 | -6.64 | 113.82 | 119.80 | 11 | 2 |
| 2 | C | 100 | TYR | CG-CD2-CE2 | -6.64 | 115.99 | 121.30 | 11 | 2 |
| 2 | B | 134 | MET | CG-SD-CE | -6.62 | 89.60 | 100.20 | 15 | 3 |
| 1 | A | 447 | SER | CB-CA-C | -6.62 | 97.52 | 110.10 | 8 | 2 |
| 2 | C | 100 | TYR | CD1-CE1-CZ | -6.60 | 113.86 | 119.80 | 7 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 2 | B | 67 | VAL | CA-CB-CG1 | -6.60 | 101.01 | 110.90 | 8 | 1 |
| 2 | C | 61 | ARG | CA-CB-CG | 6.57 | 127.86 | 113.40 | 3 | 1 |
| 2 | B | 200 | LEU | CB-CG-CD1 | 6.57 | 122.17 | 111.00 | 8 | 1 |
| 2 | B | 114 | LEU | O-C-N | -6.57 | 112.19 | 122.70 | 13 | 1 |
| 2 | C | 188 | TYR | CG-CD2-CE2 | -6.55 | 116.06 | 121.30 | 7 | 1 |
| 2 | C | 130 | TRP | CA-CB-CG | 6.55 | 126.15 | 113.70 | 5 | 3 |
| 2 | C | 176 | ALA | CB-CA-C | -6.55 | 100.28 | 110.10 | 10 | 3 |
| 2 | B | 122 | TYR | CB-CA-C | 6.55 | 123.50 | 110.40 | 11 | 3 |
| 1 | A | 389 | VAL | O-C-N | -6.54 | 112.23 | 122.70 | 9 | 1 |
| 1 | A | 478 | TYR | CG-CD1-CE1 | -6.54 | 116.07 | 121.30 | 5 | 1 |
| 2 | C | 130 | TRP | CE2-CD2-CG | -6.53 | 102.08 | 107.30 | 10 | 1 |
| 2 | C | 87 | SER | O-C-N | -6.53 | 112.26 | 122.70 | 12 | 2 |
| 1 | A | 350 | MET | O-C-N | -6.52 | 112.27 | 122.70 | 5 | 1 |
| 2 | C | 76 | GLU | OE1-CD-OE2 | -6.51 | 115.48 | 123.30 | 9 | 1 |
| 1 | A | 338 | GLU | CB-CA-C | 6.51 | 123.41 | 110.40 | 7 | 1 |
| 2 | C | 251 | PHE | CB-CG-CD1 | 6.50 | 125.35 | 120.80 | 5 | 3 |
| 1 | A | 484 | TRP | NE1-CE2-CD2 | 6.50 | 113.80 | 107.30 | 8 | 1 |
| 2 | B | 122 | TYR | CG-CD2-CE2 | -6.50 | 116.10 | 121.30 | 1 | 3 |
| 2 | C | 119 | VAL | CA-CB-CG1 | 6.50 | 120.65 | 110.90 | 9 | 2 |
| 1 | A | 341 | PHE | CZ-CE2-CD2 | -6.50 | 112.31 | 120.10 | 2 | 1 |
| 1 | A | 342 | TRP | CE2-CD2-CG | -6.49 | 102.11 | 107.30 | 8 | 2 |
| 2 | B | 137 | TYR | CG-CD1-CE1 | -6.49 | 116.11 | 121.30 | 11 | 2 |
| 2 | C | 251 | PHE | CB-CG-CD2 | 6.49 | 125.34 | 120.80 | 10 | 4 |
| 1 | A | 463 | PRO | O-C-N | -6.48 | 112.33 | 122.70 | 3 | 1 |
| 1 | A | 484 | TRP | CH2-CZ2-CE2 | 6.45 | 123.85 | 117.40 | 5 | 1 |
| 2 | C | 174 | ALA | N-CA-CB | 6.45 | 119.12 | 110.10 | 14 | 2 |
| 2 | B | 175 | ARG | NH1-CZ-NH2 | -6.44 | 112.31 | 119.40 | 14 | 2 |
| 1 | A | 478 | TYR | CZ-CE2-CD2 | 6.44 | 125.59 | 119.80 | 10 | 1 |
| 2 | B | 122 | TYR | CG-CD1-CE1 | -6.43 | 116.15 | 121.30 | 13 | 1 |
| 2 | C | 196 | LEU | CB-CG-CD2 | -6.43 | 100.07 | 111.00 | 13 | 1 |
| 2 | C | 183 | THR | CA-CB-CG2 | -6.42 | 103.41 | 112.40 | 7 | 1 |
| 2 | B | 87 | SER | O-C-N | -6.41 | 112.44 | 122.70 | 12 | 1 |
| 2 | B | 73 | ASP | CB-CG-OD1 | 6.41 | 124.06 | 118.30 | 13 | 2 |
| 1 | A | 374 | ARG | CD-NE-CZ | 6.41 | 132.57 | 123.60 | 15 | 1 |
| 1 | A | 435 | TYR | CG-CD1-CE1 | -6.40 | 116.18 | 121.30 | 5 | 2 |
| 2 | C | 85 | GLU | OE1-CD-OE2 | -6.39 | 115.63 | 123.30 | 5 | 2 |
| 1 | A | 505 | TRP | CE2-CD2-CE3 | 6.39 | 126.37 | 118.70 | 6 | 1 |
| 1 | A | 476 | TYR | CB-CG-CD1 | -6.38 | 117.17 | 121.00 | 1 | 2 |
| 2 | B | 115 | TYR | CZ-CE2-CD2 | 6.38 | 125.54 | 119.80 | 3 | 1 |
| 1 | A | 387 | HIS | CA-CB-CG | 6.37 | 124.43 | 113.60 | 6 | 1 |
| 1 | A | 467 | PHE | O-C-N | -6.37 | 112.51 | 122.70 | 6 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 2 | C | 179 | ASP | CB-CG-OD1 | 6.37 | 124.03 | 118.30 | 2 | 2 |
| 1 | A | 372 | TYR | CA-CB-CG | 6.37 | 125.50 | 113.40 | 10 | 2 |
| 2 | B | 102 | ASP | CB-CG-OD2 | -6.37 | 112.57 | 118.30 | 10 | 4 |
| 2 | B | 199 | ARG | CD-NE-CZ | 6.36 | 132.50 | 123.60 | 11 | 1 |
| 2 | C | 164 | SER | O-C-N | -6.35 | 109.03 | 121.10 | 4 | 1 |
| 2 | B | 68 | THR | CA-CB-OG1 | 6.35 | 122.33 | 109.00 | 7 | 1 |
| 2 | C | 243 | VAL | CA-CB-CG2 | -6.34 | 101.39 | 110.90 | 2 | 3 |
| 1 | A | 435 | TYR | CD1-CE1-CZ | 6.34 | 125.51 | 119.80 | 9 | 2 |
| 1 | A | 420 | PHE | CB-CA-C | 6.34 | 123.08 | 110.40 | 13 | 1 |
| 2 | C | 83 | ARG | NH1-CZ-NH2 | -6.34 | 112.43 | 119.40 | 5 | 2 |
| 2 | B | 198 | ALA | N-CA-CB | 6.33 | 118.97 | 110.10 | 3 | 2 |
| 2 | B | 79 | THR | N-CA-CB | 6.33 | 122.33 | 110.30 | 3 | 1 |
| 1 | A | 338 | GLU | N-CA-CB | 6.33 | 121.99 | 110.60 | 12 | 1 |
| 2 | B | 175 | ARG | CD-NE-CZ | 6.33 | 132.46 | 123.60 | 14 | 1 |
| 2 | B | 137 | TYR | CG-CD2-CE2 | -6.33 | 116.24 | 121.30 | 5 | 3 |
| 2 | B | 188 | TYR | CG-CD2-CE2 | -6.32 | 116.24 | 121.30 | 3 | 1 |
| 2 | B | 92 | GLU | OE1-CD-OE2 | -6.32 | 115.72 | 123.30 | 6 | 2 |
| 2 | B | 72 | TRP | NE1-CE2-CD2 | 6.30 | 113.60 | 107.30 | 8 | 1 |
| 1 | A | 389 | VAL | CA-CB-CG1 | -6.30 | 101.45 | 110.90 | 10 | 1 |
| 1 | A | 495 | PRO | N-CD-CG | 6.30 | 112.64 | 103.20 | 10 | 1 |
| 2 | B | 130 | TRP | CE3-CZ3-CH2 | 6.29 | 128.12 | 121.20 | 7 | 1 |
| 2 | B | 108 | TRP | CB-CG-CD2 | 6.28 | 134.77 | 126.60 | 2 | 1 |
| 2 | C | 73 | ASP | O-C-N | -6.28 | 112.65 | 122.70 | 10 | 1 |
| 2 | B | 195 | ARG | CG-CD-NE | -6.28 | 98.61 | 111.80 | 7 | 2 |
| 2 | C | 210 | ARG | CG-CD-NE | -6.26 | 98.65 | 111.80 | 9 | 1 |
| 1 | A | 341 | PHE | CD1-CG-CD2 | -6.25 | 110.17 | 118.30 | 13 | 1 |
| 1 | A | 334 | PHE | CG-CD1-CE1 | 6.24 | 127.67 | 120.80 | 6 | 2 |
| 2 | B | 130 | TRP | CH2-CZ2-CE2 | -6.23 | 111.17 | 117.40 | 12 | 2 |
| 2 | C | 211 | LEU | CB-CG-CD1 | 6.22 | 121.58 | 111.00 | 5 | 1 |
| 2 | C | 124 | ASP | CB-CG-OD2 | 6.21 | 123.89 | 118.30 | 11 | 2 |
| 1 | A | 447 | SER | N-CA-CB | 6.20 | 119.80 | 110.50 | 11 | 1 |
| 1 | A | 504 | ASP | CB-CG-OD2 | 6.20 | 123.88 | 118.30 | 3 | 3 |
| 2 | C | 178 | VAL | O-C-N | -6.19 | 112.79 | 122.70 | 11 | 1 |
| 2 | C | 198 | ALA | N-CA-CB | -6.18 | 101.44 | 110.10 | 13 | 2 |
| 2 | B | 251 | PHE | CB-CG-CD1 | -6.18 | 116.48 | 120.80 | 11 | 2 |
| 2 | B | 130 | TRP | CB-CG-CD1 | -6.17 | 118.98 | 127.00 | 5 | 1 |
| 2 | B | 260 | LYS | O-C-N | -6.16 | 112.85 | 122.70 | 2 | 1 |
| 1 | A | 412 | THR | O-C-N | -6.15 | 112.86 | 122.70 | 7 | 1 |
| 2 | B | 119 | VAL | O-C-N | -6.15 | 112.86 | 122.70 | 11 | 1 |
| 2 | C | 100 | TYR | CG-CD1-CE1 | 6.15 | 126.22 | 121.30 | 12 | 2 |
| 2 | B | 191 | GLU | OE1-CD-OE2 | 6.15 | 130.68 | 123.30 | 4 | 2 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 1 | A | 374 | ARG | CG-CD-NE | -6.13 | 98.92 | 111.80 | 2 | 3 |
| 1 | A | 505 | TRP | CD2-CE3-CZ3 | -6.13 | 110.83 | 118.80 | 6 | 1 |
| 1 | A | 492 | LYS | N-CA-CB | 6.12 | 121.62 | 110.60 | 2 | 1 |
| 2 | C | 72 | TRP | CB-CG-CD1 | 6.12 | 134.96 | 127.00 | 5 | 1 |
| 2 | C | 72 | TRP | CB-CA-C | 6.12 | 122.63 | 110.40 | 2 | 1 |
| 2 | B | 72 | TRP | CB-CG-CD2 | -6.12 | 118.65 | 126.60 | 8 | 2 |
| 1 | A | 392 | GLU | OE1-CD-OE2 | -6.11 | 115.97 | 123.30 | 4 | 1 |
| 2 | C | 182 | ARG | N-CA-CB | 6.10 | 121.58 | 110.60 | 13 | 1 |
| 2 | B | 97 | VAL | CA-CB-CG1 | 6.10 | 120.05 | 110.90 | 10 | 2 |
| 2 | C | 232 | ALA | N-CA-CB | -6.10 | 101.56 | 110.10 | 4 | 2 |
| 1 | A | 368 | ILE | CG1-CB-CG2 | -6.09 | 98.00 | 111.40 | 12 | 1 |
| 2 | C | 170 | MET | CB-CA-C | -6.08 | 98.23 | 110.40 | 7 | 1 |
| 2 | B | 212 | ALA | CB-CA-C | 6.08 | 119.22 | 110.10 | 10 | 1 |
| 1 | A | 342 | TRP | N-CA-CB | 6.08 | 121.54 | 110.60 | 1 | 3 |
| 1 | A | 405 | GLU | CG-CD-OE1 | -6.08 | 106.15 | 118.30 | 15 | 1 |
| 2 | C | 216 | ALA | N-CA-CB | 6.06 | 118.59 | 110.10 | 3 | 1 |
| 1 | A | 354 | PRO | O-C-N | -6.06 | 113.00 | 122.70 | 10 | 1 |
| 1 | A | 345 | ARG | NH1-CZ-NH2 | -6.06 | 112.73 | 119.40 | 8 | 2 |
| 1 | A | 456 | TRP | CD1-CG-CD2 | -6.05 | 101.46 | 106.30 | 14 | 1 |
| 2 | B | 188 | TYR | CG-CD1-CE1 | 6.05 | 126.14 | 121.30 | 12 | 1 |
| 2 | B | 258 | TYR | CD1-CE1-CZ | -6.05 | 114.36 | 119.80 | 5 | 2 |
| 2 | B | 177 | HIS | N-CA-CB | 6.04 | 121.47 | 110.60 | 10 | 1 |
| 1 | A | 328 | MET | CG-SD-CE | -6.03 | 90.55 | 100.20 | 1 | 1 |
| 1 | A | 430 | PHE | CD1-CE1-CZ | 6.03 | 127.34 | 120.10 | 6 | 1 |
| 2 | C | 246 | SER | O-C-N | -6.03 | 113.05 | 122.70 | 1 | 1 |
| 2 | B | 72 | TRP | N-CA-CB | -6.03 | 99.75 | 110.60 | 4 | 1 |
| 1 | A | 441 | GLU | O-C-N | -6.02 | 113.06 | 122.70 | 14 | 2 |
| 2 | B | 60 | LEU | CB-CG-CD2 | 6.02 | 121.23 | 111.00 | 14 | 2 |
| 2 | C | 234 | GLU | OE1-CD-OE2 | -6.01 | 116.08 | 123.30 | 14 | 2 |
| 1 | A | 477 | PHE | CB-CG-CD2 | -6.01 | 116.59 | 120.80 | 11 | 4 |
| 2 | B | 193 | ARG | NH1-CZ-NH2 | -6.00 | 112.80 | 119.40 | 12 | 1 |
| 1 | A | 476 | TYR | CG-CD2-CE2 | -6.00 | 116.50 | 121.30 | 4 | 2 |
| 2 | C | 91 | GLU | OE1-CD-OE2 | -6.00 | 116.11 | 123.30 | 4 | 2 |
| 2 | B | 120 | GLU | OE1-CD-OE2 | -6.00 | 116.11 | 123.30 | 3 | 2 |
| 2 | B | 175 | ARG | N-CA-CB | -5.99 | 99.81 | 110.60 | 4 | 1 |
| 2 | C | 195 | ARG | CD-NE-CZ | 5.99 | 131.99 | 123.60 | 6 | 1 |
| 1 | A | 456 | TRP | CB-CG-CD2 | 5.98 | 134.38 | 126.60 | 5 | 1 |
| 2 | C | 61 | ARG | NH1-CZ-NH2 | -5.98 | 112.83 | 119.40 | 4 | 2 |
| 1 | A | 365 | PRO | O-C-N | 5.97 | 132.26 | 122.70 | 13 | 1 |
| 1 | A | 323 | PHE | CB-CG-CD1 | 5.97 | 124.98 | 120.80 | 3 | 5 |
| 1 | A | 449 | TYR | CG-CD1-CE1 | -5.97 | 116.53 | 121.30 | 3 | 2 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 1 | A | 361 | TRP | CB-CG-CD2 | -5.97 | 118.84 | 126.60 | 8 | 1 |
| 2 | C | 190 | ASP | CB-CG-OD2 | 5.97 | 123.67 | 118.30 | 15 | 4 |
| 2 | B | 172 | ASP | N-CA-CB | 5.97 | 121.34 | 110.60 | 10 | 2 |
| 1 | A | 339 | ARG | NH1-CZ-NH2 | -5.96 | 112.84 | 119.40 | 2 | 1 |
| 2 | B | 253 | SER | N-CA-CB | 5.96 | 119.44 | 110.50 | 4 | 2 |
| 1 | A | 333 | MET | CG-SD-CE | -5.95 | 90.67 | 100.20 | 4 | 2 |
| 1 | A | 425 | GLY | O-C-N | -5.95 | 113.17 | 122.70 | 8 | 1 |
| 1 | A | 361 | TRP | CD2-CE3-CZ3 | -5.95 | 111.06 | 118.80 | 14 | 1 |
| 2 | B | 160 | GLN | O-C-N | -5.94 | 113.19 | 122.70 | 11 | 1 |
| 1 | A | 472 | GLU | OE1-CD-OE2 | -5.94 | 116.17 | 123.30 | 14 | 2 |
| 2 | B | 137 | TYR | CD1-CE1-CZ | 5.94 | 125.14 | 119.80 | 6 | 1 |
| 2 | C | 212 | ALA | N-CA-CB | -5.94 | 101.79 | 110.10 | 14 | 1 |
| 2 | B | 86 | MET | CA-CB-CG | 5.93 | 123.38 | 113.30 | 2 | 3 |
| 2 | B | 214 | TYR | CG-CD1-CE1 | -5.93 | 116.56 | 121.30 | 9 | 1 |
| 1 | A | 355 | MET | CG-SD-CE | -5.92 | 90.72 | 100.20 | 12 | 4 |
| 2 | B | 92 | GLU | O-C-N | -5.92 | 113.23 | 122.70 | 8 | 3 |
| 2 | C | 120 | GLU | OE1-CD-OE2 | -5.91 | 116.20 | 123.30 | 2 | 3 |
| 2 | C | 134 | MET | O-C-N | -5.91 | 113.24 | 122.70 | 3 | 1 |
| 1 | A | 397 | PRO | C-N-CA | 5.91 | 134.71 | 122.30 | 9 | 1 |
| 1 | A | 328 | MET | N-CA-CB | -5.91 | 99.96 | 110.60 | 7 | 1 |
| 2 | C | 116 | ARG | N-CA-CB | -5.91 | 99.97 | 110.60 | 14 | 1 |
| 2 | C | 98 | GLN | O-C-N | -5.90 | 109.89 | 121.10 | 11 | 1 |
| 2 | B | 192 | LEU | CB-CG-CD1 | 5.90 | 121.03 | 111.00 | 12 | 1 |
| 2 | C | 69 | GLN | CA-CB-CG | 5.90 | 126.38 | 113.40 | 5 | 1 |
| 2 | C | 172 | ASP | CB-CG-OD2 | 5.90 | 123.61 | 118.30 | 4 | 1 |
| 1 | A | 413 | ASP | CA-CB-CG | 5.90 | 126.37 | 113.40 | 10 | 1 |
| 2 | B | 71 | PHE | CD1-CE1-CZ | 5.88 | 127.16 | 120.10 | 10 | 1 |
| 2 | B | 230 | LYS | N-CA-C | 5.88 | 126.88 | 111.00 | 5 | 1 |
| 1 | A | 320 | ASP | CB-CG-OD1 | 5.88 | 123.59 | 118.30 | 14 | 2 |
| 1 | A | 361 | TRP | CB-CG-CD1 | 5.88 | 134.64 | 127.00 | 8 | 1 |
| 1 | A | 361 | TRP | N-CA-CB | 5.88 | 121.17 | 110.60 | 5 | 1 |
| 2 | C | 166 | LEU | CB-CG-CD1 | 5.86 | 120.97 | 111.00 | 11 | 1 |
| 1 | A | 435 | TYR | CB-CA-C | 5.86 | 122.12 | 110.40 | 5 | 1 |
| 2 | B | 203 | LEU | N-CA-CB | -5.86 | 98.69 | 110.40 | 11 | 1 |
| 1 | A | 505 | TRP | CB-CG-CD1 | 5.86 | 134.61 | 127.00 | 13 | 1 |
| 1 | A | 411 | PRO | N-CA-CB | -5.85 | 96.16 | 102.60 | 10 | 1 |
| 2 | C | 216 | ALA | CB-CA-C | -5.85 | 101.32 | 110.10 | 15 | 1 |
| 1 | A | 458 | GLY | O-C-N | -5.85 | 113.34 | 122.70 | 13 | 1 |
| 2 | B | 223 | SER | N-CA-CB | 5.85 | 119.28 | 110.50 | 2 | 1 |
| 1 | A | 335 | VAL | CG1-CB-CG2 | -5.85 | 101.54 | 110.90 | 12 | 1 |
| 2 | B | 108 | TRP | CB-CG-CD1 | -5.85 | 119.40 | 127.00 | 3 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 2 | C | 226 | SER | N-CA-CB | 5.85 | 119.27 | 110.50 | 10 | 1 |
| 2 | B | 251 | PHE | CD1-CE1-CZ | -5.84 | 113.09 | 120.10 | 7 | 1 |
| 2 | B | 122 | TYR | N-CA-CB | -5.84 | 100.08 | 110.60 | 8 | 1 |
| 1 | A | 318 | ILE | O-C-N | -5.84 | 113.36 | 122.70 | 3 | 1 |
| 2 | C | 89 | ASP | CB-CG-OD2 | 5.84 | 123.55 | 118.30 | 9 | 4 |
| 1 | A | 428 | TYR | CB-CA-C | -5.84 | 98.72 | 110.40 | 13 | 1 |
| 1 | A | 472 | GLU | N-CA-CB | 5.83 | 121.09 | 110.60 | 13 | 1 |
| 2 | B | 59 | LYS | O-C-N | -5.82 | 113.39 | 122.70 | 7 | 1 |
| 1 | A | 503 | ARG | CD-NE-CZ | 5.82 | 131.75 | 123.60 | 13 | 1 |
| 2 | B | 249 | VAL | CA-CB-CG2 | -5.82 | 102.18 | 110.90 | 4 | 3 |
| 1 | A | 449 | TYR | CG-CD2-CE2 | -5.82 | 116.65 | 121.30 | 7 | 2 |
| 1 | A | 410 | LEU | CB-CG-CD1 | -5.82 | 101.11 | 111.00 | 6 | 1 |
| 1 | A | 420 | PHE | CD1-CE1-CZ | -5.82 | 113.12 | 120.10 | 7 | 2 |
| 1 | A | 430 | PHE | CG-CD1-CE1 | -5.82 | 114.40 | 120.80 | 8 | 1 |
| 2 | B | 240 | LEU | CB-CA-C | -5.82 | 99.15 | 110.20 | 12 | 1 |
| 2 | B | 235 | ASP | CB-CG-OD2 | 5.81 | 123.53 | 118.30 | 10 | 2 |
| 1 | A | 469 | GLY | C-N-CA | 5.81 | 136.22 | 121.70 | 1 | 1 |
| 2 | B | 238 | GLN | N-CA-CB | 5.81 | 121.05 | 110.60 | 12 | 1 |
| 2 | C | 98 | GLN | N-CA-C | 5.80 | 126.67 | 111.00 | 12 | 1 |
| 2 | C | 145 | ARG | O-C-N | -5.80 | 113.42 | 122.70 | 13 | 1 |
| 1 | A | 353 | TYR | CZ-CE2-CD2 | 5.80 | 125.02 | 119.80 | 9 | 1 |
| 2 | B | 169 | GLU | OE1-CD-OE2 | -5.80 | 116.34 | 123.30 | 8 | 2 |
| 1 | A | 379 | PHE | CG-CD1-CE1 | -5.80 | 114.42 | 120.80 | 9 | 1 |
| 2 | B | 108 | TRP | CD1-NE1-CE2 | 5.79 | 114.21 | 109.00 | 10 | 1 |
| 2 | C | 245 | GLU | N-CA-CB | 5.79 | 121.02 | 110.60 | 11 | 1 |
| 2 | B | 156 | LEU | CB-CG-CD2 | 5.79 | 120.84 | 111.00 | 10 | 1 |
| 2 | B | 95 | ALA | CB-CA-C | 5.79 | 118.78 | 110.10 | 4 | 1 |
| 2 | B | 251 | PHE | CZ-CE2-CD2 | -5.78 | 113.16 | 120.10 | 3 | 1 |
| 1 | A | 351 | ASP | O-C-N | -5.78 | 113.37 | 123.20 | 11 | 1 |
| 1 | A | 444 | ALA | N-CA-CB | -5.78 | 102.01 | 110.10 | 1 | 1 |
| 2 | B | 141 | VAL | CA-CB-CG1 | 5.78 | 119.57 | 110.90 | 7 | 2 |
| 2 | B | 146 | ALA | CB-CA-C | 5.77 | 118.76 | 110.10 | 8 | 2 |
| 2 | C | 244 | LEU | O-C-N | -5.77 | 113.47 | 122.70 | 3 | 1 |
| 1 | A | 323 | PHE | CG-CD1-CE1 | 5.77 | 127.15 | 120.80 | 3 | 2 |
| 2 | C | 201 | GLU | O-C-N | -5.77 | 113.47 | 122.70 | 13 | 1 |
| 2 | B | 198 | ALA | O-C-N | -5.77 | 113.47 | 122.70 | 4 | 1 |
| 2 | B | 111 | GLU | O-C-N | -5.77 | 113.47 | 122.70 | 11 | 1 |
| 2 | B | 259 | THR | N-CA-CB | 5.75 | 121.23 | 110.30 | 4 | 1 |
| 2 | C | 150 | GLU | O-C-N | -5.75 | 113.42 | 123.20 | 6 | 1 |
| 1 | A | 493 | VAL | CA-CB-CG2 | -5.75 | 102.27 | 110.90 | 14 | 1 |
| 1 | A | 413 | ASP | CB-CA-C | 5.75 | 121.90 | 110.40 | 5 | 2 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 1 | A | 495 | PRO | O-C-N | -5.75 | 113.43 | 123.20 | 7 | 1 |
| 2 | B | 162 | LYS | O-C-N | -5.75 | 113.50 | 122.70 | 9 | 1 |
| 1 | A | 497 | TYR | CD1-CG-CD2 | -5.75 | 111.58 | 117.90 | 13 | 1 |
| 2 | B | 119 | VAL | CG1-CB-CG2 | -5.75 | 101.70 | 110.90 | 8 | 2 |
| 2 | C | 71 | PHE | CD1-CG-CD2 | -5.74 | 110.83 | 118.30 | 15 | 1 |
| 2 | C | 259 | THR | CA-CB-CG2 | -5.74 | 104.36 | 112.40 | 5 | 1 |
| 1 | A | 388 | TRP | N-CA-CB | 5.74 | 120.93 | 110.60 | 3 | 1 |
| 2 | B | 108 | TRP | CE3-CZ3-CH2 | -5.74 | 114.89 | 121.20 | 8 | 1 |
| 2 | B | 216 | ALA | N-CA-CB | -5.74 | 102.07 | 110.10 | 11 | 1 |
| 1 | A | 342 | TRP | CB-CA-C | -5.73 | 98.94 | 110.40 | 4 | 1 |
| 1 | A | 324 | ASP | CB-CG-OD2 | -5.73 | 113.14 | 118.30 | 10 | 2 |
| 2 | B | 240 | LEU | O-C-N | -5.73 | 113.53 | 122.70 | 4 | 1 |
| 2 | C | 159 | LEU | CB-CG-CD2 | 5.72 | 120.73 | 111.00 | 7 | 1 |
| 2 | C | 194 | GLN | CG-CD-OE1 | 5.72 | 133.04 | 121.60 | 12 | 1 |
| 1 | A | 323 | PHE | CZ-CE2-CD2 | -5.72 | 113.24 | 120.10 | 1 | 1 |
| 1 | A | 423 | PRO | N-CA-CB | 5.72 | 110.16 | 103.30 | 6 | 2 |
| 1 | A | 421 | TRP | CZ3-CH2-CZ2 | -5.72 | 114.74 | 121.60 | 14 | 1 |
| 2 | C | 108 | TRP | CZ3-CH2-CZ2 | -5.72 | 114.74 | 121.60 | 11 | 1 |
| 2 | C | 255 | LEU | CB-CG-CD2 | 5.72 | 120.72 | 111.00 | 8 | 1 |
| 2 | C | 254 | ALA | N-CA-CB | -5.72 | 102.10 | 110.10 | 9 | 2 |
| 2 | C | 116 | ARG | CD-NE-CZ | 5.71 | 131.60 | 123.60 | 3 | 1 |
| 2 | C | 235 | ASP | N-CA-CB | -5.71 | 100.32 | 110.60 | 1 | 1 |
| 2 | C | 132 | GLU | OE1-CD-OE2 | 5.71 | 130.15 | 123.30 | 2 | 3 |
| 2 | B | 166 | LEU | CB-CA-C | -5.71 | 99.35 | 110.20 | 14 | 1 |
| 2 | B | 211 | LEU | CB-CA-C | 5.70 | 121.03 | 110.20 | 2 | 1 |
| 2 | C | 130 | TRP | CB-CG-CD1 | -5.70 | 119.59 | 127.00 | 5 | 1 |
| 1 | A | 484 | TRP | CD2-CE3-CZ3 | 5.69 | 126.19 | 118.80 | 4 | 1 |
| 2 | C | 163 | LEU | O-C-N | -5.69 | 113.60 | 122.70 | 4 | 1 |
| 2 | C | 219 | THR | CA-CB-OG1 | 5.68 | 120.94 | 109.00 | 1 | 2 |
| 2 | C | 136 | LEU | CB-CG-CD1 | 5.68 | 120.66 | 111.00 | 8 | 1 |
| 2 | B | 69 | GLN | N-CA-CB | -5.67 | 100.39 | 110.60 | 4 | 1 |
| 2 | C | 104 | PHE | CZ-CE2-CD2 | -5.67 | 113.30 | 120.10 | 8 | 1 |
| 1 | A | 382 | PHE | CD1-CE1-CZ | 5.67 | 126.90 | 120.10 | 13 | 1 |
| 2 | B | 98 | GLN | N-CA-CB | 5.66 | 120.79 | 110.60 | 4 | 1 |
| 1 | A | 464 | ARG | CG-CD-NE | -5.66 | 99.92 | 111.80 | 12 | 1 |
| 1 | A | 443 | ARG | NH1-CZ-NH2 | -5.65 | 113.18 | 119.40 | 6 | 2 |
| 1 | A | 342 | TRP | CG-CD2-CE3 | -5.65 | 128.81 | 133.90 | 5 | 1 |
| 2 | B | 181 | LEU | CB-CG-CD1 | 5.65 | 120.60 | 111.00 | 14 | 1 |
| 1 | A | 341 | PHE | O-C-N | -5.64 | 113.67 | 122.70 | 15 | 1 |
| 1 | A | 498 | PRO | O-C-N | 5.64 | 131.73 | 122.70 | 15 | 1 |
| 2 | B | 163 | LEU | CB-CG-CD2 | 5.64 | 120.59 | 111.00 | 1 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 2 | C | 61 | ARG | O-C-N | -5.64 | 113.68 | 122.70 | 5 | 1 |
| 1 | A | 372 | TYR | CG-CD1-CE1 | -5.64 | 116.79 | 121.30 | 5 | 3 |
| 2 | C | 180 | ALA | N-CA-CB | 5.64 | 117.99 | 110.10 | 13 | 1 |
| 2 | B | 103 | ASP | CB-CG-OD2 | -5.63 | 113.23 | 118.30 | 5 | 2 |
| 2 | C | 72 | TRP | CD1-NE1-CE2 | 5.63 | 114.06 | 109.00 | 4 | 1 |
| 2 | C | 186 | ALA | N-CA-CB | -5.63 | 102.22 | 110.10 | 7 | 2 |
| 1 | A | 350 | MET | CA-CB-CG | -5.63 | 103.73 | 113.30 | 12 | 1 |
| 2 | B | 254 | ALA | CA-C-O | 5.62 | 131.91 | 120.10 | 11 | 1 |
| 2 | C | 108 | TRP | CD2-CE2-CZ2 | -5.62 | 115.55 | 122.30 | 12 | 1 |
| 2 | C | 160 | GLN | O-C-N | -5.62 | 113.70 | 122.70 | 4 | 1 |
| 1 | A | 462 | SER | CA-C-O | -5.62 | 108.29 | 120.10 | 7 | 1 |
| 2 | B | 236 | LEU | O-C-N | -5.62 | 113.71 | 122.70 | 8 | 1 |
| 2 | C | 119 | VAL | CG1-CB-CG2 | 5.62 | 119.90 | 110.90 | 13 | 2 |
| 1 | A | 373 | GLU | OE1-CD-OE2 | -5.62 | 116.56 | 123.30 | 2 | 1 |
| 2 | B | 128 | LYS | CB-CA-C | 5.62 | 121.63 | 110.40 | 2 | 1 |
| 2 | C | 132 | GLU | CG-CD-OE2 | 5.62 | 129.53 | 118.30 | 6 | 1 |
| 2 | B | 72 | TRP | CE3-CZ3-CH2 | 5.61 | 127.38 | 121.20 | 2 | 1 |
| 1 | A | 497 | TYR | CA-CB-CG | -5.61 | 102.74 | 113.40 | 4 | 1 |
| 2 | C | 213 | GLU | N-CA-CB | 5.61 | 120.70 | 110.60 | 9 | 1 |
| 2 | C | 181 | LEU | CB-CG-CD1 | -5.61 | 101.47 | 111.00 | 8 | 1 |
| 2 | C | 81 | GLY | O-C-N | -5.61 | 113.73 | 122.70 | 10 | 1 |
| 1 | A | 390 | PHE | CZ-CE2-CD2 | -5.61 | 113.37 | 120.10 | 14 | 1 |
| 1 | A | 326 | VAL | CB-CA-C | -5.60 | 100.75 | 111.40 | 10 | 1 |
| 2 | B | 233 | LEU | N-CA-CB | -5.60 | 99.20 | 110.40 | 2 | 1 |
| 2 | B | 258 | TYR | CG-CD2-CE2 | -5.60 | 116.82 | 121.30 | 14 | 1 |
| 2 | C | 183 | THR | O-C-N | -5.60 | 113.74 | 122.70 | 11 | 1 |
| 2 | C | 229 | ALA | CB-CA-C | 5.60 | 118.50 | 110.10 | 1 | 1 |
| 1 | A | 414 | LYS | N-CA-CB | 5.59 | 120.67 | 110.60 | 5 | 2 |
| 2 | B | 184 | HIS | O-C-N | -5.59 | 113.75 | 122.70 | 2 | 1 |
| 2 | C | 173 | ARG | CD-NE-CZ | 5.59 | 131.43 | 123.60 | 5 | 3 |
| 1 | A | 342 | TRP | CD1-CG-CD2 | -5.59 | 101.83 | 106.30 | 15 | 2 |
| 2 | B | 171 | ARG | CD-NE-CZ | 5.59 | 131.43 | 123.60 | 9 | 1 |
| 2 | C | 120 | GLU | CA-C-N | 5.59 | 132.75 | 117.10 | 1 | 2 |
| 2 | B | 198 | ALA | CB-CA-C | -5.59 | 101.72 | 110.10 | 7 | 2 |
| 2 | B | 210 | ARG | NH1-CZ-NH2 | -5.59 | 113.25 | 119.40 | 4 | 2 |
| 2 | B | 61 | ARG | NH1-CZ-NH2 | -5.58 | 113.26 | 119.40 | 4 | 1 |
| 2 | B | 179 | ASP | CB-CG-OD2 | 5.58 | 123.33 | 118.30 | 15 | 1 |
| 2 | B | 234 | GLU | OE1-CD-OE2 | -5.57 | 116.61 | 123.30 | 15 | 1 |
| 2 | C | 88 | LYS | O-C-N | -5.57 | 113.79 | 122.70 | 10 | 1 |
| 2 | C | 197 | ALA | O-C-N | -5.57 | 113.79 | 122.70 | 15 | 1 |
| 2 | B | 202 | ALA | N-CA-CB | -5.57 | 102.31 | 110.10 | 7 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 2 | B | 147 | GLU | O-C-N | -5.57 | 113.79 | 122.70 | 8 | 1 |
| 2 | C | 215 | HIS | O-C-N | -5.56 | 113.80 | 122.70 | 3 | 1 |
| 2 | C | 181 | LEU | N-CA-CB | -5.56 | 99.28 | 110.40 | 3 | 1 |
| 2 | C | 124 | ASP | O-C-N | -5.55 | 113.82 | 122.70 | 11 | 1 |
| 2 | B | 109 | GLN | CA-CB-CG | 5.55 | 125.60 | 113.40 | 5 | 1 |
| 2 | B | 257 | GLU | OE1-CD-OE2 | 5.55 | 129.96 | 123.30 | 10 | 1 |
| 1 | A | 440 | GLU | N-CA-CB | -5.54 | 100.62 | 110.60 | 10 | 1 |
| 2 | C | 170 | MET | O-C-N | 5.54 | 131.56 | 122.70 | 6 | 1 |
| 1 | A | 505 | TRP | CA-CB-CG | 5.54 | 124.22 | 113.70 | 7 | 3 |
| 2 | C | 100 | TYR | N-CA-CB | 5.53 | 120.56 | 110.60 | 7 | 1 |
| 2 | B | 231 | PRO | N-CA-CB | 5.53 | 109.94 | 103.30 | 5 | 1 |
| 2 | C | 70 | GLU | OE1-CD-OE2 | -5.53 | 116.67 | 123.30 | 3 | 2 |
| 1 | A | 431 | ARG | CD-NE-CZ | 5.52 | 131.33 | 123.60 | 1 | 1 |
| 2 | B | 224 | THR | N-CA-CB | 5.52 | 120.80 | 110.30 | 4 | 1 |
| 2 | C | 251 | PHE | CA-CB-CG | 5.52 | 127.14 | 113.90 | 4 | 1 |
| 2 | B | 165 | PRO | N-CA-CB | 5.52 | 109.92 | 103.30 | 12 | 1 |
| 1 | A | 345 | ARG | C-N-CA | 5.51 | 135.49 | 121.70 | 3 | 1 |
| 2 | C | 210 | ARG | CA-CB-CG | 5.51 | 125.52 | 113.40 | 2 | 1 |
| 2 | B | 86 | MET | O-C-N | -5.51 | 113.88 | 122.70 | 3 | 1 |
| 2 | B | 100 | TYR | CZ-CE2-CD2 | -5.51 | 114.84 | 119.80 | 8 | 2 |
| 2 | C | 237 | ARG | CB-CG-CD | 5.51 | 125.93 | 111.60 | 7 | 1 |
| 2 | B | 264 | THR | CA-CB-CG2 | -5.50 | 104.69 | 112.40 | 12 | 1 |
| 2 | B | 147 | GLU | OE1-CD-OE2 | -5.50 | 116.69 | 123.30 | 12 | 1 |
| 1 | A | 421 | TRP | CE3-CZ3-CH2 | 5.50 | 127.25 | 121.20 | 2 | 1 |
| 1 | A | 372 | TYR | CD1-CE1-CZ | 5.50 | 124.75 | 119.80 | 5 | 1 |
| 1 | A | 483 | TYR | CG-CD1-CE1 | -5.50 | 116.90 | 121.30 | 13 | 1 |
| 2 | B | 72 | TRP | O-C-N | -5.50 | 113.90 | 122.70 | 12 | 1 |
| 2 | C | 230 | LYS | CB-CA-C | 5.50 | 121.40 | 110.40 | 11 | 1 |
| 2 | C | 130 | TRP | CG-CD2-CE3 | -5.50 | 128.95 | 133.90 | 1 | 1 |
| 2 | B | 63 | GLN | O-C-N | -5.50 | 113.91 | 122.70 | 2 | 1 |
| 2 | B | 195 | ARG | CD-NE-CZ | 5.49 | 131.29 | 123.60 | 15 | 1 |
| 2 | C | 100 | TYR | CZ-CE2-CD2 | -5.49 | 114.86 | 119.80 | 13 | 1 |
| 1 | A | 475 | THR | N-CA-CB | 5.48 | 120.71 | 110.30 | 14 | 1 |
| 2 | B | 91 | GLU | OE1-CD-OE2 | -5.48 | 116.73 | 123.30 | 4 | 1 |
| 1 | A | 418 | ALA | N-CA-CB | -5.48 | 102.43 | 110.10 | 5 | 1 |
| 2 | C | 149 | GLN | N-CA-CB | 5.48 | 120.46 | 110.60 | 12 | 1 |
| 1 | A | 401 | LYS | CA-CB-CG | 5.48 | 125.45 | 113.40 | 14 | 1 |
| 2 | C | 255 | LEU | CB-CA-C | 5.48 | 120.61 | 110.20 | 5 | 1 |
| 1 | A | 329 | LEU | O-C-N | -5.47 | 113.95 | 122.70 | 8 | 1 |
| 1 | A | 409 | GLY | O-C-N | -5.47 | 113.95 | 122.70 | 4 | 2 |
| 2 | C | 56 | THR | N-CA-C | 5.47 | 125.77 | 111.00 | 6 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 2 | B | 193 | ARG | CA-CB-CG | 5.47 | 125.42 | 113.40 | 12 | 1 |
| 1 | A | 439 | ASN | N-CA-CB | -5.46 | 100.76 | 110.60 | 6 | 1 |
| 1 | A | 456 | TRP | CE2-CD2-CG | -5.46 | 102.93 | 107.30 | 6 | 1 |
| 2 | C | 178 | VAL | CA-CB-CG2 | -5.46 | 102.71 | 110.90 | 8 | 1 |
| 2 | B | 130 | TRP | CZ3-CH2-CZ2 | 5.46 | 128.15 | 121.60 | 12 | 1 |
| 2 | C | 229 | ALA | N-CA-CB | -5.46 | 102.46 | 110.10 | 6 | 1 |
| 2 | C | 223 | SER | N-CA-CB | -5.46 | 102.31 | 110.50 | 14 | 1 |
| 1 | A | 333 | MET | CA-C-O | 5.46 | 131.56 | 120.10 | 6 | 1 |
| 2 | B | 118 | LYS | CB-CA-C | 5.45 | 121.31 | 110.40 | 12 | 1 |
| 2 | B | 65 | GLY | N-CA-C | 5.45 | 126.72 | 113.10 | 9 | 1 |
| 1 | A | 382 | PHE | CG-CD1-CE1 | -5.45 | 114.81 | 120.80 | 10 | 1 |
| 2 | C | 92 | GLU | OE1-CD-OE2 | -5.45 | 116.76 | 123.30 | 4 | 1 |
| 1 | A | 480 | GLY | C-N-CA | 5.45 | 135.32 | 121.70 | 11 | 1 |
| 1 | A | 484 | TRP | CB-CG-CD2 | 5.45 | 133.68 | 126.60 | 8 | 1 |
| 2 | C | 178 | VAL | CG1-CB-CG2 | -5.44 | 102.19 | 110.90 | 5 | 1 |
| 2 | C | 82 | LEU | CB-CG-CD2 | 5.44 | 120.25 | 111.00 | 13 | 1 |
| 2 | B | 232 | ALA | C-N-CA | 5.44 | 135.30 | 121.70 | 11 | 1 |
| 2 | B | 115 | TYR | CB-CA-C | 5.43 | 121.27 | 110.40 | 3 | 1 |
| 2 | C | 206 | ASN | CA-CB-CG | 5.43 | 125.35 | 113.40 | 8 | 1 |
| 2 | B | 67 | VAL | CG1-CB-CG2 | 5.43 | 119.59 | 110.90 | 15 | 1 |
| 1 | A | 316 | PRO | N-CD-CG | 5.43 | 111.35 | 103.20 | 2 | 1 |
| 2 | B | 241 | LEU | CB-CG-CD1 | -5.43 | 101.77 | 111.00 | 11 | 1 |
| 1 | A | 334 | PHE | CD1-CG-CD2 | -5.43 | 111.24 | 118.30 | 6 | 1 |
| 1 | A | 484 | TRP | CB-CG-CD1 | -5.43 | 119.94 | 127.00 | 8 | 2 |
| 2 | C | 186 | ALA | CB-CA-C | 5.43 | 118.24 | 110.10 | 15 | 1 |
| 1 | A | 399 | TYR | CZ-CE2-CD2 | 5.42 | 124.68 | 119.80 | 2 | 1 |
| 2 | C | 240 | LEU | CB-CG-CD1 | 5.42 | 120.21 | 111.00 | 4 | 1 |
| 2 | C | 190 | ASP | O-C-N | -5.41 | 114.04 | 122.70 | 7 | 2 |
| 1 | A | 484 | TRP | CG-CD2-CE3 | 5.41 | 138.77 | 133.90 | 4 | 1 |
| 1 | A | 505 | TRP | CG-CD1-NE1 | 5.41 | 115.51 | 110.10 | 15 | 1 |
| 2 | B | 56 | THR | O-C-N | -5.41 | 114.05 | 122.70 | 8 | 1 |
| 2 | B | 97 | VAL | CG1-CB-CG2 | -5.40 | 102.25 | 110.90 | 8 | 1 |
| 1 | A | 391 | ASP | OD1-CG-OD2 | -5.40 | 113.03 | 123.30 | 4 | 1 |
| 2 | C | 188 | TYR | CD1-CE1-CZ | -5.40 | 114.94 | 119.80 | 11 | 2 |
| 1 | A | 354 | PRO | CA-N-CD | -5.40 | 103.94 | 111.50 | 12 | 1 |
| 2 | C | 142 | GLU | O-C-N | -5.40 | 110.85 | 121.10 | 5 | 1 |
| 2 | C | 258 | TYR | CD1-CG-CD2 | 5.39 | 123.83 | 117.90 | 3 | 1 |
| 1 | A | 443 | ARG | CD-NE-CZ | 5.39 | 131.14 | 123.60 | 3 | 2 |
| 2 | B | 79 | THR | CA-CB-CG2 | 5.38 | 119.94 | 112.40 | 9 | 1 |
| 2 | B | 98 | GLN | CA-C-O | -5.38 | 108.79 | 120.10 | 10 | 1 |
| 2 | B | 189 | SER | O-C-N | -5.38 | 114.08 | 122.70 | 12 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 2 | C | 101 | LEU | CB-CG-CD1 | 5.38 | 120.15 | 111.00 | 15 | 1 |
| 1 | A | 378 | LYS | N-CA-CB | 5.38 | 120.29 | 110.60 | 1 | 1 |
| 2 | B | 153 | ARG | CD-NE-CZ | 5.38 | 131.13 | 123.60 | 7 | 1 |
| 2 | C | 143 | PRO | N-CA-CB | 5.38 | 109.75 | 103.30 | 10 | 1 |
| 1 | A | 353 | TYR | CD1-CE1-CZ | -5.38 | 114.96 | 119.80 | 2 | 1 |
| 1 | A | 429 | PHE | CG-CD2-CE2 | -5.38 | 114.89 | 120.80 | 2 | 1 |
| 2 | C | 186 | ALA | O-C-N | -5.38 | 110.89 | 121.10 | 9 | 1 |
| 2 | B | 209 | ALA | N-CA-CB | -5.37 | 102.58 | 110.10 | 8 | 2 |
| 2 | C | 112 | MET | CG-SD-CE | -5.37 | 91.60 | 100.20 | 12 | 2 |
| 2 | B | 134 | MET | CB-CA-C | 5.37 | 121.15 | 110.40 | 9 | 1 |
| 2 | C | 185 | LEU | CB-CG-CD1 | -5.37 | 101.87 | 111.00 | 13 | 1 |
| 2 | C | 214 | TYR | CG-CD1-CE1 | -5.37 | 117.00 | 121.30 | 1 | 2 |
| 2 | C | 98 | GLN | CA-C-N | 5.37 | 132.14 | 117.10 | 12 | 2 |
| 2 | B | 258 | TYR | O-C-N | -5.37 | 114.11 | 122.70 | 9 | 1 |
| 2 | B | 251 | PHE | CB-CA-C | 5.36 | 121.12 | 110.40 | 2 | 1 |
| 1 | A | 340 | TRP | O-C-N | -5.36 | 114.13 | 122.70 | 10 | 1 |
| 2 | B | 218 | ALA | N-CA-CB | -5.36 | 102.60 | 110.10 | 3 | 1 |
| 1 | A | 506 | MET | CG-SD-CE | -5.35 | 91.64 | 100.20 | 9 | 3 |
| 2 | C | 190 | ASP | CB-CA-C | -5.35 | 99.70 | 110.40 | 5 | 1 |
| 2 | B | 97 | VAL | CA-CB-CG2 | -5.35 | 102.88 | 110.90 | 14 | 1 |
| 2 | C | 99 | PRO | O-C-N | 5.35 | 131.26 | 122.70 | 14 | 1 |
| 1 | A | 422 | MET | CA-CB-CG | 5.35 | 122.39 | 113.30 | 15 | 1 |
| 2 | C | 137 | TYR | CG-CD2-CE2 | -5.35 | 117.02 | 121.30 | 11 | 2 |
| 1 | A | 349 | VAL | CA-C-O | 5.34 | 131.32 | 120.10 | 9 | 1 |
| 1 | A | 483 | TYR | CZ-CE2-CD2 | 5.34 | 124.61 | 119.80 | 2 | 1 |
| 2 | B | 72 | TRP | CD1-CG-CD2 | -5.34 | 102.03 | 106.30 | 1 | 1 |
| 2 | B | 180 | ALA | N-CA-CB | -5.34 | 102.63 | 110.10 | 12 | 1 |
| 1 | A | 345 | ARG | O-C-N | -5.33 | 114.17 | 122.70 | 13 | 2 |
| 1 | A | 443 | ARG | N-CA-CB | 5.33 | 120.19 | 110.60 | 1 | 1 |
| 1 | A | 440 | GLU | OE1-CD-OE2 | -5.33 | 116.91 | 123.30 | 5 | 1 |
| 2 | B | 95 | ALA | N-CA-CB | -5.33 | 102.64 | 110.10 | 14 | 1 |
| 2 | C | 57 | PHE | N-CA-CB | 5.32 | 120.18 | 110.60 | 2 | 1 |
| 2 | B | 63 | GLN | CG-CD-OE1 | -5.32 | 110.96 | 121.60 | 4 | 1 |
| 2 | C | 59 | LYS | CB-CG-CD | 5.32 | 125.43 | 111.60 | 7 | 1 |
| 1 | A | 369 | ASN | CB-CA-C | -5.32 | 99.76 | 110.40 | 7 | 1 |
| 2 | C | 262 | LEU | CB-CA-C | -5.32 | 100.10 | 110.20 | 10 | 1 |
| 1 | A | 342 | TRP | CE2-CD2-CE3 | -5.32 | 112.32 | 118.70 | 13 | 1 |
| 1 | A | 340 | TRP | CE2-CD2-CE3 | 5.32 | 125.08 | 118.70 | 2 | 1 |
| 1 | A | 335 | VAL | CA-CB-CG2 | -5.32 | 102.93 | 110.90 | 4 | 1 |
| 2 | C | 83 | ARG | CG-CD-NE | -5.32 | 100.64 | 111.80 | 13 | 2 |
| 2 | B | 122 | TYR | CD1-CG-CD2 | 5.31 | 123.75 | 117.90 | 13 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|------------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 1 | A | 341 | PHE | CG-CD2-CE2 | 5.31 | 126.64 | 120.80 | 2 | 1 |
| 2 | C | 247 | PHE | CD1-CE1-CZ | 5.31 | 126.48 | 120.10 | 5 | 1 |
| 1 | A | 455 | VAL | CA-CB-CG2 | -5.31 | 102.93 | 110.90 | 7 | 1 |
| 2 | C | 219 | THR | OG1-CB-CG2 | -5.31 | 97.78 | 110.00 | 9 | 1 |
| 2 | B | 183 | THR | CA-CB-CG2 | -5.31 | 104.97 | 112.40 | 13 | 2 |
| 2 | C | 83 | ARG | CD-NE-CZ | 5.31 | 131.03 | 123.60 | 9 | 1 |
| 2 | C | 258 | TYR | CZ-CE2-CD2 | 5.31 | 124.58 | 119.80 | 1 | 1 |
| 1 | A | 505 | TRP | N-CA-CB | 5.30 | 120.15 | 110.60 | 12 | 1 |
| 2 | B | 197 | ALA | CB-CA-C | 5.30 | 118.05 | 110.10 | 8 | 1 |
| 2 | C | 102 | ASP | CB-CG-OD2 | 5.30 | 123.07 | 118.30 | 12 | 2 |
| 2 | C | 256 | GLU | OE1-CD-OE2 | -5.30 | 116.94 | 123.30 | 6 | 1 |
| 2 | C | 119 | VAL | CA-CB-CG2 | -5.30 | 102.95 | 110.90 | 11 | 2 |
| 2 | B | 233 | LEU | CB-CG-CD2 | -5.30 | 102.00 | 111.00 | 11 | 1 |
| 1 | A | 329 | LEU | CB-CG-CD2 | 5.30 | 120.00 | 111.00 | 12 | 1 |
| 2 | C | 221 | HIS | CA-CB-CG | -5.29 | 104.60 | 113.60 | 14 | 1 |
| 2 | B | 176 | ALA | CB-CA-C | 5.29 | 118.04 | 110.10 | 13 | 2 |
| 1 | A | 399 | TYR | CA-CB-CG | -5.29 | 103.35 | 113.40 | 13 | 1 |
| 1 | A | 330 | ARG | CB-CA-C | 5.27 | 120.95 | 110.40 | 6 | 1 |
| 2 | B | 85 | GLU | OE1-CD-OE2 | -5.27 | 116.97 | 123.30 | 2 | 1 |
| 2 | B | 127 | GLN | CG-CD-OE1 | 5.27 | 132.15 | 121.60 | 4 | 1 |
| 2 | B | 214 | TYR | N-CA-CB | -5.27 | 101.11 | 110.60 | 1 | 1 |
| 2 | B | 75 | LEU | O-C-N | -5.27 | 114.27 | 122.70 | 13 | 2 |
| 2 | C | 96 | LYS | O-C-N | -5.27 | 114.27 | 122.70 | 13 | 1 |
| 1 | A | 387 | HIS | C-N-CA | 5.27 | 134.87 | 121.70 | 7 | 1 |
| 1 | A | 407 | GLY | O-C-N | -5.26 | 114.28 | 122.70 | 3 | 1 |
| 2 | C | 71 | PHE | CG-CD2-CE2 | 5.26 | 126.59 | 120.80 | 15 | 1 |
| 1 | A | 499 | LYS | O-C-N | -5.26 | 114.28 | 122.70 | 10 | 1 |
| 1 | A | 382 | PHE | CB-CA-C | -5.26 | 99.88 | 110.40 | 12 | 1 |
| 2 | B | 108 | TRP | C-N-CA | 5.26 | 134.85 | 121.70 | 15 | 1 |
| 1 | A | 333 | MET | O-C-N | -5.26 | 114.29 | 122.70 | 6 | 1 |
| 1 | A | 482 | LYS | N-CA-CB | 5.25 | 120.05 | 110.60 | 6 | 1 |
| 2 | B | 82 | LEU | O-C-N | -5.25 | 114.30 | 122.70 | 10 | 1 |
| 1 | A | 328 | MET | CA-CB-CG | 5.25 | 122.23 | 113.30 | 13 | 1 |
| 2 | C | 221 | HIS | N-CA-CB | 5.25 | 120.04 | 110.60 | 4 | 1 |
| 1 | A | 503 | ARG | C-N-CA | 5.24 | 134.80 | 121.70 | 2 | 1 |
| 2 | C | 245 | GLU | CG-CD-OE2 | 5.24 | 128.78 | 118.30 | 8 | 1 |
| 2 | B | 100 | TYR | CD1-CG-CD2 | 5.24 | 123.66 | 117.90 | 11 | 1 |
| 1 | A | 348 | GLN | O-C-N | -5.24 | 114.32 | 122.70 | 8 | 1 |
| 2 | B | 148 | LEU | CB-CA-C | 5.23 | 120.14 | 110.20 | 1 | 1 |
| 2 | C | 262 | LEU | CB-CG-CD2 | 5.23 | 119.90 | 111.00 | 11 | 1 |
| 1 | A | 476 | TYR | CD1-CE1-CZ | -5.23 | 115.09 | 119.80 | 10 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 2 | B | 55 | SER | N-CA-CB | 5.23 | 118.35 | 110.50 | 11 | 1 |
| 1 | A | 330 | ARG | N-CA-CB | 5.23 | 120.02 | 110.60 | 7 | 1 |
| 2 | B | 179 | ASP | CB-CA-C | 5.23 | 120.86 | 110.40 | 8 | 1 |
| 2 | C | 215 | HIS | CA-CB-CG | 5.23 | 122.49 | 113.60 | 1 | 1 |
| 1 | A | 436 | TYR | CD1-CE1-CZ | -5.22 | 115.10 | 119.80 | 13 | 1 |
| 1 | A | 435 | TYR | O-C-N | -5.22 | 114.35 | 122.70 | 6 | 1 |
| 2 | C | 73 | ASP | CB-CA-C | 5.22 | 120.83 | 110.40 | 3 | 1 |
| 1 | A | 433 | ASN | N-CA-CB | 5.22 | 119.99 | 110.60 | 13 | 1 |
| 1 | A | 388 | TRP | CD1-CG-CD2 | 5.21 | 110.47 | 106.30 | 13 | 1 |
| 2 | C | 75 | LEU | CB-CG-CD1 | -5.21 | 102.14 | 111.00 | 14 | 1 |
| 1 | A | 505 | TRP | NE1-CE2-CD2 | 5.21 | 112.51 | 107.30 | 6 | 1 |
| 1 | A | 475 | THR | CA-CB-CG2 | -5.21 | 105.11 | 112.40 | 13 | 1 |
| 2 | B | 60 | LEU | CB-CG-CD1 | 5.21 | 119.86 | 111.00 | 15 | 1 |
| 2 | B | 209 | ALA | CB-CA-C | 5.21 | 117.91 | 110.10 | 1 | 1 |
| 2 | B | 191 | GLU | O-C-N | -5.21 | 114.37 | 122.70 | 9 | 1 |
| 1 | A | 477 | PHE | CD1-CG-CD2 | 5.21 | 125.07 | 118.30 | 13 | 1 |
| 2 | B | 71 | PHE | O-C-N | -5.20 | 114.37 | 122.70 | 7 | 1 |
| 2 | C | 102 | ASP | CB-CA-C | 5.20 | 120.81 | 110.40 | 7 | 1 |
| 2 | C | 192 | LEU | CB-CA-C | 5.20 | 120.09 | 110.20 | 8 | 1 |
| 1 | A | 323 | PHE | CG-CD2-CE2 | -5.20 | 115.08 | 120.80 | 11 | 1 |
| 2 | C | 108 | TRP | O-C-N | -5.20 | 114.38 | 122.70 | 5 | 2 |
| 2 | B | 132 | GLU | OE1-CD-OE2 | -5.20 | 117.06 | 123.30 | 8 | 1 |
| 2 | C | 64 | LEU | CB-CA-C | -5.20 | 100.32 | 110.20 | 7 | 1 |
| 2 | B | 114 | LEU | CA-CB-CG | 5.20 | 127.25 | 115.30 | 13 | 1 |
| 2 | B | 130 | TRP | CD1-NE1-CE2 | 5.19 | 113.67 | 109.00 | 7 | 1 |
| 2 | B | 245 | GLU | OE1-CD-OE2 | 5.19 | 129.53 | 123.30 | 3 | 1 |
| 2 | C | 214 | TYR | CD1-CE1-CZ | 5.19 | 124.47 | 119.80 | 1 | 1 |
| 1 | A | 435 | TYR | CA-CB-CG | 5.19 | 123.25 | 113.40 | 4 | 1 |
| 1 | A | 484 | TRP | CD2-CE2-CZ2 | -5.19 | 116.07 | 122.30 | 5 | 1 |
| 1 | A | 385 | ASP | CB-CA-C | 5.18 | 120.77 | 110.40 | 1 | 1 |
| 1 | A | 420 | PHE | CG-CD1-CE1 | 5.18 | 126.50 | 120.80 | 2 | 1 |
| 1 | A | 505 | TRP | CD1-CG-CD2 | 5.18 | 110.45 | 106.30 | 3 | 1 |
| 1 | A | 376 | ASP | CA-CB-CG | 5.18 | 124.80 | 113.40 | 1 | 1 |
| 1 | A | 487 | ASN | N-CA-CB | 5.18 | 119.93 | 110.60 | 12 | 2 |
| 1 | A | 478 | TYR | CD1-CE1-CZ | -5.18 | 115.14 | 119.80 | 13 | 1 |
| 2 | C | 116 | ARG | C-N-CA | 5.18 | 134.65 | 121.70 | 1 | 1 |
| 2 | C | 73 | ASP | CB-CG-OD2 | -5.17 | 113.64 | 118.30 | 10 | 1 |
| 2 | B | 202 | ALA | CB-CA-C | 5.17 | 117.86 | 110.10 | 3 | 1 |
| 2 | B | 99 | PRO | CA-N-CD | 5.17 | 118.94 | 111.70 | 15 | 1 |
| 2 | C | 86 | MET | O-C-N | -5.17 | 114.43 | 122.70 | 9 | 1 |
| 2 | B | 221 | HIS | N-CA-CB | 5.17 | 119.90 | 110.60 | 10 | 2 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 2 | C | 205 | GLU | O-C-N | -5.16 | 114.44 | 122.70 | 14 | 1 |
| 2 | C | 73 | ASP | CB-CG-OD1 | 5.16 | 122.94 | 118.30 | 1 | 1 |
| 2 | C | 146 | ALA | N-CA-CB | -5.16 | 102.88 | 110.10 | 12 | 1 |
| 1 | A | 388 | TRP | CE3-CZ3-CH2 | 5.16 | 126.88 | 121.20 | 13 | 1 |
| 1 | A | 345 | ARG | N-CA-CB | 5.16 | 119.88 | 110.60 | 13 | 1 |
| 2 | B | 105 | GLN | CB-CG-CD | 5.16 | 125.00 | 111.60 | 10 | 1 |
| 1 | A | 330 | ARG | CD-NE-CZ | 5.16 | 130.82 | 123.60 | 11 | 1 |
| 2 | B | 154 | GLN | N-CA-CB | -5.15 | 101.32 | 110.60 | 2 | 1 |
| 1 | A | 344 | VAL | O-C-N | -5.15 | 114.45 | 122.70 | 10 | 1 |
| 2 | B | 178 | VAL | CA-CB-CG1 | 5.15 | 118.63 | 110.90 | 1 | 1 |
| 2 | C | 219 | THR | N-CA-CB | 5.15 | 120.09 | 110.30 | 14 | 1 |
| 1 | A | 380 | VAL | O-C-N | -5.14 | 114.47 | 122.70 | 4 | 1 |
| 2 | C | 260 | LYS | N-CA-CB | 5.14 | 119.86 | 110.60 | 14 | 1 |
| 2 | B | 57 | PHE | CA-CB-CG | -5.14 | 101.56 | 113.90 | 8 | 1 |
| 2 | B | 229 | ALA | N-CA-CB | -5.14 | 102.90 | 110.10 | 13 | 1 |
| 2 | C | 112 | MET | CA-CB-CG | 5.14 | 122.03 | 113.30 | 3 | 1 |
| 1 | A | 420 | PHE | CG-CD2-CE2 | -5.14 | 115.15 | 120.80 | 4 | 1 |
| 2 | C | 100 | TYR | O-C-N | -5.14 | 114.48 | 122.70 | 4 | 1 |
| 2 | C | 235 | ASP | O-C-N | -5.14 | 114.48 | 122.70 | 6 | 1 |
| 2 | B | 252 | LEU | CB-CG-CD1 | -5.14 | 102.27 | 111.00 | 11 | 1 |
| 1 | A | 470 | SER | N-CA-CB | 5.14 | 118.20 | 110.50 | 12 | 1 |
| 2 | C | 132 | GLU | CA-CB-CG | 5.13 | 124.69 | 113.40 | 5 | 1 |
| 1 | A | 464 | ARG | CD-NE-CZ | 5.13 | 130.79 | 123.60 | 8 | 1 |
| 2 | C | 168 | GLU | O-C-N | -5.13 | 114.48 | 122.70 | 14 | 1 |
| 2 | B | 262 | LEU | CB-CG-CD2 | -5.13 | 102.28 | 111.00 | 2 | 1 |
| 2 | C | 220 | GLU | N-CA-CB | 5.13 | 119.83 | 110.60 | 2 | 1 |
| 2 | B | 122 | TYR | CA-CB-CG | 5.13 | 123.14 | 113.40 | 3 | 1 |
| 2 | C | 205 | GLU | CA-CB-CG | 5.13 | 124.68 | 113.40 | 9 | 1 |
| 1 | A | 393 | ALA | N-CA-CB | -5.13 | 102.92 | 110.10 | 8 | 1 |
| 2 | C | 202 | ALA | N-CA-CB | -5.12 | 102.92 | 110.10 | 8 | 1 |
| 1 | A | 460 | PRO | N-CD-CG | 5.12 | 110.89 | 103.20 | 11 | 1 |
| 2 | C | 142 | GLU | OE1-CD-OE2 | -5.12 | 117.15 | 123.30 | 10 | 1 |
| 2 | C | 164 | SER | N-CA-CB | 5.12 | 118.18 | 110.50 | 15 | 1 |
| 1 | A | 503 | ARG | CG-CD-NE | -5.12 | 101.05 | 111.80 | 7 | 1 |
| 2 | B | 126 | PHE | O-C-N | -5.12 | 114.51 | 122.70 | 9 | 1 |
| 2 | C | 89 | ASP | CA-CB-CG | -5.11 | 102.15 | 113.40 | 11 | 1 |
| 2 | C | 142 | GLU | CA-C-O | -5.11 | 109.37 | 120.10 | 5 | 1 |
| 2 | C | 111 | GLU | OE1-CD-OE2 | -5.11 | 117.17 | 123.30 | 8 | 1 |
| 2 | C | 168 | GLU | CG-CD-OE2 | 5.11 | 128.51 | 118.30 | 7 | 1 |
| 2 | B | 113 | GLU | N-CA-CB | -5.11 | 101.41 | 110.60 | 5 | 1 |
| 2 | C | 130 | TRP | CD1-CG-CD2 | 5.11 | 110.39 | 106.30 | 7 | 2 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 1 | A | 436 | TYR | CG-CD1-CE1 | -5.11 | 117.22 | 121.30 | 10 | 1 |
| 2 | B | 65 | GLY | O-C-N | -5.10 | 111.40 | 121.10 | 2 | 1 |
| 2 | C | 122 | TYR | CD1-CG-CD2 | 5.10 | 123.51 | 117.90 | 10 | 1 |
| 2 | C | 168 | GLU | OE1-CD-OE2 | -5.10 | 117.18 | 123.30 | 10 | 1 |
| 1 | A | 427 | THR | N-CA-CB | 5.10 | 119.99 | 110.30 | 6 | 1 |
| 2 | B | 73 | ASP | CB-CG-OD2 | 5.10 | 122.89 | 118.30 | 1 | 1 |
| 2 | C | 262 | LEU | N-CA-C | 5.09 | 124.75 | 111.00 | 10 | 1 |
| 2 | C | 250 | SER | N-CA-CB | -5.09 | 102.86 | 110.50 | 10 | 1 |
| 1 | A | 450 | PRO | N-CA-C | 5.09 | 125.33 | 112.10 | 10 | 1 |
| 1 | A | 421 | TRP | CA-CB-CG | 5.08 | 123.36 | 113.70 | 4 | 1 |
| 2 | C | 58 | SER | O-C-N | -5.08 | 114.57 | 122.70 | 4 | 1 |
| 2 | C | 169 | GLU | O-C-N | -5.08 | 114.57 | 122.70 | 8 | 1 |
| 1 | A | 435 | TYR | N-CA-CB | 5.08 | 119.74 | 110.60 | 8 | 2 |
| 1 | A | 455 | VAL | CG1-CB-CG2 | 5.08 | 119.02 | 110.90 | 5 | 1 |
| 1 | A | 473 | VAL | CA-CB-CG1 | 5.08 | 118.52 | 110.90 | 14 | 1 |
| 2 | C | 122 | TYR | CA-CB-CG | 5.08 | 123.04 | 113.40 | 13 | 2 |
| 1 | A | 397 | PRO | N-CD-CG | 5.08 | 110.81 | 103.20 | 11 | 1 |
| 2 | B | 219 | THR | O-C-N | -5.07 | 114.58 | 122.70 | 13 | 1 |
| 1 | A | 493 | VAL | CA-CB-CG1 | 5.07 | 118.51 | 110.90 | 2 | 1 |
| 2 | B | 55 | SER | C-N-CA | 5.07 | 134.38 | 121.70 | 5 | 1 |
| 2 | C | 63 | GLN | CG-CD-OE1 | 5.07 | 131.74 | 121.60 | 3 | 1 |
| 1 | A | 400 | PRO | N-CA-CB | 5.07 | 109.39 | 103.30 | 14 | 1 |
| 2 | B | 238 | GLN | CG-CD-OE1 | -5.07 | 111.46 | 121.60 | 15 | 1 |
| 2 | B | 158 | GLU | O-C-N | -5.07 | 114.59 | 122.70 | 4 | 1 |
| 2 | C | 121 | PRO | N-CA-CB | 5.07 | 109.38 | 103.30 | 6 | 1 |
| 2 | C | 71 | PHE | CD1-CE1-CZ | -5.07 | 114.02 | 120.10 | 15 | 1 |
| 1 | A | 426 | LYS | N-CA-CB | 5.07 | 119.72 | 110.60 | 9 | 1 |
| 2 | B | 88 | LYS | CB-CA-C | 5.06 | 120.53 | 110.40 | 5 | 1 |
| 1 | A | 323 | PHE | CD1-CE1-CZ | 5.06 | 126.17 | 120.10 | 7 | 1 |
| 1 | A | 439 | ASN | CB-CA-C | 5.06 | 120.52 | 110.40 | 12 | 1 |
| 1 | A | 391 | ASP | CB-CA-C | 5.06 | 120.52 | 110.40 | 10 | 1 |
| 1 | A | 340 | TRP | NE1-CE2-CD2 | 5.05 | 112.36 | 107.30 | 2 | 1 |
| 2 | B | 224 | THR | CA-CB-CG2 | -5.05 | 105.32 | 112.40 | 5 | 1 |
| 2 | C | 185 | LEU | O-C-N | 5.05 | 130.78 | 122.70 | 12 | 1 |
| 2 | C | 122 | TYR | C-N-CA | 5.05 | 134.32 | 121.70 | 5 | 1 |
| 2 | B | 62 | GLU | OE1-CD-OE2 | -5.05 | 117.24 | 123.30 | 8 | 1 |
| 2 | B | 210 | ARG | CB-CG-CD | 5.05 | 124.73 | 111.60 | 14 | 1 |
| 2 | C | 122 | TYR | CZ-CE2-CD2 | 5.05 | 124.34 | 119.80 | 6 | 1 |
| 2 | B | 232 | ALA | CB-CA-C | -5.04 | 102.53 | 110.10 | 14 | 1 |
| 1 | A | 402 | HIS | CA-CB-CG | 5.04 | 122.17 | 113.60 | 7 | 1 |
| 1 | A | 446 | ASP | N-CA-C | 5.04 | 124.60 | 111.00 | 1 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 2 | C | 171 | ARG | CG-CD-NE | -5.04 | 101.22 | 111.80 | 3 | 1 |
| 2 | C | 230 | LYS | N-CA-C | 5.04 | 124.59 | 111.00 | 3 | 1 |
| 2 | B | 186 | ALA | N-CA-CB | 5.04 | 117.15 | 110.10 | 4 | 1 |
| 1 | A | 405 | GLU | N-CA-CB | 5.04 | 119.66 | 110.60 | 7 | 1 |
| 2 | B | 245 | GLU | N-CA-CB | -5.04 | 101.54 | 110.60 | 7 | 1 |
| 1 | A | 399 | TYR | CG-CD1-CE1 | -5.03 | 117.28 | 121.30 | 3 | 1 |
| 2 | C | 150 | GLU | OE1-CD-OE2 | -5.03 | 117.26 | 123.30 | 6 | 1 |
| 2 | C | 130 | TRP | CH2-CZ2-CE2 | -5.03 | 112.37 | 117.40 | 8 | 1 |
| 2 | C | 188 | TYR | CZ-CE2-CD2 | 5.02 | 124.32 | 119.80 | 9 | 1 |
| 1 | A | 385 | ASP | CB-CG-OD1 | -5.02 | 113.78 | 118.30 | 6 | 1 |
| 1 | A | 428 | TYR | CD1-CG-CD2 | 5.02 | 123.42 | 117.90 | 7 | 1 |
| 1 | A | 317 | ASN | O-C-N | -5.02 | 114.67 | 122.70 | 8 | 1 |
| 2 | C | 84 | GLN | O-C-N | -5.02 | 114.67 | 122.70 | 8 | 1 |
| 2 | B | 102 | ASP | N-CA-CB | -5.02 | 101.57 | 110.60 | 3 | 1 |
| 2 | C | 218 | ALA | N-CA-CB | 5.02 | 117.12 | 110.10 | 3 | 1 |
| 1 | A | 333 | MET | CB-CA-C | 5.02 | 120.44 | 110.40 | 8 | 1 |
| 2 | C | 64 | LEU | O-C-N | -5.02 | 114.67 | 123.20 | 13 | 1 |
| 2 | C | 133 | GLU | OE1-CD-OE2 | 5.02 | 129.32 | 123.30 | 15 | 1 |
| 2 | C | 194 | GLN | C-N-CA | 5.01 | 134.24 | 121.70 | 2 | 1 |
| 2 | B | 152 | ALA | N-CA-CB | -5.01 | 103.08 | 110.10 | 2 | 1 |
| 1 | A | 459 | ILE | CA-CB-CG2 | 5.01 | 120.92 | 110.90 | 9 | 1 |
| 2 | B | 116 | ARG | CA-CB-CG | 5.01 | 124.42 | 113.40 | 1 | 1 |
| 2 | C | 176 | ALA | N-CA-CB | -5.01 | 103.09 | 110.10 | 11 | 1 |
| 2 | B | 195 | ARG | CB-CG-CD | 5.01 | 124.62 | 111.60 | 13 | 1 |
| 2 | C | 175 | ARG | CB-CG-CD | 5.01 | 124.62 | 111.60 | 9 | 1 |
| 2 | B | 66 | PRO | N-CD-CG | 5.01 | 110.71 | 103.20 | 14 | 1 |
| 2 | B | 65 | GLY | CA-C-N | 5.01 | 131.12 | 117.10 | 2 | 1 |
| 2 | B | 61 | ARG | CG-CD-NE | -5.00 | 101.29 | 111.80 | 5 | 1 |
| 2 | C | 71 | PHE | O-C-N | -5.00 | 114.69 | 122.70 | 12 | 1 |
| 1 | A | 486 | PHE | CG-CD2-CE2 | -5.00 | 115.30 | 120.80 | 9 | 1 |
| 2 | B | 150 | GLU | O-C-N | -5.00 | 114.70 | 123.20 | 11 | 1 |

There are no chirality outliers.

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

| Mol | Chain | Res | Type | Group | Models (Total) |
|-----|-------|-----|------|-----------|----------------|
| 2 | C | 199 | ARG | Sidechain | 11 |
| 1 | A | 478 | TYR | Sidechain | 9 |
| 2 | B | 188 | TYR | Sidechain | 9 |
| 1 | A | 449 | TYR | Sidechain | 8 |

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| Mol | Chain | Res | Type | Group | Models (Total) |
|-----|-------|-----|------|-----------|----------------|
| 1 | A | 428 | TYR | Sidechain | 8 |
| 1 | A | 497 | TYR | Sidechain | 7 |
| 1 | A | 503 | ARG | Sidechain | 7 |
| 2 | B | 214 | TYR | Sidechain | 7 |
| 2 | C | 137 | TYR | Sidechain | 7 |
| 1 | A | 464 | ARG | Sidechain | 6 |
| 2 | C | 175 | ARG | Sidechain | 6 |
| 2 | C | 195 | ARG | Sidechain | 6 |
| 2 | B | 115 | TYR | Sidechain | 6 |
| 1 | A | 372 | TYR | Sidechain | 6 |
| 1 | A | 343 | ARG | Sidechain | 5 |
| 2 | B | 100 | TYR | Sidechain | 5 |
| 2 | B | 173 | ARG | Sidechain | 5 |
| 2 | B | 237 | ARG | Sidechain | 5 |
| 2 | C | 115 | TYR | Sidechain | 5 |
| 2 | C | 258 | TYR | Sidechain | 5 |
| 1 | A | 435 | TYR | Sidechain | 5 |
| 1 | A | 339 | ARG | Sidechain | 5 |
| 1 | A | 399 | TYR | Sidechain | 5 |
| 2 | C | 157 | HIS | Sidechain | 5 |
| 2 | C | 61 | ARG | Sidechain | 5 |
| 2 | C | 138 | ARG | Sidechain | 5 |
| 2 | C | 171 | ARG | Sidechain | 5 |
| 2 | B | 210 | ARG | Sidechain | 5 |
| 1 | A | 436 | TYR | Sidechain | 4 |
| 2 | C | 100 | TYR | Sidechain | 4 |
| 2 | B | 145 | ARG | Sidechain | 4 |
| 2 | C | 83 | ARG | Sidechain | 4 |
| 2 | C | 122 | TYR | Sidechain | 4 |
| 1 | A | 345 | ARG | Sidechain | 4 |
| 1 | A | 476 | TYR | Sidechain | 4 |
| 2 | C | 214 | TYR | Sidechain | 4 |
| 1 | A | 437 | ARG | Sidechain | 4 |
| 2 | B | 137 | TYR | Sidechain | 4 |
| 2 | B | 258 | TYR | Sidechain | 4 |
| 1 | A | 336 | PHE | Sidechain | 3 |
| 1 | A | 362 | ARG | Sidechain | 3 |
| 2 | B | 116 | ARG | Sidechain | 3 |
| 2 | B | 122 | TYR | Sidechain | 3 |
| 2 | C | 188 | TYR | Sidechain | 3 |
| 1 | A | 330 | ARG | Sidechain | 3 |
| 2 | C | 145 | ARG | Sidechain | 3 |

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| Mol | Chain | Res | Type | Group | Models (Total) |
|-----|-------|-----|------|-----------|----------------|
| 2 | C | 193 | ARG | Sidechain | 3 |
| 2 | B | 195 | ARG | Sidechain | 3 |
| 1 | A | 467 | PHE | Sidechain | 3 |
| 2 | C | 173 | ARG | Sidechain | 3 |
| 1 | A | 353 | TYR | Sidechain | 3 |
| 2 | B | 153 | ARG | Sidechain | 3 |
| 2 | B | 175 | ARG | Sidechain | 3 |
| 2 | C | 153 | ARG | Sidechain | 3 |
| 1 | A | 477 | PHE | Sidechain | 3 |
| 2 | C | 182 | ARG | Sidechain | 3 |
| 1 | A | 402 | HIS | Sidechain | 2 |
| 2 | B | 83 | ARG | Sidechain | 2 |
| 2 | C | 237 | ARG | Sidechain | 2 |
| 1 | A | 443 | ARG | Sidechain | 2 |
| 1 | A | 486 | PHE | Sidechain | 2 |
| 2 | B | 193 | ARG | Sidechain | 2 |
| 2 | B | 171 | ARG | Sidechain | 2 |
| 2 | B | 177 | HIS | Sidechain | 2 |
| 1 | A | 387 | HIS | Sidechain | 2 |
| 1 | A | 431 | ARG | Sidechain | 2 |
| 2 | C | 210 | ARG | Sidechain | 2 |
| 1 | A | 374 | ARG | Sidechain | 2 |
| 1 | A | 334 | PHE | Sidechain | 2 |
| 2 | C | 126 | PHE | Sidechain | 2 |
| 2 | C | 71 | PHE | Sidechain | 2 |
| 1 | A | 483 | TYR | Sidechain | 1 |
| 2 | B | 182 | ARG | Sidechain | 1 |
| 1 | A | 341 | PHE | Sidechain | 1 |
| 1 | A | 394 | SER | Peptide | 1 |
| 1 | A | 465 | GLY | Peptide | 1 |
| 2 | C | 116 | ARG | Sidechain | 1 |
| 2 | C | 215 | HIS | Sidechain | 1 |
| 1 | A | 420 | PHE | Sidechain | 1 |
| 2 | B | 247 | PHE | Sidechain | 1 |
| 2 | C | 104 | PHE | Sidechain | 1 |
| 2 | C | 184 | HIS | Sidechain | 1 |
| 2 | B | 157 | HIS | Sidechain | 1 |
| 2 | B | 251 | PHE | Sidechain | 1 |
| 2 | C | 60 | LEU | Mainchain | 1 |
| 2 | C | 94 | LYS | Mainchain | 1 |
| 2 | C | 177 | HIS | Sidechain | 1 |
| 1 | A | 414 | LYS | Peptide | 1 |

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| Mol | Chain | Res | Type | Group | Models (Total) |
|-----|-------|-----|------|-----------|----------------|
| 1 | A | 429 | PHE | Sidechain | 1 |
| 1 | A | 430 | PHE | Sidechain | 1 |
| 1 | A | 438 | PHE | Sidechain | 1 |
| 2 | B | 126 | PHE | Sidechain | 1 |
| 2 | B | 138 | ARG | Sidechain | 1 |
| 2 | C | 251 | PHE | Mainchain | 1 |
| 1 | A | 342 | TRP | Peptide | 1 |
| 2 | B | 61 | ARG | Sidechain | 1 |
| 2 | B | 211 | LEU | Mainchain | 1 |
| 2 | C | 190 | ASP | Mainchain | 1 |
| 2 | C | 221 | HIS | Sidechain | 1 |
| 1 | A | 408 | ARG | Sidechain | 1 |
| 1 | A | 474 | PHE | Sidechain | 1 |
| 2 | C | 218 | ALA | Peptide | 1 |
| 2 | B | 184 | HIS | Sidechain | 1 |
| 1 | A | 381 | PHE | Sidechain | 1 |
| 1 | A | 471 | ASP | Sidechain | 1 |
| 1 | A | 508 | CYS | Peptide | 1 |
| 2 | B | 57 | PHE | Sidechain | 1 |
| 2 | B | 104 | PHE | Sidechain | 1 |

6.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|--------|----------|----------|---------|
| 1 | A | 1637 | 1565 | 1562 | 4±2 |
| 2 | B | 1753 | 1745 | 1742 | 3±2 |
| 2 | C | 1728 | 1724 | 1721 | 2±2 |
| 3 | A | 2484 | 3888 | 3888 | 35±5 |
| 3 | B | 4600 | 7200 | 7200 | 53±7 |
| 3 | C | 2944 | 4608 | 4608 | 29±5 |
| All | All | 227220 | 310950 | 310821 | 1642 |

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

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

| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:402:HIS:CE1 | 3:A:649:PX4:H12 | 0.90 | 2.00 | 7 | 5 |
| 3:B:338:PX4:H4 | 3:B:343:PX4:O3 | 0.74 | 1.82 | 2 | 1 |
| 3:C:358:PX4:H9 | 3:C:361:PX4:O3 | 0.72 | 1.85 | 6 | 1 |
| 3:B:326:PX4:O3 | 3:B:355:PX4:H3 | 0.71 | 1.84 | 5 | 3 |
| 3:C:351:PX4:O4 | 3:C:351:PX4:H4 | 0.70 | 1.86 | 13 | 2 |
| 3:B:334:PX4:O1 | 3:B:348:PX4:H4 | 0.69 | 1.87 | 15 | 2 |
| 3:B:322:PX4:O4 | 3:B:350:PX4:H11 | 0.69 | 1.86 | 1 | 1 |
| 3:A:636:PX4:O4 | 3:A:645:PX4:H11 | 0.68 | 1.88 | 1 | 1 |
| 3:B:373:PX4:H6 | 3:B:380:PX4:O4 | 0.68 | 1.89 | 5 | 1 |
| 3:B:375:PX4:O4 | 3:B:376:PX4:H5 | 0.68 | 1.88 | 3 | 1 |
| 3:B:361:PX4:H4 | 3:B:368:PX4:O3 | 0.68 | 1.89 | 10 | 2 |
| 3:B:325:PX4:O2 | 3:B:357:PX4:H3 | 0.67 | 1.88 | 13 | 1 |
| 3:A:640:PX4:H3 | 3:B:398:PX4:O6 | 0.67 | 1.88 | 13 | 1 |
| 3:B:351:PX4:H4 | 3:B:354:PX4:O4 | 0.67 | 1.90 | 15 | 2 |
| 3:B:374:PX4:O2 | 3:B:384:PX4:H6 | 0.67 | 1.89 | 1 | 3 |
| 3:A:614:PX4:H4 | 3:C:336:PX4:O4 | 0.67 | 1.88 | 6 | 5 |
| 3:A:625:PX4:O7 | 3:A:625:PX4:H3 | 0.67 | 1.90 | 2 | 2 |
| 3:B:333:PX4:O3 | 3:B:361:PX4:H12 | 0.66 | 1.89 | 14 | 1 |
| 3:B:320:PX4:H4 | 3:B:340:PX4:O4 | 0.66 | 1.90 | 5 | 1 |
| 3:B:312:PX4:O1 | 3:B:317:PX4:H4 | 0.66 | 1.90 | 10 | 2 |
| 3:B:373:PX4:H4 | 3:B:373:PX4:O4 | 0.66 | 1.90 | 1 | 3 |
| 3:C:312:PX4:O3 | 3:C:312:PX4:H6 | 0.66 | 1.91 | 1 | 2 |
| 3:B:361:PX4:O3 | 3:B:368:PX4:H3 | 0.66 | 1.90 | 11 | 3 |
| 3:B:391:PX4:H9 | 3:C:303:PX4:O5 | 0.66 | 1.91 | 2 | 1 |
| 3:B:383:PX4:O4 | 3:B:383:PX4:H3 | 0.66 | 1.90 | 2 | 2 |
| 3:A:613:PX4:O4 | 3:A:628:PX4:H4 | 0.65 | 1.92 | 9 | 2 |
| 3:A:607:PX4:H10 | 3:A:607:PX4:O2 | 0.65 | 1.92 | 1 | 1 |
| 3:C:338:PX4:O4 | 3:C:345:PX4:H9 | 0.65 | 1.92 | 12 | 1 |
| 1:A:405:GLU:OE1 | 3:A:641:PX4:H4 | 0.65 | 1.90 | 3 | 1 |
| 3:B:361:PX4:H3 | 3:B:368:PX4:O3 | 0.65 | 1.90 | 11 | 5 |
| 3:A:642:PX4:O4 | 3:A:642:PX4:H4 | 0.65 | 1.92 | 10 | 7 |
| 3:B:362:PX4:O1 | 3:B:366:PX4:H3 | 0.65 | 1.92 | 11 | 1 |
| 3:B:380:PX4:O2 | 3:B:387:PX4:H3 | 0.64 | 1.92 | 8 | 1 |
| 3:A:628:PX4:O6 | 3:A:642:PX4:H8 | 0.64 | 1.92 | 10 | 1 |
| 3:A:622:PX4:O1 | 3:A:635:PX4:H4 | 0.64 | 1.93 | 7 | 2 |
| 3:C:307:PX4:H10 | 3:C:307:PX4:O2 | 0.64 | 1.93 | 12 | 2 |
| 3:B:333:PX4:O4 | 3:B:333:PX4:H13 | 0.64 | 1.93 | 12 | 2 |
| 3:B:310:PX4:O1 | 3:B:310:PX4:H9 | 0.64 | 1.92 | 12 | 2 |
| 3:C:309:PX4:H4 | 3:C:315:PX4:O1 | 0.64 | 1.92 | 2 | 2 |
| 3:B:323:PX4:O1 | 3:B:346:PX4:H3 | 0.64 | 1.93 | 5 | 2 |
| 1:A:402:HIS:CE1 | 3:A:649:PX4:H6 | 0.64 | 2.28 | 15 | 2 |
| 3:A:632:PX4:H4 | 3:A:647:PX4:O2 | 0.64 | 1.93 | 14 | 5 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 3:A:614:PX4:O1 | 3:A:625:PX4:H9 | 0.64 | 1.93 | 3 | 2 |
| 3:A:641:PX4:H15 | 3:A:641:PX4:H10 | 0.64 | 1.69 | 12 | 1 |
| 3:A:625:PX4:O4 | 3:A:625:PX4:H3 | 0.63 | 1.93 | 7 | 8 |
| 1:A:359:GLN:OE1 | 3:A:640:PX4:H10 | 0.63 | 1.93 | 5 | 2 |
| 3:C:358:PX4:H10 | 3:C:358:PX4:H16 | 0.63 | 1.68 | 11 | 1 |
| 3:B:360:PX4:O2 | 3:B:362:PX4:H9 | 0.63 | 1.93 | 2 | 1 |
| 3:C:316:PX4:H3 | 3:C:342:PX4:O1 | 0.63 | 1.92 | 6 | 2 |
| 3:B:349:PX4:O1 | 3:B:357:PX4:H11 | 0.63 | 1.94 | 5 | 1 |
| 3:C:333:PX4:H9 | 3:C:352:PX4:O2 | 0.63 | 1.94 | 13 | 1 |
| 3:A:632:PX4:H9 | 3:A:647:PX4:O4 | 0.63 | 1.94 | 13 | 3 |
| 3:B:301:PX4:O1 | 3:B:301:PX4:H3 | 0.63 | 1.92 | 6 | 2 |
| 3:A:631:PX4:O1 | 3:A:642:PX4:H3 | 0.63 | 1.94 | 13 | 1 |
| 3:A:647:PX4:H13 | 3:A:652:PX4:O1 | 0.63 | 1.93 | 15 | 1 |
| 3:A:627:PX4:O4 | 3:A:643:PX4:H6 | 0.63 | 1.94 | 1 | 1 |
| 3:B:380:PX4:O3 | 3:B:380:PX4:H6 | 0.63 | 1.94 | 13 | 1 |
| 3:B:335:PX4:H3 | 3:B:353:PX4:O2 | 0.62 | 1.94 | 8 | 1 |
| 3:B:380:PX4:O2 | 3:B:387:PX4:H4 | 0.62 | 1.94 | 2 | 2 |
| 3:B:360:PX4:O4 | 3:B:360:PX4:H3 | 0.62 | 1.93 | 13 | 7 |
| 3:C:350:PX4:O1 | 3:C:350:PX4:H4 | 0.62 | 1.95 | 4 | 1 |
| 3:C:330:PX4:O2 | 3:C:330:PX4:H3 | 0.62 | 1.94 | 13 | 3 |
| 3:C:359:PX4:H9 | 3:C:359:PX4:O1 | 0.62 | 1.94 | 10 | 1 |
| 3:C:318:PX4:H8 | 3:C:321:PX4:C1 | 0.62 | 2.24 | 14 | 1 |
| 3:B:337:PX4:O1 | 3:B:352:PX4:H7 | 0.62 | 1.93 | 12 | 2 |
| 3:A:626:PX4:O2 | 3:A:626:PX4:H12 | 0.62 | 1.95 | 15 | 1 |
| 3:B:363:PX4:H3 | 3:B:363:PX4:O1 | 0.62 | 1.94 | 3 | 4 |
| 3:B:368:PX4:O2 | 3:B:368:PX4:H7 | 0.62 | 1.93 | 10 | 2 |
| 3:A:606:PX4:O2 | 3:A:606:PX4:H4 | 0.62 | 1.95 | 9 | 3 |
| 3:A:607:PX4:O1 | 3:A:612:PX4:H3 | 0.62 | 1.95 | 8 | 2 |
| 3:C:325:PX4:O4 | 3:C:325:PX4:H7 | 0.62 | 1.94 | 11 | 1 |
| 3:A:619:PX4:H69 | 3:A:632:PX4:H5 | 0.61 | 1.71 | 4 | 1 |
| 3:B:400:PX4:H11 | 3:C:347:PX4:O4 | 0.61 | 1.95 | 9 | 1 |
| 3:B:348:PX4:O1 | 3:B:348:PX4:H3 | 0.61 | 1.95 | 5 | 3 |
| 3:C:343:PX4:H4 | 3:C:353:PX4:O2 | 0.61 | 1.95 | 6 | 1 |
| 3:C:307:PX4:O4 | 3:C:310:PX4:H5 | 0.61 | 1.95 | 14 | 1 |
| 3:A:617:PX4:H4 | 3:A:617:PX4:O4 | 0.61 | 1.96 | 14 | 1 |
| 3:B:363:PX4:H8 | 3:C:302:PX4:O2 | 0.61 | 1.95 | 15 | 1 |
| 3:B:311:PX4:O2 | 3:B:345:PX4:H3 | 0.61 | 1.96 | 1 | 1 |
| 3:A:641:PX4:H9 | 3:A:641:PX4:O3 | 0.61 | 1.96 | 14 | 3 |
| 3:C:340:PX4:H11 | 3:C:360:PX4:O4 | 0.61 | 1.95 | 14 | 1 |
| 3:B:368:PX4:H9 | 3:B:368:PX4:O3 | 0.61 | 1.96 | 7 | 1 |
| 3:A:613:PX4:O7 | 3:A:613:PX4:H9 | 0.61 | 1.95 | 11 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 3:A:618:PX4:O3 | 3:A:633:PX4:H6 | 0.61 | 1.94 | 15 | 1 |
| 3:A:611:PX4:H5 | 3:B:394:PX4:O4 | 0.61 | 1.95 | 2 | 2 |
| 3:B:397:PX4:H7 | 3:B:397:PX4:O4 | 0.61 | 1.96 | 1 | 2 |
| 3:A:614:PX4:O4 | 3:A:614:PX4:H3 | 0.61 | 1.96 | 2 | 3 |
| 3:A:633:PX4:O2 | 3:A:638:PX4:H6 | 0.61 | 1.96 | 4 | 1 |
| 3:C:307:PX4:O1 | 3:C:310:PX4:H9 | 0.61 | 1.96 | 7 | 1 |
| 3:B:329:PX4:O3 | 3:B:329:PX4:H6 | 0.61 | 1.96 | 2 | 5 |
| 3:B:383:PX4:H9 | 3:B:383:PX4:O3 | 0.60 | 1.96 | 5 | 4 |
| 3:A:610:PX4:H4 | 3:B:389:PX4:O1 | 0.60 | 1.96 | 6 | 3 |
| 3:A:645:PX4:H3 | 3:A:646:PX4:O2 | 0.60 | 1.96 | 4 | 1 |
| 3:A:632:PX4:O4 | 3:A:632:PX4:H12 | 0.60 | 1.95 | 7 | 2 |
| 3:A:628:PX4:O8 | 3:A:642:PX4:H5 | 0.60 | 1.95 | 6 | 1 |
| 1:A:400:PRO:O | 3:A:652:PX4:H11 | 0.60 | 1.96 | 6 | 7 |
| 3:A:609:PX4:H8 | 3:B:384:PX4:O4 | 0.60 | 1.96 | 7 | 4 |
| 3:C:350:PX4:O3 | 3:C:355:PX4:H4 | 0.60 | 1.97 | 5 | 1 |
| 3:B:386:PX4:H16 | 3:B:386:PX4:H10 | 0.60 | 1.71 | 7 | 1 |
| 3:A:645:PX4:O1 | 3:A:648:PX4:H11 | 0.60 | 1.96 | 4 | 1 |
| 3:B:327:PX4:O1 | 3:B:351:PX4:H4 | 0.60 | 1.96 | 6 | 2 |
| 3:C:332:PX4:O1 | 3:C:332:PX4:H3 | 0.60 | 1.97 | 8 | 3 |
| 3:C:337:PX4:O2 | 3:C:337:PX4:H4 | 0.60 | 1.97 | 11 | 1 |
| 3:B:353:PX4:H6 | 3:B:353:PX4:O2 | 0.60 | 1.97 | 15 | 1 |
| 3:A:614:PX4:O3 | 3:A:614:PX4:H12 | 0.59 | 1.97 | 11 | 2 |
| 3:B:353:PX4:H3 | 3:B:369:PX4:O3 | 0.59 | 1.97 | 4 | 5 |
| 3:C:307:PX4:H4 | 3:C:340:PX4:O2 | 0.59 | 1.97 | 14 | 3 |
| 3:A:605:PX4:O2 | 3:A:609:PX4:H4 | 0.59 | 1.97 | 8 | 2 |
| 3:B:327:PX4:O1 | 3:B:351:PX4:H7 | 0.59 | 1.97 | 7 | 1 |
| 3:B:362:PX4:H4 | 3:B:362:PX4:O2 | 0.59 | 1.97 | 7 | 1 |
| 2:B:76:GLU:OE2 | 3:B:305:PX4:H4 | 0.59 | 1.96 | 11 | 1 |
| 3:B:389:PX4:H10 | 3:B:389:PX4:O3 | 0.59 | 1.96 | 8 | 1 |
| 3:C:323:PX4:H4 | 3:C:323:PX4:O4 | 0.59 | 1.97 | 10 | 2 |
| 3:A:647:PX4:H10 | 3:A:652:PX4:O1 | 0.59 | 1.97 | 3 | 4 |
| 3:C:349:PX4:O4 | 3:C:358:PX4:H5 | 0.59 | 1.97 | 7 | 1 |
| 3:A:631:PX4:H10 | 3:A:646:PX4:O5 | 0.59 | 1.98 | 13 | 4 |
| 3:A:640:PX4:O2 | 3:A:650:PX4:H8 | 0.59 | 1.97 | 6 | 1 |
| 3:B:320:PX4:H13 | 3:B:340:PX4:O4 | 0.59 | 1.98 | 6 | 1 |
| 3:B:376:PX4:O6 | 3:B:390:PX4:H3 | 0.59 | 1.97 | 12 | 1 |
| 3:B:305:PX4:H3 | 3:B:305:PX4:O1 | 0.59 | 1.97 | 15 | 2 |
| 1:A:400:PRO:O | 3:A:652:PX4:H5 | 0.59 | 1.97 | 8 | 3 |
| 3:B:362:PX4:H4 | 3:B:366:PX4:O4 | 0.59 | 1.97 | 14 | 1 |
| 3:C:317:PX4:O4 | 3:C:344:PX4:H10 | 0.59 | 1.97 | 12 | 2 |
| 3:C:323:PX4:O8 | 3:C:323:PX4:H6 | 0.59 | 1.98 | 12 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 3:A:648:PX4:O2 | 3:A:654:PX4:H4 | 0.59 | 1.98 | 15 | 1 |
| 3:A:605:PX4:O6 | 3:A:609:PX4:H9 | 0.59 | 1.98 | 3 | 4 |
| 3:B:392:PX4:C6 | 3:B:392:PX4:H3 | 0.59 | 2.26 | 4 | 3 |
| 3:A:612:PX4:H9 | 3:A:612:PX4:O3 | 0.59 | 1.97 | 11 | 4 |
| 3:B:393:PX4:O2 | 3:B:393:PX4:H4 | 0.58 | 1.99 | 4 | 1 |
| 3:A:613:PX4:O2 | 3:A:628:PX4:H12 | 0.58 | 1.98 | 11 | 2 |
| 3:B:309:PX4:O1 | 3:B:309:PX4:H3 | 0.58 | 1.97 | 2 | 2 |
| 3:B:338:PX4:H48 | 3:B:343:PX4:H8 | 0.58 | 1.74 | 8 | 1 |
| 3:B:365:PX4:O6 | 3:B:378:PX4:H4 | 0.58 | 1.99 | 2 | 1 |
| 3:A:606:PX4:O2 | 3:B:381:PX4:H10 | 0.58 | 1.99 | 6 | 1 |
| 3:B:320:PX4:H6 | 3:B:340:PX4:O4 | 0.58 | 1.98 | 7 | 1 |
| 3:A:632:PX4:H7 | 3:A:647:PX4:O4 | 0.58 | 1.99 | 15 | 3 |
| 3:B:363:PX4:H9 | 3:C:302:PX4:O1 | 0.58 | 1.98 | 6 | 2 |
| 3:C:353:PX4:H3 | 3:C:353:PX4:O1 | 0.58 | 1.97 | 4 | 1 |
| 3:B:363:PX4:H13 | 3:B:363:PX4:O8 | 0.58 | 1.98 | 14 | 1 |
| 3:B:360:PX4:H3 | 3:B:360:PX4:O7 | 0.58 | 1.99 | 2 | 2 |
| 3:C:305:PX4:C3 | 3:C:324:PX4:H6 | 0.58 | 2.29 | 3 | 1 |
| 3:A:618:PX4:H67 | 3:A:633:PX4:H45 | 0.58 | 1.76 | 8 | 1 |
| 1:A:402:HIS:CE1 | 3:A:649:PX4:H10 | 0.58 | 2.33 | 8 | 1 |
| 3:C:336:PX4:H15 | 3:C:355:PX4:H13 | 0.58 | 1.75 | 3 | 1 |
| 3:A:601:PX4:O1 | 3:B:377:PX4:H4 | 0.58 | 1.99 | 4 | 1 |
| 3:B:398:PX4:H3 | 3:C:357:PX4:O3 | 0.58 | 1.98 | 8 | 2 |
| 3:A:647:PX4:H3 | 3:A:652:PX4:O2 | 0.58 | 1.99 | 11 | 5 |
| 3:B:327:PX4:O2 | 3:B:351:PX4:H7 | 0.58 | 1.99 | 4 | 2 |
| 3:B:354:PX4:O4 | 3:B:354:PX4:H3 | 0.58 | 1.98 | 6 | 2 |
| 2:C:71:PHE:CE1 | 2:C:75:LEU:HD11 | 0.58 | 2.34 | 8 | 1 |
| 3:B:369:PX4:O1 | 3:B:386:PX4:H4 | 0.58 | 1.98 | 13 | 2 |
| 3:C:323:PX4:O6 | 3:C:323:PX4:H13 | 0.57 | 1.99 | 2 | 1 |
| 3:A:611:PX4:H11 | 3:B:394:PX4:O3 | 0.57 | 1.98 | 3 | 2 |
| 3:A:611:PX4:H5 | 3:B:394:PX4:O6 | 0.57 | 1.98 | 6 | 2 |
| 3:C:361:PX4:H10 | 3:C:361:PX4:O3 | 0.57 | 1.99 | 12 | 2 |
| 3:A:633:PX4:O2 | 3:A:638:PX4:H9 | 0.57 | 1.99 | 14 | 1 |
| 3:C:322:PX4:H4 | 3:C:325:PX4:O6 | 0.57 | 1.99 | 15 | 1 |
| 3:C:320:PX4:H9 | 3:C:341:PX4:O1 | 0.57 | 1.99 | 3 | 1 |
| 3:B:306:PX4:H13 | 3:B:348:PX4:O2 | 0.57 | 1.99 | 1 | 1 |
| 3:A:630:PX4:O1 | 3:A:630:PX4:H3 | 0.57 | 1.99 | 7 | 1 |
| 2:B:201:GLU:OE2 | 3:B:313:PX4:H6 | 0.57 | 2.00 | 6 | 1 |
| 3:A:613:PX4:O8 | 3:A:628:PX4:H6 | 0.57 | 1.99 | 13 | 1 |
| 3:C:313:PX4:H9 | 3:C:337:PX4:O2 | 0.57 | 2.00 | 15 | 1 |
| 2:B:120:GLU:OE2 | 3:B:311:PX4:H4 | 0.57 | 1.98 | 8 | 1 |
| 2:B:72:TRP:CD2 | 3:B:341:PX4:H13 | 0.57 | 2.34 | 12 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 3:C:347:PX4:O3 | 3:C:347:PX4:H13 | 0.57 | 2.00 | 14 | 1 |
| 3:A:609:PX4:H11 | 3:B:384:PX4:O2 | 0.57 | 1.99 | 7 | 4 |
| 3:A:623:PX4:O1 | 3:A:640:PX4:H3 | 0.57 | 1.99 | 15 | 2 |
| 3:B:374:PX4:O1 | 3:B:384:PX4:H6 | 0.57 | 2.00 | 5 | 1 |
| 3:B:301:PX4:O2 | 3:B:304:PX4:H3 | 0.57 | 2.00 | 1 | 1 |
| 3:A:604:PX4:O2 | 3:A:607:PX4:H9 | 0.57 | 2.00 | 10 | 1 |
| 3:A:607:PX4:O1 | 3:A:612:PX4:H12 | 0.56 | 2.00 | 3 | 1 |
| 3:A:633:PX4:H44 | 3:C:303:PX4:H71 | 0.56 | 1.77 | 7 | 1 |
| 3:B:306:PX4:O3 | 3:B:306:PX4:H7 | 0.56 | 1.99 | 13 | 2 |
| 3:C:352:PX4:O3 | 3:C:352:PX4:H6 | 0.56 | 1.98 | 4 | 1 |
| 3:A:610:PX4:H3 | 3:B:389:PX4:O2 | 0.56 | 2.01 | 11 | 2 |
| 3:B:335:PX4:H10 | 3:B:353:PX4:O1 | 0.56 | 2.01 | 7 | 1 |
| 3:C:339:PX4:H7 | 3:C:339:PX4:O1 | 0.56 | 2.00 | 7 | 1 |
| 3:A:618:PX4:O2 | 3:A:630:PX4:H10 | 0.56 | 2.01 | 5 | 1 |
| 3:A:626:PX4:H13 | 3:C:362:PX4:O4 | 0.56 | 1.99 | 11 | 2 |
| 3:B:316:PX4:H3 | 3:B:316:PX4:O1 | 0.56 | 2.01 | 11 | 2 |
| 3:A:605:PX4:O2 | 3:B:379:PX4:H12 | 0.56 | 2.00 | 1 | 1 |
| 3:A:604:PX4:H7 | 3:B:392:PX4:H2 | 0.56 | 1.77 | 2 | 1 |
| 3:B:375:PX4:H7 | 3:B:375:PX4:O3 | 0.56 | 2.00 | 2 | 3 |
| 3:B:390:PX4:H9 | 3:B:390:PX4:O1 | 0.56 | 1.99 | 8 | 1 |
| 2:B:142:GLU:OE2 | 3:B:328:PX4:H8 | 0.56 | 2.00 | 10 | 3 |
| 3:A:601:PX4:H12 | 3:A:601:PX4:O4 | 0.56 | 2.01 | 12 | 4 |
| 3:A:647:PX4:O3 | 3:A:647:PX4:H7 | 0.56 | 2.01 | 5 | 1 |
| 3:B:375:PX4:H9 | 3:B:375:PX4:O1 | 0.56 | 2.00 | 12 | 1 |
| 3:A:602:PX4:O4 | 3:A:602:PX4:H3 | 0.56 | 1.99 | 1 | 2 |
| 3:B:380:PX4:O8 | 3:B:387:PX4:H4 | 0.56 | 2.00 | 9 | 2 |
| 3:A:605:PX4:H13 | 3:B:379:PX4:O4 | 0.56 | 2.00 | 10 | 1 |
| 3:A:636:PX4:O2 | 3:A:645:PX4:H8 | 0.56 | 2.00 | 1 | 1 |
| 3:B:318:PX4:O3 | 3:B:318:PX4:H6 | 0.56 | 2.00 | 1 | 3 |
| 3:A:607:PX4:H3 | 3:B:392:PX4:O2 | 0.56 | 2.01 | 3 | 1 |
| 3:A:605:PX4:O3 | 3:B:379:PX4:H10 | 0.56 | 2.00 | 10 | 1 |
| 3:C:321:PX4:O1 | 3:C:350:PX4:H6 | 0.56 | 2.01 | 13 | 1 |
| 2:B:76:GLU:HB3 | 3:B:305:PX4:H13 | 0.56 | 1.77 | 6 | 1 |
| 2:B:130:TRP:CD1 | 2:C:177:HIS:CE1 | 0.56 | 2.93 | 6 | 2 |
| 3:A:608:PX4:H4 | 3:A:608:PX4:O4 | 0.56 | 2.01 | 11 | 1 |
| 3:B:323:PX4:H4 | 3:B:323:PX4:O2 | 0.56 | 1.99 | 15 | 1 |
| 3:A:624:PX4:H34 | 3:A:639:PX4:H48 | 0.56 | 1.76 | 3 | 1 |
| 3:B:363:PX4:O3 | 3:B:363:PX4:H12 | 0.55 | 2.01 | 4 | 2 |
| 3:A:633:PX4:H12 | 3:A:633:PX4:O1 | 0.55 | 2.02 | 13 | 1 |
| 1:A:443:ARG:CD | 3:A:651:PX4:H7 | 0.55 | 2.31 | 14 | 1 |
| 3:C:305:PX4:O4 | 3:C:311:PX4:H3 | 0.55 | 2.01 | 6 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 2:B:184:HIS:CD2 | 2:C:126:PHE:CD2 | 0.55 | 2.94 | 3 | 1 |
| 3:B:323:PX4:O3 | 3:B:323:PX4:H13 | 0.55 | 2.01 | 11 | 2 |
| 3:B:364:PX4:H3 | 3:C:301:PX4:O2 | 0.55 | 2.01 | 5 | 2 |
| 3:B:304:PX4:O2 | 3:B:345:PX4:H12 | 0.55 | 2.02 | 9 | 1 |
| 3:B:307:PX4:H7 | 3:B:318:PX4:O1 | 0.55 | 2.01 | 9 | 1 |
| 3:A:620:PX4:H1 | 3:A:636:PX4:H11 | 0.55 | 1.77 | 11 | 1 |
| 3:B:305:PX4:H32 | 3:B:356:PX4:H43 | 0.55 | 1.78 | 12 | 1 |
| 3:B:374:PX4:O4 | 3:B:384:PX4:H3 | 0.55 | 2.02 | 1 | 5 |
| 3:A:604:PX4:H4 | 3:B:376:PX4:O2 | 0.55 | 2.01 | 4 | 3 |
| 3:B:387:PX4:O1 | 3:B:390:PX4:H6 | 0.55 | 2.02 | 5 | 2 |
| 3:B:316:PX4:H5 | 3:B:321:PX4:O4 | 0.55 | 2.01 | 6 | 1 |
| 3:B:396:PX4:O2 | 3:B:396:PX4:H3 | 0.55 | 2.02 | 13 | 1 |
| 3:C:321:PX4:H4 | 3:C:321:PX4:O2 | 0.55 | 2.01 | 1 | 1 |
| 3:B:353:PX4:O3 | 3:B:353:PX4:H13 | 0.55 | 2.01 | 9 | 1 |
| 3:A:626:PX4:O1 | 3:A:626:PX4:H4 | 0.55 | 2.02 | 10 | 1 |
| 3:B:301:PX4:O3 | 3:B:301:PX4:H13 | 0.55 | 2.01 | 10 | 1 |
| 3:A:617:PX4:H5 | 3:A:625:PX4:O1 | 0.55 | 2.02 | 1 | 1 |
| 3:A:613:PX4:O2 | 3:A:628:PX4:H4 | 0.55 | 2.01 | 5 | 2 |
| 3:C:358:PX4:H14 | 3:C:361:PX4:H7 | 0.55 | 1.79 | 6 | 1 |
| 3:A:632:PX4:H7 | 3:A:647:PX4:O2 | 0.55 | 2.02 | 11 | 1 |
| 3:A:645:PX4:O1 | 3:A:648:PX4:H9 | 0.55 | 2.02 | 3 | 1 |
| 3:B:306:PX4:H12 | 3:B:348:PX4:O4 | 0.55 | 2.02 | 13 | 1 |
| 3:B:301:PX4:O1 | 3:B:303:PX4:H10 | 0.55 | 2.02 | 6 | 1 |
| 3:C:315:PX4:H7 | 3:C:315:PX4:O3 | 0.55 | 2.02 | 13 | 4 |
| 3:B:374:PX4:C6 | 3:B:384:PX4:H3 | 0.55 | 2.32 | 9 | 1 |
| 3:C:360:PX4:O2 | 3:C:360:PX4:H12 | 0.55 | 2.01 | 5 | 2 |
| 3:A:645:PX4:O1 | 3:A:653:PX4:H5 | 0.55 | 2.02 | 6 | 1 |
| 3:B:345:PX4:O8 | 3:B:369:PX4:H7 | 0.55 | 2.02 | 6 | 1 |
| 3:B:306:PX4:H4 | 3:B:339:PX4:O1 | 0.55 | 2.02 | 10 | 3 |
| 3:B:393:PX4:H10 | 3:B:393:PX4:O3 | 0.55 | 2.02 | 12 | 3 |
| 3:B:364:PX4:H13 | 3:C:301:PX4:O2 | 0.55 | 2.02 | 2 | 2 |
| 3:A:605:PX4:H3 | 3:B:379:PX4:O4 | 0.55 | 2.02 | 12 | 1 |
| 3:C:314:PX4:O2 | 3:C:314:PX4:H4 | 0.55 | 2.01 | 12 | 2 |
| 3:C:349:PX4:O8 | 3:C:349:PX4:H4 | 0.55 | 2.01 | 12 | 1 |
| 3:B:363:PX4:H4 | 3:B:381:PX4:O1 | 0.55 | 2.01 | 15 | 1 |
| 3:A:644:PX4:H12 | 3:A:650:PX4:H13 | 0.54 | 1.78 | 1 | 1 |
| 3:A:624:PX4:O1 | 3:A:639:PX4:H7 | 0.54 | 2.02 | 5 | 1 |
| 3:B:334:PX4:H7 | 3:B:352:PX4:O1 | 0.54 | 2.02 | 6 | 1 |
| 3:B:395:PX4:H3 | 3:C:358:PX4:O2 | 0.54 | 2.02 | 14 | 2 |
| 3:A:621:PX4:O3 | 3:A:621:PX4:H12 | 0.54 | 2.02 | 12 | 2 |
| 3:C:349:PX4:O8 | 3:C:349:PX4:H10 | 0.54 | 2.02 | 12 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 3:B:310:PX4:O8 | 3:B:358:PX4:H5 | 0.54 | 2.02 | 2 | 1 |
| 3:B:343:PX4:O4 | 3:B:343:PX4:H4 | 0.54 | 2.01 | 6 | 1 |
| 3:B:392:PX4:O1 | 3:B:394:PX4:H12 | 0.54 | 2.03 | 7 | 1 |
| 3:B:346:PX4:O4 | 3:B:346:PX4:H4 | 0.54 | 2.02 | 12 | 2 |
| 3:B:397:PX4:H9 | 3:C:312:PX4:O2 | 0.54 | 2.01 | 15 | 1 |
| 3:B:338:PX4:H10 | 3:B:338:PX4:O2 | 0.54 | 2.02 | 7 | 1 |
| 3:A:616:PX4:O2 | 3:A:634:PX4:H11 | 0.54 | 2.02 | 14 | 3 |
| 3:C:358:PX4:H10 | 3:C:358:PX4:O4 | 0.54 | 2.03 | 7 | 2 |
| 3:C:340:PX4:H4 | 3:C:360:PX4:H12 | 0.54 | 1.78 | 8 | 1 |
| 3:A:622:PX4:H10 | 3:A:622:PX4:O4 | 0.54 | 2.02 | 10 | 1 |
| 3:A:642:PX4:O1 | 3:A:651:PX4:H5 | 0.54 | 2.02 | 10 | 1 |
| 3:B:363:PX4:H8 | 3:B:381:PX4:O4 | 0.54 | 2.01 | 10 | 1 |
| 3:B:399:PX4:O4 | 3:B:399:PX4:H12 | 0.54 | 2.02 | 11 | 1 |
| 3:B:399:PX4:H13 | 3:C:357:PX4:O3 | 0.54 | 2.03 | 13 | 1 |
| 3:C:312:PX4:H7 | 3:C:312:PX4:H15 | 0.54 | 1.80 | 5 | 1 |
| 3:B:342:PX4:H4 | 3:B:342:PX4:O2 | 0.54 | 2.03 | 6 | 1 |
| 3:A:602:PX4:H6 | 3:B:372:PX4:O1 | 0.54 | 2.02 | 13 | 1 |
| 2:B:76:GLU:OE1 | 3:B:305:PX4:H9 | 0.54 | 2.03 | 8 | 1 |
| 3:B:369:PX4:O6 | 3:B:386:PX4:H13 | 0.54 | 2.02 | 5 | 1 |
| 3:B:379:PX4:H9 | 3:B:379:PX4:O3 | 0.54 | 2.03 | 5 | 2 |
| 3:B:380:PX4:H15 | 3:B:380:PX4:H3 | 0.54 | 1.79 | 15 | 1 |
| 3:A:649:PX4:O3 | 3:A:649:PX4:H13 | 0.54 | 2.02 | 2 | 2 |
| 3:B:311:PX4:O4 | 3:B:311:PX4:H4 | 0.54 | 2.01 | 4 | 2 |
| 3:B:380:PX4:O8 | 3:B:387:PX4:H10 | 0.54 | 2.03 | 10 | 3 |
| 3:B:369:PX4:O1 | 3:B:386:PX4:H7 | 0.54 | 2.03 | 11 | 1 |
| 3:A:618:PX4:H3 | 3:A:620:PX4:O1 | 0.54 | 2.02 | 5 | 3 |
| 3:A:649:PX4:O7 | 3:A:652:PX4:H7 | 0.54 | 2.03 | 5 | 1 |
| 3:B:400:PX4:O8 | 3:B:400:PX4:H7 | 0.54 | 2.02 | 6 | 1 |
| 3:B:329:PX4:O4 | 3:B:355:PX4:H3 | 0.54 | 2.03 | 12 | 2 |
| 3:B:342:PX4:O2 | 3:B:367:PX4:H3 | 0.54 | 2.02 | 13 | 1 |
| 3:B:356:PX4:H4 | 3:B:373:PX4:O1 | 0.54 | 2.03 | 14 | 1 |
| 3:A:649:PX4:O4 | 3:A:652:PX4:H8 | 0.54 | 2.02 | 1 | 1 |
| 3:C:307:PX4:O6 | 3:C:310:PX4:H8 | 0.54 | 2.03 | 1 | 2 |
| 3:B:307:PX4:O1 | 3:B:307:PX4:H3 | 0.54 | 2.03 | 4 | 2 |
| 2:C:91:GLU:OE1 | 3:C:314:PX4:H5 | 0.54 | 2.03 | 5 | 1 |
| 3:C:327:PX4:H5 | 3:C:334:PX4:O1 | 0.54 | 2.03 | 8 | 1 |
| 3:A:630:PX4:O8 | 3:A:648:PX4:H7 | 0.53 | 2.02 | 2 | 1 |
| 1:A:443:ARG:HD2 | 3:A:651:PX4:H6 | 0.53 | 1.80 | 1 | 1 |
| 3:C:352:PX4:H3 | 3:C:352:PX4:O1 | 0.53 | 2.03 | 6 | 1 |
| 2:B:72:TRP:CE2 | 3:B:341:PX4:H6 | 0.53 | 2.38 | 9 | 2 |
| 3:B:342:PX4:O4 | 3:B:350:PX4:H6 | 0.53 | 2.04 | 9 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 3:C:325:PX4:O3 | 3:C:325:PX4:H9 | 0.53 | 2.03 | 11 | 2 |
| 3:B:382:PX4:H13 | 3:B:382:PX4:C6 | 0.53 | 2.33 | 11 | 1 |
| 3:A:605:PX4:H6 | 3:B:379:PX4:O2 | 0.53 | 2.02 | 11 | 3 |
| 3:A:602:PX4:O1 | 3:B:375:PX4:H4 | 0.53 | 2.03 | 12 | 1 |
| 3:C:303:PX4:H10 | 3:C:303:PX4:O2 | 0.53 | 2.03 | 12 | 1 |
| 3:C:364:PX4:H3 | 3:C:364:PX4:O2 | 0.53 | 2.03 | 4 | 1 |
| 3:A:617:PX4:H3 | 3:A:617:PX4:O4 | 0.53 | 2.03 | 7 | 1 |
| 3:A:652:PX4:O2 | 3:A:652:PX4:H12 | 0.53 | 2.04 | 7 | 1 |
| 3:A:653:PX4:O4 | 3:A:653:PX4:H3 | 0.53 | 2.03 | 10 | 1 |
| 3:C:328:PX4:H3 | 3:C:337:PX4:O1 | 0.53 | 2.03 | 15 | 1 |
| 3:B:370:PX4:H4 | 3:B:370:PX4:O2 | 0.53 | 2.03 | 10 | 3 |
| 3:B:392:PX4:O3 | 3:B:392:PX4:H12 | 0.53 | 2.03 | 4 | 4 |
| 3:C:323:PX4:H4 | 3:C:323:PX4:C6 | 0.53 | 2.34 | 4 | 1 |
| 1:A:405:GLU:O | 3:A:641:PX4:H6 | 0.53 | 2.03 | 5 | 1 |
| 3:C:358:PX4:O8 | 3:C:361:PX4:H4 | 0.53 | 2.04 | 8 | 1 |
| 3:C:358:PX4:O1 | 3:C:361:PX4:H4 | 0.53 | 2.03 | 10 | 1 |
| 3:C:320:PX4:H3 | 3:C:330:PX4:O8 | 0.53 | 2.04 | 15 | 2 |
| 3:B:345:PX4:O4 | 3:B:345:PX4:H4 | 0.53 | 2.03 | 1 | 1 |
| 3:C:313:PX4:H3 | 3:C:313:PX4:O1 | 0.53 | 2.03 | 9 | 2 |
| 3:A:620:PX4:O3 | 3:A:620:PX4:H6 | 0.53 | 2.03 | 3 | 1 |
| 3:C:357:PX4:O1 | 3:C:357:PX4:H3 | 0.53 | 2.02 | 14 | 1 |
| 3:B:376:PX4:O1 | 3:B:390:PX4:H9 | 0.53 | 2.03 | 5 | 1 |
| 3:C:306:PX4:H12 | 3:C:306:PX4:O2 | 0.53 | 2.04 | 5 | 1 |
| 3:B:333:PX4:O1 | 3:B:361:PX4:H10 | 0.53 | 2.04 | 6 | 1 |
| 3:A:616:PX4:H4 | 3:A:616:PX4:O2 | 0.53 | 2.04 | 12 | 1 |
| 3:C:344:PX4:H7 | 3:C:364:PX4:O1 | 0.53 | 2.04 | 14 | 1 |
| 3:B:304:PX4:O1 | 3:B:304:PX4:H3 | 0.53 | 2.03 | 2 | 2 |
| 3:C:318:PX4:H5 | 3:C:321:PX4:O4 | 0.53 | 2.03 | 4 | 3 |
| 3:B:301:PX4:H4 | 3:B:303:PX4:O3 | 0.53 | 2.04 | 3 | 2 |
| 3:A:643:PX4:H12 | 3:A:643:PX4:O1 | 0.53 | 2.04 | 12 | 2 |
| 3:A:623:PX4:H3 | 3:B:398:PX4:O1 | 0.53 | 2.03 | 14 | 1 |
| 3:B:381:PX4:H4 | 3:B:381:PX4:O2 | 0.53 | 2.04 | 14 | 1 |
| 3:C:333:PX4:O4 | 3:C:333:PX4:H3 | 0.53 | 2.03 | 3 | 2 |
| 3:B:398:PX4:O2 | 3:B:398:PX4:H4 | 0.52 | 2.02 | 5 | 1 |
| 3:A:611:PX4:O4 | 3:A:611:PX4:H6 | 0.52 | 2.04 | 7 | 1 |
| 3:A:602:PX4:O2 | 3:A:604:PX4:H9 | 0.52 | 2.04 | 9 | 1 |
| 3:A:606:PX4:H3 | 3:B:383:PX4:O2 | 0.52 | 2.04 | 9 | 1 |
| 3:A:630:PX4:O3 | 3:A:648:PX4:H7 | 0.52 | 2.04 | 12 | 1 |
| 3:B:373:PX4:H3 | 3:B:380:PX4:O2 | 0.52 | 2.03 | 12 | 1 |
| 3:C:347:PX4:O2 | 3:C:347:PX4:H4 | 0.52 | 2.04 | 12 | 2 |
| 3:B:351:PX4:H7 | 3:B:354:PX4:O3 | 0.52 | 2.03 | 13 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 3:C:325:PX4:O1 | 3:C:325:PX4:H3 | 0.52 | 2.04 | 2 | 1 |
| 3:B:392:PX4:O6 | 3:B:392:PX4:H6 | 0.52 | 2.04 | 4 | 1 |
| 3:B:320:PX4:H6 | 3:B:340:PX4:O2 | 0.52 | 2.04 | 5 | 1 |
| 3:B:329:PX4:O3 | 3:B:355:PX4:H5 | 0.52 | 2.04 | 6 | 1 |
| 3:B:334:PX4:H12 | 3:B:334:PX4:O1 | 0.52 | 2.05 | 6 | 1 |
| 3:B:338:PX4:O2 | 3:B:358:PX4:H6 | 0.52 | 2.04 | 6 | 1 |
| 3:B:342:PX4:O2 | 3:B:350:PX4:H4 | 0.52 | 2.03 | 8 | 3 |
| 3:C:339:PX4:O1 | 3:C:339:PX4:H9 | 0.52 | 2.03 | 9 | 1 |
| 3:A:614:PX4:H4 | 3:A:628:PX4:O2 | 0.52 | 2.05 | 11 | 1 |
| 2:B:229:ALA:HB2 | 3:B:332:PX4:H61 | 0.52 | 1.80 | 11 | 1 |
| 3:A:636:PX4:O3 | 3:A:645:PX4:H5 | 0.52 | 2.04 | 1 | 1 |
| 3:A:646:PX4:H8 | 3:A:653:PX4:O2 | 0.52 | 2.05 | 1 | 1 |
| 3:B:396:PX4:O3 | 3:B:396:PX4:H6 | 0.52 | 2.03 | 4 | 1 |
| 3:B:356:PX4:H7 | 3:B:356:PX4:O3 | 0.52 | 2.05 | 13 | 1 |
| 3:B:332:PX4:O1 | 3:B:332:PX4:H3 | 0.52 | 2.04 | 12 | 2 |
| 3:B:352:PX4:O1 | 3:B:352:PX4:H3 | 0.52 | 2.05 | 6 | 1 |
| 3:A:644:PX4:O2 | 3:A:650:PX4:H3 | 0.52 | 2.04 | 7 | 1 |
| 3:B:353:PX4:H11 | 3:B:382:PX4:O2 | 0.52 | 2.04 | 10 | 1 |
| 3:B:400:PX4:H10 | 3:B:400:PX4:O8 | 0.52 | 2.05 | 10 | 1 |
| 3:A:648:PX4:H10 | 3:A:648:PX4:O4 | 0.52 | 2.05 | 11 | 1 |
| 3:B:312:PX4:O3 | 3:B:317:PX4:H13 | 0.52 | 2.04 | 12 | 1 |
| 3:C:312:PX4:O3 | 3:C:312:PX4:C3 | 0.52 | 2.58 | 14 | 1 |
| 3:C:313:PX4:O1 | 3:C:328:PX4:H11 | 0.52 | 2.04 | 15 | 2 |
| 3:C:346:PX4:H5 | 3:C:362:PX4:O1 | 0.52 | 2.04 | 1 | 1 |
| 3:A:611:PX4:O1 | 3:A:611:PX4:H13 | 0.52 | 2.05 | 2 | 2 |
| 3:A:614:PX4:H7 | 3:C:336:PX4:O1 | 0.52 | 2.05 | 2 | 1 |
| 3:A:625:PX4:H3 | 3:A:625:PX4:C6 | 0.52 | 2.35 | 13 | 2 |
| 3:B:378:PX4:O2 | 3:C:302:PX4:H12 | 0.52 | 2.05 | 4 | 1 |
| 3:A:642:PX4:O2 | 3:A:651:PX4:H8 | 0.52 | 2.05 | 5 | 1 |
| 2:B:80:GLU:OE1 | 3:B:305:PX4:H7 | 0.52 | 2.04 | 5 | 1 |
| 3:A:612:PX4:O2 | 3:A:612:PX4:H7 | 0.52 | 2.03 | 6 | 1 |
| 3:C:332:PX4:H6 | 3:C:335:PX4:O3 | 0.52 | 2.05 | 7 | 1 |
| 3:C:351:PX4:O2 | 3:C:359:PX4:H4 | 0.52 | 2.04 | 9 | 1 |
| 3:B:306:PX4:O1 | 3:B:306:PX4:H9 | 0.52 | 2.04 | 10 | 1 |
| 3:C:323:PX4:O2 | 3:C:342:PX4:H12 | 0.52 | 2.04 | 10 | 1 |
| 3:B:399:PX4:O2 | 3:C:326:PX4:H13 | 0.52 | 2.04 | 14 | 1 |
| 3:B:321:PX4:O2 | 3:B:321:PX4:H4 | 0.52 | 2.05 | 15 | 1 |
| 2:B:55:SER:N | 2:B:58:SER:HG | 0.52 | 2.02 | 2 | 3 |
| 3:A:614:PX4:H9 | 3:C:336:PX4:O2 | 0.52 | 2.05 | 4 | 1 |
| 3:B:311:PX4:H71 | 3:C:309:PX4:H44 | 0.52 | 1.81 | 4 | 1 |
| 3:C:328:PX4:O4 | 3:C:356:PX4:H3 | 0.52 | 2.05 | 6 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 3:A:624:PX4:O3 | 3:A:624:PX4:H9 | 0.52 | 2.04 | 10 | 1 |
| 3:A:631:PX4:O1 | 3:A:631:PX4:H9 | 0.52 | 2.04 | 12 | 1 |
| 3:A:611:PX4:P1 | 3:A:611:PX4:H13 | 0.52 | 2.45 | 13 | 1 |
| 3:A:651:PX4:O1 | 3:A:651:PX4:H4 | 0.52 | 2.05 | 13 | 1 |
| 3:B:363:PX4:H11 | 3:B:381:PX4:O4 | 0.52 | 2.05 | 5 | 2 |
| 3:B:339:PX4:H3 | 3:B:339:PX4:O1 | 0.52 | 2.04 | 5 | 1 |
| 3:C:328:PX4:O4 | 3:C:356:PX4:H6 | 0.52 | 2.05 | 5 | 1 |
| 3:A:636:PX4:O2 | 3:A:636:PX4:H7 | 0.52 | 2.05 | 6 | 2 |
| 3:B:380:PX4:O1 | 3:B:380:PX4:H3 | 0.52 | 2.05 | 6 | 1 |
| 3:A:644:PX4:H3 | 3:A:650:PX4:O2 | 0.52 | 2.04 | 14 | 2 |
| 3:B:399:PX4:O1 | 3:C:326:PX4:H13 | 0.52 | 2.05 | 8 | 1 |
| 3:A:607:PX4:P1 | 3:A:612:PX4:H3 | 0.52 | 2.44 | 9 | 1 |
| 3:B:320:PX4:O4 | 3:B:320:PX4:H3 | 0.52 | 2.05 | 11 | 1 |
| 3:A:629:PX4:O2 | 3:A:629:PX4:H4 | 0.52 | 2.03 | 12 | 1 |
| 3:A:613:PX4:O2 | 3:A:628:PX4:H6 | 0.52 | 2.05 | 14 | 1 |
| 3:B:356:PX4:H3 | 3:B:373:PX4:O2 | 0.52 | 2.05 | 15 | 1 |
| 3:B:366:PX4:H13 | 3:B:383:PX4:O1 | 0.52 | 2.05 | 3 | 1 |
| 3:B:319:PX4:O1 | 3:B:319:PX4:H3 | 0.52 | 2.04 | 10 | 2 |
| 3:A:614:PX4:O1 | 3:A:625:PX4:H4 | 0.52 | 2.04 | 6 | 3 |
| 3:C:338:PX4:O2 | 3:C:345:PX4:H9 | 0.52 | 2.05 | 11 | 1 |
| 3:B:359:PX4:O2 | 3:B:373:PX4:H13 | 0.52 | 2.04 | 14 | 1 |
| 3:B:374:PX4:O1 | 3:B:384:PX4:H11 | 0.52 | 2.05 | 14 | 1 |
| 3:B:382:PX4:H5 | 3:B:391:PX4:O1 | 0.52 | 2.04 | 15 | 1 |
| 3:B:392:PX4:O1 | 3:B:394:PX4:H10 | 0.52 | 2.05 | 10 | 1 |
| 3:A:629:PX4:O6 | 3:A:631:PX4:H12 | 0.52 | 2.05 | 9 | 3 |
| 3:B:312:PX4:H5 | 3:B:356:PX4:O1 | 0.52 | 2.05 | 3 | 1 |
| 3:A:635:PX4:O6 | 3:A:637:PX4:H8 | 0.52 | 2.05 | 5 | 1 |
| 3:B:361:PX4:H3 | 3:B:368:PX4:O1 | 0.52 | 2.04 | 7 | 1 |
| 3:C:348:PX4:O2 | 3:C:348:PX4:H10 | 0.52 | 2.04 | 8 | 1 |
| 3:C:350:PX4:O2 | 3:C:355:PX4:H4 | 0.51 | 2.04 | 1 | 1 |
| 3:B:369:PX4:O1 | 3:B:369:PX4:H13 | 0.51 | 2.06 | 9 | 2 |
| 3:B:328:PX4:H4 | 3:B:328:PX4:O2 | 0.51 | 2.04 | 11 | 1 |
| 3:B:346:PX4:H4 | 3:B:346:PX4:O2 | 0.51 | 2.05 | 13 | 1 |
| 3:C:313:PX4:H7 | 3:C:337:PX4:O3 | 0.51 | 2.05 | 14 | 1 |
| 3:B:360:PX4:O3 | 3:B:360:PX4:H9 | 0.51 | 2.06 | 1 | 2 |
| 3:B:347:PX4:O1 | 3:B:347:PX4:H3 | 0.51 | 2.06 | 13 | 2 |
| 3:C:312:PX4:H3 | 3:C:312:PX4:C6 | 0.51 | 2.36 | 4 | 1 |
| 3:B:363:PX4:H5 | 3:C:302:PX4:O2 | 0.51 | 2.05 | 14 | 1 |
| 3:B:369:PX4:H11 | 3:B:370:PX4:O6 | 0.51 | 2.05 | 14 | 1 |
| 3:A:613:PX4:O1 | 3:A:628:PX4:H4 | 0.51 | 2.05 | 1 | 1 |
| 3:B:390:PX4:H7 | 3:B:390:PX4:O3 | 0.51 | 2.05 | 3 | 4 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 3:B:370:PX4:O2 | 3:B:378:PX4:H5 | 0.51 | 2.06 | 15 | 1 |
| 3:C:327:PX4:H9 | 3:C:327:PX4:O2 | 0.51 | 2.05 | 8 | 2 |
| 3:A:606:PX4:H6 | 3:B:383:PX4:O3 | 0.51 | 2.06 | 9 | 1 |
| 3:A:618:PX4:H13 | 3:A:620:PX4:O3 | 0.51 | 2.05 | 2 | 1 |
| 3:C:351:PX4:O3 | 3:C:351:PX4:H13 | 0.51 | 2.06 | 6 | 4 |
| 3:B:367:PX4:H10 | 3:B:367:PX4:O3 | 0.51 | 2.06 | 6 | 3 |
| 3:A:644:PX4:H4 | 3:A:644:PX4:O2 | 0.51 | 2.05 | 11 | 2 |
| 3:A:614:PX4:H5 | 3:C:350:PX4:O2 | 0.51 | 2.05 | 14 | 1 |
| 3:A:621:PX4:O4 | 3:A:621:PX4:H6 | 0.51 | 2.05 | 2 | 1 |
| 3:C:302:PX4:H9 | 3:C:302:PX4:O1 | 0.51 | 2.05 | 2 | 1 |
| 3:A:627:PX4:O1 | 3:A:643:PX4:H13 | 0.51 | 2.04 | 4 | 1 |
| 3:B:341:PX4:O1 | 3:B:341:PX4:H3 | 0.51 | 2.05 | 7 | 1 |
| 3:C:342:PX4:O1 | 3:C:342:PX4:H3 | 0.51 | 2.06 | 13 | 1 |
| 3:A:610:PX4:O1 | 3:A:610:PX4:H3 | 0.51 | 2.05 | 15 | 2 |
| 2:C:173:ARG:HH11 | 2:C:177:HIS:CE1 | 0.51 | 2.24 | 14 | 1 |
| 3:A:611:PX4:C22 | 3:B:394:PX4:H44 | 0.51 | 2.36 | 10 | 1 |
| 3:A:623:PX4:H3 | 3:B:398:PX4:O8 | 0.51 | 2.05 | 11 | 1 |
| 3:B:312:PX4:H9 | 3:B:356:PX4:O1 | 0.51 | 2.05 | 2 | 1 |
| 3:C:358:PX4:O6 | 3:C:358:PX4:H8 | 0.51 | 2.06 | 2 | 2 |
| 3:B:355:PX4:O4 | 3:B:355:PX4:H4 | 0.51 | 2.06 | 8 | 1 |
| 3:A:618:PX4:O2 | 3:A:618:PX4:H4 | 0.51 | 2.05 | 10 | 1 |
| 3:B:369:PX4:O3 | 3:B:369:PX4:H13 | 0.51 | 2.06 | 14 | 1 |
| 3:C:353:PX4:O3 | 3:C:353:PX4:H12 | 0.51 | 2.06 | 6 | 1 |
| 3:B:354:PX4:O6 | 3:B:354:PX4:H12 | 0.51 | 2.06 | 7 | 1 |
| 2:B:72:TRP:NE1 | 3:B:341:PX4:H4 | 0.51 | 2.21 | 10 | 1 |
| 3:C:359:PX4:H3 | 3:C:359:PX4:O6 | 0.51 | 2.06 | 8 | 1 |
| 3:B:356:PX4:H43 | 3:C:333:PX4:H66 | 0.51 | 1.83 | 9 | 1 |
| 3:C:352:PX4:O3 | 3:C:352:PX4:H12 | 0.51 | 2.06 | 11 | 1 |
| 3:C:301:PX4:O3 | 3:C:301:PX4:H13 | 0.50 | 2.06 | 2 | 1 |
| 3:B:307:PX4:H4 | 3:B:318:PX4:O2 | 0.50 | 2.06 | 8 | 2 |
| 3:A:626:PX4:H6 | 3:C:362:PX4:O2 | 0.50 | 2.06 | 12 | 1 |
| 3:B:373:PX4:H3 | 3:B:380:PX4:O3 | 0.50 | 2.05 | 14 | 1 |
| 3:C:305:PX4:O1 | 3:C:324:PX4:H7 | 0.50 | 2.07 | 3 | 1 |
| 3:A:604:PX4:H3 | 3:B:392:PX4:O2 | 0.50 | 2.06 | 5 | 1 |
| 3:A:643:PX4:O3 | 3:A:643:PX4:H10 | 0.50 | 2.06 | 15 | 2 |
| 3:C:315:PX4:O3 | 3:C:348:PX4:H5 | 0.50 | 2.06 | 6 | 1 |
| 3:B:322:PX4:H4 | 3:B:322:PX4:O2 | 0.50 | 2.05 | 12 | 1 |
| 3:B:351:PX4:H7 | 3:B:354:PX4:H1 | 0.50 | 1.83 | 14 | 1 |
| 3:B:388:PX4:H9 | 3:B:388:PX4:O3 | 0.50 | 2.06 | 15 | 1 |
| 1:A:360:PHE:O | 3:A:644:PX4:H10 | 0.50 | 2.06 | 4 | 2 |
| 3:B:310:PX4:H9 | 3:B:310:PX4:O3 | 0.50 | 2.06 | 8 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:405:GLU:OE2 | 3:A:641:PX4:H4 | 0.50 | 2.06 | 8 | 2 |
| 3:C:338:PX4:O2 | 3:C:345:PX4:H7 | 0.50 | 2.06 | 15 | 2 |
| 3:B:400:PX4:H11 | 3:C:363:PX4:H14 | 0.50 | 1.83 | 13 | 1 |
| 3:A:645:PX4:H4 | 3:A:645:PX4:O2 | 0.50 | 2.06 | 10 | 3 |
| 3:B:308:PX4:O3 | 3:B:308:PX4:H13 | 0.50 | 2.07 | 15 | 2 |
| 1:A:358:GLY:O | 3:A:650:PX4:H4 | 0.50 | 2.06 | 15 | 1 |
| 3:A:623:PX4:H7 | 3:B:398:PX4:O1 | 0.50 | 2.06 | 15 | 1 |
| 3:A:650:PX4:O8 | 3:A:654:PX4:H11 | 0.50 | 2.07 | 2 | 1 |
| 3:B:322:PX4:O2 | 3:B:350:PX4:H11 | 0.50 | 2.07 | 4 | 2 |
| 3:A:602:PX4:O1 | 3:B:375:PX4:H3 | 0.50 | 2.07 | 13 | 1 |
| 3:B:338:PX4:H12 | 3:B:338:PX4:O3 | 0.50 | 2.07 | 4 | 3 |
| 3:B:354:PX4:H6 | 3:B:354:PX4:O6 | 0.50 | 2.07 | 2 | 1 |
| 3:A:651:PX4:O3 | 3:A:651:PX4:H7 | 0.50 | 2.07 | 3 | 3 |
| 2:B:177:HIS:CE1 | 2:C:133:GLU:OE1 | 0.50 | 2.65 | 6 | 1 |
| 3:B:359:PX4:O2 | 3:B:373:PX4:H11 | 0.50 | 2.06 | 8 | 1 |
| 3:B:309:PX4:H9 | 3:B:336:PX4:O1 | 0.50 | 2.06 | 9 | 1 |
| 3:C:304:PX4:H9 | 3:C:304:PX4:O3 | 0.50 | 2.07 | 9 | 2 |
| 3:A:654:PX4:O3 | 3:A:654:PX4:H6 | 0.50 | 2.06 | 11 | 1 |
| 3:B:351:PX4:H4 | 3:B:354:PX4:O2 | 0.50 | 2.07 | 11 | 1 |
| 3:C:331:PX4:H7 | 3:C:331:PX4:O3 | 0.50 | 2.07 | 3 | 1 |
| 3:A:615:PX4:H5 | 3:C:360:PX4:O8 | 0.50 | 2.07 | 4 | 1 |
| 3:A:654:PX4:O2 | 3:A:654:PX4:H3 | 0.50 | 2.07 | 7 | 2 |
| 3:C:344:PX4:H3 | 3:C:364:PX4:O8 | 0.50 | 2.06 | 7 | 1 |
| 3:B:359:PX4:O2 | 3:B:359:PX4:H4 | 0.50 | 2.06 | 9 | 1 |
| 3:C:320:PX4:H4 | 3:C:341:PX4:O4 | 0.50 | 2.06 | 10 | 1 |
| 3:B:337:PX4:O2 | 3:B:337:PX4:H13 | 0.50 | 2.06 | 13 | 2 |
| 3:A:616:PX4:O1 | 3:A:634:PX4:H5 | 0.50 | 2.07 | 14 | 2 |
| 3:B:334:PX4:H4 | 3:B:352:PX4:O2 | 0.50 | 2.07 | 13 | 1 |
| 3:B:306:PX4:H4 | 3:B:348:PX4:O1 | 0.50 | 2.06 | 1 | 1 |
| 3:C:354:PX4:O3 | 3:C:354:PX4:H10 | 0.50 | 2.07 | 4 | 1 |
| 3:C:320:PX4:H3 | 3:C:341:PX4:O1 | 0.50 | 2.07 | 6 | 1 |
| 1:A:484:TRP:CE2 | 1:A:498:PRO:HB3 | 0.50 | 2.41 | 7 | 2 |
| 2:B:205:GLU:OE1 | 3:B:321:PX4:H4 | 0.50 | 2.06 | 7 | 2 |
| 3:A:646:PX4:O2 | 3:A:646:PX4:H3 | 0.50 | 2.06 | 8 | 1 |
| 3:A:646:PX4:O1 | 3:A:646:PX4:H3 | 0.50 | 2.07 | 15 | 2 |
| 2:B:72:TRP:CG | 3:B:341:PX4:H13 | 0.50 | 2.42 | 12 | 1 |
| 3:B:315:PX4:H9 | 3:B:336:PX4:O6 | 0.50 | 2.07 | 2 | 1 |
| 3:C:349:PX4:O2 | 3:C:349:PX4:H4 | 0.50 | 2.06 | 7 | 2 |
| 1:A:398:GLY:O | 3:A:652:PX4:H6 | 0.50 | 2.07 | 13 | 2 |
| 2:B:263:ASN:OD1 | 3:B:331:PX4:H10 | 0.50 | 2.07 | 7 | 1 |
| 3:B:302:PX4:H72 | 3:C:306:PX4:H70 | 0.50 | 1.83 | 9 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 3:B:321:PX4:H3 | 3:B:321:PX4:O2 | 0.50 | 2.05 | 9 | 1 |
| 3:C:305:PX4:O4 | 3:C:311:PX4:H10 | 0.50 | 2.06 | 9 | 1 |
| 3:C:335:PX4:H6 | 3:C:335:PX4:O3 | 0.50 | 2.07 | 9 | 1 |
| 3:B:334:PX4:O2 | 3:B:348:PX4:H12 | 0.50 | 2.07 | 15 | 2 |
| 3:B:338:PX4:O1 | 3:B:338:PX4:H12 | 0.50 | 2.07 | 14 | 1 |
| 3:A:626:PX4:H13 | 3:C:362:PX4:C1 | 0.49 | 2.36 | 2 | 1 |
| 3:B:313:PX4:O3 | 3:B:313:PX4:H9 | 0.49 | 2.07 | 5 | 2 |
| 3:B:397:PX4:O3 | 3:B:397:PX4:H9 | 0.49 | 2.07 | 6 | 1 |
| 3:C:330:PX4:O3 | 3:C:330:PX4:H9 | 0.49 | 2.07 | 7 | 3 |
| 3:B:384:PX4:O2 | 3:B:384:PX4:H4 | 0.49 | 2.07 | 13 | 3 |
| 3:A:619:PX4:O3 | 3:A:619:PX4:H12 | 0.49 | 2.06 | 11 | 1 |
| 3:A:634:PX4:H6 | 3:A:634:PX4:O3 | 0.49 | 2.07 | 12 | 2 |
| 2:B:72:TRP:CE2 | 3:B:341:PX4:H13 | 0.49 | 2.42 | 14 | 1 |
| 3:B:320:PX4:H17 | 3:B:320:PX4:H3 | 0.49 | 1.84 | 14 | 1 |
| 3:C:313:PX4:H8 | 3:C:337:PX4:C6 | 0.49 | 2.37 | 15 | 1 |
| 3:B:382:PX4:O2 | 3:B:382:PX4:H3 | 0.49 | 2.06 | 9 | 1 |
| 3:A:620:PX4:H6 | 3:A:620:PX4:O1 | 0.49 | 2.07 | 13 | 1 |
| 3:B:351:PX4:O1 | 3:B:351:PX4:H3 | 0.49 | 2.08 | 12 | 4 |
| 3:C:336:PX4:O1 | 3:C:336:PX4:H3 | 0.49 | 2.07 | 3 | 1 |
| 3:C:326:PX4:H10 | 3:C:326:PX4:O3 | 0.49 | 2.07 | 4 | 2 |
| 3:A:640:PX4:H7 | 3:A:640:PX4:O4 | 0.49 | 2.07 | 7 | 1 |
| 3:A:616:PX4:O8 | 3:A:634:PX4:H11 | 0.49 | 2.07 | 11 | 1 |
| 3:B:327:PX4:H4 | 3:B:327:PX4:O2 | 0.49 | 2.06 | 11 | 6 |
| 3:C:361:PX4:O2 | 3:C:361:PX4:H4 | 0.49 | 2.08 | 2 | 2 |
| 3:A:620:PX4:H7 | 3:C:348:PX4:H17 | 0.49 | 1.84 | 5 | 1 |
| 3:B:339:PX4:H9 | 3:B:339:PX4:O3 | 0.49 | 2.06 | 6 | 1 |
| 3:B:361:PX4:O1 | 3:B:368:PX4:H12 | 0.49 | 2.07 | 6 | 2 |
| 3:C:364:PX4:O2 | 3:C:364:PX4:H4 | 0.49 | 2.06 | 8 | 2 |
| 2:B:225:LEU:HD23 | 2:C:82:LEU:HD21 | 0.49 | 1.84 | 10 | 1 |
| 2:B:245:GLU:O | 2:B:249:VAL:HG23 | 0.49 | 2.08 | 13 | 1 |
| 3:B:378:PX4:H3 | 3:B:378:PX4:O4 | 0.49 | 2.07 | 15 | 2 |
| 3:B:334:PX4:H10 | 3:B:334:PX4:O3 | 0.49 | 2.07 | 2 | 1 |
| 3:C:312:PX4:H3 | 3:C:312:PX4:O4 | 0.49 | 2.07 | 15 | 3 |
| 3:C:322:PX4:O4 | 3:C:351:PX4:H4 | 0.49 | 2.08 | 6 | 1 |
| 3:B:301:PX4:O1 | 3:B:303:PX4:H13 | 0.49 | 2.07 | 13 | 1 |
| 3:C:331:PX4:H10 | 3:C:331:PX4:O1 | 0.49 | 2.08 | 15 | 1 |
| 3:A:605:PX4:O3 | 3:A:605:PX4:H12 | 0.49 | 2.07 | 3 | 2 |
| 3:A:610:PX4:H13 | 3:B:389:PX4:O2 | 0.49 | 2.07 | 6 | 1 |
| 3:B:362:PX4:H8 | 3:B:366:PX4:O2 | 0.49 | 2.07 | 1 | 1 |
| 3:B:376:PX4:O3 | 3:B:376:PX4:H6 | 0.49 | 2.07 | 1 | 2 |
| 3:B:326:PX4:O1 | 3:B:355:PX4:H3 | 0.49 | 2.07 | 2 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 3:A:642:PX4:O3 | 3:A:642:PX4:H7 | 0.49 | 2.08 | 3 | 1 |
| 3:B:400:PX4:O8 | 3:B:400:PX4:H12 | 0.49 | 2.08 | 12 | 1 |
| 3:B:365:PX4:H12 | 3:B:365:PX4:O2 | 0.49 | 2.08 | 13 | 2 |
| 2:C:80:GLU:OE1 | 3:C:304:PX4:H4 | 0.49 | 2.06 | 14 | 1 |
| 3:B:353:PX4:O2 | 3:B:369:PX4:H3 | 0.49 | 2.07 | 1 | 1 |
| 3:C:362:PX4:O2 | 3:C:362:PX4:H9 | 0.49 | 2.08 | 1 | 1 |
| 3:B:325:PX4:H6 | 3:B:357:PX4:O8 | 0.49 | 2.08 | 2 | 1 |
| 3:A:610:PX4:O2 | 3:B:379:PX4:H3 | 0.49 | 2.08 | 3 | 1 |
| 3:A:645:PX4:O1 | 3:A:648:PX4:H8 | 0.49 | 2.07 | 10 | 1 |
| 3:B:332:PX4:O3 | 3:B:332:PX4:H9 | 0.49 | 2.07 | 13 | 2 |
| 3:A:638:PX4:H10 | 3:A:648:PX4:O3 | 0.49 | 2.07 | 1 | 1 |
| 3:A:614:PX4:O2 | 3:A:625:PX4:H4 | 0.49 | 2.08 | 5 | 2 |
| 3:A:649:PX4:O4 | 3:A:652:PX4:H5 | 0.49 | 2.07 | 3 | 1 |
| 3:B:306:PX4:H4 | 3:B:348:PX4:O4 | 0.49 | 2.07 | 6 | 1 |
| 3:C:346:PX4:O1 | 3:C:346:PX4:H3 | 0.49 | 2.07 | 7 | 1 |
| 3:A:605:PX4:H3 | 3:B:379:PX4:O3 | 0.49 | 2.08 | 9 | 2 |
| 3:B:356:PX4:H7 | 3:B:356:PX4:O2 | 0.49 | 2.07 | 8 | 1 |
| 3:B:387:PX4:H6 | 3:B:387:PX4:O1 | 0.49 | 2.08 | 10 | 2 |
| 3:C:344:PX4:O1 | 3:C:344:PX4:H6 | 0.49 | 2.08 | 14 | 1 |
| 3:C:354:PX4:O3 | 3:C:354:PX4:H12 | 0.49 | 2.08 | 15 | 1 |
| 3:A:611:PX4:H8 | 3:B:394:PX4:O1 | 0.49 | 2.08 | 11 | 2 |
| 3:A:635:PX4:O6 | 3:A:637:PX4:H5 | 0.49 | 2.08 | 4 | 1 |
| 3:B:400:PX4:O4 | 3:B:400:PX4:H3 | 0.49 | 2.08 | 13 | 3 |
| 3:A:640:PX4:O3 | 3:A:640:PX4:H9 | 0.49 | 2.08 | 6 | 2 |
| 3:B:386:PX4:H10 | 3:B:386:PX4:O3 | 0.49 | 2.07 | 8 | 1 |
| 3:A:631:PX4:O4 | 3:A:642:PX4:H10 | 0.49 | 2.07 | 10 | 1 |
| 3:C:349:PX4:O4 | 3:C:349:PX4:H4 | 0.49 | 2.08 | 13 | 1 |
| 3:A:615:PX4:H8 | 3:C:345:PX4:O1 | 0.48 | 2.09 | 3 | 1 |
| 3:A:650:PX4:O3 | 3:A:650:PX4:H7 | 0.48 | 2.08 | 8 | 1 |
| 3:B:362:PX4:O3 | 3:B:366:PX4:H3 | 0.48 | 2.08 | 10 | 1 |
| 3:B:396:PX4:H37 | 3:C:361:PX4:H43 | 0.48 | 1.85 | 10 | 1 |
| 3:B:359:PX4:H18 | 3:B:373:PX4:H5 | 0.48 | 1.83 | 13 | 1 |
| 3:A:620:PX4:O8 | 3:A:636:PX4:H10 | 0.48 | 2.08 | 15 | 1 |
| 3:A:621:PX4:O1 | 3:A:621:PX4:H3 | 0.48 | 2.07 | 7 | 2 |
| 3:B:356:PX4:H5 | 3:B:373:PX4:O2 | 0.48 | 2.08 | 6 | 1 |
| 3:B:336:PX4:O3 | 3:B:336:PX4:H9 | 0.48 | 2.07 | 7 | 1 |
| 3:C:329:PX4:O2 | 3:C:329:PX4:H4 | 0.48 | 2.08 | 9 | 1 |
| 3:A:610:PX4:H3 | 3:B:389:PX4:O4 | 0.48 | 2.08 | 10 | 1 |
| 3:A:623:PX4:O1 | 3:A:640:PX4:C2 | 0.48 | 2.61 | 15 | 1 |
| 3:B:374:PX4:O1 | 3:B:384:PX4:H13 | 0.48 | 2.08 | 1 | 1 |
| 3:A:631:PX4:O8 | 3:A:642:PX4:H10 | 0.48 | 2.07 | 3 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 3:C:307:PX4:H9 | 3:C:343:PX4:O2 | 0.48 | 2.07 | 3 | 1 |
| 3:A:641:PX4:O1 | 3:A:651:PX4:H3 | 0.48 | 2.08 | 4 | 1 |
| 3:B:315:PX4:H4 | 3:B:315:PX4:O4 | 0.48 | 2.07 | 4 | 1 |
| 3:B:329:PX4:O4 | 3:B:355:PX4:H8 | 0.48 | 2.07 | 5 | 1 |
| 3:A:608:PX4:H3 | 3:A:611:PX4:O1 | 0.48 | 2.08 | 7 | 1 |
| 3:B:355:PX4:O2 | 3:B:377:PX4:H12 | 0.48 | 2.08 | 8 | 1 |
| 3:C:351:PX4:O5 | 3:C:351:PX4:H12 | 0.48 | 2.08 | 9 | 1 |
| 3:A:647:PX4:H4 | 3:A:652:PX4:O1 | 0.48 | 2.08 | 15 | 1 |
| 3:B:320:PX4:O2 | 3:B:340:PX4:H8 | 0.48 | 2.07 | 1 | 1 |
| 3:B:326:PX4:O1 | 3:B:355:PX4:H9 | 0.48 | 2.08 | 3 | 3 |
| 3:C:317:PX4:H12 | 3:C:317:PX4:O3 | 0.48 | 2.09 | 9 | 3 |
| 3:A:603:PX4:H3 | 3:A:603:PX4:O1 | 0.48 | 2.08 | 8 | 1 |
| 3:C:351:PX4:O1 | 3:C:359:PX4:H6 | 0.48 | 2.09 | 11 | 1 |
| 3:B:350:PX4:O1 | 3:B:374:PX4:H13 | 0.48 | 2.09 | 13 | 1 |
| 3:B:383:PX4:H10 | 3:B:383:PX4:H14 | 0.48 | 1.83 | 1 | 1 |
| 3:C:344:PX4:O2 | 3:C:344:PX4:H4 | 0.48 | 2.09 | 1 | 2 |
| 3:A:621:PX4:O2 | 3:A:621:PX4:H6 | 0.48 | 2.09 | 3 | 1 |
| 3:B:315:PX4:H3 | 3:B:336:PX4:O1 | 0.48 | 2.09 | 10 | 2 |
| 3:A:652:PX4:O3 | 3:A:652:PX4:H13 | 0.48 | 2.09 | 10 | 2 |
| 3:B:327:PX4:O8 | 3:B:354:PX4:H13 | 0.48 | 2.08 | 10 | 1 |
| 2:C:76:GLU:OE1 | 3:C:304:PX4:H12 | 0.48 | 2.08 | 12 | 1 |
| 1:A:365:PRO:HG2 | 1:A:388:TRP:CZ2 | 0.48 | 2.43 | 1 | 1 |
| 1:A:393:ALA:O | 3:A:644:PX4:H9 | 0.48 | 2.08 | 4 | 2 |
| 3:B:338:PX4:H48 | 3:B:343:PX4:H11 | 0.48 | 1.86 | 2 | 1 |
| 3:A:644:PX4:O1 | 3:A:644:PX4:H6 | 0.48 | 2.08 | 3 | 1 |
| 3:B:325:PX4:H13 | 3:B:325:PX4:O3 | 0.48 | 2.07 | 10 | 1 |
| 2:B:72:TRP:CZ2 | 3:B:341:PX4:H6 | 0.48 | 2.43 | 14 | 2 |
| 3:B:359:PX4:O2 | 3:B:380:PX4:H4 | 0.48 | 2.09 | 1 | 1 |
| 3:B:332:PX4:H7 | 3:B:332:PX4:O3 | 0.48 | 2.09 | 3 | 1 |
| 3:B:391:PX4:H12 | 3:B:391:PX4:O3 | 0.48 | 2.09 | 15 | 3 |
| 3:B:321:PX4:O3 | 3:B:321:PX4:H9 | 0.48 | 2.08 | 6 | 1 |
| 3:C:355:PX4:H10 | 3:C:355:PX4:O3 | 0.48 | 2.09 | 6 | 4 |
| 3:A:631:PX4:O2 | 3:A:631:PX4:H7 | 0.48 | 2.09 | 8 | 1 |
| 3:B:322:PX4:O4 | 3:B:350:PX4:H5 | 0.48 | 2.09 | 4 | 1 |
| 3:B:399:PX4:O2 | 3:B:399:PX4:H4 | 0.48 | 2.08 | 7 | 1 |
| 2:B:262:LEU:O | 3:B:331:PX4:H5 | 0.48 | 2.07 | 11 | 1 |
| 3:C:345:PX4:H12 | 3:C:345:PX4:O3 | 0.48 | 2.07 | 14 | 2 |
| 3:C:358:PX4:H9 | 3:C:361:PX4:O1 | 0.48 | 2.09 | 12 | 1 |
| 2:B:221:HIS:CD2 | 2:C:86:MET:HG2 | 0.48 | 2.43 | 14 | 1 |
| 3:A:634:PX4:H3 | 3:A:634:PX4:O7 | 0.48 | 2.08 | 15 | 1 |
| 3:B:341:PX4:O2 | 3:B:346:PX4:H3 | 0.48 | 2.09 | 1 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 3:A:644:PX4:O3 | 3:A:650:PX4:H4 | 0.48 | 2.09 | 2 | 1 |
| 3:B:322:PX4:O2 | 3:B:322:PX4:H3 | 0.48 | 2.08 | 3 | 1 |
| 3:C:324:PX4:O2 | 3:C:345:PX4:H7 | 0.48 | 2.09 | 4 | 1 |
| 3:C:354:PX4:O8 | 3:C:354:PX4:H12 | 0.48 | 2.09 | 6 | 1 |
| 3:C:331:PX4:O2 | 3:C:331:PX4:H4 | 0.48 | 2.08 | 7 | 1 |
| 3:A:614:PX4:H10 | 3:A:628:PX4:O2 | 0.48 | 2.09 | 10 | 1 |
| 3:B:376:PX4:O1 | 3:B:390:PX4:H12 | 0.48 | 2.09 | 10 | 1 |
| 3:B:359:PX4:H4 | 3:B:359:PX4:O4 | 0.48 | 2.08 | 11 | 1 |
| 3:B:303:PX4:H22 | 3:C:334:PX4:H70 | 0.48 | 1.84 | 12 | 1 |
| 3:A:645:PX4:H6 | 3:A:646:PX4:O2 | 0.47 | 2.08 | 11 | 5 |
| 3:B:325:PX4:H3 | 3:B:357:PX4:O8 | 0.47 | 2.09 | 3 | 1 |
| 3:C:320:PX4:H3 | 3:C:341:PX4:O4 | 0.47 | 2.08 | 4 | 1 |
| 3:B:320:PX4:O2 | 3:B:320:PX4:H9 | 0.47 | 2.09 | 8 | 1 |
| 3:B:315:PX4:O3 | 3:B:315:PX4:H7 | 0.47 | 2.09 | 10 | 1 |
| 3:C:303:PX4:O3 | 3:C:303:PX4:H12 | 0.47 | 2.09 | 13 | 2 |
| 3:B:373:PX4:H13 | 3:B:380:PX4:O4 | 0.47 | 2.09 | 13 | 1 |
| 3:B:334:PX4:O3 | 3:B:334:PX4:H12 | 0.47 | 2.09 | 14 | 1 |
| 3:B:359:PX4:O4 | 3:B:373:PX4:H13 | 0.47 | 2.09 | 15 | 1 |
| 3:A:626:PX4:H13 | 3:C:362:PX4:H2 | 0.47 | 1.86 | 2 | 1 |
| 3:B:350:PX4:O1 | 3:B:374:PX4:H11 | 0.47 | 2.09 | 8 | 2 |
| 3:A:637:PX4:O3 | 3:A:637:PX4:H7 | 0.47 | 2.08 | 3 | 3 |
| 3:C:341:PX4:O3 | 3:C:341:PX4:H6 | 0.47 | 2.09 | 6 | 2 |
| 3:B:373:PX4:H10 | 3:B:373:PX4:O3 | 0.47 | 2.08 | 8 | 3 |
| 3:C:315:PX4:O3 | 3:C:348:PX4:H6 | 0.47 | 2.09 | 5 | 1 |
| 2:B:130:TRP:HE1 | 2:C:177:HIS:CE1 | 0.47 | 2.27 | 8 | 1 |
| 3:C:306:PX4:H12 | 3:C:306:PX4:O3 | 0.47 | 2.08 | 12 | 2 |
| 3:B:378:PX4:H5 | 3:B:386:PX4:H46 | 0.47 | 1.85 | 11 | 1 |
| 3:B:389:PX4:O2 | 3:B:389:PX4:H4 | 0.47 | 2.08 | 14 | 1 |
| 3:A:639:PX4:O1 | 3:A:639:PX4:H3 | 0.47 | 2.09 | 3 | 1 |
| 3:C:305:PX4:O2 | 3:C:305:PX4:H4 | 0.47 | 2.10 | 14 | 2 |
| 3:C:328:PX4:H10 | 3:C:328:PX4:O3 | 0.47 | 2.10 | 4 | 1 |
| 3:B:316:PX4:H3 | 3:B:316:PX4:O2 | 0.47 | 2.10 | 5 | 1 |
| 3:B:330:PX4:O4 | 3:B:330:PX4:H3 | 0.47 | 2.09 | 12 | 1 |
| 3:B:366:PX4:O3 | 3:B:366:PX4:H13 | 0.47 | 2.09 | 14 | 2 |
| 3:B:346:PX4:H10 | 3:B:346:PX4:O3 | 0.47 | 2.10 | 15 | 1 |
| 3:C:358:PX4:O3 | 3:C:358:PX4:H12 | 0.47 | 2.09 | 2 | 4 |
| 3:C:339:PX4:H10 | 3:C:339:PX4:O3 | 0.47 | 2.09 | 5 | 1 |
| 3:A:610:PX4:O3 | 3:A:610:PX4:H9 | 0.47 | 2.10 | 10 | 3 |
| 3:B:376:PX4:O2 | 3:B:392:PX4:H9 | 0.47 | 2.09 | 7 | 1 |
| 3:A:638:PX4:H7 | 3:A:648:PX4:O2 | 0.47 | 2.09 | 8 | 1 |
| 3:A:638:PX4:H6 | 3:A:638:PX4:O3 | 0.47 | 2.09 | 14 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 3:A:629:PX4:O4 | 3:A:631:PX4:H13 | 0.47 | 2.10 | 4 | 4 |
| 2:B:120:GLU:OE1 | 3:B:311:PX4:H7 | 0.47 | 2.10 | 8 | 1 |
| 3:A:604:PX4:O3 | 3:B:392:PX4:H4 | 0.47 | 2.09 | 12 | 1 |
| 3:B:399:PX4:H6 | 3:C:357:PX4:O3 | 0.47 | 2.10 | 14 | 1 |
| 3:B:320:PX4:O3 | 3:B:320:PX4:H9 | 0.47 | 2.10 | 12 | 3 |
| 3:B:333:PX4:O3 | 3:B:333:PX4:H6 | 0.47 | 2.09 | 1 | 2 |
| 3:B:320:PX4:O4 | 3:B:340:PX4:H7 | 0.47 | 2.10 | 2 | 1 |
| 3:B:367:PX4:C4 | 3:B:367:PX4:O3 | 0.47 | 2.62 | 5 | 1 |
| 3:A:631:PX4:O6 | 3:A:642:PX4:H10 | 0.47 | 2.09 | 6 | 1 |
| 3:B:365:PX4:H6 | 3:B:365:PX4:O3 | 0.47 | 2.10 | 6 | 1 |
| 3:A:628:PX4:H6 | 3:A:628:PX4:O3 | 0.47 | 2.09 | 7 | 1 |
| 3:A:642:PX4:O2 | 3:A:651:PX4:H5 | 0.47 | 2.09 | 11 | 2 |
| 3:A:632:PX4:H10 | 3:A:632:PX4:O4 | 0.47 | 2.09 | 9 | 1 |
| 3:B:323:PX4:O6 | 3:B:346:PX4:H13 | 0.47 | 2.09 | 10 | 2 |
| 3:B:335:PX4:O2 | 3:B:335:PX4:H4 | 0.47 | 2.10 | 12 | 1 |
| 3:C:331:PX4:H10 | 3:C:331:PX4:O3 | 0.47 | 2.08 | 14 | 1 |
| 3:A:613:PX4:H11 | 3:C:345:PX4:O4 | 0.47 | 2.09 | 15 | 1 |
| 3:B:399:PX4:H3 | 3:C:357:PX4:O4 | 0.47 | 2.10 | 15 | 1 |
| 3:B:372:PX4:O2 | 3:B:372:PX4:H4 | 0.47 | 2.10 | 2 | 2 |
| 3:A:632:PX4:H9 | 3:A:647:PX4:O2 | 0.47 | 2.10 | 6 | 1 |
| 3:B:352:PX4:H10 | 3:B:368:PX4:O6 | 0.47 | 2.10 | 12 | 1 |
| 3:C:311:PX4:H7 | 3:C:311:PX4:O3 | 0.47 | 2.10 | 15 | 1 |
| 3:A:626:PX4:H5 | 3:A:638:PX4:O1 | 0.47 | 2.10 | 1 | 1 |
| 3:A:633:PX4:H15 | 3:A:633:PX4:H10 | 0.47 | 1.87 | 1 | 1 |
| 3:C:306:PX4:H11 | 3:C:350:PX4:O1 | 0.47 | 2.09 | 2 | 1 |
| 3:C:350:PX4:H10 | 3:C:350:PX4:O3 | 0.47 | 2.10 | 2 | 1 |
| 3:C:320:PX4:H11 | 3:C:330:PX4:H9 | 0.47 | 1.86 | 4 | 1 |
| 3:B:338:PX4:C25 | 3:B:343:PX4:H8 | 0.47 | 2.40 | 8 | 1 |
| 3:C:316:PX4:H9 | 3:C:342:PX4:O2 | 0.47 | 2.10 | 9 | 1 |
| 3:B:336:PX4:H8 | 3:B:343:PX4:O1 | 0.47 | 2.10 | 10 | 2 |
| 3:A:602:PX4:H10 | 3:A:602:PX4:O3 | 0.47 | 2.10 | 11 | 1 |
| 3:B:351:PX4:H7 | 3:B:354:PX4:C1 | 0.47 | 2.40 | 14 | 1 |
| 1:A:392:GLU:O | 3:A:644:PX4:H9 | 0.47 | 2.10 | 1 | 1 |
| 3:B:344:PX4:O3 | 3:B:344:PX4:H7 | 0.47 | 2.10 | 1 | 2 |
| 3:B:343:PX4:C20 | 3:C:336:PX4:H70 | 0.47 | 2.40 | 2 | 1 |
| 3:A:639:PX4:H6 | 3:A:639:PX4:O3 | 0.47 | 2.10 | 13 | 5 |
| 3:B:338:PX4:P1 | 3:B:358:PX4:H6 | 0.47 | 2.50 | 6 | 1 |
| 3:C:307:PX4:H12 | 3:C:307:PX4:O3 | 0.47 | 2.10 | 6 | 1 |
| 2:B:105:GLN:OE1 | 3:B:303:PX4:H13 | 0.47 | 2.10 | 9 | 1 |
| 3:B:364:PX4:H11 | 3:C:301:PX4:O1 | 0.47 | 2.08 | 10 | 1 |
| 3:C:320:PX4:H5 | 3:C:330:PX4:O3 | 0.47 | 2.10 | 10 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 2:C:83:ARG:HA | 3:C:312:PX4:H59 | 0.47 | 1.87 | 12 | 1 |
| 3:C:339:PX4:O3 | 3:C:339:PX4:H7 | 0.47 | 2.10 | 14 | 1 |
| 3:A:641:PX4:O4 | 3:A:641:PX4:H3 | 0.47 | 2.10 | 15 | 1 |
| 3:C:363:PX4:O3 | 3:C:363:PX4:H10 | 0.46 | 2.10 | 1 | 1 |
| 3:A:627:PX4:O2 | 3:A:643:PX4:H13 | 0.46 | 2.11 | 3 | 1 |
| 3:B:338:PX4:O4 | 3:B:338:PX4:H3 | 0.46 | 2.09 | 3 | 1 |
| 3:A:631:PX4:H11 | 3:A:646:PX4:O1 | 0.46 | 2.09 | 14 | 2 |
| 3:A:604:PX4:C6 | 3:A:604:PX4:H4 | 0.46 | 2.40 | 12 | 1 |
| 3:C:323:PX4:O2 | 3:C:342:PX4:H4 | 0.46 | 2.10 | 12 | 1 |
| 3:C:327:PX4:H5 | 3:C:334:PX4:O2 | 0.46 | 2.09 | 13 | 1 |
| 3:A:618:PX4:P1 | 3:A:633:PX4:H3 | 0.46 | 2.50 | 14 | 1 |
| 1:A:368:ILE:H | 1:A:368:ILE:HD13 | 0.46 | 1.69 | 2 | 1 |
| 3:C:312:PX4:H7 | 3:C:312:PX4:C6 | 0.46 | 2.39 | 5 | 1 |
| 3:B:342:PX4:O3 | 3:B:350:PX4:H13 | 0.46 | 2.10 | 7 | 2 |
| 3:A:626:PX4:H13 | 3:C:362:PX4:O3 | 0.46 | 2.09 | 2 | 1 |
| 3:B:395:PX4:H12 | 3:C:358:PX4:O3 | 0.46 | 2.11 | 3 | 1 |
| 3:C:303:PX4:O1 | 3:C:303:PX4:H4 | 0.46 | 2.10 | 3 | 1 |
| 3:C:311:PX4:H4 | 3:C:311:PX4:O2 | 0.46 | 2.10 | 4 | 1 |
| 3:A:632:PX4:H10 | 3:A:632:PX4:O3 | 0.46 | 2.09 | 14 | 2 |
| 2:B:80:GLU:OE1 | 3:B:305:PX4:H10 | 0.46 | 2.09 | 6 | 1 |
| 3:A:614:PX4:H10 | 3:A:614:PX4:O4 | 0.46 | 2.10 | 11 | 1 |
| 3:A:624:PX4:O4 | 3:A:639:PX4:H9 | 0.46 | 2.11 | 7 | 1 |
| 2:B:72:TRP:CE2 | 3:B:341:PX4:H4 | 0.46 | 2.46 | 10 | 1 |
| 3:B:353:PX4:O2 | 3:B:369:PX4:H4 | 0.46 | 2.11 | 11 | 1 |
| 3:B:312:PX4:H12 | 3:B:312:PX4:O3 | 0.46 | 2.10 | 13 | 1 |
| 3:A:615:PX4:H12 | 3:A:615:PX4:O3 | 0.46 | 2.10 | 14 | 1 |
| 3:C:307:PX4:H9 | 3:C:343:PX4:O1 | 0.46 | 2.11 | 1 | 1 |
| 3:C:357:PX4:O3 | 3:C:357:PX4:H6 | 0.46 | 2.11 | 1 | 2 |
| 3:C:305:PX4:O2 | 3:C:311:PX4:H9 | 0.46 | 2.10 | 3 | 1 |
| 3:C:308:PX4:O1 | 3:C:308:PX4:H12 | 0.46 | 2.10 | 3 | 1 |
| 3:B:392:PX4:H3 | 3:B:392:PX4:H14 | 0.46 | 1.86 | 4 | 1 |
| 3:B:391:PX4:H4 | 3:C:303:PX4:O2 | 0.46 | 2.11 | 1 | 1 |
| 3:B:388:PX4:O3 | 3:B:388:PX4:H7 | 0.46 | 2.09 | 9 | 3 |
| 3:B:327:PX4:O2 | 3:B:327:PX4:H4 | 0.46 | 2.10 | 5 | 1 |
| 3:B:392:PX4:H3 | 3:B:392:PX4:H15 | 0.46 | 1.88 | 5 | 1 |
| 3:C:333:PX4:H29 | 3:C:333:PX4:H38 | 0.46 | 1.86 | 7 | 1 |
| 3:B:400:PX4:H9 | 3:B:400:PX4:O3 | 0.46 | 2.11 | 9 | 1 |
| 3:C:329:PX4:O1 | 3:C:354:PX4:H8 | 0.46 | 2.10 | 9 | 1 |
| 3:A:607:PX4:O2 | 3:A:612:PX4:H12 | 0.46 | 2.10 | 10 | 1 |
| 3:A:601:PX4:O2 | 3:B:372:PX4:H9 | 0.46 | 2.11 | 13 | 1 |
| 3:B:340:PX4:O4 | 3:B:340:PX4:H4 | 0.46 | 2.10 | 13 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 2:C:173:ARG:HE | 2:C:177:HIS:CD2 | 0.46 | 2.28 | 13 | 1 |
| 3:A:640:PX4:O1 | 3:A:640:PX4:H4 | 0.46 | 2.10 | 2 | 1 |
| 3:A:605:PX4:H11 | 3:B:379:PX4:O3 | 0.46 | 2.10 | 3 | 1 |
| 3:C:323:PX4:O2 | 3:C:342:PX4:H8 | 0.46 | 2.09 | 3 | 1 |
| 1:A:371:ALA:HB2 | 1:A:381:PHE:CD2 | 0.46 | 2.45 | 4 | 1 |
| 3:A:605:PX4:H13 | 3:B:379:PX4:C6 | 0.46 | 2.40 | 9 | 3 |
| 3:B:397:PX4:O1 | 3:B:397:PX4:H3 | 0.46 | 2.11 | 8 | 1 |
| 3:C:315:PX4:O4 | 3:C:315:PX4:H4 | 0.46 | 2.11 | 10 | 1 |
| 3:B:309:PX4:O3 | 3:B:309:PX4:H6 | 0.46 | 2.11 | 14 | 1 |
| 3:C:357:PX4:O3 | 3:C:357:PX4:C3 | 0.46 | 2.64 | 1 | 1 |
| 3:B:400:PX4:H9 | 3:B:400:PX4:O8 | 0.46 | 2.11 | 3 | 1 |
| 3:A:631:PX4:H8 | 3:A:646:PX4:O4 | 0.46 | 2.10 | 4 | 2 |
| 2:B:262:LEU:O | 3:B:331:PX4:H9 | 0.46 | 2.11 | 5 | 1 |
| 3:A:624:PX4:O1 | 3:A:639:PX4:H9 | 0.46 | 2.10 | 8 | 1 |
| 3:A:616:PX4:O2 | 3:A:616:PX4:H7 | 0.46 | 2.11 | 11 | 1 |
| 1:A:387:HIS:CE1 | 1:A:406:LEU:HB2 | 0.46 | 2.46 | 12 | 1 |
| 3:C:343:PX4:O3 | 3:C:343:PX4:H12 | 0.46 | 2.11 | 12 | 1 |
| 3:A:632:PX4:H9 | 3:A:647:PX4:C6 | 0.46 | 2.41 | 13 | 1 |
| 3:C:305:PX4:O6 | 3:C:311:PX4:H3 | 0.46 | 2.11 | 14 | 1 |
| 3:B:373:PX4:H13 | 3:B:380:PX4:O3 | 0.46 | 2.10 | 6 | 2 |
| 3:B:364:PX4:O3 | 3:B:364:PX4:H7 | 0.46 | 2.11 | 6 | 2 |
| 3:B:310:PX4:H9 | 3:B:310:PX4:P1 | 0.46 | 2.51 | 10 | 2 |
| 3:A:630:PX4:O2 | 3:A:633:PX4:H13 | 0.46 | 2.11 | 10 | 1 |
| 3:B:361:PX4:H4 | 3:B:368:PX4:C1 | 0.46 | 2.41 | 10 | 1 |
| 3:B:383:PX4:O3 | 3:B:383:PX4:C4 | 0.46 | 2.64 | 10 | 1 |
| 3:C:362:PX4:O3 | 3:C:362:PX4:H7 | 0.46 | 2.10 | 14 | 1 |
| 3:A:605:PX4:O3 | 3:B:379:PX4:H3 | 0.46 | 2.11 | 1 | 1 |
| 3:A:630:PX4:O3 | 3:A:630:PX4:H6 | 0.46 | 2.11 | 3 | 1 |
| 3:A:642:PX4:O3 | 3:A:642:PX4:C3 | 0.46 | 2.64 | 3 | 1 |
| 3:C:320:PX4:H8 | 3:C:330:PX4:O3 | 0.46 | 2.11 | 6 | 1 |
| 3:B:387:PX4:H7 | 3:B:390:PX4:O3 | 0.46 | 2.11 | 10 | 1 |
| 3:C:315:PX4:O2 | 3:C:315:PX4:H4 | 0.46 | 2.11 | 15 | 1 |
| 3:B:306:PX4:H3 | 3:B:339:PX4:O8 | 0.45 | 2.11 | 8 | 2 |
| 3:A:649:PX4:H18 | 3:A:649:PX4:H13 | 0.45 | 1.87 | 9 | 1 |
| 3:C:307:PX4:H4 | 3:C:343:PX4:O2 | 0.45 | 2.11 | 10 | 1 |
| 3:C:323:PX4:O2 | 3:C:342:PX4:H3 | 0.45 | 2.11 | 11 | 1 |
| 3:B:326:PX4:O4 | 3:B:326:PX4:H3 | 0.45 | 2.11 | 1 | 1 |
| 3:B:337:PX4:O1 | 3:B:337:PX4:H3 | 0.45 | 2.11 | 1 | 1 |
| 2:C:180:ALA:O | 2:C:184:HIS:CD2 | 0.45 | 2.70 | 2 | 1 |
| 3:C:320:PX4:H11 | 3:C:330:PX4:O4 | 0.45 | 2.11 | 3 | 1 |
| 3:A:620:PX4:H12 | 3:C:348:PX4:O1 | 0.45 | 2.11 | 4 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 3:C:352:PX4:O2 | 3:C:352:PX4:H3 | 0.45 | 2.11 | 8 | 1 |
| 3:B:320:PX4:O2 | 3:B:340:PX4:H7 | 0.45 | 2.10 | 11 | 1 |
| 2:B:142:GLU:OE1 | 3:B:328:PX4:H10 | 0.45 | 2.11 | 13 | 1 |
| 3:C:309:PX4:H10 | 3:C:309:PX4:O3 | 0.45 | 2.11 | 8 | 3 |
| 3:A:636:PX4:H9 | 3:A:636:PX4:O3 | 0.45 | 2.11 | 4 | 1 |
| 3:B:392:PX4:O3 | 3:B:392:PX4:C5 | 0.45 | 2.64 | 4 | 1 |
| 3:C:324:PX4:H3 | 3:C:324:PX4:O1 | 0.45 | 2.11 | 4 | 2 |
| 3:A:633:PX4:H44 | 3:A:633:PX4:H68 | 0.45 | 1.89 | 6 | 1 |
| 3:B:388:PX4:O1 | 3:B:388:PX4:H9 | 0.45 | 2.12 | 11 | 1 |
| 3:B:335:PX4:H10 | 3:B:353:PX4:O2 | 0.45 | 2.11 | 12 | 1 |
| 3:B:380:PX4:O1 | 3:B:387:PX4:H8 | 0.45 | 2.10 | 12 | 1 |
| 3:B:331:PX4:O1 | 3:B:331:PX4:H3 | 0.45 | 2.11 | 2 | 1 |
| 3:B:380:PX4:O1 | 3:B:387:PX4:H10 | 0.45 | 2.11 | 3 | 2 |
| 2:C:207:GLY:HA2 | 2:C:210:ARG:NH2 | 0.45 | 2.26 | 3 | 1 |
| 3:C:305:PX4:H6 | 3:C:324:PX4:H6 | 0.45 | 1.88 | 3 | 1 |
| 3:B:326:PX4:C1 | 3:B:355:PX4:H7 | 0.45 | 2.41 | 5 | 1 |
| 3:B:370:PX4:H6 | 3:B:386:PX4:O1 | 0.45 | 2.12 | 5 | 1 |
| 3:B:334:PX4:H10 | 3:B:334:PX4:P1 | 0.45 | 2.51 | 6 | 1 |
| 3:C:342:PX4:H9 | 3:C:342:PX4:O3 | 0.45 | 2.11 | 7 | 1 |
| 3:A:618:PX4:H3 | 3:A:620:PX4:O8 | 0.45 | 2.12 | 8 | 1 |
| 3:A:648:PX4:H72 | 3:A:653:PX4:H34 | 0.45 | 1.88 | 10 | 1 |
| 3:A:615:PX4:O1 | 3:A:615:PX4:H3 | 0.45 | 2.11 | 11 | 1 |
| 2:C:131:GLN:HA | 2:C:131:GLN:OE1 | 0.45 | 2.12 | 12 | 1 |
| 3:B:400:PX4:H3 | 3:B:400:PX4:O8 | 0.45 | 2.12 | 13 | 1 |
| 3:B:362:PX4:O3 | 3:B:362:PX4:H13 | 0.45 | 2.12 | 4 | 2 |
| 3:A:645:PX4:H6 | 3:A:646:PX4:O3 | 0.45 | 2.12 | 3 | 1 |
| 3:A:622:PX4:O4 | 3:A:622:PX4:H3 | 0.45 | 2.12 | 5 | 1 |
| 3:B:336:PX4:H72 | 3:C:305:PX4:H37 | 0.45 | 1.87 | 5 | 1 |
| 3:A:635:PX4:O6 | 3:A:637:PX4:H11 | 0.45 | 2.12 | 6 | 1 |
| 3:A:644:PX4:O2 | 3:A:650:PX4:H4 | 0.45 | 2.12 | 6 | 1 |
| 3:C:330:PX4:O2 | 3:C:330:PX4:H9 | 0.45 | 2.12 | 11 | 1 |
| 1:A:347:ASN:HA | 1:A:505:TRP:O | 0.45 | 2.12 | 12 | 1 |
| 3:B:345:PX4:O3 | 3:B:345:PX4:H7 | 0.45 | 2.12 | 14 | 1 |
| 3:C:347:PX4:O3 | 3:C:347:PX4:C5 | 0.45 | 2.64 | 14 | 1 |
| 3:A:633:PX4:C1 | 3:A:638:PX4:H6 | 0.45 | 2.42 | 5 | 1 |
| 3:A:632:PX4:H3 | 3:A:643:PX4:O1 | 0.45 | 2.12 | 9 | 2 |
| 3:B:351:PX4:H12 | 3:B:351:PX4:O3 | 0.45 | 2.12 | 9 | 1 |
| 3:B:302:PX4:O2 | 3:B:302:PX4:H7 | 0.45 | 2.11 | 11 | 1 |
| 3:A:635:PX4:O1 | 3:A:637:PX4:H5 | 0.45 | 2.12 | 15 | 1 |
| 3:B:322:PX4:H12 | 3:B:322:PX4:O3 | 0.45 | 2.11 | 1 | 1 |
| 3:C:343:PX4:H3 | 3:C:343:PX4:O1 | 0.45 | 2.12 | 5 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 3:A:610:PX4:H45 | 3:A:649:PX4:H44 | 0.45 | 1.89 | 6 | 1 |
| 3:B:342:PX4:O4 | 3:B:350:PX4:H13 | 0.45 | 2.12 | 10 | 2 |
| 3:B:364:PX4:H15 | 3:C:303:PX4:H10 | 0.45 | 1.89 | 6 | 1 |
| 3:C:316:PX4:O8 | 3:C:316:PX4:H4 | 0.45 | 2.12 | 9 | 1 |
| 3:A:611:PX4:H13 | 3:A:611:PX4:O3 | 0.45 | 2.12 | 13 | 1 |
| 3:A:618:PX4:O1 | 3:A:633:PX4:H3 | 0.45 | 2.12 | 14 | 1 |
| 3:A:637:PX4:O2 | 3:A:637:PX4:H3 | 0.45 | 2.10 | 14 | 1 |
| 3:A:650:PX4:H9 | 3:A:650:PX4:O3 | 0.45 | 2.12 | 14 | 1 |
| 3:B:373:PX4:H3 | 3:B:380:PX4:C1 | 0.45 | 2.40 | 14 | 1 |
| 3:B:400:PX4:O3 | 3:B:400:PX4:H6 | 0.45 | 2.12 | 2 | 2 |
| 2:B:76:GLU:CD | 3:B:305:PX4:H10 | 0.45 | 2.32 | 3 | 1 |
| 3:B:353:PX4:H8 | 3:B:382:PX4:O2 | 0.45 | 2.11 | 3 | 2 |
| 3:B:360:PX4:O2 | 3:B:362:PX4:H10 | 0.45 | 2.12 | 5 | 1 |
| 3:B:397:PX4:H7 | 3:C:347:PX4:H10 | 0.45 | 1.89 | 6 | 1 |
| 3:A:627:PX4:H45 | 3:A:647:PX4:H69 | 0.45 | 1.89 | 7 | 1 |
| 3:A:634:PX4:H47 | 3:A:634:PX4:H7 | 0.45 | 1.87 | 12 | 1 |
| 3:C:304:PX4:O2 | 3:C:347:PX4:H6 | 0.45 | 2.12 | 12 | 1 |
| 3:B:395:PX4:O3 | 3:B:395:PX4:H13 | 0.45 | 2.12 | 1 | 1 |
| 3:B:363:PX4:H7 | 3:C:302:PX4:O1 | 0.45 | 2.11 | 7 | 1 |
| 3:B:349:PX4:O3 | 3:B:349:PX4:H13 | 0.45 | 2.11 | 11 | 1 |
| 3:C:309:PX4:O4 | 3:C:327:PX4:H12 | 0.44 | 2.11 | 4 | 2 |
| 3:B:342:PX4:O6 | 3:B:367:PX4:H6 | 0.44 | 2.11 | 5 | 1 |
| 3:B:367:PX4:O3 | 3:B:367:PX4:H10 | 0.44 | 2.12 | 5 | 1 |
| 3:A:608:PX4:H10 | 3:A:611:PX4:O2 | 0.44 | 2.12 | 8 | 1 |
| 3:B:370:PX4:H9 | 3:B:378:PX4:H10 | 0.44 | 1.89 | 9 | 1 |
| 3:C:301:PX4:H4 | 3:C:301:PX4:O2 | 0.44 | 2.12 | 15 | 1 |
| 3:B:360:PX4:O1 | 3:B:362:PX4:H10 | 0.44 | 2.13 | 4 | 1 |
| 3:C:316:PX4:H7 | 3:C:342:PX4:P1 | 0.44 | 2.52 | 7 | 1 |
| 3:C:350:PX4:O2 | 3:C:355:PX4:H7 | 0.44 | 2.13 | 9 | 1 |
| 3:B:378:PX4:H13 | 3:B:386:PX4:O1 | 0.44 | 2.13 | 15 | 1 |
| 3:B:364:PX4:H3 | 3:B:364:PX4:O1 | 0.44 | 2.13 | 1 | 1 |
| 3:A:653:PX4:H7 | 3:A:653:PX4:O2 | 0.44 | 2.13 | 2 | 2 |
| 3:B:331:PX4:O3 | 3:B:331:PX4:H12 | 0.44 | 2.12 | 4 | 2 |
| 3:B:326:PX4:H13 | 3:B:355:PX4:O3 | 0.44 | 2.13 | 6 | 1 |
| 3:C:334:PX4:O2 | 3:C:334:PX4:H4 | 0.44 | 2.13 | 8 | 1 |
| 3:A:645:PX4:O3 | 3:A:648:PX4:H5 | 0.44 | 2.12 | 9 | 1 |
| 3:B:338:PX4:O6 | 3:B:358:PX4:H4 | 0.44 | 2.12 | 11 | 1 |
| 3:A:636:PX4:H3 | 3:A:636:PX4:C6 | 0.44 | 2.42 | 12 | 1 |
| 3:A:605:PX4:H8 | 3:B:344:PX4:C5 | 0.44 | 2.43 | 13 | 1 |
| 3:B:360:PX4:H12 | 3:B:360:PX4:O6 | 0.44 | 2.12 | 13 | 1 |
| 3:A:610:PX4:O1 | 3:B:379:PX4:H8 | 0.44 | 2.11 | 7 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 3:A:627:PX4:O6 | 3:C:361:PX4:H8 | 0.44 | 2.12 | 7 | 1 |
| 3:C:323:PX4:O3 | 3:C:323:PX4:H7 | 0.44 | 2.12 | 10 | 1 |
| 3:B:380:PX4:O6 | 3:B:387:PX4:H10 | 0.44 | 2.13 | 1 | 1 |
| 3:B:371:PX4:H6 | 3:B:371:PX4:O1 | 0.44 | 2.12 | 7 | 1 |
| 3:A:611:PX4:O3 | 3:A:611:PX4:H13 | 0.44 | 2.12 | 8 | 1 |
| 3:A:619:PX4:H4 | 3:A:632:PX4:O2 | 0.44 | 2.12 | 11 | 1 |
| 3:A:642:PX4:H69 | 3:A:648:PX4:H59 | 0.44 | 1.90 | 13 | 1 |
| 3:C:317:PX4:O6 | 3:C:344:PX4:H9 | 0.44 | 2.13 | 2 | 1 |
| 3:A:629:PX4:O6 | 3:A:631:PX4:H13 | 0.44 | 2.13 | 5 | 1 |
| 2:B:175:ARG:HG2 | 3:B:318:PX4:H13 | 0.44 | 1.89 | 7 | 1 |
| 3:C:340:PX4:H7 | 3:C:340:PX4:O3 | 0.44 | 2.13 | 9 | 2 |
| 2:B:212:ALA:HB2 | 3:B:322:PX4:H12 | 0.44 | 1.88 | 15 | 1 |
| 3:C:320:PX4:H11 | 3:C:330:PX4:O3 | 0.44 | 2.13 | 9 | 2 |
| 3:A:605:PX4:O1 | 3:A:609:PX4:H10 | 0.44 | 2.13 | 4 | 1 |
| 3:A:609:PX4:H6 | 3:A:609:PX4:O3 | 0.44 | 2.12 | 4 | 1 |
| 3:B:303:PX4:H4 | 3:B:303:PX4:O2 | 0.44 | 2.13 | 5 | 1 |
| 3:C:315:PX4:O3 | 3:C:315:PX4:H7 | 0.44 | 2.12 | 6 | 1 |
| 3:B:320:PX4:H6 | 3:B:340:PX4:C6 | 0.44 | 2.43 | 7 | 1 |
| 3:B:377:PX4:O3 | 3:B:377:PX4:H6 | 0.44 | 2.13 | 7 | 1 |
| 3:B:375:PX4:O2 | 3:B:392:PX4:H4 | 0.44 | 2.12 | 15 | 1 |
| 3:B:307:PX4:O3 | 3:B:307:PX4:H12 | 0.44 | 2.13 | 3 | 1 |
| 3:B:337:PX4:O2 | 3:B:337:PX4:H3 | 0.44 | 2.11 | 3 | 1 |
| 3:A:627:PX4:O1 | 3:A:643:PX4:H3 | 0.44 | 2.13 | 5 | 1 |
| 3:C:322:PX4:C1 | 3:C:322:PX4:H15 | 0.44 | 2.43 | 7 | 1 |
| 3:C:351:PX4:O1 | 3:C:359:PX4:H4 | 0.44 | 2.12 | 12 | 2 |
| 3:C:358:PX4:O8 | 3:C:361:PX4:H7 | 0.44 | 2.13 | 7 | 1 |
| 3:A:626:PX4:H10 | 3:C:346:PX4:H47 | 0.44 | 1.89 | 9 | 1 |
| 3:B:304:PX4:H14 | 3:B:345:PX4:H6 | 0.44 | 1.90 | 14 | 1 |
| 3:B:400:PX4:O8 | 3:B:400:PX4:H3 | 0.44 | 2.12 | 3 | 1 |
| 3:B:398:PX4:H10 | 3:B:398:PX4:O3 | 0.44 | 2.12 | 4 | 1 |
| 3:C:334:PX4:O3 | 3:C:334:PX4:H13 | 0.44 | 2.12 | 15 | 4 |
| 3:B:400:PX4:H11 | 3:C:347:PX4:C6 | 0.44 | 2.43 | 9 | 1 |
| 3:B:374:PX4:H10 | 3:B:374:PX4:O3 | 0.44 | 2.13 | 11 | 1 |
| 1:A:382:PHE:CD1 | 1:A:387:HIS:HB3 | 0.44 | 2.48 | 12 | 1 |
| 3:A:631:PX4:H45 | 3:B:381:PX4:H43 | 0.43 | 1.89 | 3 | 1 |
| 3:C:351:PX4:O1 | 3:C:351:PX4:H13 | 0.43 | 2.13 | 4 | 1 |
| 3:B:312:PX4:O2 | 3:B:317:PX4:H4 | 0.43 | 2.13 | 6 | 1 |
| 3:B:376:PX4:O1 | 3:B:390:PX4:H6 | 0.43 | 2.12 | 8 | 1 |
| 3:B:379:PX4:O1 | 3:B:379:PX4:H9 | 0.43 | 2.13 | 12 | 1 |
| 3:B:378:PX4:H4 | 3:B:386:PX4:O4 | 0.43 | 2.13 | 14 | 1 |
| 3:B:311:PX4:O1 | 3:B:345:PX4:H12 | 0.43 | 2.13 | 3 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 3:A:633:PX4:O3 | 3:A:638:PX4:H6 | 0.43 | 2.13 | 5 | 1 |
| 3:A:641:PX4:O3 | 3:A:641:PX4:C4 | 0.43 | 2.66 | 7 | 2 |
| 3:B:340:PX4:O2 | 3:B:340:PX4:H4 | 0.43 | 2.13 | 15 | 2 |
| 3:B:400:PX4:H11 | 3:C:347:PX4:O7 | 0.43 | 2.14 | 7 | 1 |
| 3:A:608:PX4:H5 | 3:A:611:PX4:H2 | 0.43 | 1.89 | 12 | 1 |
| 3:C:345:PX4:O1 | 3:C:345:PX4:H3 | 0.43 | 2.13 | 13 | 2 |
| 2:B:262:LEU:O | 3:B:331:PX4:H13 | 0.43 | 2.13 | 14 | 1 |
| 3:B:367:PX4:H13 | 3:B:377:PX4:O2 | 0.43 | 2.13 | 15 | 1 |
| 3:B:357:PX4:O4 | 3:B:357:PX4:H4 | 0.43 | 2.13 | 2 | 1 |
| 3:A:605:PX4:H8 | 3:B:379:PX4:O2 | 0.43 | 2.14 | 3 | 1 |
| 3:A:615:PX4:O2 | 3:A:615:PX4:H3 | 0.43 | 2.13 | 5 | 1 |
| 3:C:323:PX4:H16 | 3:C:323:PX4:H4 | 0.43 | 1.90 | 5 | 1 |
| 1:A:402:HIS:HE1 | 3:A:649:PX4:H12 | 0.43 | 1.62 | 7 | 1 |
| 3:C:301:PX4:C6 | 3:C:301:PX4:H2 | 0.43 | 2.43 | 8 | 1 |
| 3:C:362:PX4:O2 | 3:C:362:PX4:H4 | 0.43 | 2.13 | 10 | 1 |
| 3:A:630:PX4:H40 | 3:B:391:PX4:H72 | 0.43 | 1.90 | 14 | 1 |
| 3:A:633:PX4:O3 | 3:A:633:PX4:H10 | 0.43 | 2.13 | 3 | 2 |
| 3:B:327:PX4:O8 | 3:B:354:PX4:H5 | 0.43 | 2.13 | 5 | 1 |
| 3:C:315:PX4:C1 | 3:C:348:PX4:H6 | 0.43 | 2.44 | 5 | 1 |
| 3:C:310:PX4:H65 | 3:C:343:PX4:H71 | 0.43 | 1.89 | 10 | 1 |
| 3:B:321:PX4:H7 | 3:B:321:PX4:O3 | 0.43 | 2.13 | 12 | 1 |
| 3:A:606:PX4:O2 | 3:C:302:PX4:H10 | 0.43 | 2.13 | 15 | 1 |
| 3:C:323:PX4:H4 | 3:C:323:PX4:H16 | 0.43 | 1.90 | 4 | 1 |
| 3:B:313:PX4:O3 | 3:B:313:PX4:C4 | 0.43 | 2.66 | 5 | 1 |
| 3:B:397:PX4:O8 | 3:C:312:PX4:H17 | 0.43 | 2.13 | 5 | 1 |
| 3:B:390:PX4:O2 | 3:B:392:PX4:H6 | 0.43 | 2.14 | 7 | 1 |
| 3:B:379:PX4:O3 | 3:B:379:PX4:H9 | 0.43 | 2.14 | 9 | 1 |
| 3:B:398:PX4:C9 | 3:B:398:PX4:H26 | 0.43 | 2.43 | 9 | 1 |
| 3:B:357:PX4:O1 | 3:B:357:PX4:H4 | 0.43 | 2.13 | 1 | 1 |
| 3:A:620:PX4:H4 | 3:C:348:PX4:O1 | 0.43 | 2.14 | 3 | 1 |
| 3:A:636:PX4:O8 | 3:A:636:PX4:H15 | 0.43 | 2.13 | 4 | 1 |
| 3:B:374:PX4:O3 | 3:B:374:PX4:H7 | 0.43 | 2.14 | 4 | 1 |
| 3:B:397:PX4:H5 | 3:C:304:PX4:O1 | 0.43 | 2.14 | 4 | 1 |
| 3:A:617:PX4:O1 | 3:A:617:PX4:H3 | 0.43 | 2.13 | 9 | 1 |
| 3:B:399:PX4:O1 | 3:C:326:PX4:H3 | 0.43 | 2.14 | 9 | 1 |
| 3:B:387:PX4:O1 | 3:B:390:PX4:H9 | 0.43 | 2.13 | 10 | 1 |
| 3:A:631:PX4:O1 | 3:A:642:PX4:H10 | 0.43 | 2.13 | 15 | 1 |
| 3:C:316:PX4:H13 | 3:C:323:PX4:O1 | 0.43 | 2.14 | 15 | 1 |
| 3:A:646:PX4:H9 | 3:A:646:PX4:O3 | 0.43 | 2.14 | 14 | 2 |
| 3:B:324:PX4:H3 | 3:B:324:PX4:O1 | 0.43 | 2.13 | 5 | 1 |
| 3:B:316:PX4:H8 | 3:B:321:PX4:O1 | 0.43 | 2.13 | 6 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 3:C:310:PX4:O3 | 3:C:310:PX4:H13 | 0.43 | 2.13 | 11 | 2 |
| 3:C:318:PX4:O3 | 3:C:318:PX4:H6 | 0.43 | 2.14 | 10 | 2 |
| 1:A:399:TYR:CD1 | 1:A:401:LYS:HG3 | 0.43 | 2.48 | 12 | 1 |
| 3:A:632:PX4:O3 | 3:A:632:PX4:C4 | 0.43 | 2.67 | 12 | 1 |
| 3:B:326:PX4:O1 | 3:B:326:PX4:H3 | 0.43 | 2.13 | 12 | 1 |
| 3:B:335:PX4:O3 | 3:B:335:PX4:H7 | 0.43 | 2.13 | 12 | 1 |
| 3:B:394:PX4:O3 | 3:B:394:PX4:H7 | 0.43 | 2.14 | 12 | 1 |
| 3:C:349:PX4:H10 | 3:C:349:PX4:O8 | 0.43 | 2.14 | 13 | 1 |
| 3:A:644:PX4:H9 | 3:A:650:PX4:O1 | 0.43 | 2.14 | 14 | 1 |
| 1:A:362:ARG:NH2 | 3:A:650:PX4:H9 | 0.43 | 2.29 | 15 | 1 |
| 3:A:635:PX4:H15 | 3:A:637:PX4:H8 | 0.43 | 1.91 | 15 | 1 |
| 3:B:342:PX4:O3 | 3:B:342:PX4:H13 | 0.43 | 2.14 | 4 | 2 |
| 3:A:614:PX4:H13 | 3:A:628:PX4:O1 | 0.43 | 2.14 | 9 | 1 |
| 3:B:365:PX4:O3 | 3:B:365:PX4:H12 | 0.43 | 2.12 | 10 | 1 |
| 3:C:335:PX4:O1 | 3:C:335:PX4:H3 | 0.43 | 2.14 | 10 | 1 |
| 3:B:308:PX4:H63 | 3:B:323:PX4:H38 | 0.43 | 1.91 | 14 | 1 |
| 3:B:335:PX4:O3 | 3:B:335:PX4:H13 | 0.43 | 2.14 | 3 | 1 |
| 3:B:375:PX4:O1 | 3:B:376:PX4:H8 | 0.43 | 2.14 | 3 | 1 |
| 3:B:328:PX4:O3 | 3:B:328:PX4:H13 | 0.43 | 2.14 | 5 | 1 |
| 3:C:359:PX4:H9 | 3:C:359:PX4:O3 | 0.43 | 2.14 | 12 | 1 |
| 3:B:312:PX4:H3 | 3:B:312:PX4:C6 | 0.43 | 2.44 | 14 | 1 |
| 2:C:80:GLU:CD | 3:C:304:PX4:H4 | 0.43 | 2.34 | 14 | 1 |
| 3:A:641:PX4:C6 | 3:A:641:PX4:H3 | 0.43 | 2.44 | 1 | 1 |
| 3:B:395:PX4:H4 | 3:B:395:PX4:O2 | 0.43 | 2.13 | 7 | 2 |
| 3:B:353:PX4:O4 | 3:B:369:PX4:H10 | 0.43 | 2.14 | 3 | 1 |
| 2:C:113:GLU:OE1 | 3:C:330:PX4:H13 | 0.43 | 2.14 | 6 | 1 |
| 3:B:311:PX4:O4 | 3:B:311:PX4:H3 | 0.43 | 2.13 | 8 | 2 |
| 3:B:359:PX4:H5 | 3:B:371:PX4:H9 | 0.42 | 1.91 | 2 | 1 |
| 3:B:325:PX4:O3 | 3:B:325:PX4:H7 | 0.42 | 2.13 | 3 | 1 |
| 3:C:352:PX4:O3 | 3:C:352:PX4:C3 | 0.42 | 2.67 | 4 | 1 |
| 3:A:608:PX4:H13 | 3:A:608:PX4:O3 | 0.42 | 2.14 | 5 | 1 |
| 3:C:344:PX4:O1 | 3:C:364:PX4:H4 | 0.42 | 2.13 | 5 | 1 |
| 3:A:605:PX4:O4 | 3:A:605:PX4:H12 | 0.42 | 2.14 | 7 | 1 |
| 3:A:643:PX4:O2 | 3:A:643:PX4:H4 | 0.42 | 2.12 | 8 | 1 |
| 3:B:378:PX4:H9 | 3:B:378:PX4:O3 | 0.42 | 2.14 | 8 | 1 |
| 3:C:355:PX4:H10 | 3:C:355:PX4:O1 | 0.42 | 2.14 | 11 | 1 |
| 3:A:632:PX4:O3 | 3:A:632:PX4:H10 | 0.42 | 2.14 | 12 | 1 |
| 3:B:355:PX4:H39 | 3:B:399:PX4:H43 | 0.42 | 1.91 | 4 | 1 |
| 3:C:302:PX4:O2 | 3:C:302:PX4:H4 | 0.42 | 2.14 | 7 | 1 |
| 3:C:340:PX4:H8 | 3:C:360:PX4:C6 | 0.42 | 2.44 | 10 | 1 |
| 3:B:375:PX4:O2 | 3:B:376:PX4:H5 | 0.42 | 2.15 | 12 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 3:A:632:PX4:O1 | 3:A:632:PX4:H4 | 0.42 | 2.14 | 2 | 1 |
| 3:B:312:PX4:H15 | 3:B:312:PX4:H10 | 0.42 | 1.90 | 2 | 1 |
| 3:B:313:PX4:O1 | 3:B:313:PX4:H4 | 0.42 | 2.14 | 2 | 1 |
| 3:A:616:PX4:H3 | 3:C:356:PX4:O4 | 0.42 | 2.13 | 4 | 1 |
| 3:B:307:PX4:H4 | 3:B:318:PX4:O1 | 0.42 | 2.15 | 4 | 1 |
| 3:B:373:PX4:H13 | 3:B:380:PX4:C1 | 0.42 | 2.44 | 6 | 1 |
| 3:C:342:PX4:H3 | 3:C:342:PX4:O4 | 0.42 | 2.13 | 6 | 2 |
| 1:A:382:PHE:CD1 | 1:A:415:ILE:HD12 | 0.42 | 2.50 | 8 | 1 |
| 3:B:350:PX4:O3 | 3:B:350:PX4:H9 | 0.42 | 2.14 | 15 | 2 |
| 3:A:629:PX4:O2 | 3:A:631:PX4:H6 | 0.42 | 2.14 | 11 | 1 |
| 3:C:338:PX4:H9 | 3:C:338:PX4:O3 | 0.42 | 2.15 | 13 | 1 |
| 3:A:619:PX4:H7 | 3:B:397:PX4:O2 | 0.42 | 2.14 | 14 | 1 |
| 3:B:377:PX4:O2 | 3:B:377:PX4:H6 | 0.42 | 2.14 | 15 | 1 |
| 3:B:382:PX4:O2 | 3:B:382:PX4:H4 | 0.42 | 2.14 | 15 | 1 |
| 2:B:80:GLU:OE2 | 3:B:305:PX4:H6 | 0.42 | 2.15 | 1 | 1 |
| 3:B:320:PX4:H11 | 3:B:340:PX4:H14 | 0.42 | 1.92 | 8 | 1 |
| 3:A:636:PX4:H3 | 3:A:636:PX4:O4 | 0.42 | 2.13 | 11 | 1 |
| 3:B:306:PX4:H8 | 3:B:339:PX4:O8 | 0.42 | 2.15 | 1 | 1 |
| 1:A:360:PHE:O | 3:A:644:PX4:H12 | 0.42 | 2.14 | 3 | 1 |
| 1:A:386:LYS:HE3 | 1:A:402:HIS:CE1 | 0.42 | 2.49 | 5 | 1 |
| 3:B:357:PX4:H4 | 3:B:357:PX4:O2 | 0.42 | 2.15 | 6 | 1 |
| 3:C:306:PX4:H17 | 3:C:306:PX4:O8 | 0.42 | 2.15 | 10 | 1 |
| 3:B:350:PX4:O1 | 3:B:374:PX4:H8 | 0.42 | 2.15 | 11 | 1 |
| 3:B:400:PX4:H3 | 3:B:400:PX4:H16 | 0.42 | 1.89 | 12 | 1 |
| 3:C:351:PX4:O6 | 3:C:351:PX4:H12 | 0.42 | 2.14 | 13 | 1 |
| 3:B:353:PX4:O3 | 3:B:369:PX4:H4 | 0.42 | 2.13 | 3 | 1 |
| 3:A:653:PX4:O3 | 3:A:653:PX4:H9 | 0.42 | 2.14 | 5 | 1 |
| 3:B:316:PX4:O3 | 3:B:316:PX4:C5 | 0.42 | 2.67 | 6 | 1 |
| 3:B:389:PX4:O3 | 3:B:389:PX4:C4 | 0.42 | 2.66 | 8 | 1 |
| 3:A:626:PX4:H48 | 3:A:634:PX4:H9 | 0.42 | 1.90 | 9 | 1 |
| 3:B:311:PX4:O8 | 3:B:345:PX4:H3 | 0.42 | 2.15 | 14 | 1 |
| 3:B:316:PX4:H53 | 3:B:344:PX4:C27 | 0.42 | 2.44 | 1 | 1 |
| 3:B:369:PX4:O2 | 3:B:386:PX4:H8 | 0.42 | 2.14 | 1 | 1 |
| 3:B:302:PX4:H4 | 3:B:302:PX4:O2 | 0.42 | 2.13 | 7 | 2 |
| 3:B:334:PX4:O2 | 3:B:348:PX4:H13 | 0.42 | 2.15 | 4 | 1 |
| 3:B:337:PX4:O3 | 3:B:337:PX4:H6 | 0.42 | 2.13 | 4 | 2 |
| 3:B:363:PX4:H11 | 3:B:381:PX4:P1 | 0.42 | 2.54 | 5 | 1 |
| 3:B:386:PX4:C1 | 3:B:388:PX4:H10 | 0.42 | 2.44 | 7 | 1 |
| 3:C:340:PX4:H4 | 3:C:340:PX4:O2 | 0.42 | 2.14 | 7 | 1 |
| 3:B:378:PX4:O1 | 3:C:302:PX4:H10 | 0.42 | 2.14 | 8 | 1 |
| 3:B:333:PX4:O1 | 3:B:333:PX4:H13 | 0.42 | 2.14 | 10 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 3:A:644:PX4:H29 | 3:A:654:PX4:H8 | 0.42 | 1.92 | 11 | 1 |
| 3:A:609:PX4:H5 | 3:B:384:PX4:O4 | 0.42 | 2.14 | 13 | 1 |
| 3:B:303:PX4:H43 | 3:C:327:PX4:H72 | 0.42 | 1.92 | 13 | 1 |
| 3:B:346:PX4:O1 | 3:B:371:PX4:H3 | 0.42 | 2.14 | 13 | 1 |
| 3:C:322:PX4:O1 | 3:C:351:PX4:H10 | 0.42 | 2.15 | 2 | 1 |
| 3:C:325:PX4:H24 | 3:C:359:PX4:H22 | 0.42 | 1.92 | 2 | 1 |
| 3:A:635:PX4:O4 | 3:A:637:PX4:H12 | 0.42 | 2.14 | 6 | 1 |
| 3:B:363:PX4:H5 | 3:B:381:PX4:O1 | 0.42 | 2.15 | 6 | 1 |
| 3:A:641:PX4:O2 | 3:A:651:PX4:H10 | 0.42 | 2.14 | 8 | 1 |
| 3:B:307:PX4:H2 | 3:B:307:PX4:C6 | 0.42 | 2.44 | 10 | 1 |
| 3:B:371:PX4:H10 | 3:B:371:PX4:O1 | 0.42 | 2.15 | 11 | 1 |
| 3:C:341:PX4:O1 | 3:C:349:PX4:H5 | 0.42 | 2.15 | 12 | 1 |
| 3:A:610:PX4:H6 | 3:A:612:PX4:O2 | 0.42 | 2.14 | 13 | 1 |
| 3:B:304:PX4:H39 | 3:B:340:PX4:H72 | 0.42 | 1.90 | 13 | 1 |
| 3:A:602:PX4:O2 | 3:A:602:PX4:H4 | 0.42 | 2.14 | 14 | 1 |
| 3:B:361:PX4:H12 | 3:B:361:PX4:O3 | 0.42 | 2.14 | 1 | 1 |
| 3:B:387:PX4:C1 | 3:B:387:PX4:C6 | 0.42 | 2.98 | 1 | 1 |
| 3:C:309:PX4:H34 | 3:C:315:PX4:H33 | 0.42 | 1.91 | 4 | 1 |
| 3:B:360:PX4:O2 | 3:B:362:PX4:H12 | 0.42 | 2.15 | 10 | 1 |
| 3:B:363:PX4:O8 | 3:B:363:PX4:H13 | 0.42 | 2.15 | 15 | 1 |
| 3:A:626:PX4:H13 | 3:C:362:PX4:H17 | 0.42 | 1.91 | 1 | 1 |
| 3:A:617:PX4:H11 | 3:A:625:PX4:O1 | 0.42 | 2.15 | 2 | 1 |
| 3:B:325:PX4:H38 | 3:B:331:PX4:H64 | 0.42 | 1.91 | 3 | 1 |
| 3:A:609:PX4:O1 | 3:A:609:PX4:H6 | 0.42 | 2.15 | 5 | 2 |
| 3:B:320:PX4:O4 | 3:B:320:PX4:H7 | 0.42 | 2.15 | 8 | 1 |
| 3:B:400:PX4:H5 | 3:C:347:PX4:H2 | 0.42 | 1.89 | 9 | 1 |
| 3:A:647:PX4:H9 | 3:A:647:PX4:O3 | 0.42 | 2.14 | 13 | 1 |
| 2:C:58:SER:OG | 3:C:332:PX4:H4 | 0.42 | 2.15 | 14 | 1 |
| 3:C:325:PX4:H4 | 3:C:334:PX4:O8 | 0.41 | 2.14 | 1 | 1 |
| 3:C:316:PX4:H7 | 3:C:316:PX4:O3 | 0.41 | 2.14 | 2 | 1 |
| 3:C:362:PX4:O6 | 3:C:362:PX4:H3 | 0.41 | 2.15 | 3 | 1 |
| 3:B:385:PX4:H6 | 3:B:385:PX4:O3 | 0.41 | 2.15 | 5 | 1 |
| 3:A:623:PX4:O3 | 3:A:623:PX4:H13 | 0.41 | 2.15 | 6 | 1 |
| 3:B:341:PX4:H45 | 3:C:344:PX4:H65 | 0.41 | 1.92 | 8 | 1 |
| 3:B:390:PX4:O3 | 3:B:390:PX4:H7 | 0.41 | 2.15 | 10 | 1 |
| 3:A:620:PX4:O3 | 3:A:620:PX4:H13 | 0.41 | 2.14 | 11 | 1 |
| 3:B:359:PX4:O3 | 3:B:359:PX4:H12 | 0.41 | 2.15 | 11 | 1 |
| 3:B:338:PX4:H11 | 3:B:365:PX4:C1 | 0.41 | 2.45 | 12 | 1 |
| 3:A:616:PX4:H7 | 3:A:616:PX4:O4 | 0.41 | 2.15 | 5 | 1 |
| 3:B:334:PX4:H9 | 3:B:352:PX4:O1 | 0.41 | 2.15 | 7 | 1 |
| 3:A:601:PX4:O1 | 3:B:377:PX4:C2 | 0.41 | 2.68 | 9 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 3:C:340:PX4:H10 | 3:C:360:PX4:O8 | 0.41 | 2.15 | 9 | 1 |
| 3:B:311:PX4:O3 | 3:B:311:PX4:H12 | 0.41 | 2.15 | 10 | 1 |
| 3:B:354:PX4:O3 | 3:B:354:PX4:H7 | 0.41 | 2.16 | 11 | 1 |
| 3:C:341:PX4:O2 | 3:C:349:PX4:H8 | 0.41 | 2.15 | 12 | 1 |
| 1:A:364:LEU:HD11 | 1:A:368:ILE:CG2 | 0.41 | 2.45 | 13 | 1 |
| 3:B:374:PX4:H7 | 3:B:374:PX4:O1 | 0.41 | 2.14 | 2 | 1 |
| 3:A:634:PX4:O2 | 3:A:634:PX4:H3 | 0.41 | 2.14 | 4 | 1 |
| 3:A:603:PX4:H5 | 3:A:609:PX4:O1 | 0.41 | 2.15 | 5 | 1 |
| 3:A:633:PX4:O2 | 3:A:633:PX4:H4 | 0.41 | 2.14 | 6 | 1 |
| 3:B:356:PX4:O3 | 3:B:356:PX4:H9 | 0.41 | 2.15 | 6 | 1 |
| 1:A:402:HIS:HE1 | 3:A:649:PX4:H4 | 0.41 | 1.74 | 8 | 1 |
| 3:A:627:PX4:H10 | 3:A:627:PX4:O3 | 0.41 | 2.16 | 9 | 1 |
| 3:B:323:PX4:O5 | 3:B:323:PX4:C23 | 0.41 | 2.68 | 12 | 1 |
| 3:C:332:PX4:H9 | 3:C:332:PX4:O3 | 0.41 | 2.15 | 13 | 1 |
| 3:A:621:PX4:O4 | 3:A:621:PX4:H13 | 0.41 | 2.15 | 3 | 1 |
| 3:B:361:PX4:H4 | 3:B:368:PX4:O1 | 0.41 | 2.15 | 4 | 1 |
| 3:C:305:PX4:H7 | 3:C:305:PX4:O3 | 0.41 | 2.15 | 7 | 1 |
| 2:B:130:TRP:NE1 | 2:C:177:HIS:CE1 | 0.41 | 2.89 | 8 | 1 |
| 3:C:332:PX4:H13 | 3:C:335:PX4:O2 | 0.41 | 2.15 | 9 | 1 |
| 3:A:622:PX4:O3 | 3:A:622:PX4:H12 | 0.41 | 2.14 | 11 | 1 |
| 3:B:357:PX4:H13 | 3:B:357:PX4:O3 | 0.41 | 2.16 | 11 | 1 |
| 2:C:113:GLU:OE1 | 3:C:330:PX4:H11 | 0.41 | 2.16 | 11 | 1 |
| 3:B:378:PX4:H12 | 3:B:386:PX4:O4 | 0.41 | 2.16 | 12 | 1 |
| 3:B:380:PX4:O2 | 3:B:387:PX4:H11 | 0.41 | 2.15 | 14 | 1 |
| 3:B:322:PX4:H10 | 3:B:350:PX4:C4 | 0.41 | 2.45 | 1 | 1 |
| 3:C:345:PX4:O4 | 3:C:345:PX4:H3 | 0.41 | 2.15 | 3 | 1 |
| 3:A:618:PX4:H10 | 3:A:618:PX4:O3 | 0.41 | 2.16 | 6 | 1 |
| 3:B:337:PX4:H45 | 3:B:368:PX4:H70 | 0.41 | 1.91 | 6 | 1 |
| 3:B:338:PX4:O1 | 3:B:358:PX4:H4 | 0.41 | 2.15 | 7 | 1 |
| 3:C:344:PX4:H3 | 3:C:364:PX4:O3 | 0.41 | 2.16 | 8 | 1 |
| 3:A:616:PX4:H22 | 3:C:337:PX4:H24 | 0.41 | 1.92 | 9 | 1 |
| 3:A:626:PX4:H5 | 3:C:362:PX4:O2 | 0.41 | 2.16 | 9 | 1 |
| 3:C:309:PX4:H7 | 3:C:315:PX4:O1 | 0.41 | 2.15 | 9 | 1 |
| 3:C:337:PX4:H10 | 3:C:337:PX4:O3 | 0.41 | 2.16 | 13 | 2 |
| 3:C:320:PX4:H10 | 3:C:341:PX4:O4 | 0.41 | 2.15 | 11 | 1 |
| 2:B:72:TRP:CD1 | 3:B:341:PX4:H4 | 0.41 | 2.50 | 12 | 1 |
| 3:A:614:PX4:H12 | 3:A:614:PX4:O2 | 0.41 | 2.16 | 13 | 1 |
| 3:B:323:PX4:O4 | 3:B:323:PX4:H4 | 0.41 | 2.15 | 14 | 1 |
| 3:B:387:PX4:O6 | 3:B:390:PX4:H12 | 0.41 | 2.15 | 15 | 1 |
| 3:C:307:PX4:H2 | 3:C:343:PX4:H14 | 0.41 | 1.93 | 1 | 1 |
| 3:A:604:PX4:H7 | 3:B:392:PX4:C1 | 0.41 | 2.45 | 2 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 3:A:652:PX4:H13 | 3:A:652:PX4:O3 | 0.41 | 2.15 | 2 | 1 |
| 3:B:390:PX4:O3 | 3:B:392:PX4:H8 | 0.41 | 2.15 | 2 | 1 |
| 3:C:319:PX4:H10 | 3:C:319:PX4:O1 | 0.41 | 2.16 | 3 | 1 |
| 3:A:634:PX4:H54 | 3:A:640:PX4:H44 | 0.41 | 1.91 | 8 | 1 |
| 3:C:340:PX4:H9 | 3:C:340:PX4:O1 | 0.41 | 2.15 | 8 | 1 |
| 3:B:314:PX4:O3 | 3:B:314:PX4:H12 | 0.41 | 2.15 | 9 | 1 |
| 3:A:605:PX4:O6 | 3:A:609:PX4:H3 | 0.41 | 2.16 | 13 | 2 |
| 3:B:382:PX4:H4 | 3:B:393:PX4:O1 | 0.41 | 2.16 | 10 | 1 |
| 3:B:304:PX4:H9 | 3:B:304:PX4:O3 | 0.41 | 2.16 | 11 | 1 |
| 3:C:346:PX4:H9 | 3:C:346:PX4:O3 | 0.41 | 2.15 | 11 | 1 |
| 3:A:616:PX4:H46 | 3:A:634:PX4:H8 | 0.41 | 1.92 | 12 | 1 |
| 3:C:349:PX4:H4 | 3:C:349:PX4:O8 | 0.41 | 2.15 | 13 | 1 |
| 3:B:312:PX4:H65 | 3:C:328:PX4:H39 | 0.41 | 1.91 | 15 | 1 |
| 3:A:614:PX4:H13 | 3:A:628:PX4:O2 | 0.41 | 2.15 | 1 | 1 |
| 3:B:338:PX4:H3 | 3:B:338:PX4:C6 | 0.41 | 2.45 | 2 | 1 |
| 3:C:357:PX4:H3 | 3:C:357:PX4:O4 | 0.41 | 2.14 | 2 | 1 |
| 3:B:310:PX4:H7 | 3:B:310:PX4:O2 | 0.41 | 2.15 | 4 | 1 |
| 1:A:361:TRP:HE1 | 1:A:364:LEU:HD22 | 0.41 | 1.76 | 5 | 1 |
| 3:B:368:PX4:O3 | 3:B:368:PX4:C4 | 0.41 | 2.67 | 7 | 1 |
| 3:B:382:PX4:H4 | 3:B:393:PX4:O2 | 0.41 | 2.16 | 8 | 1 |
| 3:A:612:PX4:C1 | 3:A:612:PX4:C6 | 0.41 | 2.99 | 9 | 1 |
| 3:C:329:PX4:H7 | 3:C:329:PX4:O3 | 0.41 | 2.16 | 13 | 1 |
| 3:B:329:PX4:H3 | 3:B:329:PX4:O1 | 0.41 | 2.16 | 1 | 1 |
| 3:C:357:PX4:H3 | 3:C:357:PX4:C6 | 0.41 | 2.45 | 3 | 1 |
| 3:A:602:PX4:H57 | 3:B:357:PX4:H30 | 0.41 | 1.92 | 4 | 1 |
| 3:A:641:PX4:O3 | 3:A:641:PX4:H9 | 0.41 | 2.16 | 4 | 1 |
| 3:C:318:PX4:H6 | 3:C:318:PX4:O3 | 0.41 | 2.16 | 4 | 1 |
| 3:C:306:PX4:O2 | 3:C:336:PX4:H5 | 0.41 | 2.16 | 6 | 1 |
| 2:B:129:LYS:NZ | 2:B:132:GLU:OE1 | 0.41 | 2.50 | 9 | 1 |
| 3:A:635:PX4:O1 | 3:A:635:PX4:H3 | 0.41 | 2.16 | 10 | 1 |
| 3:B:362:PX4:H7 | 3:B:366:PX4:H2 | 0.41 | 1.91 | 12 | 1 |
| 3:B:316:PX4:O3 | 3:B:316:PX4:H12 | 0.41 | 2.16 | 13 | 1 |
| 2:C:153:ARG:O | 2:C:157:HIS:CD2 | 0.41 | 2.74 | 14 | 1 |
| 3:A:602:PX4:H8 | 3:A:603:PX4:O2 | 0.41 | 2.15 | 1 | 1 |
| 3:B:335:PX4:H4 | 3:B:335:PX4:O2 | 0.41 | 2.16 | 1 | 1 |
| 3:B:359:PX4:H10 | 3:B:359:PX4:O3 | 0.41 | 2.16 | 1 | 1 |
| 3:B:365:PX4:O3 | 3:B:365:PX4:C4 | 0.41 | 2.69 | 2 | 1 |
| 3:B:312:PX4:H8 | 3:B:356:PX4:O4 | 0.41 | 2.16 | 4 | 1 |
| 3:B:329:PX4:O4 | 3:B:355:PX4:H5 | 0.41 | 2.16 | 4 | 1 |
| 3:B:339:PX4:H4 | 3:B:360:PX4:O2 | 0.41 | 2.15 | 4 | 1 |
| 3:B:391:PX4:H13 | 3:C:303:PX4:H15 | 0.41 | 1.92 | 4 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 3:C:323:PX4:H4 | 3:C:323:PX4:C7 | 0.41 | 2.46 | 4 | 1 |
| 3:B:343:PX4:H4 | 3:B:343:PX4:O4 | 0.41 | 2.16 | 5 | 1 |
| 3:B:378:PX4:O1 | 3:B:378:PX4:H3 | 0.41 | 2.16 | 5 | 1 |
| 3:A:645:PX4:H13 | 3:A:646:PX4:O2 | 0.41 | 2.16 | 6 | 1 |
| 3:B:387:PX4:H13 | 3:B:387:PX4:O3 | 0.41 | 2.16 | 6 | 1 |
| 3:C:344:PX4:C1 | 3:C:364:PX4:H6 | 0.41 | 2.46 | 6 | 1 |
| 3:B:342:PX4:O6 | 3:B:367:PX4:H7 | 0.41 | 2.16 | 7 | 1 |
| 3:B:400:PX4:C6 | 3:B:400:PX4:H3 | 0.41 | 2.46 | 7 | 1 |
| 3:B:317:PX4:O2 | 3:B:317:PX4:H9 | 0.41 | 2.15 | 8 | 1 |
| 3:C:332:PX4:H6 | 3:C:335:PX4:O4 | 0.41 | 2.16 | 9 | 1 |
| 3:C:323:PX4:O3 | 3:C:323:PX4:C3 | 0.41 | 2.69 | 10 | 1 |
| 3:B:312:PX4:O3 | 3:B:312:PX4:C5 | 0.41 | 2.69 | 13 | 1 |
| 3:A:617:PX4:O2 | 3:A:617:PX4:H4 | 0.41 | 2.15 | 15 | 1 |
| 3:B:306:PX4:C2 | 3:B:339:PX4:O8 | 0.41 | 2.69 | 15 | 1 |
| 3:B:330:PX4:H3 | 3:B:330:PX4:H16 | 0.41 | 1.93 | 15 | 1 |
| 3:C:357:PX4:H6 | 3:C:357:PX4:O3 | 0.41 | 2.15 | 15 | 1 |
| 3:A:625:PX4:H12 | 3:A:625:PX4:O3 | 0.41 | 2.16 | 2 | 1 |
| 3:C:323:PX4:H19 | 3:C:342:PX4:H27 | 0.41 | 1.93 | 4 | 1 |
| 3:A:622:PX4:H3 | 3:A:622:PX4:C6 | 0.41 | 2.46 | 5 | 1 |
| 3:B:322:PX4:O6 | 3:B:350:PX4:H5 | 0.41 | 2.15 | 5 | 1 |
| 3:B:359:PX4:O3 | 3:B:359:PX4:H10 | 0.41 | 2.16 | 8 | 1 |
| 1:A:362:ARG:HE | 3:A:650:PX4:C6 | 0.41 | 2.28 | 11 | 1 |
| 3:A:605:PX4:H3 | 3:B:379:PX4:C6 | 0.41 | 2.46 | 12 | 1 |
| 3:B:314:PX4:O1 | 3:B:314:PX4:H3 | 0.41 | 2.15 | 13 | 1 |
| 3:B:375:PX4:H9 | 3:B:375:PX4:O3 | 0.40 | 2.16 | 1 | 1 |
| 3:B:392:PX4:H15 | 3:B:392:PX4:H13 | 0.40 | 1.93 | 3 | 1 |
| 3:C:316:PX4:H13 | 3:C:342:PX4:O1 | 0.40 | 2.16 | 3 | 1 |
| 3:B:387:PX4:O1 | 3:B:387:PX4:H13 | 0.40 | 2.15 | 4 | 1 |
| 3:A:614:PX4:H12 | 3:A:614:PX4:O3 | 0.40 | 2.16 | 10 | 1 |
| 3:B:331:PX4:H4 | 3:B:331:PX4:H15 | 0.40 | 1.92 | 13 | 1 |
| 3:A:626:PX4:H4 | 3:C:346:PX4:O1 | 0.40 | 2.16 | 14 | 1 |
| 3:A:605:PX4:H12 | 3:A:605:PX4:O3 | 0.40 | 2.16 | 4 | 1 |
| 3:C:333:PX4:O3 | 3:C:333:PX4:H12 | 0.40 | 2.16 | 4 | 1 |
| 3:A:601:PX4:H11 | 3:A:601:PX4:O6 | 0.40 | 2.16 | 6 | 1 |
| 3:C:352:PX4:O4 | 3:C:352:PX4:H13 | 0.40 | 2.17 | 8 | 1 |
| 3:B:315:PX4:H10 | 3:B:336:PX4:O1 | 0.40 | 2.16 | 9 | 1 |
| 3:B:358:PX4:O3 | 3:B:358:PX4:H9 | 0.40 | 2.16 | 9 | 1 |
| 2:B:115:TYR:CE2 | 2:B:119:VAL:CG2 | 0.40 | 3.04 | 10 | 1 |
| 3:B:353:PX4:H9 | 3:B:369:PX4:O2 | 0.40 | 2.15 | 12 | 1 |
| 3:C:313:PX4:H8 | 3:C:337:PX4:H14 | 0.40 | 1.92 | 15 | 1 |
| 3:B:386:PX4:O3 | 3:B:386:PX4:H9 | 0.40 | 2.16 | 1 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 3:C:342:PX4:O3 | 3:C:342:PX4:H9 | 0.40 | 2.17 | 1 | 1 |
| 3:B:363:PX4:O2 | 3:B:368:PX4:H5 | 0.40 | 2.17 | 2 | 1 |
| 3:A:617:PX4:H26 | 3:C:355:PX4:H69 | 0.40 | 1.93 | 3 | 1 |
| 3:A:628:PX4:O3 | 3:A:628:PX4:H16 | 0.40 | 2.16 | 3 | 1 |
| 3:C:320:PX4:O3 | 3:C:320:PX4:H13 | 0.40 | 2.16 | 3 | 1 |
| 3:C:314:PX4:H13 | 3:C:314:PX4:O2 | 0.40 | 2.17 | 4 | 1 |
| 3:A:649:PX4:H58 | 3:A:649:PX4:C13 | 0.40 | 2.46 | 5 | 1 |
| 3:B:325:PX4:H11 | 3:B:357:PX4:O2 | 0.40 | 2.16 | 6 | 1 |
| 3:C:310:PX4:H13 | 3:C:310:PX4:O3 | 0.40 | 2.17 | 8 | 1 |
| 3:B:398:PX4:H6 | 3:C:357:PX4:O3 | 0.40 | 2.17 | 10 | 1 |
| 2:C:91:GLU:OE1 | 3:C:314:PX4:H6 | 0.40 | 2.17 | 10 | 1 |
| 3:C:340:PX4:H8 | 3:C:360:PX4:H14 | 0.40 | 1.92 | 10 | 1 |
| 3:C:322:PX4:O3 | 3:C:322:PX4:H13 | 0.40 | 2.16 | 11 | 1 |
| 3:B:350:PX4:O1 | 3:B:350:PX4:H3 | 0.40 | 2.17 | 13 | 1 |
| 1:A:443:ARG:HD2 | 3:A:651:PX4:H7 | 0.40 | 1.93 | 14 | 1 |
| 3:B:395:PX4:O1 | 3:C:312:PX4:H8 | 0.40 | 2.16 | 15 | 1 |
| 3:B:360:PX4:O3 | 3:B:360:PX4:C4 | 0.40 | 2.70 | 3 | 1 |
| 1:A:359:GLN:OE1 | 3:A:650:PX4:H8 | 0.40 | 2.16 | 4 | 1 |
| 3:C:315:PX4:H3 | 3:C:353:PX4:O2 | 0.40 | 2.17 | 4 | 1 |
| 3:A:649:PX4:H58 | 3:A:649:PX4:H26 | 0.40 | 1.93 | 5 | 1 |
| 3:C:317:PX4:H4 | 3:C:333:PX4:C8 | 0.40 | 2.46 | 5 | 1 |
| 3:B:375:PX4:C6 | 3:B:376:PX4:H5 | 0.40 | 2.47 | 6 | 1 |
| 3:B:387:PX4:H13 | 3:B:387:PX4:O1 | 0.40 | 2.16 | 6 | 1 |
| 3:C:344:PX4:O3 | 3:C:364:PX4:H6 | 0.40 | 2.17 | 6 | 1 |
| 3:B:363:PX4:H8 | 3:B:381:PX4:H1 | 0.40 | 1.93 | 7 | 1 |
| 2:C:226:SER:OG | 3:C:317:PX4:H10 | 0.40 | 2.16 | 11 | 1 |
| 3:B:341:PX4:H7 | 3:B:341:PX4:O4 | 0.40 | 2.16 | 12 | 1 |
| 3:B:341:PX4:H54 | 3:B:373:PX4:C11 | 0.40 | 2.46 | 14 | 1 |
| 3:A:619:PX4:H58 | 3:A:632:PX4:H8 | 0.40 | 1.93 | 15 | 1 |
| 3:B:316:PX4:H8 | 3:B:322:PX4:O1 | 0.40 | 2.16 | 1 | 1 |
| 2:C:164:SER:OG | 3:C:305:PX4:H8 | 0.40 | 2.15 | 2 | 1 |
| 3:A:607:PX4:O2 | 3:A:607:PX4:H4 | 0.40 | 2.16 | 3 | 1 |
| 3:B:368:PX4:O3 | 3:B:368:PX4:H9 | 0.40 | 2.17 | 3 | 1 |
| 3:C:332:PX4:O3 | 3:C:332:PX4:H9 | 0.40 | 2.16 | 9 | 1 |
| 3:B:396:PX4:H3 | 3:B:396:PX4:O1 | 0.40 | 2.16 | 10 | 1 |
| 3:B:356:PX4:H9 | 3:B:356:PX4:O1 | 0.40 | 2.16 | 11 | 1 |
| 3:B:399:PX4:O2 | 3:C:326:PX4:H3 | 0.40 | 2.17 | 12 | 1 |
| 1:A:364:LEU:HD11 | 1:A:368:ILE:HG21 | 0.40 | 1.93 | 13 | 1 |
| 3:B:363:PX4:H3 | 3:B:363:PX4:O4 | 0.40 | 2.17 | 13 | 1 |

6.3 Torsion angles

6.3.1 Protein backbone

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|---------------|-------------|------------|-------------|----|
| 1 | A | 194/196 (99%) | 176±3 (91±1%) | 15±3 (8±1%) | 3±1 (2±1%) | 13 | 57 |
| 2 | B | 209/211 (99%) | 205±2 (98±1%) | 4±2 (2±1%) | 0±0 (0±0%) | 50 | 82 |
| 2 | C | 207/211 (98%) | 202±2 (98±1%) | 4±2 (2±1%) | 1±1 (0±0%) | 44 | 80 |
| All | All | 9150/9270 (99%) | 8751 (96%) | 338 (4%) | 61 (1%) | 26 | 73 |

All 34 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | A | 448 | GLU | 5 |
| 1 | A | 367 | SER | 4 |
| 1 | A | 411 | PRO | 4 |
| 1 | A | 510 | SER | 3 |
| 2 | C | 65 | GLY | 3 |
| 1 | A | 491 | LEU | 3 |
| 1 | A | 322 | ASN | 3 |
| 1 | A | 472 | GLU | 2 |
| 1 | A | 446 | ASP | 2 |
| 1 | A | 466 | SER | 2 |
| 1 | A | 479 | LYS | 2 |
| 1 | A | 338 | GLU | 2 |
| 1 | A | 354 | PRO | 2 |
| 2 | B | 65 | GLY | 2 |
| 2 | C | 100 | TYR | 2 |
| 1 | A | 454 | LYS | 2 |
| 1 | A | 443 | ARG | 1 |
| 1 | A | 463 | PRO | 1 |
| 1 | A | 347 | ASN | 1 |
| 1 | A | 395 | LEU | 1 |
| 1 | A | 394 | SER | 1 |
| 1 | A | 375 | LYS | 1 |
| 2 | C | 121 | PRO | 1 |
| 1 | A | 404 | LYS | 1 |
| 1 | A | 366 | ALA | 1 |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | A | 370 | THR | 1 |
| 1 | A | 393 | ALA | 1 |
| 2 | B | 187 | PRO | 1 |
| 1 | A | 368 | ILE | 1 |
| 2 | B | 66 | PRO | 1 |
| 2 | C | 99 | PRO | 1 |
| 1 | A | 450 | PRO | 1 |
| 2 | B | 98 | GLN | 1 |
| 2 | C | 142 | GLU | 1 |

6.3.2 Protein sidechains ⓘ

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|---------------|------------|-------------|----|
| 1 | A | 169/169 (100%) | 163±3 (97±2%) | 6±3 (3±2%) | 39 | 86 |
| 2 | B | 187/187 (100%) | 182±1 (97±1%) | 5±1 (3±1%) | 49 | 91 |
| 2 | C | 184/187 (98%) | 181±1 (98±1%) | 3±1 (2±1%) | 66 | 95 |
| All | All | 8100/8145 (99%) | 7897 (97%) | 203 (3%) | 50 | 91 |

All 92 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 2 | B | 145 | ARG | 15 |
| 2 | B | 210 | ARG | 15 |
| 1 | A | 361 | TRP | 14 |
| 1 | A | 492 | LYS | 14 |
| 2 | B | 116 | ARG | 7 |
| 1 | A | 368 | ILE | 7 |
| 2 | C | 106 | LYS | 6 |
| 1 | A | 342 | TRP | 5 |
| 1 | A | 412 | THR | 5 |
| 1 | A | 422 | MET | 4 |
| 1 | A | 372 | TYR | 4 |
| 1 | A | 365 | PRO | 3 |
| 2 | B | 156 | LEU | 3 |
| 2 | C | 114 | LEU | 3 |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | A | 325 | THR | 3 |
| 1 | A | 388 | TRP | 3 |
| 2 | B | 96 | LYS | 3 |
| 2 | B | 106 | LYS | 3 |
| 2 | C | 119 | VAL | 3 |
| 1 | A | 486 | PHE | 2 |
| 1 | A | 349 | VAL | 2 |
| 2 | C | 99 | PRO | 2 |
| 1 | A | 411 | PRO | 2 |
| 2 | C | 234 | GLU | 2 |
| 1 | A | 341 | PHE | 2 |
| 1 | A | 433 | ASN | 2 |
| 1 | A | 509 | PRO | 2 |
| 2 | C | 192 | LEU | 2 |
| 2 | B | 261 | LYS | 2 |
| 1 | A | 394 | SER | 1 |
| 2 | B | 56 | THR | 1 |
| 2 | B | 68 | THR | 1 |
| 2 | C | 56 | THR | 1 |
| 2 | C | 71 | PHE | 1 |
| 2 | C | 140 | LYS | 1 |
| 2 | C | 231 | PRO | 1 |
| 2 | C | 259 | THR | 1 |
| 1 | A | 390 | PHE | 1 |
| 2 | B | 221 | HIS | 1 |
| 1 | A | 423 | PRO | 1 |
| 1 | A | 435 | TYR | 1 |
| 1 | A | 484 | TRP | 1 |
| 2 | B | 131 | GLN | 1 |
| 2 | B | 226 | SER | 1 |
| 2 | C | 121 | PRO | 1 |
| 2 | C | 123 | LEU | 1 |
| 1 | A | 397 | PRO | 1 |
| 2 | B | 87 | SER | 1 |
| 2 | B | 160 | GLN | 1 |
| 2 | B | 183 | THR | 1 |
| 2 | C | 86 | MET | 1 |
| 2 | B | 69 | GLN | 1 |
| 2 | B | 93 | VAL | 1 |
| 2 | B | 215 | HIS | 1 |
| 2 | C | 141 | VAL | 1 |
| 2 | C | 179 | ASP | 1 |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 2 | C | 214 | TYR | 1 |
| 2 | C | 213 | GLU | 1 |
| 1 | A | 370 | THR | 1 |
| 1 | A | 374 | ARG | 1 |
| 1 | A | 453 | ILE | 1 |
| 2 | B | 74 | ASN | 1 |
| 1 | A | 362 | ARG | 1 |
| 2 | B | 149 | GLN | 1 |
| 2 | C | 100 | TYR | 1 |
| 2 | C | 247 | PHE | 1 |
| 2 | C | 250 | SER | 1 |
| 1 | A | 404 | LYS | 1 |
| 2 | B | 166 | LEU | 1 |
| 2 | B | 231 | PRO | 1 |
| 2 | C | 154 | GLN | 1 |
| 2 | C | 211 | LEU | 1 |
| 2 | C | 251 | PHE | 1 |
| 2 | B | 63 | GLN | 1 |
| 2 | B | 165 | PRO | 1 |
| 2 | C | 66 | PRO | 1 |
| 2 | C | 144 | LEU | 1 |
| 1 | A | 467 | PHE | 1 |
| 2 | B | 141 | VAL | 1 |
| 2 | B | 237 | ARG | 1 |
| 2 | C | 221 | HIS | 1 |
| 1 | A | 402 | HIS | 1 |
| 2 | B | 154 | GLN | 1 |
| 2 | B | 242 | PRO | 1 |
| 2 | C | 173 | ARG | 1 |
| 2 | C | 227 | GLU | 1 |
| 2 | B | 84 | GLN | 1 |
| 2 | B | 108 | TRP | 1 |
| 2 | B | 126 | PHE | 1 |
| 2 | B | 251 | PHE | 1 |
| 1 | A | 340 | TRP | 1 |
| 2 | C | 122 | TYR | 1 |

6.3.3 RNA ⓘ

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

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

| Mol | Type | Chain | Res | Link | Bond lengths | | |
|-----|------|-------|-----|------|--------------|-----------|------------|
| | | | | | Counts | RMSZ | #Z>2 |
| 3 | PX4 | B | 326 | - | 45,45,45 | 1.08±0.14 | 3±2 (6±4%) |
| 3 | PX4 | A | 627 | - | 45,45,45 | 1.11±0.12 | 4±1 (7±3%) |
| 3 | PX4 | B | 393 | - | 45,45,45 | 1.11±0.14 | 3±2 (7±4%) |
| 3 | PX4 | B | 392 | - | 45,45,45 | 1.05±0.11 | 3±1 (6±2%) |
| 3 | PX4 | C | 336 | - | 45,45,45 | 1.06±0.08 | 3±1 (6±2%) |
| 3 | PX4 | B | 391 | - | 45,45,45 | 1.04±0.07 | 2±1 (5±2%) |
| 3 | PX4 | B | 319 | - | 45,45,45 | 1.08±0.10 | 3±1 (5±3%) |
| 3 | PX4 | A | 608 | - | 45,45,45 | 1.04±0.08 | 3±2 (6±3%) |
| 3 | PX4 | B | 304 | - | 45,45,45 | 1.03±0.13 | 2±2 (5±3%) |
| 3 | PX4 | A | 609 | - | 45,45,45 | 1.09±0.11 | 4±1 (7±3%) |
| 3 | PX4 | B | 348 | - | 45,45,45 | 1.07±0.11 | 3±1 (6±2%) |
| 3 | PX4 | B | 355 | - | 45,45,45 | 1.11±0.12 | 4±2 (8±4%) |
| 3 | PX4 | B | 305 | - | 45,45,45 | 1.09±0.08 | 3±1 (6±2%) |
| 3 | PX4 | B | 333 | - | 45,45,45 | 1.09±0.11 | 3±1 (6±3%) |
| 3 | PX4 | C | 350 | - | 45,45,45 | 1.09±0.11 | 3±1 (6±2%) |
| 3 | PX4 | B | 376 | - | 45,45,45 | 1.10±0.09 | 3±2 (7±3%) |
| 3 | PX4 | B | 317 | - | 45,45,45 | 1.05±0.11 | 3±1 (6±2%) |
| 3 | PX4 | B | 357 | - | 45,45,45 | 1.07±0.12 | 3±1 (6±3%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | |
|-----|------|-------|-----|------|--------------|-----------|------------|
| | | | | | Counts | RMSZ | #Z>2 |
| 3 | PX4 | A | 629 | - | 45,45,45 | 1.07±0.10 | 3±1 (5±2%) |
| 3 | PX4 | C | 329 | - | 45,45,45 | 1.16±0.12 | 4±2 (8±4%) |
| 3 | PX4 | B | 323 | - | 45,45,45 | 1.08±0.13 | 3±2 (6±3%) |
| 3 | PX4 | C | 342 | - | 45,45,45 | 1.04±0.13 | 3±1 (6±3%) |
| 3 | PX4 | C | 321 | - | 45,45,45 | 1.10±0.13 | 4±2 (8±4%) |
| 3 | PX4 | B | 330 | - | 45,45,45 | 1.09±0.09 | 3±1 (6±2%) |
| 3 | PX4 | A | 634 | - | 45,45,45 | 1.04±0.10 | 3±1 (6±3%) |
| 3 | PX4 | C | 319 | - | 45,45,45 | 1.04±0.10 | 3±1 (5±2%) |
| 3 | PX4 | C | 341 | - | 45,45,45 | 1.10±0.11 | 3±1 (7±2%) |
| 3 | PX4 | B | 395 | - | 45,45,45 | 1.04±0.11 | 2±1 (4±2%) |
| 3 | PX4 | C | 332 | - | 45,45,45 | 1.06±0.11 | 3±1 (7±3%) |
| 3 | PX4 | C | 310 | - | 45,45,45 | 1.06±0.11 | 3±1 (5±2%) |
| 3 | PX4 | B | 350 | - | 45,45,45 | 1.09±0.08 | 3±1 (7±3%) |
| 3 | PX4 | B | 336 | - | 45,45,45 | 1.03±0.12 | 3±2 (5±4%) |
| 3 | PX4 | C | 331 | - | 45,45,45 | 1.03±0.11 | 2±1 (5±2%) |
| 3 | PX4 | C | 355 | - | 45,45,45 | 1.11±0.11 | 4±2 (8±4%) |
| 3 | PX4 | B | 320 | - | 45,45,45 | 1.08±0.11 | 3±1 (6±2%) |
| 3 | PX4 | B | 367 | - | 45,45,45 | 1.09±0.11 | 3±1 (5±3%) |
| 3 | PX4 | A | 625 | - | 45,45,45 | 1.08±0.11 | 3±2 (6±3%) |
| 3 | PX4 | B | 344 | - | 45,45,45 | 1.07±0.12 | 4±2 (7±3%) |
| 3 | PX4 | B | 327 | - | 45,45,45 | 1.10±0.13 | 3±2 (7±3%) |
| 3 | PX4 | B | 321 | - | 45,45,45 | 1.11±0.10 | 3±2 (7±3%) |
| 3 | PX4 | C | 301 | - | 45,45,45 | 1.08±0.08 | 3±1 (7±2%) |
| 3 | PX4 | A | 631 | - | 45,45,45 | 1.11±0.12 | 3±2 (7±3%) |
| 3 | PX4 | C | 354 | - | 45,45,45 | 1.11±0.09 | 3±1 (7±3%) |
| 3 | PX4 | C | 315 | - | 45,45,45 | 1.07±0.10 | 2±1 (5±2%) |
| 3 | PX4 | A | 618 | - | 45,45,45 | 1.05±0.10 | 2±1 (5±2%) |
| 3 | PX4 | C | 353 | - | 45,45,45 | 1.08±0.10 | 3±1 (7±2%) |
| 3 | PX4 | A | 635 | - | 45,45,45 | 1.07±0.13 | 3±2 (7±4%) |
| 3 | PX4 | C | 346 | - | 45,45,45 | 1.09±0.09 | 3±2 (5±3%) |
| 3 | PX4 | B | 387 | - | 45,45,45 | 1.06±0.11 | 3±2 (5±3%) |
| 3 | PX4 | C | 340 | - | 45,45,45 | 1.06±0.09 | 3±1 (6±3%) |
| 3 | PX4 | C | 318 | - | 45,45,45 | 1.07±0.14 | 3±1 (5±2%) |
| 3 | PX4 | C | 327 | - | 45,45,45 | 1.06±0.08 | 3±1 (6±2%) |
| 3 | PX4 | C | 352 | - | 45,45,45 | 1.14±0.11 | 3±1 (7±2%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | |
|-----|------|-------|-----|------|--------------|-----------|------------|
| | | | | | Counts | RMSZ | #Z>2 |
| 3 | PX4 | A | 620 | - | 45,45,45 | 1.04±0.10 | 3±1 (5±2%) |
| 3 | PX4 | A | 633 | - | 45,45,45 | 1.07±0.13 | 3±1 (5±3%) |
| 3 | PX4 | C | 309 | - | 45,45,45 | 1.10±0.17 | 3±2 (6±4%) |
| 3 | PX4 | B | 342 | - | 45,45,45 | 1.11±0.10 | 3±2 (6±3%) |
| 3 | PX4 | C | 304 | - | 45,45,45 | 1.12±0.10 | 3±2 (7±3%) |
| 3 | PX4 | A | 602 | - | 45,45,45 | 1.08±0.11 | 3±2 (6±3%) |
| 3 | PX4 | B | 400 | - | 45,45,45 | 1.07±0.12 | 3±1 (6±3%) |
| 3 | PX4 | C | 330 | - | 45,45,45 | 1.08±0.12 | 3±2 (7±4%) |
| 3 | PX4 | B | 360 | - | 45,45,45 | 1.09±0.11 | 3±2 (7±3%) |
| 3 | PX4 | C | 364 | - | 45,45,45 | 1.10±0.11 | 3±2 (7±3%) |
| 3 | PX4 | C | 345 | - | 45,45,45 | 1.09±0.13 | 3±2 (6±3%) |
| 3 | PX4 | C | 362 | - | 45,45,45 | 1.09±0.13 | 3±2 (6±3%) |
| 3 | PX4 | A | 648 | - | 45,45,45 | 1.10±0.09 | 3±1 (7±2%) |
| 3 | PX4 | B | 310 | - | 45,45,45 | 1.10±0.16 | 3±1 (6±3%) |
| 3 | PX4 | A | 639 | - | 45,45,45 | 1.13±0.14 | 4±2 (9±4%) |
| 3 | PX4 | A | 622 | - | 45,45,45 | 1.07±0.09 | 3±1 (6±2%) |
| 3 | PX4 | B | 389 | - | 45,45,45 | 1.08±0.13 | 3±1 (6±2%) |
| 3 | PX4 | A | 649 | - | 45,45,45 | 1.08±0.12 | 3±1 (6±3%) |
| 3 | PX4 | B | 383 | - | 45,45,45 | 1.10±0.13 | 4±2 (8±3%) |
| 3 | PX4 | B | 347 | - | 45,45,45 | 1.07±0.06 | 3±1 (7±2%) |
| 3 | PX4 | C | 361 | - | 45,45,45 | 1.07±0.15 | 3±2 (5±3%) |
| 3 | PX4 | A | 642 | - | 45,45,45 | 1.08±0.09 | 3±1 (7±2%) |
| 3 | PX4 | C | 324 | - | 45,45,45 | 1.04±0.09 | 2±2 (5±3%) |
| 3 | PX4 | B | 346 | - | 45,45,45 | 1.09±0.12 | 3±1 (6±2%) |
| 3 | PX4 | A | 610 | - | 45,45,45 | 1.07±0.12 | 3±2 (6±3%) |
| 3 | PX4 | B | 318 | - | 45,45,45 | 1.04±0.11 | 3±2 (5±3%) |
| 3 | PX4 | A | 616 | - | 45,45,45 | 1.08±0.11 | 3±1 (6±2%) |
| 3 | PX4 | B | 349 | - | 45,45,45 | 1.09±0.06 | 3±1 (7±2%) |
| 3 | PX4 | B | 334 | - | 45,45,45 | 1.07±0.09 | 3±1 (6±2%) |
| 3 | PX4 | B | 379 | - | 45,45,45 | 1.06±0.10 | 3±1 (7±2%) |
| 3 | PX4 | B | 397 | - | 45,45,45 | 1.07±0.11 | 3±1 (7±2%) |
| 3 | PX4 | B | 339 | - | 45,45,45 | 1.05±0.09 | 3±1 (6±3%) |
| 3 | PX4 | C | 302 | - | 45,45,45 | 1.05±0.07 | 3±1 (7±1%) |
| 3 | PX4 | B | 322 | - | 45,45,45 | 1.10±0.12 | 3±1 (7±2%) |
| 3 | PX4 | C | 357 | - | 45,45,45 | 1.04±0.13 | 2±1 (5±2%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | |
|-----|------|-------|-----|------|--------------|-----------|------------|
| | | | | | Counts | RMSZ | #Z>2 |
| 3 | PX4 | A | 644 | - | 45,45,45 | 1.03±0.13 | 3±2 (6±3%) |
| 3 | PX4 | C | 317 | - | 45,45,45 | 1.08±0.14 | 3±2 (6±4%) |
| 3 | PX4 | B | 354 | - | 45,45,45 | 1.08±0.08 | 3±1 (6±2%) |
| 3 | PX4 | C | 314 | - | 45,45,45 | 1.06±0.11 | 2±1 (5±3%) |
| 3 | PX4 | B | 378 | - | 45,45,45 | 1.06±0.12 | 3±1 (6±2%) |
| 3 | PX4 | C | 343 | - | 45,45,45 | 1.09±0.10 | 3±1 (6±1%) |
| 3 | PX4 | C | 358 | - | 45,45,45 | 1.03±0.10 | 3±1 (5±2%) |
| 3 | PX4 | B | 302 | - | 45,45,45 | 1.09±0.13 | 3±2 (7±4%) |
| 3 | PX4 | A | 630 | - | 45,45,45 | 1.05±0.09 | 3±2 (6±3%) |
| 3 | PX4 | B | 388 | - | 45,45,45 | 1.07±0.11 | 3±2 (6±3%) |
| 3 | PX4 | C | 323 | - | 45,45,45 | 1.06±0.17 | 3±2 (6±4%) |
| 3 | PX4 | B | 311 | - | 45,45,45 | 1.15±0.12 | 4±1 (9±2%) |
| 3 | PX4 | B | 363 | - | 45,45,45 | 1.04±0.11 | 2±1 (5±2%) |
| 3 | PX4 | A | 652 | - | 45,45,45 | 1.05±0.07 | 3±1 (6±2%) |
| 3 | PX4 | B | 313 | - | 45,45,45 | 1.06±0.14 | 3±2 (6±3%) |
| 3 | PX4 | C | 334 | - | 45,45,45 | 1.05±0.14 | 3±2 (6±3%) |
| 3 | PX4 | B | 394 | - | 45,45,45 | 1.09±0.12 | 3±2 (7±3%) |
| 3 | PX4 | B | 312 | - | 45,45,45 | 1.10±0.14 | 4±2 (8±4%) |
| 3 | PX4 | B | 385 | - | 45,45,45 | 1.10±0.12 | 3±1 (7±3%) |
| 3 | PX4 | B | 356 | - | 45,45,45 | 1.04±0.14 | 3±2 (5±3%) |
| 3 | PX4 | C | 339 | - | 45,45,45 | 1.06±0.10 | 3±1 (6±2%) |
| 3 | PX4 | B | 359 | - | 45,45,45 | 1.08±0.09 | 3±1 (6±3%) |
| 3 | PX4 | B | 306 | - | 45,45,45 | 1.06±0.13 | 3±2 (6±3%) |
| 3 | PX4 | B | 390 | - | 45,45,45 | 1.07±0.10 | 3±1 (7±3%) |
| 3 | PX4 | C | 335 | - | 45,45,45 | 1.14±0.12 | 3±1 (6±3%) |
| 3 | PX4 | A | 653 | - | 45,45,45 | 1.11±0.13 | 4±2 (8±3%) |
| 3 | PX4 | B | 375 | - | 45,45,45 | 1.02±0.08 | 3±1 (5±1%) |
| 3 | PX4 | B | 364 | - | 45,45,45 | 1.07±0.14 | 3±2 (7±4%) |
| 3 | PX4 | B | 341 | - | 45,45,45 | 1.07±0.07 | 3±1 (5±3%) |
| 3 | PX4 | B | 343 | - | 45,45,45 | 1.05±0.12 | 3±1 (5±3%) |
| 3 | PX4 | B | 372 | - | 45,45,45 | 1.04±0.12 | 3±2 (6±3%) |
| 3 | PX4 | B | 370 | - | 45,45,45 | 1.06±0.10 | 3±1 (5±2%) |
| 3 | PX4 | A | 607 | - | 45,45,45 | 1.11±0.13 | 3±1 (6±2%) |
| 3 | PX4 | B | 331 | - | 45,45,45 | 1.08±0.12 | 3±2 (6±3%) |
| 3 | PX4 | B | 337 | - | 45,45,45 | 1.06±0.13 | 3±2 (7±3%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | |
|-----|------|-------|-----|------|--------------|-----------|------------|
| | | | | | Counts | RMSZ | #Z>2 |
| 3 | PX4 | A | 654 | - | 45,45,45 | 1.05±0.11 | 3±2 (6±3%) |
| 3 | PX4 | C | 305 | - | 45,45,45 | 1.09±0.13 | 3±2 (7±4%) |
| 3 | PX4 | C | 308 | - | 45,45,45 | 1.11±0.11 | 4±2 (8±3%) |
| 3 | PX4 | A | 640 | - | 45,45,45 | 1.07±0.09 | 3±1 (6±2%) |
| 3 | PX4 | A | 645 | - | 45,45,45 | 1.11±0.09 | 3±1 (6±1%) |
| 3 | PX4 | C | 347 | - | 45,45,45 | 1.08±0.14 | 3±1 (6±3%) |
| 3 | PX4 | C | 359 | - | 45,45,45 | 1.12±0.12 | 3±1 (6±3%) |
| 3 | PX4 | B | 329 | - | 45,45,45 | 1.12±0.11 | 4±1 (8±2%) |
| 3 | PX4 | C | 338 | - | 45,45,45 | 1.03±0.11 | 3±2 (6±4%) |
| 3 | PX4 | C | 328 | - | 45,45,45 | 1.10±0.11 | 3±1 (7±2%) |
| 3 | PX4 | A | 604 | - | 45,45,45 | 1.06±0.10 | 3±1 (6±2%) |
| 3 | PX4 | B | 351 | - | 45,45,45 | 1.07±0.14 | 3±2 (5±3%) |
| 3 | PX4 | C | 322 | - | 45,45,45 | 1.05±0.13 | 3±1 (6±2%) |
| 3 | PX4 | C | 312 | - | 45,45,45 | 1.08±0.11 | 3±2 (7±3%) |
| 3 | PX4 | C | 349 | - | 45,45,45 | 1.05±0.12 | 3±2 (6±4%) |
| 3 | PX4 | C | 337 | - | 45,45,45 | 1.07±0.09 | 3±2 (6±3%) |
| 3 | PX4 | B | 399 | - | 45,45,45 | 1.04±0.11 | 3±2 (6±3%) |
| 3 | PX4 | B | 362 | - | 45,45,45 | 1.06±0.11 | 3±1 (6±3%) |
| 3 | PX4 | A | 615 | - | 45,45,45 | 1.05±0.13 | 2±1 (5±3%) |
| 3 | PX4 | B | 396 | - | 45,45,45 | 1.10±0.14 | 4±2 (8±3%) |
| 3 | PX4 | A | 621 | - | 45,45,45 | 1.04±0.10 | 3±1 (5±3%) |
| 3 | PX4 | B | 374 | - | 45,45,45 | 1.08±0.14 | 3±2 (6±3%) |
| 3 | PX4 | A | 638 | - | 45,45,45 | 1.04±0.12 | 2±1 (5±3%) |
| 3 | PX4 | B | 358 | - | 45,45,45 | 1.07±0.09 | 3±1 (6±2%) |
| 3 | PX4 | B | 365 | - | 45,45,45 | 1.06±0.14 | 3±2 (6±3%) |
| 3 | PX4 | A | 601 | - | 45,45,45 | 1.10±0.08 | 3±1 (7±2%) |
| 3 | PX4 | C | 303 | - | 45,45,45 | 1.08±0.17 | 3±2 (6±3%) |
| 3 | PX4 | B | 377 | - | 45,45,45 | 1.08±0.11 | 3±1 (7±3%) |
| 3 | PX4 | B | 332 | - | 45,45,45 | 1.11±0.11 | 3±1 (7±3%) |
| 3 | PX4 | A | 650 | - | 45,45,45 | 1.07±0.08 | 3±1 (6±2%) |
| 3 | PX4 | B | 303 | - | 45,45,45 | 1.02±0.14 | 3±2 (5±3%) |
| 3 | PX4 | B | 366 | - | 45,45,45 | 1.02±0.11 | 3±1 (6±2%) |
| 3 | PX4 | B | 352 | - | 45,45,45 | 1.09±0.16 | 3±1 (6±3%) |
| 3 | PX4 | B | 328 | - | 45,45,45 | 1.10±0.08 | 3±1 (7±2%) |
| 3 | PX4 | B | 353 | - | 45,45,45 | 1.10±0.13 | 3±1 (6±3%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | |
|-----|------|-------|-----|------|--------------|-----------|------------|
| | | | | | Counts | RMSZ | #Z>2 |
| 3 | PX4 | B | 301 | - | 45,45,45 | 1.11±0.11 | 4±2 (7±3%) |
| 3 | PX4 | C | 313 | - | 45,45,45 | 1.04±0.12 | 2±2 (5±3%) |
| 3 | PX4 | B | 384 | - | 45,45,45 | 1.11±0.11 | 3±1 (7±3%) |
| 3 | PX4 | A | 617 | - | 45,45,45 | 1.08±0.10 | 3±2 (7±4%) |
| 3 | PX4 | C | 363 | - | 45,45,45 | 1.09±0.12 | 3±2 (7±3%) |
| 3 | PX4 | A | 641 | - | 45,45,45 | 1.04±0.11 | 3±1 (5±2%) |
| 3 | PX4 | B | 335 | - | 45,45,45 | 1.04±0.10 | 3±1 (5±2%) |
| 3 | PX4 | A | 612 | - | 45,45,45 | 1.02±0.11 | 2±1 (5±2%) |
| 3 | PX4 | A | 651 | - | 45,45,45 | 1.06±0.07 | 3±1 (7±2%) |
| 3 | PX4 | A | 624 | - | 45,45,45 | 1.05±0.10 | 2±2 (5±3%) |
| 3 | PX4 | B | 371 | - | 45,45,45 | 1.05±0.12 | 3±2 (5±3%) |
| 3 | PX4 | B | 314 | - | 45,45,45 | 1.11±0.11 | 3±1 (6±2%) |
| 3 | PX4 | A | 636 | - | 45,45,45 | 1.06±0.07 | 2±1 (5±2%) |
| 3 | PX4 | B | 338 | - | 45,45,45 | 1.08±0.11 | 3±1 (6±1%) |
| 3 | PX4 | C | 320 | - | 45,45,45 | 1.08±0.12 | 3±1 (5±2%) |
| 3 | PX4 | B | 308 | - | 45,45,45 | 1.10±0.13 | 4±1 (8±2%) |
| 3 | PX4 | B | 361 | - | 45,45,45 | 1.09±0.11 | 3±2 (7±4%) |
| 3 | PX4 | B | 325 | - | 45,45,45 | 1.05±0.08 | 2±2 (5±3%) |
| 3 | PX4 | C | 356 | - | 45,45,45 | 1.05±0.16 | 3±2 (6±3%) |
| 3 | PX4 | C | 311 | - | 45,45,45 | 1.06±0.09 | 3±1 (6±2%) |
| 3 | PX4 | C | 307 | - | 45,45,45 | 1.10±0.16 | 3±2 (7±4%) |
| 3 | PX4 | A | 623 | - | 45,45,45 | 1.03±0.13 | 2±2 (5±3%) |
| 3 | PX4 | A | 646 | - | 45,45,45 | 1.03±0.07 | 2±1 (4±2%) |
| 3 | PX4 | C | 344 | - | 45,45,45 | 1.02±0.14 | 3±1 (5±3%) |
| 3 | PX4 | C | 351 | - | 45,45,45 | 1.06±0.09 | 3±1 (6±2%) |
| 3 | PX4 | A | 611 | - | 45,45,45 | 1.08±0.09 | 3±1 (6±2%) |
| 3 | PX4 | C | 348 | - | 45,45,45 | 1.06±0.10 | 3±1 (6±2%) |
| 3 | PX4 | C | 325 | - | 45,45,45 | 1.06±0.11 | 3±1 (6±2%) |
| 3 | PX4 | B | 368 | - | 45,45,45 | 1.10±0.09 | 3±1 (7±2%) |
| 3 | PX4 | A | 619 | - | 45,45,45 | 1.07±0.12 | 3±1 (6±2%) |
| 3 | PX4 | A | 606 | - | 45,45,45 | 1.10±0.10 | 4±2 (8±3%) |
| 3 | PX4 | B | 345 | - | 45,45,45 | 1.09±0.14 | 3±2 (7±3%) |
| 3 | PX4 | B | 381 | - | 45,45,45 | 1.06±0.10 | 3±1 (6±2%) |
| 3 | PX4 | B | 324 | - | 45,45,45 | 1.06±0.09 | 2±1 (5±2%) |
| 3 | PX4 | C | 326 | - | 45,45,45 | 1.11±0.12 | 3±1 (7±3%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | |
|-----|------|-------|-----|------|--------------|-----------|------------|
| | | | | | Counts | RMSZ | #Z>2 |
| 3 | PX4 | B | 316 | - | 45,45,45 | 1.07±0.11 | 3±1 (7±3%) |
| 3 | PX4 | B | 386 | - | 45,45,45 | 1.06±0.12 | 3±1 (6±3%) |
| 3 | PX4 | A | 613 | - | 45,45,45 | 1.11±0.12 | 3±1 (7±2%) |
| 3 | PX4 | C | 316 | - | 45,45,45 | 1.05±0.11 | 3±1 (6±2%) |
| 3 | PX4 | B | 398 | - | 45,45,45 | 1.06±0.11 | 3±1 (6±2%) |
| 3 | PX4 | B | 307 | - | 45,45,45 | 1.08±0.08 | 4±1 (8±3%) |
| 3 | PX4 | A | 603 | - | 45,45,45 | 1.09±0.13 | 3±2 (6±3%) |
| 3 | PX4 | A | 632 | - | 45,45,45 | 1.07±0.16 | 3±1 (7±3%) |
| 3 | PX4 | C | 360 | - | 45,45,45 | 1.09±0.10 | 3±1 (7±2%) |
| 3 | PX4 | A | 637 | - | 45,45,45 | 1.06±0.10 | 3±2 (6±3%) |
| 3 | PX4 | B | 373 | - | 45,45,45 | 1.08±0.13 | 3±1 (5±2%) |
| 3 | PX4 | C | 306 | - | 45,45,45 | 1.10±0.12 | 3±1 (7±2%) |
| 3 | PX4 | A | 628 | - | 45,45,45 | 1.05±0.11 | 3±2 (6±3%) |
| 3 | PX4 | B | 309 | - | 45,45,45 | 1.07±0.10 | 3±1 (6±3%) |
| 3 | PX4 | B | 380 | - | 45,45,45 | 1.07±0.10 | 3±1 (6±2%) |
| 3 | PX4 | A | 647 | - | 45,45,45 | 1.08±0.08 | 3±2 (7±3%) |
| 3 | PX4 | B | 315 | - | 45,45,45 | 1.04±0.12 | 3±1 (6±2%) |
| 3 | PX4 | A | 643 | - | 45,45,45 | 1.04±0.13 | 3±2 (6±4%) |
| 3 | PX4 | A | 626 | - | 45,45,45 | 1.05±0.14 | 2±1 (5±3%) |
| 3 | PX4 | A | 614 | - | 45,45,45 | 1.10±0.09 | 3±1 (6±2%) |
| 3 | PX4 | B | 382 | - | 45,45,45 | 1.09±0.10 | 3±1 (7±2%) |
| 3 | PX4 | A | 605 | - | 45,45,45 | 1.11±0.09 | 3±1 (7±2%) |
| 3 | PX4 | B | 369 | - | 45,45,45 | 1.06±0.14 | 3±2 (6±4%) |
| 3 | PX4 | B | 340 | - | 45,45,45 | 1.10±0.13 | 3±2 (6±3%) |
| 3 | PX4 | C | 333 | - | 45,45,45 | 1.08±0.14 | 3±2 (6±3%) |

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

| Mol | Type | Chain | Res | Link | Bond angles | | |
|-----|------|-------|-----|------|-------------|-----------|------------|
| | | | | | Counts | RMSZ | #Z>2 |
| 3 | PX4 | B | 326 | - | 51,53,53 | 0.96±0.12 | 2±2 (4±3%) |

| Mol | Type | Chain | Res | Link | Bond angles | | |
|-----|------|-------|-----|------|-------------|-----------|------------|
| | | | | | Counts | RMSZ | #Z>2 |
| 3 | PX4 | A | 627 | - | 51,53,53 | 0.93±0.11 | 2±1 (4±2%) |
| 3 | PX4 | B | 393 | - | 51,53,53 | 0.96±0.08 | 2±1 (4±1%) |
| 3 | PX4 | B | 392 | - | 51,53,53 | 0.96±0.09 | 3±1 (4±2%) |
| 3 | PX4 | C | 336 | - | 51,53,53 | 0.93±0.10 | 2±1 (4±2%) |
| 3 | PX4 | B | 391 | - | 51,53,53 | 0.91±0.13 | 2±2 (3±3%) |
| 3 | PX4 | B | 319 | - | 51,53,53 | 1.00±0.10 | 3±2 (5±3%) |
| 3 | PX4 | A | 608 | - | 51,53,53 | 0.96±0.19 | 3±2 (4±3%) |
| 3 | PX4 | B | 304 | - | 51,53,53 | 0.94±0.10 | 2±1 (3±2%) |
| 3 | PX4 | A | 609 | - | 51,53,53 | 0.97±0.12 | 2±2 (4±3%) |
| 3 | PX4 | B | 348 | - | 51,53,53 | 0.99±0.10 | 3±1 (5±2%) |
| 3 | PX4 | B | 355 | - | 51,53,53 | 0.94±0.13 | 2±1 (4±2%) |
| 3 | PX4 | B | 305 | - | 51,53,53 | 0.95±0.08 | 3±1 (5±2%) |
| 3 | PX4 | B | 333 | - | 51,53,53 | 0.95±0.10 | 2±2 (4±3%) |
| 3 | PX4 | C | 350 | - | 51,53,53 | 1.07±0.13 | 3±2 (6±3%) |
| 3 | PX4 | B | 376 | - | 51,53,53 | 0.92±0.10 | 2±1 (4±2%) |
| 3 | PX4 | B | 317 | - | 51,53,53 | 0.91±0.10 | 2±1 (3±2%) |
| 3 | PX4 | B | 357 | - | 51,53,53 | 0.98±0.14 | 3±2 (5±4%) |
| 3 | PX4 | A | 629 | - | 51,53,53 | 0.88±0.13 | 2±1 (3±2%) |
| 3 | PX4 | C | 329 | - | 51,53,53 | 0.99±0.14 | 3±2 (5±3%) |
| 3 | PX4 | B | 323 | - | 51,53,53 | 0.90±0.08 | 2±1 (3±2%) |
| 3 | PX4 | C | 342 | - | 51,53,53 | 0.92±0.11 | 2±1 (3±2%) |
| 3 | PX4 | C | 321 | - | 51,53,53 | 0.97±0.08 | 2±1 (4±2%) |
| 3 | PX4 | B | 330 | - | 51,53,53 | 0.93±0.10 | 2±1 (3±2%) |
| 3 | PX4 | A | 634 | - | 51,53,53 | 0.95±0.12 | 2±2 (4±3%) |
| 3 | PX4 | C | 319 | - | 51,53,53 | 0.90±0.09 | 2±1 (3±1%) |
| 3 | PX4 | C | 341 | - | 51,53,53 | 0.97±0.09 | 3±1 (4±2%) |
| 3 | PX4 | B | 395 | - | 51,53,53 | 0.93±0.12 | 2±1 (4±2%) |
| 3 | PX4 | C | 332 | - | 51,53,53 | 0.97±0.14 | 2±2 (4±3%) |
| 3 | PX4 | C | 310 | - | 51,53,53 | 1.03±0.14 | 3±1 (6±2%) |
| 3 | PX4 | B | 350 | - | 51,53,53 | 0.97±0.14 | 3±2 (5±4%) |
| 3 | PX4 | B | 336 | - | 51,53,53 | 0.95±0.10 | 2±2 (3±2%) |
| 3 | PX4 | C | 331 | - | 51,53,53 | 0.92±0.11 | 2±1 (4±2%) |
| 3 | PX4 | C | 355 | - | 51,53,53 | 0.99±0.12 | 3±1 (5±2%) |
| 3 | PX4 | B | 320 | - | 51,53,53 | 0.99±0.13 | 3±2 (4±3%) |
| 3 | PX4 | B | 367 | - | 51,53,53 | 0.97±0.11 | 2±1 (4±1%) |

| Mol | Type | Chain | Res | Link | Bond angles | | |
|-----|------|-------|-----|------|-------------|-----------|------------|
| | | | | | Counts | RMSZ | #Z>2 |
| 3 | PX4 | A | 625 | - | 51,53,53 | 0.98±0.09 | 2±1 (3±2%) |
| 3 | PX4 | B | 344 | - | 51,53,53 | 1.00±0.10 | 2±1 (4±1%) |
| 3 | PX4 | B | 327 | - | 51,53,53 | 0.95±0.15 | 2±2 (4±3%) |
| 3 | PX4 | B | 321 | - | 51,53,53 | 0.95±0.13 | 3±2 (5±3%) |
| 3 | PX4 | C | 301 | - | 51,53,53 | 0.95±0.09 | 2±2 (4±3%) |
| 3 | PX4 | A | 631 | - | 51,53,53 | 0.95±0.10 | 2±1 (4±2%) |
| 3 | PX4 | C | 354 | - | 51,53,53 | 0.98±0.11 | 3±1 (5±2%) |
| 3 | PX4 | C | 315 | - | 51,53,53 | 0.97±0.10 | 3±1 (4±2%) |
| 3 | PX4 | A | 618 | - | 51,53,53 | 0.99±0.13 | 3±2 (6±3%) |
| 3 | PX4 | C | 353 | - | 51,53,53 | 0.97±0.09 | 2±1 (4±2%) |
| 3 | PX4 | A | 635 | - | 51,53,53 | 0.90±0.07 | 2±1 (3±1%) |
| 3 | PX4 | C | 346 | - | 51,53,53 | 0.97±0.09 | 2±1 (4±2%) |
| 3 | PX4 | B | 387 | - | 51,53,53 | 0.89±0.10 | 2±1 (3±2%) |
| 3 | PX4 | C | 340 | - | 51,53,53 | 0.96±0.13 | 2±2 (4±3%) |
| 3 | PX4 | C | 318 | - | 51,53,53 | 0.95±0.12 | 2±1 (4±2%) |
| 3 | PX4 | C | 327 | - | 51,53,53 | 0.97±0.13 | 3±2 (5±3%) |
| 3 | PX4 | C | 352 | - | 51,53,53 | 0.95±0.08 | 2±1 (4±2%) |
| 3 | PX4 | A | 620 | - | 51,53,53 | 0.93±0.12 | 2±1 (4±2%) |
| 3 | PX4 | A | 633 | - | 51,53,53 | 0.94±0.10 | 2±1 (3±1%) |
| 3 | PX4 | C | 309 | - | 51,53,53 | 0.93±0.11 | 2±1 (4±2%) |
| 3 | PX4 | B | 342 | - | 51,53,53 | 0.99±0.13 | 3±2 (5±3%) |
| 3 | PX4 | C | 304 | - | 51,53,53 | 0.96±0.15 | 3±2 (5±3%) |
| 3 | PX4 | A | 602 | - | 51,53,53 | 0.92±0.11 | 2±2 (4±3%) |
| 3 | PX4 | B | 400 | - | 51,53,53 | 0.93±0.11 | 2±1 (4±2%) |
| 3 | PX4 | C | 330 | - | 51,53,53 | 0.96±0.11 | 2±1 (4±1%) |
| 3 | PX4 | B | 360 | - | 51,53,53 | 0.96±0.11 | 2±2 (3±3%) |
| 3 | PX4 | C | 364 | - | 51,53,53 | 0.94±0.09 | 2±1 (4±2%) |
| 3 | PX4 | C | 345 | - | 51,53,53 | 0.95±0.13 | 2±1 (4±2%) |
| 3 | PX4 | C | 362 | - | 51,53,53 | 0.93±0.11 | 2±2 (4±3%) |
| 3 | PX4 | A | 648 | - | 51,53,53 | 0.97±0.10 | 2±1 (4±2%) |
| 3 | PX4 | B | 310 | - | 51,53,53 | 0.92±0.10 | 2±1 (3±1%) |
| 3 | PX4 | A | 639 | - | 51,53,53 | 0.93±0.08 | 2±1 (4±2%) |
| 3 | PX4 | A | 622 | - | 51,53,53 | 0.97±0.14 | 3±1 (4±2%) |
| 3 | PX4 | B | 389 | - | 51,53,53 | 0.96±0.09 | 2±1 (4±1%) |
| 3 | PX4 | A | 649 | - | 51,53,53 | 1.01±0.11 | 3±2 (5±3%) |

| Mol | Type | Chain | Res | Link | Bond angles | | |
|-----|------|-------|-----|------|-------------|-----------|------------|
| | | | | | Counts | RMSZ | #Z>2 |
| 3 | PX4 | B | 383 | - | 51,53,53 | 1.02±0.08 | 3±1 (5±2%) |
| 3 | PX4 | B | 347 | - | 51,53,53 | 0.99±0.12 | 3±1 (4±1%) |
| 3 | PX4 | C | 361 | - | 51,53,53 | 0.95±0.09 | 2±1 (4±2%) |
| 3 | PX4 | A | 642 | - | 51,53,53 | 0.98±0.11 | 3±2 (5±2%) |
| 3 | PX4 | C | 324 | - | 51,53,53 | 0.97±0.12 | 3±1 (4±2%) |
| 3 | PX4 | B | 346 | - | 51,53,53 | 0.88±0.07 | 1±1 (2±1%) |
| 3 | PX4 | A | 610 | - | 51,53,53 | 0.92±0.12 | 2±1 (3±2%) |
| 3 | PX4 | B | 318 | - | 51,53,53 | 0.94±0.12 | 2±1 (3±2%) |
| 3 | PX4 | A | 616 | - | 51,53,53 | 0.95±0.11 | 3±1 (5±2%) |
| 3 | PX4 | B | 349 | - | 51,53,53 | 0.95±0.10 | 2±1 (3±2%) |
| 3 | PX4 | B | 334 | - | 51,53,53 | 0.89±0.11 | 1±1 (2±2%) |
| 3 | PX4 | B | 379 | - | 51,53,53 | 0.96±0.11 | 2±2 (4±3%) |
| 3 | PX4 | B | 397 | - | 51,53,53 | 0.94±0.12 | 2±1 (4±2%) |
| 3 | PX4 | B | 339 | - | 51,53,53 | 0.91±0.12 | 2±1 (4±2%) |
| 3 | PX4 | C | 302 | - | 51,53,53 | 0.98±0.13 | 3±2 (5±3%) |
| 3 | PX4 | B | 322 | - | 51,53,53 | 0.92±0.12 | 2±1 (3±2%) |
| 3 | PX4 | C | 357 | - | 51,53,53 | 0.96±0.08 | 2±1 (4±2%) |
| 3 | PX4 | A | 644 | - | 51,53,53 | 0.94±0.09 | 2±1 (4±1%) |
| 3 | PX4 | C | 317 | - | 51,53,53 | 1.05±0.11 | 4±2 (7±3%) |
| 3 | PX4 | B | 354 | - | 51,53,53 | 0.97±0.12 | 2±2 (4±3%) |
| 3 | PX4 | C | 314 | - | 51,53,53 | 0.94±0.08 | 2±1 (3±2%) |
| 3 | PX4 | B | 378 | - | 51,53,53 | 0.96±0.12 | 2±1 (4±2%) |
| 3 | PX4 | C | 343 | - | 51,53,53 | 0.93±0.09 | 2±2 (4±3%) |
| 3 | PX4 | C | 358 | - | 51,53,53 | 0.99±0.10 | 2±1 (4±2%) |
| 3 | PX4 | B | 302 | - | 51,53,53 | 0.90±0.11 | 2±1 (3±2%) |
| 3 | PX4 | A | 630 | - | 51,53,53 | 0.92±0.11 | 2±1 (4±2%) |
| 3 | PX4 | B | 388 | - | 51,53,53 | 0.98±0.13 | 3±2 (4±3%) |
| 3 | PX4 | C | 323 | - | 51,53,53 | 0.96±0.10 | 2±1 (4±2%) |
| 3 | PX4 | B | 311 | - | 51,53,53 | 0.96±0.08 | 2±1 (3±2%) |
| 3 | PX4 | B | 363 | - | 51,53,53 | 0.97±0.10 | 2±1 (4±2%) |
| 3 | PX4 | A | 652 | - | 51,53,53 | 0.99±0.10 | 3±1 (5±2%) |
| 3 | PX4 | B | 313 | - | 51,53,53 | 0.98±0.10 | 2±1 (4±2%) |
| 3 | PX4 | C | 334 | - | 51,53,53 | 0.93±0.10 | 2±1 (3±2%) |
| 3 | PX4 | B | 394 | - | 51,53,53 | 0.99±0.11 | 2±1 (4±2%) |
| 3 | PX4 | B | 312 | - | 51,53,53 | 0.99±0.08 | 2±2 (4±2%) |

| Mol | Type | Chain | Res | Link | Bond angles | | |
|-----|------|-------|-----|------|-------------|-----------|------------|
| | | | | | Counts | RMSZ | #Z>2 |
| 3 | PX4 | B | 385 | - | 51,53,53 | 1.01±0.16 | 3±1 (5±2%) |
| 3 | PX4 | B | 356 | - | 51,53,53 | 0.98±0.13 | 3±2 (5±3%) |
| 3 | PX4 | C | 339 | - | 51,53,53 | 0.94±0.13 | 2±1 (3±2%) |
| 3 | PX4 | B | 359 | - | 51,53,53 | 0.95±0.10 | 2±2 (3±3%) |
| 3 | PX4 | B | 306 | - | 51,53,53 | 1.00±0.12 | 3±1 (6±2%) |
| 3 | PX4 | B | 390 | - | 51,53,53 | 0.91±0.10 | 2±1 (3±2%) |
| 3 | PX4 | C | 335 | - | 51,53,53 | 0.99±0.11 | 3±2 (6±3%) |
| 3 | PX4 | A | 653 | - | 51,53,53 | 1.00±0.12 | 2±1 (4±2%) |
| 3 | PX4 | B | 375 | - | 51,53,53 | 0.89±0.13 | 2±1 (3±2%) |
| 3 | PX4 | B | 364 | - | 51,53,53 | 0.94±0.13 | 2±1 (3±2%) |
| 3 | PX4 | B | 341 | - | 51,53,53 | 1.05±0.12 | 3±1 (6±2%) |
| 3 | PX4 | B | 343 | - | 51,53,53 | 0.95±0.09 | 2±2 (3±3%) |
| 3 | PX4 | B | 372 | - | 51,53,53 | 1.02±0.10 | 3±1 (6±2%) |
| 3 | PX4 | B | 370 | - | 51,53,53 | 0.96±0.09 | 2±1 (4±2%) |
| 3 | PX4 | A | 607 | - | 51,53,53 | 0.97±0.11 | 2±2 (4±3%) |
| 3 | PX4 | B | 331 | - | 51,53,53 | 0.89±0.13 | 2±2 (3±3%) |
| 3 | PX4 | B | 337 | - | 51,53,53 | 0.93±0.09 | 2±1 (4±2%) |
| 3 | PX4 | A | 654 | - | 51,53,53 | 0.91±0.11 | 2±1 (3±2%) |
| 3 | PX4 | C | 305 | - | 51,53,53 | 0.94±0.09 | 2±1 (4±2%) |
| 3 | PX4 | C | 308 | - | 51,53,53 | 0.92±0.13 | 2±1 (3±2%) |
| 3 | PX4 | A | 640 | - | 51,53,53 | 0.98±0.09 | 2±1 (4±2%) |
| 3 | PX4 | A | 645 | - | 51,53,53 | 0.90±0.14 | 2±2 (4±3%) |
| 3 | PX4 | C | 347 | - | 51,53,53 | 0.95±0.09 | 2±1 (4±2%) |
| 3 | PX4 | C | 359 | - | 51,53,53 | 0.85±0.11 | 1±1 (2±2%) |
| 3 | PX4 | B | 329 | - | 51,53,53 | 0.95±0.13 | 2±1 (4±2%) |
| 3 | PX4 | C | 338 | - | 51,53,53 | 0.96±0.12 | 2±1 (4±2%) |
| 3 | PX4 | C | 328 | - | 51,53,53 | 0.95±0.11 | 2±1 (4±2%) |
| 3 | PX4 | A | 604 | - | 51,53,53 | 0.96±0.09 | 3±1 (5±2%) |
| 3 | PX4 | B | 351 | - | 51,53,53 | 0.93±0.11 | 2±1 (4±2%) |
| 3 | PX4 | C | 322 | - | 51,53,53 | 0.96±0.10 | 2±1 (4±2%) |
| 3 | PX4 | C | 312 | - | 51,53,53 | 0.92±0.11 | 2±2 (4±4%) |
| 3 | PX4 | C | 349 | - | 51,53,53 | 1.00±0.14 | 3±2 (5±3%) |
| 3 | PX4 | C | 337 | - | 51,53,53 | 0.93±0.11 | 2±1 (3±2%) |
| 3 | PX4 | B | 399 | - | 51,53,53 | 0.96±0.11 | 2±1 (4±2%) |
| 3 | PX4 | B | 362 | - | 51,53,53 | 0.95±0.10 | 2±2 (4±2%) |

| Mol | Type | Chain | Res | Link | Bond angles | | |
|-----|------|-------|-----|------|-------------|-----------|------------|
| | | | | | Counts | RMSZ | #Z>2 |
| 3 | PX4 | A | 615 | - | 51,53,53 | 0.93±0.11 | 2±1 (3±2%) |
| 3 | PX4 | B | 396 | - | 51,53,53 | 0.99±0.10 | 2±1 (4±2%) |
| 3 | PX4 | A | 621 | - | 51,53,53 | 0.97±0.11 | 3±1 (5±2%) |
| 3 | PX4 | B | 374 | - | 51,53,53 | 0.92±0.10 | 2±1 (4±2%) |
| 3 | PX4 | A | 638 | - | 51,53,53 | 0.94±0.09 | 2±1 (4±2%) |
| 3 | PX4 | B | 358 | - | 51,53,53 | 0.96±0.13 | 2±2 (4±3%) |
| 3 | PX4 | B | 365 | - | 51,53,53 | 0.94±0.13 | 2±1 (3±2%) |
| 3 | PX4 | A | 601 | - | 51,53,53 | 0.97±0.14 | 3±1 (5±2%) |
| 3 | PX4 | C | 303 | - | 51,53,53 | 0.93±0.10 | 2±1 (3±2%) |
| 3 | PX4 | B | 377 | - | 51,53,53 | 0.94±0.11 | 2±1 (3±2%) |
| 3 | PX4 | B | 332 | - | 51,53,53 | 0.96±0.15 | 3±2 (5±2%) |
| 3 | PX4 | A | 650 | - | 51,53,53 | 0.94±0.12 | 2±1 (4±2%) |
| 3 | PX4 | B | 303 | - | 51,53,53 | 0.92±0.12 | 2±1 (4±2%) |
| 3 | PX4 | B | 366 | - | 51,53,53 | 0.93±0.09 | 2±1 (3±2%) |
| 3 | PX4 | B | 352 | - | 51,53,53 | 0.94±0.10 | 2±1 (3±2%) |
| 3 | PX4 | B | 328 | - | 51,53,53 | 0.95±0.07 | 2±1 (3±1%) |
| 3 | PX4 | B | 353 | - | 51,53,53 | 0.96±0.12 | 2±1 (4±2%) |
| 3 | PX4 | B | 301 | - | 51,53,53 | 0.95±0.11 | 2±1 (3±2%) |
| 3 | PX4 | C | 313 | - | 51,53,53 | 0.98±0.09 | 2±2 (4±3%) |
| 3 | PX4 | B | 384 | - | 51,53,53 | 1.03±0.10 | 3±1 (5±2%) |
| 3 | PX4 | A | 617 | - | 51,53,53 | 0.98±0.12 | 2±1 (4±2%) |
| 3 | PX4 | C | 363 | - | 51,53,53 | 1.01±0.13 | 3±2 (5±3%) |
| 3 | PX4 | A | 641 | - | 51,53,53 | 0.91±0.12 | 2±1 (3±2%) |
| 3 | PX4 | B | 335 | - | 51,53,53 | 0.94±0.12 | 2±1 (4±2%) |
| 3 | PX4 | A | 612 | - | 51,53,53 | 1.00±0.15 | 2±1 (4±2%) |
| 3 | PX4 | A | 651 | - | 51,53,53 | 1.03±0.13 | 3±1 (6±2%) |
| 3 | PX4 | A | 624 | - | 51,53,53 | 0.93±0.14 | 2±2 (4±3%) |
| 3 | PX4 | B | 371 | - | 51,53,53 | 0.96±0.12 | 2±1 (4±2%) |
| 3 | PX4 | B | 314 | - | 51,53,53 | 0.88±0.11 | 2±1 (3±1%) |
| 3 | PX4 | A | 636 | - | 51,53,53 | 0.98±0.11 | 2±1 (4±2%) |
| 3 | PX4 | B | 338 | - | 51,53,53 | 0.91±0.12 | 2±1 (4±2%) |
| 3 | PX4 | C | 320 | - | 51,53,53 | 1.00±0.10 | 3±1 (5±2%) |
| 3 | PX4 | B | 308 | - | 51,53,53 | 0.93±0.16 | 2±2 (4±4%) |
| 3 | PX4 | B | 361 | - | 51,53,53 | 0.94±0.11 | 2±2 (4±3%) |
| 3 | PX4 | B | 325 | - | 51,53,53 | 0.95±0.12 | 2±2 (3±3%) |

| Mol | Type | Chain | Res | Link | Bond angles | | |
|-----|------|-------|-----|------|-------------|-----------|------------|
| | | | | | Counts | RMSZ | #Z>2 |
| 3 | PX4 | C | 356 | - | 51,53,53 | 0.94±0.12 | 2±2 (4±2%) |
| 3 | PX4 | C | 311 | - | 51,53,53 | 1.00±0.10 | 2±1 (4±2%) |
| 3 | PX4 | C | 307 | - | 51,53,53 | 0.94±0.09 | 2±1 (3±1%) |
| 3 | PX4 | A | 623 | - | 51,53,53 | 0.95±0.09 | 2±1 (4±2%) |
| 3 | PX4 | A | 646 | - | 51,53,53 | 0.91±0.14 | 2±1 (4±2%) |
| 3 | PX4 | C | 344 | - | 51,53,53 | 0.99±0.12 | 2±1 (4±2%) |
| 3 | PX4 | C | 351 | - | 51,53,53 | 0.97±0.10 | 2±2 (4±3%) |
| 3 | PX4 | A | 611 | - | 51,53,53 | 0.93±0.13 | 2±1 (3±1%) |
| 3 | PX4 | C | 348 | - | 51,53,53 | 0.93±0.09 | 2±2 (4±3%) |
| 3 | PX4 | C | 325 | - | 51,53,53 | 0.98±0.07 | 3±1 (5±2%) |
| 3 | PX4 | B | 368 | - | 51,53,53 | 0.97±0.14 | 2±1 (4±2%) |
| 3 | PX4 | A | 619 | - | 51,53,53 | 0.93±0.09 | 2±1 (3±2%) |
| 3 | PX4 | A | 606 | - | 51,53,53 | 0.92±0.10 | 2±2 (4±3%) |
| 3 | PX4 | B | 345 | - | 51,53,53 | 0.93±0.10 | 2±1 (3±1%) |
| 3 | PX4 | B | 381 | - | 51,53,53 | 0.93±0.09 | 2±1 (3±2%) |
| 3 | PX4 | B | 324 | - | 51,53,53 | 0.91±0.10 | 2±1 (4±2%) |
| 3 | PX4 | C | 326 | - | 51,53,53 | 0.97±0.09 | 2±1 (4±2%) |
| 3 | PX4 | B | 316 | - | 51,53,53 | 0.91±0.14 | 2±1 (4±2%) |
| 3 | PX4 | B | 386 | - | 51,53,53 | 0.95±0.10 | 2±1 (3±2%) |
| 3 | PX4 | A | 613 | - | 51,53,53 | 0.88±0.08 | 2±1 (3±1%) |
| 3 | PX4 | C | 316 | - | 51,53,53 | 0.90±0.08 | 2±1 (3±2%) |
| 3 | PX4 | B | 398 | - | 51,53,53 | 0.90±0.09 | 2±1 (3±2%) |
| 3 | PX4 | B | 307 | - | 51,53,53 | 0.95±0.07 | 2±1 (4±2%) |
| 3 | PX4 | A | 603 | - | 51,53,53 | 0.97±0.12 | 3±1 (5±2%) |
| 3 | PX4 | A | 632 | - | 51,53,53 | 0.94±0.12 | 2±2 (4±3%) |
| 3 | PX4 | C | 360 | - | 51,53,53 | 0.95±0.16 | 2±1 (3±2%) |
| 3 | PX4 | A | 637 | - | 51,53,53 | 0.95±0.08 | 2±1 (4±1%) |
| 3 | PX4 | B | 373 | - | 51,53,53 | 0.95±0.09 | 2±1 (4±2%) |
| 3 | PX4 | C | 306 | - | 51,53,53 | 1.00±0.09 | 3±1 (5±2%) |
| 3 | PX4 | A | 628 | - | 51,53,53 | 0.93±0.06 | 2±1 (4±2%) |
| 3 | PX4 | B | 309 | - | 51,53,53 | 0.99±0.13 | 3±1 (5±2%) |
| 3 | PX4 | B | 380 | - | 51,53,53 | 0.98±0.12 | 3±2 (5±3%) |
| 3 | PX4 | A | 647 | - | 51,53,53 | 0.96±0.10 | 2±1 (4±2%) |
| 3 | PX4 | B | 315 | - | 51,53,53 | 0.99±0.12 | 2±1 (4±2%) |
| 3 | PX4 | A | 643 | - | 51,53,53 | 0.97±0.08 | 2±2 (4±3%) |

| Mol | Type | Chain | Res | Link | Bond angles | | |
|-----|------|-------|-----|------|-------------|-----------|------------|
| | | | | | Counts | RMSZ | #Z>2 |
| 3 | PX4 | A | 626 | - | 51,53,53 | 0.96±0.15 | 2±2 (4±2%) |
| 3 | PX4 | A | 614 | - | 51,53,53 | 0.93±0.13 | 2±2 (4±3%) |
| 3 | PX4 | B | 382 | - | 51,53,53 | 0.96±0.08 | 2±1 (4±2%) |
| 3 | PX4 | A | 605 | - | 51,53,53 | 0.97±0.12 | 3±1 (5±2%) |
| 3 | PX4 | B | 369 | - | 51,53,53 | 0.98±0.13 | 3±2 (5±3%) |
| 3 | PX4 | B | 340 | - | 51,53,53 | 0.92±0.09 | 2±1 (4±2%) |
| 3 | PX4 | C | 333 | - | 51,53,53 | 0.95±0.13 | 2±2 (4±3%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|--------------|-------|
| 3 | PX4 | C | 352 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | A | 602 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | C | 304 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 360 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 355 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | C | 350 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | C | 361 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | A | 642 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | A | 620 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | C | 301 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | A | 653 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 372 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | A | 652 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 337 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 329 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | C | 324 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | C | 323 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | C | 331 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 377 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 346 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | A | 615 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | A | 627 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 379 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | A | 651 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | A | 636 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 361 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | A | 634 | - | - | 0±0,49,49,49 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|--------------|-------|
| 3 | PX4 | B | 338 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 400 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | C | 346 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | C | 318 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | C | 349 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | A | 644 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | C | 354 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 371 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | A | 604 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 368 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 398 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 333 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 390 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | A | 617 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 380 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 358 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | A | 649 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | C | 311 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | C | 313 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | C | 327 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | C | 303 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | A | 610 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 395 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | C | 363 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 322 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | C | 364 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 310 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 347 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | C | 332 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | C | 343 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | A | 609 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | A | 613 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | C | 312 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | A | 621 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | A | 601 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 352 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 304 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | C | 337 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | A | 638 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 350 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 363 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | C | 306 | - | - | 0±0,49,49,49 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|--------------|-------|
| 3 | PX4 | B | 345 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 320 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 328 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 321 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 327 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | C | 325 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 324 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 317 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | A | 614 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 383 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | A | 629 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | C | 345 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | C | 317 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 311 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | C | 328 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | C | 319 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 396 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 384 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | A | 611 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | A | 646 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 318 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 354 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | A | 654 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | A | 606 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 342 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | C | 314 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | A | 605 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | C | 341 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | C | 360 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | C | 322 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 366 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 331 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 374 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | C | 336 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 325 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 303 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | C | 340 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | A | 632 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 301 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | A | 619 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | C | 308 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 375 | - | - | 0±0,49,49,49 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|--------------|-------|
| 3 | PX4 | A | 616 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 364 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 326 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | C | 302 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | A | 625 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 309 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | C | 309 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | C | 315 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | A | 630 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | C | 305 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 323 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | C | 326 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 365 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | C | 321 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 392 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | C | 342 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | C | 357 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 353 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | C | 307 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 378 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 370 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | C | 348 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | C | 334 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | A | 612 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 314 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | A | 635 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 399 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | A | 643 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | C | 310 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | A | 650 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | A | 628 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | A | 622 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 319 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 351 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 385 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | A | 637 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | C | 316 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 343 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | A | 626 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | A | 647 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 341 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | C | 339 | - | - | 0±0,49,49,49 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|--------------|-------|
| 3 | PX4 | C | 356 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 312 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | A | 631 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | A | 639 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | C | 330 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 336 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 340 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 335 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | C | 344 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 386 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 308 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | C | 355 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | A | 640 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 359 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 362 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | C | 362 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | A | 607 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 313 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 302 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 389 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 394 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | C | 335 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 387 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | A | 608 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | C | 329 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | A | 624 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 315 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | C | 351 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | C | 320 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 391 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 305 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | A | 645 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 332 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 357 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 330 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 307 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | C | 338 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 388 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 367 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 348 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 334 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 393 | - | - | 0±0,49,49,49 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|--------------|-------|
| 3 | PX4 | B | 339 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | A | 623 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 376 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | A | 618 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 349 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | A | 648 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 382 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | C | 333 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | C | 353 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | A | 603 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | A | 641 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | C | 358 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | A | 633 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 344 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 316 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 373 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | C | 347 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 306 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 356 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | C | 359 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 381 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 369 | - | - | 0±0,49,49,49 | - |
| 3 | PX4 | B | 397 | - | - | 0±0,49,49,49 | - |

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

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|--------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | C | 322 | PX4 | C2-C1 | 5.97 | 1.69 | 1.51 | 1 | 5 |
| 3 | B | 352 | PX4 | C2-C1 | 5.78 | 1.68 | 1.51 | 2 | 6 |
| 3 | B | 313 | PX4 | C6-C7 | 5.46 | 1.67 | 1.50 | 7 | 6 |
| 3 | B | 357 | PX4 | C8-C7 | 5.44 | 1.67 | 1.50 | 10 | 5 |
| 3 | A | 611 | PX4 | C10-C9 | 5.39 | 1.66 | 1.50 | 3 | 5 |
| 3 | B | 372 | PX4 | C8-C7 | 5.28 | 1.67 | 1.50 | 5 | 8 |
| 3 | C | 356 | PX4 | C8-C7 | 5.19 | 1.67 | 1.50 | 1 | 11 |
| 3 | A | 638 | PX4 | C8-C7 | 5.18 | 1.67 | 1.50 | 8 | 6 |
| 3 | B | 338 | PX4 | C6-C7 | 5.16 | 1.67 | 1.50 | 9 | 8 |
| 3 | B | 365 | PX4 | C6-C7 | 5.13 | 1.66 | 1.50 | 7 | 6 |
| 3 | B | 353 | PX4 | O7-C7 | 5.12 | 1.34 | 1.46 | 11 | 4 |
| 3 | B | 356 | PX4 | O7-C7 | 5.12 | 1.34 | 1.46 | 2 | 2 |
| 3 | C | 303 | PX4 | C8-C7 | 5.11 | 1.66 | 1.50 | 3 | 7 |
| 3 | B | 370 | PX4 | C6-C7 | 5.10 | 1.66 | 1.50 | 5 | 7 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | C | 352 | PX4 | C8-C7 | 5.07 | 1.66 | 1.50 | 8 | 3 |
| 3 | B | 346 | PX4 | C8-C7 | 5.06 | 1.66 | 1.50 | 7 | 5 |
| 3 | C | 346 | PX4 | C24-C23 | 5.06 | 1.65 | 1.50 | 14 | 3 |
| 3 | C | 306 | PX4 | C24-C23 | 5.03 | 1.65 | 1.50 | 4 | 3 |
| 3 | B | 386 | PX4 | C24-C23 | 5.02 | 1.65 | 1.50 | 6 | 5 |
| 3 | A | 618 | PX4 | C24-C23 | 5.00 | 1.65 | 1.50 | 10 | 3 |
| 3 | B | 388 | PX4 | C6-C7 | 5.00 | 1.66 | 1.50 | 10 | 7 |
| 3 | C | 347 | PX4 | C8-C7 | 4.99 | 1.66 | 1.50 | 5 | 7 |
| 3 | C | 309 | PX4 | C6-C7 | 4.93 | 1.66 | 1.50 | 12 | 6 |
| 3 | B | 303 | PX4 | C6-C7 | 4.92 | 1.66 | 1.50 | 5 | 9 |
| 3 | A | 631 | PX4 | O7-C23 | 4.91 | 1.20 | 1.34 | 14 | 6 |
| 3 | A | 613 | PX4 | C2-C1 | 4.90 | 1.66 | 1.51 | 8 | 7 |
| 3 | A | 603 | PX4 | C2-C1 | 4.89 | 1.66 | 1.51 | 1 | 5 |
| 3 | B | 393 | PX4 | O7-C7 | 4.87 | 1.35 | 1.46 | 11 | 3 |
| 3 | A | 645 | PX4 | C6-C7 | 4.82 | 1.65 | 1.50 | 2 | 6 |
| 3 | C | 353 | PX4 | O7-C7 | 4.79 | 1.35 | 1.46 | 1 | 3 |
| 3 | A | 612 | PX4 | C2-C1 | 4.78 | 1.65 | 1.51 | 5 | 4 |
| 3 | C | 359 | PX4 | O7-C23 | 4.78 | 1.20 | 1.34 | 11 | 3 |
| 3 | C | 352 | PX4 | C10-C9 | 4.77 | 1.64 | 1.50 | 2 | 4 |
| 3 | A | 607 | PX4 | C6-C7 | 4.73 | 1.65 | 1.50 | 15 | 5 |
| 3 | C | 333 | PX4 | C8-C7 | 4.70 | 1.65 | 1.50 | 1 | 5 |
| 3 | B | 350 | PX4 | C6-C7 | 4.69 | 1.65 | 1.50 | 13 | 9 |
| 3 | C | 305 | PX4 | C8-C7 | 4.68 | 1.65 | 1.50 | 2 | 9 |
| 3 | B | 393 | PX4 | C8-C7 | 4.67 | 1.65 | 1.50 | 6 | 6 |
| 3 | B | 301 | PX4 | C24-C23 | 4.66 | 1.64 | 1.50 | 9 | 4 |
| 3 | B | 373 | PX4 | C8-C7 | 4.65 | 1.65 | 1.50 | 14 | 6 |
| 3 | B | 343 | PX4 | C8-C7 | 4.64 | 1.65 | 1.50 | 7 | 7 |
| 3 | B | 306 | PX4 | O5-C8 | 4.63 | 1.55 | 1.45 | 4 | 1 |
| 3 | C | 313 | PX4 | C8-C7 | 4.61 | 1.65 | 1.50 | 2 | 8 |
| 3 | B | 340 | PX4 | C8-C7 | 4.61 | 1.65 | 1.50 | 15 | 7 |
| 3 | B | 318 | PX4 | C8-C7 | 4.60 | 1.65 | 1.50 | 10 | 7 |
| 3 | B | 314 | PX4 | C8-C7 | 4.58 | 1.65 | 1.50 | 9 | 8 |
| 3 | B | 324 | PX4 | C6-C7 | 4.58 | 1.65 | 1.50 | 9 | 4 |
| 3 | B | 351 | PX4 | C2-N1 | 4.58 | 1.65 | 1.51 | 1 | 4 |
| 3 | B | 308 | PX4 | C2-C1 | 4.57 | 1.65 | 1.51 | 4 | 6 |
| 3 | B | 373 | PX4 | C10-C9 | 4.56 | 1.63 | 1.50 | 9 | 4 |
| 3 | B | 381 | PX4 | C6-C7 | 4.55 | 1.65 | 1.50 | 13 | 6 |
| 3 | B | 330 | PX4 | C6-C7 | 4.55 | 1.65 | 1.50 | 2 | 7 |
| 3 | C | 351 | PX4 | C6-C7 | 4.55 | 1.65 | 1.50 | 6 | 8 |
| 3 | B | 396 | PX4 | O7-C23 | 4.55 | 1.21 | 1.34 | 3 | 5 |
| 3 | B | 385 | PX4 | C2-C1 | 4.54 | 1.65 | 1.51 | 3 | 5 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 326 | PX4 | C6-C7 | 4.53 | 1.65 | 1.50 | 10 | 8 |
| 3 | A | 619 | PX4 | C8-C7 | 4.52 | 1.64 | 1.50 | 13 | 9 |
| 3 | B | 314 | PX4 | C2-C1 | 4.52 | 1.65 | 1.51 | 3 | 6 |
| 3 | B | 342 | PX4 | O7-C7 | 4.52 | 1.36 | 1.46 | 7 | 3 |
| 3 | A | 627 | PX4 | C8-C7 | 4.49 | 1.64 | 1.50 | 6 | 9 |
| 3 | B | 331 | PX4 | C8-C7 | 4.49 | 1.64 | 1.50 | 13 | 7 |
| 3 | B | 380 | PX4 | C6-C7 | 4.49 | 1.64 | 1.50 | 3 | 6 |
| 3 | B | 338 | PX4 | C8-C7 | 4.48 | 1.64 | 1.50 | 7 | 5 |
| 3 | C | 304 | PX4 | C8-C7 | 4.48 | 1.64 | 1.50 | 2 | 6 |
| 3 | B | 322 | PX4 | C2-C1 | 4.47 | 1.64 | 1.51 | 1 | 8 |
| 3 | B | 368 | PX4 | C8-C7 | 4.45 | 1.64 | 1.50 | 2 | 7 |
| 3 | C | 343 | PX4 | C6-C7 | 4.44 | 1.64 | 1.50 | 10 | 3 |
| 3 | A | 619 | PX4 | C6-C7 | 4.44 | 1.64 | 1.50 | 5 | 6 |
| 3 | B | 319 | PX4 | C8-C7 | 4.43 | 1.64 | 1.50 | 11 | 8 |
| 3 | B | 374 | PX4 | C6-C7 | 4.44 | 1.64 | 1.50 | 15 | 7 |
| 3 | B | 315 | PX4 | C8-C7 | 4.43 | 1.64 | 1.50 | 10 | 5 |
| 3 | B | 349 | PX4 | C10-C9 | 4.43 | 1.63 | 1.50 | 2 | 2 |
| 3 | B | 333 | PX4 | C2-C1 | 4.42 | 1.64 | 1.51 | 14 | 1 |
| 3 | B | 330 | PX4 | C2-C1 | 4.41 | 1.64 | 1.51 | 1 | 7 |
| 3 | B | 351 | PX4 | C2-C1 | 4.41 | 1.64 | 1.51 | 13 | 5 |
| 3 | B | 395 | PX4 | C2-C1 | 4.40 | 1.64 | 1.51 | 11 | 2 |
| 3 | C | 323 | PX4 | C8-C7 | 4.40 | 1.64 | 1.50 | 5 | 7 |
| 3 | A | 639 | PX4 | C2-C1 | 4.40 | 1.64 | 1.51 | 9 | 9 |
| 3 | A | 632 | PX4 | C6-C7 | 4.40 | 1.64 | 1.50 | 4 | 6 |
| 3 | B | 376 | PX4 | C6-C7 | 4.38 | 1.64 | 1.50 | 12 | 6 |
| 3 | B | 332 | PX4 | C8-C7 | 4.38 | 1.64 | 1.50 | 3 | 9 |
| 3 | A | 648 | PX4 | C8-C7 | 4.38 | 1.64 | 1.50 | 4 | 6 |
| 3 | A | 650 | PX4 | C8-C7 | 4.38 | 1.64 | 1.50 | 13 | 9 |
| 3 | C | 350 | PX4 | C6-C7 | 4.38 | 1.64 | 1.50 | 1 | 10 |
| 3 | B | 380 | PX4 | C8-C7 | 4.38 | 1.64 | 1.50 | 7 | 5 |
| 3 | C | 335 | PX4 | C2-C1 | 4.37 | 1.64 | 1.51 | 5 | 9 |
| 3 | C | 320 | PX4 | C2-C1 | 4.37 | 1.64 | 1.51 | 14 | 1 |
| 3 | B | 385 | PX4 | C8-C7 | 4.37 | 1.64 | 1.50 | 14 | 6 |
| 3 | B | 308 | PX4 | C8-C7 | 4.36 | 1.64 | 1.50 | 10 | 8 |
| 3 | B | 364 | PX4 | C24-C23 | 4.36 | 1.63 | 1.50 | 4 | 4 |
| 3 | C | 314 | PX4 | C6-C7 | 4.36 | 1.64 | 1.50 | 5 | 4 |
| 3 | C | 347 | PX4 | C6-C7 | 4.36 | 1.64 | 1.50 | 3 | 6 |
| 3 | A | 641 | PX4 | C8-C7 | 4.35 | 1.64 | 1.50 | 12 | 6 |
| 3 | B | 378 | PX4 | C2-C1 | 4.34 | 1.64 | 1.51 | 9 | 4 |
| 3 | B | 347 | PX4 | C8-C7 | 4.33 | 1.64 | 1.50 | 8 | 9 |
| 3 | B | 389 | PX4 | O5-C9 | 4.33 | 1.46 | 1.33 | 10 | 2 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 304 | PX4 | O7-C23 | 4.33 | 1.22 | 1.34 | 7 | 2 |
| 3 | B | 323 | PX4 | O7-C7 | 4.33 | 1.56 | 1.46 | 1 | 5 |
| 3 | B | 327 | PX4 | C8-C7 | 4.32 | 1.64 | 1.50 | 5 | 7 |
| 3 | A | 645 | PX4 | C24-C23 | 4.32 | 1.63 | 1.50 | 10 | 5 |
| 3 | A | 635 | PX4 | O7-C23 | 4.32 | 1.22 | 1.34 | 10 | 3 |
| 3 | B | 396 | PX4 | C8-C7 | 4.32 | 1.64 | 1.50 | 13 | 5 |
| 3 | B | 380 | PX4 | C2-C1 | 4.31 | 1.64 | 1.51 | 1 | 4 |
| 3 | C | 335 | PX4 | C24-C23 | 4.31 | 1.63 | 1.50 | 14 | 3 |
| 3 | B | 305 | PX4 | C5-N1 | 4.31 | 1.37 | 1.50 | 14 | 1 |
| 3 | C | 326 | PX4 | C10-C9 | 4.31 | 1.63 | 1.50 | 2 | 5 |
| 3 | B | 333 | PX4 | C8-C7 | 4.31 | 1.64 | 1.50 | 8 | 6 |
| 3 | C | 307 | PX4 | C2-C1 | 4.31 | 1.64 | 1.51 | 8 | 5 |
| 3 | C | 361 | PX4 | C10-C9 | 4.30 | 1.63 | 1.50 | 7 | 5 |
| 3 | B | 369 | PX4 | C6-C7 | 4.30 | 1.64 | 1.50 | 15 | 7 |
| 3 | B | 327 | PX4 | C6-C7 | 4.30 | 1.64 | 1.50 | 2 | 6 |
| 3 | B | 382 | PX4 | C8-C7 | 4.30 | 1.64 | 1.50 | 9 | 6 |
| 3 | B | 398 | PX4 | C8-C7 | 4.29 | 1.64 | 1.50 | 2 | 7 |
| 3 | C | 350 | PX4 | C8-C7 | 4.29 | 1.64 | 1.50 | 8 | 8 |
| 3 | B | 312 | PX4 | C10-C9 | 4.27 | 1.63 | 1.50 | 13 | 7 |
| 3 | A | 612 | PX4 | O7-C7 | 4.26 | 1.36 | 1.46 | 5 | 2 |
| 3 | A | 648 | PX4 | C10-C9 | 4.26 | 1.63 | 1.50 | 10 | 3 |
| 3 | C | 306 | PX4 | C8-C7 | 4.26 | 1.64 | 1.50 | 11 | 9 |
| 3 | B | 390 | PX4 | C2-C1 | 4.26 | 1.64 | 1.51 | 12 | 6 |
| 3 | C | 345 | PX4 | C2-C1 | 4.26 | 1.64 | 1.51 | 7 | 8 |
| 3 | B | 346 | PX4 | C2-C1 | 4.24 | 1.64 | 1.51 | 1 | 5 |
| 3 | B | 353 | PX4 | C2-C1 | 4.24 | 1.64 | 1.51 | 12 | 6 |
| 3 | C | 336 | PX4 | O7-C7 | 4.24 | 1.36 | 1.46 | 14 | 4 |
| 3 | A | 611 | PX4 | C6-C7 | 4.24 | 1.64 | 1.50 | 11 | 7 |
| 3 | B | 362 | PX4 | O7-C7 | 4.23 | 1.36 | 1.46 | 3 | 3 |
| 3 | C | 301 | PX4 | C2-C1 | 4.23 | 1.64 | 1.51 | 5 | 8 |
| 3 | C | 317 | PX4 | O5-C8 | 4.23 | 1.35 | 1.45 | 5 | 3 |
| 3 | B | 354 | PX4 | C10-C9 | 4.23 | 1.63 | 1.50 | 15 | 4 |
| 3 | B | 305 | PX4 | C6-C7 | 4.22 | 1.64 | 1.50 | 4 | 7 |
| 3 | B | 321 | PX4 | C6-C7 | 4.22 | 1.64 | 1.50 | 1 | 8 |
| 3 | B | 367 | PX4 | C8-C7 | 4.22 | 1.64 | 1.50 | 5 | 6 |
| 3 | C | 348 | PX4 | C6-C7 | 4.22 | 1.64 | 1.50 | 15 | 7 |
| 3 | C | 357 | PX4 | C6-C7 | 4.21 | 1.64 | 1.50 | 9 | 4 |
| 3 | A | 624 | PX4 | C6-C7 | 4.21 | 1.64 | 1.50 | 2 | 7 |
| 3 | A | 629 | PX4 | C24-C23 | 4.20 | 1.62 | 1.50 | 4 | 3 |
| 3 | A | 649 | PX4 | C6-C7 | 4.20 | 1.63 | 1.50 | 9 | 7 |
| 3 | A | 639 | PX4 | C8-C7 | 4.19 | 1.63 | 1.50 | 14 | 6 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 343 | PX4 | O7-C7 | 4.18 | 1.36 | 1.46 | 15 | 3 |
| 3 | B | 333 | PX4 | C6-C7 | 4.18 | 1.63 | 1.50 | 15 | 5 |
| 3 | A | 628 | PX4 | O7-C7 | 4.18 | 1.36 | 1.46 | 2 | 2 |
| 3 | C | 313 | PX4 | C6-C7 | 4.18 | 1.63 | 1.50 | 5 | 4 |
| 3 | C | 334 | PX4 | O7-C23 | 4.18 | 1.22 | 1.34 | 8 | 3 |
| 3 | B | 360 | PX4 | C10-C9 | 4.17 | 1.62 | 1.50 | 4 | 3 |
| 3 | B | 389 | PX4 | C24-C23 | 4.17 | 1.62 | 1.50 | 13 | 2 |
| 3 | C | 360 | PX4 | C6-C7 | 4.17 | 1.63 | 1.50 | 14 | 4 |
| 3 | C | 359 | PX4 | C6-C7 | 4.17 | 1.63 | 1.50 | 9 | 8 |
| 3 | C | 357 | PX4 | C2-C1 | 4.16 | 1.63 | 1.51 | 8 | 6 |
| 3 | B | 383 | PX4 | C24-C23 | 4.16 | 1.62 | 1.50 | 8 | 5 |
| 3 | B | 384 | PX4 | C2-C1 | 4.15 | 1.63 | 1.51 | 11 | 4 |
| 3 | B | 355 | PX4 | O7-C23 | 4.15 | 1.22 | 1.34 | 12 | 4 |
| 3 | B | 324 | PX4 | C8-C7 | 4.15 | 1.63 | 1.50 | 2 | 5 |
| 3 | B | 345 | PX4 | C24-C23 | 4.14 | 1.62 | 1.50 | 1 | 4 |
| 3 | A | 637 | PX4 | C10-C9 | 4.14 | 1.62 | 1.50 | 7 | 4 |
| 3 | B | 373 | PX4 | O5-C8 | 4.14 | 1.54 | 1.45 | 4 | 3 |
| 3 | C | 343 | PX4 | O7-C7 | 4.14 | 1.36 | 1.46 | 3 | 2 |
| 3 | C | 335 | PX4 | C10-C9 | 4.13 | 1.62 | 1.50 | 13 | 7 |
| 3 | B | 349 | PX4 | C6-C7 | 4.13 | 1.63 | 1.50 | 12 | 7 |
| 3 | B | 351 | PX4 | C6-C7 | 4.13 | 1.63 | 1.50 | 3 | 6 |
| 3 | B | 316 | PX4 | C8-C7 | 4.12 | 1.63 | 1.50 | 12 | 6 |
| 3 | B | 306 | PX4 | O7-C7 | 4.12 | 1.36 | 1.46 | 8 | 4 |
| 3 | B | 309 | PX4 | C2-C1 | 4.12 | 1.63 | 1.51 | 14 | 8 |
| 3 | B | 363 | PX4 | O7-C7 | 4.12 | 1.36 | 1.46 | 13 | 4 |
| 3 | C | 308 | PX4 | O5-C8 | 4.12 | 1.54 | 1.45 | 6 | 4 |
| 3 | A | 642 | PX4 | C2-C1 | 4.11 | 1.63 | 1.51 | 15 | 2 |
| 3 | B | 387 | PX4 | C6-C7 | 4.10 | 1.63 | 1.50 | 7 | 5 |
| 3 | C | 364 | PX4 | C6-C7 | 4.10 | 1.63 | 1.50 | 9 | 7 |
| 3 | A | 605 | PX4 | C8-C7 | 4.10 | 1.63 | 1.50 | 10 | 6 |
| 3 | A | 646 | PX4 | C2-C1 | 4.10 | 1.63 | 1.51 | 12 | 7 |
| 3 | B | 382 | PX4 | C2-C1 | 4.09 | 1.63 | 1.51 | 2 | 7 |
| 3 | C | 341 | PX4 | C6-C7 | 4.09 | 1.63 | 1.50 | 5 | 7 |
| 3 | C | 362 | PX4 | C6-C7 | 4.09 | 1.63 | 1.50 | 3 | 6 |
| 3 | C | 360 | PX4 | C2-C1 | 4.09 | 1.63 | 1.51 | 1 | 3 |
| 3 | B | 394 | PX4 | C6-C7 | 4.09 | 1.63 | 1.50 | 8 | 6 |
| 3 | A | 649 | PX4 | C8-C7 | 4.09 | 1.63 | 1.50 | 15 | 5 |
| 3 | B | 383 | PX4 | C10-C9 | 4.09 | 1.62 | 1.50 | 9 | 5 |
| 3 | C | 329 | PX4 | C6-C7 | 4.09 | 1.63 | 1.50 | 3 | 9 |
| 3 | C | 336 | PX4 | C2-C1 | 4.08 | 1.63 | 1.51 | 15 | 3 |
| 3 | B | 322 | PX4 | C6-C7 | 4.08 | 1.63 | 1.50 | 1 | 7 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | C | 320 | PX4 | C10-C9 | 4.08 | 1.62 | 1.50 | 4 | 5 |
| 3 | C | 358 | PX4 | O5-C9 | 4.08 | 1.21 | 1.33 | 10 | 2 |
| 3 | B | 324 | PX4 | C24-C23 | 4.07 | 1.62 | 1.50 | 10 | 3 |
| 3 | A | 603 | PX4 | C6-C7 | 4.06 | 1.63 | 1.50 | 15 | 8 |
| 3 | B | 383 | PX4 | C6-C7 | 4.06 | 1.63 | 1.50 | 2 | 6 |
| 3 | B | 370 | PX4 | C24-C23 | 4.06 | 1.62 | 1.50 | 15 | 3 |
| 3 | A | 641 | PX4 | O5-C9 | 4.06 | 1.21 | 1.33 | 7 | 1 |
| 3 | C | 345 | PX4 | C24-C23 | 4.06 | 1.62 | 1.50 | 14 | 1 |
| 3 | B | 310 | PX4 | O5-C8 | 4.06 | 1.36 | 1.45 | 6 | 4 |
| 3 | B | 342 | PX4 | C8-C7 | 4.06 | 1.63 | 1.50 | 6 | 9 |
| 3 | C | 325 | PX4 | C10-C9 | 4.06 | 1.62 | 1.50 | 8 | 3 |
| 3 | A | 644 | PX4 | O5-C8 | 4.05 | 1.36 | 1.45 | 5 | 1 |
| 3 | A | 613 | PX4 | C6-C7 | 4.05 | 1.63 | 1.50 | 2 | 5 |
| 3 | B | 395 | PX4 | C8-C7 | 4.05 | 1.63 | 1.50 | 10 | 5 |
| 3 | C | 318 | PX4 | C8-C7 | 4.05 | 1.63 | 1.50 | 8 | 3 |
| 3 | A | 654 | PX4 | C2-C1 | 4.04 | 1.63 | 1.51 | 2 | 3 |
| 3 | B | 301 | PX4 | C8-C7 | 4.04 | 1.63 | 1.50 | 15 | 3 |
| 3 | C | 343 | PX4 | C8-C7 | 4.04 | 1.63 | 1.50 | 15 | 6 |
| 3 | A | 604 | PX4 | C8-C7 | 4.04 | 1.63 | 1.50 | 10 | 3 |
| 3 | B | 377 | PX4 | C2-C1 | 4.03 | 1.63 | 1.51 | 8 | 6 |
| 3 | C | 339 | PX4 | C2-C1 | 4.03 | 1.63 | 1.51 | 2 | 9 |
| 3 | C | 344 | PX4 | C8-C7 | 4.03 | 1.63 | 1.50 | 8 | 6 |
| 3 | A | 647 | PX4 | C2-C1 | 4.03 | 1.63 | 1.51 | 9 | 5 |
| 3 | B | 311 | PX4 | C6-C7 | 4.03 | 1.63 | 1.50 | 3 | 7 |
| 3 | A | 611 | PX4 | O5-C9 | 4.03 | 1.45 | 1.33 | 10 | 2 |
| 3 | C | 301 | PX4 | C8-C7 | 4.03 | 1.63 | 1.50 | 14 | 7 |
| 3 | A | 645 | PX4 | C2-C1 | 4.02 | 1.63 | 1.51 | 15 | 6 |
| 3 | B | 326 | PX4 | C24-C23 | 4.02 | 1.62 | 1.50 | 10 | 3 |
| 3 | C | 323 | PX4 | O5-C8 | 4.02 | 1.36 | 1.45 | 5 | 2 |
| 3 | B | 395 | PX4 | C6-C7 | 4.01 | 1.63 | 1.50 | 2 | 5 |
| 3 | B | 314 | PX4 | O7-C7 | 4.01 | 1.37 | 1.46 | 4 | 5 |
| 3 | B | 316 | PX4 | C4-N1 | 4.01 | 1.38 | 1.50 | 6 | 1 |
| 3 | B | 320 | PX4 | C6-C7 | 4.00 | 1.63 | 1.50 | 7 | 6 |
| 3 | B | 381 | PX4 | C11-C10 | 4.00 | 1.66 | 1.52 | 13 | 1 |
| 3 | B | 336 | PX4 | C8-C7 | 4.00 | 1.63 | 1.50 | 14 | 5 |
| 3 | B | 344 | PX4 | O7-C7 | 4.00 | 1.37 | 1.46 | 3 | 4 |
| 3 | C | 339 | PX4 | C6-C7 | 4.00 | 1.63 | 1.50 | 12 | 4 |
| 3 | C | 311 | PX4 | C8-C7 | 3.99 | 1.63 | 1.50 | 15 | 8 |
| 3 | B | 372 | PX4 | C6-C7 | 3.99 | 1.63 | 1.50 | 3 | 5 |
| 3 | C | 336 | PX4 | C6-C7 | 3.99 | 1.63 | 1.50 | 3 | 2 |
| 3 | B | 354 | PX4 | O7-C7 | 3.99 | 1.37 | 1.46 | 11 | 4 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 397 | PX4 | C2-C1 | 3.98 | 1.63 | 1.51 | 1 | 4 |
| 3 | B | 363 | PX4 | C6-C7 | 3.98 | 1.63 | 1.50 | 1 | 5 |
| 3 | C | 315 | PX4 | C2-N1 | 3.98 | 1.63 | 1.51 | 5 | 2 |
| 3 | C | 342 | PX4 | C8-C7 | 3.98 | 1.63 | 1.50 | 2 | 8 |
| 3 | C | 355 | PX4 | C8-C7 | 3.98 | 1.63 | 1.50 | 4 | 4 |
| 3 | B | 376 | PX4 | C2-C1 | 3.98 | 1.63 | 1.51 | 8 | 8 |
| 3 | C | 313 | PX4 | C24-C23 | 3.98 | 1.62 | 1.50 | 5 | 2 |
| 3 | C | 333 | PX4 | C3-N1 | 3.98 | 1.38 | 1.50 | 9 | 2 |
| 3 | B | 316 | PX4 | C6-C7 | 3.98 | 1.63 | 1.50 | 15 | 9 |
| 3 | B | 327 | PX4 | O7-C7 | 3.98 | 1.37 | 1.46 | 6 | 5 |
| 3 | C | 329 | PX4 | O5-C8 | 3.98 | 1.36 | 1.45 | 1 | 5 |
| 3 | C | 306 | PX4 | O7-C7 | 3.97 | 1.37 | 1.46 | 7 | 4 |
| 3 | C | 309 | PX4 | C8-C7 | 3.97 | 1.63 | 1.50 | 2 | 8 |
| 3 | B | 311 | PX4 | C8-C7 | 3.97 | 1.63 | 1.50 | 14 | 10 |
| 3 | C | 364 | PX4 | O7-C7 | 3.96 | 1.37 | 1.46 | 13 | 3 |
| 3 | A | 637 | PX4 | O7-C7 | 3.96 | 1.37 | 1.46 | 10 | 3 |
| 3 | A | 606 | PX4 | O7-C23 | 3.96 | 1.23 | 1.34 | 8 | 5 |
| 3 | A | 640 | PX4 | C10-C9 | 3.96 | 1.62 | 1.50 | 3 | 3 |
| 3 | C | 359 | PX4 | C2-C1 | 3.96 | 1.63 | 1.51 | 6 | 4 |
| 3 | C | 328 | PX4 | C2-C1 | 3.95 | 1.63 | 1.51 | 4 | 4 |
| 3 | C | 346 | PX4 | C6-C7 | 3.95 | 1.63 | 1.50 | 11 | 5 |
| 3 | C | 332 | PX4 | C24-C23 | 3.95 | 1.62 | 1.50 | 8 | 5 |
| 3 | C | 305 | PX4 | C6-C7 | 3.95 | 1.63 | 1.50 | 3 | 7 |
| 3 | C | 335 | PX4 | C6-C7 | 3.95 | 1.63 | 1.50 | 14 | 6 |
| 3 | A | 606 | PX4 | C8-C7 | 3.94 | 1.63 | 1.50 | 8 | 6 |
| 3 | B | 310 | PX4 | C6-C7 | 3.94 | 1.63 | 1.50 | 6 | 6 |
| 3 | B | 362 | PX4 | C8-C7 | 3.94 | 1.63 | 1.50 | 1 | 5 |
| 3 | A | 639 | PX4 | O7-C7 | 3.93 | 1.37 | 1.46 | 7 | 6 |
| 3 | B | 323 | PX4 | C8-C7 | 3.93 | 1.63 | 1.50 | 13 | 7 |
| 3 | C | 303 | PX4 | C6-C7 | 3.93 | 1.63 | 1.50 | 11 | 8 |
| 3 | C | 323 | PX4 | C6-C7 | 3.93 | 1.63 | 1.50 | 6 | 6 |
| 3 | C | 328 | PX4 | C8-C7 | 3.93 | 1.63 | 1.50 | 4 | 7 |
| 3 | B | 345 | PX4 | C11-C10 | 3.93 | 1.66 | 1.52 | 9 | 3 |
| 3 | B | 337 | PX4 | O5-C8 | 3.92 | 1.36 | 1.45 | 9 | 5 |
| 3 | A | 632 | PX4 | C8-C7 | 3.92 | 1.63 | 1.50 | 6 | 11 |
| 3 | B | 360 | PX4 | C6-C7 | 3.92 | 1.63 | 1.50 | 14 | 6 |
| 3 | A | 620 | PX4 | C2-C1 | 3.92 | 1.63 | 1.51 | 9 | 5 |
| 3 | B | 327 | PX4 | C2-C1 | 3.92 | 1.63 | 1.51 | 3 | 4 |
| 3 | B | 367 | PX4 | O7-C23 | 3.92 | 1.23 | 1.34 | 6 | 2 |
| 3 | C | 304 | PX4 | C11-C10 | 3.91 | 1.66 | 1.52 | 6 | 2 |
| 3 | B | 326 | PX4 | O7-C23 | 3.91 | 1.23 | 1.34 | 3 | 2 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | A | 648 | PX4 | C2-C1 | 3.91 | 1.63 | 1.51 | 5 | 6 |
| 3 | B | 378 | PX4 | C6-C7 | 3.91 | 1.63 | 1.50 | 14 | 6 |
| 3 | A | 636 | PX4 | C8-C7 | 3.91 | 1.63 | 1.50 | 12 | 3 |
| 3 | B | 356 | PX4 | C6-C7 | 3.91 | 1.63 | 1.50 | 12 | 7 |
| 3 | B | 305 | PX4 | O5-C8 | 3.91 | 1.36 | 1.45 | 13 | 2 |
| 3 | B | 374 | PX4 | C8-C7 | 3.90 | 1.63 | 1.50 | 2 | 6 |
| 3 | B | 337 | PX4 | C2-C1 | 3.90 | 1.63 | 1.51 | 14 | 4 |
| 3 | A | 637 | PX4 | C8-C7 | 3.90 | 1.63 | 1.50 | 1 | 3 |
| 3 | B | 376 | PX4 | O7-C7 | 3.90 | 1.37 | 1.46 | 2 | 5 |
| 3 | C | 322 | PX4 | C6-C7 | 3.90 | 1.63 | 1.50 | 5 | 7 |
| 3 | C | 363 | PX4 | O5-C8 | 3.90 | 1.36 | 1.45 | 4 | 2 |
| 3 | B | 386 | PX4 | C2-C1 | 3.89 | 1.63 | 1.51 | 8 | 5 |
| 3 | B | 383 | PX4 | C8-C7 | 3.89 | 1.63 | 1.50 | 9 | 9 |
| 3 | A | 605 | PX4 | C6-C7 | 3.89 | 1.63 | 1.50 | 6 | 6 |
| 3 | B | 310 | PX4 | C8-C7 | 3.88 | 1.62 | 1.50 | 5 | 8 |
| 3 | B | 384 | PX4 | C6-C7 | 3.88 | 1.62 | 1.50 | 8 | 8 |
| 3 | B | 375 | PX4 | C24-C23 | 3.88 | 1.62 | 1.50 | 7 | 2 |
| 3 | C | 359 | PX4 | C8-C7 | 3.88 | 1.62 | 1.50 | 5 | 5 |
| 3 | A | 637 | PX4 | O7-C23 | 3.87 | 1.23 | 1.34 | 3 | 1 |
| 3 | C | 307 | PX4 | C24-C23 | 3.87 | 1.61 | 1.50 | 2 | 5 |
| 3 | B | 377 | PX4 | C8-C7 | 3.87 | 1.62 | 1.50 | 8 | 8 |
| 3 | A | 633 | PX4 | C6-C7 | 3.87 | 1.62 | 1.50 | 7 | 4 |
| 3 | C | 327 | PX4 | C2-C1 | 3.87 | 1.63 | 1.51 | 4 | 6 |
| 3 | A | 651 | PX4 | C8-C7 | 3.86 | 1.62 | 1.50 | 14 | 9 |
| 3 | B | 374 | PX4 | C4-N1 | 3.86 | 1.38 | 1.50 | 5 | 1 |
| 3 | B | 364 | PX4 | C2-C1 | 3.86 | 1.63 | 1.51 | 11 | 7 |
| 3 | B | 367 | PX4 | C24-C23 | 3.86 | 1.61 | 1.50 | 5 | 3 |
| 3 | A | 649 | PX4 | O5-C8 | 3.85 | 1.53 | 1.45 | 10 | 2 |
| 3 | B | 323 | PX4 | C2-C1 | 3.85 | 1.63 | 1.51 | 10 | 3 |
| 3 | B | 390 | PX4 | C10-C9 | 3.85 | 1.61 | 1.50 | 11 | 2 |
| 3 | C | 329 | PX4 | C2-C1 | 3.85 | 1.63 | 1.51 | 3 | 6 |
| 3 | B | 332 | PX4 | C10-C9 | 3.85 | 1.61 | 1.50 | 15 | 3 |
| 3 | C | 361 | PX4 | C6-C7 | 3.85 | 1.62 | 1.50 | 3 | 4 |
| 3 | A | 622 | PX4 | O7-C7 | 3.85 | 1.37 | 1.46 | 7 | 4 |
| 3 | C | 310 | PX4 | C10-C9 | 3.85 | 1.61 | 1.50 | 10 | 2 |
| 3 | B | 302 | PX4 | C3-N1 | 3.84 | 1.61 | 1.50 | 2 | 3 |
| 3 | C | 311 | PX4 | O7-C7 | 3.84 | 1.37 | 1.46 | 4 | 3 |
| 3 | B | 323 | PX4 | C24-C23 | 3.84 | 1.61 | 1.50 | 10 | 5 |
| 3 | C | 306 | PX4 | C6-C7 | 3.84 | 1.62 | 1.50 | 14 | 8 |
| 3 | A | 604 | PX4 | C2-C1 | 3.84 | 1.62 | 1.51 | 11 | 3 |
| 3 | C | 357 | PX4 | C8-C7 | 3.83 | 1.62 | 1.50 | 5 | 7 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 350 | PX4 | O7-C7 | 3.83 | 1.37 | 1.46 | 14 | 5 |
| 3 | C | 310 | PX4 | C2-C1 | 3.83 | 1.62 | 1.51 | 1 | 8 |
| 3 | A | 611 | PX4 | O7-C7 | 3.82 | 1.37 | 1.46 | 7 | 3 |
| 3 | A | 639 | PX4 | C5-N1 | 3.82 | 1.61 | 1.50 | 5 | 5 |
| 3 | B | 347 | PX4 | C2-C1 | 3.82 | 1.62 | 1.51 | 9 | 6 |
| 3 | B | 359 | PX4 | C11-C10 | 3.82 | 1.66 | 1.52 | 14 | 1 |
| 3 | B | 320 | PX4 | C2-N1 | 3.82 | 1.63 | 1.51 | 14 | 2 |
| 3 | B | 392 | PX4 | O7-C7 | 3.82 | 1.37 | 1.46 | 5 | 4 |
| 3 | B | 393 | PX4 | C24-C23 | 3.81 | 1.61 | 1.50 | 10 | 5 |
| 3 | B | 398 | PX4 | C2-C1 | 3.81 | 1.62 | 1.51 | 5 | 5 |
| 3 | B | 338 | PX4 | C24-C23 | 3.81 | 1.61 | 1.50 | 2 | 3 |
| 3 | B | 311 | PX4 | C10-C9 | 3.81 | 1.61 | 1.50 | 3 | 3 |
| 3 | B | 312 | PX4 | C25-C24 | 3.81 | 1.66 | 1.52 | 15 | 2 |
| 3 | B | 371 | PX4 | C6-C7 | 3.81 | 1.62 | 1.50 | 14 | 7 |
| 3 | B | 399 | PX4 | C2-N1 | 3.81 | 1.63 | 1.51 | 2 | 1 |
| 3 | C | 307 | PX4 | O7-C7 | 3.81 | 1.37 | 1.46 | 6 | 2 |
| 3 | A | 631 | PX4 | C8-C7 | 3.80 | 1.62 | 1.50 | 10 | 10 |
| 3 | C | 308 | PX4 | C3-N1 | 3.80 | 1.61 | 1.50 | 13 | 4 |
| 3 | A | 618 | PX4 | C8-C7 | 3.80 | 1.62 | 1.50 | 5 | 7 |
| 3 | A | 631 | PX4 | C10-C9 | 3.80 | 1.61 | 1.50 | 10 | 1 |
| 3 | A | 635 | PX4 | C6-C7 | 3.80 | 1.62 | 1.50 | 15 | 5 |
| 3 | B | 385 | PX4 | C6-C7 | 3.80 | 1.62 | 1.50 | 7 | 6 |
| 3 | B | 392 | PX4 | C10-C9 | 3.80 | 1.61 | 1.50 | 7 | 6 |
| 3 | A | 653 | PX4 | C6-C7 | 3.79 | 1.62 | 1.50 | 7 | 8 |
| 3 | A | 612 | PX4 | O7-C23 | 3.79 | 1.23 | 1.34 | 4 | 2 |
| 3 | C | 308 | PX4 | C24-C23 | 3.79 | 1.39 | 1.50 | 4 | 5 |
| 3 | B | 348 | PX4 | O7-C7 | 3.79 | 1.37 | 1.46 | 11 | 4 |
| 3 | A | 610 | PX4 | C6-C7 | 3.79 | 1.62 | 1.50 | 9 | 7 |
| 3 | B | 321 | PX4 | C8-C7 | 3.79 | 1.62 | 1.50 | 15 | 9 |
| 3 | B | 346 | PX4 | C10-C9 | 3.79 | 1.61 | 1.50 | 10 | 5 |
| 3 | C | 354 | PX4 | C6-C7 | 3.79 | 1.62 | 1.50 | 3 | 8 |
| 3 | B | 317 | PX4 | C2-C1 | 3.79 | 1.62 | 1.51 | 6 | 6 |
| 3 | B | 371 | PX4 | O7-C7 | 3.78 | 1.37 | 1.46 | 15 | 4 |
| 3 | C | 330 | PX4 | C6-C7 | 3.78 | 1.62 | 1.50 | 3 | 9 |
| 3 | C | 310 | PX4 | C8-C7 | 3.78 | 1.62 | 1.50 | 12 | 4 |
| 3 | A | 633 | PX4 | C24-C23 | 3.77 | 1.61 | 1.50 | 6 | 5 |
| 3 | B | 399 | PX4 | C6-C7 | 3.77 | 1.62 | 1.50 | 12 | 5 |
| 3 | C | 302 | PX4 | C6-C7 | 3.77 | 1.62 | 1.50 | 3 | 4 |
| 3 | C | 307 | PX4 | C8-C7 | 3.76 | 1.62 | 1.50 | 8 | 7 |
| 3 | C | 311 | PX4 | C2-N1 | 3.77 | 1.62 | 1.51 | 3 | 3 |
| 3 | C | 335 | PX4 | O5-C8 | 3.77 | 1.53 | 1.45 | 9 | 2 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 312 | PX4 | C8-C7 | 3.76 | 1.62 | 1.50 | 6 | 7 |
| 3 | C | 326 | PX4 | C6-C7 | 3.76 | 1.62 | 1.50 | 6 | 3 |
| 3 | B | 369 | PX4 | C8-C7 | 3.75 | 1.62 | 1.50 | 10 | 4 |
| 3 | A | 650 | PX4 | C6-C7 | 3.75 | 1.62 | 1.50 | 8 | 5 |
| 3 | B | 309 | PX4 | O7-C7 | 3.75 | 1.37 | 1.46 | 3 | 4 |
| 3 | B | 331 | PX4 | C6-C7 | 3.75 | 1.62 | 1.50 | 7 | 4 |
| 3 | C | 337 | PX4 | C10-C9 | 3.75 | 1.61 | 1.50 | 1 | 4 |
| 3 | B | 348 | PX4 | C2-C1 | 3.75 | 1.62 | 1.51 | 7 | 6 |
| 3 | C | 362 | PX4 | C8-C7 | 3.75 | 1.62 | 1.50 | 14 | 6 |
| 3 | B | 380 | PX4 | C24-C23 | 3.74 | 1.61 | 1.50 | 12 | 3 |
| 3 | B | 393 | PX4 | C2-C1 | 3.74 | 1.62 | 1.51 | 13 | 6 |
| 3 | A | 615 | PX4 | C8-C7 | 3.74 | 1.62 | 1.50 | 7 | 6 |
| 3 | B | 351 | PX4 | O7-C7 | 3.74 | 1.37 | 1.46 | 13 | 4 |
| 3 | B | 334 | PX4 | O5-C8 | 3.73 | 1.36 | 1.45 | 1 | 5 |
| 3 | B | 305 | PX4 | O5-C9 | 3.73 | 1.22 | 1.33 | 10 | 4 |
| 3 | B | 392 | PX4 | O7-C23 | 3.73 | 1.23 | 1.34 | 7 | 4 |
| 3 | C | 358 | PX4 | O7-C23 | 3.73 | 1.23 | 1.34 | 2 | 2 |
| 3 | A | 608 | PX4 | C6-C7 | 3.73 | 1.62 | 1.50 | 15 | 8 |
| 3 | B | 345 | PX4 | C2-C1 | 3.72 | 1.62 | 1.51 | 2 | 4 |
| 3 | C | 333 | PX4 | C24-C23 | 3.72 | 1.61 | 1.50 | 1 | 5 |
| 3 | A | 602 | PX4 | O7-C7 | 3.72 | 1.37 | 1.46 | 2 | 4 |
| 3 | A | 616 | PX4 | C24-C23 | 3.72 | 1.61 | 1.50 | 5 | 2 |
| 3 | A | 623 | PX4 | C2-C1 | 3.72 | 1.62 | 1.51 | 4 | 3 |
| 3 | B | 312 | PX4 | C2-C1 | 3.72 | 1.62 | 1.51 | 9 | 5 |
| 3 | C | 312 | PX4 | C6-C7 | 3.72 | 1.62 | 1.50 | 1 | 6 |
| 3 | C | 326 | PX4 | C24-C23 | 3.72 | 1.61 | 1.50 | 15 | 4 |
| 3 | B | 387 | PX4 | C2-C1 | 3.72 | 1.62 | 1.51 | 15 | 4 |
| 3 | B | 351 | PX4 | C10-C9 | 3.71 | 1.61 | 1.50 | 7 | 2 |
| 3 | B | 356 | PX4 | O7-C23 | 3.71 | 1.23 | 1.34 | 5 | 2 |
| 3 | C | 356 | PX4 | C6-C7 | 3.72 | 1.62 | 1.50 | 8 | 5 |
| 3 | B | 377 | PX4 | C6-C7 | 3.71 | 1.62 | 1.50 | 5 | 8 |
| 3 | B | 328 | PX4 | C24-C23 | 3.71 | 1.61 | 1.50 | 10 | 3 |
| 3 | C | 333 | PX4 | C10-C9 | 3.71 | 1.61 | 1.50 | 11 | 3 |
| 3 | A | 607 | PX4 | C8-C7 | 3.71 | 1.62 | 1.50 | 3 | 9 |
| 3 | B | 315 | PX4 | C6-C7 | 3.71 | 1.62 | 1.50 | 13 | 6 |
| 3 | C | 349 | PX4 | O7-C23 | 3.71 | 1.23 | 1.34 | 2 | 5 |
| 3 | A | 625 | PX4 | C8-C7 | 3.71 | 1.62 | 1.50 | 8 | 6 |
| 3 | B | 319 | PX4 | C11-C10 | 3.71 | 1.65 | 1.52 | 2 | 2 |
| 3 | C | 361 | PX4 | O5-C9 | 3.71 | 1.44 | 1.33 | 1 | 2 |
| 3 | C | 363 | PX4 | C2-C1 | 3.71 | 1.62 | 1.51 | 7 | 6 |
| 3 | B | 369 | PX4 | C11-C10 | 3.70 | 1.65 | 1.52 | 13 | 2 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 317 | PX4 | C6-C7 | 3.70 | 1.62 | 1.50 | 4 | 6 |
| 3 | A | 607 | PX4 | C5-N1 | 3.70 | 1.60 | 1.50 | 11 | 2 |
| 3 | A | 626 | PX4 | C2-C1 | 3.69 | 1.62 | 1.51 | 12 | 8 |
| 3 | A | 649 | PX4 | O7-C7 | 3.69 | 1.37 | 1.46 | 12 | 4 |
| 3 | B | 346 | PX4 | C6-C7 | 3.69 | 1.62 | 1.50 | 6 | 8 |
| 3 | A | 620 | PX4 | O5-C8 | 3.69 | 1.36 | 1.45 | 6 | 2 |
| 3 | B | 345 | PX4 | O5-C8 | 3.68 | 1.53 | 1.45 | 13 | 2 |
| 3 | B | 368 | PX4 | O7-C7 | 3.68 | 1.37 | 1.46 | 12 | 3 |
| 3 | C | 303 | PX4 | C2-C1 | 3.68 | 1.62 | 1.51 | 1 | 2 |
| 3 | A | 652 | PX4 | C10-C9 | 3.68 | 1.61 | 1.50 | 13 | 5 |
| 3 | B | 308 | PX4 | C6-C7 | 3.68 | 1.62 | 1.50 | 2 | 5 |
| 3 | A | 625 | PX4 | C2-C1 | 3.68 | 1.62 | 1.51 | 7 | 3 |
| 3 | C | 328 | PX4 | C6-C7 | 3.68 | 1.62 | 1.50 | 9 | 5 |
| 3 | B | 367 | PX4 | C6-C7 | 3.68 | 1.62 | 1.50 | 14 | 3 |
| 3 | B | 322 | PX4 | C8-C7 | 3.67 | 1.62 | 1.50 | 6 | 5 |
| 3 | B | 347 | PX4 | C10-C9 | 3.67 | 1.61 | 1.50 | 7 | 4 |
| 3 | C | 348 | PX4 | C8-C7 | 3.68 | 1.62 | 1.50 | 12 | 7 |
| 3 | B | 329 | PX4 | C6-C7 | 3.67 | 1.62 | 1.50 | 5 | 6 |
| 3 | A | 627 | PX4 | C6-C7 | 3.67 | 1.62 | 1.50 | 4 | 8 |
| 3 | A | 640 | PX4 | C8-C7 | 3.67 | 1.62 | 1.50 | 6 | 8 |
| 3 | B | 359 | PX4 | C10-C9 | 3.67 | 1.61 | 1.50 | 4 | 4 |
| 3 | A | 638 | PX4 | O5-C8 | 3.67 | 1.37 | 1.45 | 15 | 3 |
| 3 | B | 326 | PX4 | C8-C7 | 3.67 | 1.62 | 1.50 | 3 | 7 |
| 3 | B | 359 | PX4 | C6-C7 | 3.67 | 1.62 | 1.50 | 9 | 6 |
| 3 | B | 343 | PX4 | C2-C1 | 3.67 | 1.62 | 1.51 | 13 | 4 |
| 3 | C | 317 | PX4 | C8-C7 | 3.67 | 1.62 | 1.50 | 6 | 9 |
| 3 | B | 306 | PX4 | C24-C23 | 3.66 | 1.61 | 1.50 | 1 | 3 |
| 3 | A | 617 | PX4 | C8-C7 | 3.66 | 1.62 | 1.50 | 11 | 10 |
| 3 | C | 325 | PX4 | O7-C23 | 3.66 | 1.23 | 1.34 | 3 | 5 |
| 3 | C | 355 | PX4 | C10-C9 | 3.66 | 1.61 | 1.50 | 9 | 4 |
| 3 | B | 302 | PX4 | C2-C1 | 3.66 | 1.62 | 1.51 | 8 | 6 |
| 3 | A | 610 | PX4 | C2-C1 | 3.65 | 1.62 | 1.51 | 1 | 2 |
| 3 | A | 649 | PX4 | C2-C1 | 3.65 | 1.62 | 1.51 | 11 | 5 |
| 3 | A | 654 | PX4 | C24-C23 | 3.65 | 1.61 | 1.50 | 14 | 3 |
| 3 | A | 613 | PX4 | O5-C8 | 3.65 | 1.53 | 1.45 | 12 | 5 |
| 3 | A | 654 | PX4 | C10-C9 | 3.65 | 1.61 | 1.50 | 6 | 4 |
| 3 | B | 313 | PX4 | C8-C7 | 3.65 | 1.62 | 1.50 | 13 | 6 |
| 3 | B | 368 | PX4 | C2-C1 | 3.65 | 1.62 | 1.51 | 3 | 6 |
| 3 | C | 352 | PX4 | C24-C23 | 3.65 | 1.40 | 1.50 | 3 | 3 |
| 3 | A | 646 | PX4 | C24-C23 | 3.65 | 1.61 | 1.50 | 9 | 2 |
| 3 | B | 372 | PX4 | C24-C23 | 3.65 | 1.61 | 1.50 | 10 | 3 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | A | 648 | PX4 | C6-C7 | 3.64 | 1.62 | 1.50 | 11 | 7 |
| 3 | C | 305 | PX4 | C25-C24 | 3.64 | 1.65 | 1.52 | 7 | 1 |
| 3 | C | 314 | PX4 | C3-N1 | 3.64 | 1.39 | 1.50 | 3 | 2 |
| 3 | C | 329 | PX4 | C8-C7 | 3.64 | 1.62 | 1.50 | 15 | 7 |
| 3 | A | 606 | PX4 | C6-C7 | 3.64 | 1.62 | 1.50 | 3 | 6 |
| 3 | A | 609 | PX4 | C8-C7 | 3.64 | 1.62 | 1.50 | 4 | 8 |
| 3 | A | 630 | PX4 | C2-C1 | 3.64 | 1.62 | 1.51 | 9 | 3 |
| 3 | C | 343 | PX4 | C2-C1 | 3.64 | 1.62 | 1.51 | 3 | 3 |
| 3 | A | 621 | PX4 | C2-C1 | 3.63 | 1.62 | 1.51 | 1 | 3 |
| 3 | B | 343 | PX4 | O7-C23 | 3.63 | 1.24 | 1.34 | 12 | 3 |
| 3 | B | 301 | PX4 | O7-C7 | 3.63 | 1.38 | 1.46 | 9 | 5 |
| 3 | B | 329 | PX4 | O7-C7 | 3.63 | 1.38 | 1.46 | 3 | 4 |
| 3 | C | 310 | PX4 | C6-C7 | 3.63 | 1.62 | 1.50 | 1 | 5 |
| 3 | C | 339 | PX4 | C8-C7 | 3.63 | 1.62 | 1.50 | 1 | 4 |
| 3 | A | 646 | PX4 | C8-C7 | 3.62 | 1.62 | 1.50 | 9 | 6 |
| 3 | B | 379 | PX4 | C8-C7 | 3.62 | 1.62 | 1.50 | 13 | 10 |
| 3 | C | 314 | PX4 | O5-C8 | 3.62 | 1.53 | 1.45 | 13 | 2 |
| 3 | C | 315 | PX4 | C8-C7 | 3.62 | 1.62 | 1.50 | 2 | 5 |
| 3 | B | 384 | PX4 | C10-C9 | 3.62 | 1.61 | 1.50 | 5 | 4 |
| 3 | B | 321 | PX4 | C2-C1 | 3.62 | 1.62 | 1.51 | 10 | 3 |
| 3 | B | 325 | PX4 | C2-C1 | 3.62 | 1.62 | 1.51 | 15 | 7 |
| 3 | B | 348 | PX4 | C8-C7 | 3.62 | 1.62 | 1.50 | 13 | 7 |
| 3 | B | 364 | PX4 | O5-C8 | 3.62 | 1.37 | 1.45 | 8 | 5 |
| 3 | A | 622 | PX4 | C6-C7 | 3.61 | 1.62 | 1.50 | 6 | 6 |
| 3 | A | 603 | PX4 | C8-C7 | 3.61 | 1.62 | 1.50 | 14 | 6 |
| 3 | B | 328 | PX4 | C2-C1 | 3.61 | 1.62 | 1.51 | 7 | 4 |
| 3 | B | 335 | PX4 | C2-C1 | 3.61 | 1.62 | 1.51 | 3 | 5 |
| 3 | C | 352 | PX4 | C6-C7 | 3.60 | 1.62 | 1.50 | 1 | 10 |
| 3 | B | 376 | PX4 | C8-C7 | 3.60 | 1.62 | 1.50 | 6 | 7 |
| 3 | C | 318 | PX4 | C24-C23 | 3.60 | 1.61 | 1.50 | 8 | 1 |
| 3 | C | 347 | PX4 | C2-N1 | 3.60 | 1.62 | 1.51 | 5 | 1 |
| 3 | C | 319 | PX4 | C8-C7 | 3.60 | 1.62 | 1.50 | 7 | 10 |
| 3 | C | 344 | PX4 | O7-C7 | 3.60 | 1.38 | 1.46 | 13 | 5 |
| 3 | C | 353 | PX4 | C2-C1 | 3.60 | 1.62 | 1.51 | 15 | 10 |
| 3 | A | 614 | PX4 | C6-C7 | 3.60 | 1.62 | 1.50 | 2 | 6 |
| 3 | B | 399 | PX4 | O7-C7 | 3.59 | 1.38 | 1.46 | 11 | 3 |
| 3 | C | 362 | PX4 | O7-C7 | 3.59 | 1.38 | 1.46 | 1 | 2 |
| 3 | B | 329 | PX4 | C10-C9 | 3.59 | 1.61 | 1.50 | 14 | 4 |
| 3 | B | 359 | PX4 | C2-C1 | 3.59 | 1.62 | 1.51 | 13 | 4 |
| 3 | C | 302 | PX4 | C2-C1 | 3.59 | 1.62 | 1.51 | 4 | 6 |
| 3 | C | 364 | PX4 | C8-C7 | 3.59 | 1.62 | 1.50 | 12 | 7 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | C | 326 | PX4 | C2-C1 | 3.59 | 1.62 | 1.51 | 2 | 3 |
| 3 | C | 347 | PX4 | C2-C1 | 3.59 | 1.62 | 1.51 | 15 | 2 |
| 3 | C | 340 | PX4 | O5-C8 | 3.58 | 1.53 | 1.45 | 2 | 3 |
| 3 | C | 359 | PX4 | C10-C9 | 3.58 | 1.61 | 1.50 | 4 | 5 |
| 3 | A | 624 | PX4 | C2-C1 | 3.58 | 1.62 | 1.51 | 3 | 5 |
| 3 | C | 355 | PX4 | O5-C9 | 3.58 | 1.22 | 1.33 | 2 | 2 |
| 3 | C | 317 | PX4 | C24-C23 | 3.58 | 1.61 | 1.50 | 13 | 5 |
| 3 | B | 389 | PX4 | C8-C7 | 3.58 | 1.62 | 1.50 | 2 | 6 |
| 3 | A | 621 | PX4 | C24-C23 | 3.57 | 1.61 | 1.50 | 13 | 2 |
| 3 | C | 317 | PX4 | C2-C1 | 3.58 | 1.62 | 1.51 | 5 | 5 |
| 3 | C | 320 | PX4 | C24-C23 | 3.57 | 1.61 | 1.50 | 7 | 4 |
| 3 | A | 618 | PX4 | C6-C7 | 3.57 | 1.62 | 1.50 | 13 | 3 |
| 3 | C | 316 | PX4 | O7-C7 | 3.57 | 1.38 | 1.46 | 10 | 2 |
| 3 | A | 619 | PX4 | O7-C7 | 3.57 | 1.38 | 1.46 | 1 | 3 |
| 3 | B | 340 | PX4 | C2-C1 | 3.57 | 1.62 | 1.51 | 3 | 4 |
| 3 | B | 307 | PX4 | O7-C7 | 3.57 | 1.38 | 1.46 | 15 | 1 |
| 3 | C | 318 | PX4 | C6-C7 | 3.57 | 1.62 | 1.50 | 14 | 7 |
| 3 | C | 341 | PX4 | C8-C7 | 3.57 | 1.62 | 1.50 | 2 | 8 |
| 3 | A | 616 | PX4 | O5-C9 | 3.57 | 1.23 | 1.33 | 14 | 1 |
| 3 | B | 361 | PX4 | C6-C7 | 3.57 | 1.62 | 1.50 | 8 | 10 |
| 3 | B | 360 | PX4 | O7-C7 | 3.56 | 1.38 | 1.46 | 7 | 4 |
| 3 | C | 358 | PX4 | C24-C23 | 3.56 | 1.61 | 1.50 | 9 | 6 |
| 3 | A | 610 | PX4 | C8-C7 | 3.56 | 1.61 | 1.50 | 13 | 5 |
| 3 | A | 626 | PX4 | C2-N1 | 3.56 | 1.62 | 1.51 | 14 | 2 |
| 3 | B | 307 | PX4 | C2-C1 | 3.56 | 1.62 | 1.51 | 4 | 5 |
| 3 | C | 360 | PX4 | C25-C24 | 3.56 | 1.65 | 1.52 | 12 | 2 |
| 3 | A | 615 | PX4 | C6-C7 | 3.55 | 1.61 | 1.50 | 6 | 4 |
| 3 | C | 321 | PX4 | O7-C7 | 3.55 | 1.38 | 1.46 | 2 | 3 |
| 3 | A | 602 | PX4 | C2-C1 | 3.55 | 1.62 | 1.51 | 1 | 8 |
| 3 | B | 342 | PX4 | C24-C23 | 3.55 | 1.61 | 1.50 | 10 | 3 |
| 3 | C | 363 | PX4 | C6-C7 | 3.55 | 1.61 | 1.50 | 14 | 3 |
| 3 | C | 320 | PX4 | C8-C7 | 3.55 | 1.61 | 1.50 | 4 | 8 |
| 3 | A | 640 | PX4 | C6-C7 | 3.54 | 1.61 | 1.50 | 4 | 5 |
| 3 | B | 318 | PX4 | C2-N1 | 3.54 | 1.62 | 1.51 | 15 | 1 |
| 3 | B | 365 | PX4 | C8-C7 | 3.54 | 1.61 | 1.50 | 4 | 5 |
| 3 | B | 377 | PX4 | C25-C24 | 3.54 | 1.65 | 1.52 | 5 | 2 |
| 3 | C | 328 | PX4 | C2-N1 | 3.54 | 1.62 | 1.51 | 3 | 2 |
| 3 | A | 620 | PX4 | C8-C7 | 3.54 | 1.61 | 1.50 | 4 | 5 |
| 3 | C | 312 | PX4 | O7-C7 | 3.54 | 1.38 | 1.46 | 12 | 2 |
| 3 | B | 328 | PX4 | C3-N1 | 3.54 | 1.60 | 1.50 | 1 | 3 |
| 3 | B | 355 | PX4 | C2-C1 | 3.54 | 1.62 | 1.51 | 10 | 5 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | C | 308 | PX4 | C2-C1 | 3.54 | 1.62 | 1.51 | 13 | 6 |
| 3 | C | 334 | PX4 | C24-C23 | 3.53 | 1.61 | 1.50 | 2 | 4 |
| 3 | A | 601 | PX4 | C10-C9 | 3.53 | 1.60 | 1.50 | 5 | 5 |
| 3 | A | 625 | PX4 | C10-C9 | 3.53 | 1.61 | 1.50 | 1 | 6 |
| 3 | B | 396 | PX4 | C6-C7 | 3.53 | 1.61 | 1.50 | 7 | 7 |
| 3 | C | 311 | PX4 | C24-C23 | 3.53 | 1.61 | 1.50 | 1 | 3 |
| 3 | B | 361 | PX4 | C8-C7 | 3.53 | 1.61 | 1.50 | 10 | 5 |
| 3 | C | 354 | PX4 | C2-C1 | 3.53 | 1.62 | 1.51 | 4 | 7 |
| 3 | A | 612 | PX4 | C6-C7 | 3.52 | 1.61 | 1.50 | 1 | 5 |
| 3 | A | 628 | PX4 | C8-C7 | 3.52 | 1.61 | 1.50 | 5 | 5 |
| 3 | B | 400 | PX4 | C2-N1 | 3.52 | 1.62 | 1.51 | 7 | 4 |
| 3 | B | 307 | PX4 | C25-C24 | 3.52 | 1.65 | 1.52 | 11 | 3 |
| 3 | B | 333 | PX4 | O5-C8 | 3.52 | 1.37 | 1.45 | 10 | 4 |
| 3 | C | 361 | PX4 | C8-C7 | 3.52 | 1.61 | 1.50 | 3 | 5 |
| 3 | C | 355 | PX4 | C4-N1 | 3.52 | 1.39 | 1.50 | 14 | 1 |
| 3 | B | 306 | PX4 | C2-C1 | 3.52 | 1.62 | 1.51 | 12 | 4 |
| 3 | C | 327 | PX4 | C6-C7 | 3.52 | 1.61 | 1.50 | 6 | 7 |
| 3 | C | 352 | PX4 | C2-C1 | 3.52 | 1.62 | 1.51 | 9 | 5 |
| 3 | B | 302 | PX4 | C6-C7 | 3.51 | 1.61 | 1.50 | 11 | 5 |
| 3 | B | 374 | PX4 | C24-C23 | 3.51 | 1.60 | 1.50 | 14 | 4 |
| 3 | C | 337 | PX4 | C8-C7 | 3.51 | 1.61 | 1.50 | 2 | 5 |
| 3 | B | 335 | PX4 | C6-C7 | 3.51 | 1.61 | 1.50 | 3 | 7 |
| 3 | A | 637 | PX4 | C6-C7 | 3.51 | 1.61 | 1.50 | 11 | 5 |
| 3 | C | 335 | PX4 | O7-C7 | 3.51 | 1.38 | 1.46 | 14 | 2 |
| 3 | A | 642 | PX4 | C24-C23 | 3.51 | 1.60 | 1.50 | 14 | 3 |
| 3 | C | 328 | PX4 | C24-C23 | 3.51 | 1.60 | 1.50 | 12 | 2 |
| 3 | C | 351 | PX4 | C24-C23 | 3.51 | 1.60 | 1.50 | 9 | 5 |
| 3 | A | 653 | PX4 | C10-C9 | 3.51 | 1.60 | 1.50 | 7 | 1 |
| 3 | B | 378 | PX4 | O5-C9 | 3.50 | 1.23 | 1.33 | 1 | 2 |
| 3 | B | 336 | PX4 | C2-C1 | 3.50 | 1.61 | 1.51 | 2 | 3 |
| 3 | B | 341 | PX4 | C2-C1 | 3.50 | 1.61 | 1.51 | 10 | 4 |
| 3 | C | 302 | PX4 | O7-C7 | 3.50 | 1.38 | 1.46 | 7 | 3 |
| 3 | C | 323 | PX4 | O5-C9 | 3.50 | 1.43 | 1.33 | 3 | 2 |
| 3 | B | 340 | PX4 | C4-N1 | 3.50 | 1.39 | 1.50 | 11 | 1 |
| 3 | B | 394 | PX4 | O7-C23 | 3.49 | 1.24 | 1.34 | 13 | 3 |
| 3 | B | 366 | PX4 | C2-N1 | 3.49 | 1.62 | 1.51 | 7 | 2 |
| 3 | B | 382 | PX4 | C4-N1 | 3.49 | 1.39 | 1.50 | 10 | 3 |
| 3 | C | 326 | PX4 | O7-C7 | 3.49 | 1.38 | 1.46 | 6 | 4 |
| 3 | B | 334 | PX4 | C2-C1 | 3.49 | 1.61 | 1.51 | 7 | 6 |
| 3 | B | 341 | PX4 | C6-C7 | 3.49 | 1.61 | 1.50 | 12 | 8 |
| 3 | B | 397 | PX4 | C10-C9 | 3.49 | 1.60 | 1.50 | 8 | 5 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | A | 605 | PX4 | C24-C23 | 3.48 | 1.60 | 1.50 | 11 | 4 |
| 3 | A | 636 | PX4 | C6-C7 | 3.48 | 1.61 | 1.50 | 7 | 7 |
| 3 | C | 334 | PX4 | C10-C9 | 3.48 | 1.60 | 1.50 | 2 | 6 |
| 3 | A | 650 | PX4 | C2-N1 | 3.48 | 1.62 | 1.51 | 6 | 3 |
| 3 | B | 363 | PX4 | C2-C1 | 3.48 | 1.61 | 1.51 | 1 | 5 |
| 3 | B | 352 | PX4 | O7-C23 | 3.48 | 1.44 | 1.34 | 4 | 3 |
| 3 | B | 396 | PX4 | C2-C1 | 3.48 | 1.61 | 1.51 | 2 | 7 |
| 3 | C | 354 | PX4 | C8-C7 | 3.48 | 1.61 | 1.50 | 10 | 10 |
| 3 | A | 653 | PX4 | O7-C7 | 3.48 | 1.38 | 1.46 | 6 | 6 |
| 3 | A | 635 | PX4 | C2-N1 | 3.47 | 1.62 | 1.51 | 3 | 1 |
| 3 | C | 356 | PX4 | C2-C1 | 3.48 | 1.61 | 1.51 | 9 | 4 |
| 3 | B | 332 | PX4 | C6-C7 | 3.47 | 1.61 | 1.50 | 4 | 7 |
| 3 | C | 331 | PX4 | C8-C7 | 3.47 | 1.61 | 1.50 | 13 | 6 |
| 3 | C | 336 | PX4 | C10-C9 | 3.47 | 1.60 | 1.50 | 8 | 6 |
| 3 | B | 334 | PX4 | C8-C7 | 3.47 | 1.61 | 1.50 | 8 | 8 |
| 3 | C | 321 | PX4 | O5-C9 | 3.47 | 1.43 | 1.33 | 12 | 3 |
| 3 | B | 309 | PX4 | C24-C23 | 3.47 | 1.60 | 1.50 | 10 | 4 |
| 3 | A | 619 | PX4 | C10-C9 | 3.47 | 1.60 | 1.50 | 1 | 5 |
| 3 | B | 311 | PX4 | C2-C1 | 3.47 | 1.61 | 1.51 | 3 | 6 |
| 3 | B | 316 | PX4 | O7-C7 | 3.47 | 1.38 | 1.46 | 9 | 4 |
| 3 | A | 610 | PX4 | C24-C23 | 3.46 | 1.60 | 1.50 | 4 | 4 |
| 3 | A | 630 | PX4 | O5-C8 | 3.46 | 1.52 | 1.45 | 14 | 3 |
| 3 | C | 315 | PX4 | O3-C1 | 3.46 | 1.30 | 1.44 | 1 | 1 |
| 3 | C | 345 | PX4 | C6-C7 | 3.46 | 1.61 | 1.50 | 14 | 7 |
| 3 | A | 623 | PX4 | C6-C7 | 3.46 | 1.61 | 1.50 | 4 | 4 |
| 3 | C | 338 | PX4 | C6-C7 | 3.46 | 1.61 | 1.50 | 5 | 3 |
| 3 | A | 616 | PX4 | C2-C1 | 3.46 | 1.61 | 1.51 | 13 | 5 |
| 3 | B | 363 | PX4 | C8-C7 | 3.46 | 1.61 | 1.50 | 15 | 8 |
| 3 | C | 343 | PX4 | C10-C9 | 3.46 | 1.60 | 1.50 | 14 | 2 |
| 3 | B | 352 | PX4 | O7-C7 | 3.46 | 1.38 | 1.46 | 2 | 4 |
| 3 | C | 363 | PX4 | C4-N1 | 3.46 | 1.40 | 1.50 | 12 | 1 |
| 3 | A | 636 | PX4 | C24-C23 | 3.45 | 1.60 | 1.50 | 5 | 6 |
| 3 | C | 308 | PX4 | C6-C7 | 3.45 | 1.61 | 1.50 | 5 | 5 |
| 3 | C | 350 | PX4 | O7-C23 | 3.45 | 1.24 | 1.34 | 15 | 4 |
| 3 | B | 340 | PX4 | O5-C9 | 3.45 | 1.23 | 1.33 | 6 | 2 |
| 3 | A | 643 | PX4 | O5-C9 | 3.45 | 1.23 | 1.33 | 3 | 2 |
| 3 | B | 322 | PX4 | C24-C23 | 3.45 | 1.60 | 1.50 | 5 | 3 |
| 3 | A | 629 | PX4 | C8-C7 | 3.45 | 1.61 | 1.50 | 13 | 6 |
| 3 | B | 314 | PX4 | C24-C23 | 3.45 | 1.60 | 1.50 | 14 | 1 |
| 3 | B | 366 | PX4 | C6-C7 | 3.45 | 1.61 | 1.50 | 15 | 3 |
| 3 | B | 400 | PX4 | C8-C7 | 3.45 | 1.61 | 1.50 | 5 | 9 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | C | 355 | PX4 | C6-C7 | 3.45 | 1.61 | 1.50 | 1 | 9 |
| 3 | A | 631 | PX4 | C2-C1 | 3.44 | 1.61 | 1.51 | 11 | 6 |
| 3 | C | 329 | PX4 | C3-N1 | 3.44 | 1.60 | 1.50 | 9 | 2 |
| 3 | B | 336 | PX4 | C6-C7 | 3.44 | 1.61 | 1.50 | 5 | 8 |
| 3 | B | 328 | PX4 | O7-C7 | 3.44 | 1.38 | 1.46 | 12 | 4 |
| 3 | B | 378 | PX4 | C8-C7 | 3.44 | 1.61 | 1.50 | 1 | 9 |
| 3 | A | 650 | PX4 | C25-C24 | 3.44 | 1.64 | 1.52 | 12 | 1 |
| 3 | C | 316 | PX4 | C24-C23 | 3.44 | 1.60 | 1.50 | 7 | 5 |
| 3 | A | 633 | PX4 | O7-C23 | 3.43 | 1.24 | 1.34 | 2 | 2 |
| 3 | A | 630 | PX4 | C8-C7 | 3.43 | 1.61 | 1.50 | 5 | 5 |
| 3 | A | 643 | PX4 | C8-C7 | 3.43 | 1.61 | 1.50 | 1 | 6 |
| 3 | B | 344 | PX4 | C24-C23 | 3.43 | 1.60 | 1.50 | 1 | 3 |
| 3 | B | 360 | PX4 | C8-C7 | 3.43 | 1.61 | 1.50 | 14 | 6 |
| 3 | B | 386 | PX4 | C8-C7 | 3.43 | 1.61 | 1.50 | 5 | 7 |
| 3 | B | 310 | PX4 | C2-C1 | 3.43 | 1.61 | 1.51 | 15 | 7 |
| 3 | B | 388 | PX4 | C8-C7 | 3.43 | 1.61 | 1.50 | 6 | 6 |
| 3 | B | 389 | PX4 | C10-C9 | 3.43 | 1.60 | 1.50 | 5 | 4 |
| 3 | A | 646 | PX4 | O7-C23 | 3.42 | 1.24 | 1.34 | 8 | 2 |
| 3 | B | 305 | PX4 | C8-C7 | 3.42 | 1.61 | 1.50 | 8 | 8 |
| 3 | B | 357 | PX4 | C6-C7 | 3.42 | 1.61 | 1.50 | 3 | 4 |
| 3 | B | 354 | PX4 | O5-C9 | 3.42 | 1.43 | 1.33 | 10 | 1 |
| 3 | B | 327 | PX4 | C10-C9 | 3.42 | 1.60 | 1.50 | 14 | 3 |
| 3 | B | 359 | PX4 | C24-C23 | 3.42 | 1.60 | 1.50 | 6 | 4 |
| 3 | B | 373 | PX4 | C2-C1 | 3.42 | 1.61 | 1.51 | 6 | 6 |
| 3 | A | 632 | PX4 | O7-C23 | 3.42 | 1.24 | 1.34 | 11 | 4 |
| 3 | B | 331 | PX4 | C2-C1 | 3.42 | 1.61 | 1.51 | 12 | 4 |
| 3 | C | 331 | PX4 | C10-C9 | 3.42 | 1.60 | 1.50 | 6 | 5 |
| 3 | C | 316 | PX4 | C8-C7 | 3.42 | 1.61 | 1.50 | 7 | 8 |
| 3 | B | 400 | PX4 | C2-C1 | 3.41 | 1.61 | 1.51 | 2 | 4 |
| 3 | B | 382 | PX4 | C6-C7 | 3.41 | 1.61 | 1.50 | 5 | 9 |
| 3 | B | 397 | PX4 | O5-C8 | 3.41 | 1.52 | 1.45 | 5 | 2 |
| 3 | A | 635 | PX4 | C24-C23 | 3.41 | 1.60 | 1.50 | 1 | 4 |
| 3 | A | 621 | PX4 | C6-C7 | 3.41 | 1.61 | 1.50 | 14 | 7 |
| 3 | B | 344 | PX4 | C2-C1 | 3.41 | 1.61 | 1.51 | 2 | 9 |
| 3 | B | 394 | PX4 | O7-C7 | 3.41 | 1.38 | 1.46 | 1 | 3 |
| 3 | C | 305 | PX4 | C2-C1 | 3.41 | 1.61 | 1.51 | 5 | 2 |
| 3 | B | 338 | PX4 | C10-C9 | 3.40 | 1.60 | 1.50 | 10 | 2 |
| 3 | B | 387 | PX4 | C8-C7 | 3.40 | 1.61 | 1.50 | 13 | 7 |
| 3 | C | 350 | PX4 | O7-C7 | 3.40 | 1.38 | 1.46 | 8 | 3 |
| 3 | C | 353 | PX4 | C24-C23 | 3.40 | 1.60 | 1.50 | 13 | 3 |
| 3 | A | 629 | PX4 | C11-C10 | 3.40 | 1.64 | 1.52 | 1 | 2 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | A | 636 | PX4 | C2-C1 | 3.40 | 1.61 | 1.51 | 14 | 5 |
| 3 | B | 379 | PX4 | C2-C1 | 3.40 | 1.61 | 1.51 | 12 | 4 |
| 3 | C | 321 | PX4 | C10-C9 | 3.40 | 1.60 | 1.50 | 3 | 4 |
| 3 | C | 342 | PX4 | C6-C7 | 3.40 | 1.61 | 1.50 | 15 | 6 |
| 3 | C | 302 | PX4 | C8-C7 | 3.40 | 1.61 | 1.50 | 1 | 7 |
| 3 | B | 347 | PX4 | C6-C7 | 3.40 | 1.61 | 1.50 | 13 | 6 |
| 3 | C | 336 | PX4 | C8-C7 | 3.40 | 1.61 | 1.50 | 10 | 7 |
| 3 | A | 640 | PX4 | O7-C23 | 3.39 | 1.43 | 1.34 | 11 | 1 |
| 3 | B | 396 | PX4 | C10-C9 | 3.39 | 1.60 | 1.50 | 10 | 5 |
| 3 | A | 636 | PX4 | O7-C7 | 3.39 | 1.38 | 1.46 | 8 | 4 |
| 3 | B | 335 | PX4 | C8-C7 | 3.39 | 1.61 | 1.50 | 4 | 5 |
| 3 | C | 335 | PX4 | C4-N1 | 3.39 | 1.59 | 1.50 | 9 | 1 |
| 3 | C | 359 | PX4 | O7-C7 | 3.39 | 1.38 | 1.46 | 4 | 3 |
| 3 | C | 303 | PX4 | O7-C7 | 3.39 | 1.38 | 1.46 | 5 | 3 |
| 3 | B | 340 | PX4 | C6-C7 | 3.39 | 1.61 | 1.50 | 11 | 4 |
| 3 | B | 328 | PX4 | C6-C7 | 3.39 | 1.61 | 1.50 | 12 | 8 |
| 3 | B | 381 | PX4 | C8-C7 | 3.39 | 1.61 | 1.50 | 11 | 7 |
| 3 | A | 601 | PX4 | O5-C8 | 3.38 | 1.37 | 1.45 | 14 | 1 |
| 3 | C | 318 | PX4 | C2-C1 | 3.39 | 1.61 | 1.51 | 10 | 3 |
| 3 | A | 635 | PX4 | C8-C7 | 3.38 | 1.61 | 1.50 | 11 | 7 |
| 3 | C | 307 | PX4 | C6-C7 | 3.38 | 1.61 | 1.50 | 1 | 5 |
| 3 | C | 316 | PX4 | O7-C23 | 3.38 | 1.24 | 1.34 | 1 | 3 |
| 3 | B | 326 | PX4 | C2-C1 | 3.38 | 1.61 | 1.51 | 6 | 3 |
| 3 | B | 358 | PX4 | C5-N1 | 3.38 | 1.59 | 1.50 | 6 | 1 |
| 3 | B | 355 | PX4 | C24-C23 | 3.38 | 1.60 | 1.50 | 4 | 5 |
| 3 | C | 325 | PX4 | C8-C7 | 3.38 | 1.61 | 1.50 | 7 | 4 |
| 3 | B | 397 | PX4 | C5-N1 | 3.38 | 1.59 | 1.50 | 10 | 1 |
| 3 | A | 609 | PX4 | C6-C7 | 3.37 | 1.61 | 1.50 | 4 | 9 |
| 3 | B | 339 | PX4 | C2-C1 | 3.37 | 1.61 | 1.51 | 1 | 5 |
| 3 | B | 355 | PX4 | C6-C7 | 3.37 | 1.61 | 1.50 | 1 | 7 |
| 3 | C | 302 | PX4 | C25-C24 | 3.37 | 1.64 | 1.52 | 9 | 3 |
| 3 | C | 304 | PX4 | C6-C7 | 3.37 | 1.61 | 1.50 | 13 | 7 |
| 3 | C | 314 | PX4 | C8-C7 | 3.37 | 1.61 | 1.50 | 8 | 9 |
| 3 | C | 341 | PX4 | O7-C7 | 3.37 | 1.38 | 1.46 | 4 | 5 |
| 3 | A | 601 | PX4 | C6-C7 | 3.36 | 1.61 | 1.50 | 6 | 9 |
| 3 | B | 353 | PX4 | C6-C7 | 3.37 | 1.61 | 1.50 | 11 | 8 |
| 3 | B | 388 | PX4 | C2-C1 | 3.37 | 1.61 | 1.51 | 2 | 7 |
| 3 | C | 326 | PX4 | P1-O1 | 3.37 | 1.39 | 1.55 | 1 | 4 |
| 3 | C | 308 | PX4 | C10-C9 | 3.36 | 1.60 | 1.50 | 14 | 4 |
| 3 | B | 342 | PX4 | C19-C18 | 3.36 | 1.68 | 1.51 | 9 | 1 |
| 3 | C | 331 | PX4 | C6-C7 | 3.36 | 1.61 | 1.50 | 4 | 6 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | C | 332 | PX4 | C2-C1 | 3.36 | 1.61 | 1.51 | 6 | 4 |
| 3 | C | 354 | PX4 | C10-C9 | 3.36 | 1.60 | 1.50 | 3 | 3 |
| 3 | B | 319 | PX4 | C24-C23 | 3.36 | 1.60 | 1.50 | 6 | 3 |
| 3 | C | 349 | PX4 | C10-C9 | 3.36 | 1.60 | 1.50 | 10 | 3 |
| 3 | A | 635 | PX4 | C2-C1 | 3.36 | 1.61 | 1.51 | 10 | 6 |
| 3 | B | 303 | PX4 | C2-C1 | 3.36 | 1.61 | 1.51 | 5 | 7 |
| 3 | A | 607 | PX4 | O5-C9 | 3.36 | 1.43 | 1.33 | 11 | 4 |
| 3 | A | 627 | PX4 | C2-C1 | 3.36 | 1.61 | 1.51 | 8 | 4 |
| 3 | B | 370 | PX4 | C10-C9 | 3.36 | 1.60 | 1.50 | 14 | 3 |
| 3 | C | 301 | PX4 | C6-C7 | 3.35 | 1.61 | 1.50 | 13 | 5 |
| 3 | C | 306 | PX4 | C5-N1 | 3.36 | 1.59 | 1.50 | 9 | 2 |
| 3 | B | 356 | PX4 | C24-C23 | 3.35 | 1.60 | 1.50 | 5 | 2 |
| 3 | B | 369 | PX4 | O7-C23 | 3.35 | 1.24 | 1.34 | 8 | 2 |
| 3 | A | 616 | PX4 | O7-C23 | 3.35 | 1.24 | 1.34 | 10 | 3 |
| 3 | B | 320 | PX4 | O7-C7 | 3.35 | 1.38 | 1.46 | 1 | 3 |
| 3 | C | 347 | PX4 | O5-C8 | 3.35 | 1.37 | 1.45 | 10 | 1 |
| 3 | A | 651 | PX4 | C10-C9 | 3.35 | 1.60 | 1.50 | 8 | 4 |
| 3 | B | 327 | PX4 | O5-C8 | 3.35 | 1.52 | 1.45 | 11 | 1 |
| 3 | A | 601 | PX4 | C2-N1 | 3.35 | 1.61 | 1.51 | 10 | 2 |
| 3 | C | 335 | PX4 | O7-C23 | 3.35 | 1.24 | 1.34 | 8 | 1 |
| 3 | A | 652 | PX4 | C8-C7 | 3.34 | 1.61 | 1.50 | 13 | 10 |
| 3 | A | 608 | PX4 | C8-C7 | 3.34 | 1.61 | 1.50 | 3 | 8 |
| 3 | C | 354 | PX4 | C24-C23 | 3.34 | 1.60 | 1.50 | 1 | 4 |
| 3 | C | 310 | PX4 | O7-C23 | 3.34 | 1.43 | 1.34 | 15 | 1 |
| 3 | A | 628 | PX4 | C2-N1 | 3.34 | 1.61 | 1.51 | 14 | 2 |
| 3 | A | 639 | PX4 | O7-C23 | 3.34 | 1.43 | 1.34 | 11 | 3 |
| 3 | C | 331 | PX4 | O7-C7 | 3.34 | 1.38 | 1.46 | 5 | 4 |
| 3 | C | 312 | PX4 | C8-C7 | 3.34 | 1.61 | 1.50 | 14 | 7 |
| 3 | C | 333 | PX4 | O7-C7 | 3.34 | 1.38 | 1.46 | 8 | 3 |
| 3 | A | 633 | PX4 | C2-N1 | 3.33 | 1.61 | 1.51 | 12 | 3 |
| 3 | A | 653 | PX4 | C8-C7 | 3.33 | 1.61 | 1.50 | 7 | 7 |
| 3 | A | 616 | PX4 | C8-C7 | 3.33 | 1.61 | 1.50 | 14 | 10 |
| 3 | C | 334 | PX4 | C8-C7 | 3.33 | 1.61 | 1.50 | 5 | 6 |
| 3 | A | 634 | PX4 | C8-C7 | 3.33 | 1.61 | 1.50 | 9 | 10 |
| 3 | B | 314 | PX4 | C3-N1 | 3.33 | 1.59 | 1.50 | 7 | 2 |
| 3 | B | 376 | PX4 | C24-C23 | 3.33 | 1.60 | 1.50 | 5 | 4 |
| 3 | B | 328 | PX4 | C2-N1 | 3.33 | 1.61 | 1.51 | 8 | 2 |
| 3 | C | 360 | PX4 | C8-C7 | 3.33 | 1.61 | 1.50 | 5 | 9 |
| 3 | C | 353 | PX4 | O5-C8 | 3.32 | 1.37 | 1.45 | 8 | 4 |
| 3 | A | 601 | PX4 | C8-C7 | 3.32 | 1.61 | 1.50 | 14 | 6 |
| 3 | A | 638 | PX4 | C4-N1 | 3.32 | 1.59 | 1.50 | 13 | 2 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 372 | PX4 | O7-C23 | 3.32 | 1.24 | 1.34 | 10 | 2 |
| 3 | C | 346 | PX4 | C10-C9 | 3.32 | 1.60 | 1.50 | 7 | 3 |
| 3 | C | 363 | PX4 | C8-C7 | 3.32 | 1.61 | 1.50 | 11 | 8 |
| 3 | B | 358 | PX4 | C2-C1 | 3.32 | 1.61 | 1.51 | 9 | 7 |
| 3 | B | 364 | PX4 | C8-C7 | 3.32 | 1.61 | 1.50 | 10 | 5 |
| 3 | A | 609 | PX4 | O7-C23 | 3.32 | 1.24 | 1.34 | 4 | 2 |
| 3 | B | 319 | PX4 | C6-C7 | 3.32 | 1.61 | 1.50 | 10 | 4 |
| 3 | B | 331 | PX4 | O7-C7 | 3.32 | 1.38 | 1.46 | 12 | 3 |
| 3 | B | 389 | PX4 | O7-C7 | 3.32 | 1.38 | 1.46 | 5 | 2 |
| 3 | A | 647 | PX4 | C8-C7 | 3.31 | 1.61 | 1.50 | 15 | 8 |
| 3 | B | 307 | PX4 | C24-C23 | 3.31 | 1.60 | 1.50 | 15 | 5 |
| 3 | B | 360 | PX4 | C2-C1 | 3.31 | 1.61 | 1.51 | 11 | 7 |
| 3 | A | 602 | PX4 | C25-C24 | 3.31 | 1.64 | 1.52 | 12 | 2 |
| 3 | C | 321 | PX4 | C5-N1 | 3.31 | 1.59 | 1.50 | 3 | 3 |
| 3 | C | 333 | PX4 | O5-C8 | 3.31 | 1.52 | 1.45 | 1 | 3 |
| 3 | C | 345 | PX4 | C8-C7 | 3.31 | 1.61 | 1.50 | 6 | 7 |
| 3 | B | 304 | PX4 | O5-C9 | 3.31 | 1.43 | 1.33 | 10 | 2 |
| 3 | B | 325 | PX4 | C10-C9 | 3.31 | 1.60 | 1.50 | 2 | 3 |
| 3 | B | 371 | PX4 | C2-C1 | 3.31 | 1.61 | 1.51 | 15 | 2 |
| 3 | C | 338 | PX4 | C8-C7 | 3.31 | 1.61 | 1.50 | 8 | 6 |
| 3 | A | 645 | PX4 | C5-N1 | 3.31 | 1.59 | 1.50 | 7 | 3 |
| 3 | B | 333 | PX4 | C24-C23 | 3.31 | 1.60 | 1.50 | 12 | 5 |
| 3 | B | 380 | PX4 | O5-C9 | 3.31 | 1.43 | 1.33 | 1 | 5 |
| 3 | A | 627 | PX4 | C11-C10 | 3.31 | 1.64 | 1.52 | 13 | 2 |
| 3 | A | 653 | PX4 | C24-C23 | 3.31 | 1.60 | 1.50 | 12 | 2 |
| 3 | C | 333 | PX4 | C6-C7 | 3.31 | 1.61 | 1.50 | 6 | 6 |
| 3 | C | 335 | PX4 | C8-C7 | 3.31 | 1.61 | 1.50 | 1 | 7 |
| 3 | B | 301 | PX4 | O5-C8 | 3.30 | 1.52 | 1.45 | 6 | 2 |
| 3 | B | 351 | PX4 | C8-C7 | 3.30 | 1.61 | 1.50 | 4 | 2 |
| 3 | B | 358 | PX4 | C10-C9 | 3.30 | 1.60 | 1.50 | 14 | 2 |
| 3 | B | 389 | PX4 | O7-C23 | 3.30 | 1.24 | 1.34 | 12 | 1 |
| 3 | A | 642 | PX4 | C8-C7 | 3.30 | 1.61 | 1.50 | 15 | 6 |
| 3 | C | 357 | PX4 | O7-C23 | 3.30 | 1.43 | 1.34 | 14 | 2 |
| 3 | B | 311 | PX4 | O7-C7 | 3.30 | 1.38 | 1.46 | 9 | 3 |
| 3 | B | 374 | PX4 | C2-C1 | 3.30 | 1.61 | 1.51 | 2 | 6 |
| 3 | C | 358 | PX4 | O7-C7 | 3.30 | 1.38 | 1.46 | 6 | 2 |
| 3 | C | 307 | PX4 | O5-C8 | 3.30 | 1.37 | 1.45 | 9 | 4 |
| 3 | A | 617 | PX4 | C11-C10 | 3.30 | 1.64 | 1.52 | 11 | 2 |
| 3 | A | 653 | PX4 | C11-C10 | 3.30 | 1.64 | 1.52 | 12 | 1 |
| 3 | B | 362 | PX4 | C2-C1 | 3.30 | 1.61 | 1.51 | 6 | 5 |
| 3 | B | 316 | PX4 | O5-C8 | 3.29 | 1.52 | 1.45 | 6 | 7 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 383 | PX4 | C2-C1 | 3.30 | 1.61 | 1.51 | 5 | 4 |
| 3 | C | 319 | PX4 | C6-C7 | 3.29 | 1.61 | 1.50 | 14 | 3 |
| 3 | A | 622 | PX4 | C10-C9 | 3.29 | 1.60 | 1.50 | 5 | 3 |
| 3 | C | 322 | PX4 | O7-C7 | 3.29 | 1.38 | 1.46 | 4 | 2 |
| 3 | B | 325 | PX4 | C8-C7 | 3.29 | 1.61 | 1.50 | 3 | 7 |
| 3 | B | 330 | PX4 | C24-C23 | 3.29 | 1.60 | 1.50 | 15 | 3 |
| 3 | B | 335 | PX4 | C24-C23 | 3.29 | 1.60 | 1.50 | 2 | 2 |
| 3 | C | 310 | PX4 | C2-N1 | 3.29 | 1.61 | 1.51 | 3 | 1 |
| 3 | C | 337 | PX4 | C6-C7 | 3.29 | 1.61 | 1.50 | 14 | 5 |
| 3 | A | 604 | PX4 | C6-C7 | 3.29 | 1.61 | 1.50 | 6 | 4 |
| 3 | A | 609 | PX4 | C2-C1 | 3.29 | 1.61 | 1.51 | 13 | 7 |
| 3 | A | 602 | PX4 | C6-C7 | 3.29 | 1.61 | 1.50 | 7 | 3 |
| 3 | B | 336 | PX4 | C5-N1 | 3.29 | 1.59 | 1.50 | 7 | 1 |
| 3 | B | 375 | PX4 | C10-C9 | 3.29 | 1.60 | 1.50 | 2 | 5 |
| 3 | A | 607 | PX4 | O7-C7 | 3.28 | 1.38 | 1.46 | 9 | 3 |
| 3 | A | 625 | PX4 | O5-C8 | 3.28 | 1.52 | 1.45 | 13 | 2 |
| 3 | C | 302 | PX4 | C4-N1 | 3.29 | 1.59 | 1.50 | 10 | 2 |
| 3 | B | 339 | PX4 | C6-C7 | 3.28 | 1.61 | 1.50 | 13 | 10 |
| 3 | C | 342 | PX4 | O5-C8 | 3.29 | 1.52 | 1.45 | 2 | 2 |
| 3 | A | 652 | PX4 | C11-C10 | 3.28 | 1.64 | 1.52 | 3 | 3 |
| 3 | B | 333 | PX4 | O5-C9 | 3.28 | 1.42 | 1.33 | 3 | 2 |
| 3 | B | 340 | PX4 | C24-C23 | 3.28 | 1.60 | 1.50 | 13 | 5 |
| 3 | A | 616 | PX4 | C6-C7 | 3.28 | 1.61 | 1.50 | 15 | 5 |
| 3 | B | 320 | PX4 | C8-C7 | 3.28 | 1.61 | 1.50 | 13 | 4 |
| 3 | B | 342 | PX4 | C6-C7 | 3.28 | 1.61 | 1.50 | 6 | 5 |
| 3 | B | 389 | PX4 | C6-C7 | 3.28 | 1.61 | 1.50 | 15 | 4 |
| 3 | C | 351 | PX4 | C4-N1 | 3.28 | 1.40 | 1.50 | 1 | 1 |
| 3 | B | 369 | PX4 | C2-C1 | 3.27 | 1.61 | 1.51 | 5 | 4 |
| 3 | B | 398 | PX4 | C24-C23 | 3.27 | 1.60 | 1.50 | 13 | 2 |
| 3 | B | 310 | PX4 | C10-C9 | 3.27 | 1.60 | 1.50 | 10 | 5 |
| 3 | C | 328 | PX4 | C10-C9 | 3.27 | 1.60 | 1.50 | 1 | 5 |
| 3 | B | 355 | PX4 | C10-C9 | 3.27 | 1.60 | 1.50 | 2 | 5 |
| 3 | C | 318 | PX4 | O5-C8 | 3.27 | 1.52 | 1.45 | 15 | 1 |
| 3 | A | 601 | PX4 | O7-C7 | 3.26 | 1.38 | 1.46 | 12 | 4 |
| 3 | A | 629 | PX4 | C6-C7 | 3.26 | 1.61 | 1.50 | 8 | 2 |
| 3 | C | 321 | PX4 | O7-C23 | 3.26 | 1.25 | 1.34 | 8 | 3 |
| 3 | C | 309 | PX4 | C2-N1 | 3.26 | 1.61 | 1.51 | 14 | 2 |
| 3 | C | 315 | PX4 | C6-C7 | 3.26 | 1.61 | 1.50 | 9 | 7 |
| 3 | A | 605 | PX4 | O5-C8 | 3.25 | 1.52 | 1.45 | 5 | 5 |
| 3 | A | 653 | PX4 | O5-C8 | 3.26 | 1.37 | 1.45 | 15 | 2 |
| 3 | B | 304 | PX4 | C2-C1 | 3.26 | 1.61 | 1.51 | 1 | 7 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 312 | PX4 | O7-C7 | 3.26 | 1.38 | 1.46 | 9 | 6 |
| 3 | C | 336 | PX4 | O7-C23 | 3.26 | 1.25 | 1.34 | 13 | 2 |
| 3 | A | 617 | PX4 | C6-C7 | 3.25 | 1.61 | 1.50 | 8 | 6 |
| 3 | A | 643 | PX4 | O5-C8 | 3.25 | 1.37 | 1.45 | 7 | 3 |
| 3 | C | 320 | PX4 | O5-C9 | 3.25 | 1.23 | 1.33 | 13 | 2 |
| 3 | A | 617 | PX4 | C2-C1 | 3.25 | 1.61 | 1.51 | 1 | 4 |
| 3 | A | 613 | PX4 | C8-C7 | 3.25 | 1.61 | 1.50 | 12 | 7 |
| 3 | A | 652 | PX4 | C6-C7 | 3.25 | 1.61 | 1.50 | 15 | 6 |
| 3 | B | 339 | PX4 | C8-C7 | 3.25 | 1.61 | 1.50 | 4 | 9 |
| 3 | B | 333 | PX4 | O7-C7 | 3.25 | 1.39 | 1.46 | 13 | 4 |
| 3 | B | 364 | PX4 | C6-C7 | 3.25 | 1.61 | 1.50 | 8 | 6 |
| 3 | B | 391 | PX4 | C2-C1 | 3.25 | 1.61 | 1.51 | 11 | 4 |
| 3 | C | 350 | PX4 | C2-N1 | 3.25 | 1.61 | 1.51 | 14 | 1 |
| 3 | B | 342 | PX4 | C10-C9 | 3.25 | 1.60 | 1.50 | 9 | 4 |
| 3 | B | 356 | PX4 | C10-C9 | 3.25 | 1.60 | 1.50 | 6 | 4 |
| 3 | B | 368 | PX4 | C6-C7 | 3.25 | 1.61 | 1.50 | 11 | 5 |
| 3 | B | 317 | PX4 | O5-C9 | 3.25 | 1.42 | 1.33 | 14 | 2 |
| 3 | C | 317 | PX4 | O7-C23 | 3.25 | 1.25 | 1.34 | 6 | 2 |
| 3 | C | 344 | PX4 | C24-C23 | 3.25 | 1.60 | 1.50 | 9 | 4 |
| 3 | B | 307 | PX4 | C11-C10 | 3.24 | 1.64 | 1.52 | 9 | 5 |
| 3 | B | 345 | PX4 | C4-N1 | 3.24 | 1.40 | 1.50 | 1 | 1 |
| 3 | A | 615 | PX4 | C2-C1 | 3.24 | 1.61 | 1.51 | 7 | 2 |
| 3 | B | 378 | PX4 | C4-N1 | 3.24 | 1.40 | 1.50 | 9 | 2 |
| 3 | C | 314 | PX4 | C10-C9 | 3.24 | 1.60 | 1.50 | 8 | 2 |
| 3 | C | 329 | PX4 | O5-C9 | 3.24 | 1.23 | 1.33 | 3 | 3 |
| 3 | A | 604 | PX4 | C10-C9 | 3.23 | 1.60 | 1.50 | 5 | 6 |
| 3 | A | 614 | PX4 | C2-C1 | 3.23 | 1.61 | 1.51 | 8 | 5 |
| 3 | A | 642 | PX4 | O7-C7 | 3.23 | 1.39 | 1.46 | 7 | 3 |
| 3 | A | 645 | PX4 | C8-C7 | 3.23 | 1.60 | 1.50 | 1 | 5 |
| 3 | B | 340 | PX4 | C10-C9 | 3.23 | 1.60 | 1.50 | 12 | 5 |
| 3 | C | 338 | PX4 | C10-C9 | 3.23 | 1.60 | 1.50 | 14 | 3 |
| 3 | A | 610 | PX4 | O5-C8 | 3.23 | 1.52 | 1.45 | 1 | 2 |
| 3 | A | 629 | PX4 | O7-C23 | 3.23 | 1.25 | 1.34 | 13 | 2 |
| 3 | B | 319 | PX4 | C2-C1 | 3.23 | 1.61 | 1.51 | 3 | 3 |
| 3 | B | 302 | PX4 | C8-C7 | 3.23 | 1.60 | 1.50 | 6 | 5 |
| 3 | B | 345 | PX4 | C10-C9 | 3.23 | 1.60 | 1.50 | 11 | 4 |
| 3 | C | 323 | PX4 | C2-C1 | 3.23 | 1.61 | 1.51 | 1 | 2 |
| 3 | A | 633 | PX4 | C8-C7 | 3.23 | 1.60 | 1.50 | 2 | 6 |
| 3 | C | 326 | PX4 | O5-C8 | 3.23 | 1.38 | 1.45 | 13 | 3 |
| 3 | C | 317 | PX4 | C10-C9 | 3.23 | 1.60 | 1.50 | 5 | 3 |
| 3 | B | 301 | PX4 | C6-C7 | 3.22 | 1.60 | 1.50 | 2 | 6 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 342 | PX4 | C2-C1 | 3.22 | 1.61 | 1.51 | 1 | 3 |
| 3 | B | 386 | PX4 | O7-C7 | 3.22 | 1.39 | 1.46 | 6 | 5 |
| 3 | C | 322 | PX4 | C10-C9 | 3.22 | 1.60 | 1.50 | 2 | 6 |
| 3 | B | 389 | PX4 | C4-N1 | 3.22 | 1.59 | 1.50 | 5 | 2 |
| 3 | C | 340 | PX4 | C2-C1 | 3.22 | 1.61 | 1.51 | 10 | 6 |
| 3 | C | 341 | PX4 | C10-C9 | 3.22 | 1.60 | 1.50 | 12 | 5 |
| 3 | C | 347 | PX4 | O7-C23 | 3.22 | 1.25 | 1.34 | 15 | 3 |
| 3 | B | 361 | PX4 | C10-C9 | 3.22 | 1.60 | 1.50 | 2 | 4 |
| 3 | B | 336 | PX4 | C2-N1 | 3.22 | 1.61 | 1.51 | 15 | 2 |
| 3 | A | 637 | PX4 | C2-C1 | 3.22 | 1.61 | 1.51 | 3 | 6 |
| 3 | A | 610 | PX4 | O7-C7 | 3.21 | 1.39 | 1.46 | 6 | 2 |
| 3 | A | 624 | PX4 | O7-C23 | 3.22 | 1.43 | 1.34 | 6 | 2 |
| 3 | B | 329 | PX4 | C24-C23 | 3.21 | 1.60 | 1.50 | 8 | 2 |
| 3 | B | 357 | PX4 | C10-C9 | 3.21 | 1.60 | 1.50 | 10 | 3 |
| 3 | B | 361 | PX4 | C11-C10 | 3.21 | 1.64 | 1.52 | 10 | 2 |
| 3 | A | 641 | PX4 | C2-N1 | 3.21 | 1.61 | 1.51 | 5 | 2 |
| 3 | A | 643 | PX4 | C2-C1 | 3.21 | 1.61 | 1.51 | 7 | 5 |
| 3 | C | 361 | PX4 | C2-C1 | 3.21 | 1.61 | 1.51 | 12 | 4 |
| 3 | A | 604 | PX4 | O5-C8 | 3.21 | 1.38 | 1.45 | 7 | 3 |
| 3 | C | 329 | PX4 | C2-N1 | 3.21 | 1.61 | 1.51 | 10 | 2 |
| 3 | B | 333 | PX4 | C4-N1 | 3.21 | 1.59 | 1.50 | 15 | 2 |
| 3 | B | 349 | PX4 | O7-C23 | 3.21 | 1.43 | 1.34 | 9 | 3 |
| 3 | B | 307 | PX4 | O5-C8 | 3.20 | 1.38 | 1.45 | 14 | 5 |
| 3 | B | 400 | PX4 | C6-C7 | 3.20 | 1.60 | 1.50 | 5 | 4 |
| 3 | C | 341 | PX4 | O4-C6 | 3.20 | 1.32 | 1.44 | 8 | 1 |
| 3 | C | 363 | PX4 | C5-N1 | 3.20 | 1.59 | 1.50 | 9 | 2 |
| 3 | A | 642 | PX4 | C10-C9 | 3.20 | 1.60 | 1.50 | 1 | 3 |
| 3 | B | 308 | PX4 | O5-C9 | 3.20 | 1.24 | 1.33 | 3 | 2 |
| 3 | B | 358 | PX4 | C8-C7 | 3.20 | 1.60 | 1.50 | 2 | 6 |
| 3 | B | 386 | PX4 | C6-C7 | 3.20 | 1.60 | 1.50 | 2 | 7 |
| 3 | C | 323 | PX4 | C24-C23 | 3.20 | 1.60 | 1.50 | 5 | 4 |
| 3 | B | 307 | PX4 | C8-C7 | 3.20 | 1.60 | 1.50 | 11 | 5 |
| 3 | B | 351 | PX4 | C25-C24 | 3.20 | 1.63 | 1.52 | 12 | 2 |
| 3 | C | 332 | PX4 | O5-C8 | 3.20 | 1.52 | 1.45 | 6 | 3 |
| 3 | C | 340 | PX4 | C8-C7 | 3.20 | 1.60 | 1.50 | 13 | 6 |
| 3 | A | 605 | PX4 | O7-C7 | 3.20 | 1.39 | 1.46 | 11 | 2 |
| 3 | A | 602 | PX4 | C24-C23 | 3.20 | 1.60 | 1.50 | 15 | 5 |
| 3 | B | 362 | PX4 | C10-C9 | 3.20 | 1.60 | 1.50 | 8 | 2 |
| 3 | B | 369 | PX4 | O5-C8 | 3.19 | 1.52 | 1.45 | 14 | 4 |
| 3 | B | 380 | PX4 | O7-C23 | 3.19 | 1.25 | 1.34 | 9 | 1 |
| 3 | C | 330 | PX4 | C8-C7 | 3.19 | 1.60 | 1.50 | 11 | 4 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 355 | PX4 | C3-N1 | 3.19 | 1.59 | 1.50 | 8 | 4 |
| 3 | A | 632 | PX4 | O5-C8 | 3.19 | 1.38 | 1.45 | 4 | 3 |
| 3 | A | 639 | PX4 | C10-C9 | 3.19 | 1.60 | 1.50 | 2 | 6 |
| 3 | B | 309 | PX4 | C8-C7 | 3.19 | 1.60 | 1.50 | 15 | 2 |
| 3 | B | 329 | PX4 | C8-C7 | 3.19 | 1.60 | 1.50 | 2 | 8 |
| 3 | B | 392 | PX4 | C6-C7 | 3.19 | 1.60 | 1.50 | 7 | 3 |
| 3 | B | 393 | PX4 | O7-C23 | 3.19 | 1.25 | 1.34 | 5 | 3 |
| 3 | A | 623 | PX4 | C8-C7 | 3.19 | 1.60 | 1.50 | 2 | 4 |
| 3 | B | 343 | PX4 | C3-N1 | 3.19 | 1.40 | 1.50 | 1 | 1 |
| 3 | B | 397 | PX4 | C8-C7 | 3.19 | 1.60 | 1.50 | 14 | 5 |
| 3 | B | 399 | PX4 | C8-C7 | 3.19 | 1.60 | 1.50 | 6 | 8 |
| 3 | C | 358 | PX4 | C6-C7 | 3.19 | 1.60 | 1.50 | 6 | 4 |
| 3 | A | 602 | PX4 | O5-C8 | 3.19 | 1.52 | 1.45 | 14 | 3 |
| 3 | B | 315 | PX4 | C24-C23 | 3.19 | 1.59 | 1.50 | 2 | 4 |
| 3 | C | 337 | PX4 | C24-C23 | 3.19 | 1.59 | 1.50 | 9 | 5 |
| 3 | A | 652 | PX4 | O7-C23 | 3.18 | 1.43 | 1.34 | 4 | 1 |
| 3 | B | 370 | PX4 | C2-C1 | 3.18 | 1.61 | 1.51 | 11 | 3 |
| 3 | B | 371 | PX4 | C24-C23 | 3.18 | 1.59 | 1.50 | 3 | 3 |
| 3 | C | 340 | PX4 | O7-C7 | 3.18 | 1.39 | 1.46 | 6 | 6 |
| 3 | B | 352 | PX4 | C6-C7 | 3.18 | 1.60 | 1.50 | 13 | 10 |
| 3 | A | 616 | PX4 | O5-C8 | 3.18 | 1.52 | 1.45 | 8 | 3 |
| 3 | B | 355 | PX4 | C8-C7 | 3.18 | 1.60 | 1.50 | 1 | 6 |
| 3 | B | 317 | PX4 | O7-C7 | 3.18 | 1.39 | 1.46 | 14 | 5 |
| 3 | B | 360 | PX4 | O5-C9 | 3.18 | 1.42 | 1.33 | 5 | 1 |
| 3 | A | 606 | PX4 | C2-C1 | 3.17 | 1.60 | 1.51 | 7 | 6 |
| 3 | A | 629 | PX4 | O7-C7 | 3.17 | 1.39 | 1.46 | 1 | 3 |
| 3 | B | 346 | PX4 | C4-N1 | 3.17 | 1.40 | 1.50 | 2 | 1 |
| 3 | B | 343 | PX4 | C6-C7 | 3.17 | 1.60 | 1.50 | 5 | 5 |
| 3 | B | 391 | PX4 | C6-C7 | 3.17 | 1.60 | 1.50 | 10 | 9 |
| 3 | C | 330 | PX4 | C10-C9 | 3.17 | 1.41 | 1.50 | 9 | 4 |
| 3 | A | 607 | PX4 | C4-N1 | 3.17 | 1.59 | 1.50 | 2 | 3 |
| 3 | C | 354 | PX4 | O5-C9 | 3.17 | 1.24 | 1.33 | 15 | 3 |
| 3 | C | 342 | PX4 | C10-C9 | 3.17 | 1.59 | 1.50 | 15 | 5 |
| 3 | C | 342 | PX4 | C24-C23 | 3.17 | 1.59 | 1.50 | 10 | 3 |
| 3 | A | 612 | PX4 | C2-N1 | 3.16 | 1.61 | 1.51 | 11 | 2 |
| 3 | B | 337 | PX4 | C6-C7 | 3.16 | 1.60 | 1.50 | 15 | 5 |
| 3 | A | 621 | PX4 | O7-C7 | 3.16 | 1.39 | 1.46 | 14 | 1 |
| 3 | B | 346 | PX4 | O5-C8 | 3.16 | 1.52 | 1.45 | 13 | 4 |
| 3 | B | 350 | PX4 | C2-C1 | 3.16 | 1.60 | 1.51 | 5 | 5 |
| 3 | B | 353 | PX4 | C8-C7 | 3.16 | 1.60 | 1.50 | 7 | 6 |
| 3 | B | 391 | PX4 | C10-C9 | 3.16 | 1.59 | 1.50 | 4 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | C | 311 | PX4 | C3-N1 | 3.16 | 1.40 | 1.50 | 8 | 1 |
| 3 | A | 604 | PX4 | C25-C24 | 3.16 | 1.63 | 1.52 | 13 | 1 |
| 3 | A | 618 | PX4 | C4-N1 | 3.16 | 1.40 | 1.50 | 14 | 2 |
| 3 | B | 355 | PX4 | C4-N1 | 3.16 | 1.59 | 1.50 | 12 | 3 |
| 3 | C | 348 | PX4 | C2-N1 | 3.16 | 1.61 | 1.51 | 7 | 1 |
| 3 | B | 370 | PX4 | C8-C7 | 3.15 | 1.60 | 1.50 | 6 | 7 |
| 3 | B | 392 | PX4 | C8-C7 | 3.15 | 1.60 | 1.50 | 5 | 7 |
| 3 | A | 623 | PX4 | O5-C8 | 3.15 | 1.38 | 1.45 | 7 | 1 |
| 3 | A | 633 | PX4 | C2-C1 | 3.15 | 1.60 | 1.51 | 7 | 4 |
| 3 | B | 397 | PX4 | O7-C7 | 3.15 | 1.39 | 1.46 | 6 | 5 |
| 3 | C | 316 | PX4 | C2-C1 | 3.15 | 1.60 | 1.51 | 4 | 4 |
| 3 | A | 615 | PX4 | C25-C24 | 3.15 | 1.63 | 1.52 | 2 | 3 |
| 3 | B | 350 | PX4 | C11-C10 | 3.15 | 1.63 | 1.52 | 15 | 3 |
| 3 | B | 385 | PX4 | O7-C7 | 3.15 | 1.39 | 1.46 | 5 | 6 |
| 3 | C | 352 | PX4 | O7-C23 | 3.15 | 1.25 | 1.34 | 15 | 3 |
| 3 | A | 653 | PX4 | C3-N1 | 3.15 | 1.59 | 1.50 | 12 | 1 |
| 3 | B | 390 | PX4 | C6-C7 | 3.15 | 1.60 | 1.50 | 4 | 7 |
| 3 | B | 383 | PX4 | O5-C8 | 3.14 | 1.52 | 1.45 | 14 | 7 |
| 3 | B | 400 | PX4 | C10-C9 | 3.14 | 1.59 | 1.50 | 1 | 3 |
| 3 | B | 362 | PX4 | C6-C7 | 3.14 | 1.60 | 1.50 | 8 | 3 |
| 3 | C | 334 | PX4 | O7-C7 | 3.14 | 1.39 | 1.46 | 2 | 5 |
| 3 | B | 344 | PX4 | C11-C10 | 3.14 | 1.63 | 1.52 | 12 | 3 |
| 3 | B | 366 | PX4 | O7-C23 | 3.14 | 1.25 | 1.34 | 14 | 2 |
| 3 | A | 602 | PX4 | C8-C7 | 3.14 | 1.60 | 1.50 | 1 | 4 |
| 3 | B | 341 | PX4 | C8-C7 | 3.14 | 1.60 | 1.50 | 5 | 5 |
| 3 | C | 324 | PX4 | C6-C7 | 3.14 | 1.60 | 1.50 | 7 | 3 |
| 3 | A | 617 | PX4 | C24-C23 | 3.14 | 1.59 | 1.50 | 7 | 2 |
| 3 | B | 306 | PX4 | C10-C9 | 3.13 | 1.59 | 1.50 | 3 | 4 |
| 3 | B | 332 | PX4 | C2-C1 | 3.13 | 1.60 | 1.51 | 3 | 6 |
| 3 | B | 347 | PX4 | O5-C8 | 3.13 | 1.38 | 1.45 | 9 | 2 |
| 3 | B | 350 | PX4 | C8-C7 | 3.13 | 1.60 | 1.50 | 3 | 7 |
| 3 | B | 397 | PX4 | C6-C7 | 3.13 | 1.60 | 1.50 | 12 | 4 |
| 3 | C | 323 | PX4 | O7-C7 | 3.13 | 1.39 | 1.46 | 2 | 4 |
| 3 | B | 302 | PX4 | O5-C9 | 3.13 | 1.24 | 1.33 | 6 | 4 |
| 3 | B | 333 | PX4 | C10-C9 | 3.13 | 1.59 | 1.50 | 11 | 2 |
| 3 | B | 366 | PX4 | C8-C7 | 3.13 | 1.60 | 1.50 | 8 | 8 |
| 3 | B | 387 | PX4 | O7-C7 | 3.13 | 1.39 | 1.46 | 3 | 3 |
| 3 | A | 626 | PX4 | C8-C7 | 3.13 | 1.60 | 1.50 | 11 | 5 |
| 3 | B | 340 | PX4 | C11-C10 | 3.13 | 1.63 | 1.52 | 7 | 2 |
| 3 | C | 351 | PX4 | C11-C10 | 3.13 | 1.63 | 1.52 | 2 | 2 |
| 3 | B | 310 | PX4 | C25-C24 | 3.13 | 1.63 | 1.52 | 13 | 2 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | C | 309 | PX4 | O7-C7 | 3.12 | 1.39 | 1.46 | 15 | 3 |
| 3 | C | 360 | PX4 | C24-C23 | 3.12 | 1.59 | 1.50 | 10 | 5 |
| 3 | A | 611 | PX4 | C25-C24 | 3.12 | 1.63 | 1.52 | 5 | 3 |
| 3 | A | 628 | PX4 | C25-C24 | 3.12 | 1.63 | 1.52 | 13 | 1 |
| 3 | C | 337 | PX4 | O7-C23 | 3.12 | 1.25 | 1.34 | 2 | 4 |
| 3 | C | 357 | PX4 | C11-C10 | 3.12 | 1.63 | 1.52 | 2 | 1 |
| 3 | A | 620 | PX4 | C2-N1 | 3.12 | 1.61 | 1.51 | 12 | 4 |
| 3 | B | 391 | PX4 | C25-C24 | 3.12 | 1.63 | 1.52 | 15 | 1 |
| 3 | C | 353 | PX4 | C10-C9 | 3.12 | 1.59 | 1.50 | 10 | 6 |
| 3 | A | 630 | PX4 | C6-C7 | 3.11 | 1.60 | 1.50 | 3 | 6 |
| 3 | A | 642 | PX4 | C6-C7 | 3.11 | 1.60 | 1.50 | 11 | 7 |
| 3 | B | 365 | PX4 | C2-C1 | 3.11 | 1.60 | 1.51 | 13 | 5 |
| 3 | C | 329 | PX4 | C11-C10 | 3.11 | 1.63 | 1.52 | 11 | 2 |
| 3 | A | 614 | PX4 | O7-C7 | 3.11 | 1.39 | 1.46 | 1 | 5 |
| 3 | A | 635 | PX4 | C5-N1 | 3.11 | 1.59 | 1.50 | 7 | 2 |
| 3 | A | 643 | PX4 | C2-N1 | 3.11 | 1.61 | 1.51 | 4 | 2 |
| 3 | B | 381 | PX4 | P1-O1 | 3.11 | 1.40 | 1.55 | 2 | 2 |
| 3 | A | 644 | PX4 | C2-C1 | 3.11 | 1.60 | 1.51 | 4 | 7 |
| 3 | B | 379 | PX4 | C11-C10 | 3.11 | 1.63 | 1.52 | 9 | 4 |
| 3 | B | 389 | PX4 | C2-N1 | 3.11 | 1.60 | 1.51 | 1 | 2 |
| 3 | B | 390 | PX4 | O7-C23 | 3.11 | 1.25 | 1.34 | 10 | 4 |
| 3 | C | 324 | PX4 | O5-C9 | 3.11 | 1.24 | 1.33 | 1 | 2 |
| 3 | B | 359 | PX4 | O7-C7 | 3.11 | 1.39 | 1.46 | 10 | 3 |
| 3 | A | 625 | PX4 | C6-C7 | 3.10 | 1.60 | 1.50 | 3 | 6 |
| 3 | A | 614 | PX4 | C24-C23 | 3.10 | 1.59 | 1.50 | 1 | 3 |
| 3 | A | 647 | PX4 | C10-C9 | 3.10 | 1.59 | 1.50 | 3 | 3 |
| 3 | B | 367 | PX4 | C2-C1 | 3.10 | 1.60 | 1.51 | 1 | 3 |
| 3 | B | 379 | PX4 | C3-N1 | 3.10 | 1.41 | 1.50 | 1 | 2 |
| 3 | C | 304 | PX4 | O5-C8 | 3.10 | 1.38 | 1.45 | 8 | 3 |
| 3 | C | 315 | PX4 | C24-C23 | 3.10 | 1.59 | 1.50 | 9 | 1 |
| 3 | C | 348 | PX4 | O7-C7 | 3.10 | 1.39 | 1.46 | 6 | 1 |
| 3 | A | 614 | PX4 | O5-C9 | 3.10 | 1.42 | 1.33 | 5 | 1 |
| 3 | B | 349 | PX4 | C25-C24 | 3.09 | 1.63 | 1.52 | 6 | 7 |
| 3 | C | 325 | PX4 | C2-C1 | 3.09 | 1.60 | 1.51 | 1 | 3 |
| 3 | C | 301 | PX4 | C11-C10 | 3.09 | 1.63 | 1.52 | 8 | 2 |
| 3 | C | 349 | PX4 | O5-C8 | 3.09 | 1.38 | 1.45 | 4 | 2 |
| 3 | A | 605 | PX4 | C10-C9 | 3.09 | 1.59 | 1.50 | 5 | 4 |
| 3 | A | 618 | PX4 | C10-C9 | 3.09 | 1.59 | 1.50 | 2 | 4 |
| 3 | B | 368 | PX4 | C10-C9 | 3.09 | 1.59 | 1.50 | 15 | 2 |
| 3 | B | 384 | PX4 | C3-N1 | 3.09 | 1.59 | 1.50 | 12 | 2 |
| 3 | C | 355 | PX4 | C11-C10 | 3.09 | 1.63 | 1.52 | 8 | 3 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 384 | PX4 | C24-C23 | 3.09 | 1.59 | 1.50 | 5 | 4 |
| 3 | C | 318 | PX4 | O5-C9 | 3.09 | 1.42 | 1.33 | 9 | 2 |
| 3 | B | 382 | PX4 | O5-C8 | 3.08 | 1.38 | 1.45 | 3 | 2 |
| 3 | C | 350 | PX4 | C24-C23 | 3.09 | 1.59 | 1.50 | 14 | 1 |
| 3 | A | 613 | PX4 | O7-C23 | 3.08 | 1.25 | 1.34 | 10 | 6 |
| 3 | B | 334 | PX4 | C10-C9 | 3.08 | 1.59 | 1.50 | 6 | 3 |
| 3 | B | 381 | PX4 | C10-C9 | 3.08 | 1.59 | 1.50 | 15 | 2 |
| 3 | C | 349 | PX4 | C8-C7 | 3.08 | 1.60 | 1.50 | 14 | 3 |
| 3 | A | 609 | PX4 | O5-C9 | 3.08 | 1.24 | 1.33 | 7 | 3 |
| 3 | B | 306 | PX4 | C6-C7 | 3.08 | 1.60 | 1.50 | 13 | 3 |
| 3 | B | 354 | PX4 | C6-C7 | 3.08 | 1.60 | 1.50 | 3 | 6 |
| 3 | B | 364 | PX4 | C10-C9 | 3.08 | 1.59 | 1.50 | 11 | 3 |
| 3 | C | 341 | PX4 | C2-C1 | 3.08 | 1.60 | 1.51 | 7 | 4 |
| 3 | C | 362 | PX4 | O5-C9 | 3.08 | 1.42 | 1.33 | 14 | 3 |
| 3 | B | 308 | PX4 | O7-C23 | 3.08 | 1.25 | 1.34 | 3 | 3 |
| 3 | B | 317 | PX4 | O7-C23 | 3.08 | 1.25 | 1.34 | 9 | 2 |
| 3 | B | 383 | PX4 | C4-N1 | 3.08 | 1.58 | 1.50 | 4 | 3 |
| 3 | B | 398 | PX4 | C6-C7 | 3.08 | 1.60 | 1.50 | 10 | 4 |
| 3 | C | 303 | PX4 | O5-C8 | 3.08 | 1.38 | 1.45 | 15 | 2 |
| 3 | C | 309 | PX4 | C2-C1 | 3.08 | 1.60 | 1.51 | 15 | 4 |
| 3 | B | 305 | PX4 | C4-N1 | 3.08 | 1.58 | 1.50 | 14 | 1 |
| 3 | C | 354 | PX4 | O7-C7 | 3.08 | 1.39 | 1.46 | 10 | 2 |
| 3 | A | 651 | PX4 | C11-C10 | 3.07 | 1.63 | 1.52 | 1 | 1 |
| 3 | B | 345 | PX4 | C6-C7 | 3.07 | 1.60 | 1.50 | 13 | 4 |
| 3 | C | 334 | PX4 | C6-C7 | 3.07 | 1.60 | 1.50 | 5 | 3 |
| 3 | A | 615 | PX4 | C10-C9 | 3.07 | 1.59 | 1.50 | 2 | 3 |
| 3 | C | 319 | PX4 | C2-C1 | 3.07 | 1.60 | 1.51 | 14 | 6 |
| 3 | C | 328 | PX4 | O5-C9 | 3.07 | 1.42 | 1.33 | 15 | 3 |
| 3 | B | 345 | PX4 | O7-C23 | 3.07 | 1.25 | 1.34 | 11 | 1 |
| 3 | A | 616 | PX4 | C25-C24 | 3.07 | 1.63 | 1.52 | 10 | 3 |
| 3 | B | 329 | PX4 | C2-C1 | 3.07 | 1.60 | 1.51 | 2 | 7 |
| 3 | C | 314 | PX4 | C24-C23 | 3.07 | 1.59 | 1.50 | 8 | 2 |
| 3 | B | 312 | PX4 | O5-C8 | 3.07 | 1.52 | 1.45 | 3 | 3 |
| 3 | B | 325 | PX4 | C24-C23 | 3.07 | 1.59 | 1.50 | 10 | 3 |
| 3 | C | 320 | PX4 | C6-C7 | 3.07 | 1.60 | 1.50 | 2 | 6 |
| 3 | C | 351 | PX4 | C8-C7 | 3.07 | 1.60 | 1.50 | 8 | 4 |
| 3 | C | 362 | PX4 | O7-C23 | 3.07 | 1.25 | 1.34 | 10 | 2 |
| 3 | B | 379 | PX4 | C6-C7 | 3.07 | 1.60 | 1.50 | 8 | 6 |
| 3 | A | 612 | PX4 | C8-C7 | 3.06 | 1.60 | 1.50 | 2 | 4 |
| 3 | C | 304 | PX4 | O7-C23 | 3.06 | 1.25 | 1.34 | 13 | 4 |
| 3 | B | 321 | PX4 | C11-C10 | 3.06 | 1.63 | 1.52 | 6 | 4 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 361 | PX4 | O5-C8 | 3.06 | 1.38 | 1.45 | 5 | 1 |
| 3 | B | 367 | PX4 | O7-C7 | 3.06 | 1.39 | 1.46 | 6 | 2 |
| 3 | B | 371 | PX4 | C5-N1 | 3.06 | 1.58 | 1.50 | 11 | 1 |
| 3 | C | 341 | PX4 | O5-C8 | 3.06 | 1.38 | 1.45 | 7 | 6 |
| 3 | A | 616 | PX4 | C10-C9 | 3.06 | 1.59 | 1.50 | 2 | 1 |
| 3 | A | 603 | PX4 | O7-C23 | 3.06 | 1.25 | 1.34 | 15 | 2 |
| 3 | B | 369 | PX4 | O7-C7 | 3.06 | 1.39 | 1.46 | 13 | 1 |
| 3 | B | 349 | PX4 | O7-C7 | 3.06 | 1.39 | 1.46 | 10 | 2 |
| 3 | B | 370 | PX4 | O5-C8 | 3.06 | 1.38 | 1.45 | 15 | 3 |
| 3 | B | 384 | PX4 | C8-C7 | 3.06 | 1.60 | 1.50 | 4 | 7 |
| 3 | B | 386 | PX4 | O7-C23 | 3.06 | 1.25 | 1.34 | 5 | 1 |
| 3 | B | 386 | PX4 | O5-C8 | 3.06 | 1.52 | 1.45 | 14 | 3 |
| 3 | C | 326 | PX4 | O7-C23 | 3.06 | 1.42 | 1.34 | 15 | 3 |
| 3 | C | 359 | PX4 | C24-C23 | 3.06 | 1.59 | 1.50 | 7 | 3 |
| 3 | A | 653 | PX4 | C25-C24 | 3.05 | 1.63 | 1.52 | 9 | 3 |
| 3 | C | 305 | PX4 | O5-C9 | 3.05 | 1.42 | 1.33 | 5 | 1 |
| 3 | B | 313 | PX4 | O5-C8 | 3.05 | 1.38 | 1.45 | 13 | 1 |
| 3 | C | 317 | PX4 | C2-N1 | 3.05 | 1.60 | 1.51 | 3 | 1 |
| 3 | C | 337 | PX4 | C2-C1 | 3.05 | 1.60 | 1.51 | 5 | 4 |
| 3 | B | 329 | PX4 | C25-C24 | 3.05 | 1.63 | 1.52 | 10 | 1 |
| 3 | B | 339 | PX4 | C10-C9 | 3.05 | 1.59 | 1.50 | 15 | 2 |
| 3 | C | 341 | PX4 | C24-C23 | 3.05 | 1.59 | 1.50 | 1 | 2 |
| 3 | C | 336 | PX4 | C24-C23 | 3.05 | 1.59 | 1.50 | 15 | 6 |
| 3 | C | 358 | PX4 | C4-N1 | 3.05 | 1.58 | 1.50 | 12 | 2 |
| 3 | A | 614 | PX4 | C8-C7 | 3.04 | 1.60 | 1.50 | 6 | 5 |
| 3 | A | 611 | PX4 | C8-C7 | 3.04 | 1.60 | 1.50 | 12 | 6 |
| 3 | A | 619 | PX4 | C2-N1 | 3.04 | 1.60 | 1.51 | 12 | 2 |
| 3 | B | 321 | PX4 | O7-C23 | 3.04 | 1.25 | 1.34 | 2 | 3 |
| 3 | A | 644 | PX4 | C10-C9 | 3.04 | 1.59 | 1.50 | 6 | 3 |
| 3 | B | 313 | PX4 | O5-C9 | 3.04 | 1.42 | 1.33 | 13 | 1 |
| 3 | B | 352 | PX4 | C10-C9 | 3.04 | 1.59 | 1.50 | 9 | 2 |
| 3 | B | 374 | PX4 | C11-C10 | 3.04 | 1.63 | 1.52 | 14 | 2 |
| 3 | B | 385 | PX4 | O7-C23 | 3.04 | 1.25 | 1.34 | 4 | 2 |
| 3 | A | 607 | PX4 | C2-C1 | 3.04 | 1.60 | 1.51 | 15 | 1 |
| 3 | C | 343 | PX4 | C24-C23 | 3.04 | 1.59 | 1.50 | 7 | 4 |
| 3 | B | 318 | PX4 | C10-C9 | 3.04 | 1.59 | 1.50 | 2 | 3 |
| 3 | B | 337 | PX4 | C10-C9 | 3.03 | 1.41 | 1.50 | 4 | 3 |
| 3 | B | 378 | PX4 | O5-C8 | 3.03 | 1.51 | 1.45 | 1 | 2 |
| 3 | C | 342 | PX4 | O7-C7 | 3.03 | 1.39 | 1.46 | 8 | 2 |
| 3 | B | 366 | PX4 | C2-C1 | 3.03 | 1.60 | 1.51 | 13 | 6 |
| 3 | B | 344 | PX4 | C2-N1 | 3.03 | 1.60 | 1.51 | 2 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | C | 301 | PX4 | C10-C9 | 3.03 | 1.59 | 1.50 | 4 | 7 |
| 3 | B | 309 | PX4 | O7-C23 | 3.03 | 1.25 | 1.34 | 6 | 2 |
| 3 | B | 357 | PX4 | O7-C23 | 3.03 | 1.25 | 1.34 | 3 | 2 |
| 3 | B | 390 | PX4 | C8-C7 | 3.03 | 1.60 | 1.50 | 5 | 8 |
| 3 | A | 634 | PX4 | C2-C1 | 3.03 | 1.60 | 1.51 | 6 | 6 |
| 3 | C | 316 | PX4 | C6-C7 | 3.02 | 1.60 | 1.50 | 14 | 7 |
| 3 | A | 617 | PX4 | P1-O1 | 3.02 | 1.41 | 1.55 | 14 | 3 |
| 3 | A | 647 | PX4 | C24-C23 | 3.02 | 1.59 | 1.50 | 10 | 5 |
| 3 | B | 341 | PX4 | C24-C23 | 3.02 | 1.59 | 1.50 | 15 | 3 |
| 3 | B | 353 | PX4 | P1-O1 | 3.02 | 1.41 | 1.55 | 15 | 2 |
| 3 | B | 390 | PX4 | C25-C24 | 3.02 | 1.63 | 1.52 | 11 | 2 |
| 3 | A | 605 | PX4 | C2-C1 | 3.02 | 1.60 | 1.51 | 2 | 3 |
| 3 | A | 626 | PX4 | O5-C8 | 3.02 | 1.38 | 1.45 | 2 | 2 |
| 3 | B | 316 | PX4 | C5-N1 | 3.02 | 1.58 | 1.50 | 7 | 2 |
| 3 | B | 348 | PX4 | C10-C9 | 3.02 | 1.59 | 1.50 | 1 | 2 |
| 3 | C | 323 | PX4 | C25-C24 | 3.02 | 1.63 | 1.52 | 4 | 2 |
| 3 | A | 623 | PX4 | O5-C9 | 3.01 | 1.42 | 1.33 | 10 | 2 |
| 3 | A | 643 | PX4 | C5-N1 | 3.01 | 1.58 | 1.50 | 9 | 2 |
| 3 | B | 339 | PX4 | C11-C10 | 3.01 | 1.63 | 1.52 | 3 | 1 |
| 3 | C | 313 | PX4 | C5-N1 | 3.01 | 1.58 | 1.50 | 4 | 2 |
| 3 | C | 338 | PX4 | C2-C1 | 3.01 | 1.60 | 1.51 | 8 | 3 |
| 3 | C | 342 | PX4 | C2-C1 | 3.01 | 1.60 | 1.51 | 6 | 5 |
| 3 | A | 628 | PX4 | C2-C1 | 3.01 | 1.60 | 1.51 | 4 | 3 |
| 3 | B | 313 | PX4 | C11-C10 | 3.01 | 1.63 | 1.52 | 9 | 3 |
| 3 | C | 340 | PX4 | C6-C7 | 3.01 | 1.60 | 1.50 | 15 | 5 |
| 3 | A | 633 | PX4 | O7-C7 | 3.01 | 1.39 | 1.46 | 7 | 3 |
| 3 | A | 639 | PX4 | C24-C23 | 3.01 | 1.59 | 1.50 | 9 | 3 |
| 3 | B | 304 | PX4 | C6-C7 | 3.01 | 1.60 | 1.50 | 7 | 4 |
| 3 | B | 354 | PX4 | C8-C7 | 3.01 | 1.60 | 1.50 | 13 | 4 |
| 3 | B | 359 | PX4 | C2-N1 | 3.01 | 1.60 | 1.51 | 11 | 1 |
| 3 | B | 381 | PX4 | C2-N1 | 3.01 | 1.42 | 1.51 | 6 | 1 |
| 3 | B | 358 | PX4 | C6-C7 | 3.01 | 1.60 | 1.50 | 6 | 9 |
| 3 | A | 648 | PX4 | O5-C8 | 3.01 | 1.51 | 1.45 | 13 | 4 |
| 3 | B | 368 | PX4 | C11-C10 | 3.01 | 1.63 | 1.52 | 8 | 2 |
| 3 | B | 303 | PX4 | C24-C23 | 3.01 | 1.59 | 1.50 | 14 | 2 |
| 3 | B | 318 | PX4 | C5-N1 | 3.01 | 1.41 | 1.50 | 6 | 2 |
| 3 | A | 622 | PX4 | C24-C23 | 3.00 | 1.59 | 1.50 | 12 | 2 |
| 3 | B | 354 | PX4 | C24-C23 | 3.00 | 1.59 | 1.50 | 6 | 2 |
| 3 | A | 644 | PX4 | O7-C23 | 3.00 | 1.25 | 1.34 | 7 | 3 |
| 3 | B | 308 | PX4 | C10-C9 | 3.00 | 1.59 | 1.50 | 6 | 2 |
| 3 | B | 394 | PX4 | O5-C9 | 3.00 | 1.24 | 1.33 | 12 | 2 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 398 | PX4 | C10-C9 | 3.00 | 1.59 | 1.50 | 5 | 3 |
| 3 | B | 306 | PX4 | C5-N1 | 3.00 | 1.41 | 1.50 | 5 | 1 |
| 3 | B | 333 | PX4 | P1-O1 | 3.00 | 1.41 | 1.55 | 1 | 1 |
| 3 | C | 331 | PX4 | C2-C1 | 3.00 | 1.60 | 1.51 | 6 | 3 |
| 3 | C | 356 | PX4 | O7-C23 | 3.00 | 1.25 | 1.34 | 4 | 3 |
| 3 | B | 346 | PX4 | O5-C9 | 3.00 | 1.42 | 1.33 | 6 | 4 |
| 3 | B | 366 | PX4 | C24-C23 | 3.00 | 1.59 | 1.50 | 8 | 3 |
| 3 | C | 303 | PX4 | C2-N1 | 2.99 | 1.60 | 1.51 | 5 | 4 |
| 3 | A | 630 | PX4 | C3-N1 | 2.99 | 1.58 | 1.50 | 3 | 1 |
| 3 | A | 639 | PX4 | C6-C7 | 2.99 | 1.60 | 1.50 | 3 | 5 |
| 3 | A | 618 | PX4 | C5-N1 | 2.99 | 1.41 | 1.50 | 1 | 1 |
| 3 | A | 640 | PX4 | O5-C8 | 2.99 | 1.38 | 1.45 | 6 | 3 |
| 3 | B | 324 | PX4 | O7-C7 | 2.99 | 1.39 | 1.46 | 8 | 2 |
| 3 | B | 324 | PX4 | C28-C27 | 2.99 | 1.66 | 1.51 | 12 | 3 |
| 3 | B | 325 | PX4 | O7-C7 | 2.99 | 1.39 | 1.46 | 12 | 2 |
| 3 | B | 382 | PX4 | C2-N1 | 2.99 | 1.60 | 1.51 | 12 | 2 |
| 3 | C | 338 | PX4 | O5-C8 | 2.99 | 1.38 | 1.45 | 12 | 1 |
| 3 | A | 648 | PX4 | O7-C7 | 2.99 | 1.39 | 1.46 | 9 | 4 |
| 3 | B | 313 | PX4 | C25-C24 | 2.99 | 1.63 | 1.52 | 9 | 5 |
| 3 | B | 360 | PX4 | C17-C16 | 2.99 | 1.66 | 1.51 | 14 | 1 |
| 3 | B | 393 | PX4 | C4-N1 | 2.99 | 1.41 | 1.50 | 10 | 1 |
| 3 | B | 330 | PX4 | C8-C7 | 2.98 | 1.60 | 1.50 | 9 | 4 |
| 3 | B | 379 | PX4 | O7-C7 | 2.99 | 1.39 | 1.46 | 9 | 5 |
| 3 | C | 353 | PX4 | C6-C7 | 2.99 | 1.60 | 1.50 | 4 | 7 |
| 3 | C | 306 | PX4 | O5-C8 | 2.98 | 1.38 | 1.45 | 15 | 1 |
| 3 | C | 348 | PX4 | P1-O1 | 2.98 | 1.41 | 1.55 | 13 | 3 |
| 3 | C | 363 | PX4 | C3-N1 | 2.98 | 1.58 | 1.50 | 8 | 2 |
| 3 | A | 635 | PX4 | O7-C7 | 2.98 | 1.39 | 1.46 | 8 | 2 |
| 3 | A | 638 | PX4 | C6-C7 | 2.98 | 1.60 | 1.50 | 3 | 6 |
| 3 | A | 640 | PX4 | C2-N1 | 2.98 | 1.60 | 1.51 | 8 | 2 |
| 3 | B | 328 | PX4 | C8-C7 | 2.98 | 1.60 | 1.50 | 11 | 8 |
| 3 | B | 394 | PX4 | C24-C23 | 2.98 | 1.59 | 1.50 | 4 | 2 |
| 3 | B | 331 | PX4 | O5-C8 | 2.98 | 1.38 | 1.45 | 10 | 5 |
| 3 | B | 394 | PX4 | C2-N1 | 2.98 | 1.60 | 1.51 | 3 | 2 |
| 3 | C | 301 | PX4 | O7-C23 | 2.98 | 1.25 | 1.34 | 2 | 1 |
| 3 | B | 368 | PX4 | C4-N1 | 2.98 | 1.41 | 1.50 | 4 | 2 |
| 3 | C | 345 | PX4 | C10-C9 | 2.98 | 1.59 | 1.50 | 13 | 3 |
| 3 | C | 345 | PX4 | C25-C24 | 2.98 | 1.63 | 1.52 | 7 | 2 |
| 3 | C | 353 | PX4 | O5-C9 | 2.98 | 1.24 | 1.33 | 1 | 3 |
| 3 | B | 360 | PX4 | C24-C23 | 2.97 | 1.59 | 1.50 | 10 | 2 |
| 3 | C | 318 | PX4 | C3-N1 | 2.98 | 1.58 | 1.50 | 12 | 3 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 304 | PX4 | C8-C7 | 2.97 | 1.60 | 1.50 | 14 | 5 |
| 3 | B | 318 | PX4 | P1-O1 | 2.97 | 1.41 | 1.55 | 9 | 2 |
| 3 | B | 399 | PX4 | C11-C10 | 2.97 | 1.63 | 1.52 | 6 | 2 |
| 3 | B | 332 | PX4 | O5-C9 | 2.97 | 1.42 | 1.33 | 8 | 4 |
| 3 | B | 388 | PX4 | P1-O1 | 2.97 | 1.41 | 1.55 | 7 | 4 |
| 3 | B | 390 | PX4 | C2-N1 | 2.97 | 1.42 | 1.51 | 8 | 1 |
| 3 | B | 353 | PX4 | O5-C9 | 2.97 | 1.42 | 1.33 | 6 | 1 |
| 3 | B | 309 | PX4 | C4-N1 | 2.97 | 1.58 | 1.50 | 11 | 6 |
| 3 | B | 344 | PX4 | C8-C7 | 2.97 | 1.60 | 1.50 | 7 | 8 |
| 3 | B | 345 | PX4 | C8-C7 | 2.97 | 1.60 | 1.50 | 8 | 7 |
| 3 | B | 354 | PX4 | P1-O3 | 2.97 | 1.47 | 1.59 | 2 | 1 |
| 3 | B | 391 | PX4 | O5-C9 | 2.97 | 1.42 | 1.33 | 12 | 2 |
| 3 | B | 324 | PX4 | C25-C24 | 2.97 | 1.63 | 1.52 | 15 | 2 |
| 3 | B | 330 | PX4 | O5-C8 | 2.97 | 1.51 | 1.45 | 6 | 2 |
| 3 | C | 312 | PX4 | C2-C1 | 2.97 | 1.60 | 1.51 | 13 | 6 |
| 3 | A | 617 | PX4 | C10-C9 | 2.96 | 1.59 | 1.50 | 13 | 5 |
| 3 | A | 627 | PX4 | C24-C23 | 2.96 | 1.59 | 1.50 | 6 | 6 |
| 3 | C | 340 | PX4 | C24-C23 | 2.96 | 1.59 | 1.50 | 6 | 2 |
| 3 | B | 318 | PX4 | C2-C1 | 2.96 | 1.60 | 1.51 | 12 | 6 |
| 3 | A | 613 | PX4 | O7-C7 | 2.96 | 1.39 | 1.46 | 5 | 3 |
| 3 | B | 349 | PX4 | C18-C17 | 2.96 | 1.66 | 1.51 | 1 | 1 |
| 3 | A | 630 | PX4 | C11-C10 | 2.96 | 1.63 | 1.52 | 5 | 2 |
| 3 | A | 634 | PX4 | O5-C9 | 2.96 | 1.42 | 1.33 | 2 | 3 |
| 3 | C | 315 | PX4 | O7-C7 | 2.96 | 1.39 | 1.46 | 5 | 4 |
| 3 | C | 323 | PX4 | C2-N1 | 2.96 | 1.60 | 1.51 | 6 | 2 |
| 3 | A | 640 | PX4 | C2-C1 | 2.96 | 1.60 | 1.51 | 2 | 4 |
| 3 | A | 643 | PX4 | C6-C7 | 2.96 | 1.60 | 1.50 | 4 | 4 |
| 3 | A | 646 | PX4 | O5-C8 | 2.96 | 1.38 | 1.45 | 13 | 1 |
| 3 | A | 647 | PX4 | C5-N1 | 2.96 | 1.41 | 1.50 | 5 | 1 |
| 3 | B | 347 | PX4 | C24-C23 | 2.96 | 1.59 | 1.50 | 6 | 1 |
| 3 | B | 383 | PX4 | O7-C23 | 2.95 | 1.25 | 1.34 | 12 | 2 |
| 3 | B | 389 | PX4 | C25-C24 | 2.95 | 1.63 | 1.52 | 15 | 2 |
| 3 | C | 343 | PX4 | O7-C23 | 2.96 | 1.25 | 1.34 | 5 | 4 |
| 3 | B | 323 | PX4 | C6-C7 | 2.95 | 1.60 | 1.50 | 8 | 2 |
| 3 | A | 606 | PX4 | C11-C10 | 2.95 | 1.63 | 1.52 | 14 | 5 |
| 3 | A | 607 | PX4 | C10-C9 | 2.95 | 1.59 | 1.50 | 7 | 2 |
| 3 | B | 317 | PX4 | C25-C24 | 2.95 | 1.63 | 1.52 | 9 | 1 |
| 3 | B | 319 | PX4 | O7-C7 | 2.95 | 1.39 | 1.46 | 2 | 1 |
| 3 | B | 329 | PX4 | C11-C10 | 2.95 | 1.63 | 1.52 | 15 | 4 |
| 3 | B | 304 | PX4 | O5-C8 | 2.95 | 1.38 | 1.45 | 5 | 1 |
| 3 | A | 644 | PX4 | C6-C7 | 2.95 | 1.60 | 1.50 | 5 | 3 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 311 | PX4 | C5-N1 | 2.95 | 1.58 | 1.50 | 7 | 5 |
| 3 | B | 388 | PX4 | C11-C10 | 2.95 | 1.63 | 1.52 | 10 | 3 |
| 3 | A | 651 | PX4 | O5-C8 | 2.95 | 1.51 | 1.45 | 1 | 5 |
| 3 | B | 331 | PX4 | C24-C23 | 2.95 | 1.59 | 1.50 | 14 | 2 |
| 3 | A | 651 | PX4 | O5-C9 | 2.94 | 1.41 | 1.33 | 6 | 2 |
| 3 | B | 367 | PX4 | C11-C10 | 2.94 | 1.63 | 1.52 | 15 | 2 |
| 3 | C | 306 | PX4 | C10-C9 | 2.94 | 1.59 | 1.50 | 1 | 3 |
| 3 | C | 352 | PX4 | O7-C7 | 2.94 | 1.39 | 1.46 | 3 | 1 |
| 3 | B | 323 | PX4 | O4-C6 | 2.94 | 1.33 | 1.44 | 7 | 1 |
| 3 | A | 604 | PX4 | C5-N1 | 2.94 | 1.58 | 1.50 | 9 | 3 |
| 3 | B | 307 | PX4 | C10-C9 | 2.94 | 1.59 | 1.50 | 13 | 5 |
| 3 | B | 337 | PX4 | C3-N1 | 2.94 | 1.41 | 1.50 | 9 | 3 |
| 3 | A | 603 | PX4 | O7-C7 | 2.94 | 1.39 | 1.46 | 5 | 2 |
| 3 | C | 361 | PX4 | C11-C10 | 2.94 | 1.63 | 1.52 | 3 | 1 |
| 3 | A | 608 | PX4 | C24-C23 | 2.94 | 1.59 | 1.50 | 6 | 2 |
| 3 | A | 627 | PX4 | C5-N1 | 2.94 | 1.58 | 1.50 | 13 | 2 |
| 3 | B | 303 | PX4 | O5-C8 | 2.93 | 1.38 | 1.45 | 14 | 1 |
| 3 | B | 327 | PX4 | C2-N1 | 2.93 | 1.60 | 1.51 | 4 | 1 |
| 3 | B | 359 | PX4 | O5-C8 | 2.93 | 1.51 | 1.45 | 10 | 2 |
| 3 | B | 389 | PX4 | C11-C10 | 2.93 | 1.62 | 1.52 | 10 | 2 |
| 3 | C | 363 | PX4 | C24-C23 | 2.93 | 1.59 | 1.50 | 6 | 1 |
| 3 | B | 315 | PX4 | O5-C9 | 2.93 | 1.41 | 1.33 | 12 | 2 |
| 3 | B | 360 | PX4 | O5-C8 | 2.93 | 1.38 | 1.45 | 9 | 3 |
| 3 | B | 304 | PX4 | C11-C10 | 2.93 | 1.62 | 1.52 | 5 | 1 |
| 3 | B | 339 | PX4 | O5-C8 | 2.93 | 1.38 | 1.45 | 3 | 2 |
| 3 | B | 386 | PX4 | C10-C9 | 2.93 | 1.59 | 1.50 | 11 | 3 |
| 3 | C | 307 | PX4 | C10-C9 | 2.93 | 1.59 | 1.50 | 2 | 3 |
| 3 | C | 360 | PX4 | O7-C7 | 2.93 | 1.39 | 1.46 | 6 | 2 |
| 3 | C | 338 | PX4 | O7-C7 | 2.93 | 1.39 | 1.46 | 7 | 1 |
| 3 | C | 349 | PX4 | C6-C7 | 2.93 | 1.60 | 1.50 | 10 | 7 |
| 3 | A | 605 | PX4 | C11-C10 | 2.92 | 1.62 | 1.52 | 15 | 2 |
| 3 | C | 309 | PX4 | P1-O1 | 2.92 | 1.41 | 1.55 | 7 | 4 |
| 3 | C | 325 | PX4 | C25-C24 | 2.92 | 1.62 | 1.52 | 12 | 3 |
| 3 | C | 337 | PX4 | C25-C24 | 2.92 | 1.62 | 1.52 | 12 | 1 |
| 3 | C | 344 | PX4 | C6-C7 | 2.92 | 1.59 | 1.50 | 7 | 6 |
| 3 | A | 652 | PX4 | C24-C23 | 2.92 | 1.59 | 1.50 | 5 | 4 |
| 3 | B | 306 | PX4 | C8-C7 | 2.92 | 1.59 | 1.50 | 5 | 5 |
| 3 | B | 322 | PX4 | O7-C23 | 2.92 | 1.26 | 1.34 | 4 | 3 |
| 3 | B | 356 | PX4 | C4-N1 | 2.92 | 1.58 | 1.50 | 2 | 2 |
| 3 | A | 645 | PX4 | C25-C24 | 2.92 | 1.62 | 1.52 | 3 | 2 |
| 3 | A | 649 | PX4 | C24-C23 | 2.92 | 1.59 | 1.50 | 2 | 2 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 311 | PX4 | C24-C23 | 2.92 | 1.59 | 1.50 | 11 | 6 |
| 3 | B | 338 | PX4 | O7-C7 | 2.92 | 1.39 | 1.46 | 2 | 1 |
| 3 | B | 368 | PX4 | C5-N1 | 2.92 | 1.58 | 1.50 | 6 | 1 |
| 3 | A | 634 | PX4 | C11-C10 | 2.92 | 1.62 | 1.52 | 14 | 4 |
| 3 | B | 332 | PX4 | C24-C23 | 2.92 | 1.59 | 1.50 | 11 | 1 |
| 3 | B | 394 | PX4 | O5-C8 | 2.92 | 1.51 | 1.45 | 9 | 3 |
| 3 | C | 311 | PX4 | C2-C1 | 2.91 | 1.60 | 1.51 | 6 | 5 |
| 3 | C | 346 | PX4 | O7-C7 | 2.91 | 1.39 | 1.46 | 7 | 4 |
| 3 | C | 356 | PX4 | C24-C23 | 2.91 | 1.59 | 1.50 | 8 | 2 |
| 3 | A | 621 | PX4 | C8-C7 | 2.91 | 1.59 | 1.50 | 3 | 4 |
| 3 | B | 303 | PX4 | C2-N1 | 2.91 | 1.60 | 1.51 | 13 | 1 |
| 3 | B | 388 | PX4 | O7-C23 | 2.91 | 1.26 | 1.34 | 13 | 3 |
| 3 | C | 346 | PX4 | C2-C1 | 2.91 | 1.60 | 1.51 | 2 | 2 |
| 3 | C | 364 | PX4 | C2-C1 | 2.91 | 1.60 | 1.51 | 1 | 3 |
| 3 | B | 387 | PX4 | C25-C24 | 2.91 | 1.62 | 1.52 | 11 | 1 |
| 3 | A | 628 | PX4 | C6-C7 | 2.91 | 1.59 | 1.50 | 7 | 5 |
| 3 | A | 646 | PX4 | O7-C7 | 2.91 | 1.39 | 1.46 | 13 | 2 |
| 3 | C | 309 | PX4 | C3-N1 | 2.91 | 1.58 | 1.50 | 7 | 1 |
| 3 | C | 344 | PX4 | C11-C10 | 2.91 | 1.62 | 1.52 | 8 | 2 |
| 3 | A | 601 | PX4 | C24-C23 | 2.91 | 1.59 | 1.50 | 3 | 3 |
| 3 | A | 648 | PX4 | O7-C23 | 2.91 | 1.26 | 1.34 | 13 | 5 |
| 3 | B | 335 | PX4 | C10-C9 | 2.91 | 1.59 | 1.50 | 9 | 3 |
| 3 | B | 378 | PX4 | O7-C7 | 2.91 | 1.39 | 1.46 | 8 | 3 |
| 3 | A | 620 | PX4 | O5-C9 | 2.90 | 1.24 | 1.33 | 13 | 1 |
| 3 | A | 638 | PX4 | C11-C10 | 2.90 | 1.62 | 1.52 | 13 | 1 |
| 3 | B | 345 | PX4 | C25-C24 | 2.90 | 1.62 | 1.52 | 2 | 3 |
| 3 | A | 653 | PX4 | C2-C1 | 2.90 | 1.60 | 1.51 | 8 | 6 |
| 3 | C | 312 | PX4 | C10-C9 | 2.90 | 1.59 | 1.50 | 7 | 4 |
| 3 | C | 349 | PX4 | C2-C1 | 2.90 | 1.60 | 1.51 | 1 | 3 |
| 3 | B | 381 | PX4 | C3-N1 | 2.90 | 1.58 | 1.50 | 15 | 2 |
| 3 | B | 363 | PX4 | C24-C23 | 2.90 | 1.59 | 1.50 | 4 | 2 |
| 3 | B | 366 | PX4 | C5-N1 | 2.90 | 1.58 | 1.50 | 6 | 2 |
| 3 | B | 375 | PX4 | O7-C7 | 2.90 | 1.39 | 1.46 | 11 | 3 |
| 3 | C | 334 | PX4 | P1-O1 | 2.90 | 1.41 | 1.55 | 14 | 3 |
| 3 | B | 354 | PX4 | O7-C23 | 2.90 | 1.26 | 1.34 | 3 | 3 |
| 3 | C | 317 | PX4 | C6-C7 | 2.90 | 1.59 | 1.50 | 7 | 5 |
| 3 | B | 357 | PX4 | O7-C7 | 2.90 | 1.39 | 1.46 | 1 | 3 |
| 3 | C | 352 | PX4 | O5-C8 | 2.90 | 1.51 | 1.45 | 8 | 4 |
| 3 | B | 305 | PX4 | C2-C1 | 2.89 | 1.60 | 1.51 | 2 | 3 |
| 3 | B | 323 | PX4 | C2-N1 | 2.89 | 1.60 | 1.51 | 12 | 1 |
| 3 | B | 371 | PX4 | C11-C10 | 2.89 | 1.62 | 1.52 | 13 | 4 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 356 | PX4 | C2-C1 | 2.89 | 1.60 | 1.51 | 3 | 6 |
| 3 | A | 622 | PX4 | C8-C7 | 2.89 | 1.59 | 1.50 | 4 | 7 |
| 3 | B | 376 | PX4 | C10-C9 | 2.89 | 1.59 | 1.50 | 4 | 3 |
| 3 | B | 301 | PX4 | C2-N1 | 2.89 | 1.60 | 1.51 | 9 | 1 |
| 3 | B | 319 | PX4 | O5-C8 | 2.89 | 1.51 | 1.45 | 14 | 3 |
| 3 | B | 337 | PX4 | O7-C7 | 2.89 | 1.53 | 1.46 | 10 | 3 |
| 3 | A | 623 | PX4 | O7-C7 | 2.88 | 1.39 | 1.46 | 4 | 2 |
| 3 | A | 601 | PX4 | O5-C9 | 2.88 | 1.25 | 1.33 | 2 | 1 |
| 3 | B | 321 | PX4 | C24-C23 | 2.88 | 1.59 | 1.50 | 14 | 4 |
| 3 | C | 333 | PX4 | C2-C1 | 2.88 | 1.60 | 1.51 | 2 | 3 |
| 3 | A | 626 | PX4 | O7-C23 | 2.88 | 1.26 | 1.34 | 13 | 3 |
| 3 | C | 301 | PX4 | C25-C24 | 2.88 | 1.62 | 1.52 | 9 | 2 |
| 3 | A | 614 | PX4 | O5-C8 | 2.88 | 1.51 | 1.45 | 14 | 2 |
| 3 | A | 639 | PX4 | C25-C24 | 2.88 | 1.62 | 1.52 | 14 | 2 |
| 3 | C | 302 | PX4 | C2-N1 | 2.88 | 1.60 | 1.51 | 15 | 3 |
| 3 | B | 366 | PX4 | C11-C10 | 2.88 | 1.62 | 1.52 | 11 | 2 |
| 3 | C | 324 | PX4 | O7-C7 | 2.88 | 1.39 | 1.46 | 11 | 2 |
| 3 | C | 331 | PX4 | O5-C8 | 2.88 | 1.38 | 1.45 | 4 | 3 |
| 3 | B | 395 | PX4 | O5-C9 | 2.88 | 1.41 | 1.33 | 12 | 2 |
| 3 | C | 336 | PX4 | C3-N1 | 2.88 | 1.58 | 1.50 | 11 | 1 |
| 3 | C | 349 | PX4 | O7-C7 | 2.88 | 1.39 | 1.46 | 5 | 2 |
| 3 | B | 342 | PX4 | O5-C8 | 2.88 | 1.38 | 1.45 | 6 | 1 |
| 3 | B | 307 | PX4 | C6-C7 | 2.88 | 1.59 | 1.50 | 1 | 4 |
| 3 | C | 364 | PX4 | O5-C8 | 2.88 | 1.38 | 1.45 | 2 | 2 |
| 3 | A | 638 | PX4 | C24-C23 | 2.87 | 1.59 | 1.50 | 12 | 1 |
| 3 | B | 351 | PX4 | O5-C9 | 2.87 | 1.41 | 1.33 | 2 | 2 |
| 3 | B | 363 | PX4 | C10-C9 | 2.87 | 1.59 | 1.50 | 13 | 3 |
| 3 | B | 385 | PX4 | O5-C8 | 2.87 | 1.51 | 1.45 | 2 | 2 |
| 3 | C | 361 | PX4 | O5-C8 | 2.87 | 1.38 | 1.45 | 4 | 1 |
| 3 | C | 363 | PX4 | O7-C7 | 2.87 | 1.39 | 1.46 | 9 | 4 |
| 3 | B | 302 | PX4 | O7-C7 | 2.87 | 1.39 | 1.46 | 1 | 4 |
| 3 | B | 366 | PX4 | O7-C7 | 2.87 | 1.39 | 1.46 | 8 | 2 |
| 3 | B | 368 | PX4 | P1-O1 | 2.87 | 1.42 | 1.55 | 12 | 4 |
| 3 | B | 350 | PX4 | C10-C9 | 2.87 | 1.59 | 1.50 | 1 | 5 |
| 3 | C | 305 | PX4 | C11-C10 | 2.87 | 1.62 | 1.52 | 8 | 6 |
| 3 | A | 605 | PX4 | O7-C23 | 2.87 | 1.26 | 1.34 | 9 | 6 |
| 3 | B | 396 | PX4 | O7-C7 | 2.87 | 1.39 | 1.46 | 15 | 2 |
| 3 | B | 358 | PX4 | O7-C7 | 2.87 | 1.39 | 1.46 | 3 | 3 |
| 3 | C | 303 | PX4 | C11-C10 | 2.87 | 1.62 | 1.52 | 15 | 2 |
| 3 | B | 394 | PX4 | C8-C7 | 2.87 | 1.59 | 1.50 | 12 | 4 |
| 3 | B | 398 | PX4 | C2-N1 | 2.87 | 1.60 | 1.51 | 6 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | C | 330 | PX4 | O7-C23 | 2.87 | 1.26 | 1.34 | 5 | 4 |
| 3 | A | 607 | PX4 | C24-C23 | 2.86 | 1.59 | 1.50 | 14 | 3 |
| 3 | C | 337 | PX4 | O5-C9 | 2.86 | 1.25 | 1.33 | 3 | 5 |
| 3 | A | 628 | PX4 | C11-C10 | 2.86 | 1.62 | 1.52 | 15 | 3 |
| 3 | C | 305 | PX4 | O5-C8 | 2.86 | 1.51 | 1.45 | 8 | 2 |
| 3 | A | 623 | PX4 | C25-C24 | 2.86 | 1.62 | 1.52 | 13 | 1 |
| 3 | B | 318 | PX4 | O5-C8 | 2.86 | 1.51 | 1.45 | 10 | 3 |
| 3 | B | 317 | PX4 | C10-C9 | 2.86 | 1.59 | 1.50 | 1 | 2 |
| 3 | C | 340 | PX4 | C10-C9 | 2.86 | 1.59 | 1.50 | 5 | 3 |
| 3 | A | 610 | PX4 | C10-C9 | 2.86 | 1.59 | 1.50 | 4 | 2 |
| 3 | B | 306 | PX4 | O7-C23 | 2.86 | 1.26 | 1.34 | 7 | 2 |
| 3 | B | 317 | PX4 | C24-C23 | 2.86 | 1.59 | 1.50 | 14 | 2 |
| 3 | B | 338 | PX4 | C5-N1 | 2.85 | 1.41 | 1.50 | 15 | 2 |
| 3 | B | 373 | PX4 | C6-C7 | 2.85 | 1.59 | 1.50 | 11 | 4 |
| 3 | B | 337 | PX4 | C8-C7 | 2.85 | 1.59 | 1.50 | 13 | 10 |
| 3 | B | 352 | PX4 | C8-C7 | 2.85 | 1.59 | 1.50 | 7 | 6 |
| 3 | C | 348 | PX4 | O7-C23 | 2.85 | 1.42 | 1.34 | 2 | 2 |
| 3 | B | 364 | PX4 | O5-C9 | 2.85 | 1.41 | 1.33 | 8 | 2 |
| 3 | C | 328 | PX4 | O7-C7 | 2.85 | 1.39 | 1.46 | 8 | 4 |
| 3 | B | 335 | PX4 | O7-C7 | 2.85 | 1.39 | 1.46 | 5 | 1 |
| 3 | C | 321 | PX4 | C26-C25 | 2.85 | 1.65 | 1.51 | 9 | 1 |
| 3 | A | 610 | PX4 | O5-C9 | 2.84 | 1.41 | 1.33 | 2 | 4 |
| 3 | A | 602 | PX4 | P1-O1 | 2.84 | 1.42 | 1.55 | 12 | 3 |
| 3 | A | 638 | PX4 | O5-C9 | 2.84 | 1.41 | 1.33 | 7 | 1 |
| 3 | A | 642 | PX4 | O5-C8 | 2.84 | 1.38 | 1.45 | 14 | 4 |
| 3 | B | 312 | PX4 | C6-C7 | 2.84 | 1.59 | 1.50 | 9 | 4 |
| 3 | B | 327 | PX4 | C11-C10 | 2.84 | 1.62 | 1.52 | 1 | 2 |
| 3 | C | 339 | PX4 | C3-N1 | 2.84 | 1.41 | 1.50 | 5 | 2 |
| 3 | B | 328 | PX4 | P1-O1 | 2.84 | 1.42 | 1.55 | 11 | 3 |
| 3 | C | 308 | PX4 | C8-C7 | 2.84 | 1.59 | 1.50 | 1 | 9 |
| 3 | A | 627 | PX4 | O5-C8 | 2.84 | 1.38 | 1.45 | 3 | 3 |
| 3 | A | 633 | PX4 | O5-C9 | 2.84 | 1.41 | 1.33 | 14 | 2 |
| 3 | C | 303 | PX4 | C10-C9 | 2.84 | 1.58 | 1.50 | 10 | 2 |
| 3 | C | 309 | PX4 | O5-C9 | 2.84 | 1.41 | 1.33 | 15 | 1 |
| 3 | C | 325 | PX4 | O7-C7 | 2.84 | 1.39 | 1.46 | 4 | 1 |
| 3 | B | 388 | PX4 | C10-C9 | 2.84 | 1.58 | 1.50 | 6 | 5 |
| 3 | B | 393 | PX4 | C15-C14 | 2.84 | 1.65 | 1.51 | 10 | 1 |
| 3 | C | 357 | PX4 | O7-C7 | 2.84 | 1.39 | 1.46 | 10 | 4 |
| 3 | A | 625 | PX4 | C25-C24 | 2.83 | 1.62 | 1.52 | 7 | 1 |
| 3 | B | 333 | PX4 | O7-C23 | 2.83 | 1.26 | 1.34 | 4 | 3 |
| 3 | C | 312 | PX4 | C24-C23 | 2.83 | 1.58 | 1.50 | 14 | 4 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | A | 618 | PX4 | O7-C23 | 2.83 | 1.42 | 1.34 | 4 | 2 |
| 3 | C | 310 | PX4 | P1-O1 | 2.83 | 1.42 | 1.55 | 13 | 3 |
| 3 | A | 627 | PX4 | C25-C24 | 2.83 | 1.62 | 1.52 | 7 | 1 |
| 3 | C | 312 | PX4 | P1-O2 | 2.83 | 1.41 | 1.50 | 14 | 2 |
| 3 | C | 315 | PX4 | C10-C9 | 2.83 | 1.58 | 1.50 | 2 | 2 |
| 3 | C | 342 | PX4 | C11-C10 | 2.83 | 1.62 | 1.52 | 7 | 2 |
| 3 | A | 641 | PX4 | C5-N1 | 2.83 | 1.58 | 1.50 | 4 | 2 |
| 3 | B | 341 | PX4 | C10-C9 | 2.83 | 1.58 | 1.50 | 2 | 4 |
| 3 | A | 621 | PX4 | C3-N1 | 2.82 | 1.58 | 1.50 | 1 | 3 |
| 3 | A | 629 | PX4 | C2-C1 | 2.82 | 1.59 | 1.51 | 9 | 6 |
| 3 | A | 645 | PX4 | C10-C9 | 2.82 | 1.58 | 1.50 | 15 | 4 |
| 3 | B | 302 | PX4 | C10-C9 | 2.82 | 1.58 | 1.50 | 15 | 3 |
| 3 | B | 354 | PX4 | C25-C24 | 2.82 | 1.62 | 1.52 | 1 | 1 |
| 3 | B | 357 | PX4 | C24-C23 | 2.82 | 1.58 | 1.50 | 12 | 1 |
| 3 | C | 304 | PX4 | C2-C1 | 2.82 | 1.59 | 1.51 | 6 | 5 |
| 3 | C | 319 | PX4 | C10-C9 | 2.82 | 1.58 | 1.50 | 5 | 2 |
| 3 | A | 634 | PX4 | C6-C7 | 2.82 | 1.59 | 1.50 | 1 | 5 |
| 3 | A | 648 | PX4 | P1-O4 | 2.82 | 1.48 | 1.59 | 12 | 1 |
| 3 | B | 334 | PX4 | P1-O2 | 2.82 | 1.41 | 1.50 | 5 | 2 |
| 3 | C | 315 | PX4 | O7-C23 | 2.82 | 1.26 | 1.34 | 4 | 3 |
| 3 | A | 610 | PX4 | C15-C14 | 2.82 | 1.65 | 1.51 | 6 | 1 |
| 3 | B | 326 | PX4 | C25-C24 | 2.82 | 1.62 | 1.52 | 6 | 3 |
| 3 | B | 332 | PX4 | C4-N1 | 2.82 | 1.41 | 1.50 | 9 | 1 |
| 3 | B | 371 | PX4 | C8-C7 | 2.82 | 1.59 | 1.50 | 2 | 5 |
| 3 | B | 379 | PX4 | C5-N1 | 2.82 | 1.58 | 1.50 | 10 | 1 |
| 3 | C | 313 | PX4 | O7-C7 | 2.82 | 1.40 | 1.46 | 3 | 1 |
| 3 | C | 354 | PX4 | C3-N1 | 2.82 | 1.41 | 1.50 | 4 | 2 |
| 3 | C | 356 | PX4 | C10-C9 | 2.82 | 1.58 | 1.50 | 8 | 1 |
| 3 | B | 311 | PX4 | O5-C9 | 2.81 | 1.25 | 1.33 | 15 | 2 |
| 3 | B | 356 | PX4 | O5-C8 | 2.81 | 1.51 | 1.45 | 12 | 2 |
| 3 | B | 360 | PX4 | C2-N1 | 2.81 | 1.60 | 1.51 | 15 | 2 |
| 3 | B | 394 | PX4 | C2-C1 | 2.81 | 1.59 | 1.51 | 2 | 6 |
| 3 | C | 305 | PX4 | O7-C7 | 2.81 | 1.40 | 1.46 | 8 | 3 |
| 3 | C | 321 | PX4 | C6-C7 | 2.81 | 1.59 | 1.50 | 10 | 3 |
| 3 | B | 301 | PX4 | C10-C9 | 2.81 | 1.58 | 1.50 | 12 | 5 |
| 3 | B | 359 | PX4 | P1-O1 | 2.81 | 1.42 | 1.55 | 8 | 3 |
| 3 | C | 327 | PX4 | C24-C23 | 2.81 | 1.58 | 1.50 | 1 | 3 |
| 3 | A | 634 | PX4 | C24-C23 | 2.81 | 1.58 | 1.50 | 10 | 1 |
| 3 | C | 346 | PX4 | C8-C7 | 2.81 | 1.59 | 1.50 | 11 | 3 |
| 3 | B | 328 | PX4 | C10-C9 | 2.81 | 1.58 | 1.50 | 4 | 5 |
| 3 | A | 618 | PX4 | C2-C1 | 2.81 | 1.59 | 1.51 | 6 | 2 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | C | 344 | PX4 | C2-C1 | 2.81 | 1.59 | 1.51 | 10 | 2 |
| 3 | C | 358 | PX4 | C10-C9 | 2.81 | 1.58 | 1.50 | 12 | 2 |
| 3 | A | 647 | PX4 | O5-C9 | 2.81 | 1.41 | 1.33 | 14 | 2 |
| 3 | B | 321 | PX4 | C4-N1 | 2.81 | 1.41 | 1.50 | 1 | 2 |
| 3 | B | 379 | PX4 | C24-C23 | 2.81 | 1.58 | 1.50 | 8 | 4 |
| 3 | B | 381 | PX4 | O7-C23 | 2.81 | 1.26 | 1.34 | 10 | 3 |
| 3 | B | 382 | PX4 | O5-C9 | 2.81 | 1.41 | 1.33 | 13 | 4 |
| 3 | B | 389 | PX4 | C2-C1 | 2.81 | 1.59 | 1.51 | 4 | 5 |
| 3 | C | 348 | PX4 | C24-C23 | 2.81 | 1.58 | 1.50 | 10 | 1 |
| 3 | C | 363 | PX4 | C25-C24 | 2.81 | 1.62 | 1.52 | 11 | 4 |
| 3 | B | 383 | PX4 | C5-N1 | 2.81 | 1.41 | 1.50 | 2 | 1 |
| 3 | B | 375 | PX4 | C8-C7 | 2.81 | 1.59 | 1.50 | 9 | 3 |
| 3 | C | 359 | PX4 | O5-C9 | 2.80 | 1.25 | 1.33 | 15 | 3 |
| 3 | A | 608 | PX4 | C25-C24 | 2.80 | 1.62 | 1.52 | 2 | 3 |
| 3 | B | 301 | PX4 | C4-N1 | 2.80 | 1.58 | 1.50 | 5 | 3 |
| 3 | B | 301 | PX4 | O5-C9 | 2.80 | 1.25 | 1.33 | 14 | 1 |
| 3 | B | 359 | PX4 | C4-N1 | 2.80 | 1.41 | 1.50 | 14 | 3 |
| 3 | B | 364 | PX4 | O7-C23 | 2.80 | 1.26 | 1.34 | 9 | 1 |
| 3 | C | 337 | PX4 | P1-O2 | 2.80 | 1.41 | 1.50 | 1 | 2 |
| 3 | A | 654 | PX4 | C8-C7 | 2.80 | 1.59 | 1.50 | 13 | 10 |
| 3 | A | 635 | PX4 | C25-C24 | 2.80 | 1.62 | 1.52 | 1 | 1 |
| 3 | A | 654 | PX4 | C6-C7 | 2.80 | 1.59 | 1.50 | 10 | 8 |
| 3 | B | 391 | PX4 | C24-C23 | 2.80 | 1.58 | 1.50 | 1 | 2 |
| 3 | C | 338 | PX4 | C4-N1 | 2.80 | 1.58 | 1.50 | 13 | 1 |
| 3 | A | 627 | PX4 | O7-C23 | 2.80 | 1.26 | 1.34 | 4 | 2 |
| 3 | B | 305 | PX4 | P1-O1 | 2.80 | 1.42 | 1.55 | 4 | 5 |
| 3 | B | 322 | PX4 | O5-C8 | 2.80 | 1.51 | 1.45 | 8 | 4 |
| 3 | B | 364 | PX4 | C11-C10 | 2.80 | 1.62 | 1.52 | 1 | 3 |
| 3 | A | 616 | PX4 | O7-C7 | 2.80 | 1.53 | 1.46 | 11 | 2 |
| 3 | B | 345 | PX4 | C2-N1 | 2.80 | 1.60 | 1.51 | 15 | 1 |
| 3 | C | 330 | PX4 | C24-C23 | 2.79 | 1.58 | 1.50 | 14 | 3 |
| 3 | C | 355 | PX4 | C24-C23 | 2.80 | 1.58 | 1.50 | 9 | 4 |
| 3 | A | 605 | PX4 | O5-C9 | 2.79 | 1.25 | 1.33 | 5 | 3 |
| 3 | A | 614 | PX4 | C3-N1 | 2.79 | 1.58 | 1.50 | 10 | 2 |
| 3 | A | 645 | PX4 | P1-O4 | 2.79 | 1.70 | 1.59 | 6 | 1 |
| 3 | A | 604 | PX4 | C34-C33 | 2.79 | 1.65 | 1.51 | 8 | 1 |
| 3 | B | 337 | PX4 | O7-C23 | 2.79 | 1.26 | 1.34 | 13 | 2 |
| 3 | B | 372 | PX4 | C10-C9 | 2.79 | 1.58 | 1.50 | 13 | 2 |
| 3 | C | 324 | PX4 | C8-C7 | 2.79 | 1.59 | 1.50 | 15 | 5 |
| 3 | B | 371 | PX4 | O7-C23 | 2.79 | 1.26 | 1.34 | 2 | 2 |
| 3 | C | 339 | PX4 | C24-C23 | 2.79 | 1.58 | 1.50 | 12 | 3 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | A | 620 | PX4 | C6-C7 | 2.79 | 1.59 | 1.50 | 1 | 5 |
| 3 | A | 627 | PX4 | C3-N1 | 2.79 | 1.58 | 1.50 | 9 | 2 |
| 3 | B | 393 | PX4 | C5-N1 | 2.79 | 1.41 | 1.50 | 2 | 3 |
| 3 | C | 346 | PX4 | C4-N1 | 2.79 | 1.58 | 1.50 | 8 | 2 |
| 3 | B | 371 | PX4 | C10-C9 | 2.79 | 1.58 | 1.50 | 10 | 2 |
| 3 | C | 320 | PX4 | O7-C7 | 2.79 | 1.53 | 1.46 | 10 | 3 |
| 3 | A | 606 | PX4 | C15-C14 | 2.79 | 1.65 | 1.51 | 2 | 1 |
| 3 | B | 373 | PX4 | C5-N1 | 2.79 | 1.58 | 1.50 | 9 | 2 |
| 3 | B | 387 | PX4 | C11-C10 | 2.79 | 1.62 | 1.52 | 10 | 2 |
| 3 | B | 385 | PX4 | C10-C9 | 2.79 | 1.58 | 1.50 | 3 | 4 |
| 3 | B | 400 | PX4 | C11-C10 | 2.79 | 1.62 | 1.52 | 11 | 2 |
| 3 | C | 361 | PX4 | P1-O1 | 2.79 | 1.42 | 1.55 | 2 | 3 |
| 3 | C | 308 | PX4 | C25-C24 | 2.79 | 1.62 | 1.52 | 3 | 2 |
| 3 | C | 313 | PX4 | C20-C19 | 2.79 | 1.65 | 1.51 | 7 | 1 |
| 3 | C | 364 | PX4 | C10-C9 | 2.79 | 1.58 | 1.50 | 3 | 1 |
| 3 | A | 641 | PX4 | C6-C7 | 2.79 | 1.59 | 1.50 | 10 | 4 |
| 3 | A | 646 | PX4 | C6-C7 | 2.79 | 1.59 | 1.50 | 8 | 3 |
| 3 | A | 652 | PX4 | C25-C24 | 2.78 | 1.62 | 1.52 | 3 | 2 |
| 3 | B | 302 | PX4 | C24-C23 | 2.78 | 1.58 | 1.50 | 10 | 2 |
| 3 | B | 324 | PX4 | O5-C8 | 2.78 | 1.38 | 1.45 | 3 | 2 |
| 3 | C | 312 | PX4 | O7-C23 | 2.79 | 1.26 | 1.34 | 13 | 2 |
| 3 | B | 343 | PX4 | C26-C25 | 2.78 | 1.65 | 1.51 | 10 | 1 |
| 3 | B | 386 | PX4 | C3-N1 | 2.78 | 1.58 | 1.50 | 5 | 1 |
| 3 | C | 311 | PX4 | C10-C9 | 2.78 | 1.58 | 1.50 | 12 | 1 |
| 3 | C | 322 | PX4 | P1-O1 | 2.78 | 1.42 | 1.55 | 5 | 4 |
| 3 | B | 334 | PX4 | C6-C7 | 2.78 | 1.59 | 1.50 | 6 | 5 |
| 3 | B | 360 | PX4 | O7-C23 | 2.78 | 1.26 | 1.34 | 12 | 2 |
| 3 | A | 606 | PX4 | C4-N1 | 2.78 | 1.41 | 1.50 | 11 | 2 |
| 3 | A | 608 | PX4 | C4-N1 | 2.78 | 1.58 | 1.50 | 6 | 2 |
| 3 | B | 352 | PX4 | C2-N1 | 2.78 | 1.59 | 1.51 | 5 | 1 |
| 3 | B | 379 | PX4 | C10-C9 | 2.78 | 1.58 | 1.50 | 14 | 1 |
| 3 | C | 330 | PX4 | O5-C9 | 2.78 | 1.25 | 1.33 | 2 | 2 |
| 3 | A | 632 | PX4 | C24-C23 | 2.78 | 1.58 | 1.50 | 6 | 5 |
| 3 | A | 628 | PX4 | C10-C9 | 2.77 | 1.58 | 1.50 | 6 | 3 |
| 3 | A | 637 | PX4 | C25-C24 | 2.77 | 1.62 | 1.52 | 11 | 3 |
| 3 | A | 638 | PX4 | P1-O1 | 2.77 | 1.42 | 1.55 | 10 | 3 |
| 3 | B | 397 | PX4 | C3-N1 | 2.77 | 1.58 | 1.50 | 8 | 3 |
| 3 | B | 398 | PX4 | P1-O4 | 2.77 | 1.48 | 1.59 | 13 | 1 |
| 3 | A | 622 | PX4 | C2-C1 | 2.77 | 1.59 | 1.51 | 15 | 5 |
| 3 | A | 634 | PX4 | O3-C1 | 2.77 | 1.33 | 1.44 | 9 | 1 |
| 3 | A | 630 | PX4 | C34-C33 | 2.77 | 1.65 | 1.51 | 6 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | C | 333 | PX4 | O5-C9 | 2.77 | 1.25 | 1.33 | 15 | 1 |
| 3 | C | 330 | PX4 | C4-N1 | 2.77 | 1.58 | 1.50 | 11 | 1 |
| 3 | A | 602 | PX4 | C3-N1 | 2.77 | 1.58 | 1.50 | 3 | 1 |
| 3 | B | 341 | PX4 | C2-N1 | 2.77 | 1.59 | 1.51 | 11 | 3 |
| 3 | C | 327 | PX4 | C10-C9 | 2.77 | 1.58 | 1.50 | 13 | 3 |
| 3 | A | 641 | PX4 | C10-C9 | 2.77 | 1.58 | 1.50 | 7 | 4 |
| 3 | C | 332 | PX4 | C6-C7 | 2.77 | 1.59 | 1.50 | 2 | 8 |
| 3 | B | 306 | PX4 | C11-C10 | 2.77 | 1.62 | 1.52 | 14 | 1 |
| 3 | B | 350 | PX4 | C24-C23 | 2.77 | 1.58 | 1.50 | 7 | 3 |
| 3 | C | 355 | PX4 | C25-C24 | 2.77 | 1.62 | 1.52 | 8 | 3 |
| 3 | A | 641 | PX4 | C2-C1 | 2.76 | 1.59 | 1.51 | 6 | 4 |
| 3 | B | 338 | PX4 | C2-C1 | 2.76 | 1.59 | 1.51 | 12 | 3 |
| 3 | C | 348 | PX4 | C34-C33 | 2.77 | 1.65 | 1.51 | 11 | 1 |
| 3 | C | 357 | PX4 | C24-C23 | 2.77 | 1.58 | 1.50 | 15 | 3 |
| 3 | B | 340 | PX4 | C25-C24 | 2.76 | 1.62 | 1.52 | 11 | 5 |
| 3 | B | 348 | PX4 | C28-C27 | 2.76 | 1.65 | 1.51 | 14 | 1 |
| 3 | C | 318 | PX4 | C16-C15 | 2.76 | 1.65 | 1.51 | 14 | 1 |
| 3 | A | 614 | PX4 | C25-C24 | 2.76 | 1.62 | 1.52 | 11 | 1 |
| 3 | B | 305 | PX4 | C2-N1 | 2.76 | 1.59 | 1.51 | 2 | 4 |
| 3 | C | 342 | PX4 | P1-O1 | 2.76 | 1.42 | 1.55 | 8 | 2 |
| 3 | A | 627 | PX4 | O3-C1 | 2.76 | 1.33 | 1.44 | 5 | 1 |
| 3 | A | 628 | PX4 | O5-C8 | 2.76 | 1.39 | 1.45 | 12 | 3 |
| 3 | A | 642 | PX4 | O5-C9 | 2.76 | 1.25 | 1.33 | 6 | 6 |
| 3 | A | 652 | PX4 | O5-C8 | 2.76 | 1.51 | 1.45 | 12 | 4 |
| 3 | C | 306 | PX4 | C2-C1 | 2.76 | 1.59 | 1.51 | 3 | 4 |
| 3 | B | 330 | PX4 | O7-C7 | 2.76 | 1.40 | 1.46 | 15 | 3 |
| 3 | B | 359 | PX4 | P1-O3 | 2.76 | 1.70 | 1.59 | 5 | 2 |
| 3 | B | 355 | PX4 | O7-C7 | 2.76 | 1.40 | 1.46 | 7 | 3 |
| 3 | B | 395 | PX4 | O7-C7 | 2.76 | 1.40 | 1.46 | 9 | 2 |
| 3 | C | 349 | PX4 | O5-C9 | 2.76 | 1.25 | 1.33 | 2 | 3 |
| 3 | C | 316 | PX4 | C27-C26 | 2.76 | 1.65 | 1.51 | 11 | 1 |
| 3 | A | 630 | PX4 | C24-C23 | 2.75 | 1.58 | 1.50 | 1 | 3 |
| 3 | B | 352 | PX4 | P1-O4 | 2.76 | 1.48 | 1.59 | 8 | 1 |
| 3 | C | 322 | PX4 | C24-C23 | 2.76 | 1.58 | 1.50 | 7 | 5 |
| 3 | C | 339 | PX4 | C2-N1 | 2.76 | 1.59 | 1.51 | 3 | 3 |
| 3 | B | 369 | PX4 | P1-O4 | 2.75 | 1.48 | 1.59 | 1 | 1 |
| 3 | B | 308 | PX4 | O5-C8 | 2.75 | 1.51 | 1.45 | 11 | 2 |
| 3 | B | 367 | PX4 | C4-N1 | 2.75 | 1.58 | 1.50 | 12 | 3 |
| 3 | B | 370 | PX4 | C2-N1 | 2.75 | 1.59 | 1.51 | 5 | 3 |
| 3 | C | 301 | PX4 | C4-N1 | 2.75 | 1.58 | 1.50 | 9 | 2 |
| 3 | A | 613 | PX4 | C2-N1 | 2.75 | 1.59 | 1.51 | 11 | 4 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | A | 616 | PX4 | C3-N1 | 2.75 | 1.58 | 1.50 | 13 | 1 |
| 3 | A | 638 | PX4 | C25-C24 | 2.75 | 1.62 | 1.52 | 12 | 2 |
| 3 | B | 338 | PX4 | O7-C23 | 2.75 | 1.26 | 1.34 | 3 | 1 |
| 3 | B | 364 | PX4 | C2-N1 | 2.75 | 1.59 | 1.51 | 9 | 1 |
| 3 | C | 304 | PX4 | C4-N1 | 2.75 | 1.42 | 1.50 | 3 | 4 |
| 3 | B | 393 | PX4 | O5-C8 | 2.75 | 1.39 | 1.45 | 14 | 3 |
| 3 | A | 654 | PX4 | O7-C7 | 2.75 | 1.40 | 1.46 | 8 | 4 |
| 3 | B | 306 | PX4 | O5-C9 | 2.75 | 1.41 | 1.33 | 7 | 3 |
| 3 | C | 332 | PX4 | C25-C24 | 2.75 | 1.62 | 1.52 | 7 | 3 |
| 3 | C | 363 | PX4 | P1-O1 | 2.75 | 1.42 | 1.55 | 15 | 2 |
| 3 | A | 628 | PX4 | P1-O1 | 2.75 | 1.42 | 1.55 | 14 | 4 |
| 3 | A | 643 | PX4 | C25-C24 | 2.75 | 1.62 | 1.52 | 7 | 3 |
| 3 | B | 316 | PX4 | O5-C9 | 2.75 | 1.25 | 1.33 | 14 | 2 |
| 3 | B | 320 | PX4 | C10-C9 | 2.75 | 1.42 | 1.50 | 7 | 1 |
| 3 | C | 361 | PX4 | C3-N1 | 2.75 | 1.42 | 1.50 | 1 | 2 |
| 3 | C | 348 | PX4 | O5-C8 | 2.74 | 1.51 | 1.45 | 15 | 2 |
| 3 | C | 355 | PX4 | C2-C1 | 2.74 | 1.59 | 1.51 | 1 | 5 |
| 3 | C | 362 | PX4 | C24-C23 | 2.74 | 1.58 | 1.50 | 5 | 4 |
| 3 | A | 608 | PX4 | O7-C7 | 2.74 | 1.40 | 1.46 | 6 | 3 |
| 3 | A | 643 | PX4 | O7-C23 | 2.74 | 1.26 | 1.34 | 8 | 1 |
| 3 | B | 344 | PX4 | O5-C9 | 2.74 | 1.25 | 1.33 | 5 | 1 |
| 3 | B | 305 | PX4 | O7-C7 | 2.74 | 1.40 | 1.46 | 15 | 3 |
| 3 | B | 346 | PX4 | C3-N1 | 2.74 | 1.42 | 1.50 | 1 | 2 |
| 3 | A | 609 | PX4 | C24-C23 | 2.74 | 1.58 | 1.50 | 15 | 6 |
| 3 | B | 323 | PX4 | O5-C8 | 2.74 | 1.39 | 1.45 | 8 | 2 |
| 3 | C | 312 | PX4 | P1-O1 | 2.74 | 1.42 | 1.55 | 5 | 4 |
| 3 | C | 342 | PX4 | O7-C23 | 2.74 | 1.26 | 1.34 | 11 | 2 |
| 3 | C | 347 | PX4 | O7-C7 | 2.74 | 1.40 | 1.46 | 12 | 3 |
| 3 | B | 310 | PX4 | O5-C9 | 2.73 | 1.41 | 1.33 | 14 | 1 |
| 3 | B | 334 | PX4 | P1-O1 | 2.73 | 1.42 | 1.55 | 5 | 4 |
| 3 | B | 367 | PX4 | P1-O2 | 2.73 | 1.41 | 1.50 | 1 | 1 |
| 3 | C | 306 | PX4 | O7-C23 | 2.73 | 1.26 | 1.34 | 4 | 2 |
| 3 | C | 329 | PX4 | C24-C23 | 2.74 | 1.58 | 1.50 | 2 | 2 |
| 3 | C | 353 | PX4 | C11-C10 | 2.73 | 1.62 | 1.52 | 11 | 4 |
| 3 | A | 619 | PX4 | O5-C8 | 2.73 | 1.51 | 1.45 | 15 | 3 |
| 3 | B | 319 | PX4 | O5-C9 | 2.73 | 1.25 | 1.33 | 15 | 2 |
| 3 | B | 328 | PX4 | C11-C10 | 2.73 | 1.62 | 1.52 | 8 | 2 |
| 3 | A | 624 | PX4 | C5-N1 | 2.73 | 1.57 | 1.50 | 2 | 1 |
| 3 | B | 318 | PX4 | C25-C24 | 2.73 | 1.62 | 1.52 | 1 | 2 |
| 3 | B | 365 | PX4 | O7-C7 | 2.73 | 1.40 | 1.46 | 15 | 2 |
| 3 | A | 642 | PX4 | C11-C10 | 2.73 | 1.62 | 1.52 | 1 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 318 | PX4 | C4-N1 | 2.73 | 1.42 | 1.50 | 9 | 1 |
| 3 | B | 381 | PX4 | C2-C1 | 2.73 | 1.59 | 1.51 | 11 | 7 |
| 3 | C | 361 | PX4 | C25-C24 | 2.73 | 1.62 | 1.52 | 13 | 2 |
| 3 | C | 348 | PX4 | C2-C1 | 2.73 | 1.59 | 1.51 | 14 | 8 |
| 3 | C | 362 | PX4 | C2-C1 | 2.73 | 1.59 | 1.51 | 7 | 2 |
| 3 | A | 613 | PX4 | C25-C24 | 2.73 | 1.62 | 1.52 | 8 | 2 |
| 3 | B | 329 | PX4 | O7-C23 | 2.73 | 1.26 | 1.34 | 9 | 2 |
| 3 | B | 362 | PX4 | C24-C23 | 2.73 | 1.58 | 1.50 | 3 | 3 |
| 3 | B | 364 | PX4 | C3-N1 | 2.73 | 1.57 | 1.50 | 6 | 1 |
| 3 | C | 323 | PX4 | P1-O1 | 2.73 | 1.42 | 1.55 | 4 | 5 |
| 3 | A | 626 | PX4 | C24-C23 | 2.73 | 1.58 | 1.50 | 15 | 1 |
| 3 | B | 381 | PX4 | C24-C23 | 2.73 | 1.58 | 1.50 | 2 | 3 |
| 3 | B | 385 | PX4 | C11-C10 | 2.73 | 1.62 | 1.52 | 8 | 2 |
| 3 | B | 340 | PX4 | C34-C33 | 2.72 | 1.65 | 1.51 | 10 | 1 |
| 3 | C | 306 | PX4 | C3-N1 | 2.72 | 1.57 | 1.50 | 10 | 3 |
| 3 | C | 363 | PX4 | C15-C14 | 2.72 | 1.65 | 1.51 | 7 | 1 |
| 3 | B | 356 | PX4 | C11-C10 | 2.72 | 1.62 | 1.52 | 5 | 1 |
| 3 | A | 633 | PX4 | C10-C9 | 2.72 | 1.58 | 1.50 | 9 | 2 |
| 3 | A | 635 | PX4 | C11-C10 | 2.72 | 1.62 | 1.52 | 9 | 3 |
| 3 | A | 644 | PX4 | C2-N1 | 2.72 | 1.59 | 1.51 | 15 | 2 |
| 3 | B | 350 | PX4 | O5-C8 | 2.72 | 1.39 | 1.45 | 9 | 2 |
| 3 | A | 606 | PX4 | O5-C9 | 2.72 | 1.41 | 1.33 | 15 | 3 |
| 3 | B | 377 | PX4 | C34-C33 | 2.72 | 1.65 | 1.51 | 12 | 1 |
| 3 | A | 654 | PX4 | O5-C8 | 2.72 | 1.51 | 1.45 | 8 | 1 |
| 3 | C | 325 | PX4 | C6-C7 | 2.72 | 1.59 | 1.50 | 8 | 6 |
| 3 | C | 351 | PX4 | C10-C9 | 2.72 | 1.58 | 1.50 | 10 | 5 |
| 3 | B | 349 | PX4 | C8-C7 | 2.72 | 1.59 | 1.50 | 14 | 7 |
| 3 | B | 389 | PX4 | C33-C32 | 2.72 | 1.65 | 1.51 | 3 | 1 |
| 3 | A | 608 | PX4 | O5-C8 | 2.72 | 1.51 | 1.45 | 6 | 3 |
| 3 | B | 344 | PX4 | C10-C9 | 2.72 | 1.58 | 1.50 | 10 | 3 |
| 3 | B | 367 | PX4 | O5-C8 | 2.71 | 1.51 | 1.45 | 11 | 4 |
| 3 | B | 310 | PX4 | C3-N1 | 2.71 | 1.57 | 1.50 | 1 | 2 |
| 3 | B | 349 | PX4 | C2-C1 | 2.71 | 1.59 | 1.51 | 12 | 4 |
| 3 | B | 397 | PX4 | C4-N1 | 2.71 | 1.57 | 1.50 | 3 | 1 |
| 3 | C | 310 | PX4 | C4-N1 | 2.71 | 1.42 | 1.50 | 3 | 1 |
| 3 | A | 632 | PX4 | O5-C9 | 2.71 | 1.25 | 1.33 | 3 | 2 |
| 3 | B | 308 | PX4 | O7-C7 | 2.71 | 1.40 | 1.46 | 6 | 7 |
| 3 | B | 349 | PX4 | P1-O1 | 2.71 | 1.42 | 1.55 | 7 | 3 |
| 3 | C | 362 | PX4 | P1-O1 | 2.71 | 1.42 | 1.55 | 6 | 3 |
| 3 | A | 612 | PX4 | C24-C23 | 2.71 | 1.42 | 1.50 | 3 | 1 |
| 3 | B | 307 | PX4 | P1-O1 | 2.71 | 1.42 | 1.55 | 2 | 7 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 382 | PX4 | O7-C7 | 2.71 | 1.40 | 1.46 | 2 | 3 |
| 3 | A | 645 | PX4 | C3-N1 | 2.71 | 1.42 | 1.50 | 9 | 1 |
| 3 | A | 623 | PX4 | P1-O3 | 2.71 | 1.48 | 1.59 | 7 | 1 |
| 3 | A | 650 | PX4 | C10-C9 | 2.71 | 1.58 | 1.50 | 4 | 1 |
| 3 | B | 323 | PX4 | O7-C23 | 2.71 | 1.41 | 1.34 | 8 | 1 |
| 3 | B | 359 | PX4 | O7-C23 | 2.71 | 1.26 | 1.34 | 7 | 2 |
| 3 | B | 383 | PX4 | P1-O1 | 2.71 | 1.42 | 1.55 | 1 | 2 |
| 3 | B | 392 | PX4 | P1-O4 | 2.71 | 1.70 | 1.59 | 9 | 1 |
| 3 | B | 357 | PX4 | C25-C24 | 2.71 | 1.62 | 1.52 | 13 | 2 |
| 3 | C | 305 | PX4 | C2-N1 | 2.71 | 1.43 | 1.51 | 11 | 1 |
| 3 | C | 321 | PX4 | C8-C7 | 2.71 | 1.59 | 1.50 | 12 | 5 |
| 3 | C | 322 | PX4 | C8-C7 | 2.71 | 1.59 | 1.50 | 12 | 3 |
| 3 | C | 352 | PX4 | P1-O1 | 2.71 | 1.42 | 1.55 | 15 | 4 |
| 3 | B | 336 | PX4 | O7-C23 | 2.71 | 1.26 | 1.34 | 13 | 3 |
| 3 | B | 354 | PX4 | C2-C1 | 2.71 | 1.59 | 1.51 | 1 | 3 |
| 3 | B | 399 | PX4 | C10-C9 | 2.71 | 1.42 | 1.50 | 14 | 4 |
| 3 | B | 363 | PX4 | C4-N1 | 2.70 | 1.42 | 1.50 | 7 | 1 |
| 3 | B | 365 | PX4 | C10-C9 | 2.70 | 1.58 | 1.50 | 15 | 4 |
| 3 | B | 399 | PX4 | C2-C1 | 2.70 | 1.59 | 1.51 | 7 | 4 |
| 3 | C | 322 | PX4 | C4-N1 | 2.70 | 1.57 | 1.50 | 10 | 1 |
| 3 | A | 617 | PX4 | C25-C24 | 2.70 | 1.62 | 1.52 | 4 | 1 |
| 3 | B | 315 | PX4 | C2-C1 | 2.70 | 1.59 | 1.51 | 3 | 3 |
| 3 | C | 324 | PX4 | C24-C23 | 2.70 | 1.58 | 1.50 | 12 | 4 |
| 3 | B | 332 | PX4 | O5-C8 | 2.70 | 1.51 | 1.45 | 11 | 2 |
| 3 | B | 349 | PX4 | P1-O3 | 2.70 | 1.48 | 1.59 | 13 | 1 |
| 3 | B | 377 | PX4 | C2-N1 | 2.70 | 1.59 | 1.51 | 2 | 2 |
| 3 | B | 379 | PX4 | C28-C27 | 2.70 | 1.65 | 1.51 | 12 | 2 |
| 3 | C | 325 | PX4 | C11-C10 | 2.70 | 1.62 | 1.52 | 7 | 4 |
| 3 | A | 604 | PX4 | C3-N1 | 2.70 | 1.42 | 1.50 | 6 | 1 |
| 3 | A | 644 | PX4 | C24-C23 | 2.70 | 1.58 | 1.50 | 2 | 3 |
| 3 | B | 341 | PX4 | C3-N1 | 2.70 | 1.42 | 1.50 | 15 | 1 |
| 3 | C | 324 | PX4 | C2-C1 | 2.70 | 1.59 | 1.51 | 10 | 3 |
| 3 | C | 325 | PX4 | O5-C9 | 2.70 | 1.41 | 1.33 | 14 | 2 |
| 3 | A | 631 | PX4 | C4-N1 | 2.70 | 1.57 | 1.50 | 2 | 4 |
| 3 | A | 631 | PX4 | C6-C7 | 2.70 | 1.59 | 1.50 | 7 | 3 |
| 3 | B | 317 | PX4 | C8-C7 | 2.70 | 1.59 | 1.50 | 2 | 7 |
| 3 | B | 322 | PX4 | C10-C9 | 2.70 | 1.58 | 1.50 | 11 | 1 |
| 3 | B | 372 | PX4 | O7-C7 | 2.70 | 1.40 | 1.46 | 7 | 3 |
| 3 | C | 323 | PX4 | C3-N1 | 2.70 | 1.42 | 1.50 | 6 | 2 |
| 3 | C | 346 | PX4 | P1-O3 | 2.70 | 1.48 | 1.59 | 5 | 2 |
| 3 | A | 624 | PX4 | O5-C9 | 2.70 | 1.25 | 1.33 | 8 | 2 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | C | 349 | PX4 | C2-N1 | 2.69 | 1.59 | 1.51 | 13 | 3 |
| 3 | C | 362 | PX4 | C25-C24 | 2.70 | 1.62 | 1.52 | 15 | 3 |
| 3 | B | 339 | PX4 | O7-C7 | 2.69 | 1.40 | 1.46 | 14 | 3 |
| 3 | B | 348 | PX4 | C24-C23 | 2.69 | 1.58 | 1.50 | 13 | 2 |
| 3 | A | 609 | PX4 | C18-C17 | 2.69 | 1.65 | 1.51 | 12 | 2 |
| 3 | A | 649 | PX4 | C5-N1 | 2.69 | 1.57 | 1.50 | 6 | 1 |
| 3 | B | 322 | PX4 | C25-C24 | 2.69 | 1.62 | 1.52 | 7 | 3 |
| 3 | C | 347 | PX4 | C3-N1 | 2.69 | 1.57 | 1.50 | 15 | 2 |
| 3 | A | 645 | PX4 | O5-C8 | 2.69 | 1.39 | 1.45 | 8 | 1 |
| 3 | A | 651 | PX4 | O7-C23 | 2.69 | 1.41 | 1.34 | 7 | 2 |
| 3 | B | 324 | PX4 | P1-O3 | 2.69 | 1.48 | 1.59 | 5 | 1 |
| 3 | B | 384 | PX4 | C4-N1 | 2.69 | 1.57 | 1.50 | 13 | 2 |
| 3 | C | 327 | PX4 | C8-C7 | 2.69 | 1.59 | 1.50 | 1 | 4 |
| 3 | A | 622 | PX4 | C3-N1 | 2.69 | 1.57 | 1.50 | 14 | 2 |
| 3 | B | 369 | PX4 | C24-C23 | 2.69 | 1.58 | 1.50 | 8 | 1 |
| 3 | B | 342 | PX4 | C3-N1 | 2.69 | 1.57 | 1.50 | 10 | 2 |
| 3 | B | 349 | PX4 | C3-N1 | 2.69 | 1.42 | 1.50 | 7 | 1 |
| 3 | C | 313 | PX4 | O5-C8 | 2.69 | 1.39 | 1.45 | 5 | 3 |
| 3 | A | 610 | PX4 | C4-N1 | 2.68 | 1.57 | 1.50 | 5 | 1 |
| 3 | B | 372 | PX4 | C2-C1 | 2.68 | 1.59 | 1.51 | 10 | 6 |
| 3 | B | 360 | PX4 | C5-N1 | 2.68 | 1.57 | 1.50 | 1 | 1 |
| 3 | B | 366 | PX4 | C25-C24 | 2.68 | 1.62 | 1.52 | 13 | 2 |
| 3 | C | 359 | PX4 | C3-N1 | 2.68 | 1.57 | 1.50 | 8 | 3 |
| 3 | A | 654 | PX4 | P1-O1 | 2.68 | 1.42 | 1.55 | 13 | 3 |
| 3 | C | 325 | PX4 | O5-C8 | 2.68 | 1.51 | 1.45 | 12 | 1 |
| 3 | B | 349 | PX4 | C34-C33 | 2.68 | 1.65 | 1.51 | 6 | 2 |
| 3 | C | 321 | PX4 | P1-O1 | 2.68 | 1.42 | 1.55 | 7 | 4 |
| 3 | C | 355 | PX4 | C31-C30 | 2.68 | 1.65 | 1.51 | 10 | 1 |
| 3 | A | 604 | PX4 | C11-C10 | 2.68 | 1.62 | 1.52 | 13 | 3 |
| 3 | A | 638 | PX4 | O7-C7 | 2.68 | 1.40 | 1.46 | 14 | 2 |
| 3 | B | 322 | PX4 | O5-C9 | 2.68 | 1.25 | 1.33 | 7 | 3 |
| 3 | A | 619 | PX4 | C2-C1 | 2.68 | 1.59 | 1.51 | 9 | 2 |
| 3 | A | 651 | PX4 | O7-C7 | 2.68 | 1.40 | 1.46 | 5 | 3 |
| 3 | B | 368 | PX4 | O7-C23 | 2.68 | 1.26 | 1.34 | 8 | 3 |
| 3 | C | 314 | PX4 | C4-N1 | 2.68 | 1.42 | 1.50 | 3 | 1 |
| 3 | B | 361 | PX4 | C25-C24 | 2.68 | 1.62 | 1.52 | 4 | 1 |
| 3 | C | 315 | PX4 | C25-C24 | 2.68 | 1.62 | 1.52 | 12 | 3 |
| 3 | B | 339 | PX4 | C3-N1 | 2.67 | 1.57 | 1.50 | 6 | 1 |
| 3 | C | 343 | PX4 | C2-N1 | 2.67 | 1.59 | 1.51 | 1 | 2 |
| 3 | C | 354 | PX4 | C11-C10 | 2.67 | 1.62 | 1.52 | 1 | 1 |
| 3 | B | 372 | PX4 | P1-O1 | 2.67 | 1.43 | 1.55 | 12 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | C | 307 | PX4 | P1-O1 | 2.67 | 1.43 | 1.55 | 1 | 1 |
| 3 | C | 335 | PX4 | C3-N1 | 2.67 | 1.57 | 1.50 | 4 | 2 |
| 3 | C | 345 | PX4 | O7-C23 | 2.67 | 1.26 | 1.34 | 14 | 3 |
| 3 | A | 601 | PX4 | P1-O2 | 2.67 | 1.41 | 1.50 | 15 | 2 |
| 3 | A | 606 | PX4 | C24-C23 | 2.67 | 1.58 | 1.50 | 13 | 1 |
| 3 | A | 647 | PX4 | O7-C7 | 2.67 | 1.40 | 1.46 | 11 | 3 |
| 3 | A | 650 | PX4 | O5-C8 | 2.67 | 1.39 | 1.45 | 12 | 2 |
| 3 | B | 303 | PX4 | C8-C7 | 2.67 | 1.59 | 1.50 | 8 | 4 |
| 3 | A | 625 | PX4 | P1-O2 | 2.67 | 1.41 | 1.50 | 7 | 2 |
| 3 | B | 334 | PX4 | C24-C23 | 2.67 | 1.58 | 1.50 | 11 | 1 |
| 3 | B | 339 | PX4 | C25-C24 | 2.67 | 1.62 | 1.52 | 3 | 1 |
| 3 | B | 378 | PX4 | C11-C10 | 2.67 | 1.62 | 1.52 | 5 | 1 |
| 3 | C | 317 | PX4 | O7-C7 | 2.67 | 1.40 | 1.46 | 15 | 2 |
| 3 | A | 603 | PX4 | P1-O2 | 2.67 | 1.41 | 1.50 | 11 | 2 |
| 3 | B | 302 | PX4 | P1-O4 | 2.67 | 1.48 | 1.59 | 3 | 2 |
| 3 | B | 312 | PX4 | C24-C23 | 2.67 | 1.58 | 1.50 | 8 | 4 |
| 3 | C | 311 | PX4 | C6-C7 | 2.67 | 1.59 | 1.50 | 11 | 4 |
| 3 | C | 330 | PX4 | C2-N1 | 2.67 | 1.43 | 1.51 | 5 | 3 |
| 3 | C | 360 | PX4 | C3-N1 | 2.67 | 1.42 | 1.50 | 8 | 1 |
| 3 | A | 618 | PX4 | C11-C10 | 2.66 | 1.62 | 1.52 | 8 | 1 |
| 3 | B | 320 | PX4 | C4-N1 | 2.66 | 1.57 | 1.50 | 8 | 2 |
| 3 | B | 320 | PX4 | C11-C10 | 2.66 | 1.61 | 1.52 | 5 | 1 |
| 3 | B | 339 | PX4 | O5-C9 | 2.66 | 1.25 | 1.33 | 9 | 1 |
| 3 | B | 392 | PX4 | C25-C24 | 2.67 | 1.62 | 1.52 | 9 | 1 |
| 3 | B | 355 | PX4 | C11-C10 | 2.66 | 1.61 | 1.52 | 6 | 2 |
| 3 | B | 367 | PX4 | C2-N1 | 2.66 | 1.59 | 1.51 | 3 | 2 |
| 3 | C | 310 | PX4 | C3-N1 | 2.66 | 1.57 | 1.50 | 5 | 2 |
| 3 | C | 339 | PX4 | O7-C7 | 2.66 | 1.40 | 1.46 | 8 | 5 |
| 3 | A | 633 | PX4 | O5-C8 | 2.66 | 1.39 | 1.45 | 10 | 1 |
| 3 | A | 609 | PX4 | C11-C10 | 2.66 | 1.61 | 1.52 | 13 | 3 |
| 3 | A | 644 | PX4 | C8-C7 | 2.66 | 1.59 | 1.50 | 3 | 2 |
| 3 | A | 647 | PX4 | C2-N1 | 2.66 | 1.59 | 1.51 | 10 | 3 |
| 3 | A | 647 | PX4 | C6-C7 | 2.66 | 1.59 | 1.50 | 12 | 4 |
| 3 | B | 317 | PX4 | O5-C8 | 2.66 | 1.39 | 1.45 | 7 | 2 |
| 3 | B | 377 | PX4 | C15-C14 | 2.66 | 1.65 | 1.51 | 12 | 1 |
| 3 | C | 318 | PX4 | P1-O1 | 2.66 | 1.43 | 1.55 | 1 | 3 |
| 3 | B | 344 | PX4 | P1-O1 | 2.66 | 1.43 | 1.55 | 5 | 5 |
| 3 | A | 633 | PX4 | C11-C10 | 2.66 | 1.61 | 1.52 | 3 | 3 |
| 3 | C | 331 | PX4 | C5-N1 | 2.66 | 1.57 | 1.50 | 12 | 1 |
| 3 | C | 358 | PX4 | O5-C8 | 2.66 | 1.51 | 1.45 | 8 | 1 |
| 3 | C | 359 | PX4 | P1-O4 | 2.66 | 1.49 | 1.59 | 7 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 367 | PX4 | C3-N1 | 2.66 | 1.42 | 1.50 | 12 | 2 |
| 3 | C | 307 | PX4 | C25-C24 | 2.66 | 1.61 | 1.52 | 11 | 1 |
| 3 | A | 604 | PX4 | C24-C23 | 2.66 | 1.58 | 1.50 | 8 | 3 |
| 3 | B | 390 | PX4 | O7-C7 | 2.66 | 1.40 | 1.46 | 4 | 2 |
| 3 | B | 392 | PX4 | O5-C9 | 2.66 | 1.25 | 1.33 | 5 | 1 |
| 3 | C | 321 | PX4 | C4-N1 | 2.66 | 1.57 | 1.50 | 6 | 2 |
| 3 | A | 639 | PX4 | P1-O1 | 2.66 | 1.43 | 1.55 | 6 | 7 |
| 3 | B | 309 | PX4 | C11-C10 | 2.66 | 1.61 | 1.52 | 14 | 2 |
| 3 | B | 337 | PX4 | O5-C9 | 2.66 | 1.41 | 1.33 | 8 | 2 |
| 3 | C | 301 | PX4 | C24-C23 | 2.66 | 1.58 | 1.50 | 12 | 3 |
| 3 | C | 332 | PX4 | O4-C6 | 2.66 | 1.34 | 1.44 | 7 | 1 |
| 3 | C | 354 | PX4 | C20-C19 | 2.65 | 1.65 | 1.51 | 8 | 1 |
| 3 | C | 361 | PX4 | C4-N1 | 2.65 | 1.42 | 1.50 | 13 | 2 |
| 3 | A | 630 | PX4 | O7-C23 | 2.65 | 1.26 | 1.34 | 4 | 3 |
| 3 | B | 379 | PX4 | C25-C24 | 2.65 | 1.61 | 1.52 | 7 | 2 |
| 3 | C | 304 | PX4 | C10-C9 | 2.65 | 1.58 | 1.50 | 6 | 4 |
| 3 | C | 359 | PX4 | C4-N1 | 2.65 | 1.57 | 1.50 | 14 | 1 |
| 3 | B | 353 | PX4 | C31-C30 | 2.65 | 1.65 | 1.51 | 12 | 1 |
| 3 | C | 332 | PX4 | C8-C7 | 2.65 | 1.59 | 1.50 | 15 | 5 |
| 3 | B | 336 | PX4 | O5-C9 | 2.65 | 1.41 | 1.33 | 13 | 1 |
| 3 | B | 348 | PX4 | C6-C7 | 2.65 | 1.59 | 1.50 | 11 | 6 |
| 3 | C | 342 | PX4 | C25-C24 | 2.65 | 1.61 | 1.52 | 7 | 3 |
| 3 | A | 640 | PX4 | C25-C24 | 2.65 | 1.61 | 1.52 | 5 | 3 |
| 3 | B | 334 | PX4 | O7-C7 | 2.65 | 1.52 | 1.46 | 1 | 1 |
| 3 | B | 388 | PX4 | C3-N1 | 2.65 | 1.42 | 1.50 | 1 | 2 |
| 3 | A | 632 | PX4 | O7-C7 | 2.65 | 1.40 | 1.46 | 4 | 4 |
| 3 | B | 347 | PX4 | C25-C24 | 2.65 | 1.61 | 1.52 | 1 | 2 |
| 3 | B | 317 | PX4 | P1-O1 | 2.65 | 1.43 | 1.55 | 15 | 5 |
| 3 | C | 351 | PX4 | O7-C23 | 2.65 | 1.26 | 1.34 | 10 | 1 |
| 3 | C | 353 | PX4 | C8-C7 | 2.65 | 1.59 | 1.50 | 11 | 4 |
| 3 | A | 613 | PX4 | C24-C23 | 2.65 | 1.58 | 1.50 | 1 | 4 |
| 3 | B | 329 | PX4 | C5-N1 | 2.65 | 1.42 | 1.50 | 7 | 1 |
| 3 | B | 321 | PX4 | C25-C24 | 2.64 | 1.61 | 1.52 | 1 | 2 |
| 3 | B | 400 | PX4 | C25-C24 | 2.64 | 1.61 | 1.52 | 15 | 2 |
| 3 | C | 338 | PX4 | C11-C10 | 2.64 | 1.61 | 1.52 | 2 | 3 |
| 3 | A | 615 | PX4 | O7-C7 | 2.64 | 1.40 | 1.46 | 15 | 2 |
| 3 | C | 309 | PX4 | O5-C8 | 2.64 | 1.51 | 1.45 | 3 | 2 |
| 3 | C | 339 | PX4 | O5-C8 | 2.64 | 1.51 | 1.45 | 15 | 3 |
| 3 | C | 360 | PX4 | O5-C8 | 2.64 | 1.51 | 1.45 | 14 | 2 |
| 3 | A | 632 | PX4 | C4-N1 | 2.64 | 1.57 | 1.50 | 7 | 2 |
| 3 | B | 308 | PX4 | C24-C23 | 2.64 | 1.43 | 1.50 | 7 | 6 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 397 | PX4 | O5-C9 | 2.64 | 1.41 | 1.33 | 14 | 3 |
| 3 | C | 302 | PX4 | O3-C1 | 2.64 | 1.34 | 1.44 | 4 | 1 |
| 3 | C | 334 | PX4 | C4-N1 | 2.64 | 1.42 | 1.50 | 9 | 2 |
| 3 | A | 635 | PX4 | C33-C32 | 2.64 | 1.64 | 1.51 | 11 | 1 |
| 3 | B | 310 | PX4 | C2-N1 | 2.64 | 1.59 | 1.51 | 10 | 2 |
| 3 | B | 338 | PX4 | C25-C24 | 2.64 | 1.61 | 1.52 | 1 | 1 |
| 3 | B | 390 | PX4 | O5-C8 | 2.64 | 1.51 | 1.45 | 15 | 1 |
| 3 | C | 347 | PX4 | C24-C23 | 2.64 | 1.58 | 1.50 | 9 | 2 |
| 3 | A | 624 | PX4 | C8-C7 | 2.63 | 1.59 | 1.50 | 12 | 5 |
| 3 | B | 329 | PX4 | O5-C8 | 2.63 | 1.51 | 1.45 | 2 | 1 |
| 3 | B | 371 | PX4 | C3-N1 | 2.63 | 1.57 | 1.50 | 5 | 1 |
| 3 | B | 400 | PX4 | P1-O1 | 2.63 | 1.43 | 1.55 | 3 | 2 |
| 3 | B | 400 | PX4 | C4-N1 | 2.63 | 1.42 | 1.50 | 12 | 1 |
| 3 | C | 324 | PX4 | O7-C23 | 2.63 | 1.41 | 1.34 | 4 | 1 |
| 3 | C | 360 | PX4 | P1-O1 | 2.63 | 1.43 | 1.55 | 4 | 2 |
| 3 | B | 311 | PX4 | O5-C8 | 2.63 | 1.51 | 1.45 | 5 | 4 |
| 3 | B | 315 | PX4 | C4-N1 | 2.63 | 1.57 | 1.50 | 12 | 2 |
| 3 | B | 332 | PX4 | C11-C10 | 2.63 | 1.61 | 1.52 | 1 | 4 |
| 3 | B | 336 | PX4 | C10-C9 | 2.63 | 1.58 | 1.50 | 2 | 1 |
| 3 | B | 388 | PX4 | O7-C7 | 2.63 | 1.40 | 1.46 | 15 | 2 |
| 3 | A | 653 | PX4 | P1-O1 | 2.63 | 1.43 | 1.55 | 6 | 2 |
| 3 | B | 301 | PX4 | P1-O1 | 2.63 | 1.43 | 1.55 | 12 | 4 |
| 3 | B | 384 | PX4 | P1-O3 | 2.63 | 1.49 | 1.59 | 12 | 2 |
| 3 | B | 334 | PX4 | C25-C24 | 2.63 | 1.61 | 1.52 | 7 | 2 |
| 3 | B | 363 | PX4 | C5-N1 | 2.63 | 1.42 | 1.50 | 4 | 1 |
| 3 | B | 391 | PX4 | O7-C7 | 2.63 | 1.40 | 1.46 | 1 | 2 |
| 3 | C | 351 | PX4 | C2-C1 | 2.63 | 1.59 | 1.51 | 2 | 6 |
| 3 | C | 359 | PX4 | C28-C27 | 2.63 | 1.64 | 1.51 | 5 | 1 |
| 3 | C | 361 | PX4 | C24-C23 | 2.63 | 1.58 | 1.50 | 6 | 3 |
| 3 | B | 389 | PX4 | P1-O1 | 2.63 | 1.43 | 1.55 | 2 | 4 |
| 3 | A | 620 | PX4 | C4-N1 | 2.63 | 1.57 | 1.50 | 3 | 1 |
| 3 | B | 314 | PX4 | C25-C24 | 2.63 | 1.61 | 1.52 | 9 | 2 |
| 3 | C | 355 | PX4 | O5-C8 | 2.62 | 1.39 | 1.45 | 14 | 4 |
| 3 | A | 617 | PX4 | C4-N1 | 2.62 | 1.57 | 1.50 | 7 | 3 |
| 3 | A | 617 | PX4 | C15-C14 | 2.62 | 1.64 | 1.51 | 9 | 1 |
| 3 | A | 626 | PX4 | C10-C9 | 2.62 | 1.58 | 1.50 | 14 | 2 |
| 3 | B | 360 | PX4 | C25-C24 | 2.62 | 1.61 | 1.52 | 13 | 2 |
| 3 | B | 375 | PX4 | C25-C24 | 2.62 | 1.61 | 1.52 | 3 | 4 |
| 3 | C | 308 | PX4 | C5-N1 | 2.62 | 1.57 | 1.50 | 14 | 2 |
| 3 | B | 349 | PX4 | C4-N1 | 2.62 | 1.42 | 1.50 | 9 | 3 |
| 3 | A | 604 | PX4 | O7-C7 | 2.62 | 1.40 | 1.46 | 3 | 3 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 322 | PX4 | O7-C7 | 2.62 | 1.40 | 1.46 | 8 | 3 |
| 3 | B | 326 | PX4 | C10-C9 | 2.62 | 1.58 | 1.50 | 2 | 2 |
| 3 | B | 358 | PX4 | O7-C23 | 2.62 | 1.26 | 1.34 | 3 | 1 |
| 3 | C | 356 | PX4 | O5-C8 | 2.62 | 1.51 | 1.45 | 11 | 2 |
| 3 | A | 641 | PX4 | P1-O2 | 2.62 | 1.41 | 1.50 | 1 | 1 |
| 3 | A | 652 | PX4 | O5-C9 | 2.62 | 1.25 | 1.33 | 10 | 1 |
| 3 | A | 638 | PX4 | C2-C1 | 2.62 | 1.59 | 1.51 | 12 | 3 |
| 3 | B | 327 | PX4 | C24-C23 | 2.61 | 1.58 | 1.50 | 8 | 1 |
| 3 | B | 353 | PX4 | C24-C23 | 2.61 | 1.58 | 1.50 | 11 | 3 |
| 3 | A | 620 | PX4 | C10-C9 | 2.61 | 1.58 | 1.50 | 7 | 2 |
| 3 | B | 368 | PX4 | P1-O4 | 2.61 | 1.49 | 1.59 | 10 | 1 |
| 3 | B | 391 | PX4 | C8-C7 | 2.61 | 1.59 | 1.50 | 15 | 3 |
| 3 | A | 651 | PX4 | C6-C7 | 2.61 | 1.59 | 1.50 | 2 | 5 |
| 3 | B | 377 | PX4 | C11-C10 | 2.61 | 1.61 | 1.52 | 13 | 2 |
| 3 | C | 318 | PX4 | C20-C19 | 2.61 | 1.64 | 1.51 | 15 | 1 |
| 3 | A | 612 | PX4 | O5-C8 | 2.61 | 1.51 | 1.45 | 15 | 3 |
| 3 | A | 639 | PX4 | C28-C27 | 2.61 | 1.64 | 1.51 | 3 | 1 |
| 3 | C | 303 | PX4 | P1-O1 | 2.61 | 1.43 | 1.55 | 15 | 4 |
| 3 | C | 313 | PX4 | P1-O1 | 2.61 | 1.43 | 1.55 | 11 | 3 |
| 3 | B | 354 | PX4 | C4-N1 | 2.61 | 1.57 | 1.50 | 5 | 2 |
| 3 | B | 398 | PX4 | O5-C8 | 2.61 | 1.51 | 1.45 | 9 | 4 |
| 3 | C | 360 | PX4 | C10-C9 | 2.61 | 1.58 | 1.50 | 13 | 5 |
| 3 | A | 606 | PX4 | C2-N1 | 2.61 | 1.59 | 1.51 | 6 | 2 |
| 3 | B | 354 | PX4 | C5-N1 | 2.61 | 1.42 | 1.50 | 10 | 2 |
| 3 | A | 608 | PX4 | C2-C1 | 2.60 | 1.59 | 1.51 | 12 | 4 |
| 3 | B | 339 | PX4 | C15-C14 | 2.60 | 1.64 | 1.51 | 14 | 1 |
| 3 | B | 344 | PX4 | C6-C7 | 2.60 | 1.59 | 1.50 | 5 | 6 |
| 3 | B | 367 | PX4 | C10-C9 | 2.60 | 1.58 | 1.50 | 2 | 2 |
| 3 | A | 640 | PX4 | C24-C23 | 2.60 | 1.58 | 1.50 | 4 | 1 |
| 3 | B | 373 | PX4 | P1-O1 | 2.60 | 1.43 | 1.55 | 2 | 4 |
| 3 | B | 303 | PX4 | C10-C9 | 2.60 | 1.58 | 1.50 | 15 | 3 |
| 3 | B | 350 | PX4 | C4-N1 | 2.60 | 1.42 | 1.50 | 6 | 1 |
| 3 | B | 376 | PX4 | C5-N1 | 2.60 | 1.42 | 1.50 | 1 | 1 |
| 3 | C | 308 | PX4 | C28-C27 | 2.60 | 1.64 | 1.51 | 11 | 1 |
| 3 | C | 314 | PX4 | C5-N1 | 2.60 | 1.57 | 1.50 | 4 | 2 |
| 3 | C | 325 | PX4 | C4-N1 | 2.60 | 1.42 | 1.50 | 6 | 1 |
| 3 | C | 355 | PX4 | C5-N1 | 2.60 | 1.57 | 1.50 | 7 | 1 |
| 3 | C | 321 | PX4 | C24-C23 | 2.60 | 1.58 | 1.50 | 15 | 5 |
| 3 | C | 338 | PX4 | O7-C23 | 2.60 | 1.41 | 1.34 | 9 | 2 |
| 3 | C | 348 | PX4 | C3-N1 | 2.60 | 1.42 | 1.50 | 13 | 1 |
| 3 | C | 364 | PX4 | O7-C23 | 2.60 | 1.26 | 1.34 | 1 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | A | 638 | PX4 | C3-N1 | 2.60 | 1.57 | 1.50 | 4 | 1 |
| 3 | B | 303 | PX4 | O7-C7 | 2.60 | 1.40 | 1.46 | 15 | 3 |
| 3 | B | 367 | PX4 | C5-N1 | 2.60 | 1.57 | 1.50 | 6 | 1 |
| 3 | A | 638 | PX4 | C2-N1 | 2.60 | 1.59 | 1.51 | 5 | 1 |
| 3 | B | 313 | PX4 | C5-N1 | 2.60 | 1.57 | 1.50 | 11 | 2 |
| 3 | B | 342 | PX4 | O7-C23 | 2.59 | 1.26 | 1.34 | 10 | 2 |
| 3 | B | 345 | PX4 | O5-C9 | 2.60 | 1.25 | 1.33 | 12 | 3 |
| 3 | B | 313 | PX4 | C24-C23 | 2.59 | 1.58 | 1.50 | 5 | 1 |
| 3 | B | 347 | PX4 | P1-O1 | 2.59 | 1.43 | 1.55 | 5 | 2 |
| 3 | B | 353 | PX4 | C19-C18 | 2.59 | 1.64 | 1.51 | 9 | 1 |
| 3 | C | 302 | PX4 | C3-N1 | 2.59 | 1.42 | 1.50 | 8 | 2 |
| 3 | A | 603 | PX4 | O5-C8 | 2.59 | 1.39 | 1.45 | 1 | 2 |
| 3 | B | 331 | PX4 | C3-N1 | 2.59 | 1.57 | 1.50 | 8 | 1 |
| 3 | B | 378 | PX4 | C24-C23 | 2.59 | 1.58 | 1.50 | 15 | 4 |
| 3 | C | 355 | PX4 | O7-C23 | 2.59 | 1.26 | 1.34 | 14 | 1 |
| 3 | C | 357 | PX4 | C10-C9 | 2.59 | 1.58 | 1.50 | 10 | 2 |
| 3 | B | 305 | PX4 | P1-O2 | 2.59 | 1.41 | 1.50 | 12 | 1 |
| 3 | A | 631 | PX4 | C2-N1 | 2.59 | 1.59 | 1.51 | 9 | 2 |
| 3 | B | 311 | PX4 | C11-C10 | 2.59 | 1.61 | 1.52 | 6 | 2 |
| 3 | C | 337 | PX4 | O7-C7 | 2.59 | 1.40 | 1.46 | 11 | 3 |
| 3 | C | 354 | PX4 | C2-N1 | 2.59 | 1.59 | 1.51 | 9 | 1 |
| 3 | C | 356 | PX4 | O7-C7 | 2.59 | 1.40 | 1.46 | 2 | 2 |
| 3 | B | 314 | PX4 | O5-C8 | 2.59 | 1.39 | 1.45 | 11 | 5 |
| 3 | B | 315 | PX4 | C5-N1 | 2.59 | 1.42 | 1.50 | 7 | 1 |
| 3 | B | 326 | PX4 | C32-C31 | 2.59 | 1.64 | 1.51 | 3 | 1 |
| 3 | A | 606 | PX4 | P1-O1 | 2.59 | 1.43 | 1.55 | 9 | 2 |
| 3 | B | 392 | PX4 | C2-C1 | 2.59 | 1.59 | 1.51 | 13 | 5 |
| 3 | C | 348 | PX4 | C10-C9 | 2.59 | 1.58 | 1.50 | 4 | 2 |
| 3 | A | 624 | PX4 | C10-C9 | 2.59 | 1.58 | 1.50 | 9 | 1 |
| 3 | B | 398 | PX4 | C11-C10 | 2.59 | 1.61 | 1.52 | 13 | 2 |
| 3 | C | 346 | PX4 | C20-C19 | 2.59 | 1.64 | 1.51 | 8 | 1 |
| 3 | A | 632 | PX4 | C30-C29 | 2.58 | 1.64 | 1.51 | 12 | 1 |
| 3 | A | 603 | PX4 | C3-N1 | 2.58 | 1.57 | 1.50 | 7 | 1 |
| 3 | A | 610 | PX4 | P1-O1 | 2.58 | 1.43 | 1.55 | 8 | 2 |
| 3 | A | 619 | PX4 | C5-N1 | 2.58 | 1.42 | 1.50 | 8 | 1 |
| 3 | B | 304 | PX4 | C14-C13 | 2.58 | 1.64 | 1.51 | 4 | 1 |
| 3 | B | 322 | PX4 | C11-C10 | 2.58 | 1.61 | 1.52 | 1 | 1 |
| 3 | B | 330 | PX4 | P1-O1 | 2.58 | 1.43 | 1.55 | 6 | 2 |
| 3 | B | 395 | PX4 | C24-C23 | 2.58 | 1.58 | 1.50 | 6 | 4 |
| 3 | C | 313 | PX4 | C2-C1 | 2.58 | 1.59 | 1.51 | 8 | 5 |
| 3 | C | 346 | PX4 | P1-O1 | 2.58 | 1.43 | 1.55 | 3 | 4 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | C | 346 | PX4 | C3-N1 | 2.58 | 1.42 | 1.50 | 6 | 1 |
| 3 | A | 626 | PX4 | C25-C24 | 2.58 | 1.61 | 1.52 | 10 | 2 |
| 3 | B | 316 | PX4 | C2-C1 | 2.58 | 1.59 | 1.51 | 2 | 5 |
| 3 | C | 339 | PX4 | C10-C9 | 2.58 | 1.58 | 1.50 | 10 | 2 |
| 3 | A | 612 | PX4 | P1-O1 | 2.58 | 1.43 | 1.55 | 2 | 4 |
| 3 | A | 634 | PX4 | C20-C19 | 2.58 | 1.64 | 1.51 | 3 | 1 |
| 3 | B | 301 | PX4 | O7-C23 | 2.58 | 1.27 | 1.34 | 5 | 3 |
| 3 | B | 324 | PX4 | C11-C10 | 2.58 | 1.61 | 1.52 | 13 | 1 |
| 3 | C | 364 | PX4 | C3-N1 | 2.58 | 1.42 | 1.50 | 3 | 2 |
| 3 | A | 642 | PX4 | C4-N1 | 2.58 | 1.57 | 1.50 | 4 | 2 |
| 3 | A | 637 | PX4 | P1-O3 | 2.57 | 1.49 | 1.59 | 3 | 1 |
| 3 | A | 650 | PX4 | C15-C14 | 2.57 | 1.64 | 1.51 | 3 | 1 |
| 3 | B | 327 | PX4 | C3-N1 | 2.57 | 1.57 | 1.50 | 9 | 3 |
| 3 | B | 330 | PX4 | C4-N1 | 2.57 | 1.57 | 1.50 | 12 | 2 |
| 3 | A | 640 | PX4 | C11-C10 | 2.57 | 1.61 | 1.52 | 6 | 1 |
| 3 | B | 356 | PX4 | C25-C24 | 2.57 | 1.61 | 1.52 | 9 | 1 |
| 3 | C | 346 | PX4 | C2-N1 | 2.57 | 1.59 | 1.51 | 12 | 1 |
| 3 | B | 382 | PX4 | C10-C9 | 2.57 | 1.58 | 1.50 | 5 | 2 |
| 3 | C | 317 | PX4 | P1-O1 | 2.57 | 1.43 | 1.55 | 3 | 2 |
| 3 | A | 627 | PX4 | P1-O1 | 2.57 | 1.43 | 1.55 | 8 | 5 |
| 3 | C | 321 | PX4 | C11-C10 | 2.57 | 1.61 | 1.52 | 9 | 3 |
| 3 | C | 327 | PX4 | O5-C9 | 2.57 | 1.40 | 1.33 | 4 | 2 |
| 3 | C | 352 | PX4 | C3-N1 | 2.57 | 1.57 | 1.50 | 11 | 1 |
| 3 | C | 359 | PX4 | O5-C8 | 2.57 | 1.39 | 1.45 | 4 | 1 |
| 3 | B | 372 | PX4 | P1-O3 | 2.57 | 1.49 | 1.59 | 5 | 1 |
| 3 | B | 340 | PX4 | O7-C23 | 2.57 | 1.27 | 1.34 | 2 | 1 |
| 3 | C | 303 | PX4 | C5-N1 | 2.57 | 1.57 | 1.50 | 1 | 1 |
| 3 | B | 346 | PX4 | C11-C10 | 2.57 | 1.61 | 1.52 | 15 | 1 |
| 3 | B | 371 | PX4 | C4-N1 | 2.56 | 1.42 | 1.50 | 14 | 1 |
| 3 | C | 305 | PX4 | C13-C12 | 2.57 | 1.64 | 1.51 | 2 | 2 |
| 3 | A | 623 | PX4 | C10-C9 | 2.56 | 1.58 | 1.50 | 14 | 2 |
| 3 | A | 650 | PX4 | C4-N1 | 2.56 | 1.42 | 1.50 | 2 | 2 |
| 3 | B | 386 | PX4 | P1-O1 | 2.56 | 1.43 | 1.55 | 15 | 1 |
| 3 | B | 396 | PX4 | O5-C8 | 2.56 | 1.39 | 1.45 | 6 | 3 |
| 3 | C | 357 | PX4 | C34-C33 | 2.56 | 1.64 | 1.51 | 5 | 1 |
| 3 | A | 645 | PX4 | C2-N1 | 2.56 | 1.59 | 1.51 | 4 | 1 |
| 3 | B | 308 | PX4 | C11-C10 | 2.56 | 1.61 | 1.52 | 3 | 5 |
| 3 | C | 319 | PX4 | O7-C7 | 2.56 | 1.40 | 1.46 | 10 | 1 |
| 3 | A | 611 | PX4 | C5-N1 | 2.56 | 1.57 | 1.50 | 7 | 2 |
| 3 | C | 310 | PX4 | C28-C27 | 2.56 | 1.64 | 1.51 | 3 | 1 |
| 3 | C | 337 | PX4 | C4-N1 | 2.56 | 1.57 | 1.50 | 15 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | A | 635 | PX4 | C10-C9 | 2.56 | 1.58 | 1.50 | 4 | 4 |
| 3 | A | 647 | PX4 | O3-C1 | 2.56 | 1.34 | 1.44 | 1 | 1 |
| 3 | A | 644 | PX4 | C25-C24 | 2.56 | 1.61 | 1.52 | 14 | 1 |
| 3 | C | 316 | PX4 | C25-C24 | 2.56 | 1.61 | 1.52 | 6 | 3 |
| 3 | A | 642 | PX4 | O3-C1 | 2.56 | 1.34 | 1.44 | 4 | 1 |
| 3 | B | 301 | PX4 | C2-C1 | 2.56 | 1.59 | 1.51 | 8 | 4 |
| 3 | B | 317 | PX4 | C29-C28 | 2.56 | 1.64 | 1.51 | 8 | 1 |
| 3 | B | 348 | PX4 | P1-O1 | 2.56 | 1.43 | 1.55 | 4 | 3 |
| 3 | B | 373 | PX4 | C24-C23 | 2.56 | 1.58 | 1.50 | 12 | 1 |
| 3 | B | 374 | PX4 | O5-C9 | 2.56 | 1.25 | 1.33 | 13 | 2 |
| 3 | B | 387 | PX4 | C3-N1 | 2.56 | 1.42 | 1.50 | 13 | 1 |
| 3 | B | 344 | PX4 | O5-C8 | 2.55 | 1.50 | 1.45 | 6 | 2 |
| 3 | B | 381 | PX4 | O7-C7 | 2.55 | 1.40 | 1.46 | 14 | 3 |
| 3 | C | 318 | PX4 | O7-C23 | 2.56 | 1.27 | 1.34 | 11 | 2 |
| 3 | C | 330 | PX4 | O7-C7 | 2.56 | 1.40 | 1.46 | 15 | 4 |
| 3 | B | 321 | PX4 | O7-C7 | 2.55 | 1.40 | 1.46 | 4 | 1 |
| 3 | B | 344 | PX4 | P1-O4 | 2.55 | 1.49 | 1.59 | 12 | 1 |
| 3 | B | 385 | PX4 | C4-N1 | 2.55 | 1.57 | 1.50 | 4 | 1 |
| 3 | C | 364 | PX4 | C5-N1 | 2.55 | 1.57 | 1.50 | 13 | 2 |
| 3 | A | 628 | PX4 | C5-N1 | 2.55 | 1.57 | 1.50 | 15 | 3 |
| 3 | B | 375 | PX4 | O5-C9 | 2.55 | 1.40 | 1.33 | 6 | 2 |
| 3 | B | 377 | PX4 | C10-C9 | 2.55 | 1.58 | 1.50 | 10 | 2 |
| 3 | B | 380 | PX4 | C11-C10 | 2.55 | 1.61 | 1.52 | 2 | 3 |
| 3 | C | 315 | PX4 | C2-C1 | 2.55 | 1.59 | 1.51 | 3 | 2 |
| 3 | A | 624 | PX4 | O5-C8 | 2.55 | 1.50 | 1.45 | 9 | 1 |
| 3 | B | 305 | PX4 | C10-C9 | 2.55 | 1.58 | 1.50 | 1 | 1 |
| 3 | C | 326 | PX4 | P1-O4 | 2.55 | 1.49 | 1.59 | 7 | 1 |
| 3 | C | 350 | PX4 | O3-C1 | 2.55 | 1.34 | 1.44 | 14 | 1 |
| 3 | B | 325 | PX4 | C2-N1 | 2.55 | 1.59 | 1.51 | 10 | 1 |
| 3 | B | 384 | PX4 | O7-C7 | 2.55 | 1.40 | 1.46 | 10 | 2 |
| 3 | B | 400 | PX4 | O7-C7 | 2.55 | 1.40 | 1.46 | 4 | 4 |
| 3 | C | 321 | PX4 | C2-C1 | 2.55 | 1.59 | 1.51 | 2 | 5 |
| 3 | A | 650 | PX4 | P1-O1 | 2.55 | 1.43 | 1.55 | 10 | 2 |
| 3 | B | 400 | PX4 | C5-N1 | 2.55 | 1.57 | 1.50 | 9 | 2 |
| 3 | B | 311 | PX4 | O7-C23 | 2.55 | 1.27 | 1.34 | 3 | 3 |
| 3 | C | 323 | PX4 | C10-C9 | 2.55 | 1.58 | 1.50 | 8 | 2 |
| 3 | B | 314 | PX4 | C10-C9 | 2.55 | 1.58 | 1.50 | 10 | 5 |
| 3 | B | 325 | PX4 | O7-C23 | 2.54 | 1.27 | 1.34 | 9 | 3 |
| 3 | B | 369 | PX4 | C10-C9 | 2.55 | 1.58 | 1.50 | 10 | 2 |
| 3 | A | 637 | PX4 | C3-N1 | 2.54 | 1.57 | 1.50 | 11 | 2 |
| 3 | B | 373 | PX4 | P1-O4 | 2.54 | 1.49 | 1.59 | 6 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 323 | PX4 | C10-C9 | 2.54 | 1.58 | 1.50 | 7 | 1 |
| 3 | B | 396 | PX4 | C33-C32 | 2.54 | 1.64 | 1.51 | 2 | 1 |
| 3 | B | 396 | PX4 | C24-C23 | 2.54 | 1.58 | 1.50 | 6 | 2 |
| 3 | B | 359 | PX4 | C5-N1 | 2.54 | 1.57 | 1.50 | 15 | 1 |
| 3 | C | 310 | PX4 | O4-C6 | 2.54 | 1.35 | 1.44 | 4 | 1 |
| 3 | C | 320 | PX4 | C3-N1 | 2.54 | 1.42 | 1.50 | 11 | 3 |
| 3 | C | 332 | PX4 | O7-C23 | 2.54 | 1.41 | 1.34 | 6 | 1 |
| 3 | A | 641 | PX4 | O7-C23 | 2.54 | 1.27 | 1.34 | 5 | 2 |
| 3 | B | 365 | PX4 | C4-N1 | 2.54 | 1.57 | 1.50 | 8 | 2 |
| 3 | C | 310 | PX4 | P1-O2 | 2.54 | 1.42 | 1.50 | 6 | 2 |
| 3 | C | 345 | PX4 | C29-C28 | 2.54 | 1.64 | 1.51 | 13 | 1 |
| 3 | A | 608 | PX4 | O7-C23 | 2.54 | 1.27 | 1.34 | 11 | 1 |
| 3 | B | 313 | PX4 | P1-O4 | 2.54 | 1.49 | 1.59 | 7 | 1 |
| 3 | A | 631 | PX4 | P1-O1 | 2.54 | 1.43 | 1.55 | 1 | 3 |
| 3 | A | 651 | PX4 | C25-C24 | 2.54 | 1.61 | 1.52 | 13 | 2 |
| 3 | B | 399 | PX4 | C13-C12 | 2.54 | 1.64 | 1.51 | 13 | 1 |
| 3 | C | 346 | PX4 | C32-C31 | 2.54 | 1.64 | 1.51 | 15 | 1 |
| 3 | B | 362 | PX4 | C2-N1 | 2.54 | 1.43 | 1.51 | 7 | 4 |
| 3 | C | 326 | PX4 | C3-N1 | 2.53 | 1.42 | 1.50 | 13 | 2 |
| 3 | A | 613 | PX4 | P1-O1 | 2.53 | 1.43 | 1.55 | 10 | 3 |
| 3 | A | 626 | PX4 | C6-C7 | 2.53 | 1.58 | 1.50 | 11 | 2 |
| 3 | B | 361 | PX4 | C2-C1 | 2.53 | 1.59 | 1.51 | 5 | 6 |
| 3 | B | 384 | PX4 | P1-O1 | 2.53 | 1.43 | 1.55 | 14 | 3 |
| 3 | B | 393 | PX4 | C6-C7 | 2.53 | 1.58 | 1.50 | 2 | 4 |
| 3 | C | 304 | PX4 | C24-C23 | 2.53 | 1.58 | 1.50 | 5 | 3 |
| 3 | C | 327 | PX4 | C5-N1 | 2.53 | 1.57 | 1.50 | 2 | 3 |
| 3 | B | 397 | PX4 | O7-C23 | 2.53 | 1.41 | 1.34 | 15 | 2 |
| 3 | C | 332 | PX4 | C11-C10 | 2.53 | 1.61 | 1.52 | 9 | 1 |
| 3 | C | 339 | PX4 | P1-O4 | 2.53 | 1.49 | 1.59 | 11 | 1 |
| 3 | C | 355 | PX4 | C2-N1 | 2.53 | 1.59 | 1.51 | 15 | 2 |
| 3 | C | 356 | PX4 | P1-O4 | 2.53 | 1.49 | 1.59 | 2 | 1 |
| 3 | C | 358 | PX4 | P1-O3 | 2.53 | 1.49 | 1.59 | 4 | 1 |
| 3 | B | 352 | PX4 | C25-C24 | 2.53 | 1.61 | 1.52 | 14 | 2 |
| 3 | A | 649 | PX4 | O3-C1 | 2.53 | 1.34 | 1.44 | 7 | 1 |
| 3 | B | 384 | PX4 | O3-C1 | 2.53 | 1.34 | 1.44 | 1 | 1 |
| 3 | B | 395 | PX4 | C25-C24 | 2.53 | 1.61 | 1.52 | 5 | 2 |
| 3 | C | 301 | PX4 | C5-N1 | 2.53 | 1.57 | 1.50 | 15 | 4 |
| 3 | C | 337 | PX4 | P1-O3 | 2.53 | 1.49 | 1.59 | 12 | 1 |
| 3 | A | 625 | PX4 | C11-C10 | 2.53 | 1.61 | 1.52 | 15 | 4 |
| 3 | A | 641 | PX4 | O7-C7 | 2.53 | 1.40 | 1.46 | 6 | 2 |
| 3 | C | 326 | PX4 | C8-C7 | 2.53 | 1.58 | 1.50 | 11 | 6 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | C | 343 | PX4 | C4-N1 | 2.53 | 1.57 | 1.50 | 4 | 2 |
| 3 | A | 631 | PX4 | C25-C24 | 2.53 | 1.61 | 1.52 | 12 | 3 |
| 3 | A | 618 | PX4 | C3-N1 | 2.52 | 1.57 | 1.50 | 6 | 2 |
| 3 | A | 639 | PX4 | C2-N1 | 2.53 | 1.59 | 1.51 | 2 | 1 |
| 3 | B | 337 | PX4 | P1-O1 | 2.53 | 1.43 | 1.55 | 2 | 3 |
| 3 | B | 388 | PX4 | C12-C11 | 2.52 | 1.64 | 1.51 | 5 | 1 |
| 3 | C | 336 | PX4 | C11-C10 | 2.53 | 1.61 | 1.52 | 12 | 2 |
| 3 | C | 352 | PX4 | C11-C10 | 2.53 | 1.61 | 1.52 | 3 | 3 |
| 3 | A | 601 | PX4 | C3-N1 | 2.52 | 1.42 | 1.50 | 5 | 1 |
| 3 | B | 329 | PX4 | P1-O3 | 2.52 | 1.49 | 1.59 | 9 | 1 |
| 3 | A | 650 | PX4 | C24-C23 | 2.52 | 1.58 | 1.50 | 7 | 3 |
| 3 | B | 314 | PX4 | C6-C7 | 2.52 | 1.58 | 1.50 | 2 | 3 |
| 3 | B | 316 | PX4 | C11-C10 | 2.52 | 1.61 | 1.52 | 10 | 3 |
| 3 | B | 337 | PX4 | C25-C24 | 2.52 | 1.61 | 1.52 | 6 | 2 |
| 3 | C | 302 | PX4 | P1-O1 | 2.52 | 1.43 | 1.55 | 10 | 4 |
| 3 | C | 327 | PX4 | C2-N1 | 2.52 | 1.43 | 1.51 | 1 | 1 |
| 3 | A | 647 | PX4 | O7-C23 | 2.52 | 1.27 | 1.34 | 11 | 1 |
| 3 | A | 605 | PX4 | P1-O1 | 2.52 | 1.43 | 1.55 | 15 | 4 |
| 3 | B | 359 | PX4 | C8-C7 | 2.52 | 1.58 | 1.50 | 7 | 6 |
| 3 | C | 320 | PX4 | C25-C24 | 2.52 | 1.61 | 1.52 | 4 | 1 |
| 3 | B | 309 | PX4 | C2-N1 | 2.52 | 1.59 | 1.51 | 4 | 1 |
| 3 | B | 338 | PX4 | P1-O1 | 2.52 | 1.43 | 1.55 | 4 | 4 |
| 3 | B | 365 | PX4 | P1-O3 | 2.52 | 1.49 | 1.59 | 9 | 1 |
| 3 | B | 378 | PX4 | C10-C9 | 2.52 | 1.58 | 1.50 | 10 | 1 |
| 3 | B | 381 | PX4 | C19-C18 | 2.52 | 1.64 | 1.51 | 15 | 1 |
| 3 | C | 310 | PX4 | C11-C10 | 2.52 | 1.61 | 1.52 | 11 | 2 |
| 3 | B | 352 | PX4 | O3-C1 | 2.52 | 1.34 | 1.44 | 9 | 1 |
| 3 | A | 639 | PX4 | C17-C16 | 2.51 | 1.64 | 1.51 | 6 | 1 |
| 3 | B | 301 | PX4 | C27-C26 | 2.51 | 1.64 | 1.51 | 14 | 1 |
| 3 | B | 389 | PX4 | C3-N1 | 2.52 | 1.57 | 1.50 | 15 | 3 |
| 3 | C | 319 | PX4 | P1-O1 | 2.51 | 1.43 | 1.55 | 11 | 4 |
| 3 | C | 361 | PX4 | P1-O4 | 2.52 | 1.49 | 1.59 | 12 | 1 |
| 3 | A | 605 | PX4 | C4-N1 | 2.51 | 1.42 | 1.50 | 3 | 1 |
| 3 | B | 318 | PX4 | C11-C10 | 2.51 | 1.61 | 1.52 | 9 | 3 |
| 3 | B | 347 | PX4 | C5-N1 | 2.51 | 1.42 | 1.50 | 6 | 3 |
| 3 | B | 354 | PX4 | P1-O1 | 2.51 | 1.43 | 1.55 | 1 | 4 |
| 3 | C | 320 | PX4 | C2-N1 | 2.51 | 1.59 | 1.51 | 3 | 3 |
| 3 | C | 350 | PX4 | O4-C6 | 2.51 | 1.35 | 1.44 | 10 | 2 |
| 3 | C | 364 | PX4 | P1-O1 | 2.51 | 1.43 | 1.55 | 11 | 4 |
| 3 | A | 603 | PX4 | C10-C9 | 2.51 | 1.58 | 1.50 | 6 | 4 |
| 3 | C | 308 | PX4 | C2-N1 | 2.51 | 1.59 | 1.51 | 7 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | C | 313 | PX4 | C10-C9 | 2.51 | 1.58 | 1.50 | 15 | 1 |
| 3 | C | 309 | PX4 | C10-C9 | 2.51 | 1.58 | 1.50 | 7 | 3 |
| 3 | C | 310 | PX4 | C29-C28 | 2.51 | 1.64 | 1.51 | 8 | 1 |
| 3 | C | 360 | PX4 | P1-O4 | 2.51 | 1.69 | 1.59 | 2 | 1 |
| 3 | B | 368 | PX4 | O5-C8 | 2.51 | 1.39 | 1.45 | 7 | 1 |
| 3 | B | 377 | PX4 | O5-C9 | 2.51 | 1.40 | 1.33 | 4 | 1 |
| 3 | B | 383 | PX4 | O5-C9 | 2.51 | 1.40 | 1.33 | 14 | 1 |
| 3 | C | 319 | PX4 | C25-C24 | 2.51 | 1.61 | 1.52 | 4 | 2 |
| 3 | A | 625 | PX4 | P1-O1 | 2.51 | 1.43 | 1.55 | 12 | 4 |
| 3 | B | 391 | PX4 | C16-C15 | 2.51 | 1.64 | 1.51 | 3 | 1 |
| 3 | C | 328 | PX4 | O7-C23 | 2.51 | 1.27 | 1.34 | 9 | 1 |
| 3 | C | 335 | PX4 | O4-C6 | 2.51 | 1.35 | 1.44 | 8 | 1 |
| 3 | B | 332 | PX4 | O7-C7 | 2.51 | 1.40 | 1.46 | 2 | 4 |
| 3 | B | 358 | PX4 | C15-C14 | 2.51 | 1.64 | 1.51 | 11 | 1 |
| 3 | B | 375 | PX4 | C6-C7 | 2.51 | 1.58 | 1.50 | 8 | 3 |
| 3 | B | 391 | PX4 | P1-O3 | 2.51 | 1.49 | 1.59 | 15 | 2 |
| 3 | A | 651 | PX4 | C2-C1 | 2.51 | 1.58 | 1.51 | 13 | 2 |
| 3 | A | 647 | PX4 | C18-C17 | 2.50 | 1.64 | 1.51 | 12 | 1 |
| 3 | A | 653 | PX4 | O5-C9 | 2.50 | 1.26 | 1.33 | 9 | 2 |
| 3 | A | 601 | PX4 | C11-C10 | 2.50 | 1.61 | 1.52 | 4 | 2 |
| 3 | A | 637 | PX4 | O3-C1 | 2.50 | 1.34 | 1.44 | 14 | 1 |
| 3 | A | 608 | PX4 | P1-O4 | 2.50 | 1.49 | 1.59 | 4 | 2 |
| 3 | A | 639 | PX4 | C4-N1 | 2.50 | 1.57 | 1.50 | 13 | 2 |
| 3 | A | 653 | PX4 | C17-C16 | 2.50 | 1.64 | 1.51 | 14 | 1 |
| 3 | B | 301 | PX4 | C3-N1 | 2.50 | 1.42 | 1.50 | 1 | 1 |
| 3 | B | 353 | PX4 | C25-C24 | 2.50 | 1.61 | 1.52 | 12 | 2 |
| 3 | C | 318 | PX4 | C34-C33 | 2.50 | 1.64 | 1.51 | 14 | 1 |
| 3 | C | 344 | PX4 | C10-C9 | 2.50 | 1.58 | 1.50 | 8 | 2 |
| 3 | C | 350 | PX4 | C11-C10 | 2.50 | 1.61 | 1.52 | 13 | 3 |
| 3 | B | 302 | PX4 | C25-C24 | 2.50 | 1.61 | 1.52 | 12 | 1 |
| 3 | B | 361 | PX4 | O7-C7 | 2.50 | 1.40 | 1.46 | 11 | 6 |
| 3 | B | 377 | PX4 | O7-C7 | 2.50 | 1.40 | 1.46 | 14 | 4 |
| 3 | B | 377 | PX4 | C17-C16 | 2.50 | 1.64 | 1.51 | 7 | 1 |
| 3 | C | 302 | PX4 | P1-O2 | 2.50 | 1.42 | 1.50 | 14 | 1 |
| 3 | A | 615 | PX4 | C24-C23 | 2.50 | 1.58 | 1.50 | 8 | 1 |
| 3 | B | 354 | PX4 | C11-C10 | 2.50 | 1.61 | 1.52 | 4 | 2 |
| 3 | A | 604 | PX4 | C4-N1 | 2.50 | 1.57 | 1.50 | 3 | 2 |
| 3 | B | 346 | PX4 | C24-C23 | 2.50 | 1.58 | 1.50 | 8 | 3 |
| 3 | C | 333 | PX4 | C4-N1 | 2.50 | 1.42 | 1.50 | 15 | 2 |
| 3 | C | 343 | PX4 | P1-O1 | 2.50 | 1.43 | 1.55 | 7 | 6 |
| 3 | A | 611 | PX4 | C28-C27 | 2.50 | 1.64 | 1.51 | 15 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 343 | PX4 | C2-N1 | 2.50 | 1.59 | 1.51 | 5 | 2 |
| 3 | B | 348 | PX4 | C5-N1 | 2.50 | 1.57 | 1.50 | 4 | 1 |
| 3 | B | 366 | PX4 | C34-C33 | 2.50 | 1.64 | 1.51 | 13 | 1 |
| 3 | B | 350 | PX4 | C2-N1 | 2.50 | 1.59 | 1.51 | 7 | 1 |
| 3 | B | 385 | PX4 | O5-C9 | 2.50 | 1.26 | 1.33 | 9 | 2 |
| 3 | C | 305 | PX4 | O7-C23 | 2.50 | 1.41 | 1.34 | 12 | 2 |
| 3 | C | 338 | PX4 | C25-C24 | 2.50 | 1.61 | 1.52 | 5 | 3 |
| 3 | C | 339 | PX4 | O5-C9 | 2.50 | 1.40 | 1.33 | 7 | 2 |
| 3 | B | 328 | PX4 | P1-O4 | 2.49 | 1.49 | 1.59 | 15 | 1 |
| 3 | B | 354 | PX4 | O5-C8 | 2.49 | 1.39 | 1.45 | 14 | 1 |
| 3 | A | 641 | PX4 | C4-N1 | 2.49 | 1.57 | 1.50 | 7 | 1 |
| 3 | B | 394 | PX4 | C25-C24 | 2.49 | 1.61 | 1.52 | 12 | 1 |
| 3 | B | 357 | PX4 | C2-C1 | 2.49 | 1.58 | 1.51 | 10 | 5 |
| 3 | B | 397 | PX4 | P1-O2 | 2.49 | 1.42 | 1.50 | 11 | 2 |
| 3 | A | 614 | PX4 | C10-C9 | 2.49 | 1.43 | 1.50 | 1 | 3 |
| 3 | A | 619 | PX4 | C3-N1 | 2.49 | 1.57 | 1.50 | 10 | 3 |
| 3 | A | 632 | PX4 | C11-C10 | 2.49 | 1.61 | 1.52 | 5 | 3 |
| 3 | B | 318 | PX4 | C6-C7 | 2.49 | 1.58 | 1.50 | 1 | 3 |
| 3 | C | 355 | PX4 | P1-O1 | 2.49 | 1.43 | 1.55 | 6 | 3 |
| 3 | B | 333 | PX4 | C25-C24 | 2.49 | 1.61 | 1.52 | 14 | 1 |
| 3 | A | 635 | PX4 | P1-O1 | 2.49 | 1.43 | 1.55 | 12 | 2 |
| 3 | B | 334 | PX4 | C2-N1 | 2.49 | 1.59 | 1.51 | 12 | 2 |
| 3 | B | 355 | PX4 | C25-C24 | 2.49 | 1.61 | 1.52 | 8 | 1 |
| 3 | B | 384 | PX4 | O5-C9 | 2.49 | 1.40 | 1.33 | 13 | 2 |
| 3 | C | 318 | PX4 | P1-O2 | 2.49 | 1.42 | 1.50 | 1 | 2 |
| 3 | A | 641 | PX4 | C17-C16 | 2.49 | 1.64 | 1.51 | 3 | 1 |
| 3 | A | 646 | PX4 | C10-C9 | 2.49 | 1.57 | 1.50 | 15 | 1 |
| 3 | A | 645 | PX4 | C28-C27 | 2.49 | 1.64 | 1.51 | 8 | 1 |
| 3 | B | 321 | PX4 | C28-C27 | 2.49 | 1.64 | 1.51 | 13 | 1 |
| 3 | B | 331 | PX4 | C5-N1 | 2.49 | 1.57 | 1.50 | 3 | 2 |
| 3 | B | 302 | PX4 | C30-C29 | 2.49 | 1.64 | 1.51 | 7 | 1 |
| 3 | B | 343 | PX4 | C4-N1 | 2.49 | 1.57 | 1.50 | 15 | 2 |
| 3 | C | 330 | PX4 | C2-C1 | 2.49 | 1.58 | 1.51 | 9 | 3 |
| 3 | B | 346 | PX4 | P1-O1 | 2.49 | 1.43 | 1.55 | 7 | 3 |
| 3 | C | 338 | PX4 | P1-O1 | 2.49 | 1.43 | 1.55 | 4 | 2 |
| 3 | C | 329 | PX4 | O7-C7 | 2.48 | 1.40 | 1.46 | 11 | 5 |
| 3 | B | 321 | PX4 | P1-O2 | 2.48 | 1.42 | 1.50 | 10 | 1 |
| 3 | B | 346 | PX4 | C31-C30 | 2.48 | 1.64 | 1.51 | 2 | 1 |
| 3 | C | 333 | PX4 | P1-O1 | 2.48 | 1.43 | 1.55 | 9 | 3 |
| 3 | B | 388 | PX4 | O5-C9 | 2.48 | 1.26 | 1.33 | 11 | 1 |
| 3 | C | 304 | PX4 | C25-C24 | 2.48 | 1.61 | 1.52 | 9 | 2 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | C | 311 | PX4 | P1-O2 | 2.48 | 1.42 | 1.50 | 14 | 3 |
| 3 | C | 344 | PX4 | C3-N1 | 2.48 | 1.42 | 1.50 | 9 | 1 |
| 3 | B | 326 | PX4 | C4-N1 | 2.48 | 1.57 | 1.50 | 13 | 3 |
| 3 | C | 308 | PX4 | O7-C7 | 2.48 | 1.40 | 1.46 | 1 | 2 |
| 3 | C | 360 | PX4 | C11-C10 | 2.48 | 1.61 | 1.52 | 7 | 1 |
| 3 | A | 615 | PX4 | O5-C8 | 2.48 | 1.39 | 1.45 | 14 | 2 |
| 3 | A | 632 | PX4 | C3-N1 | 2.48 | 1.42 | 1.50 | 2 | 1 |
| 3 | B | 323 | PX4 | C3-N1 | 2.48 | 1.42 | 1.50 | 13 | 2 |
| 3 | B | 312 | PX4 | C4-N1 | 2.48 | 1.57 | 1.50 | 2 | 1 |
| 3 | B | 348 | PX4 | P1-O4 | 2.48 | 1.49 | 1.59 | 9 | 1 |
| 3 | B | 366 | PX4 | C3-N1 | 2.48 | 1.42 | 1.50 | 15 | 1 |
| 3 | B | 377 | PX4 | O7-C23 | 2.48 | 1.27 | 1.34 | 8 | 1 |
| 3 | C | 332 | PX4 | C2-N1 | 2.48 | 1.59 | 1.51 | 8 | 2 |
| 3 | C | 338 | PX4 | C34-C33 | 2.48 | 1.64 | 1.51 | 5 | 1 |
| 3 | C | 339 | PX4 | C5-N1 | 2.48 | 1.42 | 1.50 | 13 | 1 |
| 3 | C | 344 | PX4 | O5-C9 | 2.48 | 1.40 | 1.33 | 13 | 1 |
| 3 | C | 354 | PX4 | P1-O1 | 2.48 | 1.43 | 1.55 | 4 | 1 |
| 3 | A | 631 | PX4 | O7-C7 | 2.48 | 1.40 | 1.46 | 4 | 2 |
| 3 | A | 643 | PX4 | C10-C9 | 2.48 | 1.57 | 1.50 | 8 | 3 |
| 3 | B | 315 | PX4 | C15-C14 | 2.48 | 1.64 | 1.51 | 7 | 1 |
| 3 | C | 320 | PX4 | P1-O3 | 2.48 | 1.49 | 1.59 | 4 | 1 |
| 3 | B | 384 | PX4 | O4-C6 | 2.47 | 1.54 | 1.44 | 14 | 1 |
| 3 | C | 356 | PX4 | C4-N1 | 2.48 | 1.42 | 1.50 | 13 | 1 |
| 3 | A | 625 | PX4 | C4-N1 | 2.47 | 1.42 | 1.50 | 5 | 1 |
| 3 | A | 634 | PX4 | C25-C24 | 2.47 | 1.61 | 1.52 | 5 | 3 |
| 3 | A | 625 | PX4 | C24-C23 | 2.47 | 1.43 | 1.50 | 5 | 1 |
| 3 | A | 646 | PX4 | P1-O1 | 2.47 | 1.43 | 1.55 | 14 | 1 |
| 3 | B | 362 | PX4 | C4-N1 | 2.47 | 1.57 | 1.50 | 6 | 2 |
| 3 | B | 365 | PX4 | P1-O1 | 2.47 | 1.43 | 1.55 | 10 | 3 |
| 3 | B | 381 | PX4 | C20-C19 | 2.47 | 1.64 | 1.51 | 2 | 1 |
| 3 | C | 329 | PX4 | C4-N1 | 2.47 | 1.42 | 1.50 | 8 | 3 |
| 3 | C | 334 | PX4 | C2-C1 | 2.47 | 1.58 | 1.51 | 2 | 4 |
| 3 | C | 352 | PX4 | C25-C24 | 2.47 | 1.61 | 1.52 | 3 | 2 |
| 3 | B | 313 | PX4 | O7-C7 | 2.47 | 1.40 | 1.46 | 15 | 2 |
| 3 | C | 358 | PX4 | C3-N1 | 2.47 | 1.57 | 1.50 | 6 | 2 |
| 3 | A | 603 | PX4 | C24-C23 | 2.47 | 1.57 | 1.50 | 4 | 3 |
| 3 | A | 614 | PX4 | C33-C32 | 2.47 | 1.64 | 1.51 | 3 | 1 |
| 3 | A | 621 | PX4 | C31-C30 | 2.47 | 1.64 | 1.51 | 2 | 2 |
| 3 | B | 310 | PX4 | C5-N1 | 2.47 | 1.42 | 1.50 | 6 | 1 |
| 3 | C | 341 | PX4 | C5-N1 | 2.47 | 1.57 | 1.50 | 3 | 1 |
| 3 | A | 645 | PX4 | P1-O1 | 2.47 | 1.43 | 1.55 | 12 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | C | 311 | PX4 | O7-C23 | 2.47 | 1.41 | 1.34 | 4 | 2 |
| 3 | A | 628 | PX4 | C24-C23 | 2.47 | 1.57 | 1.50 | 4 | 2 |
| 3 | A | 615 | PX4 | P1-O1 | 2.47 | 1.43 | 1.55 | 11 | 3 |
| 3 | A | 644 | PX4 | C31-C30 | 2.47 | 1.64 | 1.51 | 2 | 1 |
| 3 | B | 304 | PX4 | C3-N1 | 2.47 | 1.57 | 1.50 | 14 | 1 |
| 3 | B | 364 | PX4 | P1-O2 | 2.47 | 1.42 | 1.50 | 5 | 1 |
| 3 | B | 394 | PX4 | C5-N1 | 2.47 | 1.57 | 1.50 | 13 | 1 |
| 3 | B | 365 | PX4 | O7-C23 | 2.47 | 1.27 | 1.34 | 15 | 2 |
| 3 | B | 375 | PX4 | C27-C26 | 2.47 | 1.64 | 1.51 | 4 | 1 |
| 3 | B | 387 | PX4 | O5-C9 | 2.47 | 1.40 | 1.33 | 2 | 1 |
| 3 | B | 308 | PX4 | C4-N1 | 2.46 | 1.57 | 1.50 | 2 | 2 |
| 3 | B | 345 | PX4 | P1-O1 | 2.46 | 1.43 | 1.55 | 5 | 3 |
| 3 | B | 382 | PX4 | C21-C20 | 2.46 | 1.66 | 1.51 | 15 | 1 |
| 3 | A | 611 | PX4 | C2-C1 | 2.46 | 1.58 | 1.51 | 13 | 3 |
| 3 | A | 614 | PX4 | C28-C27 | 2.46 | 1.64 | 1.51 | 5 | 1 |
| 3 | B | 358 | PX4 | C25-C24 | 2.46 | 1.61 | 1.52 | 15 | 2 |
| 3 | B | 364 | PX4 | O7-C7 | 2.46 | 1.52 | 1.46 | 13 | 2 |
| 3 | B | 399 | PX4 | C24-C23 | 2.46 | 1.57 | 1.50 | 12 | 2 |
| 3 | B | 314 | PX4 | C2-N1 | 2.46 | 1.59 | 1.51 | 15 | 1 |
| 3 | C | 330 | PX4 | C3-N1 | 2.46 | 1.42 | 1.50 | 15 | 3 |
| 3 | A | 615 | PX4 | C27-C26 | 2.46 | 1.64 | 1.51 | 14 | 1 |
| 3 | A | 620 | PX4 | C24-C23 | 2.46 | 1.57 | 1.50 | 15 | 4 |
| 3 | A | 640 | PX4 | C5-N1 | 2.46 | 1.57 | 1.50 | 15 | 2 |
| 3 | A | 649 | PX4 | P1-O1 | 2.46 | 1.43 | 1.55 | 8 | 1 |
| 3 | B | 331 | PX4 | O7-C23 | 2.46 | 1.41 | 1.34 | 9 | 3 |
| 3 | B | 353 | PX4 | C10-C9 | 2.46 | 1.57 | 1.50 | 4 | 2 |
| 3 | B | 361 | PX4 | C4-N1 | 2.46 | 1.57 | 1.50 | 5 | 1 |
| 3 | B | 387 | PX4 | O5-C8 | 2.46 | 1.39 | 1.45 | 13 | 2 |
| 3 | A | 637 | PX4 | C31-C30 | 2.46 | 1.64 | 1.51 | 12 | 3 |
| 3 | A | 648 | PX4 | O5-C9 | 2.46 | 1.26 | 1.33 | 1 | 1 |
| 3 | A | 653 | PX4 | C2-N1 | 2.46 | 1.59 | 1.51 | 8 | 1 |
| 3 | B | 324 | PX4 | O7-C23 | 2.46 | 1.27 | 1.34 | 4 | 3 |
| 3 | C | 310 | PX4 | O5-C8 | 2.46 | 1.39 | 1.45 | 6 | 3 |
| 3 | B | 304 | PX4 | C12-C11 | 2.46 | 1.64 | 1.51 | 3 | 1 |
| 3 | A | 622 | PX4 | O5-C8 | 2.45 | 1.39 | 1.45 | 10 | 3 |
| 3 | B | 308 | PX4 | C25-C24 | 2.45 | 1.61 | 1.52 | 8 | 3 |
| 3 | B | 326 | PX4 | O5-C8 | 2.46 | 1.50 | 1.45 | 14 | 4 |
| 3 | B | 374 | PX4 | O5-C8 | 2.46 | 1.39 | 1.45 | 14 | 4 |
| 3 | C | 360 | PX4 | C4-N1 | 2.46 | 1.57 | 1.50 | 5 | 3 |
| 3 | B | 374 | PX4 | C10-C9 | 2.45 | 1.57 | 1.50 | 14 | 1 |
| 3 | B | 378 | PX4 | C20-C19 | 2.45 | 1.64 | 1.51 | 9 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | C | 302 | PX4 | C24-C23 | 2.45 | 1.57 | 1.50 | 12 | 1 |
| 3 | C | 320 | PX4 | C16-C15 | 2.45 | 1.64 | 1.51 | 1 | 1 |
| 3 | A | 636 | PX4 | C19-C18 | 2.45 | 1.64 | 1.51 | 2 | 1 |
| 3 | B | 326 | PX4 | P1-O1 | 2.45 | 1.44 | 1.55 | 2 | 2 |
| 3 | B | 327 | PX4 | C5-N1 | 2.45 | 1.42 | 1.50 | 15 | 3 |
| 3 | C | 327 | PX4 | O7-C7 | 2.45 | 1.40 | 1.46 | 5 | 4 |
| 3 | C | 359 | PX4 | C13-C12 | 2.45 | 1.64 | 1.51 | 10 | 1 |
| 3 | A | 622 | PX4 | C25-C24 | 2.45 | 1.61 | 1.52 | 4 | 3 |
| 3 | B | 336 | PX4 | O7-C7 | 2.45 | 1.40 | 1.46 | 12 | 1 |
| 3 | C | 306 | PX4 | P1-O1 | 2.45 | 1.44 | 1.55 | 5 | 3 |
| 3 | C | 357 | PX4 | C5-N1 | 2.45 | 1.57 | 1.50 | 6 | 1 |
| 3 | B | 302 | PX4 | C4-N1 | 2.45 | 1.57 | 1.50 | 4 | 1 |
| 3 | B | 336 | PX4 | C11-C10 | 2.45 | 1.61 | 1.52 | 13 | 1 |
| 3 | A | 613 | PX4 | C3-N1 | 2.45 | 1.42 | 1.50 | 6 | 1 |
| 3 | B | 309 | PX4 | O5-C8 | 2.45 | 1.50 | 1.45 | 5 | 1 |
| 3 | B | 321 | PX4 | C3-N1 | 2.45 | 1.57 | 1.50 | 4 | 2 |
| 3 | A | 602 | PX4 | C10-C9 | 2.44 | 1.57 | 1.50 | 10 | 4 |
| 3 | A | 624 | PX4 | C17-C16 | 2.44 | 1.63 | 1.51 | 2 | 1 |
| 3 | B | 312 | PX4 | P1-O4 | 2.44 | 1.49 | 1.59 | 12 | 2 |
| 3 | B | 371 | PX4 | C13-C12 | 2.44 | 1.63 | 1.51 | 11 | 1 |
| 3 | B | 375 | PX4 | C2-N1 | 2.45 | 1.58 | 1.51 | 11 | 4 |
| 3 | C | 308 | PX4 | P1-O1 | 2.44 | 1.44 | 1.55 | 2 | 4 |
| 3 | B | 316 | PX4 | C24-C23 | 2.44 | 1.57 | 1.50 | 5 | 4 |
| 3 | B | 338 | PX4 | C2-N1 | 2.44 | 1.58 | 1.51 | 3 | 2 |
| 3 | C | 328 | PX4 | P1-O1 | 2.44 | 1.44 | 1.55 | 3 | 3 |
| 3 | A | 639 | PX4 | C20-C19 | 2.44 | 1.63 | 1.51 | 6 | 1 |
| 3 | A | 644 | PX4 | C5-N1 | 2.44 | 1.42 | 1.50 | 11 | 2 |
| 3 | B | 301 | PX4 | C5-N1 | 2.44 | 1.42 | 1.50 | 4 | 2 |
| 3 | B | 328 | PX4 | C25-C24 | 2.44 | 1.61 | 1.52 | 13 | 1 |
| 3 | B | 337 | PX4 | C24-C23 | 2.44 | 1.57 | 1.50 | 2 | 1 |
| 3 | B | 349 | PX4 | O5-C8 | 2.44 | 1.50 | 1.45 | 5 | 1 |
| 3 | B | 368 | PX4 | C24-C23 | 2.44 | 1.57 | 1.50 | 12 | 2 |
| 3 | B | 380 | PX4 | C4-N1 | 2.44 | 1.57 | 1.50 | 8 | 1 |
| 3 | A | 645 | PX4 | O7-C7 | 2.44 | 1.40 | 1.46 | 11 | 3 |
| 3 | B | 382 | PX4 | O7-C23 | 2.44 | 1.41 | 1.34 | 5 | 3 |
| 3 | A | 611 | PX4 | C3-N1 | 2.44 | 1.57 | 1.50 | 13 | 2 |
| 3 | B | 349 | PX4 | C24-C23 | 2.44 | 1.57 | 1.50 | 10 | 2 |
| 3 | A | 615 | PX4 | C32-C31 | 2.43 | 1.63 | 1.51 | 8 | 2 |
| 3 | B | 352 | PX4 | C11-C10 | 2.43 | 1.61 | 1.52 | 3 | 1 |
| 3 | B | 372 | PX4 | O5-C9 | 2.44 | 1.40 | 1.33 | 1 | 2 |
| 3 | B | 340 | PX4 | O7-C7 | 2.43 | 1.40 | 1.46 | 3 | 2 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 376 | PX4 | C3-N1 | 2.43 | 1.57 | 1.50 | 1 | 1 |
| 3 | B | 393 | PX4 | O5-C9 | 2.43 | 1.26 | 1.33 | 2 | 3 |
| 3 | A | 653 | PX4 | O7-C23 | 2.43 | 1.27 | 1.34 | 3 | 4 |
| 3 | B | 306 | PX4 | C34-C33 | 2.43 | 1.63 | 1.51 | 8 | 1 |
| 3 | B | 324 | PX4 | C2-C1 | 2.43 | 1.58 | 1.51 | 8 | 2 |
| 3 | B | 328 | PX4 | P1-O3 | 2.43 | 1.49 | 1.59 | 13 | 1 |
| 3 | B | 358 | PX4 | C12-C11 | 2.43 | 1.63 | 1.51 | 12 | 1 |
| 3 | B | 387 | PX4 | P1-O1 | 2.43 | 1.44 | 1.55 | 3 | 2 |
| 3 | B | 398 | PX4 | P1-O1 | 2.43 | 1.44 | 1.55 | 10 | 1 |
| 3 | C | 324 | PX4 | C5-N1 | 2.43 | 1.42 | 1.50 | 8 | 2 |
| 3 | C | 358 | PX4 | C8-C7 | 2.43 | 1.58 | 1.50 | 3 | 1 |
| 3 | B | 336 | PX4 | P1-O1 | 2.43 | 1.44 | 1.55 | 1 | 2 |
| 3 | B | 343 | PX4 | C5-N1 | 2.43 | 1.42 | 1.50 | 7 | 2 |
| 3 | B | 357 | PX4 | C14-C13 | 2.43 | 1.63 | 1.51 | 1 | 1 |
| 3 | C | 327 | PX4 | C25-C24 | 2.43 | 1.61 | 1.52 | 11 | 2 |
| 3 | A | 619 | PX4 | P1-O2 | 2.43 | 1.42 | 1.50 | 7 | 3 |
| 3 | A | 639 | PX4 | C11-C10 | 2.43 | 1.61 | 1.52 | 13 | 1 |
| 3 | A | 639 | PX4 | P1-O3 | 2.43 | 1.49 | 1.59 | 14 | 1 |
| 3 | C | 350 | PX4 | C2-C1 | 2.43 | 1.58 | 1.51 | 9 | 7 |
| 3 | B | 304 | PX4 | C2-N1 | 2.43 | 1.44 | 1.51 | 7 | 4 |
| 3 | B | 341 | PX4 | C4-N1 | 2.43 | 1.57 | 1.50 | 5 | 1 |
| 3 | B | 391 | PX4 | P1-O1 | 2.43 | 1.44 | 1.55 | 9 | 1 |
| 3 | C | 303 | PX4 | C18-C17 | 2.43 | 1.63 | 1.51 | 3 | 1 |
| 3 | C | 326 | PX4 | C25-C24 | 2.43 | 1.61 | 1.52 | 3 | 2 |
| 3 | A | 651 | PX4 | C19-C18 | 2.43 | 1.63 | 1.51 | 15 | 1 |
| 3 | A | 631 | PX4 | O5-C9 | 2.43 | 1.40 | 1.33 | 9 | 1 |
| 3 | B | 356 | PX4 | P1-O1 | 2.43 | 1.44 | 1.55 | 8 | 4 |
| 3 | B | 400 | PX4 | C24-C23 | 2.43 | 1.57 | 1.50 | 7 | 3 |
| 3 | C | 302 | PX4 | O5-C8 | 2.43 | 1.50 | 1.45 | 2 | 3 |
| 3 | C | 303 | PX4 | C24-C23 | 2.42 | 1.43 | 1.50 | 4 | 2 |
| 3 | C | 326 | PX4 | P1-O3 | 2.42 | 1.49 | 1.59 | 12 | 1 |
| 3 | C | 344 | PX4 | C2-N1 | 2.42 | 1.44 | 1.51 | 10 | 3 |
| 3 | C | 345 | PX4 | C31-C30 | 2.43 | 1.63 | 1.51 | 4 | 1 |
| 3 | A | 640 | PX4 | C4-N1 | 2.42 | 1.43 | 1.50 | 11 | 2 |
| 3 | C | 303 | PX4 | O7-C23 | 2.42 | 1.41 | 1.34 | 10 | 3 |
| 3 | A | 644 | PX4 | C33-C32 | 2.42 | 1.63 | 1.51 | 14 | 1 |
| 3 | C | 307 | PX4 | C3-N1 | 2.42 | 1.57 | 1.50 | 9 | 3 |
| 3 | C | 321 | PX4 | C25-C24 | 2.42 | 1.61 | 1.52 | 5 | 3 |
| 3 | C | 313 | PX4 | O7-C23 | 2.42 | 1.27 | 1.34 | 14 | 3 |
| 3 | C | 325 | PX4 | P1-O1 | 2.42 | 1.44 | 1.55 | 6 | 2 |
| 3 | C | 341 | PX4 | C25-C24 | 2.42 | 1.61 | 1.52 | 11 | 3 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | C | 356 | PX4 | O5-C9 | 2.42 | 1.26 | 1.33 | 4 | 1 |
| 3 | B | 302 | PX4 | C15-C14 | 2.42 | 1.63 | 1.51 | 4 | 2 |
| 3 | B | 373 | PX4 | O5-C9 | 2.42 | 1.40 | 1.33 | 10 | 1 |
| 3 | B | 387 | PX4 | C30-C29 | 2.42 | 1.63 | 1.51 | 11 | 2 |
| 3 | C | 304 | PX4 | C13-C12 | 2.42 | 1.63 | 1.51 | 12 | 1 |
| 3 | C | 314 | PX4 | C27-C26 | 2.42 | 1.63 | 1.51 | 12 | 1 |
| 3 | A | 649 | PX4 | C14-C13 | 2.42 | 1.63 | 1.51 | 11 | 1 |
| 3 | C | 325 | PX4 | C24-C23 | 2.42 | 1.57 | 1.50 | 14 | 2 |
| 3 | A | 602 | PX4 | C4-N1 | 2.42 | 1.57 | 1.50 | 12 | 1 |
| 3 | A | 624 | PX4 | P1-O1 | 2.42 | 1.44 | 1.55 | 9 | 3 |
| 3 | A | 634 | PX4 | C10-C9 | 2.42 | 1.57 | 1.50 | 8 | 3 |
| 3 | B | 319 | PX4 | C2-N1 | 2.42 | 1.44 | 1.51 | 2 | 1 |
| 3 | B | 366 | PX4 | P1-O1 | 2.42 | 1.44 | 1.55 | 3 | 2 |
| 3 | B | 399 | PX4 | C25-C24 | 2.42 | 1.61 | 1.52 | 5 | 1 |
| 3 | C | 301 | PX4 | C15-C14 | 2.42 | 1.63 | 1.51 | 12 | 1 |
| 3 | B | 321 | PX4 | C10-C9 | 2.42 | 1.57 | 1.50 | 3 | 2 |
| 3 | A | 606 | PX4 | P1-O2 | 2.41 | 1.42 | 1.50 | 14 | 1 |
| 3 | A | 609 | PX4 | C3-N1 | 2.42 | 1.43 | 1.50 | 13 | 2 |
| 3 | B | 333 | PX4 | C29-C28 | 2.42 | 1.63 | 1.51 | 2 | 1 |
| 3 | B | 361 | PX4 | C29-C28 | 2.42 | 1.63 | 1.51 | 8 | 1 |
| 3 | B | 391 | PX4 | C5-N1 | 2.42 | 1.57 | 1.50 | 13 | 2 |
| 3 | B | 395 | PX4 | C10-C9 | 2.42 | 1.57 | 1.50 | 1 | 4 |
| 3 | C | 360 | PX4 | O7-C23 | 2.42 | 1.27 | 1.34 | 9 | 2 |
| 3 | A | 622 | PX4 | O4-C6 | 2.41 | 1.53 | 1.44 | 7 | 1 |
| 3 | B | 384 | PX4 | C20-C19 | 2.41 | 1.63 | 1.51 | 8 | 1 |
| 3 | C | 312 | PX4 | C11-C10 | 2.42 | 1.61 | 1.52 | 10 | 3 |
| 3 | A | 601 | PX4 | P1-O1 | 2.41 | 1.44 | 1.55 | 4 | 5 |
| 3 | A | 627 | PX4 | O5-C9 | 2.41 | 1.40 | 1.33 | 10 | 2 |
| 3 | A | 615 | PX4 | C19-C18 | 2.41 | 1.63 | 1.51 | 11 | 1 |
| 3 | B | 309 | PX4 | C3-N1 | 2.41 | 1.57 | 1.50 | 2 | 1 |
| 3 | B | 347 | PX4 | O7-C7 | 2.41 | 1.52 | 1.46 | 8 | 4 |
| 3 | B | 357 | PX4 | C2-N1 | 2.41 | 1.58 | 1.51 | 4 | 3 |
| 3 | C | 324 | PX4 | C2-N1 | 2.41 | 1.44 | 1.51 | 13 | 1 |
| 3 | A | 621 | PX4 | C5-N1 | 2.41 | 1.57 | 1.50 | 9 | 1 |
| 3 | A | 638 | PX4 | C5-N1 | 2.41 | 1.43 | 1.50 | 3 | 2 |
| 3 | C | 314 | PX4 | C2-C1 | 2.41 | 1.58 | 1.51 | 10 | 2 |
| 3 | C | 345 | PX4 | O7-C7 | 2.41 | 1.40 | 1.46 | 4 | 1 |
| 3 | C | 349 | PX4 | C4-N1 | 2.41 | 1.57 | 1.50 | 7 | 1 |
| 3 | B | 342 | PX4 | C11-C10 | 2.41 | 1.61 | 1.52 | 9 | 2 |
| 3 | B | 375 | PX4 | C4-N1 | 2.41 | 1.57 | 1.50 | 9 | 2 |
| 3 | B | 320 | PX4 | P1-O4 | 2.41 | 1.50 | 1.59 | 13 | 2 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | C | 314 | PX4 | O7-C23 | 2.41 | 1.27 | 1.34 | 1 | 1 |
| 3 | C | 326 | PX4 | C2-N1 | 2.41 | 1.58 | 1.51 | 9 | 1 |
| 3 | A | 609 | PX4 | C5-N1 | 2.41 | 1.57 | 1.50 | 5 | 3 |
| 3 | B | 399 | PX4 | C4-N1 | 2.41 | 1.43 | 1.50 | 2 | 2 |
| 3 | C | 304 | PX4 | O3-C1 | 2.41 | 1.35 | 1.44 | 4 | 1 |
| 3 | C | 327 | PX4 | C4-N1 | 2.41 | 1.57 | 1.50 | 15 | 3 |
| 3 | A | 605 | PX4 | C5-N1 | 2.40 | 1.57 | 1.50 | 9 | 1 |
| 3 | A | 626 | PX4 | C4-N1 | 2.41 | 1.57 | 1.50 | 2 | 1 |
| 3 | B | 322 | PX4 | C5-N1 | 2.41 | 1.43 | 1.50 | 4 | 1 |
| 3 | B | 334 | PX4 | C4-N1 | 2.41 | 1.43 | 1.50 | 7 | 1 |
| 3 | B | 351 | PX4 | O5-C8 | 2.41 | 1.39 | 1.45 | 12 | 1 |
| 3 | B | 397 | PX4 | C24-C23 | 2.40 | 1.57 | 1.50 | 11 | 4 |
| 3 | B | 365 | PX4 | O3-C1 | 2.40 | 1.35 | 1.44 | 5 | 1 |
| 3 | B | 370 | PX4 | C11-C10 | 2.40 | 1.61 | 1.52 | 4 | 1 |
| 3 | C | 340 | PX4 | P1-O1 | 2.40 | 1.44 | 1.55 | 8 | 4 |
| 3 | B | 331 | PX4 | C10-C9 | 2.40 | 1.57 | 1.50 | 9 | 3 |
| 3 | B | 383 | PX4 | C25-C24 | 2.40 | 1.61 | 1.52 | 2 | 2 |
| 3 | B | 395 | PX4 | P1-O2 | 2.40 | 1.42 | 1.50 | 2 | 1 |
| 3 | C | 307 | PX4 | O7-C23 | 2.40 | 1.41 | 1.34 | 10 | 2 |
| 3 | C | 350 | PX4 | P1-O1 | 2.40 | 1.44 | 1.55 | 9 | 2 |
| 3 | A | 626 | PX4 | O3-C1 | 2.40 | 1.35 | 1.44 | 13 | 1 |
| 3 | A | 644 | PX4 | P1-O1 | 2.40 | 1.44 | 1.55 | 6 | 4 |
| 3 | B | 316 | PX4 | C10-C9 | 2.40 | 1.57 | 1.50 | 3 | 1 |
| 3 | A | 612 | PX4 | C10-C9 | 2.40 | 1.57 | 1.50 | 9 | 1 |
| 3 | B | 390 | PX4 | C30-C29 | 2.40 | 1.63 | 1.51 | 13 | 1 |
| 3 | B | 363 | PX4 | O7-C23 | 2.40 | 1.27 | 1.34 | 2 | 2 |
| 3 | C | 358 | PX4 | C2-C1 | 2.40 | 1.58 | 1.51 | 3 | 6 |
| 3 | B | 322 | PX4 | P1-O1 | 2.40 | 1.44 | 1.55 | 3 | 2 |
| 3 | B | 344 | PX4 | C20-C19 | 2.40 | 1.63 | 1.51 | 5 | 1 |
| 3 | C | 332 | PX4 | C31-C30 | 2.40 | 1.63 | 1.51 | 10 | 1 |
| 3 | C | 334 | PX4 | C2-N1 | 2.40 | 1.58 | 1.51 | 6 | 2 |
| 3 | C | 335 | PX4 | O5-C9 | 2.40 | 1.40 | 1.33 | 11 | 1 |
| 3 | C | 354 | PX4 | C16-C15 | 2.40 | 1.63 | 1.51 | 14 | 1 |
| 3 | A | 629 | PX4 | O5-C8 | 2.39 | 1.50 | 1.45 | 3 | 2 |
| 3 | B | 309 | PX4 | C5-N1 | 2.39 | 1.57 | 1.50 | 5 | 1 |
| 3 | B | 330 | PX4 | C25-C24 | 2.39 | 1.61 | 1.52 | 5 | 1 |
| 3 | A | 653 | PX4 | O4-C6 | 2.39 | 1.35 | 1.44 | 3 | 1 |
| 3 | B | 329 | PX4 | O3-C1 | 2.39 | 1.35 | 1.44 | 12 | 1 |
| 3 | B | 357 | PX4 | P1-O1 | 2.39 | 1.44 | 1.55 | 12 | 3 |
| 3 | C | 324 | PX4 | C26-C25 | 2.39 | 1.63 | 1.51 | 6 | 1 |
| 3 | C | 340 | PX4 | C31-C30 | 2.39 | 1.63 | 1.51 | 11 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | C | 356 | PX4 | C11-C10 | 2.39 | 1.61 | 1.52 | 8 | 1 |
| 3 | B | 324 | PX4 | C4-N1 | 2.39 | 1.43 | 1.50 | 1 | 2 |
| 3 | B | 330 | PX4 | C3-N1 | 2.39 | 1.56 | 1.50 | 7 | 1 |
| 3 | B | 381 | PX4 | O5-C8 | 2.39 | 1.39 | 1.45 | 12 | 1 |
| 3 | C | 314 | PX4 | P1-O4 | 2.39 | 1.50 | 1.59 | 9 | 1 |
| 3 | A | 606 | PX4 | O5-C8 | 2.39 | 1.50 | 1.45 | 9 | 2 |
| 3 | B | 348 | PX4 | C25-C24 | 2.39 | 1.61 | 1.52 | 8 | 3 |
| 3 | C | 312 | PX4 | C32-C31 | 2.39 | 1.63 | 1.51 | 5 | 1 |
| 3 | C | 338 | PX4 | P1-O2 | 2.39 | 1.42 | 1.50 | 7 | 2 |
| 3 | C | 352 | PX4 | P1-O4 | 2.39 | 1.68 | 1.59 | 8 | 1 |
| 3 | B | 353 | PX4 | O5-C8 | 2.39 | 1.50 | 1.45 | 12 | 1 |
| 3 | A | 603 | PX4 | C11-C10 | 2.39 | 1.60 | 1.52 | 7 | 2 |
| 3 | B | 307 | PX4 | C3-N1 | 2.39 | 1.56 | 1.50 | 7 | 2 |
| 3 | B | 353 | PX4 | C3-N1 | 2.39 | 1.56 | 1.50 | 7 | 2 |
| 3 | B | 400 | PX4 | C18-C17 | 2.39 | 1.63 | 1.51 | 12 | 1 |
| 3 | C | 348 | PX4 | P1-O2 | 2.39 | 1.42 | 1.50 | 11 | 2 |
| 3 | C | 356 | PX4 | C25-C24 | 2.39 | 1.60 | 1.52 | 10 | 1 |
| 3 | B | 344 | PX4 | C3-N1 | 2.39 | 1.56 | 1.50 | 14 | 2 |
| 3 | C | 363 | PX4 | O7-C23 | 2.39 | 1.41 | 1.34 | 9 | 2 |
| 3 | C | 304 | PX4 | O8-C23 | 2.39 | 1.15 | 1.22 | 2 | 1 |
| 3 | C | 311 | PX4 | C25-C24 | 2.39 | 1.60 | 1.52 | 1 | 1 |
| 3 | A | 602 | PX4 | C11-C10 | 2.39 | 1.60 | 1.52 | 2 | 2 |
| 3 | C | 312 | PX4 | C4-N1 | 2.39 | 1.43 | 1.50 | 9 | 1 |
| 3 | C | 345 | PX4 | P1-O1 | 2.39 | 1.44 | 1.55 | 8 | 3 |
| 3 | A | 604 | PX4 | O7-C23 | 2.38 | 1.27 | 1.34 | 8 | 1 |
| 3 | A | 643 | PX4 | C24-C23 | 2.39 | 1.57 | 1.50 | 11 | 2 |
| 3 | C | 305 | PX4 | P1-O4 | 2.39 | 1.50 | 1.59 | 1 | 2 |
| 3 | C | 362 | PX4 | C27-C26 | 2.39 | 1.63 | 1.51 | 11 | 1 |
| 3 | A | 646 | PX4 | C5-N1 | 2.38 | 1.56 | 1.50 | 1 | 3 |
| 3 | B | 315 | PX4 | O5-C8 | 2.38 | 1.39 | 1.45 | 11 | 3 |
| 3 | A | 607 | PX4 | O7-C23 | 2.38 | 1.41 | 1.34 | 9 | 3 |
| 3 | A | 648 | PX4 | O4-C6 | 2.38 | 1.35 | 1.44 | 2 | 1 |
| 3 | B | 301 | PX4 | C11-C10 | 2.38 | 1.60 | 1.52 | 1 | 4 |
| 3 | B | 363 | PX4 | C11-C10 | 2.38 | 1.60 | 1.52 | 14 | 1 |
| 3 | C | 334 | PX4 | C11-C10 | 2.38 | 1.60 | 1.52 | 9 | 1 |
| 3 | C | 350 | PX4 | C10-C9 | 2.38 | 1.57 | 1.50 | 11 | 2 |
| 3 | B | 327 | PX4 | O7-C23 | 2.38 | 1.27 | 1.34 | 13 | 1 |
| 3 | B | 338 | PX4 | C18-C17 | 2.38 | 1.63 | 1.51 | 10 | 1 |
| 3 | B | 358 | PX4 | O5-C9 | 2.38 | 1.26 | 1.33 | 4 | 1 |
| 3 | B | 371 | PX4 | C25-C24 | 2.38 | 1.60 | 1.52 | 14 | 1 |
| 3 | B | 356 | PX4 | C33-C32 | 2.38 | 1.63 | 1.51 | 10 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | C | 328 | PX4 | O5-C8 | 2.38 | 1.39 | 1.45 | 12 | 2 |
| 3 | B | 369 | PX4 | C25-C24 | 2.38 | 1.60 | 1.52 | 8 | 2 |
| 3 | B | 376 | PX4 | O5-C8 | 2.38 | 1.39 | 1.45 | 7 | 1 |
| 3 | B | 324 | PX4 | C16-C15 | 2.38 | 1.63 | 1.51 | 3 | 1 |
| 3 | B | 326 | PX4 | O5-C9 | 2.38 | 1.26 | 1.33 | 9 | 1 |
| 3 | B | 382 | PX4 | P1-O1 | 2.38 | 1.44 | 1.55 | 2 | 2 |
| 3 | B | 390 | PX4 | P1-O3 | 2.38 | 1.50 | 1.59 | 2 | 1 |
| 3 | B | 390 | PX4 | C4-N1 | 2.38 | 1.43 | 1.50 | 6 | 3 |
| 3 | B | 396 | PX4 | C18-C17 | 2.38 | 1.63 | 1.51 | 5 | 1 |
| 3 | C | 349 | PX4 | P1-O4 | 2.38 | 1.68 | 1.59 | 15 | 1 |
| 3 | A | 602 | PX4 | C19-C18 | 2.38 | 1.63 | 1.51 | 15 | 1 |
| 3 | B | 333 | PX4 | C5-N1 | 2.38 | 1.43 | 1.50 | 13 | 3 |
| 3 | A | 610 | PX4 | C25-C24 | 2.37 | 1.60 | 1.52 | 12 | 2 |
| 3 | A | 652 | PX4 | C2-C1 | 2.38 | 1.58 | 1.51 | 7 | 2 |
| 3 | B | 320 | PX4 | C24-C23 | 2.38 | 1.57 | 1.50 | 3 | 1 |
| 3 | B | 326 | PX4 | C34-C33 | 2.38 | 1.63 | 1.51 | 13 | 1 |
| 3 | B | 380 | PX4 | C10-C9 | 2.38 | 1.57 | 1.50 | 10 | 2 |
| 3 | A | 640 | PX4 | P1-O4 | 2.37 | 1.68 | 1.59 | 6 | 1 |
| 3 | A | 647 | PX4 | C3-N1 | 2.37 | 1.43 | 1.50 | 6 | 1 |
| 3 | A | 648 | PX4 | C24-C23 | 2.37 | 1.57 | 1.50 | 14 | 3 |
| 3 | B | 325 | PX4 | C27-C26 | 2.37 | 1.63 | 1.51 | 10 | 1 |
| 3 | B | 328 | PX4 | C16-C15 | 2.37 | 1.63 | 1.51 | 9 | 1 |
| 3 | B | 362 | PX4 | P1-O1 | 2.37 | 1.44 | 1.55 | 12 | 3 |
| 3 | A | 629 | PX4 | C10-C9 | 2.37 | 1.57 | 1.50 | 13 | 2 |
| 3 | B | 309 | PX4 | C6-C7 | 2.37 | 1.58 | 1.50 | 11 | 3 |
| 3 | B | 323 | PX4 | C27-C26 | 2.37 | 1.63 | 1.51 | 7 | 1 |
| 3 | B | 399 | PX4 | O7-C23 | 2.37 | 1.27 | 1.34 | 2 | 1 |
| 3 | C | 341 | PX4 | O5-C9 | 2.37 | 1.40 | 1.33 | 10 | 1 |
| 3 | A | 603 | PX4 | C25-C24 | 2.37 | 1.60 | 1.52 | 8 | 2 |
| 3 | A | 636 | PX4 | C25-C24 | 2.37 | 1.60 | 1.52 | 7 | 2 |
| 3 | B | 344 | PX4 | C18-C17 | 2.37 | 1.63 | 1.51 | 7 | 1 |
| 3 | B | 376 | PX4 | P1-O1 | 2.37 | 1.44 | 1.55 | 1 | 4 |
| 3 | B | 386 | PX4 | C11-C10 | 2.37 | 1.60 | 1.52 | 9 | 1 |
| 3 | C | 311 | PX4 | C11-C10 | 2.37 | 1.60 | 1.52 | 14 | 1 |
| 3 | C | 330 | PX4 | O5-C8 | 2.37 | 1.50 | 1.45 | 6 | 2 |
| 3 | B | 387 | PX4 | C24-C23 | 2.37 | 1.57 | 1.50 | 2 | 1 |
| 3 | C | 355 | PX4 | C3-N1 | 2.37 | 1.43 | 1.50 | 15 | 2 |
| 3 | B | 312 | PX4 | C20-C19 | 2.37 | 1.63 | 1.51 | 12 | 1 |
| 3 | B | 371 | PX4 | C30-C29 | 2.37 | 1.63 | 1.51 | 2 | 1 |
| 3 | B | 392 | PX4 | C5-N1 | 2.37 | 1.56 | 1.50 | 6 | 1 |
| 3 | A | 639 | PX4 | O5-C8 | 2.37 | 1.50 | 1.45 | 13 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 308 | PX4 | C32-C31 | 2.37 | 1.63 | 1.51 | 7 | 1 |
| 3 | C | 313 | PX4 | C31-C30 | 2.37 | 1.63 | 1.51 | 11 | 1 |
| 3 | C | 331 | PX4 | C12-C11 | 2.37 | 1.63 | 1.51 | 8 | 1 |
| 3 | B | 400 | PX4 | C31-C30 | 2.36 | 1.63 | 1.51 | 15 | 1 |
| 3 | C | 328 | PX4 | C26-C25 | 2.36 | 1.63 | 1.51 | 1 | 1 |
| 3 | C | 329 | PX4 | P1-O1 | 2.36 | 1.44 | 1.55 | 1 | 4 |
| 3 | C | 335 | PX4 | C2-N1 | 2.36 | 1.44 | 1.51 | 11 | 2 |
| 3 | C | 349 | PX4 | C24-C23 | 2.36 | 1.57 | 1.50 | 15 | 4 |
| 3 | A | 626 | PX4 | P1-O4 | 2.36 | 1.50 | 1.59 | 10 | 1 |
| 3 | A | 632 | PX4 | C33-C32 | 2.36 | 1.63 | 1.51 | 13 | 1 |
| 3 | B | 380 | PX4 | P1-O1 | 2.36 | 1.44 | 1.55 | 8 | 2 |
| 3 | C | 353 | PX4 | C4-N1 | 2.36 | 1.43 | 1.50 | 14 | 2 |
| 3 | A | 617 | PX4 | O3-C1 | 2.36 | 1.35 | 1.44 | 5 | 1 |
| 3 | A | 617 | PX4 | C3-N1 | 2.36 | 1.56 | 1.50 | 6 | 3 |
| 3 | A | 630 | PX4 | C5-N1 | 2.36 | 1.56 | 1.50 | 11 | 2 |
| 3 | B | 340 | PX4 | P1-O3 | 2.36 | 1.50 | 1.59 | 9 | 1 |
| 3 | B | 376 | PX4 | C11-C10 | 2.36 | 1.60 | 1.52 | 1 | 1 |
| 3 | C | 307 | PX4 | C11-C10 | 2.36 | 1.60 | 1.52 | 1 | 2 |
| 3 | C | 305 | PX4 | C10-C9 | 2.36 | 1.57 | 1.50 | 12 | 3 |
| 3 | C | 331 | PX4 | C24-C23 | 2.36 | 1.57 | 1.50 | 15 | 1 |
| 3 | B | 321 | PX4 | C5-N1 | 2.36 | 1.43 | 1.50 | 8 | 1 |
| 3 | B | 347 | PX4 | O7-C23 | 2.36 | 1.27 | 1.34 | 1 | 2 |
| 3 | C | 332 | PX4 | P1-O3 | 2.36 | 1.50 | 1.59 | 8 | 1 |
| 3 | C | 334 | PX4 | C26-C25 | 2.36 | 1.63 | 1.51 | 1 | 2 |
| 3 | A | 623 | PX4 | C11-C10 | 2.36 | 1.60 | 1.52 | 13 | 1 |
| 3 | A | 614 | PX4 | O7-C23 | 2.36 | 1.27 | 1.34 | 12 | 2 |
| 3 | A | 629 | PX4 | C3-N1 | 2.36 | 1.56 | 1.50 | 13 | 2 |
| 3 | B | 305 | PX4 | O7-C23 | 2.36 | 1.27 | 1.34 | 12 | 1 |
| 3 | B | 309 | PX4 | P1-O1 | 2.36 | 1.44 | 1.55 | 1 | 2 |
| 3 | B | 364 | PX4 | C28-C27 | 2.36 | 1.63 | 1.51 | 5 | 1 |
| 3 | A | 605 | PX4 | P1-O4 | 2.35 | 1.68 | 1.59 | 9 | 1 |
| 3 | A | 644 | PX4 | C28-C27 | 2.36 | 1.63 | 1.51 | 12 | 1 |
| 3 | A | 654 | PX4 | C5-N1 | 2.36 | 1.43 | 1.50 | 7 | 1 |
| 3 | B | 348 | PX4 | O5-C9 | 2.35 | 1.40 | 1.33 | 3 | 1 |
| 3 | A | 635 | PX4 | O3-C1 | 2.35 | 1.35 | 1.44 | 12 | 1 |
| 3 | A | 645 | PX4 | C32-C31 | 2.35 | 1.63 | 1.51 | 14 | 1 |
| 3 | B | 323 | PX4 | P1-O1 | 2.35 | 1.44 | 1.55 | 1 | 2 |
| 3 | B | 377 | PX4 | C3-N1 | 2.35 | 1.43 | 1.50 | 12 | 1 |
| 3 | B | 399 | PX4 | O5-C9 | 2.35 | 1.26 | 1.33 | 4 | 2 |
| 3 | A | 601 | PX4 | C4-N1 | 2.35 | 1.43 | 1.50 | 5 | 2 |
| 3 | A | 626 | PX4 | C14-C13 | 2.35 | 1.63 | 1.51 | 15 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | A | 643 | PX4 | P1-O4 | 2.35 | 1.50 | 1.59 | 14 | 1 |
| 3 | B | 342 | PX4 | C4-N1 | 2.35 | 1.43 | 1.50 | 5 | 1 |
| 3 | A | 611 | PX4 | P1-O1 | 2.35 | 1.44 | 1.55 | 3 | 2 |
| 3 | A | 622 | PX4 | P1-O1 | 2.35 | 1.44 | 1.55 | 8 | 3 |
| 3 | A | 631 | PX4 | C11-C10 | 2.35 | 1.60 | 1.52 | 9 | 1 |
| 3 | A | 649 | PX4 | O5-C9 | 2.35 | 1.26 | 1.33 | 10 | 2 |
| 3 | A | 651 | PX4 | C20-C19 | 2.35 | 1.63 | 1.51 | 4 | 1 |
| 3 | B | 330 | PX4 | C10-C9 | 2.35 | 1.57 | 1.50 | 4 | 3 |
| 3 | B | 358 | PX4 | O5-C8 | 2.35 | 1.39 | 1.45 | 15 | 1 |
| 3 | B | 360 | PX4 | C11-C10 | 2.35 | 1.60 | 1.52 | 4 | 2 |
| 3 | B | 365 | PX4 | O5-C9 | 2.35 | 1.40 | 1.33 | 9 | 1 |
| 3 | B | 378 | PX4 | P1-O1 | 2.35 | 1.44 | 1.55 | 13 | 5 |
| 3 | B | 397 | PX4 | C2-N1 | 2.35 | 1.58 | 1.51 | 5 | 2 |
| 3 | A | 623 | PX4 | C24-C23 | 2.35 | 1.57 | 1.50 | 2 | 2 |
| 3 | B | 302 | PX4 | C26-C25 | 2.35 | 1.63 | 1.51 | 15 | 1 |
| 3 | B | 388 | PX4 | C24-C23 | 2.35 | 1.43 | 1.50 | 3 | 1 |
| 3 | B | 394 | PX4 | P1-O1 | 2.35 | 1.44 | 1.55 | 9 | 3 |
| 3 | A | 614 | PX4 | C4-N1 | 2.34 | 1.43 | 1.50 | 4 | 1 |
| 3 | A | 653 | PX4 | P1-O4 | 2.35 | 1.50 | 1.59 | 2 | 1 |
| 3 | B | 320 | PX4 | C2-C1 | 2.35 | 1.58 | 1.51 | 10 | 4 |
| 3 | C | 354 | PX4 | O7-C23 | 2.35 | 1.27 | 1.34 | 13 | 1 |
| 3 | B | 331 | PX4 | C11-C10 | 2.35 | 1.43 | 1.52 | 7 | 2 |
| 3 | B | 308 | PX4 | P1-O1 | 2.34 | 1.44 | 1.55 | 8 | 1 |
| 3 | B | 352 | PX4 | C26-C25 | 2.34 | 1.63 | 1.51 | 8 | 1 |
| 3 | B | 383 | PX4 | C3-N1 | 2.34 | 1.56 | 1.50 | 9 | 2 |
| 3 | B | 385 | PX4 | C24-C23 | 2.35 | 1.57 | 1.50 | 9 | 2 |
| 3 | B | 394 | PX4 | C10-C9 | 2.35 | 1.57 | 1.50 | 9 | 2 |
| 3 | B | 391 | PX4 | C11-C10 | 2.34 | 1.60 | 1.52 | 7 | 1 |
| 3 | C | 313 | PX4 | C11-C10 | 2.34 | 1.60 | 1.52 | 15 | 1 |
| 3 | C | 326 | PX4 | C33-C32 | 2.34 | 1.63 | 1.51 | 14 | 1 |
| 3 | C | 342 | PX4 | C4-N1 | 2.34 | 1.43 | 1.50 | 7 | 1 |
| 3 | A | 611 | PX4 | O5-C8 | 2.34 | 1.39 | 1.45 | 12 | 2 |
| 3 | B | 306 | PX4 | C25-C24 | 2.34 | 1.60 | 1.52 | 7 | 1 |
| 3 | B | 338 | PX4 | O5-C8 | 2.34 | 1.39 | 1.45 | 9 | 1 |
| 3 | C | 331 | PX4 | C25-C24 | 2.34 | 1.60 | 1.52 | 9 | 2 |
| 3 | C | 339 | PX4 | P1-O2 | 2.34 | 1.42 | 1.50 | 12 | 1 |
| 3 | B | 341 | PX4 | O5-C8 | 2.34 | 1.50 | 1.45 | 8 | 3 |
| 3 | B | 360 | PX4 | C28-C27 | 2.34 | 1.63 | 1.51 | 4 | 1 |
| 3 | B | 365 | PX4 | C25-C24 | 2.34 | 1.60 | 1.52 | 15 | 1 |
| 3 | C | 348 | PX4 | C25-C24 | 2.34 | 1.60 | 1.52 | 9 | 2 |
| 3 | B | 309 | PX4 | C14-C13 | 2.34 | 1.63 | 1.51 | 5 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 311 | PX4 | P1-O1 | 2.34 | 1.44 | 1.55 | 8 | 5 |
| 3 | B | 337 | PX4 | P1-O4 | 2.34 | 1.50 | 1.59 | 15 | 1 |
| 3 | A | 641 | PX4 | C24-C23 | 2.34 | 1.57 | 1.50 | 11 | 2 |
| 3 | B | 327 | PX4 | P1-O4 | 2.34 | 1.50 | 1.59 | 14 | 2 |
| 3 | B | 385 | PX4 | C25-C24 | 2.34 | 1.60 | 1.52 | 11 | 3 |
| 3 | B | 386 | PX4 | O6-C9 | 2.34 | 1.29 | 1.22 | 14 | 1 |
| 3 | B | 390 | PX4 | C24-C23 | 2.34 | 1.57 | 1.50 | 14 | 1 |
| 3 | A | 602 | PX4 | C32-C31 | 2.34 | 1.63 | 1.51 | 14 | 2 |
| 3 | A | 611 | PX4 | C24-C23 | 2.34 | 1.57 | 1.50 | 4 | 2 |
| 3 | A | 607 | PX4 | P1-O1 | 2.34 | 1.44 | 1.55 | 12 | 3 |
| 3 | A | 607 | PX4 | O5-C8 | 2.34 | 1.50 | 1.45 | 9 | 1 |
| 3 | A | 617 | PX4 | C27-C26 | 2.34 | 1.63 | 1.51 | 10 | 1 |
| 3 | A | 620 | PX4 | C30-C29 | 2.34 | 1.63 | 1.51 | 7 | 1 |
| 3 | B | 342 | PX4 | C2-N1 | 2.34 | 1.58 | 1.51 | 1 | 1 |
| 3 | B | 392 | PX4 | O5-C8 | 2.34 | 1.50 | 1.45 | 9 | 1 |
| 3 | B | 394 | PX4 | P1-O3 | 2.34 | 1.50 | 1.59 | 8 | 1 |
| 3 | B | 400 | PX4 | O5-C9 | 2.34 | 1.40 | 1.33 | 3 | 1 |
| 3 | A | 624 | PX4 | O7-C7 | 2.34 | 1.41 | 1.46 | 1 | 1 |
| 3 | B | 368 | PX4 | C2-N1 | 2.34 | 1.58 | 1.51 | 5 | 2 |
| 3 | B | 373 | PX4 | O7-C7 | 2.34 | 1.41 | 1.46 | 10 | 1 |
| 3 | B | 398 | PX4 | O7-C23 | 2.34 | 1.27 | 1.34 | 5 | 3 |
| 3 | C | 336 | PX4 | O5-C9 | 2.34 | 1.40 | 1.33 | 10 | 3 |
| 3 | B | 313 | PX4 | C2-C1 | 2.34 | 1.58 | 1.51 | 2 | 4 |
| 3 | C | 303 | PX4 | C4-N1 | 2.34 | 1.56 | 1.50 | 7 | 2 |
| 3 | A | 608 | PX4 | C30-C29 | 2.33 | 1.63 | 1.51 | 14 | 1 |
| 3 | A | 620 | PX4 | C17-C16 | 2.33 | 1.63 | 1.51 | 5 | 1 |
| 3 | A | 623 | PX4 | P1-O4 | 2.33 | 1.68 | 1.59 | 13 | 2 |
| 3 | B | 308 | PX4 | P1-O2 | 2.33 | 1.42 | 1.50 | 13 | 1 |
| 3 | B | 318 | PX4 | C24-C23 | 2.33 | 1.57 | 1.50 | 3 | 1 |
| 3 | B | 359 | PX4 | O5-C9 | 2.33 | 1.26 | 1.33 | 7 | 1 |
| 3 | B | 373 | PX4 | C13-C12 | 2.33 | 1.63 | 1.51 | 5 | 1 |
| 3 | C | 343 | PX4 | C25-C24 | 2.33 | 1.60 | 1.52 | 14 | 1 |
| 3 | C | 358 | PX4 | C25-C24 | 2.33 | 1.60 | 1.52 | 7 | 2 |
| 3 | C | 339 | PX4 | O7-C23 | 2.33 | 1.27 | 1.34 | 1 | 2 |
| 3 | A | 606 | PX4 | O7-C7 | 2.33 | 1.41 | 1.46 | 11 | 1 |
| 3 | B | 306 | PX4 | P1-O4 | 2.33 | 1.50 | 1.59 | 9 | 1 |
| 3 | B | 339 | PX4 | C4-N1 | 2.33 | 1.43 | 1.50 | 15 | 1 |
| 3 | B | 355 | PX4 | C2-N1 | 2.33 | 1.58 | 1.51 | 1 | 1 |
| 3 | A | 621 | PX4 | O4-C6 | 2.33 | 1.35 | 1.44 | 6 | 1 |
| 3 | A | 643 | PX4 | O7-C7 | 2.33 | 1.41 | 1.46 | 7 | 1 |
| 3 | A | 653 | PX4 | C4-N1 | 2.33 | 1.56 | 1.50 | 5 | 2 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 303 | PX4 | P1-O1 | 2.33 | 1.44 | 1.55 | 9 | 4 |
| 3 | B | 362 | PX4 | O7-C23 | 2.33 | 1.27 | 1.34 | 6 | 3 |
| 3 | C | 305 | PX4 | C24-C23 | 2.33 | 1.57 | 1.50 | 13 | 2 |
| 3 | C | 343 | PX4 | C11-C10 | 2.33 | 1.60 | 1.52 | 13 | 2 |
| 3 | B | 332 | PX4 | P1-O1 | 2.33 | 1.44 | 1.55 | 12 | 3 |
| 3 | B | 368 | PX4 | C17-C16 | 2.33 | 1.63 | 1.51 | 9 | 1 |
| 3 | C | 309 | PX4 | O7-C23 | 2.33 | 1.27 | 1.34 | 7 | 2 |
| 3 | B | 307 | PX4 | C27-C26 | 2.33 | 1.63 | 1.51 | 11 | 3 |
| 3 | B | 376 | PX4 | O7-C23 | 2.33 | 1.27 | 1.34 | 4 | 2 |
| 3 | B | 358 | PX4 | C4-N1 | 2.33 | 1.56 | 1.50 | 11 | 2 |
| 3 | B | 377 | PX4 | C24-C23 | 2.33 | 1.57 | 1.50 | 1 | 2 |
| 3 | C | 337 | PX4 | C32-C31 | 2.33 | 1.63 | 1.51 | 14 | 1 |
| 3 | C | 346 | PX4 | O5-C8 | 2.33 | 1.40 | 1.45 | 8 | 3 |
| 3 | A | 616 | PX4 | P1-O1 | 2.32 | 1.44 | 1.55 | 8 | 2 |
| 3 | A | 621 | PX4 | C19-C18 | 2.32 | 1.63 | 1.51 | 5 | 1 |
| 3 | A | 650 | PX4 | O5-C9 | 2.32 | 1.40 | 1.33 | 13 | 2 |
| 3 | B | 310 | PX4 | C13-C12 | 2.32 | 1.63 | 1.51 | 3 | 1 |
| 3 | B | 335 | PX4 | C27-C26 | 2.32 | 1.63 | 1.51 | 11 | 1 |
| 3 | C | 357 | PX4 | C29-C28 | 2.33 | 1.63 | 1.51 | 10 | 1 |
| 3 | A | 636 | PX4 | O7-C23 | 2.32 | 1.27 | 1.34 | 13 | 1 |
| 3 | B | 377 | PX4 | C19-C18 | 2.32 | 1.63 | 1.51 | 10 | 1 |
| 3 | B | 390 | PX4 | P1-O1 | 2.32 | 1.44 | 1.55 | 12 | 1 |
| 3 | C | 304 | PX4 | O7-C7 | 2.32 | 1.41 | 1.46 | 2 | 3 |
| 3 | C | 350 | PX4 | P1-O4 | 2.32 | 1.68 | 1.59 | 11 | 1 |
| 3 | C | 360 | PX4 | C16-C15 | 2.32 | 1.63 | 1.51 | 6 | 2 |
| 3 | B | 313 | PX4 | C10-C9 | 2.32 | 1.57 | 1.50 | 5 | 2 |
| 3 | B | 368 | PX4 | C32-C31 | 2.32 | 1.63 | 1.51 | 15 | 1 |
| 3 | B | 382 | PX4 | C17-C16 | 2.32 | 1.63 | 1.51 | 9 | 1 |
| 3 | C | 314 | PX4 | C25-C24 | 2.32 | 1.60 | 1.52 | 9 | 1 |
| 3 | A | 635 | PX4 | C14-C13 | 2.32 | 1.63 | 1.51 | 11 | 1 |
| 3 | B | 301 | PX4 | C31-C30 | 2.32 | 1.63 | 1.51 | 1 | 1 |
| 3 | C | 364 | PX4 | C4-N1 | 2.32 | 1.43 | 1.50 | 12 | 5 |
| 3 | A | 636 | PX4 | C28-C27 | 2.32 | 1.63 | 1.51 | 3 | 1 |
| 3 | B | 303 | PX4 | C25-C24 | 2.32 | 1.60 | 1.52 | 15 | 1 |
| 3 | A | 602 | PX4 | P1-O2 | 2.32 | 1.42 | 1.50 | 9 | 1 |
| 3 | A | 624 | PX4 | C2-N1 | 2.32 | 1.58 | 1.51 | 15 | 1 |
| 3 | A | 648 | PX4 | P1-O1 | 2.32 | 1.44 | 1.55 | 9 | 4 |
| 3 | B | 327 | PX4 | C25-C24 | 2.32 | 1.60 | 1.52 | 14 | 3 |
| 3 | B | 357 | PX4 | O5-C8 | 2.32 | 1.50 | 1.45 | 12 | 3 |
| 3 | C | 307 | PX4 | C2-N1 | 2.32 | 1.44 | 1.51 | 3 | 2 |
| 3 | B | 391 | PX4 | O7-C23 | 2.32 | 1.27 | 1.34 | 9 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | C | 347 | PX4 | P1-O2 | 2.32 | 1.42 | 1.50 | 8 | 1 |
| 3 | A | 607 | PX4 | C25-C24 | 2.32 | 1.60 | 1.52 | 13 | 4 |
| 3 | A | 603 | PX4 | P1-O1 | 2.32 | 1.44 | 1.55 | 12 | 2 |
| 3 | A | 610 | PX4 | C3-N1 | 2.32 | 1.56 | 1.50 | 12 | 2 |
| 3 | A | 625 | PX4 | O5-C9 | 2.32 | 1.26 | 1.33 | 8 | 3 |
| 3 | B | 328 | PX4 | O4-C6 | 2.32 | 1.35 | 1.44 | 9 | 1 |
| 3 | B | 321 | PX4 | C2-N1 | 2.32 | 1.58 | 1.51 | 10 | 2 |
| 3 | C | 328 | PX4 | C25-C24 | 2.32 | 1.60 | 1.52 | 2 | 2 |
| 3 | A | 652 | PX4 | C29-C28 | 2.31 | 1.63 | 1.51 | 14 | 1 |
| 3 | B | 342 | PX4 | C13-C12 | 2.31 | 1.63 | 1.51 | 7 | 2 |
| 3 | B | 350 | PX4 | P1-O1 | 2.31 | 1.44 | 1.55 | 11 | 4 |
| 3 | C | 311 | PX4 | P1-O1 | 2.31 | 1.44 | 1.55 | 7 | 1 |
| 3 | C | 316 | PX4 | C26-C25 | 2.31 | 1.63 | 1.51 | 10 | 1 |
| 3 | C | 338 | PX4 | C2-N1 | 2.31 | 1.58 | 1.51 | 7 | 1 |
| 3 | C | 351 | PX4 | O3-C1 | 2.31 | 1.35 | 1.44 | 3 | 2 |
| 3 | C | 363 | PX4 | P1-O4 | 2.31 | 1.50 | 1.59 | 1 | 1 |
| 3 | B | 378 | PX4 | C15-C14 | 2.31 | 1.63 | 1.51 | 2 | 1 |
| 3 | B | 384 | PX4 | O7-C23 | 2.31 | 1.40 | 1.34 | 2 | 1 |
| 3 | C | 304 | PX4 | P1-O1 | 2.31 | 1.44 | 1.55 | 2 | 2 |
| 3 | C | 324 | PX4 | C29-C28 | 2.31 | 1.63 | 1.51 | 15 | 1 |
| 3 | B | 312 | PX4 | C15-C14 | 2.31 | 1.63 | 1.51 | 10 | 1 |
| 3 | B | 331 | PX4 | C33-C32 | 2.31 | 1.63 | 1.51 | 14 | 1 |
| 3 | C | 340 | PX4 | C3-N1 | 2.31 | 1.43 | 1.50 | 9 | 1 |
| 3 | B | 309 | PX4 | C13-C12 | 2.31 | 1.63 | 1.51 | 14 | 1 |
| 3 | B | 344 | PX4 | C4-N1 | 2.31 | 1.43 | 1.50 | 14 | 1 |
| 3 | B | 322 | PX4 | C3-N1 | 2.31 | 1.56 | 1.50 | 5 | 2 |
| 3 | B | 330 | PX4 | O7-C23 | 2.31 | 1.27 | 1.34 | 9 | 2 |
| 3 | B | 355 | PX4 | P1-O1 | 2.31 | 1.44 | 1.55 | 11 | 4 |
| 3 | B | 367 | PX4 | C13-C12 | 2.31 | 1.63 | 1.51 | 13 | 1 |
| 3 | C | 347 | PX4 | C13-C12 | 2.31 | 1.63 | 1.51 | 13 | 1 |
| 3 | B | 356 | PX4 | C32-C31 | 2.30 | 1.63 | 1.51 | 9 | 1 |
| 3 | A | 631 | PX4 | O3-C1 | 2.30 | 1.35 | 1.44 | 8 | 1 |
| 3 | A | 649 | PX4 | C18-C17 | 2.30 | 1.63 | 1.51 | 2 | 2 |
| 3 | A | 604 | PX4 | C2-N1 | 2.30 | 1.58 | 1.51 | 6 | 1 |
| 3 | A | 630 | PX4 | C25-C24 | 2.30 | 1.60 | 1.52 | 4 | 2 |
| 3 | A | 651 | PX4 | C2-N1 | 2.30 | 1.58 | 1.51 | 1 | 1 |
| 3 | B | 322 | PX4 | C4-N1 | 2.30 | 1.56 | 1.50 | 4 | 1 |
| 3 | C | 322 | PX4 | C3-N1 | 2.30 | 1.56 | 1.50 | 14 | 3 |
| 3 | A | 651 | PX4 | C5-N1 | 2.30 | 1.43 | 1.50 | 3 | 1 |
| 3 | A | 612 | PX4 | C25-C24 | 2.30 | 1.60 | 1.52 | 7 | 3 |
| 3 | A | 615 | PX4 | C3-N1 | 2.30 | 1.43 | 1.50 | 7 | 3 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | A | 628 | PX4 | O4-C6 | 2.30 | 1.35 | 1.44 | 14 | 1 |
| 3 | A | 638 | PX4 | C27-C26 | 2.30 | 1.63 | 1.51 | 11 | 1 |
| 3 | B | 325 | PX4 | C25-C24 | 2.30 | 1.60 | 1.52 | 3 | 2 |
| 3 | B | 302 | PX4 | C28-C27 | 2.30 | 1.63 | 1.51 | 13 | 1 |
| 3 | B | 336 | PX4 | C24-C23 | 2.30 | 1.57 | 1.50 | 13 | 1 |
| 3 | C | 322 | PX4 | C5-N1 | 2.30 | 1.56 | 1.50 | 7 | 1 |
| 3 | A | 650 | PX4 | C19-C18 | 2.30 | 1.63 | 1.51 | 1 | 1 |
| 3 | C | 332 | PX4 | O7-C7 | 2.30 | 1.52 | 1.46 | 9 | 2 |
| 3 | C | 353 | PX4 | P1-O1 | 2.30 | 1.44 | 1.55 | 8 | 2 |
| 3 | A | 621 | PX4 | P1-O3 | 2.30 | 1.50 | 1.59 | 1 | 1 |
| 3 | A | 622 | PX4 | C14-C13 | 2.30 | 1.63 | 1.51 | 15 | 1 |
| 3 | A | 625 | PX4 | P1-O4 | 2.30 | 1.50 | 1.59 | 10 | 1 |
| 3 | A | 625 | PX4 | C26-C25 | 2.30 | 1.63 | 1.51 | 3 | 1 |
| 3 | B | 398 | PX4 | O7-C7 | 2.30 | 1.41 | 1.46 | 12 | 4 |
| 3 | C | 310 | PX4 | C24-C23 | 2.30 | 1.57 | 1.50 | 13 | 1 |
| 3 | C | 323 | PX4 | C12-C11 | 2.30 | 1.63 | 1.51 | 6 | 1 |
| 3 | B | 336 | PX4 | C26-C25 | 2.30 | 1.63 | 1.51 | 11 | 1 |
| 3 | C | 332 | PX4 | C3-N1 | 2.30 | 1.43 | 1.50 | 9 | 1 |
| 3 | C | 338 | PX4 | C33-C32 | 2.30 | 1.63 | 1.51 | 2 | 1 |
| 3 | A | 621 | PX4 | O5-C8 | 2.29 | 1.50 | 1.45 | 10 | 3 |
| 3 | A | 625 | PX4 | O7-C23 | 2.29 | 1.27 | 1.34 | 9 | 1 |
| 3 | B | 307 | PX4 | C26-C25 | 2.29 | 1.63 | 1.51 | 14 | 1 |
| 3 | C | 311 | PX4 | C5-N1 | 2.30 | 1.56 | 1.50 | 12 | 1 |
| 3 | C | 361 | PX4 | C19-C18 | 2.30 | 1.63 | 1.51 | 1 | 1 |
| 3 | B | 343 | PX4 | O4-C6 | 2.29 | 1.35 | 1.44 | 4 | 1 |
| 3 | B | 398 | PX4 | C4-N1 | 2.29 | 1.43 | 1.50 | 13 | 1 |
| 3 | C | 322 | PX4 | O5-C8 | 2.29 | 1.40 | 1.45 | 4 | 1 |
| 3 | A | 651 | PX4 | C24-C23 | 2.29 | 1.57 | 1.50 | 1 | 3 |
| 3 | A | 651 | PX4 | C16-C15 | 2.29 | 1.63 | 1.51 | 3 | 1 |
| 3 | B | 306 | PX4 | C2-N1 | 2.29 | 1.44 | 1.51 | 6 | 3 |
| 3 | B | 329 | PX4 | P1-O2 | 2.29 | 1.42 | 1.50 | 14 | 2 |
| 3 | C | 316 | PX4 | C4-N1 | 2.29 | 1.43 | 1.50 | 10 | 1 |
| 3 | C | 336 | PX4 | P1-O1 | 2.29 | 1.44 | 1.55 | 1 | 3 |
| 3 | C | 345 | PX4 | O5-C9 | 2.29 | 1.40 | 1.33 | 6 | 2 |
| 3 | A | 606 | PX4 | O4-C6 | 2.29 | 1.35 | 1.44 | 5 | 1 |
| 3 | A | 630 | PX4 | C10-C9 | 2.29 | 1.57 | 1.50 | 7 | 3 |
| 3 | B | 305 | PX4 | C11-C10 | 2.29 | 1.60 | 1.52 | 12 | 1 |
| 3 | B | 307 | PX4 | C5-N1 | 2.29 | 1.56 | 1.50 | 15 | 3 |
| 3 | B | 357 | PX4 | O5-C9 | 2.29 | 1.40 | 1.33 | 6 | 1 |
| 3 | B | 361 | PX4 | O5-C9 | 2.29 | 1.40 | 1.33 | 5 | 2 |
| 3 | B | 367 | PX4 | C29-C28 | 2.29 | 1.63 | 1.51 | 8 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 395 | PX4 | C31-C30 | 2.29 | 1.63 | 1.51 | 2 | 1 |
| 3 | C | 318 | PX4 | C25-C24 | 2.29 | 1.60 | 1.52 | 14 | 3 |
| 3 | C | 319 | PX4 | O7-C23 | 2.29 | 1.27 | 1.34 | 14 | 4 |
| 3 | A | 624 | PX4 | C24-C23 | 2.29 | 1.57 | 1.50 | 6 | 2 |
| 3 | B | 337 | PX4 | C2-N1 | 2.29 | 1.58 | 1.51 | 8 | 3 |
| 3 | B | 340 | PX4 | P1-O1 | 2.29 | 1.44 | 1.55 | 12 | 1 |
| 3 | B | 380 | PX4 | C2-N1 | 2.29 | 1.58 | 1.51 | 6 | 1 |
| 3 | B | 394 | PX4 | C3-N1 | 2.29 | 1.56 | 1.50 | 5 | 2 |
| 3 | C | 302 | PX4 | O5-C9 | 2.29 | 1.26 | 1.33 | 5 | 1 |
| 3 | B | 365 | PX4 | P1-O2 | 2.29 | 1.42 | 1.50 | 9 | 2 |
| 3 | B | 368 | PX4 | O5-C9 | 2.29 | 1.40 | 1.33 | 4 | 2 |
| 3 | C | 303 | PX4 | C15-C14 | 2.29 | 1.63 | 1.51 | 3 | 1 |
| 3 | C | 321 | PX4 | C34-C33 | 2.29 | 1.63 | 1.51 | 2 | 1 |
| 3 | C | 345 | PX4 | C2-N1 | 2.29 | 1.58 | 1.51 | 15 | 1 |
| 3 | C | 349 | PX4 | P1-O2 | 2.29 | 1.42 | 1.50 | 14 | 1 |
| 3 | A | 631 | PX4 | O5-C8 | 2.29 | 1.40 | 1.45 | 2 | 2 |
| 3 | A | 645 | PX4 | O5-C9 | 2.29 | 1.40 | 1.33 | 15 | 2 |
| 3 | B | 317 | PX4 | C11-C10 | 2.29 | 1.60 | 1.52 | 2 | 1 |
| 3 | B | 338 | PX4 | C33-C32 | 2.29 | 1.63 | 1.51 | 6 | 1 |
| 3 | B | 351 | PX4 | P1-O1 | 2.29 | 1.44 | 1.55 | 12 | 1 |
| 3 | C | 364 | PX4 | C25-C24 | 2.29 | 1.60 | 1.52 | 5 | 2 |
| 3 | B | 311 | PX4 | C13-C12 | 2.28 | 1.63 | 1.51 | 9 | 1 |
| 3 | B | 324 | PX4 | C34-C33 | 2.28 | 1.63 | 1.51 | 11 | 1 |
| 3 | B | 327 | PX4 | P1-O1 | 2.29 | 1.44 | 1.55 | 7 | 3 |
| 3 | A | 642 | PX4 | O7-C23 | 2.28 | 1.27 | 1.34 | 3 | 2 |
| 3 | B | 338 | PX4 | C3-N1 | 2.28 | 1.56 | 1.50 | 4 | 2 |
| 3 | B | 338 | PX4 | O4-C6 | 2.28 | 1.36 | 1.44 | 13 | 1 |
| 3 | B | 361 | PX4 | C20-C19 | 2.28 | 1.63 | 1.51 | 13 | 1 |
| 3 | A | 611 | PX4 | C2-N1 | 2.28 | 1.44 | 1.51 | 2 | 2 |
| 3 | B | 303 | PX4 | O7-C23 | 2.28 | 1.27 | 1.34 | 6 | 1 |
| 3 | B | 315 | PX4 | O7-C23 | 2.28 | 1.27 | 1.34 | 6 | 3 |
| 3 | B | 339 | PX4 | C24-C23 | 2.28 | 1.57 | 1.50 | 11 | 2 |
| 3 | B | 379 | PX4 | P1-O1 | 2.28 | 1.44 | 1.55 | 7 | 1 |
| 3 | B | 392 | PX4 | C17-C16 | 2.28 | 1.63 | 1.51 | 6 | 1 |
| 3 | A | 618 | PX4 | C25-C24 | 2.28 | 1.60 | 1.52 | 1 | 1 |
| 3 | A | 637 | PX4 | C2-N1 | 2.28 | 1.58 | 1.51 | 2 | 1 |
| 3 | B | 315 | PX4 | C30-C29 | 2.28 | 1.63 | 1.51 | 7 | 1 |
| 3 | C | 324 | PX4 | C10-C9 | 2.28 | 1.57 | 1.50 | 1 | 2 |
| 3 | C | 336 | PX4 | C5-N1 | 2.28 | 1.56 | 1.50 | 8 | 1 |
| 3 | B | 326 | PX4 | C11-C10 | 2.28 | 1.60 | 1.52 | 5 | 1 |
| 3 | A | 610 | PX4 | O7-C23 | 2.28 | 1.27 | 1.34 | 12 | 2 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | A | 619 | PX4 | P1-O1 | 2.28 | 1.44 | 1.55 | 9 | 1 |
| 3 | A | 642 | PX4 | C2-N1 | 2.28 | 1.44 | 1.51 | 14 | 1 |
| 3 | A | 654 | PX4 | O5-C9 | 2.28 | 1.26 | 1.33 | 3 | 1 |
| 3 | B | 348 | PX4 | C11-C10 | 2.28 | 1.60 | 1.52 | 8 | 2 |
| 3 | B | 369 | PX4 | O5-C9 | 2.28 | 1.40 | 1.33 | 6 | 3 |
| 3 | C | 337 | PX4 | C3-N1 | 2.28 | 1.56 | 1.50 | 11 | 1 |
| 3 | A | 619 | PX4 | O5-C9 | 2.28 | 1.40 | 1.33 | 14 | 1 |
| 3 | B | 323 | PX4 | C11-C10 | 2.28 | 1.60 | 1.52 | 4 | 2 |
| 3 | B | 323 | PX4 | C13-C12 | 2.28 | 1.63 | 1.51 | 4 | 1 |
| 3 | B | 354 | PX4 | C2-N1 | 2.28 | 1.58 | 1.51 | 8 | 2 |
| 3 | B | 370 | PX4 | C33-C32 | 2.28 | 1.63 | 1.51 | 10 | 1 |
| 3 | C | 314 | PX4 | C11-C10 | 2.28 | 1.60 | 1.52 | 14 | 2 |
| 3 | C | 317 | PX4 | P1-O4 | 2.28 | 1.50 | 1.59 | 5 | 2 |
| 3 | C | 324 | PX4 | O5-C8 | 2.28 | 1.40 | 1.45 | 7 | 2 |
| 3 | C | 364 | PX4 | C11-C10 | 2.28 | 1.60 | 1.52 | 14 | 2 |
| 3 | A | 614 | PX4 | C31-C30 | 2.28 | 1.63 | 1.51 | 9 | 1 |
| 3 | B | 335 | PX4 | O7-C23 | 2.28 | 1.27 | 1.34 | 11 | 2 |
| 3 | B | 361 | PX4 | C2-N1 | 2.28 | 1.58 | 1.51 | 8 | 1 |
| 3 | B | 378 | PX4 | C2-N1 | 2.28 | 1.58 | 1.51 | 2 | 1 |
| 3 | B | 394 | PX4 | C11-C10 | 2.28 | 1.60 | 1.52 | 4 | 3 |
| 3 | C | 346 | PX4 | C30-C29 | 2.28 | 1.63 | 1.51 | 3 | 1 |
| 3 | A | 623 | PX4 | O7-C23 | 2.28 | 1.27 | 1.34 | 7 | 2 |
| 3 | B | 349 | PX4 | C16-C15 | 2.28 | 1.63 | 1.51 | 8 | 1 |
| 3 | C | 312 | PX4 | C3-N1 | 2.28 | 1.56 | 1.50 | 7 | 1 |
| 3 | C | 362 | PX4 | C3-N1 | 2.28 | 1.43 | 1.50 | 9 | 2 |
| 3 | B | 388 | PX4 | O5-C8 | 2.27 | 1.40 | 1.45 | 7 | 1 |
| 3 | C | 305 | PX4 | C3-N1 | 2.28 | 1.43 | 1.50 | 7 | 1 |
| 3 | B | 366 | PX4 | C28-C27 | 2.27 | 1.63 | 1.51 | 1 | 1 |
| 3 | B | 372 | PX4 | C2-N1 | 2.27 | 1.58 | 1.51 | 1 | 2 |
| 3 | C | 335 | PX4 | C25-C24 | 2.27 | 1.60 | 1.52 | 6 | 1 |
| 3 | A | 610 | PX4 | P1-O3 | 2.27 | 1.50 | 1.59 | 4 | 1 |
| 3 | A | 622 | PX4 | C4-N1 | 2.27 | 1.43 | 1.50 | 11 | 2 |
| 3 | B | 314 | PX4 | C5-N1 | 2.27 | 1.43 | 1.50 | 15 | 1 |
| 3 | C | 322 | PX4 | O5-C9 | 2.27 | 1.26 | 1.33 | 15 | 3 |
| 3 | C | 338 | PX4 | C26-C25 | 2.27 | 1.63 | 1.51 | 12 | 1 |
| 3 | C | 356 | PX4 | C2-N1 | 2.27 | 1.58 | 1.51 | 13 | 2 |
| 3 | A | 614 | PX4 | C5-N1 | 2.27 | 1.43 | 1.50 | 4 | 2 |
| 3 | A | 621 | PX4 | C25-C24 | 2.27 | 1.60 | 1.52 | 9 | 1 |
| 3 | A | 637 | PX4 | C24-C23 | 2.27 | 1.57 | 1.50 | 5 | 1 |
| 3 | B | 343 | PX4 | O5-C8 | 2.27 | 1.40 | 1.45 | 7 | 1 |
| 3 | B | 356 | PX4 | C16-C15 | 2.27 | 1.63 | 1.51 | 12 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 396 | PX4 | O6-C9 | 2.27 | 1.15 | 1.22 | 8 | 2 |
| 3 | C | 347 | PX4 | P1-O1 | 2.27 | 1.44 | 1.55 | 6 | 4 |
| 3 | A | 648 | PX4 | C11-C10 | 2.27 | 1.60 | 1.52 | 9 | 2 |
| 3 | B | 329 | PX4 | C26-C25 | 2.27 | 1.63 | 1.51 | 11 | 2 |
| 3 | B | 392 | PX4 | C24-C23 | 2.27 | 1.57 | 1.50 | 12 | 1 |
| 3 | C | 301 | PX4 | C2-N1 | 2.27 | 1.58 | 1.51 | 6 | 2 |
| 3 | A | 615 | PX4 | C29-C28 | 2.27 | 1.63 | 1.51 | 9 | 1 |
| 3 | A | 629 | PX4 | C5-N1 | 2.27 | 1.56 | 1.50 | 8 | 1 |
| 3 | B | 304 | PX4 | C30-C29 | 2.27 | 1.63 | 1.51 | 10 | 1 |
| 3 | B | 311 | PX4 | O4-C6 | 2.27 | 1.36 | 1.44 | 12 | 1 |
| 3 | B | 315 | PX4 | C19-C18 | 2.27 | 1.63 | 1.51 | 3 | 1 |
| 3 | B | 342 | PX4 | P1-O1 | 2.27 | 1.44 | 1.55 | 14 | 3 |
| 3 | A | 625 | PX4 | O7-C7 | 2.27 | 1.51 | 1.46 | 10 | 1 |
| 3 | A | 641 | PX4 | C11-C10 | 2.27 | 1.60 | 1.52 | 15 | 2 |
| 3 | A | 654 | PX4 | C3-N1 | 2.27 | 1.56 | 1.50 | 8 | 1 |
| 3 | B | 319 | PX4 | P1-O1 | 2.27 | 1.44 | 1.55 | 2 | 4 |
| 3 | B | 327 | PX4 | C20-C19 | 2.27 | 1.63 | 1.51 | 1 | 2 |
| 3 | B | 339 | PX4 | O3-C1 | 2.27 | 1.35 | 1.44 | 4 | 1 |
| 3 | A | 610 | PX4 | C11-C10 | 2.26 | 1.60 | 1.52 | 12 | 2 |
| 3 | B | 329 | PX4 | O5-C9 | 2.26 | 1.40 | 1.33 | 9 | 3 |
| 3 | B | 353 | PX4 | P1-O3 | 2.27 | 1.68 | 1.59 | 7 | 1 |
| 3 | B | 384 | PX4 | O5-C8 | 2.27 | 1.50 | 1.45 | 4 | 2 |
| 3 | C | 347 | PX4 | C10-C9 | 2.27 | 1.57 | 1.50 | 7 | 2 |
| 3 | A | 618 | PX4 | O7-C7 | 2.26 | 1.41 | 1.46 | 15 | 2 |
| 3 | B | 315 | PX4 | C12-C11 | 2.26 | 1.63 | 1.51 | 12 | 1 |
| 3 | B | 329 | PX4 | P1-O1 | 2.26 | 1.44 | 1.55 | 2 | 2 |
| 3 | B | 372 | PX4 | C3-N1 | 2.26 | 1.56 | 1.50 | 5 | 1 |
| 3 | C | 359 | PX4 | C25-C24 | 2.26 | 1.60 | 1.52 | 4 | 1 |
| 3 | A | 653 | PX4 | C5-N1 | 2.26 | 1.56 | 1.50 | 6 | 1 |
| 3 | B | 379 | PX4 | C2-N1 | 2.26 | 1.44 | 1.51 | 4 | 2 |
| 3 | B | 384 | PX4 | C18-C17 | 2.26 | 1.63 | 1.51 | 3 | 1 |
| 3 | B | 387 | PX4 | C31-C30 | 2.26 | 1.63 | 1.51 | 15 | 1 |
| 3 | C | 332 | PX4 | C16-C15 | 2.26 | 1.63 | 1.51 | 3 | 1 |
| 3 | A | 617 | PX4 | O7-C7 | 2.26 | 1.41 | 1.46 | 12 | 2 |
| 3 | B | 326 | PX4 | O7-C7 | 2.26 | 1.41 | 1.46 | 3 | 1 |
| 3 | B | 357 | PX4 | C12-C11 | 2.26 | 1.63 | 1.51 | 5 | 1 |
| 3 | B | 367 | PX4 | C27-C26 | 2.26 | 1.63 | 1.51 | 6 | 1 |
| 3 | B | 382 | PX4 | C29-C28 | 2.26 | 1.63 | 1.51 | 4 | 1 |
| 3 | A | 611 | PX4 | C32-C31 | 2.26 | 1.63 | 1.51 | 15 | 1 |
| 3 | B | 398 | PX4 | O5-C9 | 2.26 | 1.26 | 1.33 | 9 | 1 |
| 3 | A | 621 | PX4 | O3-C1 | 2.26 | 1.35 | 1.44 | 15 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 327 | PX4 | O5-C9 | 2.26 | 1.26 | 1.33 | 12 | 1 |
| 3 | C | 314 | PX4 | P1-O2 | 2.26 | 1.43 | 1.50 | 13 | 1 |
| 3 | B | 375 | PX4 | C11-C10 | 2.26 | 1.60 | 1.52 | 15 | 1 |
| 3 | C | 362 | PX4 | C12-C11 | 2.26 | 1.63 | 1.51 | 1 | 1 |
| 3 | A | 606 | PX4 | P1-O3 | 2.26 | 1.50 | 1.59 | 11 | 2 |
| 3 | B | 396 | PX4 | P1-O4 | 2.26 | 1.50 | 1.59 | 3 | 1 |
| 3 | C | 329 | PX4 | O7-C23 | 2.26 | 1.27 | 1.34 | 12 | 2 |
| 3 | C | 361 | PX4 | C5-N1 | 2.26 | 1.56 | 1.50 | 1 | 1 |
| 3 | A | 637 | PX4 | C20-C19 | 2.25 | 1.63 | 1.51 | 15 | 2 |
| 3 | A | 650 | PX4 | O7-C7 | 2.25 | 1.41 | 1.46 | 1 | 2 |
| 3 | B | 323 | PX4 | C5-N1 | 2.25 | 1.43 | 1.50 | 1 | 2 |
| 3 | A | 614 | PX4 | C2-N1 | 2.25 | 1.58 | 1.51 | 5 | 2 |
| 3 | A | 624 | PX4 | C11-C10 | 2.25 | 1.60 | 1.52 | 2 | 1 |
| 3 | A | 649 | PX4 | C11-C10 | 2.25 | 1.60 | 1.52 | 13 | 3 |
| 3 | B | 339 | PX4 | C26-C25 | 2.25 | 1.63 | 1.51 | 14 | 1 |
| 3 | B | 388 | PX4 | C19-C18 | 2.25 | 1.63 | 1.51 | 6 | 1 |
| 3 | C | 312 | PX4 | C25-C24 | 2.25 | 1.60 | 1.52 | 5 | 1 |
| 3 | C | 332 | PX4 | C10-C9 | 2.25 | 1.57 | 1.50 | 12 | 2 |
| 3 | B | 309 | PX4 | C31-C30 | 2.25 | 1.63 | 1.51 | 6 | 1 |
| 3 | B | 320 | PX4 | O3-C1 | 2.25 | 1.35 | 1.44 | 4 | 1 |
| 3 | B | 336 | PX4 | C4-N1 | 2.25 | 1.43 | 1.50 | 2 | 3 |
| 3 | B | 350 | PX4 | C17-C16 | 2.25 | 1.63 | 1.51 | 2 | 1 |
| 3 | A | 623 | PX4 | P1-O1 | 2.25 | 1.44 | 1.55 | 11 | 2 |
| 3 | B | 369 | PX4 | O3-C1 | 2.25 | 1.35 | 1.44 | 6 | 1 |
| 3 | B | 396 | PX4 | C34-C33 | 2.25 | 1.63 | 1.51 | 13 | 1 |
| 3 | C | 302 | PX4 | C18-C17 | 2.25 | 1.63 | 1.51 | 7 | 1 |
| 3 | C | 306 | PX4 | C14-C13 | 2.25 | 1.63 | 1.51 | 14 | 1 |
| 3 | B | 371 | PX4 | P1-O1 | 2.25 | 1.44 | 1.55 | 1 | 2 |
| 3 | C | 322 | PX4 | O7-C23 | 2.25 | 1.27 | 1.34 | 7 | 2 |
| 3 | C | 356 | PX4 | P1-O1 | 2.25 | 1.44 | 1.55 | 15 | 3 |
| 3 | C | 357 | PX4 | P1-O2 | 2.25 | 1.43 | 1.50 | 15 | 2 |
| 3 | A | 618 | PX4 | P1-O3 | 2.25 | 1.50 | 1.59 | 15 | 1 |
| 3 | A | 620 | PX4 | C3-N1 | 2.25 | 1.56 | 1.50 | 9 | 1 |
| 3 | B | 304 | PX4 | O7-C7 | 2.25 | 1.51 | 1.46 | 13 | 2 |
| 3 | B | 359 | PX4 | C3-N1 | 2.25 | 1.56 | 1.50 | 15 | 1 |
| 3 | C | 302 | PX4 | O7-C23 | 2.25 | 1.40 | 1.34 | 14 | 4 |
| 3 | C | 343 | PX4 | C20-C19 | 2.25 | 1.63 | 1.51 | 6 | 1 |
| 3 | A | 642 | PX4 | O4-C6 | 2.25 | 1.36 | 1.44 | 6 | 1 |
| 3 | A | 642 | PX4 | P1-O1 | 2.25 | 1.44 | 1.55 | 14 | 1 |
| 3 | A | 654 | PX4 | C11-C10 | 2.25 | 1.60 | 1.52 | 8 | 1 |
| 3 | B | 318 | PX4 | O7-C7 | 2.25 | 1.41 | 1.46 | 2 | 2 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 318 | PX4 | O5-C9 | 2.25 | 1.39 | 1.33 | 2 | 1 |
| 3 | B | 361 | PX4 | C3-N1 | 2.25 | 1.43 | 1.50 | 5 | 1 |
| 3 | B | 385 | PX4 | P1-O1 | 2.25 | 1.44 | 1.55 | 5 | 3 |
| 3 | C | 340 | PX4 | C20-C19 | 2.25 | 1.63 | 1.51 | 5 | 1 |
| 3 | C | 359 | PX4 | C11-C10 | 2.25 | 1.60 | 1.52 | 15 | 1 |
| 3 | B | 349 | PX4 | P1-O2 | 2.25 | 1.43 | 1.50 | 1 | 1 |
| 3 | C | 336 | PX4 | C2-N1 | 2.25 | 1.58 | 1.51 | 1 | 2 |
| 3 | A | 627 | PX4 | C2-N1 | 2.24 | 1.58 | 1.51 | 8 | 2 |
| 3 | B | 312 | PX4 | C11-C10 | 2.24 | 1.60 | 1.52 | 10 | 2 |
| 3 | B | 320 | PX4 | O7-C23 | 2.25 | 1.27 | 1.34 | 2 | 2 |
| 3 | B | 330 | PX4 | O6-C9 | 2.24 | 1.15 | 1.22 | 15 | 1 |
| 3 | B | 344 | PX4 | C5-N1 | 2.24 | 1.56 | 1.50 | 7 | 1 |
| 3 | B | 362 | PX4 | C12-C11 | 2.24 | 1.62 | 1.51 | 3 | 1 |
| 3 | B | 376 | PX4 | C31-C30 | 2.24 | 1.62 | 1.51 | 2 | 1 |
| 3 | C | 320 | PX4 | P1-O1 | 2.25 | 1.44 | 1.55 | 4 | 1 |
| 3 | A | 607 | PX4 | C32-C31 | 2.24 | 1.62 | 1.51 | 3 | 1 |
| 3 | A | 624 | PX4 | C4-N1 | 2.24 | 1.56 | 1.50 | 10 | 1 |
| 3 | A | 604 | PX4 | O3-C1 | 2.24 | 1.35 | 1.44 | 9 | 1 |
| 3 | A | 606 | PX4 | C10-C9 | 2.24 | 1.57 | 1.50 | 2 | 2 |
| 3 | A | 610 | PX4 | C33-C32 | 2.24 | 1.62 | 1.51 | 5 | 1 |
| 3 | B | 326 | PX4 | C33-C32 | 2.24 | 1.62 | 1.51 | 7 | 1 |
| 3 | B | 373 | PX4 | C31-C30 | 2.24 | 1.62 | 1.51 | 4 | 1 |
| 3 | B | 385 | PX4 | P1-O2 | 2.24 | 1.43 | 1.50 | 2 | 1 |
| 3 | B | 396 | PX4 | C2-N1 | 2.24 | 1.44 | 1.51 | 5 | 2 |
| 3 | C | 306 | PX4 | P1-O2 | 2.24 | 1.43 | 1.50 | 11 | 1 |
| 3 | C | 328 | PX4 | O4-C6 | 2.24 | 1.36 | 1.44 | 5 | 1 |
| 3 | A | 622 | PX4 | P1-O2 | 2.24 | 1.43 | 1.50 | 14 | 1 |
| 3 | B | 304 | PX4 | P1-O1 | 2.24 | 1.45 | 1.55 | 4 | 2 |
| 3 | B | 374 | PX4 | C12-C11 | 2.24 | 1.62 | 1.51 | 2 | 1 |
| 3 | A | 621 | PX4 | P1-O2 | 2.24 | 1.43 | 1.50 | 7 | 1 |
| 3 | B | 393 | PX4 | C27-C26 | 2.24 | 1.62 | 1.51 | 1 | 1 |
| 3 | B | 374 | PX4 | O7-C7 | 2.24 | 1.41 | 1.46 | 6 | 2 |
| 3 | B | 381 | PX4 | C25-C24 | 2.24 | 1.60 | 1.52 | 4 | 2 |
| 3 | B | 396 | PX4 | C3-N1 | 2.24 | 1.56 | 1.50 | 10 | 1 |
| 3 | C | 318 | PX4 | O7-C7 | 2.24 | 1.41 | 1.46 | 7 | 1 |
| 3 | C | 343 | PX4 | O3-C1 | 2.24 | 1.53 | 1.44 | 11 | 1 |
| 3 | C | 344 | PX4 | P1-O1 | 2.24 | 1.45 | 1.55 | 3 | 3 |
| 3 | B | 307 | PX4 | O5-C9 | 2.24 | 1.26 | 1.33 | 3 | 2 |
| 3 | B | 324 | PX4 | C14-C13 | 2.24 | 1.62 | 1.51 | 1 | 1 |
| 3 | B | 327 | PX4 | P1-O3 | 2.24 | 1.50 | 1.59 | 2 | 1 |
| 3 | B | 345 | PX4 | C3-N1 | 2.24 | 1.56 | 1.50 | 12 | 3 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 389 | PX4 | C29-C28 | 2.24 | 1.62 | 1.51 | 14 | 2 |
| 3 | C | 307 | PX4 | O5-C9 | 2.24 | 1.39 | 1.33 | 8 | 2 |
| 3 | C | 309 | PX4 | C24-C23 | 2.24 | 1.57 | 1.50 | 15 | 2 |
| 3 | C | 314 | PX4 | C20-C19 | 2.24 | 1.62 | 1.51 | 8 | 1 |
| 3 | A | 635 | PX4 | O5-C8 | 2.24 | 1.40 | 1.45 | 5 | 1 |
| 3 | A | 601 | PX4 | C2-C1 | 2.23 | 1.58 | 1.51 | 2 | 4 |
| 3 | A | 614 | PX4 | P1-O1 | 2.23 | 1.45 | 1.55 | 15 | 1 |
| 3 | B | 302 | PX4 | O5-C8 | 2.23 | 1.40 | 1.45 | 13 | 1 |
| 3 | B | 395 | PX4 | O4-C6 | 2.24 | 1.36 | 1.44 | 1 | 1 |
| 3 | C | 338 | PX4 | C12-C11 | 2.24 | 1.62 | 1.51 | 14 | 1 |
| 3 | B | 310 | PX4 | C20-C19 | 2.23 | 1.62 | 1.51 | 9 | 1 |
| 3 | B | 323 | PX4 | C25-C24 | 2.23 | 1.60 | 1.52 | 3 | 2 |
| 3 | B | 351 | PX4 | C4-N1 | 2.23 | 1.56 | 1.50 | 2 | 2 |
| 3 | B | 354 | PX4 | C12-C11 | 2.23 | 1.62 | 1.51 | 8 | 1 |
| 3 | B | 373 | PX4 | C11-C10 | 2.23 | 1.60 | 1.52 | 2 | 1 |
| 3 | C | 321 | PX4 | C30-C29 | 2.23 | 1.62 | 1.51 | 5 | 1 |
| 3 | C | 364 | PX4 | C24-C23 | 2.23 | 1.57 | 1.50 | 6 | 1 |
| 3 | C | 301 | PX4 | O7-C7 | 2.23 | 1.41 | 1.46 | 3 | 2 |
| 3 | B | 397 | PX4 | C33-C32 | 2.23 | 1.62 | 1.51 | 14 | 1 |
| 3 | C | 338 | PX4 | C30-C29 | 2.23 | 1.62 | 1.51 | 3 | 1 |
| 3 | C | 352 | PX4 | O5-C9 | 2.23 | 1.39 | 1.33 | 8 | 1 |
| 3 | B | 303 | PX4 | C32-C31 | 2.23 | 1.62 | 1.51 | 5 | 1 |
| 3 | B | 308 | PX4 | P1-O3 | 2.23 | 1.50 | 1.59 | 10 | 1 |
| 3 | B | 312 | PX4 | P1-O1 | 2.23 | 1.45 | 1.55 | 2 | 4 |
| 3 | C | 361 | PX4 | O7-C7 | 2.23 | 1.41 | 1.46 | 1 | 1 |
| 3 | C | 363 | PX4 | O5-C9 | 2.23 | 1.39 | 1.33 | 15 | 1 |
| 3 | A | 640 | PX4 | C28-C27 | 2.23 | 1.62 | 1.51 | 7 | 1 |
| 3 | C | 321 | PX4 | C31-C30 | 2.23 | 1.62 | 1.51 | 15 | 1 |
| 3 | A | 652 | PX4 | O7-C7 | 2.23 | 1.41 | 1.46 | 7 | 2 |
| 3 | B | 324 | PX4 | C12-C11 | 2.23 | 1.62 | 1.51 | 6 | 1 |
| 3 | B | 364 | PX4 | C17-C16 | 2.23 | 1.62 | 1.51 | 15 | 1 |
| 3 | B | 378 | PX4 | O7-C23 | 2.23 | 1.28 | 1.34 | 11 | 1 |
| 3 | C | 351 | PX4 | C18-C17 | 2.23 | 1.62 | 1.51 | 7 | 1 |
| 3 | B | 369 | PX4 | C17-C16 | 2.23 | 1.62 | 1.51 | 11 | 1 |
| 3 | C | 361 | PX4 | C2-N1 | 2.23 | 1.58 | 1.51 | 6 | 1 |
| 3 | B | 390 | PX4 | C5-N1 | 2.23 | 1.56 | 1.50 | 13 | 2 |
| 3 | C | 305 | PX4 | C28-C27 | 2.23 | 1.62 | 1.51 | 2 | 1 |
| 3 | A | 636 | PX4 | C11-C10 | 2.23 | 1.60 | 1.52 | 10 | 1 |
| 3 | B | 313 | PX4 | C17-C16 | 2.23 | 1.62 | 1.51 | 12 | 1 |
| 3 | B | 328 | PX4 | C28-C27 | 2.23 | 1.62 | 1.51 | 13 | 1 |
| 3 | B | 399 | PX4 | P1-O1 | 2.23 | 1.45 | 1.55 | 1 | 2 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | C | 358 | PX4 | P1-O1 | 2.23 | 1.45 | 1.55 | 4 | 2 |
| 3 | A | 652 | PX4 | P1-O1 | 2.22 | 1.45 | 1.55 | 2 | 2 |
| 3 | A | 649 | PX4 | C20-C19 | 2.22 | 1.62 | 1.51 | 2 | 1 |
| 3 | B | 308 | PX4 | O3-C1 | 2.22 | 1.35 | 1.44 | 8 | 1 |
| 3 | C | 306 | PX4 | O4-C6 | 2.22 | 1.36 | 1.44 | 7 | 1 |
| 3 | C | 309 | PX4 | C26-C25 | 2.22 | 1.62 | 1.51 | 3 | 1 |
| 3 | C | 351 | PX4 | O5-C9 | 2.22 | 1.26 | 1.33 | 5 | 1 |
| 3 | B | 310 | PX4 | C11-C10 | 2.22 | 1.60 | 1.52 | 9 | 1 |
| 3 | B | 339 | PX4 | O7-C23 | 2.22 | 1.28 | 1.34 | 7 | 1 |
| 3 | B | 369 | PX4 | P1-O1 | 2.22 | 1.45 | 1.55 | 7 | 4 |
| 3 | B | 397 | PX4 | P1-O1 | 2.22 | 1.45 | 1.55 | 13 | 2 |
| 3 | C | 315 | PX4 | O5-C9 | 2.22 | 1.39 | 1.33 | 15 | 1 |
| 3 | A | 643 | PX4 | P1-O2 | 2.22 | 1.43 | 1.50 | 14 | 2 |
| 3 | C | 317 | PX4 | O5-C9 | 2.22 | 1.39 | 1.33 | 13 | 1 |
| 3 | A | 609 | PX4 | P1-O1 | 2.22 | 1.45 | 1.55 | 2 | 2 |
| 3 | A | 623 | PX4 | C34-C33 | 2.22 | 1.62 | 1.51 | 8 | 1 |
| 3 | B | 302 | PX4 | P1-O1 | 2.22 | 1.45 | 1.55 | 15 | 1 |
| 3 | B | 305 | PX4 | C24-C23 | 2.22 | 1.57 | 1.50 | 1 | 1 |
| 3 | B | 343 | PX4 | C11-C10 | 2.22 | 1.60 | 1.52 | 8 | 1 |
| 3 | B | 347 | PX4 | O5-C9 | 2.22 | 1.39 | 1.33 | 12 | 2 |
| 3 | B | 360 | PX4 | C33-C32 | 2.22 | 1.62 | 1.51 | 1 | 1 |
| 3 | C | 324 | PX4 | C17-C16 | 2.22 | 1.62 | 1.51 | 8 | 1 |
| 3 | C | 327 | PX4 | C16-C15 | 2.22 | 1.62 | 1.51 | 7 | 2 |
| 3 | A | 629 | PX4 | P1-O1 | 2.22 | 1.45 | 1.55 | 5 | 3 |
| 3 | A | 643 | PX4 | C17-C16 | 2.22 | 1.62 | 1.51 | 4 | 1 |
| 3 | B | 319 | PX4 | C10-C9 | 2.22 | 1.57 | 1.50 | 13 | 5 |
| 3 | A | 646 | PX4 | C15-C14 | 2.22 | 1.62 | 1.51 | 14 | 1 |
| 3 | A | 652 | PX4 | O8-C23 | 2.22 | 1.29 | 1.22 | 9 | 1 |
| 3 | B | 351 | PX4 | C11-C10 | 2.22 | 1.60 | 1.52 | 9 | 2 |
| 3 | B | 383 | PX4 | C31-C30 | 2.22 | 1.62 | 1.51 | 7 | 1 |
| 3 | C | 307 | PX4 | C15-C14 | 2.22 | 1.62 | 1.51 | 6 | 1 |
| 3 | B | 320 | PX4 | C15-C14 | 2.22 | 1.62 | 1.51 | 6 | 2 |
| 3 | A | 613 | PX4 | O5-C9 | 2.21 | 1.26 | 1.33 | 9 | 1 |
| 3 | B | 331 | PX4 | C12-C11 | 2.22 | 1.62 | 1.51 | 8 | 1 |
| 3 | B | 361 | PX4 | C19-C18 | 2.22 | 1.62 | 1.51 | 11 | 1 |
| 3 | B | 355 | PX4 | C34-C33 | 2.21 | 1.62 | 1.51 | 13 | 1 |
| 3 | B | 305 | PX4 | C20-C19 | 2.21 | 1.62 | 1.51 | 8 | 1 |
| 3 | B | 315 | PX4 | P1-O1 | 2.21 | 1.45 | 1.55 | 2 | 2 |
| 3 | A | 608 | PX4 | C10-C9 | 2.21 | 1.57 | 1.50 | 8 | 2 |
| 3 | A | 609 | PX4 | O7-C7 | 2.21 | 1.41 | 1.46 | 15 | 2 |
| 3 | B | 356 | PX4 | C19-C18 | 2.21 | 1.62 | 1.51 | 15 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 380 | PX4 | O7-C7 | 2.21 | 1.41 | 1.46 | 2 | 1 |
| 3 | B | 382 | PX4 | C5-N1 | 2.21 | 1.56 | 1.50 | 7 | 1 |
| 3 | B | 396 | PX4 | C29-C28 | 2.21 | 1.62 | 1.51 | 13 | 1 |
| 3 | C | 307 | PX4 | C12-C11 | 2.21 | 1.62 | 1.51 | 11 | 1 |
| 3 | C | 363 | PX4 | C10-C9 | 2.21 | 1.57 | 1.50 | 10 | 3 |
| 3 | A | 642 | PX4 | C16-C15 | 2.21 | 1.62 | 1.51 | 15 | 1 |
| 3 | B | 304 | PX4 | C10-C9 | 2.21 | 1.57 | 1.50 | 2 | 2 |
| 3 | B | 361 | PX4 | C24-C23 | 2.21 | 1.57 | 1.50 | 11 | 2 |
| 3 | B | 362 | PX4 | P1-O2 | 2.21 | 1.43 | 1.50 | 2 | 3 |
| 3 | C | 308 | PX4 | O7-C23 | 2.21 | 1.28 | 1.34 | 7 | 1 |
| 3 | A | 610 | PX4 | C2-N1 | 2.21 | 1.58 | 1.51 | 10 | 1 |
| 3 | A | 621 | PX4 | C2-N1 | 2.21 | 1.58 | 1.51 | 7 | 1 |
| 3 | B | 305 | PX4 | C25-C24 | 2.21 | 1.60 | 1.52 | 12 | 1 |
| 3 | B | 320 | PX4 | C21-C20 | 2.21 | 1.65 | 1.51 | 12 | 1 |
| 3 | B | 333 | PX4 | C3-N1 | 2.21 | 1.43 | 1.50 | 8 | 1 |
| 3 | B | 352 | PX4 | O5-C8 | 2.21 | 1.50 | 1.45 | 15 | 2 |
| 3 | C | 317 | PX4 | C25-C24 | 2.21 | 1.60 | 1.52 | 9 | 3 |
| 3 | B | 393 | PX4 | C13-C12 | 2.21 | 1.62 | 1.51 | 15 | 1 |
| 3 | C | 316 | PX4 | O5-C8 | 2.21 | 1.50 | 1.45 | 5 | 1 |
| 3 | C | 321 | PX4 | O5-C8 | 2.21 | 1.40 | 1.45 | 12 | 2 |
| 3 | A | 635 | PX4 | O5-C9 | 2.21 | 1.39 | 1.33 | 15 | 3 |
| 3 | A | 638 | PX4 | C10-C9 | 2.21 | 1.57 | 1.50 | 3 | 1 |
| 3 | B | 301 | PX4 | P1-O2 | 2.21 | 1.43 | 1.50 | 12 | 1 |
| 3 | B | 322 | PX4 | P1-O2 | 2.21 | 1.43 | 1.50 | 9 | 1 |
| 3 | C | 346 | PX4 | C11-C10 | 2.21 | 1.60 | 1.52 | 14 | 2 |
| 3 | A | 603 | PX4 | C5-N1 | 2.21 | 1.56 | 1.50 | 1 | 1 |
| 3 | A | 636 | PX4 | C4-N1 | 2.21 | 1.56 | 1.50 | 7 | 2 |
| 3 | B | 322 | PX4 | C2-N1 | 2.21 | 1.44 | 1.51 | 14 | 2 |
| 3 | B | 334 | PX4 | C18-C17 | 2.21 | 1.62 | 1.51 | 11 | 2 |
| 3 | B | 351 | PX4 | C27-C26 | 2.21 | 1.62 | 1.51 | 6 | 2 |
| 3 | B | 358 | PX4 | C2-N1 | 2.21 | 1.58 | 1.51 | 1 | 1 |
| 3 | C | 328 | PX4 | P1-O2 | 2.21 | 1.43 | 1.50 | 2 | 1 |
| 3 | C | 356 | PX4 | C27-C26 | 2.21 | 1.62 | 1.51 | 8 | 1 |
| 3 | A | 636 | PX4 | P1-O1 | 2.21 | 1.45 | 1.55 | 7 | 2 |
| 3 | A | 640 | PX4 | C19-C18 | 2.21 | 1.62 | 1.51 | 3 | 1 |
| 3 | B | 330 | PX4 | C28-C27 | 2.21 | 1.62 | 1.51 | 14 | 1 |
| 3 | B | 365 | PX4 | C5-N1 | 2.21 | 1.56 | 1.50 | 9 | 5 |
| 3 | B | 376 | PX4 | C33-C32 | 2.20 | 1.62 | 1.51 | 9 | 1 |
| 3 | B | 393 | PX4 | C11-C10 | 2.21 | 1.60 | 1.52 | 14 | 3 |
| 3 | B | 390 | PX4 | C3-N1 | 2.20 | 1.56 | 1.50 | 1 | 2 |
| 3 | B | 398 | PX4 | C34-C33 | 2.20 | 1.62 | 1.51 | 9 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | C | 304 | PX4 | C3-N1 | 2.21 | 1.56 | 1.50 | 8 | 1 |
| 3 | A | 619 | PX4 | C11-C10 | 2.20 | 1.60 | 1.52 | 5 | 1 |
| 3 | A | 647 | PX4 | C25-C24 | 2.20 | 1.60 | 1.52 | 15 | 1 |
| 3 | B | 320 | PX4 | C3-N1 | 2.20 | 1.43 | 1.50 | 9 | 3 |
| 3 | A | 633 | PX4 | C31-C30 | 2.20 | 1.62 | 1.51 | 2 | 1 |
| 3 | A | 643 | PX4 | C12-C11 | 2.20 | 1.62 | 1.51 | 1 | 1 |
| 3 | B | 323 | PX4 | P1-O4 | 2.20 | 1.50 | 1.59 | 4 | 1 |
| 3 | B | 374 | PX4 | C25-C24 | 2.20 | 1.60 | 1.52 | 3 | 1 |
| 3 | B | 395 | PX4 | O3-C1 | 2.20 | 1.35 | 1.44 | 9 | 1 |
| 3 | C | 324 | PX4 | C25-C24 | 2.20 | 1.60 | 1.52 | 5 | 1 |
| 3 | B | 316 | PX4 | C17-C16 | 2.20 | 1.62 | 1.51 | 14 | 1 |
| 3 | B | 323 | PX4 | O5-C9 | 2.20 | 1.39 | 1.33 | 1 | 1 |
| 3 | B | 346 | PX4 | C29-C28 | 2.20 | 1.62 | 1.51 | 13 | 2 |
| 3 | B | 378 | PX4 | C3-N1 | 2.20 | 1.56 | 1.50 | 1 | 1 |
| 3 | B | 379 | PX4 | O5-C8 | 2.20 | 1.40 | 1.45 | 5 | 1 |
| 3 | C | 326 | PX4 | C11-C10 | 2.20 | 1.60 | 1.52 | 1 | 1 |
| 3 | B | 350 | PX4 | C25-C24 | 2.20 | 1.60 | 1.52 | 12 | 1 |
| 3 | B | 352 | PX4 | C3-N1 | 2.20 | 1.56 | 1.50 | 15 | 1 |
| 3 | B | 353 | PX4 | C11-C10 | 2.20 | 1.60 | 1.52 | 6 | 1 |
| 3 | B | 377 | PX4 | P1-O1 | 2.20 | 1.45 | 1.55 | 10 | 1 |
| 3 | B | 381 | PX4 | C14-C13 | 2.20 | 1.62 | 1.51 | 14 | 1 |
| 3 | B | 389 | PX4 | C5-N1 | 2.20 | 1.56 | 1.50 | 11 | 1 |
| 3 | C | 343 | PX4 | O5-C8 | 2.20 | 1.40 | 1.45 | 15 | 3 |
| 3 | C | 345 | PX4 | P1-O4 | 2.20 | 1.50 | 1.59 | 12 | 2 |
| 3 | C | 363 | PX4 | C11-C10 | 2.20 | 1.60 | 1.52 | 10 | 1 |
| 3 | A | 611 | PX4 | C13-C12 | 2.20 | 1.62 | 1.51 | 11 | 1 |
| 3 | B | 340 | PX4 | C3-N1 | 2.20 | 1.56 | 1.50 | 13 | 1 |
| 3 | B | 358 | PX4 | C28-C27 | 2.20 | 1.62 | 1.51 | 4 | 1 |
| 3 | B | 400 | PX4 | O5-C8 | 2.20 | 1.40 | 1.45 | 14 | 3 |
| 3 | C | 319 | PX4 | C13-C12 | 2.20 | 1.62 | 1.51 | 9 | 1 |
| 3 | C | 321 | PX4 | C33-C32 | 2.20 | 1.62 | 1.51 | 1 | 1 |
| 3 | A | 629 | PX4 | O5-C9 | 2.20 | 1.39 | 1.33 | 12 | 1 |
| 3 | C | 328 | PX4 | C29-C28 | 2.20 | 1.62 | 1.51 | 8 | 1 |
| 3 | B | 394 | PX4 | C4-N1 | 2.19 | 1.56 | 1.50 | 4 | 2 |
| 3 | B | 395 | PX4 | P1-O3 | 2.19 | 1.50 | 1.59 | 13 | 1 |
| 3 | C | 305 | PX4 | P1-O1 | 2.20 | 1.45 | 1.55 | 12 | 3 |
| 3 | C | 339 | PX4 | P1-O1 | 2.20 | 1.45 | 1.55 | 8 | 1 |
| 3 | C | 355 | PX4 | C20-C19 | 2.20 | 1.62 | 1.51 | 11 | 1 |
| 3 | C | 360 | PX4 | C27-C26 | 2.20 | 1.62 | 1.51 | 14 | 1 |
| 3 | C | 362 | PX4 | C4-N1 | 2.20 | 1.56 | 1.50 | 4 | 1 |
| 3 | C | 362 | PX4 | P1-O2 | 2.20 | 1.43 | 1.50 | 8 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | A | 612 | PX4 | C11-C10 | 2.19 | 1.60 | 1.52 | 7 | 1 |
| 3 | A | 619 | PX4 | C19-C18 | 2.19 | 1.62 | 1.51 | 15 | 1 |
| 3 | B | 309 | PX4 | C10-C9 | 2.19 | 1.57 | 1.50 | 5 | 2 |
| 3 | B | 325 | PX4 | C6-C7 | 2.19 | 1.57 | 1.50 | 4 | 2 |
| 3 | B | 334 | PX4 | C28-C27 | 2.19 | 1.62 | 1.51 | 13 | 1 |
| 3 | B | 354 | PX4 | O3-C1 | 2.19 | 1.36 | 1.44 | 3 | 1 |
| 3 | C | 309 | PX4 | P1-O4 | 2.19 | 1.50 | 1.59 | 6 | 1 |
| 3 | C | 331 | PX4 | P1-O1 | 2.19 | 1.45 | 1.55 | 3 | 2 |
| 3 | A | 613 | PX4 | C10-C9 | 2.19 | 1.57 | 1.50 | 12 | 2 |
| 3 | B | 361 | PX4 | P1-O1 | 2.19 | 1.45 | 1.55 | 5 | 1 |
| 3 | C | 328 | PX4 | C17-C16 | 2.19 | 1.62 | 1.51 | 5 | 1 |
| 3 | C | 351 | PX4 | O5-C8 | 2.19 | 1.40 | 1.45 | 3 | 3 |
| 3 | B | 310 | PX4 | C24-C23 | 2.19 | 1.57 | 1.50 | 4 | 1 |
| 3 | B | 312 | PX4 | O7-C23 | 2.19 | 1.28 | 1.34 | 2 | 2 |
| 3 | C | 307 | PX4 | C32-C31 | 2.19 | 1.62 | 1.51 | 7 | 1 |
| 3 | C | 331 | PX4 | P1-O4 | 2.19 | 1.50 | 1.59 | 14 | 1 |
| 3 | A | 606 | PX4 | C25-C24 | 2.19 | 1.60 | 1.52 | 12 | 2 |
| 3 | A | 627 | PX4 | C10-C9 | 2.19 | 1.57 | 1.50 | 10 | 2 |
| 3 | B | 318 | PX4 | P1-O2 | 2.19 | 1.43 | 1.50 | 9 | 1 |
| 3 | B | 350 | PX4 | C5-N1 | 2.19 | 1.56 | 1.50 | 2 | 1 |
| 3 | B | 374 | PX4 | O7-C23 | 2.19 | 1.28 | 1.34 | 12 | 2 |
| 3 | C | 348 | PX4 | C11-C10 | 2.19 | 1.60 | 1.52 | 9 | 4 |
| 3 | A | 604 | PX4 | P1-O1 | 2.19 | 1.45 | 1.55 | 9 | 2 |
| 3 | A | 629 | PX4 | P1-O2 | 2.19 | 1.43 | 1.50 | 5 | 1 |
| 3 | C | 326 | PX4 | C13-C12 | 2.19 | 1.62 | 1.51 | 4 | 1 |
| 3 | C | 326 | PX4 | C4-N1 | 2.19 | 1.56 | 1.50 | 14 | 1 |
| 3 | C | 362 | PX4 | C20-C19 | 2.19 | 1.62 | 1.51 | 12 | 1 |
| 3 | B | 364 | PX4 | P1-O1 | 2.19 | 1.45 | 1.55 | 2 | 2 |
| 3 | C | 337 | PX4 | P1-O1 | 2.19 | 1.45 | 1.55 | 2 | 3 |
| 3 | A | 651 | PX4 | P1-O1 | 2.18 | 1.45 | 1.55 | 12 | 1 |
| 3 | A | 654 | PX4 | C25-C24 | 2.18 | 1.60 | 1.52 | 8 | 2 |
| 3 | C | 323 | PX4 | C13-C12 | 2.18 | 1.62 | 1.51 | 11 | 1 |
| 3 | C | 325 | PX4 | C13-C12 | 2.18 | 1.62 | 1.51 | 1 | 1 |
| 3 | B | 362 | PX4 | C5-N1 | 2.18 | 1.56 | 1.50 | 10 | 1 |
| 3 | C | 341 | PX4 | C13-C12 | 2.18 | 1.62 | 1.51 | 1 | 1 |
| 3 | A | 647 | PX4 | C4-N1 | 2.18 | 1.56 | 1.50 | 5 | 3 |
| 3 | A | 651 | PX4 | C12-C11 | 2.18 | 1.62 | 1.51 | 11 | 1 |
| 3 | B | 384 | PX4 | C30-C29 | 2.18 | 1.62 | 1.51 | 8 | 1 |
| 3 | B | 362 | PX4 | C25-C24 | 2.18 | 1.60 | 1.52 | 9 | 1 |
| 3 | B | 387 | PX4 | C4-N1 | 2.18 | 1.56 | 1.50 | 7 | 2 |
| 3 | C | 364 | PX4 | C19-C18 | 2.18 | 1.62 | 1.51 | 5 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | A | 617 | PX4 | C34-C33 | 2.18 | 1.62 | 1.51 | 9 | 1 |
| 3 | A | 621 | PX4 | C14-C13 | 2.18 | 1.62 | 1.51 | 1 | 1 |
| 3 | A | 650 | PX4 | C5-N1 | 2.18 | 1.56 | 1.50 | 3 | 1 |
| 3 | C | 319 | PX4 | C11-C10 | 2.18 | 1.60 | 1.52 | 10 | 1 |
| 3 | C | 324 | PX4 | C16-C15 | 2.18 | 1.62 | 1.51 | 3 | 1 |
| 3 | C | 347 | PX4 | C4-N1 | 2.18 | 1.56 | 1.50 | 2 | 1 |
| 3 | A | 633 | PX4 | C5-N1 | 2.18 | 1.56 | 1.50 | 11 | 1 |
| 3 | C | 301 | PX4 | C3-N1 | 2.18 | 1.56 | 1.50 | 10 | 1 |
| 3 | B | 312 | PX4 | C13-C12 | 2.18 | 1.62 | 1.51 | 11 | 1 |
| 3 | B | 361 | PX4 | C5-N1 | 2.18 | 1.56 | 1.50 | 6 | 1 |
| 3 | B | 372 | PX4 | C13-C12 | 2.18 | 1.62 | 1.51 | 1 | 1 |
| 3 | B | 373 | PX4 | C25-C24 | 2.18 | 1.60 | 1.52 | 7 | 1 |
| 3 | C | 315 | PX4 | P1-O1 | 2.18 | 1.45 | 1.55 | 15 | 3 |
| 3 | C | 321 | PX4 | O4-C6 | 2.18 | 1.36 | 1.44 | 3 | 1 |
| 3 | C | 324 | PX4 | C3-N1 | 2.18 | 1.56 | 1.50 | 7 | 1 |
| 3 | C | 355 | PX4 | C29-C28 | 2.18 | 1.62 | 1.51 | 12 | 1 |
| 3 | B | 374 | PX4 | C17-C16 | 2.18 | 1.62 | 1.51 | 14 | 1 |
| 3 | B | 397 | PX4 | C11-C10 | 2.18 | 1.60 | 1.52 | 8 | 1 |
| 3 | B | 380 | PX4 | C3-N1 | 2.18 | 1.56 | 1.50 | 1 | 1 |
| 3 | B | 393 | PX4 | P1-O1 | 2.18 | 1.45 | 1.55 | 4 | 2 |
| 3 | C | 349 | PX4 | C11-C10 | 2.18 | 1.60 | 1.52 | 12 | 3 |
| 3 | A | 650 | PX4 | C2-C1 | 2.18 | 1.57 | 1.51 | 6 | 2 |
| 3 | A | 652 | PX4 | C26-C25 | 2.17 | 1.62 | 1.51 | 12 | 1 |
| 3 | C | 312 | PX4 | C28-C27 | 2.18 | 1.62 | 1.51 | 4 | 1 |
| 3 | A | 649 | PX4 | C4-N1 | 2.17 | 1.43 | 1.50 | 12 | 1 |
| 3 | B | 352 | PX4 | C24-C23 | 2.17 | 1.57 | 1.50 | 14 | 1 |
| 3 | B | 365 | PX4 | C24-C23 | 2.17 | 1.57 | 1.50 | 11 | 1 |
| 3 | B | 380 | PX4 | C25-C24 | 2.17 | 1.60 | 1.52 | 4 | 1 |
| 3 | B | 366 | PX4 | C10-C9 | 2.17 | 1.57 | 1.50 | 2 | 1 |
| 3 | B | 382 | PX4 | C12-C11 | 2.17 | 1.62 | 1.51 | 10 | 1 |
| 3 | C | 321 | PX4 | C32-C31 | 2.17 | 1.62 | 1.51 | 7 | 1 |
| 3 | C | 347 | PX4 | C16-C15 | 2.17 | 1.62 | 1.51 | 9 | 1 |
| 3 | B | 309 | PX4 | C25-C24 | 2.17 | 1.60 | 1.52 | 11 | 2 |
| 3 | B | 313 | PX4 | O7-C23 | 2.17 | 1.28 | 1.34 | 6 | 2 |
| 3 | B | 328 | PX4 | O7-C23 | 2.17 | 1.28 | 1.34 | 6 | 2 |
| 3 | B | 336 | PX4 | C16-C15 | 2.17 | 1.62 | 1.51 | 1 | 1 |
| 3 | A | 615 | PX4 | O5-C9 | 2.17 | 1.27 | 1.33 | 12 | 1 |
| 3 | B | 338 | PX4 | C30-C29 | 2.17 | 1.62 | 1.51 | 8 | 2 |
| 3 | B | 359 | PX4 | C25-C24 | 2.17 | 1.60 | 1.52 | 9 | 1 |
| 3 | B | 375 | PX4 | O7-C23 | 2.17 | 1.28 | 1.34 | 3 | 1 |
| 3 | B | 385 | PX4 | C5-N1 | 2.17 | 1.43 | 1.50 | 13 | 2 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | C | 317 | PX4 | C3-N1 | 2.17 | 1.56 | 1.50 | 3 | 1 |
| 3 | A | 644 | PX4 | C4-N1 | 2.17 | 1.56 | 1.50 | 6 | 1 |
| 3 | C | 340 | PX4 | C25-C24 | 2.17 | 1.60 | 1.52 | 5 | 1 |
| 3 | B | 380 | PX4 | C15-C14 | 2.17 | 1.62 | 1.51 | 4 | 1 |
| 3 | B | 345 | PX4 | C19-C18 | 2.17 | 1.62 | 1.51 | 9 | 1 |
| 3 | C | 326 | PX4 | O6-C9 | 2.17 | 1.29 | 1.22 | 3 | 1 |
| 3 | A | 623 | PX4 | C4-N1 | 2.17 | 1.56 | 1.50 | 13 | 1 |
| 3 | A | 630 | PX4 | O4-C6 | 2.17 | 1.36 | 1.44 | 14 | 1 |
| 3 | A | 649 | PX4 | C10-C9 | 2.17 | 1.57 | 1.50 | 10 | 1 |
| 3 | C | 328 | PX4 | C34-C33 | 2.17 | 1.62 | 1.51 | 15 | 1 |
| 3 | C | 330 | PX4 | C18-C17 | 2.17 | 1.62 | 1.51 | 5 | 1 |
| 3 | A | 634 | PX4 | O7-C23 | 2.17 | 1.28 | 1.34 | 5 | 1 |
| 3 | A | 643 | PX4 | P1-O3 | 2.17 | 1.50 | 1.59 | 3 | 1 |
| 3 | B | 334 | PX4 | P1-O3 | 2.17 | 1.50 | 1.59 | 3 | 2 |
| 3 | B | 335 | PX4 | C16-C15 | 2.17 | 1.62 | 1.51 | 10 | 1 |
| 3 | B | 335 | PX4 | C11-C10 | 2.17 | 1.60 | 1.52 | 14 | 1 |
| 3 | B | 343 | PX4 | P1-O2 | 2.17 | 1.43 | 1.50 | 10 | 1 |
| 3 | B | 359 | PX4 | O4-C6 | 2.17 | 1.36 | 1.44 | 7 | 1 |
| 3 | C | 333 | PX4 | O7-C23 | 2.17 | 1.28 | 1.34 | 1 | 3 |
| 3 | A | 637 | PX4 | C27-C26 | 2.17 | 1.62 | 1.51 | 14 | 1 |
| 3 | A | 639 | PX4 | C18-C17 | 2.16 | 1.62 | 1.51 | 4 | 1 |
| 3 | A | 644 | PX4 | O7-C7 | 2.16 | 1.41 | 1.46 | 2 | 2 |
| 3 | B | 312 | PX4 | C2-N1 | 2.16 | 1.44 | 1.51 | 5 | 1 |
| 3 | C | 341 | PX4 | P1-O3 | 2.16 | 1.50 | 1.59 | 5 | 1 |
| 3 | C | 354 | PX4 | C4-N1 | 2.17 | 1.43 | 1.50 | 6 | 1 |
| 3 | B | 385 | PX4 | C15-C14 | 2.16 | 1.62 | 1.51 | 11 | 1 |
| 3 | B | 329 | PX4 | C15-C14 | 2.16 | 1.62 | 1.51 | 1 | 1 |
| 3 | A | 626 | PX4 | P1-O1 | 2.16 | 1.45 | 1.55 | 1 | 3 |
| 3 | A | 649 | PX4 | P1-O4 | 2.16 | 1.67 | 1.59 | 7 | 1 |
| 3 | A | 654 | PX4 | C2-N1 | 2.16 | 1.58 | 1.51 | 10 | 1 |
| 3 | B | 330 | PX4 | C2-N1 | 2.16 | 1.58 | 1.51 | 15 | 3 |
| 3 | C | 347 | PX4 | C18-C17 | 2.16 | 1.62 | 1.51 | 9 | 2 |
| 3 | B | 348 | PX4 | O7-C23 | 2.16 | 1.28 | 1.34 | 4 | 1 |
| 3 | B | 356 | PX4 | C2-N1 | 2.16 | 1.44 | 1.51 | 9 | 1 |
| 3 | A | 612 | PX4 | C34-C33 | 2.16 | 1.62 | 1.51 | 12 | 1 |
| 3 | A | 620 | PX4 | O7-C7 | 2.16 | 1.41 | 1.46 | 13 | 2 |
| 3 | A | 635 | PX4 | C3-N1 | 2.16 | 1.43 | 1.50 | 4 | 1 |
| 3 | B | 369 | PX4 | P1-O2 | 2.16 | 1.43 | 1.50 | 8 | 2 |
| 3 | C | 329 | PX4 | C28-C27 | 2.16 | 1.62 | 1.51 | 10 | 1 |
| 3 | C | 354 | PX4 | C17-C16 | 2.16 | 1.62 | 1.51 | 14 | 1 |
| 3 | C | 355 | PX4 | C15-C14 | 2.16 | 1.62 | 1.51 | 12 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | C | 364 | PX4 | C17-C16 | 2.16 | 1.62 | 1.51 | 5 | 1 |
| 3 | A | 610 | PX4 | C5-N1 | 2.16 | 1.56 | 1.50 | 4 | 2 |
| 3 | B | 346 | PX4 | C25-C24 | 2.16 | 1.60 | 1.52 | 11 | 1 |
| 3 | C | 301 | PX4 | P1-O1 | 2.16 | 1.45 | 1.55 | 9 | 1 |
| 3 | A | 654 | PX4 | C4-N1 | 2.16 | 1.43 | 1.50 | 14 | 1 |
| 3 | C | 318 | PX4 | C2-N1 | 2.16 | 1.44 | 1.51 | 15 | 2 |
| 3 | C | 347 | PX4 | C19-C18 | 2.16 | 1.62 | 1.51 | 9 | 1 |
| 3 | B | 371 | PX4 | C2-N1 | 2.16 | 1.44 | 1.51 | 1 | 1 |
| 3 | B | 393 | PX4 | C18-C17 | 2.16 | 1.62 | 1.51 | 9 | 1 |
| 3 | B | 399 | PX4 | C19-C18 | 2.16 | 1.62 | 1.51 | 9 | 1 |
| 3 | C | 326 | PX4 | C29-C28 | 2.16 | 1.62 | 1.51 | 12 | 1 |
| 3 | A | 632 | PX4 | C10-C9 | 2.16 | 1.57 | 1.50 | 15 | 2 |
| 3 | C | 359 | PX4 | P1-O1 | 2.16 | 1.45 | 1.55 | 7 | 1 |
| 3 | B | 314 | PX4 | P1-O1 | 2.15 | 1.45 | 1.55 | 11 | 1 |
| 3 | B | 361 | PX4 | C26-C25 | 2.15 | 1.62 | 1.51 | 10 | 1 |
| 3 | B | 370 | PX4 | O7-C23 | 2.15 | 1.28 | 1.34 | 3 | 1 |
| 3 | A | 616 | PX4 | C4-N1 | 2.15 | 1.56 | 1.50 | 6 | 2 |
| 3 | A | 633 | PX4 | P1-O1 | 2.15 | 1.45 | 1.55 | 13 | 2 |
| 3 | B | 319 | PX4 | C5-N1 | 2.15 | 1.56 | 1.50 | 12 | 1 |
| 3 | B | 397 | PX4 | C31-C30 | 2.15 | 1.62 | 1.51 | 14 | 1 |
| 3 | B | 362 | PX4 | C16-C15 | 2.15 | 1.62 | 1.51 | 1 | 1 |
| 3 | B | 366 | PX4 | P1-O4 | 2.15 | 1.51 | 1.59 | 7 | 1 |
| 3 | C | 333 | PX4 | C20-C19 | 2.15 | 1.62 | 1.51 | 1 | 1 |
| 3 | C | 353 | PX4 | C3-N1 | 2.15 | 1.43 | 1.50 | 5 | 1 |
| 3 | A | 621 | PX4 | P1-O1 | 2.15 | 1.45 | 1.55 | 12 | 2 |
| 3 | A | 638 | PX4 | O7-C23 | 2.15 | 1.28 | 1.34 | 3 | 1 |
| 3 | B | 375 | PX4 | P1-O4 | 2.15 | 1.51 | 1.59 | 15 | 1 |
| 3 | A | 608 | PX4 | O4-C6 | 2.15 | 1.36 | 1.44 | 13 | 2 |
| 3 | B | 320 | PX4 | C19-C18 | 2.15 | 1.62 | 1.51 | 13 | 1 |
| 3 | B | 321 | PX4 | O5-C8 | 2.15 | 1.50 | 1.45 | 4 | 1 |
| 3 | B | 357 | PX4 | P1-O4 | 2.15 | 1.51 | 1.59 | 15 | 1 |
| 3 | B | 358 | PX4 | C24-C23 | 2.15 | 1.56 | 1.50 | 10 | 2 |
| 3 | C | 311 | PX4 | C33-C32 | 2.15 | 1.62 | 1.51 | 5 | 2 |
| 3 | A | 624 | PX4 | C28-C27 | 2.15 | 1.62 | 1.51 | 15 | 1 |
| 3 | A | 630 | PX4 | C19-C18 | 2.15 | 1.62 | 1.51 | 15 | 2 |
| 3 | B | 363 | PX4 | C25-C24 | 2.15 | 1.60 | 1.52 | 11 | 1 |
| 3 | B | 396 | PX4 | C27-C26 | 2.15 | 1.62 | 1.51 | 11 | 1 |
| 3 | B | 399 | PX4 | O5-C8 | 2.15 | 1.40 | 1.45 | 2 | 1 |
| 3 | C | 338 | PX4 | O5-C9 | 2.15 | 1.27 | 1.33 | 7 | 1 |
| 3 | A | 642 | PX4 | C25-C24 | 2.15 | 1.60 | 1.52 | 5 | 1 |
| 3 | A | 646 | PX4 | C25-C24 | 2.14 | 1.60 | 1.52 | 6 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 326 | PX4 | P1-O2 | 2.14 | 1.43 | 1.50 | 2 | 1 |
| 3 | B | 345 | PX4 | O3-C1 | 2.14 | 1.36 | 1.44 | 15 | 1 |
| 3 | B | 393 | PX4 | C3-N1 | 2.14 | 1.43 | 1.50 | 5 | 1 |
| 3 | C | 312 | PX4 | P1-O3 | 2.14 | 1.51 | 1.59 | 1 | 1 |
| 3 | C | 319 | PX4 | O5-C8 | 2.14 | 1.40 | 1.45 | 3 | 2 |
| 3 | C | 354 | PX4 | O8-C23 | 2.14 | 1.16 | 1.22 | 7 | 1 |
| 3 | C | 364 | PX4 | C28-C27 | 2.14 | 1.62 | 1.51 | 15 | 1 |
| 3 | A | 639 | PX4 | P1-O2 | 2.14 | 1.43 | 1.50 | 3 | 1 |
| 3 | A | 612 | PX4 | C4-N1 | 2.14 | 1.56 | 1.50 | 4 | 1 |
| 3 | A | 621 | PX4 | C4-N1 | 2.14 | 1.43 | 1.50 | 15 | 1 |
| 3 | A | 640 | PX4 | O5-C9 | 2.14 | 1.39 | 1.33 | 14 | 3 |
| 3 | A | 645 | PX4 | C31-C30 | 2.14 | 1.62 | 1.51 | 12 | 1 |
| 3 | B | 327 | PX4 | C16-C15 | 2.14 | 1.62 | 1.51 | 2 | 1 |
| 3 | B | 330 | PX4 | P1-O4 | 2.14 | 1.51 | 1.59 | 3 | 1 |
| 3 | B | 306 | PX4 | C32-C31 | 2.14 | 1.62 | 1.51 | 5 | 1 |
| 3 | B | 314 | PX4 | P1-O4 | 2.14 | 1.51 | 1.59 | 13 | 1 |
| 3 | B | 375 | PX4 | C5-N1 | 2.14 | 1.56 | 1.50 | 14 | 1 |
| 3 | C | 319 | PX4 | C15-C14 | 2.14 | 1.62 | 1.51 | 3 | 1 |
| 3 | B | 313 | PX4 | C2-N1 | 2.14 | 1.58 | 1.51 | 7 | 2 |
| 3 | B | 380 | PX4 | C18-C17 | 2.14 | 1.62 | 1.51 | 5 | 1 |
| 3 | B | 396 | PX4 | O5-C9 | 2.14 | 1.39 | 1.33 | 4 | 2 |
| 3 | C | 332 | PX4 | C4-N1 | 2.14 | 1.43 | 1.50 | 2 | 2 |
| 3 | C | 345 | PX4 | O5-C8 | 2.14 | 1.49 | 1.45 | 3 | 2 |
| 3 | C | 347 | PX4 | C12-C11 | 2.14 | 1.62 | 1.51 | 8 | 1 |
| 3 | B | 347 | PX4 | P1-O3 | 2.14 | 1.67 | 1.59 | 15 | 2 |
| 3 | B | 336 | PX4 | P1-O3 | 2.14 | 1.51 | 1.59 | 13 | 1 |
| 3 | B | 350 | PX4 | C26-C25 | 2.14 | 1.62 | 1.51 | 12 | 1 |
| 3 | B | 365 | PX4 | C2-N1 | 2.14 | 1.58 | 1.51 | 3 | 1 |
| 3 | C | 314 | PX4 | C34-C33 | 2.14 | 1.62 | 1.51 | 12 | 1 |
| 3 | C | 341 | PX4 | O7-C23 | 2.14 | 1.28 | 1.34 | 2 | 1 |
| 3 | B | 364 | PX4 | C31-C30 | 2.14 | 1.62 | 1.51 | 1 | 1 |
| 3 | C | 312 | PX4 | P1-O4 | 2.14 | 1.51 | 1.59 | 1 | 1 |
| 3 | C | 333 | PX4 | C34-C33 | 2.14 | 1.62 | 1.51 | 15 | 1 |
| 3 | A | 645 | PX4 | C11-C10 | 2.13 | 1.60 | 1.52 | 1 | 1 |
| 3 | B | 306 | PX4 | O8-C23 | 2.14 | 1.16 | 1.22 | 12 | 1 |
| 3 | B | 314 | PX4 | C34-C33 | 2.14 | 1.62 | 1.51 | 10 | 1 |
| 3 | C | 338 | PX4 | C13-C12 | 2.14 | 1.62 | 1.51 | 8 | 1 |
| 3 | A | 651 | PX4 | C17-C16 | 2.13 | 1.62 | 1.51 | 8 | 1 |
| 3 | B | 342 | PX4 | C28-C27 | 2.13 | 1.62 | 1.51 | 10 | 1 |
| 3 | B | 355 | PX4 | O5-C8 | 2.13 | 1.49 | 1.45 | 6 | 2 |
| 3 | B | 387 | PX4 | C20-C19 | 2.13 | 1.62 | 1.51 | 3 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | C | 324 | PX4 | P1-O3 | 2.14 | 1.67 | 1.59 | 12 | 2 |
| 3 | C | 334 | PX4 | C3-N1 | 2.13 | 1.56 | 1.50 | 10 | 1 |
| 3 | C | 330 | PX4 | C11-C10 | 2.13 | 1.60 | 1.52 | 8 | 1 |
| 3 | C | 332 | PX4 | O5-C9 | 2.13 | 1.39 | 1.33 | 1 | 1 |
| 3 | C | 341 | PX4 | C27-C26 | 2.13 | 1.62 | 1.51 | 5 | 2 |
| 3 | C | 344 | PX4 | O7-C23 | 2.13 | 1.28 | 1.34 | 5 | 1 |
| 3 | A | 633 | PX4 | P1-O2 | 2.13 | 1.43 | 1.50 | 3 | 1 |
| 3 | C | 335 | PX4 | C13-C12 | 2.13 | 1.62 | 1.51 | 14 | 2 |
| 3 | C | 338 | PX4 | C5-N1 | 2.13 | 1.56 | 1.50 | 5 | 1 |
| 3 | A | 648 | PX4 | P1-O2 | 2.13 | 1.43 | 1.50 | 5 | 1 |
| 3 | A | 651 | PX4 | C4-N1 | 2.13 | 1.56 | 1.50 | 2 | 1 |
| 3 | B | 329 | PX4 | C33-C32 | 2.13 | 1.62 | 1.51 | 15 | 1 |
| 3 | B | 360 | PX4 | P1-O1 | 2.13 | 1.45 | 1.55 | 14 | 3 |
| 3 | B | 392 | PX4 | C11-C10 | 2.13 | 1.60 | 1.52 | 12 | 1 |
| 3 | C | 302 | PX4 | C31-C30 | 2.13 | 1.62 | 1.51 | 10 | 1 |
| 3 | C | 319 | PX4 | C24-C23 | 2.13 | 1.56 | 1.50 | 15 | 1 |
| 3 | B | 351 | PX4 | C24-C23 | 2.13 | 1.56 | 1.50 | 4 | 1 |
| 3 | B | 311 | PX4 | P1-O4 | 2.13 | 1.51 | 1.59 | 5 | 1 |
| 3 | B | 314 | PX4 | C11-C10 | 2.13 | 1.60 | 1.52 | 14 | 2 |
| 3 | B | 317 | PX4 | C17-C16 | 2.13 | 1.62 | 1.51 | 9 | 1 |
| 3 | B | 337 | PX4 | C4-N1 | 2.13 | 1.56 | 1.50 | 8 | 1 |
| 3 | B | 341 | PX4 | C27-C26 | 2.13 | 1.62 | 1.51 | 3 | 1 |
| 3 | B | 343 | PX4 | C10-C9 | 2.13 | 1.56 | 1.50 | 10 | 2 |
| 3 | C | 320 | PX4 | C4-N1 | 2.13 | 1.56 | 1.50 | 11 | 1 |
| 3 | C | 329 | PX4 | C10-C9 | 2.13 | 1.56 | 1.50 | 13 | 1 |
| 3 | C | 304 | PX4 | P1-O4 | 2.13 | 1.51 | 1.59 | 12 | 1 |
| 3 | C | 360 | PX4 | C17-C16 | 2.13 | 1.62 | 1.51 | 3 | 1 |
| 3 | A | 622 | PX4 | C15-C14 | 2.13 | 1.62 | 1.51 | 2 | 1 |
| 3 | A | 634 | PX4 | P1-O1 | 2.13 | 1.45 | 1.55 | 9 | 1 |
| 3 | A | 641 | PX4 | P1-O1 | 2.13 | 1.45 | 1.55 | 1 | 2 |
| 3 | A | 653 | PX4 | C33-C32 | 2.13 | 1.62 | 1.51 | 3 | 1 |
| 3 | B | 311 | PX4 | P1-O2 | 2.13 | 1.43 | 1.50 | 1 | 1 |
| 3 | B | 335 | PX4 | C28-C27 | 2.13 | 1.62 | 1.51 | 8 | 1 |
| 3 | B | 348 | PX4 | C18-C17 | 2.13 | 1.62 | 1.51 | 12 | 1 |
| 3 | B | 349 | PX4 | C28-C27 | 2.13 | 1.62 | 1.51 | 4 | 1 |
| 3 | C | 308 | PX4 | C14-C13 | 2.13 | 1.62 | 1.51 | 12 | 1 |
| 3 | B | 347 | PX4 | C28-C27 | 2.13 | 1.62 | 1.51 | 5 | 1 |
| 3 | B | 396 | PX4 | C14-C13 | 2.13 | 1.62 | 1.51 | 13 | 1 |
| 3 | C | 345 | PX4 | C5-N1 | 2.13 | 1.43 | 1.50 | 2 | 1 |
| 3 | C | 364 | PX4 | O5-C9 | 2.13 | 1.27 | 1.33 | 4 | 1 |
| 3 | A | 617 | PX4 | P1-O3 | 2.13 | 1.51 | 1.59 | 10 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 301 | PX4 | C25-C24 | 2.13 | 1.60 | 1.52 | 8 | 1 |
| 3 | B | 372 | PX4 | C30-C29 | 2.13 | 1.62 | 1.51 | 14 | 1 |
| 3 | C | 325 | PX4 | C14-C13 | 2.13 | 1.62 | 1.51 | 13 | 1 |
| 3 | A | 608 | PX4 | C5-N1 | 2.12 | 1.43 | 1.50 | 8 | 1 |
| 3 | A | 604 | PX4 | P1-O4 | 2.12 | 1.51 | 1.59 | 10 | 1 |
| 3 | B | 317 | PX4 | C27-C26 | 2.12 | 1.62 | 1.51 | 2 | 1 |
| 3 | B | 351 | PX4 | C3-N1 | 2.12 | 1.56 | 1.50 | 9 | 1 |
| 3 | B | 376 | PX4 | C4-N1 | 2.12 | 1.56 | 1.50 | 1 | 1 |
| 3 | B | 383 | PX4 | C11-C10 | 2.12 | 1.60 | 1.52 | 8 | 1 |
| 3 | B | 315 | PX4 | O4-C6 | 2.12 | 1.36 | 1.44 | 3 | 1 |
| 3 | B | 315 | PX4 | C10-C9 | 2.12 | 1.56 | 1.50 | 8 | 2 |
| 3 | C | 344 | PX4 | C12-C11 | 2.12 | 1.62 | 1.51 | 15 | 1 |
| 3 | C | 354 | PX4 | C5-N1 | 2.12 | 1.43 | 1.50 | 8 | 1 |
| 3 | C | 358 | PX4 | C13-C12 | 2.12 | 1.62 | 1.51 | 10 | 1 |
| 3 | B | 320 | PX4 | P1-O1 | 2.12 | 1.45 | 1.55 | 11 | 2 |
| 3 | B | 353 | PX4 | C15-C14 | 2.12 | 1.62 | 1.51 | 2 | 1 |
| 3 | C | 348 | PX4 | C17-C16 | 2.12 | 1.62 | 1.51 | 10 | 1 |
| 3 | A | 621 | PX4 | C17-C16 | 2.12 | 1.62 | 1.51 | 14 | 1 |
| 3 | B | 374 | PX4 | C16-C15 | 2.12 | 1.62 | 1.51 | 1 | 1 |
| 3 | B | 380 | PX4 | O3-C1 | 2.12 | 1.53 | 1.44 | 5 | 1 |
| 3 | C | 340 | PX4 | P1-O2 | 2.12 | 1.43 | 1.50 | 2 | 1 |
| 3 | C | 340 | PX4 | C30-C29 | 2.12 | 1.62 | 1.51 | 6 | 1 |
| 3 | A | 613 | PX4 | C28-C27 | 2.12 | 1.62 | 1.51 | 3 | 1 |
| 3 | B | 373 | PX4 | O7-C23 | 2.12 | 1.28 | 1.34 | 7 | 1 |
| 3 | B | 375 | PX4 | C2-C1 | 2.12 | 1.57 | 1.51 | 4 | 2 |
| 3 | B | 396 | PX4 | P1-O2 | 2.12 | 1.43 | 1.50 | 11 | 1 |
| 3 | A | 619 | PX4 | C17-C16 | 2.12 | 1.62 | 1.51 | 1 | 1 |
| 3 | A | 632 | PX4 | P1-O1 | 2.12 | 1.45 | 1.55 | 6 | 2 |
| 3 | C | 303 | PX4 | O5-C9 | 2.12 | 1.27 | 1.33 | 7 | 1 |
| 3 | A | 637 | PX4 | C5-N1 | 2.12 | 1.56 | 1.50 | 5 | 1 |
| 3 | B | 316 | PX4 | C3-N1 | 2.12 | 1.43 | 1.50 | 13 | 1 |
| 3 | B | 373 | PX4 | C4-N1 | 2.12 | 1.43 | 1.50 | 12 | 1 |
| 3 | C | 344 | PX4 | C4-N1 | 2.12 | 1.56 | 1.50 | 2 | 1 |
| 3 | B | 327 | PX4 | O3-C1 | 2.12 | 1.36 | 1.44 | 7 | 1 |
| 3 | B | 388 | PX4 | C16-C15 | 2.12 | 1.62 | 1.51 | 7 | 1 |
| 3 | B | 306 | PX4 | C14-C13 | 2.11 | 1.62 | 1.51 | 13 | 1 |
| 3 | A | 622 | PX4 | C5-N1 | 2.11 | 1.43 | 1.50 | 3 | 1 |
| 3 | A | 624 | PX4 | C25-C24 | 2.11 | 1.59 | 1.52 | 2 | 1 |
| 3 | B | 336 | PX4 | C19-C18 | 2.11 | 1.62 | 1.51 | 12 | 1 |
| 3 | B | 362 | PX4 | C15-C14 | 2.11 | 1.62 | 1.51 | 14 | 1 |
| 3 | B | 377 | PX4 | C12-C11 | 2.11 | 1.62 | 1.51 | 14 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 394 | PX4 | C12-C11 | 2.11 | 1.62 | 1.51 | 13 | 1 |
| 3 | C | 317 | PX4 | C11-C10 | 2.11 | 1.44 | 1.52 | 11 | 1 |
| 3 | C | 338 | PX4 | C24-C23 | 2.11 | 1.56 | 1.50 | 14 | 2 |
| 3 | C | 344 | PX4 | C30-C29 | 2.11 | 1.62 | 1.51 | 14 | 1 |
| 3 | C | 351 | PX4 | C17-C16 | 2.11 | 1.62 | 1.51 | 8 | 1 |
| 3 | A | 653 | PX4 | C28-C27 | 2.11 | 1.62 | 1.51 | 10 | 1 |
| 3 | B | 302 | PX4 | C2-N1 | 2.11 | 1.45 | 1.51 | 7 | 1 |
| 3 | B | 315 | PX4 | O7-C7 | 2.11 | 1.41 | 1.46 | 3 | 3 |
| 3 | B | 332 | PX4 | C3-N1 | 2.11 | 1.43 | 1.50 | 11 | 1 |
| 3 | B | 335 | PX4 | C3-N1 | 2.11 | 1.56 | 1.50 | 2 | 1 |
| 3 | C | 351 | PX4 | P1-O2 | 2.11 | 1.43 | 1.50 | 14 | 2 |
| 3 | C | 306 | PX4 | C15-C14 | 2.11 | 1.62 | 1.51 | 10 | 1 |
| 3 | C | 331 | PX4 | C31-C30 | 2.11 | 1.62 | 1.51 | 2 | 1 |
| 3 | B | 302 | PX4 | C19-C18 | 2.11 | 1.62 | 1.51 | 12 | 1 |
| 3 | B | 345 | PX4 | O7-C7 | 2.11 | 1.41 | 1.46 | 6 | 1 |
| 3 | B | 330 | PX4 | C11-C10 | 2.11 | 1.59 | 1.52 | 2 | 1 |
| 3 | B | 335 | PX4 | P1-O1 | 2.11 | 1.45 | 1.55 | 13 | 5 |
| 3 | B | 355 | PX4 | C15-C14 | 2.11 | 1.62 | 1.51 | 14 | 1 |
| 3 | B | 342 | PX4 | C25-C24 | 2.11 | 1.59 | 1.52 | 15 | 1 |
| 3 | B | 358 | PX4 | P1-O1 | 2.11 | 1.45 | 1.55 | 13 | 1 |
| 3 | B | 370 | PX4 | O7-C7 | 2.11 | 1.51 | 1.46 | 13 | 2 |
| 3 | B | 387 | PX4 | O3-C1 | 2.11 | 1.36 | 1.44 | 7 | 1 |
| 3 | C | 314 | PX4 | P1-O1 | 2.11 | 1.45 | 1.55 | 4 | 1 |
| 3 | C | 338 | PX4 | P1-O4 | 2.11 | 1.51 | 1.59 | 7 | 1 |
| 3 | B | 394 | PX4 | C21-C20 | 2.11 | 1.64 | 1.51 | 3 | 1 |
| 3 | C | 312 | PX4 | C2-N1 | 2.11 | 1.57 | 1.51 | 15 | 1 |
| 3 | C | 319 | PX4 | O5-C9 | 2.11 | 1.27 | 1.33 | 13 | 1 |
| 3 | C | 352 | PX4 | C5-N1 | 2.11 | 1.56 | 1.50 | 11 | 1 |
| 3 | C | 364 | PX4 | P1-O4 | 2.11 | 1.51 | 1.59 | 12 | 1 |
| 3 | A | 603 | PX4 | C14-C13 | 2.11 | 1.62 | 1.51 | 4 | 1 |
| 3 | A | 620 | PX4 | O7-C23 | 2.11 | 1.28 | 1.34 | 12 | 1 |
| 3 | B | 310 | PX4 | C4-N1 | 2.11 | 1.43 | 1.50 | 6 | 1 |
| 3 | C | 309 | PX4 | C18-C17 | 2.11 | 1.62 | 1.51 | 13 | 1 |
| 3 | C | 324 | PX4 | P1-O1 | 2.11 | 1.45 | 1.55 | 15 | 1 |
| 3 | A | 627 | PX4 | C16-C15 | 2.11 | 1.62 | 1.51 | 14 | 1 |
| 3 | C | 301 | PX4 | C30-C29 | 2.11 | 1.62 | 1.51 | 11 | 1 |
| 3 | C | 326 | PX4 | C12-C11 | 2.11 | 1.62 | 1.51 | 2 | 1 |
| 3 | A | 623 | PX4 | C3-N1 | 2.10 | 1.43 | 1.50 | 7 | 3 |
| 3 | A | 637 | PX4 | C32-C31 | 2.10 | 1.62 | 1.51 | 14 | 1 |
| 3 | B | 373 | PX4 | C26-C25 | 2.10 | 1.62 | 1.51 | 2 | 1 |
| 3 | B | 398 | PX4 | C30-C29 | 2.10 | 1.62 | 1.51 | 1 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | C | 328 | PX4 | C4-N1 | 2.11 | 1.56 | 1.50 | 6 | 1 |
| 3 | C | 364 | PX4 | C20-C19 | 2.11 | 1.62 | 1.51 | 9 | 1 |
| 3 | A | 636 | PX4 | C5-N1 | 2.10 | 1.43 | 1.50 | 10 | 2 |
| 3 | A | 604 | PX4 | C15-C14 | 2.10 | 1.62 | 1.51 | 1 | 1 |
| 3 | A | 608 | PX4 | C28-C27 | 2.10 | 1.62 | 1.51 | 11 | 1 |
| 3 | A | 611 | PX4 | C12-C11 | 2.10 | 1.62 | 1.51 | 12 | 1 |
| 3 | A | 649 | PX4 | O4-C6 | 2.10 | 1.36 | 1.44 | 8 | 1 |
| 3 | A | 653 | PX4 | C18-C17 | 2.10 | 1.62 | 1.51 | 15 | 1 |
| 3 | B | 305 | PX4 | C30-C29 | 2.10 | 1.62 | 1.51 | 13 | 1 |
| 3 | B | 320 | PX4 | C17-C16 | 2.10 | 1.62 | 1.51 | 11 | 1 |
| 3 | B | 326 | PX4 | C35-C34 | 2.10 | 1.64 | 1.51 | 15 | 1 |
| 3 | B | 372 | PX4 | C16-C15 | 2.10 | 1.62 | 1.51 | 1 | 1 |
| 3 | B | 364 | PX4 | C18-C17 | 2.10 | 1.62 | 1.51 | 9 | 1 |
| 3 | B | 372 | PX4 | C11-C10 | 2.10 | 1.59 | 1.52 | 11 | 1 |
| 3 | B | 375 | PX4 | C16-C15 | 2.10 | 1.62 | 1.51 | 8 | 1 |
| 3 | B | 376 | PX4 | C25-C24 | 2.10 | 1.59 | 1.52 | 11 | 1 |
| 3 | B | 390 | PX4 | C26-C25 | 2.10 | 1.62 | 1.51 | 15 | 2 |
| 3 | B | 397 | PX4 | C26-C25 | 2.10 | 1.62 | 1.51 | 4 | 1 |
| 3 | C | 327 | PX4 | C3-N1 | 2.10 | 1.56 | 1.50 | 15 | 1 |
| 3 | C | 310 | PX4 | O7-C7 | 2.10 | 1.41 | 1.46 | 8 | 1 |
| 3 | C | 337 | PX4 | O5-C8 | 2.10 | 1.49 | 1.45 | 1 | 2 |
| 3 | B | 315 | PX4 | C13-C12 | 2.10 | 1.62 | 1.51 | 1 | 1 |
| 3 | B | 338 | PX4 | C4-N1 | 2.10 | 1.43 | 1.50 | 11 | 1 |
| 3 | C | 316 | PX4 | O6-C9 | 2.10 | 1.28 | 1.22 | 4 | 1 |
| 3 | C | 323 | PX4 | C11-C10 | 2.10 | 1.59 | 1.52 | 6 | 2 |
| 3 | C | 341 | PX4 | P1-O1 | 2.10 | 1.45 | 1.55 | 8 | 1 |
| 3 | B | 349 | PX4 | C17-C16 | 2.10 | 1.62 | 1.51 | 6 | 1 |
| 3 | C | 345 | PX4 | C28-C27 | 2.10 | 1.62 | 1.51 | 15 | 1 |
| 3 | A | 650 | PX4 | P1-O3 | 2.10 | 1.51 | 1.59 | 14 | 1 |
| 3 | B | 371 | PX4 | C26-C25 | 2.10 | 1.62 | 1.51 | 4 | 1 |
| 3 | C | 322 | PX4 | P1-O4 | 2.10 | 1.51 | 1.59 | 7 | 1 |
| 3 | A | 631 | PX4 | C26-C25 | 2.10 | 1.62 | 1.51 | 2 | 1 |
| 3 | B | 311 | PX4 | C26-C25 | 2.10 | 1.62 | 1.51 | 2 | 1 |
| 3 | B | 343 | PX4 | C28-C27 | 2.10 | 1.62 | 1.51 | 2 | 1 |
| 3 | C | 318 | PX4 | C11-C10 | 2.10 | 1.59 | 1.52 | 6 | 1 |
| 3 | C | 323 | PX4 | C5-N1 | 2.10 | 1.56 | 1.50 | 14 | 1 |
| 3 | C | 330 | PX4 | C32-C31 | 2.10 | 1.62 | 1.51 | 9 | 1 |
| 3 | A | 620 | PX4 | C25-C24 | 2.10 | 1.59 | 1.52 | 8 | 1 |
| 3 | A | 644 | PX4 | C11-C10 | 2.10 | 1.59 | 1.52 | 11 | 1 |
| 3 | B | 341 | PX4 | O7-C23 | 2.10 | 1.28 | 1.34 | 8 | 1 |
| 3 | C | 349 | PX4 | P1-O1 | 2.10 | 1.45 | 1.55 | 10 | 2 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 365 | PX4 | C17-C16 | 2.10 | 1.62 | 1.51 | 3 | 1 |
| 3 | B | 370 | PX4 | C5-N1 | 2.09 | 1.43 | 1.50 | 15 | 1 |
| 3 | B | 394 | PX4 | P1-O2 | 2.09 | 1.43 | 1.50 | 14 | 1 |
| 3 | C | 307 | PX4 | C20-C19 | 2.10 | 1.62 | 1.51 | 1 | 1 |
| 3 | C | 332 | PX4 | P1-O2 | 2.10 | 1.43 | 1.50 | 10 | 1 |
| 3 | A | 608 | PX4 | C11-C10 | 2.09 | 1.59 | 1.52 | 5 | 1 |
| 3 | A | 637 | PX4 | P1-O1 | 2.09 | 1.45 | 1.55 | 10 | 2 |
| 3 | A | 642 | PX4 | C31-C30 | 2.09 | 1.62 | 1.51 | 7 | 1 |
| 3 | A | 607 | PX4 | C2-N1 | 2.09 | 1.57 | 1.51 | 10 | 1 |
| 3 | A | 619 | PX4 | C29-C28 | 2.09 | 1.62 | 1.51 | 12 | 1 |
| 3 | B | 368 | PX4 | C3-N1 | 2.09 | 1.56 | 1.50 | 14 | 1 |
| 3 | C | 303 | PX4 | C25-C24 | 2.09 | 1.59 | 1.52 | 1 | 1 |
| 3 | C | 304 | PX4 | C2-N1 | 2.09 | 1.57 | 1.51 | 6 | 1 |
| 3 | A | 641 | PX4 | C20-C19 | 2.09 | 1.62 | 1.51 | 15 | 1 |
| 3 | A | 608 | PX4 | P1-O1 | 2.09 | 1.45 | 1.55 | 13 | 1 |
| 3 | A | 618 | PX4 | C28-C27 | 2.09 | 1.62 | 1.51 | 9 | 1 |
| 3 | A | 624 | PX4 | C19-C18 | 2.09 | 1.62 | 1.51 | 8 | 1 |
| 3 | A | 647 | PX4 | P1-O3 | 2.09 | 1.51 | 1.59 | 15 | 1 |
| 3 | B | 339 | PX4 | P1-O2 | 2.09 | 1.43 | 1.50 | 13 | 1 |
| 3 | A | 650 | PX4 | C11-C10 | 2.09 | 1.59 | 1.52 | 5 | 1 |
| 3 | B | 312 | PX4 | C26-C25 | 2.09 | 1.62 | 1.51 | 6 | 1 |
| 3 | B | 320 | PX4 | O5-C9 | 2.09 | 1.27 | 1.33 | 14 | 1 |
| 3 | B | 369 | PX4 | C3-N1 | 2.09 | 1.56 | 1.50 | 14 | 2 |
| 3 | B | 369 | PX4 | C2-N1 | 2.09 | 1.57 | 1.51 | 8 | 1 |
| 3 | B | 385 | PX4 | C14-C13 | 2.09 | 1.62 | 1.51 | 1 | 1 |
| 3 | B | 387 | PX4 | P1-O3 | 2.09 | 1.51 | 1.59 | 14 | 1 |
| 3 | B | 399 | PX4 | C31-C30 | 2.09 | 1.62 | 1.51 | 9 | 1 |
| 3 | C | 349 | PX4 | C20-C19 | 2.09 | 1.62 | 1.51 | 3 | 1 |
| 3 | C | 358 | PX4 | C20-C19 | 2.09 | 1.62 | 1.51 | 2 | 1 |
| 3 | A | 604 | PX4 | C32-C31 | 2.09 | 1.62 | 1.51 | 15 | 2 |
| 3 | A | 630 | PX4 | C33-C32 | 2.09 | 1.62 | 1.51 | 3 | 1 |
| 3 | A | 631 | PX4 | C29-C28 | 2.09 | 1.62 | 1.51 | 14 | 1 |
| 3 | B | 301 | PX4 | P1-O3 | 2.09 | 1.51 | 1.59 | 12 | 1 |
| 3 | B | 320 | PX4 | C28-C27 | 2.09 | 1.62 | 1.51 | 7 | 1 |
| 3 | B | 345 | PX4 | C5-N1 | 2.09 | 1.56 | 1.50 | 1 | 1 |
| 3 | B | 364 | PX4 | O3-C1 | 2.09 | 1.36 | 1.44 | 15 | 1 |
| 3 | B | 390 | PX4 | C11-C10 | 2.09 | 1.59 | 1.52 | 15 | 3 |
| 3 | B | 396 | PX4 | P1-O3 | 2.09 | 1.67 | 1.59 | 4 | 1 |
| 3 | C | 329 | PX4 | C36-C35 | 2.09 | 1.65 | 1.50 | 1 | 1 |
| 3 | A | 629 | PX4 | C4-N1 | 2.09 | 1.56 | 1.50 | 3 | 1 |
| 3 | B | 379 | PX4 | C19-C18 | 2.09 | 1.62 | 1.51 | 6 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | C | 309 | PX4 | O4-C6 | 2.09 | 1.36 | 1.44 | 15 | 1 |
| 3 | A | 609 | PX4 | C10-C9 | 2.09 | 1.56 | 1.50 | 6 | 3 |
| 3 | A | 634 | PX4 | C3-N1 | 2.09 | 1.56 | 1.50 | 5 | 1 |
| 3 | A | 652 | PX4 | C17-C16 | 2.09 | 1.62 | 1.51 | 7 | 1 |
| 3 | B | 331 | PX4 | O5-C9 | 2.09 | 1.27 | 1.33 | 11 | 1 |
| 3 | B | 320 | PX4 | C5-N1 | 2.09 | 1.56 | 1.50 | 6 | 1 |
| 3 | B | 326 | PX4 | C17-C16 | 2.09 | 1.62 | 1.51 | 5 | 1 |
| 3 | C | 306 | PX4 | C12-C11 | 2.09 | 1.62 | 1.51 | 10 | 1 |
| 3 | C | 346 | PX4 | C21-C20 | 2.09 | 1.64 | 1.51 | 9 | 1 |
| 3 | B | 316 | PX4 | C21-C20 | 2.08 | 1.64 | 1.51 | 14 | 1 |
| 3 | B | 332 | PX4 | C25-C24 | 2.09 | 1.59 | 1.52 | 10 | 2 |
| 3 | B | 319 | PX4 | P1-O2 | 2.08 | 1.43 | 1.50 | 4 | 1 |
| 3 | B | 335 | PX4 | C25-C24 | 2.08 | 1.59 | 1.52 | 14 | 1 |
| 3 | B | 336 | PX4 | C28-C27 | 2.09 | 1.62 | 1.51 | 5 | 1 |
| 3 | A | 628 | PX4 | C28-C27 | 2.08 | 1.62 | 1.51 | 15 | 1 |
| 3 | A | 639 | PX4 | C30-C29 | 2.08 | 1.62 | 1.51 | 13 | 1 |
| 3 | C | 342 | PX4 | O5-C9 | 2.09 | 1.27 | 1.33 | 4 | 1 |
| 3 | A | 631 | PX4 | C27-C26 | 2.08 | 1.62 | 1.51 | 15 | 1 |
| 3 | B | 350 | PX4 | O4-C6 | 2.08 | 1.36 | 1.44 | 8 | 1 |
| 3 | B | 356 | PX4 | C12-C11 | 2.08 | 1.62 | 1.51 | 13 | 1 |
| 3 | C | 302 | PX4 | C17-C16 | 2.08 | 1.62 | 1.51 | 1 | 1 |
| 3 | C | 354 | PX4 | O5-C8 | 2.08 | 1.40 | 1.45 | 5 | 1 |
| 3 | C | 355 | PX4 | O7-C7 | 2.08 | 1.41 | 1.46 | 2 | 1 |
| 3 | A | 604 | PX4 | C19-C18 | 2.08 | 1.62 | 1.51 | 13 | 1 |
| 3 | B | 369 | PX4 | C34-C33 | 2.08 | 1.62 | 1.51 | 2 | 1 |
| 3 | B | 384 | PX4 | P1-O2 | 2.08 | 1.43 | 1.50 | 2 | 1 |
| 3 | B | 399 | PX4 | C16-C15 | 2.08 | 1.62 | 1.51 | 15 | 1 |
| 3 | A | 625 | PX4 | O3-C1 | 2.08 | 1.36 | 1.44 | 8 | 2 |
| 3 | A | 632 | PX4 | C2-C1 | 2.08 | 1.57 | 1.51 | 5 | 1 |
| 3 | B | 318 | PX4 | O3-C1 | 2.08 | 1.36 | 1.44 | 3 | 1 |
| 3 | B | 348 | PX4 | P1-O3 | 2.08 | 1.51 | 1.59 | 7 | 1 |
| 3 | A | 647 | PX4 | C11-C10 | 2.08 | 1.59 | 1.52 | 2 | 2 |
| 3 | B | 351 | PX4 | C5-N1 | 2.08 | 1.56 | 1.50 | 3 | 2 |
| 3 | B | 368 | PX4 | C25-C24 | 2.08 | 1.59 | 1.52 | 7 | 1 |
| 3 | B | 400 | PX4 | O4-C6 | 2.08 | 1.36 | 1.44 | 4 | 1 |
| 3 | B | 391 | PX4 | C15-C14 | 2.08 | 1.62 | 1.51 | 5 | 1 |
| 3 | C | 343 | PX4 | C5-N1 | 2.08 | 1.56 | 1.50 | 5 | 1 |
| 3 | C | 347 | PX4 | O6-C9 | 2.08 | 1.28 | 1.22 | 1 | 1 |
| 3 | B | 304 | PX4 | C25-C24 | 2.08 | 1.59 | 1.52 | 4 | 1 |
| 3 | B | 323 | PX4 | C28-C27 | 2.08 | 1.62 | 1.51 | 6 | 1 |
| 3 | A | 617 | PX4 | O7-C23 | 2.08 | 1.40 | 1.34 | 12 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | A | 618 | PX4 | O5-C8 | 2.08 | 1.40 | 1.45 | 5 | 1 |
| 3 | B | 370 | PX4 | O4-C6 | 2.08 | 1.36 | 1.44 | 14 | 1 |
| 3 | C | 334 | PX4 | C25-C24 | 2.08 | 1.59 | 1.52 | 6 | 1 |
| 3 | C | 354 | PX4 | P1-O3 | 2.08 | 1.67 | 1.59 | 10 | 1 |
| 3 | C | 359 | PX4 | C32-C31 | 2.08 | 1.62 | 1.51 | 14 | 1 |
| 3 | A | 614 | PX4 | O4-C6 | 2.08 | 1.52 | 1.44 | 15 | 2 |
| 3 | A | 647 | PX4 | O8-C23 | 2.08 | 1.16 | 1.22 | 5 | 1 |
| 3 | B | 337 | PX4 | C33-C32 | 2.08 | 1.62 | 1.51 | 8 | 2 |
| 3 | B | 387 | PX4 | C10-C9 | 2.08 | 1.56 | 1.50 | 8 | 1 |
| 3 | B | 392 | PX4 | C26-C25 | 2.08 | 1.62 | 1.51 | 14 | 1 |
| 3 | A | 617 | PX4 | C5-N1 | 2.07 | 1.44 | 1.50 | 10 | 1 |
| 3 | A | 626 | PX4 | C11-C10 | 2.07 | 1.59 | 1.52 | 13 | 1 |
| 3 | B | 336 | PX4 | C25-C24 | 2.07 | 1.59 | 1.52 | 8 | 2 |
| 3 | B | 360 | PX4 | O4-C6 | 2.07 | 1.36 | 1.44 | 5 | 1 |
| 3 | B | 362 | PX4 | C11-C10 | 2.07 | 1.59 | 1.52 | 13 | 2 |
| 3 | B | 366 | PX4 | C4-N1 | 2.07 | 1.44 | 1.50 | 13 | 2 |
| 3 | C | 334 | PX4 | C15-C14 | 2.07 | 1.62 | 1.51 | 15 | 1 |
| 3 | B | 331 | PX4 | O4-C6 | 2.07 | 1.36 | 1.44 | 7 | 1 |
| 3 | B | 308 | PX4 | C20-C19 | 2.07 | 1.62 | 1.51 | 12 | 1 |
| 3 | B | 324 | PX4 | P1-O1 | 2.07 | 1.45 | 1.55 | 12 | 1 |
| 3 | B | 340 | PX4 | C30-C29 | 2.07 | 1.62 | 1.51 | 11 | 2 |
| 3 | B | 352 | PX4 | C5-N1 | 2.07 | 1.56 | 1.50 | 12 | 1 |
| 3 | B | 353 | PX4 | C4-N1 | 2.07 | 1.56 | 1.50 | 7 | 1 |
| 3 | C | 339 | PX4 | P1-O3 | 2.07 | 1.51 | 1.59 | 12 | 1 |
| 3 | C | 339 | PX4 | C17-C16 | 2.07 | 1.62 | 1.51 | 13 | 1 |
| 3 | C | 343 | PX4 | C27-C26 | 2.07 | 1.62 | 1.51 | 13 | 1 |
| 3 | C | 360 | PX4 | O5-C9 | 2.07 | 1.27 | 1.33 | 12 | 1 |
| 3 | C | 362 | PX4 | C19-C18 | 2.07 | 1.62 | 1.51 | 1 | 1 |
| 3 | B | 323 | PX4 | C15-C14 | 2.07 | 1.62 | 1.51 | 12 | 1 |
| 3 | B | 341 | PX4 | C25-C24 | 2.07 | 1.59 | 1.52 | 13 | 1 |
| 3 | B | 381 | PX4 | P1-O2 | 2.07 | 1.43 | 1.50 | 1 | 1 |
| 3 | C | 306 | PX4 | C18-C17 | 2.07 | 1.62 | 1.51 | 15 | 1 |
| 3 | C | 356 | PX4 | O3-C1 | 2.07 | 1.36 | 1.44 | 6 | 1 |
| 3 | C | 343 | PX4 | C3-N1 | 2.07 | 1.44 | 1.50 | 3 | 2 |
| 3 | A | 628 | PX4 | P1-O3 | 2.07 | 1.51 | 1.59 | 4 | 1 |
| 3 | B | 317 | PX4 | O6-C9 | 2.07 | 1.16 | 1.22 | 6 | 1 |
| 3 | B | 320 | PX4 | O5-C8 | 2.07 | 1.49 | 1.45 | 6 | 1 |
| 3 | B | 347 | PX4 | O3-C1 | 2.07 | 1.36 | 1.44 | 5 | 1 |
| 3 | C | 318 | PX4 | C4-N1 | 2.07 | 1.44 | 1.50 | 15 | 1 |
| 3 | A | 639 | PX4 | C15-C14 | 2.07 | 1.62 | 1.51 | 10 | 1 |
| 3 | C | 308 | PX4 | O5-C9 | 2.07 | 1.39 | 1.33 | 7 | 2 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | C | 316 | PX4 | P1-O1 | 2.07 | 1.45 | 1.55 | 13 | 2 |
| 3 | C | 363 | PX4 | C18-C17 | 2.07 | 1.62 | 1.51 | 2 | 1 |
| 3 | A | 620 | PX4 | P1-O1 | 2.07 | 1.45 | 1.55 | 11 | 2 |
| 3 | A | 652 | PX4 | C2-N1 | 2.07 | 1.45 | 1.51 | 5 | 1 |
| 3 | A | 654 | PX4 | O4-C6 | 2.07 | 1.36 | 1.44 | 4 | 1 |
| 3 | B | 314 | PX4 | C32-C31 | 2.07 | 1.62 | 1.51 | 11 | 1 |
| 3 | B | 368 | PX4 | C27-C26 | 2.07 | 1.62 | 1.51 | 12 | 1 |
| 3 | B | 375 | PX4 | C13-C12 | 2.07 | 1.62 | 1.51 | 3 | 1 |
| 3 | C | 351 | PX4 | C15-C14 | 2.07 | 1.41 | 1.51 | 1 | 1 |
| 3 | A | 606 | PX4 | C29-C28 | 2.06 | 1.62 | 1.51 | 9 | 1 |
| 3 | B | 337 | PX4 | C32-C31 | 2.06 | 1.62 | 1.51 | 11 | 1 |
| 3 | B | 360 | PX4 | O3-C1 | 2.06 | 1.36 | 1.44 | 7 | 1 |
| 3 | A | 605 | PX4 | C21-C20 | 2.06 | 1.64 | 1.51 | 4 | 1 |
| 3 | B | 364 | PX4 | C34-C33 | 2.06 | 1.62 | 1.51 | 11 | 1 |
| 3 | A | 616 | PX4 | C28-C27 | 2.06 | 1.62 | 1.51 | 7 | 2 |
| 3 | A | 637 | PX4 | O5-C8 | 2.06 | 1.40 | 1.45 | 5 | 1 |
| 3 | B | 318 | PX4 | O7-C23 | 2.06 | 1.28 | 1.34 | 11 | 1 |
| 3 | B | 328 | PX4 | O5-C9 | 2.06 | 1.39 | 1.33 | 14 | 1 |
| 3 | B | 336 | PX4 | C12-C11 | 2.06 | 1.62 | 1.51 | 9 | 1 |
| 3 | B | 377 | PX4 | P1-O2 | 2.06 | 1.43 | 1.50 | 1 | 1 |
| 3 | B | 358 | PX4 | C11-C10 | 2.06 | 1.59 | 1.52 | 9 | 1 |
| 3 | B | 368 | PX4 | C13-C12 | 2.06 | 1.62 | 1.51 | 13 | 1 |
| 3 | B | 379 | PX4 | C4-N1 | 2.06 | 1.56 | 1.50 | 9 | 1 |
| 3 | C | 327 | PX4 | O8-C23 | 2.06 | 1.16 | 1.22 | 5 | 1 |
| 3 | A | 609 | PX4 | C25-C24 | 2.06 | 1.59 | 1.52 | 4 | 1 |
| 3 | A | 630 | PX4 | P1-O1 | 2.06 | 1.45 | 1.55 | 14 | 2 |
| 3 | A | 641 | PX4 | C18-C17 | 2.06 | 1.62 | 1.51 | 4 | 1 |
| 3 | B | 307 | PX4 | C31-C30 | 2.06 | 1.62 | 1.51 | 11 | 1 |
| 3 | B | 386 | PX4 | C2-N1 | 2.06 | 1.57 | 1.51 | 7 | 1 |
| 3 | B | 310 | PX4 | P1-O1 | 2.06 | 1.45 | 1.55 | 7 | 2 |
| 3 | B | 390 | PX4 | O5-C9 | 2.06 | 1.27 | 1.33 | 8 | 1 |
| 3 | C | 341 | PX4 | C11-C10 | 2.06 | 1.59 | 1.52 | 10 | 1 |
| 3 | A | 651 | PX4 | C18-C17 | 2.06 | 1.62 | 1.51 | 7 | 1 |
| 3 | B | 321 | PX4 | O5-C9 | 2.06 | 1.39 | 1.33 | 1 | 1 |
| 3 | B | 359 | PX4 | P1-O2 | 2.06 | 1.43 | 1.50 | 10 | 1 |
| 3 | B | 375 | PX4 | C30-C29 | 2.06 | 1.62 | 1.51 | 9 | 1 |
| 3 | C | 363 | PX4 | C27-C26 | 2.06 | 1.62 | 1.51 | 4 | 1 |
| 3 | A | 619 | PX4 | C25-C24 | 2.06 | 1.44 | 1.52 | 10 | 1 |
| 3 | A | 647 | PX4 | O5-C8 | 2.06 | 1.40 | 1.45 | 3 | 2 |
| 3 | B | 303 | PX4 | C34-C33 | 2.06 | 1.62 | 1.51 | 1 | 1 |
| 3 | B | 316 | PX4 | P1-O2 | 2.06 | 1.43 | 1.50 | 7 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 325 | PX4 | C19-C18 | 2.06 | 1.62 | 1.51 | 12 | 1 |
| 3 | C | 302 | PX4 | C34-C33 | 2.06 | 1.62 | 1.51 | 2 | 1 |
| 3 | C | 323 | PX4 | P1-O2 | 2.06 | 1.43 | 1.50 | 6 | 1 |
| 3 | B | 352 | PX4 | P1-O3 | 2.06 | 1.67 | 1.59 | 12 | 1 |
| 3 | A | 632 | PX4 | C25-C24 | 2.06 | 1.59 | 1.52 | 2 | 1 |
| 3 | A | 648 | PX4 | C2-N1 | 2.06 | 1.45 | 1.51 | 2 | 1 |
| 3 | B | 344 | PX4 | C19-C18 | 2.06 | 1.62 | 1.51 | 7 | 1 |
| 3 | C | 309 | PX4 | O3-C1 | 2.06 | 1.36 | 1.44 | 2 | 1 |
| 3 | B | 331 | PX4 | P1-O1 | 2.06 | 1.45 | 1.55 | 13 | 2 |
| 3 | B | 340 | PX4 | C20-C19 | 2.06 | 1.62 | 1.51 | 10 | 2 |
| 3 | B | 380 | PX4 | C30-C29 | 2.06 | 1.62 | 1.51 | 8 | 1 |
| 3 | C | 330 | PX4 | P1-O1 | 2.06 | 1.45 | 1.55 | 4 | 2 |
| 3 | A | 606 | PX4 | C27-C26 | 2.05 | 1.62 | 1.51 | 15 | 1 |
| 3 | A | 618 | PX4 | O5-C9 | 2.06 | 1.39 | 1.33 | 11 | 1 |
| 3 | C | 304 | PX4 | C28-C27 | 2.06 | 1.62 | 1.51 | 10 | 1 |
| 3 | A | 626 | PX4 | C34-C33 | 2.05 | 1.62 | 1.51 | 1 | 1 |
| 3 | B | 341 | PX4 | P1-O4 | 2.05 | 1.51 | 1.59 | 15 | 1 |
| 3 | B | 345 | PX4 | C14-C13 | 2.05 | 1.62 | 1.51 | 2 | 1 |
| 3 | B | 369 | PX4 | C15-C14 | 2.05 | 1.62 | 1.51 | 13 | 1 |
| 3 | C | 363 | PX4 | C17-C16 | 2.05 | 1.62 | 1.51 | 10 | 1 |
| 3 | A | 612 | PX4 | C14-C13 | 2.05 | 1.62 | 1.51 | 7 | 1 |
| 3 | B | 302 | PX4 | C17-C16 | 2.05 | 1.62 | 1.51 | 6 | 1 |
| 3 | B | 372 | PX4 | C25-C24 | 2.05 | 1.59 | 1.52 | 8 | 1 |
| 3 | C | 348 | PX4 | P1-O3 | 2.05 | 1.51 | 1.59 | 7 | 1 |
| 3 | B | 355 | PX4 | C31-C30 | 2.05 | 1.62 | 1.51 | 14 | 1 |
| 3 | B | 392 | PX4 | C33-C32 | 2.05 | 1.62 | 1.51 | 6 | 1 |
| 3 | A | 626 | PX4 | O7-C7 | 2.05 | 1.41 | 1.46 | 7 | 1 |
| 3 | A | 644 | PX4 | C32-C31 | 2.05 | 1.62 | 1.51 | 11 | 1 |
| 3 | B | 312 | PX4 | C27-C26 | 2.05 | 1.62 | 1.51 | 7 | 1 |
| 3 | B | 332 | PX4 | C13-C12 | 2.05 | 1.62 | 1.51 | 11 | 2 |
| 3 | B | 302 | PX4 | O7-C23 | 2.05 | 1.28 | 1.34 | 12 | 1 |
| 3 | B | 358 | PX4 | C34-C33 | 2.05 | 1.62 | 1.51 | 14 | 1 |
| 3 | B | 377 | PX4 | O4-C6 | 2.05 | 1.36 | 1.44 | 11 | 1 |
| 3 | C | 311 | PX4 | O5-C9 | 2.05 | 1.27 | 1.33 | 3 | 2 |
| 3 | B | 306 | PX4 | C28-C27 | 2.05 | 1.62 | 1.51 | 14 | 1 |
| 3 | B | 323 | PX4 | C4-N1 | 2.05 | 1.55 | 1.50 | 15 | 1 |
| 3 | B | 330 | PX4 | P1-O2 | 2.05 | 1.43 | 1.50 | 15 | 1 |
| 3 | C | 351 | PX4 | C34-C33 | 2.05 | 1.62 | 1.51 | 15 | 1 |
| 3 | A | 637 | PX4 | C4-N1 | 2.04 | 1.55 | 1.50 | 1 | 1 |
| 3 | B | 335 | PX4 | C2-N1 | 2.04 | 1.57 | 1.51 | 10 | 2 |
| 3 | B | 368 | PX4 | C26-C25 | 2.04 | 1.62 | 1.51 | 5 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 380 | PX4 | C33-C32 | 2.04 | 1.61 | 1.51 | 13 | 1 |
| 3 | C | 301 | PX4 | O5-C8 | 2.04 | 1.49 | 1.45 | 4 | 1 |
| 3 | C | 343 | PX4 | C12-C11 | 2.04 | 1.61 | 1.51 | 12 | 1 |
| 3 | A | 605 | PX4 | C12-C11 | 2.04 | 1.61 | 1.51 | 11 | 1 |
| 3 | A | 637 | PX4 | C30-C29 | 2.04 | 1.61 | 1.51 | 14 | 1 |
| 3 | A | 644 | PX4 | P1-O2 | 2.04 | 1.43 | 1.50 | 6 | 1 |
| 3 | A | 645 | PX4 | C33-C32 | 2.04 | 1.61 | 1.51 | 9 | 1 |
| 3 | B | 319 | PX4 | C27-C26 | 2.04 | 1.61 | 1.51 | 6 | 1 |
| 3 | B | 329 | PX4 | C17-C16 | 2.04 | 1.61 | 1.51 | 7 | 1 |
| 3 | B | 342 | PX4 | P1-O3 | 2.04 | 1.67 | 1.59 | 5 | 1 |
| 3 | B | 355 | PX4 | P1-O3 | 2.04 | 1.51 | 1.59 | 7 | 1 |
| 3 | C | 321 | PX4 | P1-O2 | 2.04 | 1.43 | 1.50 | 11 | 1 |
| 3 | A | 619 | PX4 | C13-C12 | 2.04 | 1.61 | 1.51 | 13 | 1 |
| 3 | A | 630 | PX4 | O5-C9 | 2.04 | 1.27 | 1.33 | 3 | 1 |
| 3 | B | 308 | PX4 | C3-N1 | 2.04 | 1.44 | 1.50 | 4 | 1 |
| 3 | B | 325 | PX4 | C17-C16 | 2.04 | 1.61 | 1.51 | 11 | 1 |
| 3 | B | 383 | PX4 | P1-O4 | 2.04 | 1.51 | 1.59 | 11 | 1 |
| 3 | C | 312 | PX4 | O5-C9 | 2.04 | 1.27 | 1.33 | 14 | 1 |
| 3 | C | 330 | PX4 | C14-C13 | 2.04 | 1.61 | 1.51 | 9 | 1 |
| 3 | C | 313 | PX4 | C25-C24 | 2.04 | 1.59 | 1.52 | 11 | 1 |
| 3 | C | 314 | PX4 | O5-C9 | 2.04 | 1.39 | 1.33 | 1 | 1 |
| 3 | C | 316 | PX4 | C10-C9 | 2.04 | 1.56 | 1.50 | 15 | 1 |
| 3 | C | 355 | PX4 | C33-C32 | 2.04 | 1.61 | 1.51 | 13 | 1 |
| 3 | C | 364 | PX4 | O3-C1 | 2.04 | 1.36 | 1.44 | 1 | 1 |
| 3 | B | 368 | PX4 | C30-C29 | 2.04 | 1.61 | 1.51 | 14 | 1 |
| 3 | B | 382 | PX4 | C24-C23 | 2.04 | 1.56 | 1.50 | 4 | 1 |
| 3 | C | 352 | PX4 | C31-C30 | 2.04 | 1.61 | 1.51 | 9 | 1 |
| 3 | A | 650 | PX4 | O4-C6 | 2.04 | 1.36 | 1.44 | 4 | 1 |
| 3 | B | 316 | PX4 | O7-C23 | 2.04 | 1.28 | 1.34 | 6 | 1 |
| 3 | B | 357 | PX4 | C34-C33 | 2.04 | 1.61 | 1.51 | 11 | 1 |
| 3 | C | 303 | PX4 | C30-C29 | 2.04 | 1.41 | 1.51 | 5 | 1 |
| 3 | C | 358 | PX4 | C19-C18 | 2.04 | 1.61 | 1.51 | 3 | 1 |
| 3 | C | 360 | PX4 | C12-C11 | 2.04 | 1.61 | 1.51 | 4 | 1 |
| 3 | A | 603 | PX4 | C2-N1 | 2.04 | 1.45 | 1.51 | 8 | 1 |
| 3 | A | 612 | PX4 | C5-N1 | 2.04 | 1.55 | 1.50 | 11 | 1 |
| 3 | A | 650 | PX4 | C16-C15 | 2.04 | 1.61 | 1.51 | 14 | 1 |
| 3 | B | 343 | PX4 | C13-C12 | 2.04 | 1.61 | 1.51 | 5 | 1 |
| 3 | B | 355 | PX4 | C13-C12 | 2.04 | 1.61 | 1.51 | 9 | 1 |
| 3 | B | 370 | PX4 | C14-C13 | 2.03 | 1.61 | 1.51 | 11 | 2 |
| 3 | B | 376 | PX4 | C20-C19 | 2.03 | 1.61 | 1.51 | 15 | 2 |
| 3 | B | 380 | PX4 | C19-C18 | 2.04 | 1.61 | 1.51 | 3 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 386 | PX4 | C5-N1 | 2.04 | 1.55 | 1.50 | 3 | 2 |
| 3 | B | 331 | PX4 | P1-O3 | 2.03 | 1.51 | 1.59 | 1 | 1 |
| 3 | B | 341 | PX4 | C28-C27 | 2.03 | 1.61 | 1.51 | 8 | 1 |
| 3 | B | 377 | PX4 | C20-C19 | 2.03 | 1.61 | 1.51 | 5 | 1 |
| 3 | B | 398 | PX4 | P1-O3 | 2.03 | 1.51 | 1.59 | 9 | 1 |
| 3 | C | 306 | PX4 | C33-C32 | 2.03 | 1.61 | 1.51 | 4 | 1 |
| 3 | C | 362 | PX4 | P1-O4 | 2.03 | 1.51 | 1.59 | 9 | 1 |
| 3 | C | 363 | PX4 | C28-C27 | 2.03 | 1.61 | 1.51 | 12 | 1 |
| 3 | A | 601 | PX4 | C16-C15 | 2.03 | 1.61 | 1.51 | 13 | 1 |
| 3 | A | 613 | PX4 | C4-N1 | 2.03 | 1.55 | 1.50 | 10 | 1 |
| 3 | C | 307 | PX4 | C27-C26 | 2.03 | 1.61 | 1.51 | 8 | 1 |
| 3 | C | 309 | PX4 | P1-O3 | 2.03 | 1.51 | 1.59 | 3 | 1 |
| 3 | A | 620 | PX4 | O3-C1 | 2.03 | 1.36 | 1.44 | 10 | 1 |
| 3 | B | 353 | PX4 | C18-C17 | 2.03 | 1.61 | 1.51 | 11 | 1 |
| 3 | A | 622 | PX4 | O7-C23 | 2.03 | 1.40 | 1.34 | 13 | 1 |
| 3 | C | 362 | PX4 | O3-C1 | 2.03 | 1.52 | 1.44 | 5 | 1 |
| 3 | C | 364 | PX4 | C27-C26 | 2.03 | 1.61 | 1.51 | 5 | 1 |
| 3 | A | 629 | PX4 | C32-C31 | 2.03 | 1.61 | 1.51 | 8 | 1 |
| 3 | B | 332 | PX4 | C19-C18 | 2.03 | 1.61 | 1.51 | 9 | 1 |
| 3 | B | 341 | PX4 | P1-O1 | 2.03 | 1.45 | 1.55 | 8 | 1 |
| 3 | B | 392 | PX4 | P1-O1 | 2.03 | 1.45 | 1.55 | 11 | 2 |
| 3 | C | 302 | PX4 | C10-C9 | 2.03 | 1.56 | 1.50 | 13 | 1 |
| 3 | C | 325 | PX4 | O4-C6 | 2.03 | 1.36 | 1.44 | 2 | 1 |
| 3 | C | 325 | PX4 | O3-C1 | 2.03 | 1.36 | 1.44 | 5 | 1 |
| 3 | A | 618 | PX4 | P1-O1 | 2.03 | 1.45 | 1.55 | 3 | 1 |
| 3 | A | 606 | PX4 | C19-C18 | 2.03 | 1.61 | 1.51 | 1 | 1 |
| 3 | A | 642 | PX4 | P1-O2 | 2.03 | 1.43 | 1.50 | 9 | 1 |
| 3 | B | 310 | PX4 | P1-O4 | 2.03 | 1.51 | 1.59 | 13 | 1 |
| 3 | B | 310 | PX4 | C29-C28 | 2.03 | 1.61 | 1.51 | 5 | 1 |
| 3 | B | 331 | PX4 | C25-C24 | 2.03 | 1.59 | 1.52 | 11 | 1 |
| 3 | B | 343 | PX4 | C33-C32 | 2.03 | 1.61 | 1.51 | 11 | 1 |
| 3 | C | 305 | PX4 | C26-C25 | 2.03 | 1.61 | 1.51 | 2 | 1 |
| 3 | C | 344 | PX4 | C29-C28 | 2.03 | 1.61 | 1.51 | 9 | 1 |
| 3 | A | 607 | PX4 | P1-O3 | 2.02 | 1.51 | 1.59 | 10 | 1 |
| 3 | A | 639 | PX4 | C3-N1 | 2.02 | 1.44 | 1.50 | 8 | 1 |
| 3 | A | 645 | PX4 | C4-N1 | 2.03 | 1.55 | 1.50 | 12 | 1 |
| 3 | B | 350 | PX4 | C3-N1 | 2.02 | 1.44 | 1.50 | 7 | 1 |
| 3 | B | 321 | PX4 | P1-O1 | 2.02 | 1.46 | 1.55 | 14 | 1 |
| 3 | B | 338 | PX4 | C20-C19 | 2.02 | 1.61 | 1.51 | 1 | 1 |
| 3 | B | 351 | PX4 | O7-C23 | 2.02 | 1.40 | 1.34 | 3 | 1 |
| 3 | B | 354 | PX4 | C18-C17 | 2.02 | 1.61 | 1.51 | 4 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 354 | PX4 | C3-N1 | 2.03 | 1.44 | 1.50 | 8 | 1 |
| 3 | B | 383 | PX4 | C33-C32 | 2.03 | 1.61 | 1.51 | 3 | 1 |
| 3 | C | 315 | PX4 | C12-C11 | 2.02 | 1.61 | 1.51 | 12 | 1 |
| 3 | C | 341 | PX4 | C20-C19 | 2.03 | 1.61 | 1.51 | 7 | 1 |
| 3 | B | 383 | PX4 | O7-C7 | 2.02 | 1.41 | 1.46 | 12 | 1 |
| 3 | C | 319 | PX4 | P1-O3 | 2.02 | 1.67 | 1.59 | 11 | 1 |
| 3 | C | 338 | PX4 | C19-C18 | 2.02 | 1.61 | 1.51 | 4 | 1 |
| 3 | C | 348 | PX4 | O3-C1 | 2.02 | 1.36 | 1.44 | 3 | 1 |
| 3 | A | 648 | PX4 | C34-C33 | 2.02 | 1.61 | 1.51 | 6 | 1 |
| 3 | A | 618 | PX4 | O4-C6 | 2.02 | 1.52 | 1.44 | 10 | 1 |
| 3 | A | 619 | PX4 | P1-O3 | 2.02 | 1.51 | 1.59 | 8 | 1 |
| 3 | B | 302 | PX4 | C29-C28 | 2.02 | 1.61 | 1.51 | 11 | 1 |
| 3 | B | 313 | PX4 | C27-C26 | 2.02 | 1.61 | 1.51 | 1 | 1 |
| 3 | A | 644 | PX4 | C13-C12 | 2.02 | 1.61 | 1.51 | 13 | 1 |
| 3 | B | 313 | PX4 | P1-O1 | 2.02 | 1.46 | 1.55 | 15 | 1 |
| 3 | B | 357 | PX4 | C28-C27 | 2.02 | 1.61 | 1.51 | 9 | 1 |
| 3 | C | 330 | PX4 | C33-C32 | 2.02 | 1.61 | 1.51 | 3 | 1 |
| 3 | C | 332 | PX4 | P1-O1 | 2.02 | 1.46 | 1.55 | 10 | 2 |
| 3 | C | 340 | PX4 | O6-C9 | 2.02 | 1.28 | 1.22 | 15 | 1 |
| 3 | C | 351 | PX4 | C3-N1 | 2.02 | 1.55 | 1.50 | 4 | 1 |
| 3 | A | 642 | PX4 | C28-C27 | 2.02 | 1.61 | 1.51 | 9 | 1 |
| 3 | B | 303 | PX4 | C29-C28 | 2.02 | 1.61 | 1.51 | 5 | 1 |
| 3 | B | 317 | PX4 | C5-N1 | 2.02 | 1.55 | 1.50 | 11 | 1 |
| 3 | B | 335 | PX4 | C17-C16 | 2.02 | 1.61 | 1.51 | 6 | 1 |
| 3 | B | 338 | PX4 | O5-C9 | 2.02 | 1.39 | 1.33 | 11 | 1 |
| 3 | C | 336 | PX4 | C17-C16 | 2.02 | 1.61 | 1.51 | 15 | 1 |
| 3 | C | 340 | PX4 | C5-N1 | 2.02 | 1.44 | 1.50 | 5 | 1 |
| 3 | B | 391 | PX4 | C2-N1 | 2.02 | 1.57 | 1.51 | 7 | 2 |
| 3 | B | 396 | PX4 | C13-C12 | 2.02 | 1.61 | 1.51 | 6 | 1 |
| 3 | C | 318 | PX4 | C29-C28 | 2.02 | 1.61 | 1.51 | 6 | 1 |
| 3 | C | 327 | PX4 | P1-O2 | 2.02 | 1.43 | 1.50 | 4 | 1 |
| 3 | C | 351 | PX4 | P1-O1 | 2.02 | 1.46 | 1.55 | 3 | 1 |
| 3 | C | 349 | PX4 | C25-C24 | 2.02 | 1.59 | 1.52 | 10 | 1 |
| 3 | C | 352 | PX4 | C27-C26 | 2.02 | 1.61 | 1.51 | 2 | 1 |
| 3 | A | 621 | PX4 | C30-C29 | 2.02 | 1.61 | 1.51 | 13 | 1 |
| 3 | A | 632 | PX4 | C13-C12 | 2.02 | 1.61 | 1.51 | 11 | 1 |
| 3 | A | 628 | PX4 | C32-C31 | 2.02 | 1.61 | 1.51 | 6 | 1 |
| 3 | A | 637 | PX4 | C17-C16 | 2.02 | 1.61 | 1.51 | 14 | 1 |
| 3 | B | 315 | PX4 | C11-C10 | 2.02 | 1.59 | 1.52 | 2 | 1 |
| 3 | B | 324 | PX4 | C2-N1 | 2.02 | 1.45 | 1.51 | 4 | 1 |
| 3 | B | 323 | PX4 | C14-C13 | 2.02 | 1.61 | 1.51 | 7 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 353 | PX4 | C5-N1 | 2.02 | 1.44 | 1.50 | 12 | 1 |
| 3 | C | 345 | PX4 | O3-C1 | 2.02 | 1.36 | 1.44 | 15 | 1 |
| 3 | A | 602 | PX4 | C12-C11 | 2.01 | 1.61 | 1.51 | 11 | 1 |
| 3 | B | 332 | PX4 | C16-C15 | 2.01 | 1.61 | 1.51 | 14 | 1 |
| 3 | B | 374 | PX4 | C3-N1 | 2.02 | 1.55 | 1.50 | 4 | 2 |
| 3 | C | 307 | PX4 | P1-O3 | 2.02 | 1.51 | 1.59 | 4 | 1 |
| 3 | C | 362 | PX4 | C10-C9 | 2.01 | 1.56 | 1.50 | 13 | 1 |
| 3 | A | 622 | PX4 | C19-C18 | 2.01 | 1.61 | 1.51 | 15 | 1 |
| 3 | A | 646 | PX4 | C26-C25 | 2.01 | 1.61 | 1.51 | 10 | 1 |
| 3 | B | 330 | PX4 | C5-N1 | 2.01 | 1.55 | 1.50 | 1 | 1 |
| 3 | B | 337 | PX4 | C5-N1 | 2.01 | 1.44 | 1.50 | 13 | 1 |
| 3 | C | 316 | PX4 | P1-O3 | 2.01 | 1.51 | 1.59 | 8 | 1 |
| 3 | C | 340 | PX4 | C15-C14 | 2.01 | 1.61 | 1.51 | 5 | 1 |
| 3 | A | 606 | PX4 | C3-N1 | 2.01 | 1.44 | 1.50 | 12 | 1 |
| 3 | A | 615 | PX4 | P1-O3 | 2.01 | 1.51 | 1.59 | 9 | 1 |
| 3 | B | 341 | PX4 | O4-C6 | 2.01 | 1.37 | 1.44 | 9 | 1 |
| 3 | B | 367 | PX4 | O8-C23 | 2.01 | 1.28 | 1.22 | 4 | 1 |
| 3 | C | 309 | PX4 | C11-C10 | 2.01 | 1.59 | 1.52 | 2 | 1 |
| 3 | C | 340 | PX4 | C19-C18 | 2.01 | 1.61 | 1.51 | 9 | 1 |
| 3 | B | 370 | PX4 | C30-C29 | 2.01 | 1.61 | 1.51 | 7 | 1 |
| 3 | B | 379 | PX4 | O7-C23 | 2.01 | 1.40 | 1.34 | 4 | 1 |
| 3 | B | 387 | PX4 | O7-C23 | 2.01 | 1.28 | 1.34 | 11 | 1 |
| 3 | C | 321 | PX4 | P1-O4 | 2.01 | 1.51 | 1.59 | 10 | 1 |
| 3 | C | 356 | PX4 | C19-C18 | 2.01 | 1.61 | 1.51 | 4 | 1 |
| 3 | A | 625 | PX4 | C3-N1 | 2.01 | 1.55 | 1.50 | 15 | 1 |
| 3 | A | 644 | PX4 | C17-C16 | 2.01 | 1.61 | 1.51 | 15 | 1 |
| 3 | B | 325 | PX4 | O4-C6 | 2.01 | 1.52 | 1.44 | 9 | 1 |
| 3 | B | 346 | PX4 | O7-C23 | 2.01 | 1.28 | 1.34 | 2 | 1 |
| 3 | B | 347 | PX4 | C11-C10 | 2.01 | 1.59 | 1.52 | 13 | 1 |
| 3 | C | 325 | PX4 | C20-C19 | 2.01 | 1.61 | 1.51 | 9 | 1 |
| 3 | C | 333 | PX4 | C2-N1 | 2.01 | 1.57 | 1.51 | 12 | 1 |
| 3 | C | 352 | PX4 | C34-C33 | 2.01 | 1.61 | 1.51 | 6 | 1 |
| 3 | C | 352 | PX4 | C12-C11 | 2.01 | 1.61 | 1.51 | 10 | 1 |
| 3 | A | 614 | PX4 | C18-C17 | 2.01 | 1.61 | 1.51 | 12 | 1 |
| 3 | A | 646 | PX4 | C31-C30 | 2.01 | 1.61 | 1.51 | 9 | 1 |
| 3 | A | 620 | PX4 | P1-O2 | 2.01 | 1.43 | 1.50 | 11 | 1 |
| 3 | A | 628 | PX4 | C4-N1 | 2.01 | 1.55 | 1.50 | 6 | 1 |
| 3 | B | 363 | PX4 | P1-O1 | 2.01 | 1.46 | 1.55 | 11 | 2 |
| 3 | C | 308 | PX4 | C11-C10 | 2.01 | 1.59 | 1.52 | 13 | 1 |
| 3 | B | 370 | PX4 | C13-C12 | 2.01 | 1.61 | 1.51 | 7 | 1 |
| 3 | C | 311 | PX4 | C12-C11 | 2.01 | 1.61 | 1.51 | 1 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | A | 632 | PX4 | C12-C11 | 2.01 | 1.61 | 1.51 | 15 | 1 |
| 3 | A | 634 | PX4 | O4-C6 | 2.01 | 1.37 | 1.44 | 7 | 1 |
| 3 | B | 357 | PX4 | C11-C10 | 2.01 | 1.59 | 1.52 | 10 | 1 |
| 3 | B | 393 | PX4 | C17-C16 | 2.01 | 1.61 | 1.51 | 5 | 1 |
| 3 | B | 358 | PX4 | C19-C18 | 2.01 | 1.61 | 1.51 | 11 | 1 |
| 3 | B | 399 | PX4 | C5-N1 | 2.01 | 1.55 | 1.50 | 3 | 1 |
| 3 | B | 399 | PX4 | C29-C28 | 2.01 | 1.61 | 1.51 | 5 | 1 |
| 3 | C | 309 | PX4 | C5-N1 | 2.01 | 1.44 | 1.50 | 6 | 1 |
| 3 | C | 352 | PX4 | O8-C23 | 2.01 | 1.16 | 1.22 | 6 | 1 |
| 3 | C | 364 | PX4 | C30-C29 | 2.01 | 1.61 | 1.51 | 15 | 1 |
| 3 | A | 643 | PX4 | C3-N1 | 2.00 | 1.55 | 1.50 | 3 | 1 |
| 3 | B | 374 | PX4 | C13-C12 | 2.00 | 1.61 | 1.51 | 9 | 1 |
| 3 | C | 329 | PX4 | P1-O3 | 2.00 | 1.51 | 1.59 | 2 | 1 |
| 3 | A | 627 | PX4 | C28-C27 | 2.00 | 1.61 | 1.51 | 12 | 1 |
| 3 | B | 308 | PX4 | C13-C12 | 2.00 | 1.61 | 1.51 | 12 | 1 |
| 3 | B | 321 | PX4 | O8-C23 | 2.00 | 1.28 | 1.22 | 1 | 1 |
| 3 | B | 341 | PX4 | O7-C7 | 2.00 | 1.41 | 1.46 | 13 | 1 |
| 3 | B | 374 | PX4 | C2-N1 | 2.00 | 1.57 | 1.51 | 13 | 1 |
| 3 | B | 362 | PX4 | C3-N1 | 2.00 | 1.55 | 1.50 | 15 | 1 |
| 3 | B | 387 | PX4 | C2-N1 | 2.00 | 1.57 | 1.51 | 13 | 1 |
| 3 | B | 399 | PX4 | O3-C1 | 2.00 | 1.36 | 1.44 | 10 | 1 |
| 3 | C | 328 | PX4 | C15-C14 | 2.00 | 1.61 | 1.51 | 5 | 1 |
| 3 | C | 350 | PX4 | C3-N1 | 2.00 | 1.44 | 1.50 | 2 | 1 |
| 3 | A | 602 | PX4 | O4-C6 | 2.00 | 1.37 | 1.44 | 1 | 1 |
| 3 | B | 384 | PX4 | C15-C14 | 2.00 | 1.61 | 1.51 | 4 | 1 |
| 3 | B | 396 | PX4 | C15-C14 | 2.00 | 1.61 | 1.51 | 7 | 1 |
| 3 | C | 332 | PX4 | C5-N1 | 2.00 | 1.44 | 1.50 | 5 | 1 |
| 3 | B | 313 | PX4 | C4-N1 | 2.00 | 1.55 | 1.50 | 12 | 1 |
| 3 | C | 317 | PX4 | C5-N1 | 2.00 | 1.44 | 1.50 | 5 | 1 |
| 3 | C | 327 | PX4 | P1-O1 | 2.00 | 1.46 | 1.55 | 3 | 1 |

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

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | C | 349 | PX4 | C7-O7-C23 | 5.89 | 103.71 | 117.80 | 4 | 6 |
| 3 | A | 653 | PX4 | O7-C23-C24 | 5.81 | 98.91 | 111.48 | 12 | 5 |
| 3 | B | 343 | PX4 | C7-O7-C23 | 5.60 | 104.38 | 117.80 | 4 | 5 |
| 3 | C | 318 | PX4 | C7-O7-C23 | 5.56 | 104.48 | 117.80 | 15 | 4 |
| 3 | B | 341 | PX4 | C7-O7-C23 | 5.54 | 104.54 | 117.80 | 11 | 9 |
| 3 | B | 342 | PX4 | O7-C23-C24 | 5.50 | 99.59 | 111.48 | 1 | 5 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 385 | PX4 | O7-C23-C24 | 5.35 | 99.91 | 111.48 | 3 | 6 |
| 3 | A | 636 | PX4 | C7-O7-C23 | 5.34 | 105.02 | 117.80 | 2 | 3 |
| 3 | A | 612 | PX4 | C7-O7-C23 | 5.30 | 105.11 | 117.80 | 12 | 8 |
| 3 | B | 329 | PX4 | C8-C7-C6 | 5.24 | 99.56 | 111.78 | 6 | 3 |
| 3 | C | 310 | PX4 | O7-C23-C24 | 5.18 | 100.27 | 111.48 | 1 | 8 |
| 3 | B | 341 | PX4 | O5-C8-C7 | 5.18 | 123.32 | 108.40 | 6 | 6 |
| 3 | A | 622 | PX4 | O7-C23-C24 | 5.11 | 100.42 | 111.48 | 6 | 5 |
| 3 | C | 311 | PX4 | C7-O7-C23 | 5.05 | 105.72 | 117.80 | 1 | 7 |
| 3 | B | 379 | PX4 | O7-C23-C24 | 5.01 | 100.63 | 111.48 | 3 | 8 |
| 3 | C | 320 | PX4 | O5-C8-C7 | 5.02 | 122.85 | 108.40 | 1 | 6 |
| 3 | B | 372 | PX4 | O7-C23-C24 | 5.00 | 100.66 | 111.48 | 15 | 6 |
| 3 | C | 361 | PX4 | O5-C8-C7 | 4.98 | 122.77 | 108.40 | 12 | 2 |
| 3 | B | 330 | PX4 | C7-O7-C23 | 4.97 | 105.89 | 117.80 | 4 | 8 |
| 3 | B | 348 | PX4 | C7-O7-C23 | 4.95 | 129.64 | 117.80 | 9 | 3 |
| 3 | A | 651 | PX4 | O7-C23-C24 | 4.91 | 100.87 | 111.48 | 12 | 5 |
| 3 | C | 325 | PX4 | C8-C7-C6 | 4.90 | 100.35 | 111.78 | 11 | 1 |
| 3 | C | 360 | PX4 | O7-C23-C24 | 4.85 | 100.98 | 111.48 | 2 | 3 |
| 3 | B | 340 | PX4 | O7-C23-C24 | 4.84 | 101.02 | 111.48 | 9 | 2 |
| 3 | A | 608 | PX4 | C7-O7-C23 | 4.83 | 106.25 | 117.80 | 7 | 4 |
| 3 | C | 327 | PX4 | C7-O7-C23 | 4.82 | 106.26 | 117.80 | 4 | 4 |
| 3 | B | 313 | PX4 | C7-O7-C23 | 4.81 | 106.29 | 117.80 | 7 | 2 |
| 3 | C | 324 | PX4 | C7-O7-C23 | 4.80 | 106.30 | 117.80 | 12 | 6 |
| 3 | B | 331 | PX4 | C7-O7-C23 | 4.79 | 106.34 | 117.80 | 14 | 3 |
| 3 | B | 378 | PX4 | O7-C23-C24 | 4.76 | 101.19 | 111.48 | 3 | 3 |
| 3 | A | 614 | PX4 | O7-C23-C24 | 4.75 | 101.20 | 111.48 | 3 | 3 |
| 3 | B | 384 | PX4 | O5-C8-C7 | 4.72 | 122.01 | 108.40 | 9 | 6 |
| 3 | B | 399 | PX4 | C8-C7-C6 | 4.69 | 122.71 | 111.78 | 15 | 3 |
| 3 | B | 328 | PX4 | C7-O7-C23 | 4.66 | 106.65 | 117.80 | 6 | 5 |
| 3 | A | 616 | PX4 | C7-O7-C23 | 4.65 | 106.66 | 117.80 | 6 | 7 |
| 3 | B | 320 | PX4 | O7-C23-C24 | 4.65 | 101.41 | 111.48 | 6 | 4 |
| 3 | B | 319 | PX4 | C7-O7-C23 | 4.65 | 106.67 | 117.80 | 1 | 11 |
| 3 | C | 344 | PX4 | O7-C23-C24 | 4.64 | 101.44 | 111.48 | 7 | 5 |
| 3 | C | 353 | PX4 | O7-C23-C24 | 4.64 | 101.45 | 111.48 | 14 | 3 |
| 3 | B | 349 | PX4 | O7-C23-C24 | 4.64 | 101.45 | 111.48 | 10 | 2 |
| 3 | B | 325 | PX4 | O7-C23-C24 | 4.63 | 101.46 | 111.48 | 12 | 2 |
| 3 | C | 302 | PX4 | O5-C8-C7 | 4.60 | 121.66 | 108.40 | 6 | 9 |
| 3 | C | 344 | PX4 | C7-O7-C23 | 4.59 | 106.81 | 117.80 | 15 | 3 |
| 3 | A | 653 | PX4 | O5-C8-C7 | 4.58 | 121.59 | 108.40 | 14 | 9 |
| 3 | A | 612 | PX4 | C5-N1-C4 | 4.55 | 120.93 | 108.98 | 11 | 3 |
| 3 | A | 626 | PX4 | O7-C23-C24 | 4.54 | 101.66 | 111.48 | 4 | 7 |
| 3 | C | 329 | PX4 | C7-O7-C23 | 4.54 | 106.94 | 117.80 | 5 | 4 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | A | 620 | PX4 | O7-C23-C24 | 4.52 | 101.70 | 111.48 | 13 | 4 |
| 3 | C | 360 | PX4 | C5-N1-C3 | 4.52 | 97.10 | 108.98 | 13 | 2 |
| 3 | A | 601 | PX4 | C8-C7-C6 | 4.52 | 101.25 | 111.78 | 11 | 5 |
| 3 | B | 344 | PX4 | C8-C7-C6 | 4.52 | 101.25 | 111.78 | 13 | 3 |
| 3 | B | 328 | PX4 | O7-C23-O8 | 4.51 | 134.25 | 123.70 | 10 | 1 |
| 3 | C | 346 | PX4 | C7-O7-C23 | 4.50 | 107.03 | 117.80 | 5 | 4 |
| 3 | A | 605 | PX4 | O7-C23-O8 | 4.49 | 134.19 | 123.70 | 10 | 8 |
| 3 | C | 339 | PX4 | O7-C23-C24 | 4.47 | 101.81 | 111.48 | 3 | 4 |
| 3 | B | 354 | PX4 | O5-C8-C7 | 4.46 | 121.24 | 108.40 | 13 | 4 |
| 3 | C | 363 | PX4 | O7-C23-C24 | 4.45 | 101.84 | 111.48 | 9 | 7 |
| 3 | A | 637 | PX4 | O5-C8-C7 | 4.44 | 121.20 | 108.40 | 10 | 5 |
| 3 | C | 363 | PX4 | O7-C23-O8 | 4.44 | 134.09 | 123.70 | 9 | 2 |
| 3 | A | 651 | PX4 | C8-C7-C6 | 4.43 | 101.47 | 111.78 | 3 | 5 |
| 3 | B | 308 | PX4 | C5-N1-C4 | 4.42 | 97.36 | 108.98 | 13 | 3 |
| 3 | B | 356 | PX4 | C7-O7-C23 | 4.42 | 107.21 | 117.80 | 12 | 4 |
| 3 | C | 309 | PX4 | C8-C7-C6 | 4.42 | 101.48 | 111.78 | 11 | 1 |
| 3 | B | 399 | PX4 | C7-O7-C23 | 4.41 | 107.23 | 117.80 | 8 | 5 |
| 3 | C | 333 | PX4 | O7-C23-O8 | 4.40 | 133.99 | 123.70 | 1 | 1 |
| 3 | B | 369 | PX4 | C4-N1-C3 | 4.40 | 97.42 | 108.98 | 12 | 2 |
| 3 | C | 329 | PX4 | O5-C8-C7 | 4.38 | 121.03 | 108.40 | 1 | 6 |
| 3 | B | 318 | PX4 | C7-O7-C23 | 4.37 | 107.33 | 117.80 | 5 | 4 |
| 3 | B | 315 | PX4 | O7-C23-C24 | 4.36 | 102.04 | 111.48 | 4 | 1 |
| 3 | C | 348 | PX4 | O5-C8-C7 | 4.36 | 120.98 | 108.40 | 11 | 6 |
| 3 | C | 355 | PX4 | C7-O7-C23 | 4.36 | 107.37 | 117.80 | 8 | 4 |
| 3 | A | 605 | PX4 | O7-C23-C24 | 4.35 | 102.07 | 111.48 | 10 | 5 |
| 3 | C | 338 | PX4 | O5-C8-C7 | 4.34 | 120.92 | 108.40 | 14 | 4 |
| 3 | B | 316 | PX4 | C7-O7-C23 | 4.33 | 107.44 | 117.80 | 11 | 4 |
| 3 | A | 612 | PX4 | O5-C8-C7 | 4.32 | 120.85 | 108.40 | 3 | 6 |
| 3 | A | 611 | PX4 | O5-C8-C7 | 4.32 | 120.84 | 108.40 | 10 | 5 |
| 3 | A | 640 | PX4 | C7-O7-C23 | 4.32 | 107.46 | 117.80 | 14 | 5 |
| 3 | C | 363 | PX4 | C7-O7-C23 | 4.32 | 107.46 | 117.80 | 11 | 3 |
| 3 | C | 336 | PX4 | O7-C23-C24 | 4.31 | 102.15 | 111.48 | 13 | 4 |
| 3 | A | 650 | PX4 | O5-C8-C7 | 4.31 | 120.82 | 108.40 | 5 | 3 |
| 3 | B | 396 | PX4 | C8-C7-C6 | 4.31 | 101.74 | 111.78 | 12 | 4 |
| 3 | C | 329 | PX4 | O7-C23-C24 | 4.31 | 102.16 | 111.48 | 1 | 7 |
| 3 | A | 625 | PX4 | C8-C7-C6 | 4.30 | 101.75 | 111.78 | 6 | 1 |
| 3 | C | 339 | PX4 | C7-O7-C23 | 4.30 | 107.50 | 117.80 | 13 | 3 |
| 3 | B | 365 | PX4 | O7-C23-C24 | 4.30 | 102.18 | 111.48 | 2 | 3 |
| 3 | B | 381 | PX4 | O5-C8-C7 | 4.29 | 120.77 | 108.40 | 5 | 4 |
| 3 | A | 610 | PX4 | O7-C23-C24 | 4.27 | 102.24 | 111.48 | 4 | 3 |
| 3 | B | 323 | PX4 | C7-O7-C23 | 4.27 | 107.58 | 117.80 | 8 | 3 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 359 | PX4 | C5-N1-C4 | 4.27 | 97.77 | 108.98 | 3 | 2 |
| 3 | B | 338 | PX4 | O7-C23-C24 | 4.26 | 102.26 | 111.48 | 11 | 4 |
| 3 | A | 649 | PX4 | C7-O7-C23 | 4.26 | 107.60 | 117.80 | 7 | 3 |
| 3 | C | 331 | PX4 | C7-O7-C23 | 4.26 | 107.61 | 117.80 | 13 | 2 |
| 3 | B | 380 | PX4 | C7-O7-C23 | 4.25 | 107.62 | 117.80 | 11 | 6 |
| 3 | C | 351 | PX4 | O7-C23-C24 | 4.25 | 102.30 | 111.48 | 4 | 5 |
| 3 | B | 316 | PX4 | C8-C7-C6 | 4.24 | 101.89 | 111.78 | 11 | 1 |
| 3 | C | 331 | PX4 | C1-C2-N1 | 4.24 | 129.44 | 115.82 | 12 | 1 |
| 3 | A | 633 | PX4 | C7-O7-C23 | 4.24 | 107.66 | 117.80 | 15 | 3 |
| 3 | A | 625 | PX4 | C7-O7-C23 | 4.23 | 107.66 | 117.80 | 5 | 4 |
| 3 | A | 621 | PX4 | O7-C23-C24 | 4.23 | 102.33 | 111.48 | 5 | 6 |
| 3 | B | 369 | PX4 | C7-O7-C23 | 4.23 | 107.68 | 117.80 | 12 | 5 |
| 3 | C | 304 | PX4 | O7-C23-C24 | 4.22 | 102.34 | 111.48 | 12 | 4 |
| 3 | B | 354 | PX4 | C8-C7-C6 | 4.22 | 121.61 | 111.78 | 4 | 3 |
| 3 | B | 337 | PX4 | C8-C7-C6 | 4.21 | 101.96 | 111.78 | 15 | 5 |
| 3 | C | 338 | PX4 | C7-O7-C23 | 4.21 | 107.71 | 117.80 | 3 | 3 |
| 3 | B | 360 | PX4 | C7-O7-C23 | 4.20 | 107.73 | 117.80 | 13 | 4 |
| 3 | C | 338 | PX4 | O7-C23-C24 | 4.20 | 102.40 | 111.48 | 10 | 4 |
| 3 | C | 310 | PX4 | C7-O7-C23 | 4.20 | 107.75 | 117.80 | 1 | 5 |
| 3 | C | 350 | PX4 | C7-O7-C23 | 4.20 | 127.84 | 117.80 | 1 | 8 |
| 3 | C | 360 | PX4 | C7-O7-C23 | 4.20 | 107.75 | 117.80 | 2 | 4 |
| 3 | B | 326 | PX4 | O7-C23-C24 | 4.19 | 102.41 | 111.48 | 14 | 5 |
| 3 | C | 350 | PX4 | O7-C23-C24 | 4.19 | 102.42 | 111.48 | 11 | 5 |
| 3 | B | 353 | PX4 | O5-C8-C7 | 4.18 | 120.45 | 108.40 | 13 | 3 |
| 3 | C | 346 | PX4 | O5-C8-C7 | 4.18 | 120.44 | 108.40 | 11 | 4 |
| 3 | B | 360 | PX4 | O5-C8-C7 | 4.16 | 120.39 | 108.40 | 7 | 2 |
| 3 | C | 303 | PX4 | C7-O7-C23 | 4.16 | 107.84 | 117.80 | 11 | 7 |
| 3 | C | 351 | PX4 | C7-O7-C23 | 4.16 | 107.83 | 117.80 | 12 | 4 |
| 3 | B | 315 | PX4 | O5-C8-C7 | 4.16 | 120.39 | 108.40 | 13 | 3 |
| 3 | A | 611 | PX4 | C7-O7-C23 | 4.15 | 107.86 | 117.80 | 14 | 4 |
| 3 | A | 615 | PX4 | C7-O7-C23 | 4.15 | 107.86 | 117.80 | 15 | 3 |
| 3 | C | 326 | PX4 | C7-O7-C23 | 4.15 | 107.86 | 117.80 | 6 | 5 |
| 3 | C | 344 | PX4 | C5-N1-C3 | 4.15 | 119.88 | 108.98 | 1 | 3 |
| 3 | B | 396 | PX4 | O5-C8-C7 | 4.14 | 120.34 | 108.40 | 2 | 5 |
| 3 | C | 335 | PX4 | C7-O7-C23 | 4.14 | 107.88 | 117.80 | 3 | 4 |
| 3 | A | 624 | PX4 | C1-C2-N1 | 4.14 | 129.10 | 115.82 | 3 | 5 |
| 3 | B | 394 | PX4 | C5-N1-C3 | 4.14 | 119.85 | 108.98 | 3 | 5 |
| 3 | C | 342 | PX4 | C7-O7-C23 | 4.14 | 107.89 | 117.80 | 7 | 3 |
| 3 | A | 649 | PX4 | O7-C23-C24 | 4.14 | 102.53 | 111.48 | 2 | 3 |
| 3 | B | 364 | PX4 | C8-C7-C6 | 4.13 | 102.15 | 111.78 | 15 | 3 |
| 3 | C | 342 | PX4 | C5-N1-C4 | 4.13 | 119.83 | 108.98 | 15 | 2 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | A | 631 | PX4 | O7-C23-C24 | 4.13 | 102.54 | 111.48 | 1 | 6 |
| 3 | C | 319 | PX4 | C7-O7-C23 | 4.13 | 107.91 | 117.80 | 13 | 5 |
| 3 | B | 309 | PX4 | C7-O7-C23 | 4.13 | 127.67 | 117.80 | 10 | 7 |
| 3 | C | 313 | PX4 | O5-C8-C7 | 4.12 | 120.28 | 108.40 | 5 | 6 |
| 3 | A | 608 | PX4 | O5-C9-C10 | 4.12 | 99.27 | 111.83 | 2 | 5 |
| 3 | B | 306 | PX4 | O7-C23-C24 | 4.12 | 102.57 | 111.48 | 5 | 1 |
| 3 | A | 642 | PX4 | C5-N1-C3 | 4.12 | 98.16 | 108.98 | 14 | 3 |
| 3 | A | 635 | PX4 | O5-C8-C7 | 4.11 | 120.25 | 108.40 | 11 | 1 |
| 3 | C | 336 | PX4 | C7-O7-C23 | 4.11 | 107.96 | 117.80 | 12 | 3 |
| 3 | B | 308 | PX4 | C7-O7-C23 | 4.11 | 107.97 | 117.80 | 11 | 2 |
| 3 | C | 337 | PX4 | C7-O7-C23 | 4.11 | 107.97 | 117.80 | 9 | 4 |
| 3 | B | 318 | PX4 | O7-C23-C24 | 4.10 | 102.61 | 111.48 | 3 | 6 |
| 3 | C | 314 | PX4 | O7-C23-C24 | 4.10 | 102.61 | 111.48 | 12 | 1 |
| 3 | C | 355 | PX4 | O7-C23-C24 | 4.09 | 102.62 | 111.48 | 12 | 5 |
| 3 | B | 315 | PX4 | C7-O7-C23 | 4.09 | 108.00 | 117.80 | 12 | 9 |
| 3 | B | 360 | PX4 | O5-C9-O6 | 4.09 | 133.86 | 123.63 | 12 | 3 |
| 3 | A | 606 | PX4 | O7-C23-C24 | 4.09 | 102.64 | 111.48 | 4 | 4 |
| 3 | B | 341 | PX4 | O7-C23-C24 | 4.09 | 102.64 | 111.48 | 15 | 4 |
| 3 | B | 333 | PX4 | C5-N1-C4 | 4.08 | 119.70 | 108.98 | 6 | 3 |
| 3 | C | 309 | PX4 | O7-C23-C24 | 4.07 | 102.67 | 111.48 | 10 | 2 |
| 3 | B | 368 | PX4 | O7-C23-C24 | 4.07 | 102.68 | 111.48 | 3 | 7 |
| 3 | C | 335 | PX4 | O7-C23-C24 | 4.07 | 102.68 | 111.48 | 10 | 3 |
| 3 | C | 345 | PX4 | C5-N1-C3 | 4.07 | 119.66 | 108.98 | 10 | 3 |
| 3 | C | 328 | PX4 | O7-C23-C24 | 4.06 | 102.69 | 111.48 | 10 | 6 |
| 3 | A | 639 | PX4 | C7-O7-C23 | 4.06 | 108.08 | 117.80 | 13 | 3 |
| 3 | B | 328 | PX4 | O7-C23-C24 | 4.05 | 102.71 | 111.48 | 5 | 6 |
| 3 | C | 313 | PX4 | C7-O7-C23 | 4.05 | 108.10 | 117.80 | 2 | 4 |
| 3 | C | 353 | PX4 | O5-C8-C7 | 4.04 | 120.06 | 108.40 | 12 | 4 |
| 3 | A | 617 | PX4 | O7-C23-C24 | 4.04 | 102.75 | 111.48 | 5 | 6 |
| 3 | A | 636 | PX4 | C8-C7-C6 | 4.04 | 121.19 | 111.78 | 14 | 5 |
| 3 | C | 361 | PX4 | C8-C7-C6 | 4.04 | 102.38 | 111.78 | 8 | 5 |
| 3 | B | 389 | PX4 | O7-C23-C24 | 4.02 | 102.78 | 111.48 | 12 | 3 |
| 3 | C | 308 | PX4 | O5-C9-C10 | 4.02 | 99.58 | 111.83 | 9 | 2 |
| 3 | B | 347 | PX4 | C7-O7-C23 | 4.02 | 108.18 | 117.80 | 15 | 7 |
| 3 | B | 307 | PX4 | C7-O7-C23 | 4.01 | 108.19 | 117.80 | 1 | 2 |
| 3 | A | 652 | PX4 | C7-O7-C23 | 4.01 | 108.20 | 117.80 | 12 | 6 |
| 3 | A | 651 | PX4 | O7-C23-O8 | 4.01 | 133.07 | 123.70 | 12 | 4 |
| 3 | B | 304 | PX4 | C8-C7-C6 | 4.01 | 121.12 | 111.78 | 12 | 4 |
| 3 | B | 350 | PX4 | O7-C23-C24 | 4.01 | 102.81 | 111.48 | 2 | 1 |
| 3 | C | 315 | PX4 | O7-C23-C24 | 4.01 | 102.81 | 111.48 | 14 | 5 |
| 3 | C | 343 | PX4 | O5-C8-C7 | 4.00 | 119.93 | 108.40 | 11 | 6 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | A | 633 | PX4 | O5-C8-C7 | 4.00 | 119.93 | 108.40 | 4 | 1 |
| 3 | A | 622 | PX4 | C7-O7-C23 | 4.00 | 108.23 | 117.80 | 13 | 3 |
| 3 | B | 388 | PX4 | C8-C7-C6 | 4.00 | 121.10 | 111.78 | 13 | 5 |
| 3 | C | 307 | PX4 | O5-C8-C7 | 3.99 | 119.90 | 108.40 | 8 | 10 |
| 3 | A | 652 | PX4 | O5-C8-C7 | 3.99 | 119.89 | 108.40 | 9 | 5 |
| 3 | B | 311 | PX4 | O7-C23-C24 | 3.99 | 102.85 | 111.48 | 3 | 4 |
| 3 | C | 321 | PX4 | O5-C8-C7 | 3.99 | 119.88 | 108.40 | 12 | 4 |
| 3 | C | 350 | PX4 | C5-N1-C3 | 3.97 | 98.55 | 108.98 | 7 | 1 |
| 3 | C | 332 | PX4 | C7-O7-C23 | 3.97 | 108.30 | 117.80 | 15 | 3 |
| 3 | B | 312 | PX4 | C5-N1-C3 | 3.96 | 98.57 | 108.98 | 13 | 2 |
| 3 | B | 348 | PX4 | O7-C23-C24 | 3.96 | 102.91 | 111.48 | 12 | 3 |
| 3 | C | 354 | PX4 | C8-C7-C6 | 3.96 | 121.02 | 111.78 | 6 | 5 |
| 3 | B | 306 | PX4 | O5-C8-C7 | 3.96 | 119.80 | 108.40 | 5 | 9 |
| 3 | B | 348 | PX4 | C8-C7-C6 | 3.96 | 121.01 | 111.78 | 2 | 4 |
| 3 | C | 306 | PX4 | O7-C23-C24 | 3.96 | 102.92 | 111.48 | 9 | 3 |
| 3 | C | 317 | PX4 | C7-O7-C23 | 3.96 | 127.26 | 117.80 | 4 | 4 |
| 3 | B | 388 | PX4 | O7-C23-C24 | 3.95 | 102.93 | 111.48 | 1 | 5 |
| 3 | A | 618 | PX4 | O5-C8-C7 | 3.95 | 119.79 | 108.40 | 1 | 9 |
| 3 | C | 358 | PX4 | O7-C23-C24 | 3.95 | 102.93 | 111.48 | 8 | 4 |
| 3 | B | 393 | PX4 | O7-C23-C24 | 3.95 | 102.94 | 111.48 | 10 | 4 |
| 3 | C | 350 | PX4 | C5-N1-C4 | 3.95 | 98.61 | 108.98 | 13 | 1 |
| 3 | A | 607 | PX4 | O5-C9-C10 | 3.94 | 99.81 | 111.83 | 6 | 3 |
| 3 | B | 386 | PX4 | O7-C23-C24 | 3.94 | 102.95 | 111.48 | 14 | 6 |
| 3 | B | 336 | PX4 | C1-C2-N1 | 3.93 | 128.45 | 115.82 | 8 | 2 |
| 3 | A | 622 | PX4 | C8-C7-C6 | 3.93 | 120.95 | 111.78 | 13 | 6 |
| 3 | A | 651 | PX4 | C7-O7-C23 | 3.93 | 108.39 | 117.80 | 14 | 2 |
| 3 | B | 384 | PX4 | C7-O7-C23 | 3.92 | 108.41 | 117.80 | 13 | 6 |
| 3 | B | 327 | PX4 | C7-O7-C23 | 3.92 | 108.41 | 117.80 | 10 | 3 |
| 3 | C | 358 | PX4 | C8-C7-C6 | 3.92 | 120.92 | 111.78 | 1 | 2 |
| 3 | A | 627 | PX4 | C7-O7-C23 | 3.92 | 108.42 | 117.80 | 6 | 4 |
| 3 | B | 346 | PX4 | C7-O7-C23 | 3.92 | 108.42 | 117.80 | 7 | 1 |
| 3 | B | 327 | PX4 | C5-N1-C4 | 3.91 | 98.69 | 108.98 | 3 | 3 |
| 3 | B | 382 | PX4 | O7-C23-C24 | 3.91 | 103.01 | 111.48 | 3 | 4 |
| 3 | B | 345 | PX4 | C4-N1-C3 | 3.90 | 119.23 | 108.98 | 3 | 1 |
| 3 | C | 313 | PX4 | O5-C9-O6 | 3.90 | 133.39 | 123.63 | 14 | 2 |
| 3 | B | 367 | PX4 | C7-O7-C23 | 3.90 | 108.47 | 117.80 | 1 | 7 |
| 3 | C | 352 | PX4 | C7-O7-C23 | 3.89 | 108.49 | 117.80 | 4 | 5 |
| 3 | A | 630 | PX4 | C8-C7-C6 | 3.88 | 102.73 | 111.78 | 3 | 5 |
| 3 | B | 372 | PX4 | O7-C23-O8 | 3.89 | 132.79 | 123.70 | 15 | 5 |
| 3 | B | 362 | PX4 | O5-C8-C7 | 3.88 | 119.59 | 108.40 | 7 | 6 |
| 3 | C | 304 | PX4 | O5-C8-C7 | 3.88 | 119.59 | 108.40 | 12 | 2 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | C | 364 | PX4 | O5-C8-C7 | 3.88 | 119.57 | 108.40 | 6 | 4 |
| 3 | B | 349 | PX4 | O5-C8-C7 | 3.88 | 119.57 | 108.40 | 14 | 3 |
| 3 | B | 393 | PX4 | C7-O7-C23 | 3.87 | 108.53 | 117.80 | 12 | 1 |
| 3 | C | 310 | PX4 | C5-N1-C4 | 3.87 | 98.80 | 108.98 | 4 | 1 |
| 3 | B | 344 | PX4 | O5-C8-C7 | 3.87 | 119.56 | 108.40 | 5 | 4 |
| 3 | A | 609 | PX4 | C7-O7-C23 | 3.87 | 108.53 | 117.80 | 6 | 3 |
| 3 | B | 336 | PX4 | O7-C23-O8 | 3.87 | 132.75 | 123.70 | 14 | 2 |
| 3 | B | 392 | PX4 | C7-O7-C23 | 3.87 | 108.54 | 117.80 | 10 | 7 |
| 3 | B | 334 | PX4 | C7-O7-C23 | 3.87 | 108.54 | 117.80 | 14 | 3 |
| 3 | B | 306 | PX4 | C7-O7-C23 | 3.86 | 108.55 | 117.80 | 14 | 5 |
| 3 | B | 322 | PX4 | O7-C23-O8 | 3.86 | 132.74 | 123.70 | 12 | 2 |
| 3 | B | 399 | PX4 | O7-C23-C24 | 3.86 | 103.13 | 111.48 | 15 | 7 |
| 3 | B | 389 | PX4 | C7-O7-C23 | 3.86 | 108.56 | 117.80 | 9 | 8 |
| 3 | B | 308 | PX4 | O7-C23-C24 | 3.86 | 103.14 | 111.48 | 9 | 5 |
| 3 | B | 385 | PX4 | O5-C8-C7 | 3.86 | 119.51 | 108.40 | 7 | 1 |
| 3 | A | 604 | PX4 | O7-C23-C24 | 3.85 | 103.15 | 111.48 | 3 | 4 |
| 3 | B | 310 | PX4 | C5-N1-C4 | 3.85 | 98.86 | 108.98 | 4 | 3 |
| 3 | B | 326 | PX4 | C4-N1-C3 | 3.85 | 119.09 | 108.98 | 4 | 2 |
| 3 | C | 354 | PX4 | O7-C23-C24 | 3.85 | 103.15 | 111.48 | 13 | 7 |
| 3 | C | 320 | PX4 | C8-C7-C6 | 3.84 | 120.75 | 111.78 | 15 | 2 |
| 3 | C | 357 | PX4 | O7-C23-C24 | 3.84 | 103.17 | 111.48 | 10 | 5 |
| 3 | A | 626 | PX4 | O7-C23-O8 | 3.83 | 132.66 | 123.70 | 13 | 2 |
| 3 | B | 307 | PX4 | O5-C8-C7 | 3.83 | 119.44 | 108.40 | 14 | 5 |
| 3 | B | 352 | PX4 | O5-C8-C7 | 3.83 | 119.44 | 108.40 | 15 | 5 |
| 3 | B | 361 | PX4 | O7-C23-C24 | 3.83 | 103.20 | 111.48 | 12 | 5 |
| 3 | B | 351 | PX4 | O5-C8-C7 | 3.82 | 119.42 | 108.40 | 2 | 6 |
| 3 | B | 301 | PX4 | C7-O7-C23 | 3.82 | 108.65 | 117.80 | 3 | 2 |
| 3 | B | 353 | PX4 | O7-C23-O8 | 3.82 | 132.64 | 123.70 | 14 | 3 |
| 3 | B | 398 | PX4 | C7-O7-C23 | 3.82 | 108.66 | 117.80 | 5 | 6 |
| 3 | A | 636 | PX4 | O7-C23-O8 | 3.82 | 132.63 | 123.70 | 10 | 1 |
| 3 | B | 332 | PX4 | C7-O7-C23 | 3.81 | 108.67 | 117.80 | 1 | 5 |
| 3 | C | 307 | PX4 | O7-C23-C24 | 3.82 | 103.23 | 111.48 | 8 | 4 |
| 3 | B | 365 | PX4 | O7-C23-O8 | 3.81 | 132.62 | 123.70 | 15 | 3 |
| 3 | B | 385 | PX4 | C5-N1-C4 | 3.80 | 118.97 | 108.98 | 8 | 1 |
| 3 | B | 304 | PX4 | C7-O7-C23 | 3.80 | 108.71 | 117.80 | 11 | 7 |
| 3 | A | 610 | PX4 | C7-O7-C23 | 3.79 | 108.71 | 117.80 | 1 | 4 |
| 3 | A | 626 | PX4 | O5-C8-C7 | 3.79 | 119.33 | 108.40 | 2 | 3 |
| 3 | C | 322 | PX4 | C8-C7-C6 | 3.79 | 102.94 | 111.78 | 7 | 2 |
| 3 | A | 633 | PX4 | O7-C23-C24 | 3.79 | 103.28 | 111.48 | 5 | 6 |
| 3 | B | 344 | PX4 | O5-C9-C10 | 3.79 | 100.28 | 111.83 | 3 | 3 |
| 3 | B | 306 | PX4 | C8-C7-C6 | 3.79 | 102.95 | 111.78 | 9 | 4 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 360 | PX4 | O7-C23-C24 | 3.78 | 103.29 | 111.48 | 1 | 3 |
| 3 | A | 654 | PX4 | C7-O7-C23 | 3.78 | 108.74 | 117.80 | 6 | 7 |
| 3 | A | 603 | PX4 | O5-C8-C7 | 3.78 | 119.30 | 108.40 | 14 | 4 |
| 3 | A | 619 | PX4 | C1-C2-N1 | 3.78 | 127.95 | 115.82 | 9 | 3 |
| 3 | B | 364 | PX4 | O7-C23-C24 | 3.78 | 103.31 | 111.48 | 13 | 5 |
| 3 | A | 603 | PX4 | O7-C23-O8 | 3.77 | 132.53 | 123.70 | 12 | 7 |
| 3 | A | 641 | PX4 | O7-C23-C24 | 3.77 | 103.32 | 111.48 | 4 | 3 |
| 3 | B | 339 | PX4 | C7-O7-C23 | 3.77 | 108.77 | 117.80 | 1 | 6 |
| 3 | B | 381 | PX4 | C4-N1-C3 | 3.77 | 99.07 | 108.98 | 14 | 2 |
| 3 | A | 602 | PX4 | C7-O7-C23 | 3.76 | 108.79 | 117.80 | 11 | 5 |
| 3 | B | 334 | PX4 | C8-C7-C6 | 3.76 | 103.01 | 111.78 | 7 | 2 |
| 3 | B | 398 | PX4 | O5-C8-C7 | 3.76 | 119.24 | 108.40 | 4 | 5 |
| 3 | A | 604 | PX4 | C7-O7-C23 | 3.75 | 108.82 | 117.80 | 6 | 8 |
| 3 | B | 388 | PX4 | O5-C8-C7 | 3.75 | 119.21 | 108.40 | 15 | 3 |
| 3 | B | 356 | PX4 | O7-C23-O8 | 3.75 | 132.47 | 123.70 | 4 | 2 |
| 3 | A | 646 | PX4 | C5-N1-C3 | 3.75 | 99.13 | 108.98 | 12 | 5 |
| 3 | A | 646 | PX4 | C5-N1-C4 | 3.74 | 99.14 | 108.98 | 6 | 2 |
| 3 | C | 305 | PX4 | O5-C9-C10 | 3.74 | 100.42 | 111.83 | 14 | 2 |
| 3 | C | 324 | PX4 | O5-C8-C7 | 3.74 | 119.18 | 108.40 | 10 | 4 |
| 3 | A | 621 | PX4 | C7-O7-C23 | 3.74 | 108.84 | 117.80 | 5 | 6 |
| 3 | A | 644 | PX4 | C4-N1-C3 | 3.74 | 99.16 | 108.98 | 11 | 1 |
| 3 | B | 312 | PX4 | O7-C23-C24 | 3.73 | 103.40 | 111.48 | 12 | 1 |
| 3 | B | 376 | PX4 | C7-O7-C23 | 3.73 | 108.86 | 117.80 | 6 | 3 |
| 3 | C | 364 | PX4 | O7-C23-O8 | 3.73 | 132.44 | 123.70 | 2 | 3 |
| 3 | B | 358 | PX4 | C7-O7-C23 | 3.73 | 108.86 | 117.80 | 4 | 4 |
| 3 | B | 379 | PX4 | C7-O7-C23 | 3.73 | 126.72 | 117.80 | 4 | 4 |
| 3 | B | 380 | PX4 | C5-N1-C3 | 3.73 | 99.19 | 108.98 | 2 | 3 |
| 3 | C | 301 | PX4 | O5-C8-C7 | 3.72 | 119.13 | 108.40 | 15 | 4 |
| 3 | C | 305 | PX4 | O7-C23-O8 | 3.73 | 132.41 | 123.70 | 13 | 1 |
| 3 | C | 350 | PX4 | O5-C8-C7 | 3.72 | 119.13 | 108.40 | 10 | 8 |
| 3 | C | 353 | PX4 | C1-C2-N1 | 3.72 | 127.77 | 115.82 | 3 | 4 |
| 3 | C | 321 | PX4 | O7-C23-C24 | 3.71 | 103.45 | 111.48 | 6 | 5 |
| 3 | B | 313 | PX4 | O7-C23-C24 | 3.71 | 103.45 | 111.48 | 10 | 2 |
| 3 | B | 308 | PX4 | O7-C23-O8 | 3.71 | 132.37 | 123.70 | 3 | 3 |
| 3 | B | 320 | PX4 | C7-O7-C23 | 3.70 | 108.94 | 117.80 | 5 | 6 |
| 3 | A | 647 | PX4 | C8-C7-C6 | 3.70 | 103.17 | 111.78 | 10 | 2 |
| 3 | B | 367 | PX4 | C8-O5-C9 | 3.69 | 103.63 | 117.12 | 15 | 1 |
| 3 | C | 317 | PX4 | C8-C7-C6 | 3.69 | 120.39 | 111.78 | 4 | 9 |
| 3 | C | 310 | PX4 | O5-C8-C7 | 3.69 | 119.03 | 108.40 | 5 | 6 |
| 3 | A | 634 | PX4 | O5-C9-O6 | 3.69 | 132.85 | 123.63 | 4 | 2 |
| 3 | B | 371 | PX4 | C7-O7-C23 | 3.69 | 108.97 | 117.80 | 7 | 3 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 335 | PX4 | C5-N1-C3 | 3.68 | 118.65 | 108.98 | 8 | 3 |
| 3 | B | 313 | PX4 | O7-C23-O8 | 3.68 | 132.31 | 123.70 | 14 | 4 |
| 3 | C | 330 | PX4 | C8-C7-C6 | 3.68 | 103.20 | 111.78 | 12 | 4 |
| 3 | C | 333 | PX4 | C4-N1-C3 | 3.68 | 99.32 | 108.98 | 14 | 2 |
| 3 | C | 332 | PX4 | O5-C9-C10 | 3.67 | 100.66 | 111.83 | 2 | 4 |
| 3 | A | 645 | PX4 | O7-C23-C24 | 3.66 | 103.55 | 111.48 | 8 | 3 |
| 3 | C | 358 | PX4 | C26-C25-C24 | 3.66 | 99.67 | 113.13 | 11 | 1 |
| 3 | A | 603 | PX4 | O7-C23-C24 | 3.66 | 103.56 | 111.48 | 15 | 3 |
| 3 | A | 638 | PX4 | C4-N1-C3 | 3.66 | 99.36 | 108.98 | 2 | 2 |
| 3 | A | 631 | PX4 | C7-O7-C23 | 3.66 | 109.04 | 117.80 | 7 | 3 |
| 3 | B | 394 | PX4 | C1-C2-N1 | 3.65 | 127.55 | 115.82 | 4 | 1 |
| 3 | A | 608 | PX4 | O5-C9-O6 | 3.65 | 132.77 | 123.63 | 2 | 2 |
| 3 | B | 375 | PX4 | C7-O7-C23 | 3.65 | 109.06 | 117.80 | 7 | 6 |
| 3 | A | 607 | PX4 | O7-C23-C24 | 3.65 | 103.58 | 111.48 | 14 | 4 |
| 3 | A | 632 | PX4 | C8-C7-C6 | 3.65 | 103.28 | 111.78 | 11 | 2 |
| 3 | B | 364 | PX4 | C7-O7-C23 | 3.65 | 109.07 | 117.80 | 7 | 5 |
| 3 | B | 400 | PX4 | O7-C23-C24 | 3.64 | 103.60 | 111.48 | 5 | 5 |
| 3 | B | 311 | PX4 | O7-C23-O8 | 3.64 | 132.21 | 123.70 | 3 | 2 |
| 3 | B | 397 | PX4 | O7-C23-C24 | 3.64 | 103.61 | 111.48 | 2 | 5 |
| 3 | B | 341 | PX4 | O5-C9-O6 | 3.64 | 132.73 | 123.63 | 6 | 4 |
| 3 | C | 328 | PX4 | O5-C8-C7 | 3.64 | 118.89 | 108.40 | 9 | 6 |
| 3 | B | 353 | PX4 | C4-N1-C3 | 3.64 | 99.42 | 108.98 | 4 | 3 |
| 3 | C | 312 | PX4 | C7-O7-C23 | 3.64 | 109.09 | 117.80 | 12 | 2 |
| 3 | B | 309 | PX4 | C8-C7-C6 | 3.63 | 103.31 | 111.78 | 10 | 3 |
| 3 | B | 392 | PX4 | O5-C8-C7 | 3.63 | 118.87 | 108.40 | 8 | 6 |
| 3 | A | 643 | PX4 | C7-O7-C23 | 3.63 | 109.11 | 117.80 | 4 | 4 |
| 3 | B | 356 | PX4 | C8-C7-C6 | 3.63 | 103.32 | 111.78 | 12 | 4 |
| 3 | C | 358 | PX4 | C7-O7-C23 | 3.63 | 109.11 | 117.80 | 9 | 4 |
| 3 | B | 376 | PX4 | O7-C23-O8 | 3.62 | 132.18 | 123.70 | 15 | 3 |
| 3 | B | 354 | PX4 | C7-O7-C23 | 3.62 | 109.13 | 117.80 | 8 | 3 |
| 3 | B | 329 | PX4 | C5-N1-C4 | 3.61 | 99.49 | 108.98 | 13 | 3 |
| 3 | B | 372 | PX4 | C4-N1-C3 | 3.61 | 99.49 | 108.98 | 12 | 3 |
| 3 | C | 324 | PX4 | C5-N1-C3 | 3.61 | 99.49 | 108.98 | 7 | 1 |
| 3 | A | 654 | PX4 | O5-C9-O6 | 3.61 | 132.66 | 123.63 | 6 | 2 |
| 3 | B | 353 | PX4 | C5-N1-C3 | 3.61 | 118.45 | 108.98 | 11 | 5 |
| 3 | B | 319 | PX4 | O7-C23-C24 | 3.61 | 103.68 | 111.48 | 4 | 5 |
| 3 | A | 642 | PX4 | O7-C23-C24 | 3.60 | 103.70 | 111.48 | 15 | 1 |
| 3 | C | 340 | PX4 | C7-O7-C23 | 3.60 | 109.18 | 117.80 | 1 | 2 |
| 3 | B | 355 | PX4 | O7-C23-C24 | 3.60 | 103.70 | 111.48 | 12 | 6 |
| 3 | A | 640 | PX4 | C4-N1-C3 | 3.59 | 99.54 | 108.98 | 12 | 1 |
| 3 | A | 635 | PX4 | C5-N1-C3 | 3.59 | 118.41 | 108.98 | 1 | 2 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 308 | PX4 | O5-C9-O6 | 3.59 | 132.60 | 123.63 | 3 | 3 |
| 3 | B | 317 | PX4 | C4-N1-C3 | 3.59 | 99.56 | 108.98 | 3 | 2 |
| 3 | B | 319 | PX4 | O7-C23-O8 | 3.59 | 132.09 | 123.70 | 10 | 3 |
| 3 | A | 624 | PX4 | C7-O7-C23 | 3.58 | 109.22 | 117.80 | 2 | 3 |
| 3 | C | 307 | PX4 | C7-O7-C23 | 3.59 | 109.22 | 117.80 | 4 | 2 |
| 3 | B | 359 | PX4 | C4-N1-C3 | 3.58 | 118.39 | 108.98 | 3 | 3 |
| 3 | A | 617 | PX4 | O5-C9-C10 | 3.58 | 100.92 | 111.83 | 8 | 1 |
| 3 | A | 623 | PX4 | C8-C7-C6 | 3.58 | 120.13 | 111.78 | 7 | 4 |
| 3 | B | 338 | PX4 | O5-C8-C7 | 3.58 | 118.72 | 108.40 | 7 | 5 |
| 3 | C | 303 | PX4 | O5-C8-C7 | 3.58 | 118.71 | 108.40 | 12 | 4 |
| 3 | B | 390 | PX4 | C7-O7-C23 | 3.58 | 109.24 | 117.80 | 8 | 2 |
| 3 | C | 331 | PX4 | C5-N1-C3 | 3.57 | 99.59 | 108.98 | 15 | 1 |
| 3 | A | 608 | PX4 | O5-C8-C7 | 3.57 | 118.69 | 108.40 | 2 | 4 |
| 3 | B | 332 | PX4 | O5-C8-C7 | 3.57 | 118.69 | 108.40 | 13 | 4 |
| 3 | B | 377 | PX4 | O5-C8-C7 | 3.57 | 118.69 | 108.40 | 11 | 4 |
| 3 | C | 347 | PX4 | O7-C23-O8 | 3.57 | 132.05 | 123.70 | 15 | 3 |
| 3 | B | 395 | PX4 | O7-C23-C24 | 3.57 | 103.76 | 111.48 | 11 | 6 |
| 3 | C | 362 | PX4 | O7-C23-C24 | 3.56 | 103.77 | 111.48 | 6 | 5 |
| 3 | B | 335 | PX4 | C7-O7-C23 | 3.56 | 109.27 | 117.80 | 3 | 3 |
| 3 | C | 320 | PX4 | C7-O7-C23 | 3.56 | 109.27 | 117.80 | 10 | 6 |
| 3 | C | 326 | PX4 | O5-C8-C7 | 3.56 | 118.66 | 108.40 | 11 | 4 |
| 3 | A | 612 | PX4 | O7-C23-O8 | 3.55 | 132.00 | 123.70 | 14 | 1 |
| 3 | A | 629 | PX4 | O5-C8-C7 | 3.55 | 118.62 | 108.40 | 9 | 3 |
| 3 | C | 325 | PX4 | O7-C23-O8 | 3.54 | 131.99 | 123.70 | 9 | 6 |
| 3 | B | 336 | PX4 | C4-N1-C3 | 3.54 | 118.28 | 108.98 | 2 | 2 |
| 3 | C | 332 | PX4 | C5-N1-C4 | 3.54 | 118.28 | 108.98 | 8 | 2 |
| 3 | B | 342 | PX4 | C11-C10-C9 | 3.54 | 126.66 | 113.69 | 7 | 2 |
| 3 | B | 387 | PX4 | O7-C23-O8 | 3.54 | 131.98 | 123.70 | 12 | 2 |
| 3 | A | 640 | PX4 | O5-C8-C7 | 3.54 | 118.59 | 108.40 | 9 | 4 |
| 3 | A | 645 | PX4 | C8-O5-C9 | 3.53 | 130.04 | 117.12 | 1 | 3 |
| 3 | A | 652 | PX4 | O7-C23-C24 | 3.53 | 103.84 | 111.48 | 6 | 4 |
| 3 | B | 347 | PX4 | C4-N1-C3 | 3.53 | 99.70 | 108.98 | 4 | 4 |
| 3 | C | 311 | PX4 | O5-C8-C7 | 3.53 | 118.58 | 108.40 | 14 | 4 |
| 3 | C | 355 | PX4 | O5-C9-C10 | 3.53 | 101.07 | 111.83 | 9 | 4 |
| 3 | C | 322 | PX4 | O7-C23-C24 | 3.53 | 103.84 | 111.48 | 4 | 4 |
| 3 | C | 323 | PX4 | O5-C9-C10 | 3.53 | 101.08 | 111.83 | 3 | 3 |
| 3 | C | 306 | PX4 | O5-C8-C7 | 3.53 | 118.56 | 108.40 | 12 | 2 |
| 3 | C | 308 | PX4 | O7-C23-C24 | 3.52 | 103.86 | 111.48 | 9 | 2 |
| 3 | C | 347 | PX4 | C7-O7-C23 | 3.52 | 109.36 | 117.80 | 8 | 3 |
| 3 | B | 366 | PX4 | C8-C7-C6 | 3.52 | 103.58 | 111.78 | 15 | 1 |
| 3 | B | 395 | PX4 | O7-C7-C8 | 3.52 | 120.97 | 108.34 | 3 | 3 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | C | 364 | PX4 | C8-C7-C6 | 3.52 | 103.58 | 111.78 | 10 | 3 |
| 3 | A | 633 | PX4 | C5-N1-C4 | 3.52 | 99.74 | 108.98 | 15 | 1 |
| 3 | A | 621 | PX4 | O7-C23-O8 | 3.51 | 131.92 | 123.70 | 1 | 6 |
| 3 | C | 333 | PX4 | C7-O7-C23 | 3.51 | 109.39 | 117.80 | 13 | 3 |
| 3 | B | 324 | PX4 | O5-C8-C7 | 3.51 | 118.51 | 108.40 | 11 | 3 |
| 3 | C | 349 | PX4 | O5-C9-O6 | 3.51 | 132.40 | 123.63 | 15 | 3 |
| 3 | B | 312 | PX4 | C4-N1-C3 | 3.50 | 99.77 | 108.98 | 3 | 4 |
| 3 | B | 353 | PX4 | O7-C23-C24 | 3.50 | 103.90 | 111.48 | 9 | 1 |
| 3 | B | 383 | PX4 | C8-C7-C6 | 3.50 | 103.62 | 111.78 | 8 | 3 |
| 3 | B | 379 | PX4 | O5-C8-C7 | 3.50 | 118.48 | 108.40 | 12 | 2 |
| 3 | C | 328 | PX4 | C4-N1-C3 | 3.50 | 118.17 | 108.98 | 6 | 4 |
| 3 | A | 615 | PX4 | O7-C23-C24 | 3.50 | 103.92 | 111.48 | 7 | 2 |
| 3 | A | 622 | PX4 | C4-N1-C3 | 3.50 | 99.79 | 108.98 | 13 | 2 |
| 3 | C | 354 | PX4 | C7-O7-C23 | 3.50 | 109.43 | 117.80 | 15 | 4 |
| 3 | C | 333 | PX4 | C8-C7-C6 | 3.49 | 103.64 | 111.78 | 2 | 4 |
| 3 | C | 355 | PX4 | O5-C9-O6 | 3.49 | 132.36 | 123.63 | 9 | 2 |
| 3 | B | 310 | PX4 | C7-O7-C23 | 3.49 | 109.44 | 117.80 | 12 | 3 |
| 3 | C | 321 | PX4 | C8-C7-C6 | 3.49 | 103.65 | 111.78 | 10 | 4 |
| 3 | C | 334 | PX4 | C5-N1-C3 | 3.49 | 99.81 | 108.98 | 13 | 3 |
| 3 | A | 607 | PX4 | C7-O7-C23 | 3.49 | 109.45 | 117.80 | 6 | 6 |
| 3 | B | 313 | PX4 | O5-C8-C7 | 3.49 | 118.45 | 108.40 | 12 | 3 |
| 3 | B | 332 | PX4 | O7-C23-C24 | 3.48 | 103.94 | 111.48 | 7 | 5 |
| 3 | B | 380 | PX4 | O5-C8-C7 | 3.48 | 118.44 | 108.40 | 10 | 8 |
| 3 | C | 342 | PX4 | O7-C23-C24 | 3.48 | 103.94 | 111.48 | 3 | 3 |
| 3 | B | 381 | PX4 | C1-C2-N1 | 3.48 | 126.99 | 115.82 | 6 | 3 |
| 3 | B | 301 | PX4 | C4-N1-C3 | 3.47 | 99.85 | 108.98 | 14 | 2 |
| 3 | B | 367 | PX4 | O7-C23-C24 | 3.47 | 103.97 | 111.48 | 11 | 3 |
| 3 | C | 305 | PX4 | O5-C8-C7 | 3.47 | 118.41 | 108.40 | 15 | 4 |
| 3 | B | 366 | PX4 | C5-N1-C3 | 3.47 | 99.86 | 108.98 | 9 | 3 |
| 3 | C | 340 | PX4 | C8-C7-C6 | 3.47 | 103.69 | 111.78 | 12 | 5 |
| 3 | B | 301 | PX4 | O5-C9-O6 | 3.47 | 132.31 | 123.63 | 15 | 1 |
| 3 | A | 615 | PX4 | O5-C8-C7 | 3.47 | 118.39 | 108.40 | 1 | 2 |
| 3 | B | 373 | PX4 | O7-C23-C24 | 3.47 | 103.98 | 111.48 | 3 | 5 |
| 3 | A | 651 | PX4 | O5-C8-C7 | 3.47 | 118.39 | 108.40 | 5 | 10 |
| 3 | C | 318 | PX4 | O5-C8-C7 | 3.47 | 118.39 | 108.40 | 14 | 4 |
| 3 | A | 629 | PX4 | C7-O7-C23 | 3.47 | 109.50 | 117.80 | 6 | 4 |
| 3 | A | 624 | PX4 | C4-N1-C3 | 3.46 | 99.88 | 108.98 | 10 | 4 |
| 3 | C | 337 | PX4 | O7-C23-C24 | 3.46 | 103.99 | 111.48 | 12 | 5 |
| 3 | A | 618 | PX4 | O7-C23-O8 | 3.46 | 131.79 | 123.70 | 12 | 3 |
| 3 | B | 350 | PX4 | O5-C9-O6 | 3.46 | 132.28 | 123.63 | 4 | 5 |
| 3 | B | 357 | PX4 | C4-N1-C3 | 3.46 | 99.89 | 108.98 | 13 | 4 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | A | 644 | PX4 | O5-C8-C7 | 3.46 | 118.36 | 108.40 | 5 | 5 |
| 3 | B | 325 | PX4 | O5-C8-C7 | 3.45 | 118.36 | 108.40 | 4 | 4 |
| 3 | B | 352 | PX4 | C8-C7-C6 | 3.46 | 103.73 | 111.78 | 5 | 3 |
| 3 | B | 375 | PX4 | O7-C23-C24 | 3.46 | 104.01 | 111.48 | 7 | 1 |
| 3 | C | 302 | PX4 | O5-C9-O6 | 3.46 | 132.27 | 123.63 | 5 | 2 |
| 3 | C | 326 | PX4 | O7-C23-O8 | 3.45 | 131.78 | 123.70 | 9 | 2 |
| 3 | B | 321 | PX4 | O5-C9-O6 | 3.45 | 132.27 | 123.63 | 8 | 3 |
| 3 | A | 643 | PX4 | C8-C7-C6 | 3.45 | 103.74 | 111.78 | 5 | 3 |
| 3 | A | 636 | PX4 | C1-C2-N1 | 3.45 | 126.89 | 115.82 | 1 | 1 |
| 3 | B | 329 | PX4 | C4-N1-C3 | 3.45 | 99.92 | 108.98 | 1 | 2 |
| 3 | B | 363 | PX4 | C11-C10-C9 | 3.45 | 101.06 | 113.69 | 7 | 2 |
| 3 | B | 378 | PX4 | O5-C9-C10 | 3.45 | 101.32 | 111.83 | 15 | 3 |
| 3 | B | 378 | PX4 | C5-N1-C3 | 3.45 | 99.92 | 108.98 | 13 | 3 |
| 3 | A | 625 | PX4 | O5-C8-C7 | 3.44 | 118.32 | 108.40 | 6 | 5 |
| 3 | B | 394 | PX4 | O5-C9-O6 | 3.44 | 132.24 | 123.63 | 1 | 3 |
| 3 | B | 309 | PX4 | O7-C23-C24 | 3.44 | 104.04 | 111.48 | 10 | 5 |
| 3 | C | 317 | PX4 | O7-C7-C6 | 3.44 | 120.69 | 108.34 | 1 | 6 |
| 3 | B | 355 | PX4 | C5-N1-C3 | 3.44 | 99.94 | 108.98 | 8 | 2 |
| 3 | A | 601 | PX4 | O5-C9-O6 | 3.44 | 132.23 | 123.63 | 6 | 2 |
| 3 | C | 306 | PX4 | C8-C7-C6 | 3.44 | 119.80 | 111.78 | 11 | 4 |
| 3 | C | 330 | PX4 | C7-O7-C23 | 3.44 | 126.03 | 117.80 | 14 | 6 |
| 3 | B | 370 | PX4 | C1-C2-N1 | 3.43 | 126.85 | 115.82 | 1 | 3 |
| 3 | A | 608 | PX4 | O7-C23-C24 | 3.43 | 104.05 | 111.48 | 13 | 2 |
| 3 | A | 638 | PX4 | C7-O7-C23 | 3.43 | 109.58 | 117.80 | 7 | 2 |
| 3 | B | 377 | PX4 | C8-C7-C6 | 3.43 | 119.79 | 111.78 | 2 | 4 |
| 3 | A | 601 | PX4 | O7-C23-C24 | 3.43 | 104.06 | 111.48 | 4 | 3 |
| 3 | A | 602 | PX4 | O5-C9-O6 | 3.43 | 132.21 | 123.63 | 9 | 2 |
| 3 | A | 649 | PX4 | C5-N1-C3 | 3.43 | 99.97 | 108.98 | 13 | 6 |
| 3 | B | 344 | PX4 | O7-C23-C24 | 3.43 | 104.06 | 111.48 | 4 | 5 |
| 3 | B | 396 | PX4 | O7-C23-C24 | 3.43 | 104.06 | 111.48 | 13 | 3 |
| 3 | C | 333 | PX4 | O5-C9-O6 | 3.43 | 132.21 | 123.63 | 4 | 1 |
| 3 | B | 334 | PX4 | O5-C8-C7 | 3.43 | 118.28 | 108.40 | 6 | 3 |
| 3 | C | 331 | PX4 | O5-C8-C7 | 3.43 | 118.28 | 108.40 | 15 | 8 |
| 3 | A | 644 | PX4 | C8-C7-C6 | 3.42 | 103.80 | 111.78 | 5 | 4 |
| 3 | A | 648 | PX4 | C7-O7-C23 | 3.42 | 109.60 | 117.80 | 1 | 5 |
| 3 | C | 340 | PX4 | O5-C8-C7 | 3.43 | 118.27 | 108.40 | 1 | 3 |
| 3 | A | 644 | PX4 | C7-O7-C23 | 3.42 | 109.60 | 117.80 | 15 | 2 |
| 3 | C | 308 | PX4 | C7-O7-C23 | 3.42 | 109.60 | 117.80 | 12 | 6 |
| 3 | A | 620 | PX4 | O5-C8-C7 | 3.42 | 118.26 | 108.40 | 12 | 5 |
| 3 | B | 346 | PX4 | C5-N1-C4 | 3.41 | 100.01 | 108.98 | 5 | 3 |
| 3 | C | 358 | PX4 | O5-C9-C10 | 3.41 | 101.43 | 111.83 | 4 | 2 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | A | 621 | PX4 | C5-N1-C3 | 3.41 | 100.01 | 108.98 | 6 | 2 |
| 3 | B | 312 | PX4 | C5-N1-C4 | 3.41 | 117.94 | 108.98 | 4 | 3 |
| 3 | A | 634 | PX4 | C4-N1-C3 | 3.41 | 117.93 | 108.98 | 8 | 3 |
| 3 | C | 358 | PX4 | O7-C23-O8 | 3.41 | 131.68 | 123.70 | 2 | 3 |
| 3 | A | 615 | PX4 | O7-C23-O8 | 3.41 | 131.67 | 123.70 | 10 | 3 |
| 3 | B | 344 | PX4 | O7-C23-O8 | 3.41 | 131.67 | 123.70 | 11 | 3 |
| 3 | B | 399 | PX4 | O5-C8-C7 | 3.41 | 118.22 | 108.40 | 14 | 2 |
| 3 | B | 336 | PX4 | O7-C23-C24 | 3.40 | 104.12 | 111.48 | 1 | 5 |
| 3 | A | 611 | PX4 | C8-C7-C6 | 3.40 | 103.85 | 111.78 | 14 | 2 |
| 3 | B | 323 | PX4 | O5-C8-C7 | 3.40 | 118.20 | 108.40 | 6 | 3 |
| 3 | A | 616 | PX4 | O5-C9-O6 | 3.40 | 132.13 | 123.63 | 1 | 4 |
| 3 | B | 310 | PX4 | C8-C7-C6 | 3.40 | 103.86 | 111.78 | 8 | 4 |
| 3 | C | 318 | PX4 | O7-C23-C24 | 3.40 | 104.13 | 111.48 | 12 | 3 |
| 3 | B | 342 | PX4 | C4-N1-C3 | 3.40 | 100.06 | 108.98 | 5 | 3 |
| 3 | B | 393 | PX4 | C25-C24-C23 | 3.40 | 101.25 | 113.69 | 15 | 1 |
| 3 | C | 324 | PX4 | O7-C23-C24 | 3.40 | 104.13 | 111.48 | 4 | 7 |
| 3 | C | 306 | PX4 | C4-N1-C3 | 3.39 | 100.06 | 108.98 | 12 | 2 |
| 3 | C | 318 | PX4 | C8-C7-C6 | 3.39 | 103.87 | 111.78 | 12 | 2 |
| 3 | C | 330 | PX4 | O7-C23-C24 | 3.39 | 104.14 | 111.48 | 11 | 6 |
| 3 | B | 354 | PX4 | O7-C23-C24 | 3.39 | 104.14 | 111.48 | 14 | 3 |
| 3 | C | 315 | PX4 | C7-O7-C23 | 3.39 | 109.68 | 117.80 | 11 | 6 |
| 3 | A | 607 | PX4 | O5-C8-C7 | 3.39 | 118.17 | 108.40 | 3 | 5 |
| 3 | A | 624 | PX4 | C5-N1-C3 | 3.39 | 100.07 | 108.98 | 11 | 2 |
| 3 | A | 654 | PX4 | C8-C7-C6 | 3.39 | 103.88 | 111.78 | 15 | 4 |
| 3 | B | 374 | PX4 | C7-O7-C23 | 3.39 | 109.68 | 117.80 | 2 | 5 |
| 3 | C | 333 | PX4 | O7-C23-C24 | 3.39 | 104.15 | 111.48 | 10 | 4 |
| 3 | A | 652 | PX4 | O5-C9-O6 | 3.39 | 132.10 | 123.63 | 10 | 3 |
| 3 | B | 397 | PX4 | O5-C8-C7 | 3.39 | 118.16 | 108.40 | 8 | 4 |
| 3 | C | 361 | PX4 | O5-C9-O6 | 3.39 | 132.10 | 123.63 | 9 | 1 |
| 3 | C | 316 | PX4 | O5-C8-C7 | 3.39 | 118.16 | 108.40 | 12 | 1 |
| 3 | C | 332 | PX4 | O7-C23-C24 | 3.39 | 104.16 | 111.48 | 2 | 1 |
| 3 | C | 306 | PX4 | C5-N1-C3 | 3.38 | 117.86 | 108.98 | 1 | 4 |
| 3 | C | 327 | PX4 | O5-C8-C7 | 3.38 | 118.15 | 108.40 | 8 | 4 |
| 3 | A | 640 | PX4 | O7-C7-C8 | 3.38 | 120.47 | 108.34 | 13 | 2 |
| 3 | B | 321 | PX4 | C4-N1-C3 | 3.38 | 117.85 | 108.98 | 12 | 3 |
| 3 | B | 362 | PX4 | C4-N1-C3 | 3.38 | 117.85 | 108.98 | 3 | 2 |
| 3 | B | 396 | PX4 | O5-C9-O6 | 3.38 | 132.08 | 123.63 | 8 | 4 |
| 3 | C | 342 | PX4 | C25-C24-C23 | 3.38 | 101.31 | 113.69 | 2 | 1 |
| 3 | B | 339 | PX4 | C8-C7-C6 | 3.38 | 103.91 | 111.78 | 7 | 5 |
| 3 | C | 301 | PX4 | C8-C7-C6 | 3.38 | 103.91 | 111.78 | 8 | 2 |
| 3 | B | 337 | PX4 | C7-O7-C23 | 3.38 | 109.71 | 117.80 | 5 | 6 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | C | 354 | PX4 | O5-C9-C10 | 3.38 | 101.54 | 111.83 | 13 | 2 |
| 3 | B | 376 | PX4 | O7-C23-C24 | 3.38 | 104.18 | 111.48 | 8 | 6 |
| 3 | A | 637 | PX4 | C7-O7-C23 | 3.37 | 109.72 | 117.80 | 9 | 5 |
| 3 | B | 393 | PX4 | C8-C7-C6 | 3.38 | 119.66 | 111.78 | 15 | 2 |
| 3 | C | 301 | PX4 | O7-C23-C24 | 3.37 | 104.18 | 111.48 | 13 | 5 |
| 3 | B | 347 | PX4 | O5-C8-C7 | 3.37 | 118.11 | 108.40 | 3 | 3 |
| 3 | A | 628 | PX4 | C7-O7-C23 | 3.37 | 109.73 | 117.80 | 4 | 3 |
| 3 | B | 395 | PX4 | C8-O5-C9 | 3.37 | 104.80 | 117.12 | 14 | 1 |
| 3 | B | 317 | PX4 | C7-O7-C23 | 3.37 | 109.74 | 117.80 | 15 | 6 |
| 3 | C | 329 | PX4 | O7-C23-O8 | 3.37 | 131.58 | 123.70 | 14 | 3 |
| 3 | B | 301 | PX4 | C5-N1-C3 | 3.36 | 100.14 | 108.98 | 13 | 2 |
| 3 | B | 310 | PX4 | C5-N1-C3 | 3.36 | 117.81 | 108.98 | 5 | 2 |
| 3 | B | 373 | PX4 | O5-C9-C10 | 3.37 | 101.57 | 111.83 | 4 | 4 |
| 3 | B | 361 | PX4 | C7-O7-C23 | 3.36 | 109.74 | 117.80 | 6 | 6 |
| 3 | C | 354 | PX4 | C5-N1-C3 | 3.36 | 117.81 | 108.98 | 3 | 3 |
| 3 | C | 356 | PX4 | O5-C9-C10 | 3.36 | 101.58 | 111.83 | 14 | 2 |
| 3 | B | 335 | PX4 | O7-C23-O8 | 3.36 | 131.56 | 123.70 | 5 | 3 |
| 3 | C | 306 | PX4 | C7-O7-C23 | 3.36 | 109.76 | 117.80 | 6 | 4 |
| 3 | C | 358 | PX4 | O5-C9-O6 | 3.36 | 132.03 | 123.63 | 10 | 1 |
| 3 | B | 347 | PX4 | O7-C23-C24 | 3.36 | 104.22 | 111.48 | 6 | 4 |
| 3 | A | 648 | PX4 | O5-C9-C10 | 3.36 | 101.60 | 111.83 | 4 | 1 |
| 3 | B | 366 | PX4 | C26-C25-C24 | 3.36 | 100.79 | 113.13 | 8 | 2 |
| 3 | B | 372 | PX4 | C7-O7-C23 | 3.36 | 125.83 | 117.80 | 7 | 4 |
| 3 | B | 386 | PX4 | C5-N1-C3 | 3.36 | 100.16 | 108.98 | 15 | 2 |
| 3 | C | 311 | PX4 | O5-C9-C10 | 3.36 | 101.60 | 111.83 | 6 | 4 |
| 3 | B | 373 | PX4 | C7-O7-C23 | 3.35 | 109.77 | 117.80 | 11 | 6 |
| 3 | A | 608 | PX4 | C8-C7-C6 | 3.35 | 103.97 | 111.78 | 2 | 3 |
| 3 | B | 301 | PX4 | C8-C7-C6 | 3.35 | 103.97 | 111.78 | 11 | 2 |
| 3 | A | 618 | PX4 | C7-O7-C23 | 3.35 | 109.78 | 117.80 | 10 | 5 |
| 3 | C | 345 | PX4 | O5-C9-O6 | 3.35 | 132.01 | 123.63 | 9 | 3 |
| 3 | A | 607 | PX4 | C8-C7-C6 | 3.35 | 119.59 | 111.78 | 5 | 2 |
| 3 | B | 355 | PX4 | C4-N1-C3 | 3.35 | 100.18 | 108.98 | 6 | 4 |
| 3 | A | 636 | PX4 | O7-C23-C24 | 3.34 | 104.25 | 111.48 | 15 | 5 |
| 3 | A | 647 | PX4 | C7-O7-C23 | 3.34 | 109.79 | 117.80 | 4 | 7 |
| 3 | B | 356 | PX4 | O5-C8-C7 | 3.34 | 118.03 | 108.40 | 15 | 3 |
| 3 | C | 323 | PX4 | O5-C8-C7 | 3.34 | 118.03 | 108.40 | 13 | 6 |
| 3 | A | 601 | PX4 | O7-C7-C6 | 3.34 | 120.33 | 108.34 | 7 | 3 |
| 3 | C | 338 | PX4 | O7-C23-O8 | 3.34 | 131.52 | 123.70 | 15 | 1 |
| 3 | A | 628 | PX4 | O7-C23-O8 | 3.34 | 131.51 | 123.70 | 10 | 3 |
| 3 | B | 396 | PX4 | C7-O7-C23 | 3.34 | 109.81 | 117.80 | 8 | 4 |
| 3 | C | 307 | PX4 | C1-C2-N1 | 3.33 | 126.52 | 115.82 | 10 | 2 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | C | 309 | PX4 | O5-C8-C7 | 3.33 | 118.00 | 108.40 | 8 | 3 |
| 3 | C | 323 | PX4 | C8-C7-C6 | 3.33 | 119.56 | 111.78 | 8 | 2 |
| 3 | C | 334 | PX4 | O7-C23-O8 | 3.33 | 131.50 | 123.70 | 2 | 1 |
| 3 | C | 348 | PX4 | C7-O7-C23 | 3.33 | 109.82 | 117.80 | 8 | 6 |
| 3 | B | 358 | PX4 | O7-C23-C24 | 3.33 | 104.28 | 111.48 | 9 | 4 |
| 3 | B | 393 | PX4 | O7-C23-O8 | 3.33 | 131.49 | 123.70 | 5 | 2 |
| 3 | C | 349 | PX4 | C4-N1-C2 | 3.33 | 123.14 | 109.91 | 15 | 2 |
| 3 | A | 610 | PX4 | O5-C9-O6 | 3.33 | 131.95 | 123.63 | 7 | 1 |
| 3 | B | 331 | PX4 | C4-N1-C3 | 3.33 | 100.24 | 108.98 | 8 | 1 |
| 3 | A | 613 | PX4 | O7-C23-O8 | 3.32 | 131.47 | 123.70 | 1 | 2 |
| 3 | B | 311 | PX4 | O5-C8-C7 | 3.32 | 117.98 | 108.40 | 6 | 5 |
| 3 | B | 339 | PX4 | O7-C23-O8 | 3.32 | 131.48 | 123.70 | 9 | 3 |
| 3 | B | 347 | PX4 | C5-N1-C3 | 3.32 | 100.25 | 108.98 | 15 | 3 |
| 3 | C | 305 | PX4 | C7-O7-C23 | 3.32 | 109.85 | 117.80 | 11 | 5 |
| 3 | C | 353 | PX4 | C8-O5-C9 | 3.32 | 104.98 | 117.12 | 2 | 4 |
| 3 | C | 339 | PX4 | O7-C23-O8 | 3.32 | 131.46 | 123.70 | 10 | 4 |
| 3 | B | 357 | PX4 | O7-C23-C24 | 3.32 | 104.30 | 111.48 | 11 | 4 |
| 3 | C | 364 | PX4 | C5-N1-C3 | 3.32 | 100.26 | 108.98 | 9 | 3 |
| 3 | B | 341 | PX4 | C4-N1-C3 | 3.32 | 100.27 | 108.98 | 13 | 4 |
| 3 | A | 640 | PX4 | O7-C23-C24 | 3.31 | 104.32 | 111.48 | 12 | 6 |
| 3 | C | 315 | PX4 | O5-C9-O6 | 3.31 | 131.91 | 123.63 | 3 | 1 |
| 3 | A | 635 | PX4 | O5-C9-O6 | 3.31 | 131.91 | 123.63 | 10 | 3 |
| 3 | B | 333 | PX4 | C7-O7-C23 | 3.31 | 109.88 | 117.80 | 10 | 3 |
| 3 | C | 316 | PX4 | O7-C23-C24 | 3.31 | 104.32 | 111.48 | 10 | 4 |
| 3 | C | 342 | PX4 | O5-C8-C7 | 3.31 | 117.94 | 108.40 | 5 | 2 |
| 3 | B | 374 | PX4 | C8-C7-C6 | 3.31 | 104.07 | 111.78 | 1 | 6 |
| 3 | B | 397 | PX4 | C5-N1-C4 | 3.31 | 100.29 | 108.98 | 10 | 2 |
| 3 | C | 363 | PX4 | O5-C8-C7 | 3.31 | 117.94 | 108.40 | 7 | 6 |
| 3 | B | 400 | PX4 | C5-N1-C4 | 3.31 | 117.66 | 108.98 | 7 | 3 |
| 3 | C | 311 | PX4 | O5-C9-O6 | 3.31 | 131.90 | 123.63 | 1 | 2 |
| 3 | A | 601 | PX4 | C5-N1-C4 | 3.30 | 100.30 | 108.98 | 12 | 2 |
| 3 | A | 652 | PX4 | C8-C7-C6 | 3.30 | 119.49 | 111.78 | 6 | 3 |
| 3 | B | 391 | PX4 | O5-C9-C10 | 3.30 | 101.76 | 111.83 | 7 | 1 |
| 3 | A | 648 | PX4 | O5-C9-O6 | 3.30 | 131.88 | 123.63 | 2 | 4 |
| 3 | B | 318 | PX4 | C5-N1-C3 | 3.30 | 117.65 | 108.98 | 14 | 2 |
| 3 | B | 378 | PX4 | C5-N1-C4 | 3.30 | 100.31 | 108.98 | 5 | 3 |
| 3 | C | 357 | PX4 | O7-C23-O8 | 3.30 | 131.42 | 123.70 | 1 | 3 |
| 3 | B | 345 | PX4 | C7-O7-C23 | 3.29 | 109.91 | 117.80 | 7 | 4 |
| 3 | A | 647 | PX4 | O5-C8-C7 | 3.29 | 117.89 | 108.40 | 5 | 5 |
| 3 | B | 311 | PX4 | C8-C7-C6 | 3.29 | 104.11 | 111.78 | 4 | 2 |
| 3 | B | 316 | PX4 | C5-N1-C3 | 3.29 | 100.33 | 108.98 | 8 | 2 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 398 | PX4 | C8-O5-C9 | 3.29 | 105.08 | 117.12 | 3 | 3 |
| 3 | C | 314 | PX4 | O5-C8-C7 | 3.29 | 117.89 | 108.40 | 10 | 6 |
| 3 | C | 342 | PX4 | O7-C7-C8 | 3.29 | 120.15 | 108.34 | 4 | 3 |
| 3 | B | 309 | PX4 | O7-C23-O8 | 3.29 | 131.40 | 123.70 | 3 | 4 |
| 3 | A | 636 | PX4 | O5-C9-C10 | 3.29 | 101.81 | 111.83 | 1 | 3 |
| 3 | A | 648 | PX4 | C8-C7-C6 | 3.29 | 104.12 | 111.78 | 14 | 1 |
| 3 | A | 653 | PX4 | C7-O7-C23 | 3.29 | 109.93 | 117.80 | 13 | 3 |
| 3 | B | 307 | PX4 | O7-C23-C24 | 3.29 | 104.37 | 111.48 | 10 | 3 |
| 3 | B | 359 | PX4 | C8-C7-C6 | 3.29 | 119.45 | 111.78 | 2 | 3 |
| 3 | B | 385 | PX4 | C7-O7-C23 | 3.29 | 109.93 | 117.80 | 9 | 1 |
| 3 | A | 618 | PX4 | O5-C9-C10 | 3.28 | 101.83 | 111.83 | 10 | 3 |
| 3 | B | 314 | PX4 | O7-C23-C24 | 3.28 | 104.38 | 111.48 | 10 | 4 |
| 3 | B | 325 | PX4 | O7-C23-O8 | 3.28 | 131.38 | 123.70 | 9 | 4 |
| 3 | B | 319 | PX4 | O5-C9-C10 | 3.27 | 101.86 | 111.83 | 15 | 1 |
| 3 | B | 372 | PX4 | C5-N1-C4 | 3.27 | 117.58 | 108.98 | 12 | 3 |
| 3 | B | 329 | PX4 | C7-O7-C23 | 3.27 | 109.96 | 117.80 | 11 | 4 |
| 3 | C | 317 | PX4 | C5-N1-C3 | 3.27 | 100.38 | 108.98 | 15 | 4 |
| 3 | B | 343 | PX4 | C16-C15-C14 | 3.27 | 130.90 | 114.37 | 12 | 1 |
| 3 | B | 335 | PX4 | O5-C8-C7 | 3.27 | 117.81 | 108.40 | 6 | 6 |
| 3 | A | 618 | PX4 | O7-C23-C24 | 3.27 | 104.42 | 111.48 | 8 | 5 |
| 3 | A | 642 | PX4 | C7-O7-C23 | 3.26 | 109.99 | 117.80 | 6 | 6 |
| 3 | B | 343 | PX4 | O7-C7-C8 | 3.26 | 120.04 | 108.34 | 5 | 2 |
| 3 | B | 365 | PX4 | O5-C9-C10 | 3.26 | 101.89 | 111.83 | 15 | 2 |
| 3 | A | 640 | PX4 | C8-C7-C6 | 3.26 | 104.19 | 111.78 | 10 | 4 |
| 3 | C | 307 | PX4 | C11-C10-C9 | 3.26 | 101.76 | 113.69 | 9 | 1 |
| 3 | C | 302 | PX4 | O5-C9-C10 | 3.26 | 101.91 | 111.83 | 5 | 3 |
| 3 | A | 630 | PX4 | O7-C23-C24 | 3.25 | 104.44 | 111.48 | 13 | 3 |
| 3 | B | 351 | PX4 | C7-O7-C23 | 3.25 | 110.01 | 117.80 | 7 | 6 |
| 3 | C | 349 | PX4 | C4-N1-C3 | 3.25 | 100.43 | 108.98 | 3 | 2 |
| 3 | B | 361 | PX4 | C1-C2-N1 | 3.25 | 126.26 | 115.82 | 14 | 2 |
| 3 | A | 637 | PX4 | O7-C23-C24 | 3.25 | 104.45 | 111.48 | 7 | 2 |
| 3 | B | 345 | PX4 | O5-C8-C7 | 3.25 | 117.77 | 108.40 | 14 | 6 |
| 3 | A | 641 | PX4 | O5-C9-C10 | 3.25 | 101.93 | 111.83 | 15 | 2 |
| 3 | B | 320 | PX4 | O5-C9-O6 | 3.25 | 131.76 | 123.63 | 9 | 2 |
| 3 | B | 306 | PX4 | O7-C23-O8 | 3.25 | 131.30 | 123.70 | 7 | 6 |
| 3 | A | 603 | PX4 | O7-C7-C8 | 3.25 | 119.99 | 108.34 | 15 | 1 |
| 3 | A | 634 | PX4 | O5-C8-C7 | 3.24 | 117.75 | 108.40 | 11 | 7 |
| 3 | B | 309 | PX4 | O4-P1-O2 | 3.24 | 121.79 | 108.94 | 1 | 1 |
| 3 | C | 319 | PX4 | C5-N1-C3 | 3.24 | 100.45 | 108.98 | 4 | 1 |
| 3 | B | 312 | PX4 | O5-C9-C10 | 3.24 | 101.95 | 111.83 | 15 | 4 |
| 3 | B | 313 | PX4 | O5-C9-O6 | 3.24 | 131.73 | 123.63 | 10 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 377 | PX4 | O5-C9-C10 | 3.24 | 101.95 | 111.83 | 7 | 4 |
| 3 | C | 316 | PX4 | C7-O7-C23 | 3.24 | 110.04 | 117.80 | 5 | 1 |
| 3 | B | 329 | PX4 | O7-C23-O8 | 3.24 | 131.28 | 123.70 | 9 | 1 |
| 3 | C | 339 | PX4 | C8-C7-C6 | 3.24 | 104.23 | 111.78 | 1 | 2 |
| 3 | A | 616 | PX4 | O7-C23-O8 | 3.24 | 131.27 | 123.70 | 10 | 4 |
| 3 | B | 394 | PX4 | C8-C7-C6 | 3.24 | 104.24 | 111.78 | 12 | 5 |
| 3 | C | 362 | PX4 | C5-N1-C4 | 3.24 | 100.47 | 108.98 | 15 | 3 |
| 3 | A | 643 | PX4 | O5-C8-C7 | 3.23 | 117.72 | 108.40 | 3 | 6 |
| 3 | C | 344 | PX4 | C8-C7-C6 | 3.24 | 119.33 | 111.78 | 12 | 2 |
| 3 | C | 349 | PX4 | C5-N1-C3 | 3.23 | 100.48 | 108.98 | 1 | 1 |
| 3 | B | 383 | PX4 | O5-C9-O6 | 3.23 | 131.71 | 123.63 | 10 | 3 |
| 3 | B | 393 | PX4 | O7-C7-C8 | 3.23 | 119.94 | 108.34 | 11 | 3 |
| 3 | B | 329 | PX4 | C8-O5-C9 | 3.23 | 105.31 | 117.12 | 1 | 2 |
| 3 | B | 384 | PX4 | O7-C23-C24 | 3.23 | 104.49 | 111.48 | 10 | 6 |
| 3 | B | 358 | PX4 | O7-C23-O8 | 3.23 | 131.26 | 123.70 | 3 | 3 |
| 3 | B | 391 | PX4 | O7-C23-C24 | 3.23 | 104.50 | 111.48 | 12 | 5 |
| 3 | C | 346 | PX4 | O7-C7-C6 | 3.23 | 119.92 | 108.34 | 10 | 2 |
| 3 | A | 650 | PX4 | C7-O7-C23 | 3.23 | 110.08 | 117.80 | 4 | 2 |
| 3 | B | 366 | PX4 | C5-N1-C4 | 3.23 | 100.50 | 108.98 | 5 | 2 |
| 3 | B | 384 | PX4 | C8-C7-C6 | 3.23 | 104.26 | 111.78 | 15 | 2 |
| 3 | C | 351 | PX4 | O5-C9-O6 | 3.23 | 131.69 | 123.63 | 2 | 2 |
| 3 | C | 352 | PX4 | O5-C9-C10 | 3.22 | 102.00 | 111.83 | 13 | 2 |
| 3 | B | 384 | PX4 | O7-C23-O8 | 3.22 | 131.24 | 123.70 | 10 | 3 |
| 3 | C | 341 | PX4 | C5-N1-C3 | 3.22 | 100.51 | 108.98 | 3 | 2 |
| 3 | B | 321 | PX4 | O5-C8-C7 | 3.22 | 117.68 | 108.40 | 8 | 3 |
| 3 | B | 312 | PX4 | C8-C7-C6 | 3.22 | 119.28 | 111.78 | 9 | 3 |
| 3 | B | 329 | PX4 | C5-N1-C3 | 3.22 | 117.42 | 108.98 | 12 | 1 |
| 3 | B | 317 | PX4 | C8-C7-C6 | 3.21 | 104.29 | 111.78 | 15 | 3 |
| 3 | B | 364 | PX4 | O5-C8-C7 | 3.21 | 117.66 | 108.40 | 4 | 1 |
| 3 | C | 328 | PX4 | C7-O7-C23 | 3.21 | 110.11 | 117.80 | 3 | 3 |
| 3 | B | 371 | PX4 | O5-C8-C7 | 3.21 | 117.66 | 108.40 | 1 | 4 |
| 3 | C | 335 | PX4 | O5-C8-C7 | 3.21 | 117.66 | 108.40 | 9 | 8 |
| 3 | A | 640 | PX4 | C12-C11-C10 | 3.21 | 101.34 | 113.13 | 5 | 1 |
| 3 | A | 622 | PX4 | O5-C8-C7 | 3.20 | 117.64 | 108.40 | 1 | 6 |
| 3 | A | 627 | PX4 | O7-C23-C24 | 3.20 | 104.55 | 111.48 | 8 | 7 |
| 3 | B | 357 | PX4 | O5-C8-C7 | 3.21 | 117.64 | 108.40 | 4 | 5 |
| 3 | C | 322 | PX4 | C7-O7-C23 | 3.20 | 110.13 | 117.80 | 9 | 5 |
| 3 | C | 324 | PX4 | C8-C7-C6 | 3.20 | 119.26 | 111.78 | 8 | 4 |
| 3 | C | 340 | PX4 | O7-C7-C8 | 3.20 | 119.84 | 108.34 | 1 | 3 |
| 3 | C | 362 | PX4 | C8-C7-C6 | 3.21 | 104.31 | 111.78 | 11 | 2 |
| 3 | B | 301 | PX4 | O7-C23-O8 | 3.20 | 131.19 | 123.70 | 4 | 2 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 328 | PX4 | C5-N1-C4 | 3.20 | 117.39 | 108.98 | 4 | 1 |
| 3 | A | 616 | PX4 | O7-C7-C8 | 3.20 | 119.83 | 108.34 | 14 | 4 |
| 3 | C | 355 | PX4 | O5-C8-C7 | 3.20 | 117.62 | 108.40 | 4 | 7 |
| 3 | B | 334 | PX4 | O7-C23-C24 | 3.20 | 104.56 | 111.48 | 15 | 3 |
| 3 | B | 343 | PX4 | C1-C2-N1 | 3.20 | 126.09 | 115.82 | 15 | 2 |
| 3 | C | 341 | PX4 | C7-O7-C23 | 3.20 | 110.14 | 117.80 | 7 | 3 |
| 3 | C | 350 | PX4 | O7-C23-O8 | 3.20 | 131.18 | 123.70 | 11 | 4 |
| 3 | C | 358 | PX4 | C25-C24-C23 | 3.20 | 101.97 | 113.69 | 1 | 1 |
| 3 | B | 384 | PX4 | C4-N1-C3 | 3.20 | 100.58 | 108.98 | 2 | 3 |
| 3 | C | 317 | PX4 | C11-C10-C9 | 3.20 | 125.40 | 113.69 | 4 | 3 |
| 3 | C | 360 | PX4 | O5-C8-C7 | 3.20 | 117.61 | 108.40 | 15 | 2 |
| 3 | B | 388 | PX4 | C5-N1-C4 | 3.19 | 100.59 | 108.98 | 2 | 1 |
| 3 | C | 323 | PX4 | C7-O7-C23 | 3.19 | 110.16 | 117.80 | 13 | 4 |
| 3 | A | 619 | PX4 | C7-O7-C23 | 3.19 | 110.16 | 117.80 | 5 | 3 |
| 3 | B | 321 | PX4 | C7-O7-C23 | 3.19 | 125.43 | 117.80 | 10 | 5 |
| 3 | A | 621 | PX4 | O5-C8-C7 | 3.19 | 117.58 | 108.40 | 4 | 2 |
| 3 | B | 391 | PX4 | C26-C25-C24 | 3.19 | 124.84 | 113.13 | 7 | 1 |
| 3 | C | 306 | PX4 | O7-C23-O8 | 3.18 | 131.15 | 123.70 | 4 | 4 |
| 3 | A | 614 | PX4 | C5-N1-C4 | 3.18 | 117.32 | 108.98 | 2 | 3 |
| 3 | B | 382 | PX4 | O7-C7-C6 | 3.18 | 96.94 | 108.34 | 1 | 2 |
| 3 | B | 383 | PX4 | O5-C9-C10 | 3.18 | 102.15 | 111.83 | 14 | 5 |
| 3 | C | 340 | PX4 | O5-C9-C10 | 3.18 | 102.15 | 111.83 | 12 | 1 |
| 3 | A | 624 | PX4 | O7-C23-O8 | 3.18 | 131.13 | 123.70 | 2 | 2 |
| 3 | B | 302 | PX4 | C7-O7-C23 | 3.17 | 110.20 | 117.80 | 2 | 3 |
| 3 | C | 343 | PX4 | C8-C7-C6 | 3.17 | 104.39 | 111.78 | 4 | 2 |
| 3 | C | 349 | PX4 | C5-N1-C4 | 3.17 | 117.31 | 108.98 | 9 | 7 |
| 3 | C | 317 | PX4 | O5-C8-C7 | 3.17 | 117.54 | 108.40 | 7 | 7 |
| 3 | B | 335 | PX4 | O5-C9-C10 | 3.17 | 102.17 | 111.83 | 2 | 2 |
| 3 | B | 342 | PX4 | C7-O7-C23 | 3.17 | 110.21 | 117.80 | 12 | 6 |
| 3 | B | 400 | PX4 | O5-C9-C10 | 3.17 | 102.17 | 111.83 | 12 | 2 |
| 3 | B | 362 | PX4 | O7-C23-O8 | 3.17 | 131.11 | 123.70 | 7 | 5 |
| 3 | B | 395 | PX4 | O5-C8-C7 | 3.17 | 117.52 | 108.40 | 8 | 3 |
| 3 | C | 323 | PX4 | C5-N1-C3 | 3.17 | 117.29 | 108.98 | 9 | 2 |
| 3 | C | 323 | PX4 | O7-C23-C24 | 3.17 | 104.63 | 111.48 | 13 | 3 |
| 3 | C | 363 | PX4 | C4-N1-C3 | 3.17 | 100.66 | 108.98 | 1 | 2 |
| 3 | A | 639 | PX4 | O7-C7-C6 | 3.16 | 119.70 | 108.34 | 7 | 3 |
| 3 | B | 331 | PX4 | C5-N1-C4 | 3.16 | 100.67 | 108.98 | 6 | 3 |
| 3 | C | 341 | PX4 | O7-C23-O8 | 3.16 | 131.10 | 123.70 | 6 | 3 |
| 3 | C | 314 | PX4 | C7-O7-C23 | 3.16 | 110.23 | 117.80 | 1 | 5 |
| 3 | B | 383 | PX4 | O7-C23-O8 | 3.16 | 131.09 | 123.70 | 2 | 1 |
| 3 | C | 345 | PX4 | O5-C8-C7 | 3.16 | 117.51 | 108.40 | 2 | 4 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | A | 601 | PX4 | C7-O7-C23 | 3.16 | 110.24 | 117.80 | 15 | 5 |
| 3 | A | 602 | PX4 | C5-N1-C4 | 3.16 | 100.68 | 108.98 | 15 | 1 |
| 3 | A | 630 | PX4 | O5-C9-O6 | 3.16 | 131.53 | 123.63 | 11 | 4 |
| 3 | C | 357 | PX4 | C7-O7-C23 | 3.16 | 110.24 | 117.80 | 14 | 5 |
| 3 | A | 615 | PX4 | C5-N1-C4 | 3.16 | 100.69 | 108.98 | 2 | 3 |
| 3 | B | 315 | PX4 | C5-N1-C4 | 3.16 | 117.27 | 108.98 | 2 | 2 |
| 3 | A | 623 | PX4 | O5-C8-C7 | 3.15 | 117.48 | 108.40 | 2 | 2 |
| 3 | C | 329 | PX4 | C5-N1-C3 | 3.15 | 100.70 | 108.98 | 15 | 4 |
| 3 | C | 362 | PX4 | O7-C23-O8 | 3.15 | 131.07 | 123.70 | 10 | 3 |
| 3 | A | 614 | PX4 | O8-C23-C24 | 3.15 | 136.10 | 123.78 | 3 | 1 |
| 3 | A | 619 | PX4 | O5-C9-C10 | 3.15 | 102.24 | 111.83 | 11 | 3 |
| 3 | B | 382 | PX4 | C5-N1-C4 | 3.15 | 117.24 | 108.98 | 5 | 1 |
| 3 | B | 399 | PX4 | O5-C9-C10 | 3.15 | 102.24 | 111.83 | 5 | 2 |
| 3 | C | 330 | PX4 | O5-C8-C7 | 3.15 | 117.47 | 108.40 | 15 | 3 |
| 3 | A | 642 | PX4 | C4-N1-C3 | 3.14 | 100.72 | 108.98 | 3 | 3 |
| 3 | A | 646 | PX4 | C7-O7-C23 | 3.14 | 110.27 | 117.80 | 5 | 4 |
| 3 | A | 653 | PX4 | C4-N1-C3 | 3.14 | 117.23 | 108.98 | 13 | 1 |
| 3 | B | 320 | PX4 | O5-C8-C7 | 3.14 | 117.46 | 108.40 | 14 | 3 |
| 3 | B | 347 | PX4 | O7-C23-O8 | 3.14 | 131.06 | 123.70 | 1 | 3 |
| 3 | B | 385 | PX4 | O5-C9-C10 | 3.14 | 102.25 | 111.83 | 5 | 3 |
| 3 | C | 355 | PX4 | C25-C24-C23 | 3.14 | 125.21 | 113.69 | 14 | 1 |
| 3 | B | 348 | PX4 | C4-N1-C3 | 3.14 | 100.73 | 108.98 | 1 | 2 |
| 3 | B | 375 | PX4 | O7-C7-C8 | 3.14 | 119.61 | 108.34 | 6 | 2 |
| 3 | B | 393 | PX4 | C12-C11-C10 | 3.14 | 101.59 | 113.13 | 6 | 2 |
| 3 | A | 606 | PX4 | C8-C7-C6 | 3.14 | 104.47 | 111.78 | 1 | 4 |
| 3 | A | 634 | PX4 | O5-C9-C10 | 3.14 | 102.27 | 111.83 | 4 | 3 |
| 3 | B | 316 | PX4 | O5-C8-C7 | 3.14 | 117.44 | 108.40 | 3 | 2 |
| 3 | C | 326 | PX4 | C5-N1-C4 | 3.14 | 100.74 | 108.98 | 15 | 3 |
| 3 | C | 356 | PX4 | C8-C7-C6 | 3.13 | 119.09 | 111.78 | 5 | 4 |
| 3 | B | 352 | PX4 | O7-C23-C24 | 3.13 | 104.71 | 111.48 | 4 | 2 |
| 3 | A | 632 | PX4 | O5-C8-C7 | 3.13 | 117.42 | 108.40 | 2 | 5 |
| 3 | B | 378 | PX4 | C8-C7-C6 | 3.13 | 104.49 | 111.78 | 11 | 3 |
| 3 | B | 397 | PX4 | O7-C23-O8 | 3.13 | 131.02 | 123.70 | 11 | 1 |
| 3 | C | 350 | PX4 | O7-C7-C8 | 3.13 | 119.57 | 108.34 | 12 | 3 |
| 3 | C | 322 | PX4 | C11-C10-C9 | 3.13 | 125.15 | 113.69 | 8 | 2 |
| 3 | C | 353 | PX4 | O7-C7-C8 | 3.13 | 119.56 | 108.34 | 7 | 2 |
| 3 | A | 642 | PX4 | O5-C8-C7 | 3.12 | 117.40 | 108.40 | 15 | 6 |
| 3 | B | 320 | PX4 | O7-C23-O8 | 3.12 | 131.01 | 123.70 | 10 | 2 |
| 3 | B | 392 | PX4 | C4-N1-C3 | 3.12 | 117.18 | 108.98 | 6 | 3 |
| 3 | C | 362 | PX4 | O5-C9-C10 | 3.12 | 102.31 | 111.83 | 13 | 2 |
| 3 | C | 341 | PX4 | O5-C8-C7 | 3.12 | 117.40 | 108.40 | 3 | 6 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 301 | PX4 | C3-N1-C2 | 3.12 | 122.31 | 109.91 | 11 | 1 |
| 3 | B | 350 | PX4 | C7-O7-C23 | 3.12 | 110.34 | 117.80 | 2 | 7 |
| 3 | B | 392 | PX4 | C8-C7-C6 | 3.12 | 104.52 | 111.78 | 10 | 2 |
| 3 | B | 302 | PX4 | O7-C23-C24 | 3.12 | 104.74 | 111.48 | 13 | 4 |
| 3 | B | 341 | PX4 | C12-C11-C10 | 3.12 | 101.68 | 113.13 | 7 | 2 |
| 3 | B | 391 | PX4 | C5-N1-C4 | 3.11 | 100.80 | 108.98 | 7 | 4 |
| 3 | B | 326 | PX4 | C7-O7-C23 | 3.11 | 110.35 | 117.80 | 5 | 4 |
| 3 | A | 653 | PX4 | O7-C23-O8 | 3.11 | 130.98 | 123.70 | 12 | 4 |
| 3 | C | 346 | PX4 | O7-C23-C24 | 3.11 | 104.75 | 111.48 | 14 | 3 |
| 3 | B | 382 | PX4 | O5-C9-C10 | 3.11 | 102.36 | 111.83 | 8 | 4 |
| 3 | B | 362 | PX4 | C1-C2-N1 | 3.11 | 125.80 | 115.82 | 14 | 1 |
| 3 | C | 310 | PX4 | C8-C7-C6 | 3.11 | 104.54 | 111.78 | 4 | 4 |
| 3 | B | 341 | PX4 | O5-C9-C10 | 3.11 | 102.36 | 111.83 | 14 | 2 |
| 3 | B | 382 | PX4 | O5-C8-C7 | 3.11 | 117.35 | 108.40 | 2 | 5 |
| 3 | A | 632 | PX4 | O5-C9-C10 | 3.10 | 102.37 | 111.83 | 6 | 1 |
| 3 | A | 608 | PX4 | O7-C7-C8 | 3.10 | 119.47 | 108.34 | 7 | 2 |
| 3 | A | 637 | PX4 | P1-O3-C1 | 3.10 | 136.03 | 121.26 | 12 | 2 |
| 3 | B | 318 | PX4 | O5-C8-C7 | 3.10 | 117.34 | 108.40 | 9 | 4 |
| 3 | B | 324 | PX4 | C7-O7-C23 | 3.10 | 110.38 | 117.80 | 2 | 3 |
| 3 | B | 383 | PX4 | O7-C23-C24 | 3.10 | 104.78 | 111.48 | 11 | 5 |
| 3 | C | 340 | PX4 | C1-C2-N1 | 3.10 | 125.77 | 115.82 | 12 | 1 |
| 3 | A | 624 | PX4 | O7-C23-C24 | 3.10 | 104.78 | 111.48 | 2 | 5 |
| 3 | B | 368 | PX4 | C8-O5-C9 | 3.10 | 105.79 | 117.12 | 4 | 1 |
| 3 | A | 650 | PX4 | O7-C23-O8 | 3.10 | 130.94 | 123.70 | 14 | 3 |
| 3 | B | 321 | PX4 | C8-C7-C6 | 3.10 | 119.00 | 111.78 | 9 | 6 |
| 3 | B | 334 | PX4 | O7-C23-O8 | 3.10 | 130.94 | 123.70 | 11 | 2 |
| 3 | B | 370 | PX4 | O7-C23-C24 | 3.10 | 104.78 | 111.48 | 3 | 5 |
| 3 | C | 335 | PX4 | O5-C9-O6 | 3.10 | 131.37 | 123.63 | 14 | 2 |
| 3 | B | 365 | PX4 | C1-C2-N1 | 3.09 | 125.75 | 115.82 | 13 | 1 |
| 3 | B | 387 | PX4 | O7-C23-C24 | 3.09 | 104.79 | 111.48 | 2 | 3 |
| 3 | B | 383 | PX4 | C4-N1-C3 | 3.09 | 100.85 | 108.98 | 5 | 2 |
| 3 | A | 634 | PX4 | O3-C1-C2 | 3.09 | 124.53 | 109.65 | 2 | 2 |
| 3 | B | 358 | PX4 | C1-C2-N1 | 3.09 | 125.74 | 115.82 | 1 | 1 |
| 3 | B | 369 | PX4 | O7-C23-O8 | 3.09 | 130.93 | 123.70 | 2 | 4 |
| 3 | C | 327 | PX4 | O7-C23-C24 | 3.09 | 104.80 | 111.48 | 7 | 6 |
| 3 | C | 313 | PX4 | O7-C23-C24 | 3.08 | 104.81 | 111.48 | 2 | 3 |
| 3 | B | 309 | PX4 | C12-C11-C10 | 3.08 | 124.45 | 113.13 | 5 | 1 |
| 3 | B | 304 | PX4 | O7-C23-O8 | 3.08 | 130.91 | 123.70 | 8 | 2 |
| 3 | B | 358 | PX4 | O5-C9-C10 | 3.08 | 102.44 | 111.83 | 7 | 2 |
| 3 | C | 364 | PX4 | C7-O7-C23 | 3.08 | 110.42 | 117.80 | 8 | 7 |
| 3 | B | 356 | PX4 | C5-N1-C3 | 3.08 | 100.89 | 108.98 | 14 | 4 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 391 | PX4 | C7-O7-C23 | 3.08 | 110.43 | 117.80 | 8 | 1 |
| 3 | A | 617 | PX4 | C5-N1-C3 | 3.08 | 100.89 | 108.98 | 7 | 2 |
| 3 | B | 363 | PX4 | C8-C7-C6 | 3.08 | 118.96 | 111.78 | 9 | 3 |
| 3 | B | 373 | PX4 | C8-C7-C6 | 3.08 | 104.61 | 111.78 | 8 | 2 |
| 3 | B | 372 | PX4 | O5-C9-C10 | 3.08 | 102.45 | 111.83 | 11 | 4 |
| 3 | B | 385 | PX4 | C4-N1-C3 | 3.08 | 100.89 | 108.98 | 6 | 3 |
| 3 | B | 388 | PX4 | C11-C10-C9 | 3.08 | 102.42 | 113.69 | 9 | 3 |
| 3 | A | 622 | PX4 | C5-N1-C4 | 3.08 | 117.06 | 108.98 | 10 | 2 |
| 3 | C | 319 | PX4 | O5-C8-C7 | 3.08 | 117.26 | 108.40 | 5 | 4 |
| 3 | B | 359 | PX4 | O5-C8-C7 | 3.07 | 117.26 | 108.40 | 9 | 3 |
| 3 | C | 334 | PX4 | O5-C8-C7 | 3.07 | 117.26 | 108.40 | 6 | 3 |
| 3 | C | 357 | PX4 | C5-N1-C4 | 3.08 | 117.06 | 108.98 | 13 | 2 |
| 3 | A | 614 | PX4 | O7-C23-O8 | 3.07 | 130.89 | 123.70 | 10 | 3 |
| 3 | A | 644 | PX4 | O7-C23-C24 | 3.07 | 104.83 | 111.48 | 3 | 3 |
| 3 | C | 334 | PX4 | O7-C7-C6 | 3.07 | 119.37 | 108.34 | 12 | 1 |
| 3 | A | 617 | PX4 | O5-C8-C7 | 3.07 | 117.25 | 108.40 | 1 | 5 |
| 3 | B | 351 | PX4 | C5-N1-C3 | 3.07 | 100.91 | 108.98 | 10 | 2 |
| 3 | B | 357 | PX4 | C8-O5-C9 | 3.07 | 105.89 | 117.12 | 10 | 2 |
| 3 | C | 316 | PX4 | C1-C2-N1 | 3.07 | 125.68 | 115.82 | 12 | 1 |
| 3 | C | 335 | PX4 | C25-C24-C23 | 3.07 | 102.43 | 113.69 | 4 | 1 |
| 3 | C | 341 | PX4 | O7-C23-C24 | 3.07 | 104.84 | 111.48 | 7 | 4 |
| 3 | B | 332 | PX4 | O5-C9-O6 | 3.07 | 131.30 | 123.63 | 2 | 2 |
| 3 | B | 371 | PX4 | O5-C9-C10 | 3.07 | 102.48 | 111.83 | 14 | 2 |
| 3 | A | 609 | PX4 | O5-C9-O6 | 3.06 | 131.29 | 123.63 | 7 | 2 |
| 3 | A | 647 | PX4 | O5-C9-C10 | 3.06 | 102.49 | 111.83 | 3 | 1 |
| 3 | A | 652 | PX4 | O5-C9-C10 | 3.06 | 102.49 | 111.83 | 3 | 3 |
| 3 | B | 348 | PX4 | O7-C7-C6 | 3.06 | 119.33 | 108.34 | 13 | 3 |
| 3 | B | 368 | PX4 | O3-P1-O2 | 3.06 | 96.80 | 108.94 | 1 | 1 |
| 3 | C | 336 | PX4 | O5-C8-C7 | 3.06 | 117.22 | 108.40 | 2 | 7 |
| 3 | A | 633 | PX4 | C8-C7-C6 | 3.06 | 118.92 | 111.78 | 4 | 1 |
| 3 | C | 315 | PX4 | O7-C7-C6 | 3.06 | 119.32 | 108.34 | 1 | 1 |
| 3 | B | 350 | PX4 | O5-C9-C10 | 3.06 | 102.51 | 111.83 | 4 | 3 |
| 3 | A | 645 | PX4 | C7-O7-C23 | 3.06 | 110.48 | 117.80 | 11 | 3 |
| 3 | B | 340 | PX4 | C26-C25-C24 | 3.06 | 101.90 | 113.13 | 3 | 1 |
| 3 | B | 350 | PX4 | C8-C7-C6 | 3.06 | 104.66 | 111.78 | 6 | 3 |
| 3 | B | 354 | PX4 | P1-O3-C1 | 3.06 | 135.81 | 121.26 | 3 | 1 |
| 3 | B | 391 | PX4 | C8-C7-C6 | 3.06 | 104.65 | 111.78 | 4 | 3 |
| 3 | B | 385 | PX4 | C11-C10-C9 | 3.06 | 102.49 | 113.69 | 9 | 1 |
| 3 | C | 305 | PX4 | C4-N1-C3 | 3.06 | 117.01 | 108.98 | 7 | 2 |
| 3 | C | 352 | PX4 | O7-C23-O8 | 3.06 | 130.85 | 123.70 | 4 | 3 |
| 3 | B | 303 | PX4 | O7-C23-C24 | 3.06 | 104.87 | 111.48 | 11 | 6 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 308 | PX4 | O5-C9-C10 | 3.05 | 102.52 | 111.83 | 6 | 3 |
| 3 | B | 356 | PX4 | O7-C23-C24 | 3.05 | 104.88 | 111.48 | 4 | 5 |
| 3 | B | 371 | PX4 | O7-C23-C24 | 3.05 | 104.87 | 111.48 | 7 | 3 |
| 3 | B | 372 | PX4 | O5-C8-C7 | 3.05 | 117.19 | 108.40 | 5 | 2 |
| 3 | C | 336 | PX4 | C5-N1-C3 | 3.05 | 100.96 | 108.98 | 12 | 3 |
| 3 | C | 353 | PX4 | O7-C23-O8 | 3.05 | 130.84 | 123.70 | 14 | 1 |
| 3 | B | 349 | PX4 | C7-O7-C23 | 3.05 | 110.50 | 117.80 | 11 | 5 |
| 3 | A | 606 | PX4 | C7-O7-C23 | 3.05 | 110.50 | 117.80 | 11 | 3 |
| 3 | A | 649 | PX4 | C4-N1-C3 | 3.05 | 116.98 | 108.98 | 4 | 3 |
| 3 | C | 347 | PX4 | O5-C9-C10 | 3.05 | 102.54 | 111.83 | 8 | 1 |
| 3 | A | 639 | PX4 | C8-C7-C6 | 3.05 | 104.68 | 111.78 | 14 | 2 |
| 3 | B | 355 | PX4 | O5-C8-C7 | 3.05 | 117.18 | 108.40 | 2 | 6 |
| 3 | C | 316 | PX4 | C8-O5-C9 | 3.05 | 105.98 | 117.12 | 12 | 1 |
| 3 | C | 356 | PX4 | C7-O7-C23 | 3.05 | 110.50 | 117.80 | 9 | 3 |
| 3 | C | 320 | PX4 | O5-C9-O6 | 3.05 | 131.25 | 123.63 | 2 | 3 |
| 3 | C | 358 | PX4 | C1-C2-N1 | 3.05 | 125.60 | 115.82 | 2 | 1 |
| 3 | C | 326 | PX4 | O7-C23-C24 | 3.04 | 104.90 | 111.48 | 9 | 6 |
| 3 | C | 340 | PX4 | O7-C23-O8 | 3.04 | 130.82 | 123.70 | 11 | 1 |
| 3 | A | 608 | PX4 | C5-N1-C3 | 3.04 | 100.99 | 108.98 | 2 | 2 |
| 3 | C | 346 | PX4 | C5-N1-C3 | 3.04 | 100.98 | 108.98 | 12 | 1 |
| 3 | B | 367 | PX4 | O5-C9-O6 | 3.04 | 131.24 | 123.63 | 4 | 3 |
| 3 | A | 625 | PX4 | C26-C25-C24 | 3.04 | 101.96 | 113.13 | 11 | 1 |
| 3 | B | 303 | PX4 | C1-C2-N1 | 3.04 | 125.57 | 115.82 | 9 | 3 |
| 3 | B | 303 | PX4 | O5-C9-O6 | 3.04 | 131.23 | 123.63 | 5 | 1 |
| 3 | B | 370 | PX4 | O5-C8-C7 | 3.04 | 117.16 | 108.40 | 2 | 5 |
| 3 | C | 347 | PX4 | O7-C23-C24 | 3.04 | 104.91 | 111.48 | 11 | 5 |
| 3 | A | 623 | PX4 | C7-O7-C23 | 3.04 | 110.53 | 117.80 | 1 | 3 |
| 3 | A | 641 | PX4 | C5-N1-C4 | 3.04 | 116.95 | 108.98 | 8 | 1 |
| 3 | C | 364 | PX4 | O5-C9-C10 | 3.04 | 102.58 | 111.83 | 14 | 2 |
| 3 | B | 369 | PX4 | O7-C23-C24 | 3.03 | 104.92 | 111.48 | 15 | 5 |
| 3 | C | 359 | PX4 | C8-C7-C6 | 3.04 | 118.86 | 111.78 | 12 | 2 |
| 3 | A | 604 | PX4 | C4-N1-C3 | 3.03 | 101.01 | 108.98 | 12 | 2 |
| 3 | B | 358 | PX4 | C4-N1-C3 | 3.03 | 116.94 | 108.98 | 1 | 2 |
| 3 | B | 307 | PX4 | C8-C7-C6 | 3.03 | 118.85 | 111.78 | 13 | 1 |
| 3 | B | 368 | PX4 | C8-C7-C6 | 3.03 | 104.72 | 111.78 | 3 | 3 |
| 3 | C | 318 | PX4 | C8-O5-C9 | 3.03 | 106.04 | 117.12 | 10 | 1 |
| 3 | C | 357 | PX4 | C12-C11-C10 | 3.03 | 124.26 | 113.13 | 9 | 2 |
| 3 | A | 627 | PX4 | O5-C8-C7 | 3.03 | 117.12 | 108.40 | 14 | 4 |
| 3 | B | 394 | PX4 | O7-C23-C24 | 3.03 | 104.93 | 111.48 | 2 | 1 |
| 3 | C | 309 | PX4 | C5-N1-C3 | 3.02 | 101.03 | 108.98 | 14 | 3 |
| 3 | C | 335 | PX4 | C8-C7-C6 | 3.02 | 104.74 | 111.78 | 4 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 348 | PX4 | O5-C8-C7 | 3.02 | 117.10 | 108.40 | 15 | 7 |
| 3 | C | 348 | PX4 | O5-C9-C10 | 3.02 | 102.62 | 111.83 | 9 | 2 |
| 3 | C | 345 | PX4 | C5-N1-C2 | 3.02 | 97.91 | 109.91 | 10 | 1 |
| 3 | B | 306 | PX4 | C5-N1-C3 | 3.02 | 101.05 | 108.98 | 15 | 2 |
| 3 | B | 305 | PX4 | O7-C23-C24 | 3.01 | 104.96 | 111.48 | 9 | 5 |
| 3 | C | 344 | PX4 | O5-C8-C7 | 3.01 | 117.08 | 108.40 | 3 | 2 |
| 3 | B | 301 | PX4 | O5-C8-C7 | 3.01 | 117.08 | 108.40 | 8 | 4 |
| 3 | B | 339 | PX4 | O5-C8-C7 | 3.01 | 117.08 | 108.40 | 3 | 3 |
| 3 | B | 345 | PX4 | C8-C7-C6 | 3.01 | 104.77 | 111.78 | 6 | 4 |
| 3 | B | 374 | PX4 | O5-C9-O6 | 3.01 | 131.16 | 123.63 | 1 | 1 |
| 3 | C | 317 | PX4 | O7-C23-O8 | 3.01 | 130.74 | 123.70 | 4 | 4 |
| 3 | C | 332 | PX4 | O5-C9-O6 | 3.01 | 131.16 | 123.63 | 10 | 5 |
| 3 | C | 309 | PX4 | C7-O7-C23 | 3.01 | 110.60 | 117.80 | 8 | 4 |
| 3 | A | 623 | PX4 | C5-N1-C3 | 3.01 | 116.87 | 108.98 | 4 | 4 |
| 3 | C | 310 | PX4 | C5-N1-C3 | 3.00 | 101.08 | 108.98 | 5 | 4 |
| 3 | C | 350 | PX4 | C1-C2-N1 | 3.00 | 125.46 | 115.82 | 13 | 2 |
| 3 | A | 603 | PX4 | C1-C2-N1 | 3.00 | 125.46 | 115.82 | 5 | 2 |
| 3 | A | 619 | PX4 | O5-C8-C7 | 3.00 | 117.05 | 108.40 | 8 | 3 |
| 3 | A | 651 | PX4 | C5-N1-C3 | 3.00 | 116.86 | 108.98 | 1 | 4 |
| 3 | B | 375 | PX4 | C4-N1-C3 | 3.00 | 116.86 | 108.98 | 13 | 1 |
| 3 | B | 343 | PX4 | O5-C8-C7 | 3.00 | 117.05 | 108.40 | 3 | 3 |
| 3 | C | 344 | PX4 | C5-N1-C4 | 3.00 | 101.09 | 108.98 | 1 | 2 |
| 3 | C | 352 | PX4 | O7-C23-C24 | 3.00 | 104.99 | 111.48 | 14 | 5 |
| 3 | A | 603 | PX4 | O5-C9-O6 | 3.00 | 131.13 | 123.63 | 5 | 6 |
| 3 | A | 635 | PX4 | C4-N1-C3 | 3.00 | 101.10 | 108.98 | 10 | 4 |
| 3 | B | 386 | PX4 | O5-C8-C7 | 3.00 | 117.04 | 108.40 | 7 | 1 |
| 3 | B | 305 | PX4 | C4-N1-C3 | 3.00 | 101.10 | 108.98 | 4 | 6 |
| 3 | B | 311 | PX4 | O7-C7-C8 | 3.00 | 119.10 | 108.34 | 7 | 1 |
| 3 | B | 327 | PX4 | C4-N1-C3 | 3.00 | 116.85 | 108.98 | 1 | 4 |
| 3 | A | 609 | PX4 | O5-C8-C7 | 3.00 | 117.04 | 108.40 | 5 | 5 |
| 3 | C | 354 | PX4 | O5-C8-C7 | 3.00 | 117.04 | 108.40 | 14 | 4 |
| 3 | C | 355 | PX4 | O8-C23-C24 | 3.00 | 135.50 | 123.78 | 12 | 1 |
| 3 | B | 303 | PX4 | C7-O7-C23 | 2.99 | 110.63 | 117.80 | 1 | 3 |
| 3 | B | 326 | PX4 | C8-C7-C6 | 2.99 | 104.81 | 111.78 | 10 | 1 |
| 3 | B | 396 | PX4 | O5-C9-C10 | 2.99 | 102.71 | 111.83 | 8 | 2 |
| 3 | C | 309 | PX4 | O7-C7-C8 | 2.99 | 119.08 | 108.34 | 14 | 4 |
| 3 | C | 355 | PX4 | C4-N1-C2 | 2.99 | 98.01 | 109.91 | 12 | 1 |
| 3 | B | 320 | PX4 | C5-N1-C4 | 2.99 | 116.83 | 108.98 | 9 | 3 |
| 3 | B | 390 | PX4 | O5-C9-O6 | 2.99 | 131.11 | 123.63 | 8 | 1 |
| 3 | B | 400 | PX4 | O5-C8-C7 | 2.99 | 117.02 | 108.40 | 8 | 5 |
| 3 | B | 314 | PX4 | C8-C7-C6 | 2.99 | 104.82 | 111.78 | 14 | 4 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | C | 350 | PX4 | C8-C7-C6 | 2.99 | 118.75 | 111.78 | 11 | 2 |
| 3 | B | 358 | PX4 | C5-N1-C3 | 2.98 | 116.81 | 108.98 | 1 | 4 |
| 3 | B | 341 | PX4 | O7-C23-O8 | 2.98 | 130.68 | 123.70 | 15 | 2 |
| 3 | B | 324 | PX4 | O7-C23-O8 | 2.98 | 130.67 | 123.70 | 10 | 1 |
| 3 | B | 368 | PX4 | O7-C23-O8 | 2.98 | 130.68 | 123.70 | 8 | 4 |
| 3 | B | 372 | PX4 | O5-C9-O6 | 2.98 | 131.08 | 123.63 | 2 | 5 |
| 3 | A | 617 | PX4 | C7-O7-C23 | 2.98 | 124.92 | 117.80 | 4 | 5 |
| 3 | B | 329 | PX4 | C11-C10-C9 | 2.98 | 102.78 | 113.69 | 14 | 2 |
| 3 | B | 379 | PX4 | O5-C9-C10 | 2.98 | 102.75 | 111.83 | 9 | 2 |
| 3 | A | 613 | PX4 | O5-C8-C7 | 2.98 | 116.98 | 108.40 | 5 | 3 |
| 3 | B | 345 | PX4 | C1-C2-N1 | 2.98 | 125.38 | 115.82 | 6 | 2 |
| 3 | C | 337 | PX4 | O5-C8-C7 | 2.98 | 116.98 | 108.40 | 4 | 1 |
| 3 | B | 344 | PX4 | C5-N1-C4 | 2.98 | 101.16 | 108.98 | 10 | 1 |
| 3 | B | 349 | PX4 | O5-C9-O6 | 2.97 | 131.07 | 123.63 | 4 | 1 |
| 3 | B | 381 | PX4 | O7-C23-O8 | 2.97 | 130.66 | 123.70 | 4 | 1 |
| 3 | C | 304 | PX4 | C1-C2-N1 | 2.97 | 125.37 | 115.82 | 4 | 3 |
| 3 | A | 642 | PX4 | O5-C9-C10 | 2.97 | 102.77 | 111.83 | 13 | 6 |
| 3 | B | 311 | PX4 | C11-C10-C9 | 2.97 | 124.58 | 113.69 | 9 | 1 |
| 3 | B | 353 | PX4 | C5-N1-C4 | 2.97 | 101.17 | 108.98 | 2 | 2 |
| 3 | B | 385 | PX4 | C8-C7-C6 | 2.97 | 104.85 | 111.78 | 6 | 2 |
| 3 | C | 303 | PX4 | O5-C9-C10 | 2.97 | 102.77 | 111.83 | 10 | 3 |
| 3 | B | 370 | PX4 | C7-O7-C23 | 2.97 | 110.69 | 117.80 | 8 | 3 |
| 3 | A | 636 | PX4 | C5-N1-C4 | 2.97 | 116.77 | 108.98 | 14 | 2 |
| 3 | B | 353 | PX4 | C7-O7-C23 | 2.97 | 110.69 | 117.80 | 8 | 7 |
| 3 | A | 650 | PX4 | O5-C9-O6 | 2.97 | 131.05 | 123.63 | 2 | 2 |
| 3 | B | 314 | PX4 | O7-C23-O8 | 2.97 | 130.64 | 123.70 | 14 | 2 |
| 3 | B | 378 | PX4 | C7-O7-C23 | 2.97 | 110.69 | 117.80 | 13 | 7 |
| 3 | C | 316 | PX4 | C5-N1-C3 | 2.97 | 101.18 | 108.98 | 13 | 1 |
| 3 | A | 616 | PX4 | O5-C9-C10 | 2.97 | 102.79 | 111.83 | 9 | 1 |
| 3 | B | 305 | PX4 | C7-O7-C23 | 2.96 | 110.70 | 117.80 | 1 | 7 |
| 3 | B | 313 | PX4 | C4-N1-C3 | 2.96 | 101.19 | 108.98 | 9 | 3 |
| 3 | B | 330 | PX4 | O5-C8-C7 | 2.97 | 116.94 | 108.40 | 8 | 3 |
| 3 | B | 391 | PX4 | C5-N1-C3 | 2.97 | 101.19 | 108.98 | 5 | 1 |
| 3 | C | 326 | PX4 | C8-C7-C6 | 2.97 | 104.87 | 111.78 | 15 | 2 |
| 3 | C | 341 | PX4 | O5-C9-C10 | 2.97 | 102.79 | 111.83 | 1 | 2 |
| 3 | C | 320 | PX4 | O7-C23-C24 | 2.96 | 105.07 | 111.48 | 14 | 3 |
| 3 | C | 335 | PX4 | P1-O4-C6 | 2.96 | 138.33 | 121.35 | 13 | 1 |
| 3 | B | 350 | PX4 | C5-N1-C3 | 2.96 | 116.75 | 108.98 | 4 | 1 |
| 3 | C | 327 | PX4 | O7-C7-C6 | 2.96 | 118.97 | 108.34 | 14 | 2 |
| 3 | B | 379 | PX4 | O7-C7-C8 | 2.96 | 118.96 | 108.34 | 4 | 2 |
| 3 | C | 325 | PX4 | O7-C23-C24 | 2.96 | 105.08 | 111.48 | 10 | 5 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | C | 356 | PX4 | O7-C23-C24 | 2.96 | 105.08 | 111.48 | 7 | 3 |
| 3 | B | 345 | PX4 | O7-C23-C24 | 2.96 | 105.08 | 111.48 | 5 | 3 |
| 3 | B | 363 | PX4 | O7-C23-O8 | 2.96 | 130.62 | 123.70 | 6 | 3 |
| 3 | B | 365 | PX4 | C7-O7-C23 | 2.96 | 110.72 | 117.80 | 2 | 5 |
| 3 | C | 318 | PX4 | C4-N1-C3 | 2.96 | 101.20 | 108.98 | 5 | 3 |
| 3 | A | 625 | PX4 | C4-N1-C3 | 2.96 | 101.21 | 108.98 | 1 | 2 |
| 3 | B | 304 | PX4 | C4-N1-C3 | 2.96 | 101.21 | 108.98 | 10 | 2 |
| 3 | C | 304 | PX4 | C11-C10-C9 | 2.96 | 102.86 | 113.69 | 11 | 3 |
| 3 | C | 359 | PX4 | O5-C8-C7 | 2.96 | 116.92 | 108.40 | 7 | 2 |
| 3 | B | 362 | PX4 | O5-C9-C10 | 2.96 | 102.82 | 111.83 | 14 | 2 |
| 3 | C | 356 | PX4 | C1-C2-N1 | 2.96 | 125.31 | 115.82 | 5 | 2 |
| 3 | B | 354 | PX4 | C8-O5-C9 | 2.95 | 127.92 | 117.12 | 1 | 2 |
| 3 | A | 604 | PX4 | C8-C7-C6 | 2.95 | 104.90 | 111.78 | 13 | 3 |
| 3 | B | 323 | PX4 | C5-N1-C4 | 2.95 | 101.22 | 108.98 | 15 | 2 |
| 3 | A | 612 | PX4 | C8-C7-C6 | 2.95 | 118.66 | 111.78 | 13 | 3 |
| 3 | A | 615 | PX4 | C5-N1-C3 | 2.95 | 116.73 | 108.98 | 10 | 3 |
| 3 | C | 309 | PX4 | C5-N1-C4 | 2.95 | 101.23 | 108.98 | 5 | 3 |
| 3 | B | 379 | PX4 | C25-C24-C23 | 2.95 | 124.49 | 113.69 | 13 | 1 |
| 3 | B | 394 | PX4 | O5-C8-C7 | 2.94 | 116.89 | 108.40 | 5 | 3 |
| 3 | A | 601 | PX4 | O5-C8-C7 | 2.94 | 116.88 | 108.40 | 9 | 6 |
| 3 | B | 373 | PX4 | O7-C23-O8 | 2.94 | 130.58 | 123.70 | 10 | 2 |
| 3 | C | 329 | PX4 | C1-C2-N1 | 2.94 | 125.27 | 115.82 | 7 | 2 |
| 3 | A | 621 | PX4 | C5-N1-C2 | 2.94 | 121.60 | 109.91 | 1 | 1 |
| 3 | B | 351 | PX4 | C12-C11-C10 | 2.94 | 102.32 | 113.13 | 14 | 1 |
| 3 | C | 325 | PX4 | O5-C9-O6 | 2.94 | 130.99 | 123.63 | 12 | 4 |
| 3 | B | 390 | PX4 | O5-C8-C7 | 2.94 | 116.87 | 108.40 | 7 | 6 |
| 3 | A | 645 | PX4 | C4-N1-C3 | 2.94 | 101.26 | 108.98 | 11 | 3 |
| 3 | B | 361 | PX4 | C8-C7-C6 | 2.94 | 104.94 | 111.78 | 4 | 2 |
| 3 | C | 335 | PX4 | C5-N1-C3 | 2.94 | 116.69 | 108.98 | 7 | 3 |
| 3 | B | 368 | PX4 | O5-C8-C7 | 2.94 | 116.86 | 108.40 | 14 | 6 |
| 3 | B | 376 | PX4 | C5-N1-C4 | 2.94 | 101.26 | 108.98 | 8 | 3 |
| 3 | B | 305 | PX4 | C1-C2-N1 | 2.94 | 125.24 | 115.82 | 10 | 2 |
| 3 | B | 387 | PX4 | O7-C7-C8 | 2.94 | 118.88 | 108.34 | 8 | 2 |
| 3 | B | 322 | PX4 | C7-O7-C23 | 2.93 | 110.77 | 117.80 | 12 | 6 |
| 3 | B | 330 | PX4 | O7-C23-O8 | 2.93 | 130.56 | 123.70 | 9 | 3 |
| 3 | C | 360 | PX4 | O5-C9-O6 | 2.93 | 130.97 | 123.63 | 5 | 1 |
| 3 | A | 610 | PX4 | O5-C9-C10 | 2.93 | 102.89 | 111.83 | 10 | 2 |
| 3 | C | 317 | PX4 | C8-O5-C9 | 2.93 | 127.83 | 117.12 | 5 | 2 |
| 3 | C | 349 | PX4 | C8-C7-C6 | 2.93 | 118.62 | 111.78 | 9 | 3 |
| 3 | A | 605 | PX4 | C8-C7-C6 | 2.93 | 118.61 | 111.78 | 7 | 2 |
| 3 | B | 362 | PX4 | C7-O7-C23 | 2.93 | 110.78 | 117.80 | 2 | 4 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | C | 334 | PX4 | C5-N1-C4 | 2.93 | 101.28 | 108.98 | 6 | 4 |
| 3 | C | 353 | PX4 | O5-C9-O6 | 2.93 | 130.96 | 123.63 | 4 | 2 |
| 3 | B | 345 | PX4 | C5-N1-C3 | 2.93 | 101.28 | 108.98 | 9 | 1 |
| 3 | B | 355 | PX4 | C7-O7-C23 | 2.93 | 110.79 | 117.80 | 6 | 1 |
| 3 | B | 370 | PX4 | C8-C7-C6 | 2.93 | 104.96 | 111.78 | 10 | 2 |
| 3 | B | 374 | PX4 | O7-C7-C8 | 2.93 | 118.85 | 108.34 | 13 | 2 |
| 3 | C | 301 | PX4 | C1-C2-N1 | 2.93 | 125.22 | 115.82 | 8 | 3 |
| 3 | C | 352 | PX4 | O5-C8-C7 | 2.93 | 116.84 | 108.40 | 10 | 4 |
| 3 | A | 637 | PX4 | O7-C7-C6 | 2.93 | 118.84 | 108.34 | 3 | 1 |
| 3 | B | 342 | PX4 | O7-C23-O8 | 2.93 | 130.54 | 123.70 | 1 | 6 |
| 3 | B | 388 | PX4 | O7-C23-O8 | 2.93 | 130.54 | 123.70 | 12 | 3 |
| 3 | B | 394 | PX4 | C7-O7-C23 | 2.93 | 110.79 | 117.80 | 2 | 1 |
| 3 | A | 607 | PX4 | O5-C9-O6 | 2.92 | 130.94 | 123.63 | 6 | 1 |
| 3 | A | 603 | PX4 | O5-C9-C10 | 2.92 | 102.92 | 111.83 | 4 | 4 |
| 3 | A | 625 | PX4 | O7-C23-C24 | 2.92 | 105.16 | 111.48 | 12 | 2 |
| 3 | B | 306 | PX4 | C5-N1-C4 | 2.92 | 101.30 | 108.98 | 10 | 2 |
| 3 | B | 363 | PX4 | O7-C23-C24 | 2.92 | 105.16 | 111.48 | 7 | 5 |
| 3 | B | 370 | PX4 | O5-C9-O6 | 2.92 | 130.94 | 123.63 | 3 | 4 |
| 3 | B | 377 | PX4 | C5-N1-C2 | 2.92 | 121.53 | 109.91 | 11 | 1 |
| 3 | B | 311 | PX4 | O5-C9-O6 | 2.92 | 130.94 | 123.63 | 5 | 2 |
| 3 | B | 341 | PX4 | C8-C7-C6 | 2.92 | 104.97 | 111.78 | 3 | 2 |
| 3 | C | 345 | PX4 | O7-C23-C24 | 2.92 | 105.16 | 111.48 | 15 | 3 |
| 3 | A | 643 | PX4 | O7-C23-O8 | 2.92 | 130.53 | 123.70 | 1 | 3 |
| 3 | B | 307 | PX4 | O5-C9-O6 | 2.92 | 130.93 | 123.63 | 2 | 2 |
| 3 | B | 340 | PX4 | C5-N1-C3 | 2.92 | 101.31 | 108.98 | 13 | 1 |
| 3 | B | 363 | PX4 | O5-C9-C10 | 2.92 | 102.93 | 111.83 | 14 | 3 |
| 3 | A | 620 | PX4 | C5-N1-C3 | 2.92 | 116.64 | 108.98 | 4 | 3 |
| 3 | B | 369 | PX4 | O5-C9-O6 | 2.92 | 130.93 | 123.63 | 11 | 3 |
| 3 | A | 654 | PX4 | O7-C23-C24 | 2.92 | 105.17 | 111.48 | 12 | 3 |
| 3 | B | 306 | PX4 | C11-C10-C9 | 2.91 | 103.01 | 113.69 | 8 | 1 |
| 3 | B | 311 | PX4 | C7-O7-C23 | 2.92 | 110.82 | 117.80 | 12 | 4 |
| 3 | C | 322 | PX4 | O7-C23-O8 | 2.91 | 130.52 | 123.70 | 7 | 4 |
| 3 | B | 361 | PX4 | O5-C8-C7 | 2.91 | 116.79 | 108.40 | 13 | 3 |
| 3 | A | 630 | PX4 | C8-O5-C9 | 2.91 | 106.48 | 117.12 | 11 | 2 |
| 3 | B | 302 | PX4 | O5-C8-C7 | 2.91 | 116.79 | 108.40 | 1 | 4 |
| 3 | B | 374 | PX4 | O3-C1-C2 | 2.91 | 123.66 | 109.65 | 3 | 1 |
| 3 | B | 368 | PX4 | O5-C9-O6 | 2.91 | 130.91 | 123.63 | 1 | 1 |
| 3 | C | 324 | PX4 | C12-C11-C10 | 2.91 | 123.81 | 113.13 | 5 | 3 |
| 3 | C | 325 | PX4 | O5-C8-C7 | 2.91 | 116.78 | 108.40 | 5 | 4 |
| 3 | A | 608 | PX4 | C8-O5-C9 | 2.91 | 106.49 | 117.12 | 2 | 3 |
| 3 | A | 628 | PX4 | O7-C23-C24 | 2.91 | 105.19 | 111.48 | 14 | 2 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 330 | PX4 | C5-N1-C3 | 2.90 | 101.35 | 108.98 | 7 | 2 |
| 3 | B | 347 | PX4 | O7-C7-C8 | 2.90 | 118.76 | 108.34 | 6 | 4 |
| 3 | C | 332 | PX4 | C8-C7-C6 | 2.90 | 105.01 | 111.78 | 15 | 2 |
| 3 | C | 330 | PX4 | O5-C9-O6 | 2.90 | 130.89 | 123.63 | 11 | 3 |
| 3 | C | 335 | PX4 | O7-C23-O8 | 2.90 | 130.49 | 123.70 | 3 | 3 |
| 3 | B | 311 | PX4 | C4-N1-C3 | 2.90 | 116.59 | 108.98 | 8 | 1 |
| 3 | B | 368 | PX4 | C26-C25-C24 | 2.90 | 123.78 | 113.13 | 15 | 1 |
| 3 | B | 391 | PX4 | C11-C10-C9 | 2.90 | 103.06 | 113.69 | 2 | 1 |
| 3 | B | 397 | PX4 | C7-O7-C23 | 2.90 | 110.85 | 117.80 | 5 | 4 |
| 3 | A | 629 | PX4 | C5-N1-C4 | 2.90 | 101.36 | 108.98 | 9 | 1 |
| 3 | A | 639 | PX4 | C5-N1-C4 | 2.90 | 101.36 | 108.98 | 5 | 3 |
| 3 | C | 320 | PX4 | C5-N1-C3 | 2.90 | 116.59 | 108.98 | 13 | 1 |
| 3 | A | 647 | PX4 | C31-C30-C29 | 2.90 | 99.72 | 114.37 | 13 | 1 |
| 3 | A | 648 | PX4 | C5-N1-C3 | 2.90 | 101.36 | 108.98 | 12 | 3 |
| 3 | B | 374 | PX4 | O5-C8-C7 | 2.90 | 116.75 | 108.40 | 15 | 4 |
| 3 | B | 378 | PX4 | C1-C2-N1 | 2.90 | 125.12 | 115.82 | 10 | 1 |
| 3 | A | 626 | PX4 | O5-C9-C10 | 2.90 | 103.00 | 111.83 | 3 | 3 |
| 3 | B | 325 | PX4 | O5-C9-C10 | 2.90 | 103.00 | 111.83 | 8 | 1 |
| 3 | B | 341 | PX4 | C25-C24-C23 | 2.90 | 124.31 | 113.69 | 2 | 1 |
| 3 | B | 367 | PX4 | C8-C7-C6 | 2.89 | 105.04 | 111.78 | 6 | 7 |
| 3 | C | 353 | PX4 | C7-O7-C23 | 2.89 | 110.87 | 117.80 | 7 | 5 |
| 3 | B | 371 | PX4 | C8-C7-C6 | 2.89 | 105.04 | 111.78 | 13 | 3 |
| 3 | A | 631 | PX4 | O5-C8-C7 | 2.89 | 116.73 | 108.40 | 10 | 5 |
| 3 | A | 653 | PX4 | O5-C9-O6 | 2.89 | 130.86 | 123.63 | 10 | 1 |
| 3 | A | 606 | PX4 | O7-C23-O8 | 2.89 | 130.46 | 123.70 | 10 | 4 |
| 3 | A | 623 | PX4 | O7-C23-O8 | 2.89 | 130.46 | 123.70 | 13 | 4 |
| 3 | B | 370 | PX4 | O7-C7-C8 | 2.89 | 118.70 | 108.34 | 5 | 1 |
| 3 | C | 312 | PX4 | O5-C8-C7 | 2.89 | 116.72 | 108.40 | 2 | 3 |
| 3 | A | 609 | PX4 | C5-N1-C4 | 2.89 | 101.40 | 108.98 | 10 | 4 |
| 3 | C | 362 | PX4 | C7-O7-C23 | 2.89 | 110.89 | 117.80 | 6 | 5 |
| 3 | A | 625 | PX4 | C5-N1-C3 | 2.89 | 101.40 | 108.98 | 10 | 3 |
| 3 | A | 626 | PX4 | C4-N1-C2 | 2.88 | 121.37 | 109.91 | 13 | 1 |
| 3 | B | 324 | PX4 | O7-C7-C8 | 2.88 | 118.69 | 108.34 | 9 | 2 |
| 3 | C | 362 | PX4 | O5-C8-C7 | 2.88 | 116.70 | 108.40 | 3 | 3 |
| 3 | A | 608 | PX4 | O1-P1-O2 | 2.88 | 125.85 | 112.44 | 2 | 1 |
| 3 | B | 301 | PX4 | O5-C9-C10 | 2.88 | 103.05 | 111.83 | 15 | 1 |
| 3 | C | 307 | PX4 | O7-C7-C8 | 2.88 | 118.68 | 108.34 | 14 | 1 |
| 3 | A | 602 | PX4 | O5-C8-C7 | 2.88 | 116.69 | 108.40 | 7 | 5 |
| 3 | B | 350 | PX4 | C5-N1-C4 | 2.88 | 101.42 | 108.98 | 4 | 3 |
| 3 | B | 359 | PX4 | O7-C23-C24 | 2.88 | 117.70 | 111.48 | 5 | 4 |
| 3 | B | 386 | PX4 | O5-C9-O6 | 2.88 | 130.82 | 123.63 | 6 | 2 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 387 | PX4 | C7-O7-C23 | 2.88 | 110.92 | 117.80 | 11 | 5 |
| 3 | C | 315 | PX4 | O5-C9-C10 | 2.87 | 103.07 | 111.83 | 3 | 4 |
| 3 | B | 326 | PX4 | O7-C23-O8 | 2.87 | 130.42 | 123.70 | 12 | 3 |
| 3 | B | 344 | PX4 | C8-O5-C9 | 2.87 | 127.62 | 117.12 | 12 | 2 |
| 3 | C | 350 | PX4 | O7-C7-C6 | 2.87 | 118.65 | 108.34 | 8 | 4 |
| 3 | C | 334 | PX4 | C4-N1-C3 | 2.87 | 101.43 | 108.98 | 12 | 3 |
| 3 | A | 627 | PX4 | C8-C7-C6 | 2.87 | 118.48 | 111.78 | 1 | 2 |
| 3 | C | 312 | PX4 | C8-C7-C6 | 2.87 | 105.09 | 111.78 | 13 | 3 |
| 3 | B | 366 | PX4 | O5-C8-C7 | 2.87 | 116.67 | 108.40 | 10 | 3 |
| 3 | C | 314 | PX4 | C5-N1-C3 | 2.87 | 101.44 | 108.98 | 8 | 1 |
| 3 | C | 306 | PX4 | O7-C7-C6 | 2.87 | 118.63 | 108.34 | 13 | 5 |
| 3 | C | 349 | PX4 | O5-C8-C7 | 2.87 | 116.67 | 108.40 | 6 | 3 |
| 3 | C | 341 | PX4 | O7-C7-C6 | 2.87 | 118.63 | 108.34 | 11 | 2 |
| 3 | B | 397 | PX4 | C8-C7-C6 | 2.87 | 105.10 | 111.78 | 12 | 1 |
| 3 | C | 362 | PX4 | O7-C7-C6 | 2.87 | 118.63 | 108.34 | 13 | 2 |
| 3 | A | 641 | PX4 | C7-O7-C23 | 2.87 | 110.94 | 117.80 | 11 | 3 |
| 3 | B | 380 | PX4 | C8-C7-C6 | 2.86 | 105.11 | 111.78 | 9 | 3 |
| 3 | C | 319 | PX4 | C8-C7-C6 | 2.86 | 118.46 | 111.78 | 14 | 4 |
| 3 | C | 319 | PX4 | O5-C9-C10 | 2.86 | 103.10 | 111.83 | 13 | 2 |
| 3 | C | 340 | PX4 | O7-C23-C24 | 2.87 | 105.28 | 111.48 | 9 | 5 |
| 3 | C | 326 | PX4 | C4-N1-C3 | 2.86 | 101.45 | 108.98 | 2 | 2 |
| 3 | C | 344 | PX4 | O5-C9-O6 | 2.86 | 130.79 | 123.63 | 7 | 2 |
| 3 | B | 321 | PX4 | O7-C23-C24 | 2.86 | 105.29 | 111.48 | 4 | 2 |
| 3 | C | 324 | PX4 | P1-O3-C1 | 2.86 | 134.88 | 121.26 | 5 | 1 |
| 3 | C | 333 | PX4 | C1-C2-N1 | 2.86 | 125.01 | 115.82 | 3 | 2 |
| 3 | A | 620 | PX4 | O7-C23-O8 | 2.86 | 130.39 | 123.70 | 4 | 4 |
| 3 | A | 634 | PX4 | C5-N1-C4 | 2.86 | 116.49 | 108.98 | 3 | 2 |
| 3 | B | 382 | PX4 | C7-O7-C23 | 2.86 | 110.95 | 117.80 | 1 | 1 |
| 3 | B | 395 | PX4 | C5-N1-C2 | 2.86 | 121.27 | 109.91 | 11 | 1 |
| 3 | C | 346 | PX4 | C8-C7-C6 | 2.86 | 118.45 | 111.78 | 4 | 4 |
| 3 | A | 625 | PX4 | C5-N1-C4 | 2.85 | 101.48 | 108.98 | 2 | 2 |
| 3 | A | 631 | PX4 | C1-C2-N1 | 2.85 | 124.98 | 115.82 | 9 | 2 |
| 3 | A | 640 | PX4 | C5-N1-C3 | 2.86 | 116.48 | 108.98 | 7 | 2 |
| 3 | B | 327 | PX4 | O7-C23-C24 | 2.85 | 105.31 | 111.48 | 12 | 5 |
| 3 | B | 348 | PX4 | O5-C9-O6 | 2.86 | 130.77 | 123.63 | 8 | 4 |
| 3 | B | 356 | PX4 | C4-N1-C3 | 2.86 | 116.48 | 108.98 | 5 | 2 |
| 3 | B | 389 | PX4 | O5-C8-C7 | 2.85 | 116.62 | 108.40 | 13 | 3 |
| 3 | B | 320 | PX4 | C5-N1-C3 | 2.85 | 116.47 | 108.98 | 14 | 2 |
| 3 | B | 357 | PX4 | C5-N1-C4 | 2.85 | 101.48 | 108.98 | 10 | 2 |
| 3 | A | 621 | PX4 | P1-O3-C1 | 2.85 | 134.82 | 121.26 | 12 | 2 |
| 3 | B | 344 | PX4 | C5-N1-C3 | 2.85 | 101.49 | 108.98 | 5 | 3 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 372 | PX4 | C5-N1-C3 | 2.85 | 101.49 | 108.98 | 14 | 2 |
| 3 | C | 308 | PX4 | C8-C7-C6 | 2.85 | 118.43 | 111.78 | 8 | 2 |
| 3 | B | 354 | PX4 | O7-C7-C6 | 2.85 | 118.56 | 108.34 | 8 | 1 |
| 3 | C | 306 | PX4 | O7-C7-C8 | 2.85 | 118.56 | 108.34 | 3 | 6 |
| 3 | A | 601 | PX4 | O7-C23-O8 | 2.85 | 130.36 | 123.70 | 4 | 2 |
| 3 | A | 649 | PX4 | O7-C23-O8 | 2.85 | 130.36 | 123.70 | 7 | 3 |
| 3 | B | 317 | PX4 | O5-C9-C10 | 2.85 | 103.15 | 111.83 | 3 | 1 |
| 3 | B | 382 | PX4 | C25-C24-C23 | 2.85 | 103.26 | 113.69 | 2 | 1 |
| 3 | C | 355 | PX4 | C8-C7-C6 | 2.85 | 105.14 | 111.78 | 6 | 3 |
| 3 | B | 326 | PX4 | C5-N1-C3 | 2.85 | 116.45 | 108.98 | 14 | 3 |
| 3 | A | 605 | PX4 | C4-N1-C3 | 2.84 | 101.51 | 108.98 | 14 | 2 |
| 3 | B | 319 | PX4 | C8-C7-C6 | 2.84 | 118.42 | 111.78 | 3 | 3 |
| 3 | B | 381 | PX4 | O7-C23-C24 | 2.84 | 105.33 | 111.48 | 2 | 1 |
| 3 | C | 345 | PX4 | C7-O7-C23 | 2.84 | 110.99 | 117.80 | 10 | 5 |
| 3 | A | 613 | PX4 | O5-C9-C10 | 2.84 | 103.17 | 111.83 | 9 | 1 |
| 3 | A | 638 | PX4 | O5-C8-C7 | 2.84 | 116.59 | 108.40 | 4 | 6 |
| 3 | B | 352 | PX4 | C5-N1-C3 | 2.84 | 101.51 | 108.98 | 10 | 2 |
| 3 | B | 373 | PX4 | C12-C11-C10 | 2.84 | 123.56 | 113.13 | 6 | 1 |
| 3 | C | 305 | PX4 | O5-C9-O6 | 2.84 | 130.73 | 123.63 | 14 | 2 |
| 3 | B | 391 | PX4 | C4-N1-C3 | 2.84 | 116.44 | 108.98 | 6 | 5 |
| 3 | C | 318 | PX4 | C5-N1-C3 | 2.84 | 116.44 | 108.98 | 11 | 2 |
| 3 | A | 636 | PX4 | O5-C8-C7 | 2.84 | 116.58 | 108.40 | 10 | 3 |
| 3 | B | 352 | PX4 | O5-C9-C10 | 2.84 | 103.18 | 111.83 | 4 | 3 |
| 3 | A | 632 | PX4 | C1-C2-N1 | 2.84 | 124.93 | 115.82 | 4 | 1 |
| 3 | A | 645 | PX4 | C5-N1-C3 | 2.84 | 116.43 | 108.98 | 11 | 1 |
| 3 | B | 388 | PX4 | C7-O7-C23 | 2.84 | 111.01 | 117.80 | 6 | 3 |
| 3 | B | 319 | PX4 | O5-C9-O6 | 2.84 | 130.72 | 123.63 | 15 | 3 |
| 3 | B | 318 | PX4 | C26-C25-C24 | 2.83 | 123.54 | 113.13 | 8 | 1 |
| 3 | B | 355 | PX4 | C3-N1-C2 | 2.83 | 121.18 | 109.91 | 14 | 2 |
| 3 | C | 308 | PX4 | C26-C25-C24 | 2.84 | 123.55 | 113.13 | 7 | 2 |
| 3 | C | 342 | PX4 | C3-N1-C2 | 2.84 | 121.18 | 109.91 | 11 | 1 |
| 3 | B | 368 | PX4 | O7-C7-C8 | 2.83 | 118.51 | 108.34 | 14 | 2 |
| 3 | B | 375 | PX4 | C5-N1-C3 | 2.83 | 101.53 | 108.98 | 11 | 2 |
| 3 | B | 383 | PX4 | C7-O7-C23 | 2.83 | 111.01 | 117.80 | 2 | 4 |
| 3 | B | 386 | PX4 | O7-C7-C8 | 2.83 | 118.51 | 108.34 | 10 | 2 |
| 3 | B | 309 | PX4 | O7-C7-C6 | 2.83 | 118.50 | 108.34 | 15 | 2 |
| 3 | B | 362 | PX4 | C5-N1-C4 | 2.83 | 101.55 | 108.98 | 2 | 2 |
| 3 | B | 374 | PX4 | C1-C2-N1 | 2.83 | 124.90 | 115.82 | 11 | 1 |
| 3 | C | 301 | PX4 | O5-C9-O6 | 2.83 | 130.70 | 123.63 | 5 | 2 |
| 3 | A | 616 | PX4 | O7-C23-C24 | 2.83 | 105.37 | 111.48 | 13 | 2 |
| 3 | A | 630 | PX4 | C4-N1-C3 | 2.83 | 101.55 | 108.98 | 1 | 2 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 390 | PX4 | C1-C2-N1 | 2.83 | 124.89 | 115.82 | 1 | 1 |
| 3 | B | 385 | PX4 | O1-P1-O2 | 2.82 | 125.59 | 112.44 | 15 | 1 |
| 3 | C | 329 | PX4 | C4-N1-C3 | 2.83 | 116.40 | 108.98 | 15 | 2 |
| 3 | B | 304 | PX4 | C25-C24-C23 | 2.82 | 124.04 | 113.69 | 5 | 1 |
| 3 | B | 305 | PX4 | O7-C23-O8 | 2.82 | 130.31 | 123.70 | 9 | 1 |
| 3 | B | 311 | PX4 | C5-N1-C3 | 2.82 | 116.39 | 108.98 | 9 | 3 |
| 3 | B | 379 | PX4 | C5-N1-C3 | 2.82 | 101.57 | 108.98 | 4 | 1 |
| 3 | B | 333 | PX4 | O8-C23-C24 | 2.82 | 134.81 | 123.78 | 5 | 1 |
| 3 | B | 326 | PX4 | C1-C2-N1 | 2.82 | 124.87 | 115.82 | 14 | 2 |
| 3 | B | 385 | PX4 | O7-C23-O8 | 2.82 | 130.29 | 123.70 | 12 | 3 |
| 3 | C | 304 | PX4 | O5-C9-O6 | 2.82 | 130.68 | 123.63 | 8 | 4 |
| 3 | C | 317 | PX4 | C15-C14-C13 | 2.82 | 100.13 | 114.37 | 15 | 1 |
| 3 | A | 605 | PX4 | C7-O7-C23 | 2.81 | 111.06 | 117.80 | 1 | 6 |
| 3 | A | 605 | PX4 | O5-C8-C7 | 2.81 | 116.51 | 108.40 | 6 | 3 |
| 3 | B | 369 | PX4 | O5-C8-C7 | 2.81 | 116.51 | 108.40 | 9 | 2 |
| 3 | B | 399 | PX4 | O7-C23-O8 | 2.81 | 130.28 | 123.70 | 14 | 2 |
| 3 | A | 612 | PX4 | O7-C23-C24 | 2.81 | 105.40 | 111.48 | 4 | 4 |
| 3 | A | 616 | PX4 | C5-N1-C4 | 2.81 | 101.59 | 108.98 | 1 | 3 |
| 3 | A | 639 | PX4 | O5-C8-C7 | 2.81 | 116.50 | 108.40 | 9 | 4 |
| 3 | B | 303 | PX4 | C4-N1-C3 | 2.81 | 101.59 | 108.98 | 12 | 1 |
| 3 | A | 644 | PX4 | C11-C10-C9 | 2.81 | 123.99 | 113.69 | 12 | 1 |
| 3 | B | 332 | PX4 | C5-N1-C4 | 2.81 | 116.36 | 108.98 | 1 | 2 |
| 3 | B | 357 | PX4 | O5-C9-O6 | 2.81 | 130.66 | 123.63 | 4 | 2 |
| 3 | B | 303 | PX4 | C8-C7-C6 | 2.81 | 118.33 | 111.78 | 14 | 3 |
| 3 | A | 601 | PX4 | C5-N1-C3 | 2.81 | 101.60 | 108.98 | 2 | 1 |
| 3 | A | 609 | PX4 | O7-C23-O8 | 2.81 | 130.27 | 123.70 | 13 | 3 |
| 3 | A | 614 | PX4 | C3-N1-C2 | 2.81 | 121.07 | 109.91 | 8 | 1 |
| 3 | B | 387 | PX4 | O5-C9-C10 | 2.81 | 103.28 | 111.83 | 7 | 3 |
| 3 | B | 317 | PX4 | C1-C2-N1 | 2.80 | 124.82 | 115.82 | 9 | 1 |
| 3 | B | 399 | PX4 | O5-C9-O6 | 2.80 | 130.64 | 123.63 | 5 | 3 |
| 3 | C | 316 | PX4 | C8-C7-C6 | 2.80 | 118.32 | 111.78 | 2 | 2 |
| 3 | C | 357 | PX4 | O5-C8-C7 | 2.80 | 116.48 | 108.40 | 12 | 4 |
| 3 | B | 319 | PX4 | O7-C7-C8 | 2.80 | 118.40 | 108.34 | 2 | 2 |
| 3 | B | 333 | PX4 | O7-C23-C24 | 2.80 | 105.42 | 111.48 | 7 | 3 |
| 3 | B | 314 | PX4 | C7-O7-C23 | 2.80 | 111.09 | 117.80 | 4 | 3 |
| 3 | C | 332 | PX4 | C1-C2-N1 | 2.80 | 124.82 | 115.82 | 8 | 2 |
| 3 | C | 349 | PX4 | O7-C23-C24 | 2.80 | 105.42 | 111.48 | 8 | 3 |
| 3 | C | 359 | PX4 | C29-C28-C27 | 2.80 | 100.20 | 114.37 | 9 | 1 |
| 3 | B | 344 | PX4 | O7-C7-C8 | 2.80 | 118.39 | 108.34 | 2 | 1 |
| 3 | C | 317 | PX4 | O7-C7-C8 | 2.80 | 118.39 | 108.34 | 9 | 3 |
| 3 | A | 603 | PX4 | C7-O7-C23 | 2.80 | 111.10 | 117.80 | 10 | 3 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | A | 649 | PX4 | O5-C9-C10 | 2.80 | 103.30 | 111.83 | 8 | 3 |
| 3 | B | 303 | PX4 | O5-C9-C10 | 2.80 | 103.30 | 111.83 | 13 | 2 |
| 3 | B | 383 | PX4 | C1-C2-N1 | 2.80 | 124.80 | 115.82 | 3 | 2 |
| 3 | C | 312 | PX4 | O7-C23-O8 | 2.80 | 130.25 | 123.70 | 8 | 1 |
| 3 | A | 601 | PX4 | C34-C33-C32 | 2.80 | 100.23 | 114.37 | 12 | 1 |
| 3 | A | 606 | PX4 | O7-C7-C8 | 2.80 | 118.38 | 108.34 | 1 | 4 |
| 3 | B | 387 | PX4 | O5-C9-O6 | 2.80 | 130.62 | 123.63 | 4 | 2 |
| 3 | B | 378 | PX4 | O5-C8-C7 | 2.80 | 116.46 | 108.40 | 2 | 4 |
| 3 | A | 632 | PX4 | O7-C23-O8 | 2.79 | 130.24 | 123.70 | 11 | 4 |
| 3 | B | 327 | PX4 | C26-C25-C24 | 2.79 | 102.86 | 113.13 | 7 | 1 |
| 3 | B | 336 | PX4 | O5-C9-O6 | 2.79 | 130.62 | 123.63 | 4 | 2 |
| 3 | B | 355 | PX4 | O7-C7-C8 | 2.79 | 118.37 | 108.34 | 8 | 5 |
| 3 | B | 313 | PX4 | C5-N1-C4 | 2.79 | 116.31 | 108.98 | 1 | 1 |
| 3 | B | 379 | PX4 | O7-C23-O8 | 2.79 | 130.23 | 123.70 | 3 | 1 |
| 3 | A | 603 | PX4 | C5-N1-C4 | 2.79 | 101.65 | 108.98 | 7 | 1 |
| 3 | A | 652 | PX4 | C12-C11-C10 | 2.79 | 102.88 | 113.13 | 4 | 1 |
| 3 | B | 363 | PX4 | O5-C9-O6 | 2.79 | 130.60 | 123.63 | 15 | 3 |
| 3 | A | 613 | PX4 | C8-C7-C6 | 2.79 | 105.29 | 111.78 | 3 | 2 |
| 3 | A | 613 | PX4 | O7-C23-C24 | 2.79 | 105.45 | 111.48 | 1 | 2 |
| 3 | A | 640 | PX4 | O7-C23-O8 | 2.79 | 130.22 | 123.70 | 5 | 1 |
| 3 | B | 339 | PX4 | C1-C2-N1 | 2.79 | 124.77 | 115.82 | 4 | 2 |
| 3 | B | 370 | PX4 | C5-N1-C3 | 2.79 | 101.65 | 108.98 | 3 | 3 |
| 3 | B | 385 | PX4 | O5-C9-O6 | 2.79 | 130.60 | 123.63 | 8 | 1 |
| 3 | A | 630 | PX4 | C7-O7-C23 | 2.78 | 111.13 | 117.80 | 1 | 4 |
| 3 | B | 335 | PX4 | C1-C2-N1 | 2.78 | 124.76 | 115.82 | 2 | 1 |
| 3 | B | 306 | PX4 | C8-O5-C9 | 2.78 | 106.95 | 117.12 | 5 | 2 |
| 3 | C | 315 | PX4 | O7-C23-O8 | 2.78 | 130.21 | 123.70 | 12 | 5 |
| 3 | C | 359 | PX4 | C5-N1-C4 | 2.78 | 101.67 | 108.98 | 2 | 2 |
| 3 | A | 614 | PX4 | C7-O7-C23 | 2.78 | 111.14 | 117.80 | 2 | 5 |
| 3 | B | 330 | PX4 | C4-N1-C3 | 2.78 | 101.67 | 108.98 | 14 | 1 |
| 3 | C | 317 | PX4 | O5-C9-O6 | 2.78 | 130.59 | 123.63 | 5 | 3 |
| 3 | C | 335 | PX4 | P1-O3-C1 | 2.78 | 134.50 | 121.26 | 2 | 2 |
| 3 | A | 619 | PX4 | O7-C23-O8 | 2.78 | 130.20 | 123.70 | 7 | 2 |
| 3 | B | 316 | PX4 | O7-C23-C24 | 2.78 | 105.47 | 111.48 | 13 | 5 |
| 3 | B | 339 | PX4 | O7-C23-C24 | 2.78 | 105.47 | 111.48 | 9 | 4 |
| 3 | B | 367 | PX4 | O7-C7-C6 | 2.78 | 118.32 | 108.34 | 4 | 2 |
| 3 | B | 394 | PX4 | O5-C9-C10 | 2.78 | 103.36 | 111.83 | 9 | 1 |
| 3 | B | 339 | PX4 | C5-N1-C3 | 2.78 | 116.27 | 108.98 | 4 | 2 |
| 3 | C | 320 | PX4 | O5-C9-C10 | 2.78 | 103.36 | 111.83 | 4 | 3 |
| 3 | A | 646 | PX4 | O7-C23-O8 | 2.78 | 130.19 | 123.70 | 11 | 2 |
| 3 | B | 335 | PX4 | O7-C7-C8 | 2.78 | 118.30 | 108.34 | 4 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 362 | PX4 | O7-C23-C24 | 2.78 | 105.48 | 111.48 | 10 | 2 |
| 3 | C | 312 | PX4 | O7-C7-C6 | 2.78 | 118.30 | 108.34 | 13 | 2 |
| 3 | A | 613 | PX4 | C1-C2-N1 | 2.77 | 124.72 | 115.82 | 2 | 1 |
| 3 | B | 383 | PX4 | C5-N1-C4 | 2.77 | 101.69 | 108.98 | 6 | 3 |
| 3 | C | 329 | PX4 | C25-C24-C23 | 2.77 | 103.53 | 113.69 | 6 | 3 |
| 3 | A | 635 | PX4 | O5-C9-C10 | 2.77 | 103.38 | 111.83 | 8 | 2 |
| 3 | B | 346 | PX4 | O5-C9-C10 | 2.77 | 103.39 | 111.83 | 12 | 2 |
| 3 | B | 369 | PX4 | C5-N1-C3 | 2.77 | 101.70 | 108.98 | 5 | 3 |
| 3 | B | 381 | PX4 | O5-C9-C10 | 2.77 | 103.38 | 111.83 | 6 | 4 |
| 3 | C | 303 | PX4 | C5-N1-C4 | 2.77 | 101.69 | 108.98 | 9 | 1 |
| 3 | A | 649 | PX4 | C26-C25-C24 | 2.77 | 102.95 | 113.13 | 7 | 2 |
| 3 | B | 397 | PX4 | O7-C7-C8 | 2.77 | 118.28 | 108.34 | 2 | 2 |
| 3 | C | 304 | PX4 | C3-N1-C2 | 2.77 | 120.92 | 109.91 | 1 | 1 |
| 3 | C | 310 | PX4 | C1-C2-N1 | 2.77 | 124.71 | 115.82 | 12 | 2 |
| 3 | B | 320 | PX4 | O5-C9-C10 | 2.77 | 103.40 | 111.83 | 7 | 3 |
| 3 | B | 347 | PX4 | O5-C9-C10 | 2.77 | 103.40 | 111.83 | 14 | 1 |
| 3 | B | 396 | PX4 | C5-N1-C3 | 2.77 | 101.71 | 108.98 | 12 | 2 |
| 3 | C | 315 | PX4 | C25-C24-C23 | 2.77 | 103.56 | 113.69 | 7 | 1 |
| 3 | B | 322 | PX4 | O7-C23-C24 | 2.76 | 105.50 | 111.48 | 7 | 3 |
| 3 | C | 304 | PX4 | C5-N1-C4 | 2.76 | 101.72 | 108.98 | 1 | 2 |
| 3 | B | 392 | PX4 | O5-C9-C10 | 2.76 | 103.41 | 111.83 | 15 | 3 |
| 3 | C | 302 | PX4 | O7-C23-O8 | 2.76 | 117.25 | 123.70 | 1 | 1 |
| 3 | C | 327 | PX4 | C5-N1-C3 | 2.76 | 116.23 | 108.98 | 12 | 2 |
| 3 | B | 317 | PX4 | O5-C9-O6 | 2.76 | 130.53 | 123.63 | 3 | 2 |
| 3 | B | 318 | PX4 | O5-C9-C10 | 2.76 | 103.42 | 111.83 | 9 | 3 |
| 3 | B | 396 | PX4 | O7-C23-O8 | 2.76 | 130.16 | 123.70 | 13 | 3 |
| 3 | C | 310 | PX4 | O5-C9-C10 | 2.76 | 103.42 | 111.83 | 1 | 3 |
| 3 | B | 389 | PX4 | C1-C2-N1 | 2.76 | 124.67 | 115.82 | 6 | 2 |
| 3 | C | 321 | PX4 | C7-O7-C23 | 2.76 | 111.20 | 117.80 | 1 | 4 |
| 3 | C | 327 | PX4 | C5-N1-C4 | 2.76 | 101.73 | 108.98 | 14 | 4 |
| 3 | C | 331 | PX4 | O7-C23-C24 | 2.76 | 105.51 | 111.48 | 14 | 3 |
| 3 | A | 606 | PX4 | O5-C9-C10 | 2.76 | 103.43 | 111.83 | 5 | 3 |
| 3 | A | 601 | PX4 | C1-C2-N1 | 2.76 | 124.67 | 115.82 | 5 | 2 |
| 3 | B | 321 | PX4 | C8-O5-C9 | 2.76 | 107.04 | 117.12 | 6 | 4 |
| 3 | B | 380 | PX4 | O7-C23-C24 | 2.76 | 105.52 | 111.48 | 12 | 5 |
| 3 | C | 302 | PX4 | C11-C10-C9 | 2.76 | 123.79 | 113.69 | 4 | 1 |
| 3 | C | 320 | PX4 | P1-O4-C6 | 2.76 | 137.14 | 121.35 | 5 | 1 |
| 3 | C | 348 | PX4 | O7-C23-C24 | 2.76 | 105.52 | 111.48 | 5 | 2 |
| 3 | A | 642 | PX4 | C5-N1-C4 | 2.75 | 101.74 | 108.98 | 11 | 3 |
| 3 | B | 346 | PX4 | O5-C8-C7 | 2.75 | 116.33 | 108.40 | 15 | 3 |
| 3 | C | 361 | PX4 | C8-O5-C9 | 2.75 | 127.17 | 117.12 | 5 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | A | 611 | PX4 | C5-N1-C3 | 2.75 | 116.20 | 108.98 | 5 | 2 |
| 3 | A | 622 | PX4 | O7-C23-O8 | 2.75 | 130.13 | 123.70 | 6 | 1 |
| 3 | A | 641 | PX4 | O5-C8-C7 | 2.75 | 116.32 | 108.40 | 8 | 3 |
| 3 | C | 304 | PX4 | O5-C9-C10 | 2.75 | 103.45 | 111.83 | 2 | 2 |
| 3 | C | 351 | PX4 | O7-C23-O8 | 2.75 | 130.13 | 123.70 | 11 | 4 |
| 3 | A | 626 | PX4 | C7-O7-C23 | 2.75 | 111.22 | 117.80 | 12 | 2 |
| 3 | B | 333 | PX4 | O5-C9-C10 | 2.75 | 103.46 | 111.83 | 4 | 3 |
| 3 | B | 349 | PX4 | C5-N1-C3 | 2.75 | 116.19 | 108.98 | 14 | 2 |
| 3 | C | 305 | PX4 | O7-C7-C6 | 2.75 | 98.49 | 108.34 | 10 | 1 |
| 3 | C | 308 | PX4 | O7-C7-C8 | 2.75 | 118.20 | 108.34 | 6 | 2 |
| 3 | B | 365 | PX4 | C5-N1-C4 | 2.75 | 116.19 | 108.98 | 9 | 2 |
| 3 | B | 377 | PX4 | C7-O7-C23 | 2.75 | 111.22 | 117.80 | 9 | 3 |
| 3 | C | 364 | PX4 | C4-N1-C3 | 2.75 | 101.76 | 108.98 | 9 | 2 |
| 3 | C | 305 | PX4 | C8-C7-C6 | 2.74 | 105.39 | 111.78 | 8 | 3 |
| 3 | C | 334 | PX4 | C8-C7-C6 | 2.75 | 105.38 | 111.78 | 12 | 2 |
| 3 | C | 338 | PX4 | C25-C24-C23 | 2.74 | 103.64 | 113.69 | 7 | 1 |
| 3 | A | 612 | PX4 | C5-N1-C2 | 2.74 | 99.01 | 109.91 | 15 | 1 |
| 3 | C | 305 | PX4 | O7-C23-C24 | 2.74 | 105.55 | 111.48 | 6 | 3 |
| 3 | C | 329 | PX4 | O5-C9-O6 | 2.74 | 130.49 | 123.63 | 13 | 4 |
| 3 | A | 642 | PX4 | O1-P1-O3 | 2.74 | 119.99 | 107.57 | 13 | 1 |
| 3 | B | 364 | PX4 | C1-C2-N1 | 2.74 | 124.62 | 115.82 | 9 | 2 |
| 3 | C | 356 | PX4 | O5-C9-O6 | 2.74 | 130.48 | 123.63 | 12 | 3 |
| 3 | C | 301 | PX4 | O5-C9-C10 | 2.73 | 103.50 | 111.83 | 5 | 3 |
| 3 | C | 348 | PX4 | C5-N1-C3 | 2.74 | 116.16 | 108.98 | 4 | 2 |
| 3 | A | 643 | PX4 | O7-C7-C8 | 2.73 | 118.15 | 108.34 | 14 | 3 |
| 3 | A | 645 | PX4 | O5-C8-C7 | 2.73 | 116.28 | 108.40 | 11 | 4 |
| 3 | B | 318 | PX4 | C8-C7-C6 | 2.73 | 105.41 | 111.78 | 1 | 2 |
| 3 | B | 348 | PX4 | C5-N1-C3 | 2.73 | 116.16 | 108.98 | 15 | 4 |
| 3 | B | 357 | PX4 | C5-N1-C3 | 2.73 | 101.80 | 108.98 | 13 | 1 |
| 3 | A | 604 | PX4 | C11-C10-C9 | 2.73 | 103.69 | 113.69 | 3 | 1 |
| 3 | B | 303 | PX4 | C5-N1-C4 | 2.73 | 101.81 | 108.98 | 4 | 2 |
| 3 | C | 361 | PX4 | O7-C23-C24 | 2.73 | 105.58 | 111.48 | 12 | 4 |
| 3 | B | 400 | PX4 | O7-C23-O8 | 2.73 | 130.08 | 123.70 | 13 | 1 |
| 3 | B | 332 | PX4 | C8-C7-C6 | 2.72 | 118.14 | 111.78 | 2 | 4 |
| 3 | B | 305 | PX4 | O5-C8-C7 | 2.72 | 116.25 | 108.40 | 7 | 2 |
| 3 | B | 310 | PX4 | O5-C9-C10 | 2.72 | 103.53 | 111.83 | 9 | 2 |
| 3 | C | 347 | PX4 | O1-P1-O2 | 2.72 | 125.11 | 112.44 | 6 | 2 |
| 3 | A | 652 | PX4 | C11-C10-C9 | 2.72 | 103.72 | 113.69 | 3 | 3 |
| 3 | B | 326 | PX4 | O5-C9-O6 | 2.72 | 130.44 | 123.63 | 8 | 4 |
| 3 | B | 344 | PX4 | C7-O7-C23 | 2.72 | 111.28 | 117.80 | 14 | 3 |
| 3 | A | 618 | PX4 | C11-C10-C9 | 2.72 | 123.66 | 113.69 | 6 | 2 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 390 | PX4 | C5-N1-C3 | 2.72 | 101.83 | 108.98 | 14 | 1 |
| 3 | B | 312 | PX4 | O7-C7-C8 | 2.72 | 118.10 | 108.34 | 6 | 1 |
| 3 | C | 309 | PX4 | C12-C11-C10 | 2.72 | 123.12 | 113.13 | 11 | 1 |
| 3 | C | 331 | PX4 | C8-C7-C6 | 2.72 | 105.44 | 111.78 | 2 | 3 |
| 3 | B | 322 | PX4 | C1-C2-N1 | 2.72 | 124.55 | 115.82 | 9 | 1 |
| 3 | B | 321 | PX4 | O7-C23-O8 | 2.72 | 130.06 | 123.70 | 8 | 5 |
| 3 | B | 350 | PX4 | C1-C2-N1 | 2.72 | 124.55 | 115.82 | 11 | 1 |
| 3 | B | 389 | PX4 | C11-C10-C9 | 2.71 | 123.64 | 113.69 | 1 | 1 |
| 3 | C | 331 | PX4 | C5-N1-C4 | 2.71 | 101.85 | 108.98 | 9 | 2 |
| 3 | C | 347 | PX4 | C4-N1-C3 | 2.71 | 101.85 | 108.98 | 11 | 4 |
| 3 | A | 623 | PX4 | O7-C23-C24 | 2.71 | 105.61 | 111.48 | 8 | 3 |
| 3 | A | 636 | PX4 | O6-C9-C10 | 2.71 | 134.39 | 123.78 | 1 | 1 |
| 3 | A | 641 | PX4 | C1-C2-N1 | 2.71 | 124.53 | 115.82 | 12 | 1 |
| 3 | B | 323 | PX4 | C1-C2-N1 | 2.71 | 124.53 | 115.82 | 13 | 2 |
| 3 | B | 381 | PX4 | O4-P1-O2 | 2.71 | 119.68 | 108.94 | 9 | 1 |
| 3 | A | 614 | PX4 | O7-C7-C6 | 2.71 | 118.07 | 108.34 | 11 | 1 |
| 3 | C | 360 | PX4 | O7-C23-O8 | 2.71 | 130.04 | 123.70 | 2 | 1 |
| 3 | B | 397 | PX4 | C28-C27-C26 | 2.71 | 100.67 | 114.37 | 1 | 1 |
| 3 | A | 620 | PX4 | O5-C9-C10 | 2.71 | 103.58 | 111.83 | 14 | 1 |
| 3 | B | 394 | PX4 | C5-N1-C4 | 2.71 | 101.86 | 108.98 | 7 | 3 |
| 3 | C | 323 | PX4 | C11-C10-C9 | 2.71 | 103.77 | 113.69 | 3 | 2 |
| 3 | A | 621 | PX4 | C4-N1-C3 | 2.71 | 101.86 | 108.98 | 1 | 1 |
| 3 | B | 302 | PX4 | C4-N1-C3 | 2.71 | 116.09 | 108.98 | 11 | 4 |
| 3 | B | 330 | PX4 | C8-C7-C6 | 2.71 | 105.47 | 111.78 | 13 | 4 |
| 3 | B | 400 | PX4 | O5-C9-O6 | 2.71 | 130.40 | 123.63 | 6 | 3 |
| 3 | A | 634 | PX4 | C8-C7-C6 | 2.70 | 118.09 | 111.78 | 3 | 2 |
| 3 | B | 388 | PX4 | C8-O5-C9 | 2.71 | 107.23 | 117.12 | 15 | 1 |
| 3 | C | 313 | PX4 | C11-C10-C9 | 2.71 | 123.61 | 113.69 | 7 | 1 |
| 3 | C | 336 | PX4 | O7-C23-O8 | 2.70 | 130.03 | 123.70 | 5 | 2 |
| 3 | A | 645 | PX4 | C8-C7-C6 | 2.70 | 118.09 | 111.78 | 13 | 3 |
| 3 | B | 336 | PX4 | O5-C9-C10 | 2.70 | 103.59 | 111.83 | 7 | 2 |
| 3 | A | 648 | PX4 | C12-C11-C10 | 2.70 | 103.20 | 113.13 | 2 | 4 |
| 3 | A | 613 | PX4 | C12-C11-C10 | 2.70 | 103.21 | 113.13 | 15 | 1 |
| 3 | B | 309 | PX4 | C26-C25-C24 | 2.70 | 103.21 | 113.13 | 9 | 2 |
| 3 | A | 606 | PX4 | O5-C8-C7 | 2.70 | 116.17 | 108.40 | 3 | 1 |
| 3 | A | 621 | PX4 | C8-O5-C9 | 2.70 | 107.26 | 117.12 | 11 | 1 |
| 3 | A | 632 | PX4 | C33-C32-C31 | 2.70 | 128.00 | 114.37 | 6 | 1 |
| 3 | B | 359 | PX4 | C4-N1-C2 | 2.70 | 99.19 | 109.91 | 8 | 1 |
| 3 | B | 367 | PX4 | O7-C23-O8 | 2.70 | 130.01 | 123.70 | 10 | 3 |
| 3 | B | 393 | PX4 | C31-C30-C29 | 2.70 | 100.74 | 114.37 | 3 | 1 |
| 3 | B | 398 | PX4 | C8-C7-C6 | 2.70 | 105.50 | 111.78 | 10 | 2 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | C | 346 | PX4 | P1-O3-C1 | 2.70 | 134.10 | 121.26 | 10 | 2 |
| 3 | B | 304 | PX4 | C1-C2-N1 | 2.69 | 124.47 | 115.82 | 8 | 1 |
| 3 | B | 340 | PX4 | C25-C24-C23 | 2.70 | 123.57 | 113.69 | 2 | 3 |
| 3 | B | 301 | PX4 | C5-N1-C4 | 2.69 | 101.90 | 108.98 | 8 | 2 |
| 3 | B | 323 | PX4 | C5-N1-C3 | 2.69 | 116.05 | 108.98 | 4 | 2 |
| 3 | C | 348 | PX4 | C4-N1-C3 | 2.69 | 101.90 | 108.98 | 8 | 2 |
| 3 | B | 337 | PX4 | O7-C23-C24 | 2.69 | 105.66 | 111.48 | 2 | 4 |
| 3 | B | 365 | PX4 | O5-C8-C7 | 2.69 | 116.16 | 108.40 | 13 | 6 |
| 3 | B | 396 | PX4 | C25-C24-C23 | 2.69 | 103.83 | 113.69 | 11 | 3 |
| 3 | B | 377 | PX4 | C5-N1-C4 | 2.69 | 101.91 | 108.98 | 3 | 1 |
| 3 | C | 305 | PX4 | C1-C2-N1 | 2.69 | 124.46 | 115.82 | 6 | 2 |
| 3 | C | 313 | PX4 | C5-N1-C3 | 2.69 | 101.91 | 108.98 | 10 | 3 |
| 3 | A | 653 | PX4 | O7-C7-C8 | 2.69 | 118.00 | 108.34 | 10 | 2 |
| 3 | B | 354 | PX4 | C4-N1-C3 | 2.69 | 101.91 | 108.98 | 4 | 5 |
| 3 | A | 615 | PX4 | C8-C7-C6 | 2.69 | 105.52 | 111.78 | 15 | 1 |
| 3 | A | 630 | PX4 | O7-C23-O8 | 2.69 | 129.99 | 123.70 | 4 | 3 |
| 3 | A | 604 | PX4 | O7-C7-C6 | 2.69 | 117.98 | 108.34 | 7 | 6 |
| 3 | B | 315 | PX4 | C8-O5-C9 | 2.69 | 107.29 | 117.12 | 15 | 1 |
| 3 | B | 352 | PX4 | C8-O5-C9 | 2.69 | 107.29 | 117.12 | 2 | 1 |
| 3 | A | 651 | PX4 | C8-O5-C9 | 2.69 | 107.30 | 117.12 | 14 | 1 |
| 3 | C | 327 | PX4 | O7-C23-O8 | 2.69 | 129.99 | 123.70 | 3 | 2 |
| 3 | A | 614 | PX4 | C8-C7-C6 | 2.69 | 105.52 | 111.78 | 7 | 2 |
| 3 | A | 620 | PX4 | C4-N1-C3 | 2.69 | 101.92 | 108.98 | 14 | 1 |
| 3 | A | 632 | PX4 | C12-C11-C10 | 2.69 | 122.99 | 113.13 | 14 | 1 |
| 3 | B | 375 | PX4 | C8-O5-C9 | 2.69 | 107.30 | 117.12 | 14 | 2 |
| 3 | C | 334 | PX4 | O5-C9-C10 | 2.68 | 103.65 | 111.83 | 7 | 1 |
| 3 | C | 337 | PX4 | O7-C7-C8 | 2.68 | 117.97 | 108.34 | 5 | 2 |
| 3 | A | 612 | PX4 | C8-O5-C9 | 2.68 | 107.31 | 117.12 | 2 | 2 |
| 3 | B | 358 | PX4 | C11-C10-C9 | 2.68 | 123.52 | 113.69 | 11 | 1 |
| 3 | B | 363 | PX4 | C25-C24-C23 | 2.68 | 103.86 | 113.69 | 4 | 2 |
| 3 | B | 384 | PX4 | C8-O5-C9 | 2.68 | 107.31 | 117.12 | 11 | 1 |
| 3 | B | 333 | PX4 | O5-C9-O6 | 2.68 | 130.33 | 123.63 | 9 | 1 |
| 3 | C | 312 | PX4 | O5-C9-C10 | 2.68 | 103.66 | 111.83 | 7 | 4 |
| 3 | C | 335 | PX4 | C1-C2-N1 | 2.68 | 124.43 | 115.82 | 7 | 3 |
| 3 | A | 608 | PX4 | C5-N1-C4 | 2.68 | 101.94 | 108.98 | 13 | 2 |
| 3 | A | 651 | PX4 | O5-C9-C10 | 2.68 | 103.67 | 111.83 | 8 | 1 |
| 3 | B | 307 | PX4 | C12-C11-C10 | 2.68 | 103.28 | 113.13 | 12 | 3 |
| 3 | B | 337 | PX4 | O7-C23-O8 | 2.68 | 129.97 | 123.70 | 5 | 2 |
| 3 | C | 304 | PX4 | C7-O7-C23 | 2.68 | 111.38 | 117.80 | 4 | 4 |
| 3 | C | 310 | PX4 | O7-C23-O8 | 2.68 | 129.97 | 123.70 | 1 | 4 |
| 3 | B | 349 | PX4 | C8-O5-C9 | 2.68 | 107.33 | 117.12 | 2 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 383 | PX4 | O5-C8-C7 | 2.68 | 116.12 | 108.40 | 6 | 7 |
| 3 | C | 314 | PX4 | C12-C11-C10 | 2.68 | 122.97 | 113.13 | 3 | 1 |
| 3 | C | 314 | PX4 | O7-C7-C6 | 2.68 | 98.73 | 108.34 | 7 | 1 |
| 3 | C | 352 | PX4 | C8-O5-C9 | 2.68 | 126.91 | 117.12 | 5 | 3 |
| 3 | A | 619 | PX4 | O7-C23-C24 | 2.68 | 105.69 | 111.48 | 7 | 4 |
| 3 | B | 331 | PX4 | C12-C11-C10 | 2.68 | 103.29 | 113.13 | 1 | 2 |
| 3 | B | 355 | PX4 | C5-N1-C4 | 2.68 | 116.01 | 108.98 | 7 | 1 |
| 3 | C | 347 | PX4 | C12-C11-C10 | 2.68 | 103.29 | 113.13 | 2 | 1 |
| 3 | B | 354 | PX4 | C26-C25-C24 | 2.67 | 103.30 | 113.13 | 11 | 1 |
| 3 | C | 326 | PX4 | C12-C11-C10 | 2.67 | 103.30 | 113.13 | 5 | 1 |
| 3 | C | 347 | PX4 | C3-N1-C2 | 2.67 | 120.54 | 109.91 | 1 | 1 |
| 3 | A | 613 | PX4 | C7-O7-C23 | 2.67 | 111.40 | 117.80 | 11 | 5 |
| 3 | B | 315 | PX4 | O7-C23-O8 | 2.67 | 129.95 | 123.70 | 11 | 1 |
| 3 | C | 324 | PX4 | O5-C9-C10 | 2.67 | 103.69 | 111.83 | 3 | 2 |
| 3 | C | 356 | PX4 | C5-N1-C4 | 2.67 | 101.96 | 108.98 | 9 | 3 |
| 3 | B | 336 | PX4 | C7-O7-C23 | 2.67 | 111.41 | 117.80 | 14 | 4 |
| 3 | B | 359 | PX4 | O5-C9-C10 | 2.67 | 103.70 | 111.83 | 1 | 1 |
| 3 | C | 343 | PX4 | C5-N1-C4 | 2.67 | 115.99 | 108.98 | 13 | 2 |
| 3 | C | 349 | PX4 | O5-C9-C10 | 2.67 | 103.69 | 111.83 | 15 | 2 |
| 3 | A | 631 | PX4 | C5-N1-C4 | 2.67 | 101.97 | 108.98 | 14 | 3 |
| 3 | B | 385 | PX4 | C12-C11-C10 | 2.67 | 122.93 | 113.13 | 5 | 1 |
| 3 | A | 607 | PX4 | C5-N1-C4 | 2.67 | 115.98 | 108.98 | 13 | 2 |
| 3 | B | 327 | PX4 | O5-C9-O6 | 2.67 | 130.30 | 123.63 | 10 | 2 |
| 3 | B | 364 | PX4 | C5-N1-C3 | 2.67 | 101.97 | 108.98 | 3 | 2 |
| 3 | C | 301 | PX4 | O7-C23-O8 | 2.67 | 129.94 | 123.70 | 7 | 4 |
| 3 | C | 303 | PX4 | O7-C7-C8 | 2.67 | 117.91 | 108.34 | 15 | 1 |
| 3 | C | 343 | PX4 | C7-O7-C23 | 2.67 | 111.41 | 117.80 | 9 | 5 |
| 3 | C | 320 | PX4 | C5-N1-C4 | 2.67 | 115.98 | 108.98 | 10 | 3 |
| 3 | C | 360 | PX4 | C8-C7-C6 | 2.67 | 105.57 | 111.78 | 12 | 4 |
| 3 | C | 360 | PX4 | C8-O5-C9 | 2.67 | 107.37 | 117.12 | 5 | 2 |
| 3 | B | 337 | PX4 | C8-O5-C9 | 2.67 | 107.37 | 117.12 | 4 | 1 |
| 3 | B | 393 | PX4 | C8-O5-C9 | 2.66 | 126.86 | 117.12 | 7 | 1 |
| 3 | C | 313 | PX4 | C26-C25-C24 | 2.67 | 103.33 | 113.13 | 9 | 1 |
| 3 | B | 313 | PX4 | C5-N1-C3 | 2.66 | 101.98 | 108.98 | 11 | 1 |
| 3 | A | 616 | PX4 | C25-C24-C23 | 2.66 | 103.94 | 113.69 | 15 | 1 |
| 3 | A | 637 | PX4 | C8-O5-C9 | 2.66 | 107.38 | 117.12 | 12 | 3 |
| 3 | C | 345 | PX4 | O7-C7-C6 | 2.66 | 117.90 | 108.34 | 6 | 1 |
| 3 | B | 305 | PX4 | O5-C9-O6 | 2.66 | 130.29 | 123.63 | 10 | 2 |
| 3 | B | 313 | PX4 | C26-C25-C24 | 2.66 | 122.90 | 113.13 | 5 | 1 |
| 3 | B | 333 | PX4 | P1-O3-C1 | 2.66 | 108.59 | 121.26 | 4 | 1 |
| 3 | B | 373 | PX4 | C5-N1-C3 | 2.66 | 101.99 | 108.98 | 9 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 384 | PX4 | C27-C26-C25 | 2.66 | 127.82 | 114.37 | 7 | 1 |
| 3 | C | 320 | PX4 | C25-C24-C23 | 2.66 | 103.94 | 113.69 | 10 | 1 |
| 3 | A | 616 | PX4 | O5-C8-C7 | 2.66 | 116.06 | 108.40 | 4 | 1 |
| 3 | A | 614 | PX4 | O5-C9-O6 | 2.66 | 130.27 | 123.63 | 1 | 2 |
| 3 | A | 644 | PX4 | O5-C9-O6 | 2.66 | 130.27 | 123.63 | 9 | 2 |
| 3 | B | 338 | PX4 | C8-C7-C6 | 2.66 | 117.98 | 111.78 | 13 | 5 |
| 3 | B | 354 | PX4 | O5-C9-O6 | 2.66 | 130.28 | 123.63 | 1 | 3 |
| 3 | B | 380 | PX4 | C4-N1-C3 | 2.66 | 115.96 | 108.98 | 13 | 1 |
| 3 | B | 335 | PX4 | C8-C7-C6 | 2.66 | 105.59 | 111.78 | 5 | 2 |
| 3 | B | 352 | PX4 | C7-O7-C23 | 2.66 | 111.44 | 117.80 | 12 | 2 |
| 3 | A | 625 | PX4 | C3-N1-C2 | 2.65 | 120.46 | 109.91 | 13 | 1 |
| 3 | B | 357 | PX4 | O7-C7-C8 | 2.65 | 117.87 | 108.34 | 7 | 2 |
| 3 | C | 342 | PX4 | O5-C9-C10 | 2.65 | 103.74 | 111.83 | 12 | 2 |
| 3 | C | 361 | PX4 | C1-C2-N1 | 2.66 | 124.34 | 115.82 | 15 | 1 |
| 3 | B | 338 | PX4 | O5-C9-O6 | 2.65 | 130.26 | 123.63 | 4 | 1 |
| 3 | C | 343 | PX4 | C4-N1-C3 | 2.65 | 115.94 | 108.98 | 15 | 4 |
| 3 | C | 361 | PX4 | C5-N1-C3 | 2.65 | 102.01 | 108.98 | 8 | 2 |
| 3 | A | 638 | PX4 | C11-C10-C9 | 2.65 | 103.98 | 113.69 | 14 | 1 |
| 3 | B | 337 | PX4 | O5-C8-C7 | 2.65 | 116.03 | 108.40 | 13 | 4 |
| 3 | C | 358 | PX4 | C5-N1-C3 | 2.65 | 115.94 | 108.98 | 14 | 2 |
| 3 | A | 603 | PX4 | O7-C7-C6 | 2.65 | 117.84 | 108.34 | 7 | 1 |
| 3 | A | 637 | PX4 | C8-C7-C6 | 2.65 | 105.61 | 111.78 | 10 | 1 |
| 3 | B | 370 | PX4 | O5-C9-C10 | 2.65 | 103.76 | 111.83 | 2 | 2 |
| 3 | A | 648 | PX4 | C4-N1-C3 | 2.65 | 102.02 | 108.98 | 6 | 2 |
| 3 | B | 382 | PX4 | O5-C9-O6 | 2.65 | 130.25 | 123.63 | 7 | 2 |
| 3 | B | 384 | PX4 | O5-C9-C10 | 2.65 | 103.77 | 111.83 | 6 | 2 |
| 3 | C | 363 | PX4 | C8-C7-C6 | 2.65 | 105.61 | 111.78 | 5 | 5 |
| 3 | A | 618 | PX4 | C8-C7-C6 | 2.65 | 105.62 | 111.78 | 3 | 1 |
| 3 | A | 649 | PX4 | O5-C8-C7 | 2.65 | 116.02 | 108.40 | 15 | 5 |
| 3 | B | 312 | PX4 | C7-O7-C23 | 2.64 | 111.47 | 117.80 | 10 | 2 |
| 3 | B | 333 | PX4 | C1-C2-N1 | 2.65 | 124.31 | 115.82 | 12 | 1 |
| 3 | B | 335 | PX4 | O5-C9-O6 | 2.65 | 130.25 | 123.63 | 4 | 3 |
| 3 | C | 304 | PX4 | C8-C7-C6 | 2.65 | 117.95 | 111.78 | 4 | 2 |
| 3 | C | 333 | PX4 | O7-C7-C8 | 2.65 | 117.84 | 108.34 | 3 | 1 |
| 3 | B | 345 | PX4 | C5-N1-C4 | 2.64 | 102.03 | 108.98 | 12 | 1 |
| 3 | C | 353 | PX4 | C5-N1-C4 | 2.64 | 102.03 | 108.98 | 15 | 3 |
| 3 | A | 633 | PX4 | C4-N1-C3 | 2.64 | 115.91 | 108.98 | 11 | 3 |
| 3 | B | 360 | PX4 | C8-C7-C6 | 2.64 | 105.63 | 111.78 | 1 | 1 |
| 3 | C | 328 | PX4 | C11-C10-C9 | 2.64 | 104.02 | 113.69 | 12 | 1 |
| 3 | B | 366 | PX4 | C1-C2-N1 | 2.64 | 124.29 | 115.82 | 5 | 2 |
| 3 | C | 361 | PX4 | C11-C10-C9 | 2.64 | 104.03 | 113.69 | 12 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | C | 363 | PX4 | C5-N1-C3 | 2.64 | 102.05 | 108.98 | 15 | 2 |
| 3 | B | 327 | PX4 | O5-C8-C7 | 2.64 | 116.00 | 108.40 | 14 | 1 |
| 3 | B | 395 | PX4 | O1-P1-O2 | 2.64 | 124.71 | 112.44 | 10 | 1 |
| 3 | B | 306 | PX4 | O5-C9-C10 | 2.64 | 103.80 | 111.83 | 1 | 1 |
| 3 | B | 327 | PX4 | C8-O5-C9 | 2.63 | 107.49 | 117.12 | 8 | 1 |
| 3 | C | 313 | PX4 | O7-C23-O8 | 2.64 | 129.87 | 123.70 | 6 | 1 |
| 3 | A | 638 | PX4 | O5-C9-O6 | 2.63 | 130.22 | 123.63 | 3 | 4 |
| 3 | B | 306 | PX4 | C4-N1-C3 | 2.63 | 115.89 | 108.98 | 4 | 2 |
| 3 | C | 302 | PX4 | C8-C7-C6 | 2.63 | 105.64 | 111.78 | 4 | 2 |
| 3 | A | 634 | PX4 | C7-O7-C23 | 2.63 | 111.50 | 117.80 | 2 | 1 |
| 3 | A | 637 | PX4 | O5-C9-O6 | 2.63 | 130.21 | 123.63 | 5 | 3 |
| 3 | C | 327 | PX4 | C8-C7-C6 | 2.63 | 105.65 | 111.78 | 12 | 6 |
| 3 | A | 618 | PX4 | C4-N1-C3 | 2.63 | 102.07 | 108.98 | 15 | 2 |
| 3 | A | 638 | PX4 | C5-N1-C3 | 2.63 | 102.07 | 108.98 | 4 | 1 |
| 3 | B | 308 | PX4 | C4-N1-C3 | 2.63 | 102.07 | 108.98 | 15 | 1 |
| 3 | B | 339 | PX4 | O5-C9-O6 | 2.63 | 130.20 | 123.63 | 8 | 1 |
| 3 | B | 357 | PX4 | C25-C24-C23 | 2.63 | 104.06 | 113.69 | 6 | 2 |
| 3 | C | 330 | PX4 | C5-N1-C4 | 2.63 | 102.07 | 108.98 | 15 | 2 |
| 3 | B | 374 | PX4 | C3-N1-C2 | 2.63 | 99.47 | 109.91 | 4 | 1 |
| 3 | B | 328 | PX4 | O5-C9-C10 | 2.63 | 103.83 | 111.83 | 11 | 2 |
| 3 | C | 323 | PX4 | O7-C23-O8 | 2.63 | 129.85 | 123.70 | 6 | 5 |
| 3 | C | 363 | PX4 | O5-C9-C10 | 2.63 | 103.83 | 111.83 | 15 | 2 |
| 3 | C | 307 | PX4 | C20-C19-C18 | 2.62 | 101.10 | 114.37 | 6 | 1 |
| 3 | C | 325 | PX4 | C26-C25-C24 | 2.62 | 103.48 | 113.13 | 3 | 2 |
| 3 | A | 633 | PX4 | C5-N1-C3 | 2.62 | 102.09 | 108.98 | 10 | 3 |
| 3 | C | 324 | PX4 | C4-N1-C3 | 2.62 | 102.09 | 108.98 | 9 | 1 |
| 3 | C | 352 | PX4 | C5-N1-C4 | 2.62 | 102.08 | 108.98 | 11 | 1 |
| 3 | A | 636 | PX4 | C4-N1-C3 | 2.62 | 102.09 | 108.98 | 7 | 1 |
| 3 | A | 652 | PX4 | C8-O5-C9 | 2.62 | 107.54 | 117.12 | 15 | 2 |
| 3 | B | 398 | PX4 | O7-C23-O8 | 2.62 | 129.84 | 123.70 | 5 | 3 |
| 3 | C | 317 | PX4 | C34-C33-C32 | 2.62 | 101.12 | 114.37 | 1 | 1 |
| 3 | C | 341 | PX4 | C1-C2-N1 | 2.62 | 124.24 | 115.82 | 12 | 1 |
| 3 | B | 322 | PX4 | C5-N1-C3 | 2.62 | 102.10 | 108.98 | 10 | 1 |
| 3 | B | 338 | PX4 | O6-C9-C10 | 2.62 | 113.54 | 123.78 | 1 | 1 |
| 3 | A | 641 | PX4 | O7-C23-O8 | 2.62 | 129.82 | 123.70 | 9 | 5 |
| 3 | B | 330 | PX4 | C5-N1-C4 | 2.62 | 102.10 | 108.98 | 12 | 1 |
| 3 | B | 331 | PX4 | O7-C7-C6 | 2.62 | 117.73 | 108.34 | 13 | 2 |
| 3 | B | 332 | PX4 | C1-C2-N1 | 2.62 | 124.22 | 115.82 | 1 | 2 |
| 3 | C | 351 | PX4 | O5-C8-C7 | 2.62 | 115.94 | 108.40 | 14 | 4 |
| 3 | B | 327 | PX4 | C11-C10-C9 | 2.61 | 123.27 | 113.69 | 10 | 1 |
| 3 | A | 621 | PX4 | O7-C7-C8 | 2.61 | 117.72 | 108.34 | 2 | 4 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | A | 648 | PX4 | O5-C8-C7 | 2.61 | 115.93 | 108.40 | 14 | 4 |
| 3 | B | 342 | PX4 | C8-C7-C6 | 2.61 | 105.69 | 111.78 | 15 | 2 |
| 3 | B | 365 | PX4 | C25-C24-C23 | 2.61 | 104.12 | 113.69 | 15 | 2 |
| 3 | C | 329 | PX4 | C8-C7-C6 | 2.61 | 117.88 | 111.78 | 3 | 3 |
| 3 | B | 350 | PX4 | C4-N1-C3 | 2.61 | 102.11 | 108.98 | 4 | 2 |
| 3 | B | 360 | PX4 | O7-C23-O8 | 2.61 | 129.81 | 123.70 | 1 | 5 |
| 3 | B | 380 | PX4 | O7-C23-O8 | 2.61 | 129.81 | 123.70 | 5 | 4 |
| 3 | C | 325 | PX4 | C4-N1-C3 | 2.61 | 102.12 | 108.98 | 12 | 2 |
| 3 | A | 616 | PX4 | C4-N1-C3 | 2.61 | 102.12 | 108.98 | 3 | 3 |
| 3 | A | 609 | PX4 | O1-P1-O2 | 2.61 | 124.58 | 112.44 | 12 | 1 |
| 3 | A | 624 | PX4 | O5-C9-O6 | 2.61 | 130.15 | 123.63 | 2 | 1 |
| 3 | A | 647 | PX4 | C5-N1-C4 | 2.61 | 102.12 | 108.98 | 4 | 2 |
| 3 | A | 649 | PX4 | O7-C7-C6 | 2.61 | 117.70 | 108.34 | 2 | 1 |
| 3 | A | 632 | PX4 | O7-C7-C8 | 2.61 | 117.69 | 108.34 | 3 | 3 |
| 3 | B | 323 | PX4 | O7-C23-C24 | 2.61 | 105.84 | 111.48 | 5 | 3 |
| 3 | B | 325 | PX4 | C26-C25-C24 | 2.61 | 103.55 | 113.13 | 5 | 1 |
| 3 | A | 604 | PX4 | O5-C8-C7 | 2.60 | 115.90 | 108.40 | 3 | 2 |
| 3 | A | 627 | PX4 | O4-P1-O2 | 2.60 | 98.62 | 108.94 | 8 | 1 |
| 3 | B | 375 | PX4 | C1-C2-N1 | 2.60 | 124.18 | 115.82 | 12 | 4 |
| 3 | B | 306 | PX4 | O7-C7-C6 | 2.60 | 117.68 | 108.34 | 8 | 1 |
| 3 | B | 364 | PX4 | O7-C23-O8 | 2.60 | 129.79 | 123.70 | 9 | 4 |
| 3 | C | 323 | PX4 | C3-N1-C2 | 2.60 | 120.25 | 109.91 | 2 | 1 |
| 3 | A | 602 | PX4 | O7-C7-C6 | 2.60 | 117.67 | 108.34 | 1 | 2 |
| 3 | B | 368 | PX4 | C1-C2-N1 | 2.60 | 124.17 | 115.82 | 5 | 2 |
| 3 | C | 363 | PX4 | C1-C2-N1 | 2.60 | 124.17 | 115.82 | 15 | 1 |
| 3 | A | 611 | PX4 | P1-O3-C1 | 2.60 | 133.63 | 121.26 | 10 | 2 |
| 3 | B | 316 | PX4 | O7-C7-C8 | 2.60 | 117.67 | 108.34 | 1 | 2 |
| 3 | C | 364 | PX4 | O7-C23-C24 | 2.60 | 105.86 | 111.48 | 2 | 3 |
| 3 | B | 324 | PX4 | O5-C9-O6 | 2.60 | 130.12 | 123.63 | 15 | 2 |
| 3 | C | 331 | PX4 | O5-C9-O6 | 2.60 | 130.12 | 123.63 | 3 | 1 |
| 3 | A | 611 | PX4 | O7-C23-C24 | 2.59 | 105.87 | 111.48 | 8 | 2 |
| 3 | A | 632 | PX4 | C7-O7-C23 | 2.59 | 111.59 | 117.80 | 9 | 2 |
| 3 | B | 349 | PX4 | O7-C23-O8 | 2.59 | 129.77 | 123.70 | 13 | 3 |
| 3 | C | 339 | PX4 | C5-N1-C4 | 2.59 | 102.16 | 108.98 | 11 | 3 |
| 3 | C | 345 | PX4 | O7-C7-C8 | 2.59 | 117.65 | 108.34 | 1 | 2 |
| 3 | C | 354 | PX4 | C5-N1-C4 | 2.59 | 102.16 | 108.98 | 8 | 1 |
| 3 | A | 647 | PX4 | C1-C2-N1 | 2.59 | 124.14 | 115.82 | 3 | 4 |
| 3 | B | 305 | PX4 | O7-C7-C8 | 2.59 | 117.64 | 108.34 | 3 | 1 |
| 3 | C | 314 | PX4 | O7-C7-C8 | 2.59 | 117.65 | 108.34 | 5 | 2 |
| 3 | B | 350 | PX4 | O7-C7-C6 | 2.59 | 117.64 | 108.34 | 7 | 2 |
| 3 | B | 384 | PX4 | C5-N1-C3 | 2.59 | 102.17 | 108.98 | 3 | 2 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 329 | PX4 | O5-C8-C7 | 2.59 | 115.86 | 108.40 | 9 | 2 |
| 3 | B | 337 | PX4 | C1-C2-N1 | 2.59 | 124.14 | 115.82 | 3 | 2 |
| 3 | A | 621 | PX4 | O1-P1-O2 | 2.59 | 124.49 | 112.44 | 6 | 1 |
| 3 | A | 634 | PX4 | O7-C7-C6 | 2.59 | 117.63 | 108.34 | 8 | 2 |
| 3 | B | 313 | PX4 | C8-C7-C6 | 2.59 | 117.82 | 111.78 | 7 | 3 |
| 3 | C | 309 | PX4 | O4-P1-O2 | 2.59 | 98.67 | 108.94 | 5 | 1 |
| 3 | C | 315 | PX4 | C11-C10-C9 | 2.59 | 104.21 | 113.69 | 9 | 2 |
| 3 | C | 357 | PX4 | P1-O3-C1 | 2.59 | 133.59 | 121.26 | 12 | 1 |
| 3 | A | 618 | PX4 | C5-N1-C3 | 2.59 | 102.18 | 108.98 | 10 | 1 |
| 3 | A | 609 | PX4 | C1-C2-N1 | 2.59 | 124.12 | 115.82 | 3 | 3 |
| 3 | A | 634 | PX4 | C1-C2-N1 | 2.59 | 124.12 | 115.82 | 5 | 3 |
| 3 | B | 304 | PX4 | C12-C11-C10 | 2.59 | 103.62 | 113.13 | 4 | 1 |
| 3 | C | 317 | PX4 | O7-C23-C24 | 2.59 | 105.88 | 111.48 | 2 | 3 |
| 3 | B | 322 | PX4 | C4-N1-C3 | 2.59 | 102.18 | 108.98 | 11 | 2 |
| 3 | A | 602 | PX4 | O5-C9-C10 | 2.59 | 103.95 | 111.83 | 8 | 1 |
| 3 | A | 644 | PX4 | C5-N1-C4 | 2.59 | 102.19 | 108.98 | 3 | 1 |
| 3 | A | 646 | PX4 | O7-C23-C24 | 2.58 | 105.89 | 111.48 | 5 | 5 |
| 3 | B | 307 | PX4 | C25-C24-C23 | 2.59 | 123.17 | 113.69 | 3 | 1 |
| 3 | A | 647 | PX4 | O7-C23-C24 | 2.58 | 105.89 | 111.48 | 11 | 3 |
| 3 | B | 322 | PX4 | C5-N1-C4 | 2.58 | 115.76 | 108.98 | 5 | 2 |
| 3 | B | 324 | PX4 | O7-C23-C24 | 2.58 | 105.89 | 111.48 | 6 | 3 |
| 3 | B | 353 | PX4 | O1-P1-O2 | 2.59 | 124.47 | 112.44 | 3 | 2 |
| 3 | B | 392 | PX4 | C1-C2-N1 | 2.58 | 124.11 | 115.82 | 2 | 2 |
| 3 | B | 351 | PX4 | O7-C23-C24 | 2.58 | 105.89 | 111.48 | 7 | 4 |
| 3 | A | 644 | PX4 | O1-P1-O4 | 2.58 | 119.27 | 107.57 | 4 | 1 |
| 3 | B | 306 | PX4 | C31-C30-C29 | 2.58 | 101.33 | 114.37 | 12 | 1 |
| 3 | B | 327 | PX4 | P1-O3-C1 | 2.58 | 108.98 | 121.26 | 3 | 1 |
| 3 | B | 327 | PX4 | O7-C7-C8 | 2.58 | 117.60 | 108.34 | 8 | 4 |
| 3 | B | 377 | PX4 | O7-C23-O8 | 2.58 | 129.74 | 123.70 | 13 | 1 |
| 3 | B | 389 | PX4 | C25-C24-C23 | 2.58 | 104.24 | 113.69 | 6 | 2 |
| 3 | A | 605 | PX4 | O5-C9-C10 | 2.58 | 103.98 | 111.83 | 1 | 2 |
| 3 | A | 632 | PX4 | C5-N1-C4 | 2.58 | 115.75 | 108.98 | 10 | 1 |
| 3 | B | 360 | PX4 | C1-C2-N1 | 2.58 | 124.10 | 115.82 | 5 | 2 |
| 3 | A | 640 | PX4 | O5-C9-C10 | 2.58 | 103.97 | 111.83 | 8 | 3 |
| 3 | C | 301 | PX4 | C12-C11-C10 | 2.58 | 122.60 | 113.13 | 10 | 2 |
| 3 | C | 313 | PX4 | C1-C2-N1 | 2.58 | 124.10 | 115.82 | 6 | 1 |
| 3 | C | 351 | PX4 | O5-C9-C10 | 2.58 | 119.70 | 111.83 | 14 | 2 |
| 3 | B | 373 | PX4 | C1-C2-N1 | 2.58 | 124.09 | 115.82 | 7 | 1 |
| 3 | B | 376 | PX4 | O7-C7-C8 | 2.58 | 117.59 | 108.34 | 14 | 1 |
| 3 | C | 334 | PX4 | O5-C9-O6 | 2.58 | 130.07 | 123.63 | 7 | 1 |
| 3 | B | 352 | PX4 | C11-C10-C9 | 2.58 | 123.13 | 113.69 | 6 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 310 | PX4 | O7-C23-C24 | 2.57 | 105.91 | 111.48 | 14 | 5 |
| 3 | C | 335 | PX4 | C11-C10-C9 | 2.57 | 104.26 | 113.69 | 8 | 1 |
| 3 | B | 311 | PX4 | C5-N1-C2 | 2.57 | 120.14 | 109.91 | 12 | 1 |
| 3 | B | 389 | PX4 | C5-N1-C4 | 2.57 | 102.22 | 108.98 | 10 | 4 |
| 3 | C | 311 | PX4 | O7-C23-C24 | 2.57 | 105.92 | 111.48 | 1 | 3 |
| 3 | C | 349 | PX4 | O7-C23-O8 | 2.57 | 129.72 | 123.70 | 8 | 1 |
| 3 | A | 633 | PX4 | O5-C9-O6 | 2.57 | 130.06 | 123.63 | 9 | 2 |
| 3 | B | 348 | PX4 | O5-C9-C10 | 2.57 | 103.99 | 111.83 | 15 | 3 |
| 3 | C | 363 | PX4 | C5-N1-C2 | 2.57 | 120.14 | 109.91 | 7 | 2 |
| 3 | B | 376 | PX4 | C25-C24-C23 | 2.57 | 104.27 | 113.69 | 10 | 1 |
| 3 | B | 392 | PX4 | O7-C23-C24 | 2.57 | 105.92 | 111.48 | 10 | 4 |
| 3 | A | 617 | PX4 | C8-C7-C6 | 2.57 | 105.79 | 111.78 | 9 | 2 |
| 3 | B | 346 | PX4 | C8-C7-C6 | 2.57 | 117.78 | 111.78 | 9 | 1 |
| 3 | C | 325 | PX4 | C7-O7-C23 | 2.57 | 111.64 | 117.80 | 1 | 5 |
| 3 | C | 348 | PX4 | C1-C2-N1 | 2.57 | 124.07 | 115.82 | 3 | 1 |
| 3 | C | 359 | PX4 | O5-C9-C10 | 2.57 | 104.00 | 111.83 | 2 | 1 |
| 3 | B | 359 | PX4 | O5-C9-O6 | 2.57 | 130.06 | 123.63 | 1 | 1 |
| 3 | B | 393 | PX4 | C1-C2-N1 | 2.57 | 124.07 | 115.82 | 9 | 2 |
| 3 | B | 340 | PX4 | O7-C7-C8 | 2.57 | 117.56 | 108.34 | 1 | 1 |
| 3 | B | 383 | PX4 | C8-O5-C9 | 2.57 | 107.73 | 117.12 | 7 | 1 |
| 3 | A | 614 | PX4 | O5-C8-C7 | 2.57 | 115.79 | 108.40 | 10 | 5 |
| 3 | A | 634 | PX4 | C3-N1-C2 | 2.57 | 120.11 | 109.91 | 4 | 1 |
| 3 | C | 355 | PX4 | O7-C7-C8 | 2.57 | 117.55 | 108.34 | 1 | 1 |
| 3 | B | 357 | PX4 | C7-O7-C23 | 2.57 | 111.65 | 117.80 | 1 | 2 |
| 3 | B | 324 | PX4 | C1-C2-N1 | 2.57 | 124.06 | 115.82 | 5 | 4 |
| 3 | B | 385 | PX4 | O7-C7-C6 | 2.56 | 117.54 | 108.34 | 9 | 1 |
| 3 | C | 306 | PX4 | P1-O3-C1 | 2.56 | 133.47 | 121.26 | 3 | 1 |
| 3 | C | 364 | PX4 | O5-C9-O6 | 2.57 | 130.04 | 123.63 | 5 | 2 |
| 3 | A | 631 | PX4 | O7-C23-O8 | 2.56 | 129.70 | 123.70 | 1 | 3 |
| 3 | A | 648 | PX4 | O7-C7-C6 | 2.56 | 117.54 | 108.34 | 7 | 1 |
| 3 | A | 650 | PX4 | C25-C24-C23 | 2.56 | 104.31 | 113.69 | 12 | 1 |
| 3 | C | 312 | PX4 | O7-C23-C24 | 2.56 | 117.03 | 111.48 | 2 | 2 |
| 3 | B | 304 | PX4 | O7-C23-C24 | 2.56 | 105.94 | 111.48 | 9 | 1 |
| 3 | B | 322 | PX4 | P1-O3-C1 | 2.56 | 109.07 | 121.26 | 12 | 1 |
| 3 | C | 302 | PX4 | C7-O7-C23 | 2.56 | 111.66 | 117.80 | 8 | 3 |
| 3 | B | 389 | PX4 | O7-C7-C8 | 2.56 | 117.53 | 108.34 | 14 | 2 |
| 3 | C | 321 | PX4 | C4-N1-C3 | 2.56 | 102.25 | 108.98 | 4 | 1 |
| 3 | B | 316 | PX4 | C8-O5-C9 | 2.56 | 107.76 | 117.12 | 11 | 1 |
| 3 | B | 388 | PX4 | O7-C7-C8 | 2.56 | 99.16 | 108.34 | 7 | 2 |
| 3 | B | 400 | PX4 | C5-N1-C3 | 2.56 | 102.25 | 108.98 | 9 | 2 |
| 3 | C | 312 | PX4 | C25-C24-C23 | 2.56 | 123.07 | 113.69 | 7 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | C | 322 | PX4 | C1-C2-N1 | 2.56 | 124.04 | 115.82 | 10 | 3 |
| 3 | A | 634 | PX4 | C34-C33-C32 | 2.56 | 101.44 | 114.37 | 10 | 1 |
| 3 | A | 645 | PX4 | O7-C7-C8 | 2.56 | 117.52 | 108.34 | 13 | 2 |
| 3 | B | 362 | PX4 | C8-O5-C9 | 2.56 | 107.77 | 117.12 | 6 | 1 |
| 3 | B | 390 | PX4 | O7-C7-C8 | 2.56 | 117.52 | 108.34 | 9 | 2 |
| 3 | B | 399 | PX4 | C8-O5-C9 | 2.56 | 107.77 | 117.12 | 4 | 1 |
| 3 | C | 322 | PX4 | C5-N1-C3 | 2.56 | 115.69 | 108.98 | 8 | 3 |
| 3 | A | 653 | PX4 | O5-C9-C10 | 2.56 | 104.04 | 111.83 | 7 | 1 |
| 3 | B | 340 | PX4 | C7-O7-C23 | 2.56 | 111.68 | 117.80 | 9 | 4 |
| 3 | B | 384 | PX4 | C25-C24-C23 | 2.56 | 104.33 | 113.69 | 11 | 1 |
| 3 | A | 637 | PX4 | C5-N1-C3 | 2.55 | 102.27 | 108.98 | 3 | 4 |
| 3 | B | 328 | PX4 | C5-N1-C3 | 2.55 | 115.69 | 108.98 | 1 | 2 |
| 3 | B | 333 | PX4 | O7-C23-O8 | 2.55 | 117.73 | 123.70 | 5 | 2 |
| 3 | B | 346 | PX4 | O7-C23-C24 | 2.55 | 105.96 | 111.48 | 8 | 2 |
| 3 | C | 342 | PX4 | O5-C9-O6 | 2.55 | 130.02 | 123.63 | 6 | 2 |
| 3 | C | 301 | PX4 | O7-C7-C6 | 2.55 | 117.50 | 108.34 | 4 | 1 |
| 3 | C | 351 | PX4 | C3-N1-C2 | 2.55 | 120.06 | 109.91 | 7 | 1 |
| 3 | B | 343 | PX4 | C5-N1-C3 | 2.55 | 115.68 | 108.98 | 7 | 2 |
| 3 | B | 349 | PX4 | C4-N1-C3 | 2.55 | 102.27 | 108.98 | 5 | 2 |
| 3 | C | 338 | PX4 | O7-C7-C8 | 2.55 | 117.50 | 108.34 | 13 | 5 |
| 3 | A | 639 | PX4 | C1-C2-N1 | 2.55 | 124.00 | 115.82 | 2 | 2 |
| 3 | A | 650 | PX4 | C11-C10-C9 | 2.55 | 104.35 | 113.69 | 6 | 2 |
| 3 | A | 652 | PX4 | C4-N1-C3 | 2.55 | 102.28 | 108.98 | 1 | 2 |
| 3 | B | 395 | PX4 | O1-P1-O3 | 2.55 | 119.13 | 107.57 | 5 | 1 |
| 3 | A | 609 | PX4 | C25-C24-C23 | 2.55 | 104.36 | 113.69 | 10 | 2 |
| 3 | A | 654 | PX4 | O7-C23-O8 | 2.55 | 129.66 | 123.70 | 12 | 2 |
| 3 | B | 304 | PX4 | C8-O5-C9 | 2.55 | 107.80 | 117.12 | 13 | 1 |
| 3 | B | 317 | PX4 | O1-P1-O2 | 2.55 | 124.30 | 112.44 | 7 | 1 |
| 3 | C | 328 | PX4 | C14-C13-C12 | 2.55 | 101.48 | 114.37 | 14 | 1 |
| 3 | C | 361 | PX4 | O5-C9-C10 | 2.55 | 104.06 | 111.83 | 7 | 1 |
| 3 | B | 319 | PX4 | O3-C1-C2 | 2.55 | 121.91 | 109.65 | 7 | 1 |
| 3 | B | 319 | PX4 | P1-O3-C1 | 2.55 | 133.38 | 121.26 | 11 | 1 |
| 3 | B | 342 | PX4 | O5-C8-C7 | 2.55 | 115.74 | 108.40 | 14 | 6 |
| 3 | B | 371 | PX4 | C26-C25-C24 | 2.55 | 122.49 | 113.13 | 5 | 1 |
| 3 | B | 395 | PX4 | O5-C9-C10 | 2.55 | 104.07 | 111.83 | 10 | 2 |
| 3 | B | 400 | PX4 | O7-C7-C6 | 2.55 | 99.21 | 108.34 | 11 | 1 |
| 3 | B | 367 | PX4 | C5-N1-C3 | 2.54 | 115.66 | 108.98 | 9 | 1 |
| 3 | B | 377 | PX4 | O6-C9-C10 | 2.55 | 133.74 | 123.78 | 4 | 2 |
| 3 | B | 388 | PX4 | C26-C25-C24 | 2.55 | 103.77 | 113.13 | 8 | 1 |
| 3 | C | 315 | PX4 | C8-O5-C9 | 2.55 | 107.81 | 117.12 | 12 | 2 |
| 3 | A | 610 | PX4 | C5-N1-C4 | 2.54 | 102.29 | 108.98 | 1 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | A | 615 | PX4 | C12-C11-C10 | 2.55 | 103.77 | 113.13 | 5 | 1 |
| 3 | B | 321 | PX4 | C5-N1-C4 | 2.55 | 102.29 | 108.98 | 4 | 1 |
| 3 | C | 339 | PX4 | O7-C7-C6 | 2.55 | 117.48 | 108.34 | 1 | 2 |
| 3 | A | 641 | PX4 | C11-C10-C9 | 2.54 | 104.37 | 113.69 | 12 | 1 |
| 3 | A | 645 | PX4 | O7-C23-O8 | 2.54 | 129.66 | 123.70 | 10 | 2 |
| 3 | C | 303 | PX4 | O7-C23-O8 | 2.54 | 129.66 | 123.70 | 5 | 1 |
| 3 | C | 346 | PX4 | C8-O5-C9 | 2.55 | 107.81 | 117.12 | 6 | 1 |
| 3 | A | 647 | PX4 | O7-C23-O8 | 2.54 | 129.65 | 123.70 | 15 | 1 |
| 3 | B | 332 | PX4 | C5-N1-C3 | 2.54 | 102.29 | 108.98 | 7 | 1 |
| 3 | B | 304 | PX4 | C5-N1-C3 | 2.54 | 102.30 | 108.98 | 4 | 1 |
| 3 | B | 315 | PX4 | O7-C7-C6 | 2.54 | 117.47 | 108.34 | 6 | 3 |
| 3 | A | 623 | PX4 | C1-C2-N1 | 2.54 | 123.98 | 115.82 | 5 | 3 |
| 3 | A | 630 | PX4 | O5-C9-C10 | 2.54 | 104.09 | 111.83 | 9 | 1 |
| 3 | B | 331 | PX4 | C5-N1-C3 | 2.54 | 115.65 | 108.98 | 1 | 1 |
| 3 | B | 343 | PX4 | C5-N1-C4 | 2.54 | 115.66 | 108.98 | 2 | 1 |
| 3 | B | 348 | PX4 | O7-C7-C8 | 2.54 | 117.47 | 108.34 | 8 | 3 |
| 3 | B | 389 | PX4 | O5-C9-O6 | 2.54 | 129.99 | 123.63 | 2 | 1 |
| 3 | B | 363 | PX4 | C8-O5-C9 | 2.54 | 107.83 | 117.12 | 15 | 1 |
| 3 | B | 393 | PX4 | O5-C8-C7 | 2.54 | 115.73 | 108.40 | 1 | 3 |
| 3 | B | 394 | PX4 | O7-C7-C8 | 2.54 | 99.22 | 108.34 | 2 | 2 |
| 3 | C | 345 | PX4 | C11-C10-C9 | 2.54 | 104.38 | 113.69 | 11 | 1 |
| 3 | A | 654 | PX4 | O7-C7-C8 | 2.54 | 117.45 | 108.34 | 11 | 3 |
| 3 | B | 310 | PX4 | O5-C9-O6 | 2.54 | 129.98 | 123.63 | 11 | 1 |
| 3 | B | 328 | PX4 | O5-C9-O6 | 2.54 | 129.98 | 123.63 | 5 | 1 |
| 3 | C | 347 | PX4 | C5-N1-C3 | 2.54 | 102.30 | 108.98 | 1 | 1 |
| 3 | B | 311 | PX4 | C26-C25-C24 | 2.54 | 103.80 | 113.13 | 13 | 2 |
| 3 | A | 630 | PX4 | C3-N1-C2 | 2.54 | 120.00 | 109.91 | 1 | 1 |
| 3 | A | 645 | PX4 | P1-O3-C1 | 2.54 | 133.34 | 121.26 | 8 | 1 |
| 3 | A | 650 | PX4 | O7-C7-C8 | 2.54 | 117.44 | 108.34 | 5 | 3 |
| 3 | B | 336 | PX4 | C33-C32-C31 | 2.54 | 101.54 | 114.37 | 3 | 1 |
| 3 | B | 322 | PX4 | O5-C8-C7 | 2.54 | 115.71 | 108.40 | 15 | 2 |
| 3 | B | 371 | PX4 | P1-O3-C1 | 2.54 | 133.33 | 121.26 | 11 | 1 |
| 3 | C | 345 | PX4 | C1-C2-N1 | 2.54 | 123.96 | 115.82 | 11 | 4 |
| 3 | B | 309 | PX4 | C1-C2-N1 | 2.53 | 123.96 | 115.82 | 9 | 3 |
| 3 | C | 327 | PX4 | O8-C23-C24 | 2.54 | 133.70 | 123.78 | 11 | 2 |
| 3 | C | 313 | PX4 | C4-N1-C3 | 2.53 | 102.32 | 108.98 | 14 | 1 |
| 3 | C | 351 | PX4 | C1-C2-N1 | 2.53 | 123.96 | 115.82 | 4 | 1 |
| 3 | A | 617 | PX4 | O4-P1-O2 | 2.53 | 98.90 | 108.94 | 15 | 2 |
| 3 | A | 638 | PX4 | O7-C7-C8 | 2.53 | 117.43 | 108.34 | 15 | 2 |
| 3 | A | 643 | PX4 | O1-P1-O4 | 2.53 | 119.05 | 107.57 | 5 | 2 |
| 3 | B | 326 | PX4 | O5-C8-C7 | 2.53 | 115.70 | 108.40 | 11 | 2 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 341 | PX4 | C1-C2-N1 | 2.53 | 123.95 | 115.82 | 13 | 2 |
| 3 | B | 359 | PX4 | C1-C2-N1 | 2.53 | 123.95 | 115.82 | 3 | 1 |
| 3 | C | 337 | PX4 | C25-C24-C23 | 2.53 | 104.41 | 113.69 | 2 | 2 |
| 3 | C | 337 | PX4 | O5-C9-C10 | 2.53 | 104.11 | 111.83 | 3 | 1 |
| 3 | A | 609 | PX4 | C5-N1-C3 | 2.53 | 115.62 | 108.98 | 3 | 3 |
| 3 | B | 305 | PX4 | C8-O5-C9 | 2.53 | 126.37 | 117.12 | 4 | 2 |
| 3 | C | 362 | PX4 | C1-C2-N1 | 2.53 | 123.95 | 115.82 | 10 | 3 |
| 3 | A | 632 | PX4 | C11-C10-C9 | 2.53 | 104.42 | 113.69 | 5 | 1 |
| 3 | A | 642 | PX4 | O6-C9-C10 | 2.53 | 133.68 | 123.78 | 13 | 1 |
| 3 | A | 607 | PX4 | C8-O5-C9 | 2.53 | 126.36 | 117.12 | 10 | 1 |
| 3 | B | 387 | PX4 | C1-C2-N1 | 2.53 | 123.94 | 115.82 | 2 | 1 |
| 3 | C | 311 | PX4 | O7-C7-C8 | 2.53 | 117.41 | 108.34 | 9 | 1 |
| 3 | A | 604 | PX4 | O5-C9-C10 | 2.53 | 104.14 | 111.83 | 5 | 1 |
| 3 | A | 623 | PX4 | C11-C10-C9 | 2.53 | 122.95 | 113.69 | 4 | 1 |
| 3 | A | 648 | PX4 | C8-O5-C9 | 2.53 | 126.35 | 117.12 | 6 | 2 |
| 3 | B | 392 | PX4 | C30-C29-C28 | 2.53 | 101.59 | 114.37 | 15 | 1 |
| 3 | A | 634 | PX4 | C8-O5-C9 | 2.53 | 107.89 | 117.12 | 6 | 1 |
| 3 | B | 337 | PX4 | C5-N1-C3 | 2.52 | 115.61 | 108.98 | 13 | 1 |
| 3 | B | 371 | PX4 | O7-C23-O8 | 2.53 | 129.61 | 123.70 | 7 | 2 |
| 3 | C | 332 | PX4 | O7-C23-O8 | 2.52 | 129.60 | 123.70 | 14 | 2 |
| 3 | C | 345 | PX4 | C5-N1-C4 | 2.52 | 115.60 | 108.98 | 2 | 1 |
| 3 | C | 353 | PX4 | C12-C11-C10 | 2.52 | 122.40 | 113.13 | 15 | 2 |
| 3 | B | 329 | PX4 | O5-C9-O6 | 2.52 | 129.94 | 123.63 | 8 | 1 |
| 3 | B | 337 | PX4 | C11-C10-C9 | 2.52 | 122.93 | 113.69 | 10 | 1 |
| 3 | B | 352 | PX4 | C5-N1-C4 | 2.52 | 115.60 | 108.98 | 12 | 1 |
| 3 | A | 610 | PX4 | C1-C2-N1 | 2.52 | 123.91 | 115.82 | 12 | 1 |
| 3 | A | 646 | PX4 | O5-C9-C10 | 2.52 | 104.15 | 111.83 | 6 | 1 |
| 3 | B | 351 | PX4 | C5-N1-C4 | 2.52 | 102.36 | 108.98 | 8 | 3 |
| 3 | B | 302 | PX4 | O3-P1-O2 | 2.52 | 98.95 | 108.94 | 10 | 1 |
| 3 | B | 331 | PX4 | O5-C8-C7 | 2.52 | 115.66 | 108.40 | 13 | 3 |
| 3 | B | 342 | PX4 | O5-C9-C10 | 2.52 | 104.15 | 111.83 | 13 | 1 |
| 3 | B | 359 | PX4 | O7-C23-O8 | 2.52 | 129.60 | 123.70 | 4 | 2 |
| 3 | B | 369 | PX4 | C5-N1-C2 | 2.52 | 119.92 | 109.91 | 6 | 1 |
| 3 | B | 395 | PX4 | C7-O7-C23 | 2.52 | 111.77 | 117.80 | 7 | 4 |
| 3 | A | 601 | PX4 | C8-O5-C9 | 2.52 | 107.92 | 117.12 | 14 | 2 |
| 3 | A | 604 | PX4 | C1-C2-N1 | 2.52 | 123.90 | 115.82 | 15 | 1 |
| 3 | B | 331 | PX4 | O7-C23-C24 | 2.52 | 106.04 | 111.48 | 7 | 1 |
| 3 | B | 357 | PX4 | C1-C2-N1 | 2.52 | 123.90 | 115.82 | 1 | 3 |
| 3 | B | 358 | PX4 | O5-C9-O6 | 2.52 | 129.93 | 123.63 | 7 | 3 |
| 3 | B | 389 | PX4 | C8-O5-C9 | 2.52 | 107.91 | 117.12 | 10 | 1 |
| 3 | C | 309 | PX4 | O5-C9-C10 | 2.52 | 104.15 | 111.83 | 2 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | C | 356 | PX4 | C5-N1-C3 | 2.52 | 102.36 | 108.98 | 14 | 1 |
| 3 | A | 607 | PX4 | C26-C25-C24 | 2.52 | 122.37 | 113.13 | 11 | 2 |
| 3 | A | 618 | PX4 | C3-N1-C2 | 2.52 | 119.91 | 109.91 | 5 | 1 |
| 3 | B | 362 | PX4 | C5-N1-C2 | 2.52 | 119.91 | 109.91 | 2 | 1 |
| 3 | B | 399 | PX4 | O8-C23-C24 | 2.51 | 133.62 | 123.78 | 5 | 1 |
| 3 | C | 304 | PX4 | C26-C25-C24 | 2.52 | 103.89 | 113.13 | 9 | 1 |
| 3 | C | 315 | PX4 | C1-C2-N1 | 2.52 | 123.90 | 115.82 | 2 | 1 |
| 3 | C | 322 | PX4 | O5-C9-O6 | 2.52 | 129.92 | 123.63 | 15 | 1 |
| 3 | C | 333 | PX4 | P1-O3-C1 | 2.52 | 133.23 | 121.26 | 4 | 1 |
| 3 | C | 335 | PX4 | O7-C7-C6 | 2.52 | 117.37 | 108.34 | 9 | 1 |
| 3 | A | 611 | PX4 | C25-C24-C23 | 2.51 | 104.48 | 113.69 | 6 | 1 |
| 3 | A | 612 | PX4 | O5-C9-O6 | 2.51 | 129.92 | 123.63 | 13 | 2 |
| 3 | A | 654 | PX4 | O3-C1-C2 | 2.51 | 121.75 | 109.65 | 4 | 1 |
| 3 | B | 305 | PX4 | O5-C9-C10 | 2.51 | 104.17 | 111.83 | 8 | 4 |
| 3 | B | 350 | PX4 | O5-C8-C7 | 2.51 | 115.64 | 108.40 | 8 | 1 |
| 3 | B | 390 | PX4 | C4-N1-C3 | 2.51 | 115.58 | 108.98 | 3 | 2 |
| 3 | C | 303 | PX4 | O7-C23-C24 | 2.51 | 106.05 | 111.48 | 4 | 3 |
| 3 | B | 314 | PX4 | O5-C8-C7 | 2.51 | 115.64 | 108.40 | 9 | 3 |
| 3 | A | 635 | PX4 | C7-O7-C23 | 2.51 | 111.79 | 117.80 | 1 | 3 |
| 3 | B | 339 | PX4 | C12-C11-C10 | 2.51 | 103.90 | 113.13 | 8 | 1 |
| 3 | B | 353 | PX4 | C8-C7-C6 | 2.51 | 105.93 | 111.78 | 5 | 2 |
| 3 | C | 303 | PX4 | O5-C9-O6 | 2.51 | 129.91 | 123.63 | 7 | 2 |
| 3 | C | 322 | PX4 | O5-C8-C7 | 2.51 | 115.64 | 108.40 | 10 | 2 |
| 3 | C | 326 | PX4 | O5-C9-C10 | 2.51 | 104.18 | 111.83 | 11 | 1 |
| 3 | C | 348 | PX4 | O7-C23-O8 | 2.51 | 129.57 | 123.70 | 4 | 1 |
| 3 | A | 607 | PX4 | O1-P1-O2 | 2.51 | 124.12 | 112.44 | 5 | 2 |
| 3 | A | 640 | PX4 | C5-N1-C4 | 2.51 | 102.39 | 108.98 | 7 | 2 |
| 3 | B | 316 | PX4 | C1-C2-N1 | 2.51 | 123.87 | 115.82 | 2 | 2 |
| 3 | B | 321 | PX4 | C5-N1-C3 | 2.51 | 115.56 | 108.98 | 9 | 1 |
| 3 | B | 361 | PX4 | C8-O5-C9 | 2.51 | 107.95 | 117.12 | 4 | 3 |
| 3 | C | 332 | PX4 | O5-C8-C7 | 2.51 | 115.62 | 108.40 | 10 | 1 |
| 3 | C | 312 | PX4 | C8-O5-C9 | 2.50 | 107.96 | 117.12 | 4 | 2 |
| 3 | A | 623 | PX4 | C4-N1-C3 | 2.50 | 102.41 | 108.98 | 6 | 2 |
| 3 | A | 631 | PX4 | C5-N1-C3 | 2.50 | 102.41 | 108.98 | 3 | 1 |
| 3 | C | 307 | PX4 | P1-O3-C1 | 2.50 | 133.16 | 121.26 | 11 | 1 |
| 3 | B | 361 | PX4 | O5-C9-C10 | 2.50 | 104.21 | 111.83 | 15 | 1 |
| 3 | B | 373 | PX4 | C25-C24-C23 | 2.50 | 104.53 | 113.69 | 5 | 3 |
| 3 | C | 318 | PX4 | O5-C9-C10 | 2.50 | 104.21 | 111.83 | 8 | 1 |
| 3 | C | 330 | PX4 | C5-N1-C3 | 2.50 | 102.41 | 108.98 | 11 | 3 |
| 3 | C | 341 | PX4 | C8-C7-C6 | 2.50 | 105.95 | 111.78 | 10 | 6 |
| 3 | C | 345 | PX4 | C8-C7-C6 | 2.50 | 105.95 | 111.78 | 5 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | A | 628 | PX4 | O5-C8-C7 | 2.50 | 115.60 | 108.40 | 4 | 3 |
| 3 | B | 327 | PX4 | C1-C2-N1 | 2.50 | 123.85 | 115.82 | 6 | 3 |
| 3 | C | 363 | PX4 | C8-O5-C9 | 2.50 | 107.98 | 117.12 | 15 | 2 |
| 3 | A | 607 | PX4 | C25-C24-C23 | 2.50 | 104.54 | 113.69 | 7 | 1 |
| 3 | A | 610 | PX4 | C11-C10-C9 | 2.50 | 104.54 | 113.69 | 12 | 1 |
| 3 | A | 602 | PX4 | C4-N1-C3 | 2.50 | 115.54 | 108.98 | 15 | 2 |
| 3 | A | 628 | PX4 | P1-O3-C1 | 2.50 | 109.37 | 121.26 | 11 | 1 |
| 3 | B | 306 | PX4 | O5-C9-O6 | 2.50 | 129.88 | 123.63 | 5 | 1 |
| 3 | B | 336 | PX4 | C3-N1-C2 | 2.50 | 119.84 | 109.91 | 14 | 1 |
| 3 | B | 340 | PX4 | O1-P1-O2 | 2.50 | 124.07 | 112.44 | 13 | 1 |
| 3 | B | 386 | PX4 | O1-P1-O2 | 2.50 | 124.07 | 112.44 | 13 | 3 |
| 3 | C | 318 | PX4 | O5-C9-O6 | 2.50 | 129.88 | 123.63 | 8 | 3 |
| 3 | A | 643 | PX4 | C8-O5-C9 | 2.50 | 126.24 | 117.12 | 14 | 2 |
| 3 | C | 318 | PX4 | C1-C2-N1 | 2.50 | 123.84 | 115.82 | 6 | 2 |
| 3 | A | 620 | PX4 | C5-N1-C4 | 2.49 | 102.42 | 108.98 | 2 | 3 |
| 3 | B | 317 | PX4 | O7-C7-C8 | 2.49 | 117.29 | 108.34 | 3 | 3 |
| 3 | B | 367 | PX4 | C4-N1-C3 | 2.49 | 102.42 | 108.98 | 6 | 1 |
| 3 | B | 328 | PX4 | O5-C8-C7 | 2.49 | 115.58 | 108.40 | 12 | 3 |
| 3 | B | 333 | PX4 | O5-C8-C7 | 2.49 | 115.58 | 108.40 | 14 | 4 |
| 3 | B | 355 | PX4 | C8-C7-C6 | 2.49 | 105.97 | 111.78 | 8 | 1 |
| 3 | A | 602 | PX4 | C12-C11-C10 | 2.49 | 103.98 | 113.13 | 9 | 1 |
| 3 | B | 301 | PX4 | O7-C23-C24 | 2.49 | 106.09 | 111.48 | 4 | 3 |
| 3 | B | 389 | PX4 | C4-N1-C2 | 2.49 | 119.81 | 109.91 | 13 | 1 |
| 3 | A | 602 | PX4 | C5-N1-C3 | 2.49 | 115.51 | 108.98 | 3 | 2 |
| 3 | A | 652 | PX4 | C26-C25-C24 | 2.49 | 122.27 | 113.13 | 7 | 1 |
| 3 | B | 303 | PX4 | C8-O5-C9 | 2.49 | 126.22 | 117.12 | 12 | 1 |
| 3 | B | 362 | PX4 | O3-C1-C2 | 2.49 | 121.62 | 109.65 | 9 | 1 |
| 3 | C | 324 | PX4 | C5-N1-C4 | 2.49 | 115.52 | 108.98 | 7 | 1 |
| 3 | B | 316 | PX4 | O7-C23-O8 | 2.49 | 129.52 | 123.70 | 15 | 6 |
| 3 | C | 309 | PX4 | C8-O5-C9 | 2.49 | 108.03 | 117.12 | 3 | 3 |
| 3 | C | 310 | PX4 | C29-C28-C27 | 2.49 | 101.80 | 114.37 | 12 | 1 |
| 3 | C | 361 | PX4 | O7-C23-O8 | 2.49 | 129.52 | 123.70 | 9 | 3 |
| 3 | A | 620 | PX4 | O5-C9-O6 | 2.49 | 129.84 | 123.63 | 13 | 2 |
| 3 | B | 301 | PX4 | C26-C25-C24 | 2.49 | 122.26 | 113.13 | 1 | 1 |
| 3 | A | 653 | PX4 | C8-C7-C6 | 2.48 | 117.58 | 111.78 | 14 | 2 |
| 3 | A | 611 | PX4 | C26-C25-C24 | 2.48 | 104.00 | 113.13 | 7 | 1 |
| 3 | A | 651 | PX4 | C4-N1-C3 | 2.48 | 102.45 | 108.98 | 2 | 3 |
| 3 | B | 315 | PX4 | C8-C7-C6 | 2.48 | 105.99 | 111.78 | 6 | 2 |
| 3 | B | 323 | PX4 | O7-C23-O8 | 2.48 | 129.51 | 123.70 | 9 | 2 |
| 3 | C | 324 | PX4 | O7-C23-O8 | 2.49 | 129.52 | 123.70 | 3 | 2 |
| 3 | C | 315 | PX4 | C5-N1-C4 | 2.48 | 102.45 | 108.98 | 4 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | C | 329 | PX4 | C11-C10-C9 | 2.48 | 104.59 | 113.69 | 1 | 2 |
| 3 | B | 328 | PX4 | C8-O5-C9 | 2.48 | 108.04 | 117.12 | 3 | 1 |
| 3 | C | 304 | PX4 | O7-C23-O8 | 2.48 | 129.51 | 123.70 | 9 | 1 |
| 3 | C | 361 | PX4 | O7-C7-C8 | 2.48 | 117.25 | 108.34 | 1 | 2 |
| 3 | C | 363 | PX4 | C25-C24-C23 | 2.48 | 122.80 | 113.69 | 9 | 1 |
| 3 | A | 611 | PX4 | C4-N1-C3 | 2.48 | 102.46 | 108.98 | 13 | 2 |
| 3 | A | 650 | PX4 | O7-C23-C24 | 2.48 | 106.11 | 111.48 | 1 | 2 |
| 3 | A | 616 | PX4 | O1-P1-O2 | 2.48 | 123.98 | 112.44 | 6 | 2 |
| 3 | A | 648 | PX4 | O7-C23-O8 | 2.48 | 129.50 | 123.70 | 9 | 1 |
| 3 | A | 651 | PX4 | O5-C9-O6 | 2.48 | 129.83 | 123.63 | 5 | 3 |
| 3 | B | 337 | PX4 | O5-C9-O6 | 2.48 | 129.83 | 123.63 | 4 | 2 |
| 3 | B | 373 | PX4 | O5-C8-C7 | 2.48 | 115.55 | 108.40 | 10 | 2 |
| 3 | B | 384 | PX4 | C12-C11-C10 | 2.48 | 122.24 | 113.13 | 5 | 1 |
| 3 | B | 313 | PX4 | O7-C7-C6 | 2.48 | 117.23 | 108.34 | 1 | 2 |
| 3 | B | 321 | PX4 | O5-C9-C10 | 2.48 | 104.28 | 111.83 | 4 | 3 |
| 3 | B | 345 | PX4 | O7-C7-C6 | 2.48 | 117.23 | 108.34 | 11 | 1 |
| 3 | C | 307 | PX4 | C8-O5-C9 | 2.48 | 108.06 | 117.12 | 14 | 1 |
| 3 | C | 309 | PX4 | O7-C23-O8 | 2.48 | 129.50 | 123.70 | 5 | 3 |
| 3 | B | 395 | PX4 | O7-C23-O8 | 2.48 | 129.50 | 123.70 | 4 | 2 |
| 3 | C | 308 | PX4 | O5-C9-O6 | 2.48 | 129.82 | 123.63 | 9 | 3 |
| 3 | C | 320 | PX4 | O3-P1-O2 | 2.48 | 118.75 | 108.94 | 3 | 1 |
| 3 | A | 642 | PX4 | O7-C23-O8 | 2.48 | 129.49 | 123.70 | 15 | 2 |
| 3 | C | 350 | PX4 | C12-C11-C10 | 2.48 | 104.03 | 113.13 | 14 | 3 |
| 3 | B | 356 | PX4 | O5-C9-C10 | 2.48 | 104.29 | 111.83 | 5 | 3 |
| 3 | A | 619 | PX4 | C5-N1-C4 | 2.47 | 102.48 | 108.98 | 5 | 1 |
| 3 | B | 358 | PX4 | C25-C24-C23 | 2.48 | 104.62 | 113.69 | 5 | 1 |
| 3 | B | 394 | PX4 | C13-C12-C11 | 2.48 | 126.88 | 114.37 | 4 | 1 |
| 3 | B | 398 | PX4 | C5-N1-C3 | 2.48 | 102.47 | 108.98 | 11 | 2 |
| 3 | B | 335 | PX4 | P1-O3-C1 | 2.47 | 109.48 | 121.26 | 5 | 2 |
| 3 | B | 380 | PX4 | C1-C2-N1 | 2.47 | 123.76 | 115.82 | 9 | 2 |
| 3 | C | 345 | PX4 | C15-C14-C13 | 2.47 | 101.86 | 114.37 | 5 | 2 |
| 3 | C | 303 | PX4 | C4-N1-C3 | 2.47 | 115.47 | 108.98 | 13 | 1 |
| 3 | C | 324 | PX4 | C8-O5-C9 | 2.47 | 108.08 | 117.12 | 14 | 1 |
| 3 | C | 337 | PX4 | O7-C7-C6 | 2.47 | 99.47 | 108.34 | 8 | 1 |
| 3 | A | 630 | PX4 | C11-C10-C9 | 2.47 | 104.64 | 113.69 | 14 | 1 |
| 3 | B | 328 | PX4 | C11-C10-C9 | 2.47 | 122.75 | 113.69 | 8 | 2 |
| 3 | B | 340 | PX4 | O5-C9-C10 | 2.47 | 104.30 | 111.83 | 15 | 2 |
| 3 | B | 345 | PX4 | C26-C25-C24 | 2.47 | 104.04 | 113.13 | 11 | 2 |
| 3 | B | 363 | PX4 | O5-C8-C7 | 2.47 | 115.52 | 108.40 | 14 | 3 |
| 3 | C | 302 | PX4 | C5-N1-C3 | 2.47 | 115.47 | 108.98 | 13 | 3 |
| 3 | C | 313 | PX4 | O7-C7-C8 | 2.47 | 117.21 | 108.34 | 12 | 2 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | C | 321 | PX4 | O7-C7-C8 | 2.47 | 117.21 | 108.34 | 12 | 4 |
| 3 | C | 325 | PX4 | P1-O3-C1 | 2.47 | 133.02 | 121.26 | 4 | 1 |
| 3 | C | 354 | PX4 | C12-C11-C10 | 2.47 | 104.05 | 113.13 | 15 | 1 |
| 3 | B | 309 | PX4 | O5-C9-C10 | 2.47 | 104.31 | 111.83 | 4 | 1 |
| 3 | B | 331 | PX4 | C11-C10-C9 | 2.47 | 122.74 | 113.69 | 14 | 2 |
| 3 | C | 341 | PX4 | C8-O5-C9 | 2.47 | 108.09 | 117.12 | 4 | 2 |
| 3 | B | 324 | PX4 | C17-C16-C15 | 2.47 | 101.89 | 114.37 | 13 | 1 |
| 3 | B | 345 | PX4 | C8-O5-C9 | 2.47 | 108.10 | 117.12 | 13 | 1 |
| 3 | B | 374 | PX4 | O5-C9-C10 | 2.47 | 104.31 | 111.83 | 7 | 1 |
| 3 | A | 618 | PX4 | C5-N1-C4 | 2.47 | 115.45 | 108.98 | 15 | 2 |
| 3 | A | 638 | PX4 | C5-N1-C4 | 2.47 | 102.50 | 108.98 | 3 | 2 |
| 3 | A | 650 | PX4 | O5-C9-C10 | 2.47 | 104.31 | 111.83 | 10 | 4 |
| 3 | B | 305 | PX4 | C5-N1-C4 | 2.47 | 102.50 | 108.98 | 1 | 1 |
| 3 | B | 310 | PX4 | O7-C7-C8 | 2.47 | 117.19 | 108.34 | 13 | 1 |
| 3 | C | 301 | PX4 | C7-O7-C23 | 2.47 | 111.89 | 117.80 | 8 | 2 |
| 3 | B | 325 | PX4 | C25-C24-C23 | 2.47 | 122.73 | 113.69 | 8 | 3 |
| 3 | B | 343 | PX4 | O7-C23-C24 | 2.47 | 106.15 | 111.48 | 3 | 2 |
| 3 | A | 648 | PX4 | P1-O3-C1 | 2.46 | 132.99 | 121.26 | 15 | 1 |
| 3 | B | 309 | PX4 | O7-C7-C8 | 2.46 | 117.19 | 108.34 | 14 | 1 |
| 3 | B | 326 | PX4 | O3-P1-O2 | 2.46 | 99.17 | 108.94 | 1 | 1 |
| 3 | B | 333 | PX4 | C8-C7-C6 | 2.46 | 117.53 | 111.78 | 7 | 1 |
| 3 | B | 307 | PX4 | C1-C2-N1 | 2.46 | 123.73 | 115.82 | 10 | 1 |
| 3 | B | 359 | PX4 | C5-N1-C3 | 2.46 | 102.51 | 108.98 | 1 | 1 |
| 3 | B | 375 | PX4 | O5-C9-C10 | 2.46 | 104.33 | 111.83 | 7 | 2 |
| 3 | B | 400 | PX4 | C8-C7-C6 | 2.46 | 117.53 | 111.78 | 9 | 3 |
| 3 | C | 322 | PX4 | C25-C24-C23 | 2.46 | 122.72 | 113.69 | 6 | 1 |
| 3 | A | 617 | PX4 | C12-C11-C10 | 2.46 | 104.08 | 113.13 | 1 | 1 |
| 3 | A | 628 | PX4 | O5-C9-C10 | 2.46 | 104.33 | 111.83 | 15 | 2 |
| 3 | A | 629 | PX4 | O1-P1-O2 | 2.46 | 123.90 | 112.44 | 8 | 1 |
| 3 | C | 354 | PX4 | C26-C25-C24 | 2.46 | 122.18 | 113.13 | 15 | 1 |
| 3 | B | 309 | PX4 | C5-N1-C3 | 2.46 | 102.51 | 108.98 | 5 | 2 |
| 3 | A | 634 | PX4 | O7-C23-C24 | 2.46 | 106.16 | 111.48 | 2 | 1 |
| 3 | B | 379 | PX4 | P1-O4-C6 | 2.46 | 135.45 | 121.35 | 9 | 1 |
| 3 | B | 385 | PX4 | O3-C1-C2 | 2.46 | 121.49 | 109.65 | 3 | 1 |
| 3 | B | 348 | PX4 | C5-N1-C4 | 2.46 | 102.52 | 108.98 | 12 | 2 |
| 3 | B | 362 | PX4 | C8-C7-C6 | 2.46 | 106.05 | 111.78 | 6 | 1 |
| 3 | B | 385 | PX4 | C16-C15-C14 | 2.46 | 101.94 | 114.37 | 3 | 1 |
| 3 | B | 400 | PX4 | C7-O7-C23 | 2.46 | 111.91 | 117.80 | 14 | 2 |
| 3 | C | 322 | PX4 | C5-N1-C4 | 2.46 | 102.52 | 108.98 | 1 | 1 |
| 3 | A | 629 | PX4 | C8-C7-C6 | 2.46 | 106.06 | 111.78 | 15 | 2 |
| 3 | B | 347 | PX4 | C34-C33-C32 | 2.46 | 126.79 | 114.37 | 13 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | C | 323 | PX4 | C1-C2-N1 | 2.46 | 123.71 | 115.82 | 7 | 1 |
| 3 | C | 336 | PX4 | C25-C24-C23 | 2.46 | 104.69 | 113.69 | 9 | 2 |
| 3 | A | 603 | PX4 | C4-N1-C3 | 2.46 | 102.53 | 108.98 | 11 | 2 |
| 3 | A | 602 | PX4 | C8-C7-C6 | 2.45 | 117.51 | 111.78 | 9 | 2 |
| 3 | A | 603 | PX4 | C12-C11-C10 | 2.45 | 104.11 | 113.13 | 9 | 1 |
| 3 | A | 613 | PX4 | C26-C25-C24 | 2.45 | 122.15 | 113.13 | 1 | 1 |
| 3 | B | 390 | PX4 | C8-C7-C6 | 2.45 | 117.51 | 111.78 | 5 | 2 |
| 3 | B | 329 | PX4 | O7-C23-C24 | 2.45 | 106.17 | 111.48 | 15 | 4 |
| 3 | B | 337 | PX4 | C25-C24-C23 | 2.45 | 104.70 | 113.69 | 6 | 2 |
| 3 | A | 604 | PX4 | O7-C23-O8 | 2.45 | 129.44 | 123.70 | 1 | 3 |
| 3 | A | 605 | PX4 | O7-C7-C6 | 2.45 | 117.14 | 108.34 | 8 | 5 |
| 3 | A | 619 | PX4 | C25-C24-C23 | 2.45 | 122.69 | 113.69 | 6 | 1 |
| 3 | B | 361 | PX4 | O7-C23-O8 | 2.45 | 129.44 | 123.70 | 12 | 2 |
| 3 | B | 394 | PX4 | C12-C11-C10 | 2.45 | 122.14 | 113.13 | 1 | 2 |
| 3 | C | 330 | PX4 | C26-C25-C24 | 2.45 | 122.14 | 113.13 | 14 | 1 |
| 3 | C | 357 | PX4 | C26-C25-C24 | 2.45 | 104.11 | 113.13 | 6 | 1 |
| 3 | A | 616 | PX4 | C12-C11-C10 | 2.45 | 104.12 | 113.13 | 15 | 1 |
| 3 | A | 621 | PX4 | C8-C7-C6 | 2.45 | 117.50 | 111.78 | 6 | 2 |
| 3 | A | 627 | PX4 | O7-C23-O8 | 2.45 | 129.44 | 123.70 | 1 | 2 |
| 3 | A | 644 | PX4 | O7-C23-O8 | 2.45 | 129.44 | 123.70 | 3 | 4 |
| 3 | A | 641 | PX4 | C26-C25-C24 | 2.45 | 122.13 | 113.13 | 12 | 2 |
| 3 | B | 320 | PX4 | C1-C2-N1 | 2.45 | 123.69 | 115.82 | 3 | 2 |
| 3 | C | 332 | PX4 | O7-C7-C6 | 2.45 | 117.14 | 108.34 | 6 | 2 |
| 3 | B | 329 | PX4 | C32-C31-C30 | 2.45 | 101.98 | 114.37 | 5 | 1 |
| 3 | B | 332 | PX4 | O6-C9-C10 | 2.45 | 133.37 | 123.78 | 11 | 1 |
| 3 | C | 336 | PX4 | C4-N1-C3 | 2.45 | 115.42 | 108.98 | 12 | 2 |
| 3 | C | 344 | PX4 | O7-C7-C6 | 2.45 | 117.14 | 108.34 | 5 | 2 |
| 3 | C | 357 | PX4 | O7-C7-C6 | 2.45 | 117.14 | 108.34 | 15 | 2 |
| 3 | B | 336 | PX4 | C26-C25-C24 | 2.45 | 122.13 | 113.13 | 5 | 2 |
| 3 | B | 371 | PX4 | O1-P1-O2 | 2.45 | 123.85 | 112.44 | 6 | 1 |
| 3 | C | 316 | PX4 | O5-C9-C10 | 2.45 | 104.36 | 111.83 | 1 | 4 |
| 3 | C | 325 | PX4 | C1-C2-N1 | 2.45 | 123.69 | 115.82 | 12 | 1 |
| 3 | B | 354 | PX4 | O7-C23-O8 | 2.45 | 129.43 | 123.70 | 9 | 4 |
| 3 | A | 644 | PX4 | P1-O3-C1 | 2.45 | 132.91 | 121.26 | 1 | 1 |
| 3 | B | 312 | PX4 | C12-C11-C10 | 2.45 | 104.13 | 113.13 | 14 | 1 |
| 3 | B | 340 | PX4 | O5-C9-O6 | 2.45 | 129.75 | 123.63 | 15 | 4 |
| 3 | B | 376 | PX4 | O5-C9-C10 | 2.45 | 104.37 | 111.83 | 9 | 2 |
| 3 | B | 386 | PX4 | C7-O7-C23 | 2.45 | 123.65 | 117.80 | 7 | 2 |
| 3 | A | 610 | PX4 | O5-C8-C7 | 2.44 | 115.44 | 108.40 | 9 | 2 |
| 3 | C | 303 | PX4 | C8-C7-C6 | 2.45 | 106.08 | 111.78 | 9 | 1 |
| 3 | C | 340 | PX4 | C8-O5-C9 | 2.44 | 126.06 | 117.12 | 14 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | A | 610 | PX4 | C4-N1-C3 | 2.44 | 102.56 | 108.98 | 11 | 2 |
| 3 | A | 621 | PX4 | O5-C9-O6 | 2.44 | 129.74 | 123.63 | 12 | 1 |
| 3 | A | 622 | PX4 | C5-N1-C3 | 2.44 | 102.56 | 108.98 | 15 | 2 |
| 3 | A | 643 | PX4 | C12-C11-C10 | 2.44 | 104.15 | 113.13 | 14 | 1 |
| 3 | A | 649 | PX4 | O5-C9-O6 | 2.44 | 129.74 | 123.63 | 15 | 5 |
| 3 | B | 314 | PX4 | C8-O5-C9 | 2.44 | 108.19 | 117.12 | 3 | 1 |
| 3 | B | 348 | PX4 | C13-C12-C11 | 2.44 | 102.02 | 114.37 | 7 | 1 |
| 3 | C | 344 | PX4 | O7-C23-O8 | 2.44 | 129.42 | 123.70 | 3 | 3 |
| 3 | B | 388 | PX4 | C1-C2-N1 | 2.44 | 123.66 | 115.82 | 1 | 2 |
| 3 | B | 392 | PX4 | O7-C23-O8 | 2.44 | 129.41 | 123.70 | 12 | 5 |
| 3 | B | 361 | PX4 | C3-N1-C2 | 2.44 | 100.21 | 109.91 | 7 | 1 |
| 3 | C | 314 | PX4 | C4-N1-C3 | 2.44 | 102.56 | 108.98 | 11 | 1 |
| 3 | C | 335 | PX4 | O3-C1-C2 | 2.44 | 121.39 | 109.65 | 13 | 1 |
| 3 | A | 608 | PX4 | O7-C23-O8 | 2.44 | 129.41 | 123.70 | 11 | 3 |
| 3 | A | 639 | PX4 | C3-N1-C2 | 2.44 | 100.21 | 109.91 | 2 | 3 |
| 3 | B | 369 | PX4 | C1-C2-N1 | 2.44 | 123.65 | 115.82 | 7 | 1 |
| 3 | C | 346 | PX4 | O5-C9-O6 | 2.44 | 129.73 | 123.63 | 7 | 1 |
| 3 | B | 323 | PX4 | O5-C9-O6 | 2.44 | 129.73 | 123.63 | 12 | 2 |
| 3 | A | 609 | PX4 | C8-C7-C6 | 2.44 | 106.10 | 111.78 | 7 | 1 |
| 3 | A | 626 | PX4 | O5-C9-O6 | 2.44 | 129.72 | 123.63 | 2 | 2 |
| 3 | B | 400 | PX4 | C4-N1-C3 | 2.44 | 115.38 | 108.98 | 9 | 2 |
| 3 | A | 627 | PX4 | O5-C9-C10 | 2.44 | 104.41 | 111.83 | 2 | 1 |
| 3 | B | 315 | PX4 | C16-C15-C14 | 2.44 | 102.06 | 114.37 | 6 | 1 |
| 3 | B | 330 | PX4 | O7-C23-C24 | 2.44 | 106.21 | 111.48 | 3 | 1 |
| 3 | B | 353 | PX4 | O7-C7-C8 | 2.44 | 117.08 | 108.34 | 1 | 1 |
| 3 | B | 353 | PX4 | C11-C10-C9 | 2.44 | 104.77 | 113.69 | 14 | 2 |
| 3 | C | 308 | PX4 | C8-O5-C9 | 2.44 | 108.21 | 117.12 | 5 | 2 |
| 3 | B | 366 | PX4 | O5-C9-O6 | 2.43 | 129.72 | 123.63 | 11 | 1 |
| 3 | B | 372 | PX4 | C11-C10-C9 | 2.44 | 122.62 | 113.69 | 11 | 2 |
| 3 | B | 394 | PX4 | O7-C23-O8 | 2.44 | 129.40 | 123.70 | 2 | 2 |
| 3 | B | 398 | PX4 | O5-C9-O6 | 2.44 | 129.72 | 123.63 | 11 | 2 |
| 3 | B | 346 | PX4 | C12-C11-C10 | 2.43 | 122.07 | 113.13 | 5 | 1 |
| 3 | C | 302 | PX4 | O7-C23-C24 | 2.43 | 106.21 | 111.48 | 7 | 3 |
| 3 | A | 638 | PX4 | O7-C23-C24 | 2.43 | 116.74 | 111.48 | 4 | 2 |
| 3 | C | 323 | PX4 | C4-N1-C3 | 2.43 | 102.58 | 108.98 | 14 | 1 |
| 3 | B | 378 | PX4 | C8-O5-C9 | 2.43 | 108.23 | 117.12 | 9 | 1 |
| 3 | C | 306 | PX4 | C5-N1-C4 | 2.43 | 115.36 | 108.98 | 10 | 1 |
| 3 | C | 328 | PX4 | C8-C7-C6 | 2.43 | 117.46 | 111.78 | 5 | 2 |
| 3 | A | 646 | PX4 | C12-C11-C10 | 2.43 | 104.19 | 113.13 | 8 | 2 |
| 3 | C | 340 | PX4 | O7-C7-C6 | 2.43 | 117.07 | 108.34 | 2 | 1 |
| 3 | A | 615 | PX4 | O5-C9-O6 | 2.43 | 129.71 | 123.63 | 3 | 2 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 304 | PX4 | O5-C8-C7 | 2.43 | 115.40 | 108.40 | 2 | 1 |
| 3 | B | 340 | PX4 | C8-C7-C6 | 2.43 | 106.12 | 111.78 | 5 | 4 |
| 3 | C | 346 | PX4 | C1-C2-N1 | 2.43 | 123.63 | 115.82 | 7 | 2 |
| 3 | B | 356 | PX4 | O7-C7-C8 | 2.43 | 117.06 | 108.34 | 4 | 2 |
| 3 | A | 642 | PX4 | C13-C12-C11 | 2.43 | 126.64 | 114.37 | 2 | 1 |
| 3 | B | 350 | PX4 | C8-O5-C9 | 2.43 | 108.24 | 117.12 | 8 | 2 |
| 3 | B | 388 | PX4 | O5-C9-O6 | 2.43 | 129.70 | 123.63 | 2 | 4 |
| 3 | C | 315 | PX4 | C5-N1-C3 | 2.43 | 115.35 | 108.98 | 15 | 2 |
| 3 | C | 338 | PX4 | C15-C14-C13 | 2.43 | 102.09 | 114.37 | 10 | 1 |
| 3 | A | 631 | PX4 | C25-C24-C23 | 2.43 | 104.80 | 113.69 | 12 | 1 |
| 3 | B | 356 | PX4 | C3-N1-C2 | 2.43 | 119.56 | 109.91 | 14 | 1 |
| 3 | C | 343 | PX4 | O7-C7-C8 | 2.43 | 117.05 | 108.34 | 4 | 1 |
| 3 | A | 620 | PX4 | C11-C10-C9 | 2.42 | 122.58 | 113.69 | 7 | 3 |
| 3 | C | 323 | PX4 | O5-C9-O6 | 2.42 | 129.69 | 123.63 | 13 | 1 |
| 3 | C | 340 | PX4 | O5-C9-O6 | 2.42 | 129.69 | 123.63 | 8 | 1 |
| 3 | B | 312 | PX4 | O5-C8-C7 | 2.42 | 115.38 | 108.40 | 15 | 2 |
| 3 | B | 316 | PX4 | O5-C9-O6 | 2.42 | 129.69 | 123.63 | 13 | 1 |
| 3 | B | 333 | PX4 | C11-C10-C9 | 2.42 | 122.57 | 113.69 | 11 | 2 |
| 3 | B | 333 | PX4 | C4-N1-C3 | 2.42 | 102.61 | 108.98 | 6 | 4 |
| 3 | C | 335 | PX4 | C4-N1-C3 | 2.42 | 102.61 | 108.98 | 11 | 4 |
| 3 | C | 343 | PX4 | C1-C2-N1 | 2.42 | 123.60 | 115.82 | 1 | 1 |
| 3 | C | 358 | PX4 | O5-C8-C7 | 2.42 | 101.41 | 108.40 | 12 | 5 |
| 3 | B | 368 | PX4 | C7-O7-C23 | 2.42 | 112.00 | 117.80 | 5 | 2 |
| 3 | C | 303 | PX4 | C25-C24-C23 | 2.42 | 104.82 | 113.69 | 3 | 1 |
| 3 | C | 344 | PX4 | C11-C10-C9 | 2.42 | 104.83 | 113.69 | 12 | 1 |
| 3 | A | 616 | PX4 | C11-C10-C9 | 2.42 | 104.83 | 113.69 | 13 | 2 |
| 3 | B | 331 | PX4 | C26-C25-C24 | 2.42 | 122.01 | 113.13 | 14 | 1 |
| 3 | B | 332 | PX4 | O7-C23-O8 | 2.42 | 129.36 | 123.70 | 4 | 3 |
| 3 | B | 339 | PX4 | O7-C7-C6 | 2.42 | 117.02 | 108.34 | 4 | 2 |
| 3 | B | 342 | PX4 | C26-C25-C24 | 2.42 | 104.24 | 113.13 | 13 | 1 |
| 3 | B | 395 | PX4 | C8-C7-C6 | 2.42 | 106.14 | 111.78 | 11 | 2 |
| 3 | A | 636 | PX4 | C12-C11-C10 | 2.42 | 122.01 | 113.13 | 11 | 1 |
| 3 | A | 646 | PX4 | O5-C9-O6 | 2.42 | 129.67 | 123.63 | 8 | 1 |
| 3 | A | 618 | PX4 | C8-O5-C9 | 2.42 | 108.29 | 117.12 | 6 | 1 |
| 3 | B | 310 | PX4 | O5-C8-C7 | 2.42 | 115.36 | 108.40 | 2 | 1 |
| 3 | B | 312 | PX4 | O5-C9-O6 | 2.42 | 129.67 | 123.63 | 15 | 1 |
| 3 | B | 356 | PX4 | O8-C23-C24 | 2.42 | 133.23 | 123.78 | 7 | 1 |
| 3 | B | 366 | PX4 | C7-O7-C23 | 2.41 | 112.02 | 117.80 | 9 | 5 |
| 3 | B | 398 | PX4 | C5-N1-C4 | 2.42 | 115.32 | 108.98 | 15 | 1 |
| 3 | C | 302 | PX4 | C4-N1-C3 | 2.42 | 102.63 | 108.98 | 2 | 3 |
| 3 | C | 362 | PX4 | C11-C10-C9 | 2.42 | 122.55 | 113.69 | 6 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | A | 628 | PX4 | O5-C9-O6 | 2.41 | 129.67 | 123.63 | 15 | 1 |
| 3 | A | 646 | PX4 | C4-N1-C3 | 2.41 | 102.63 | 108.98 | 10 | 1 |
| 3 | B | 324 | PX4 | C4-N1-C3 | 2.41 | 102.63 | 108.98 | 12 | 2 |
| 3 | B | 398 | PX4 | O1-P1-O2 | 2.41 | 123.67 | 112.44 | 5 | 1 |
| 3 | B | 309 | PX4 | P1-O4-C6 | 2.41 | 107.53 | 121.35 | 14 | 1 |
| 3 | B | 315 | PX4 | O4-P1-O2 | 2.41 | 99.38 | 108.94 | 1 | 1 |
| 3 | B | 335 | PX4 | C26-C25-C24 | 2.41 | 121.99 | 113.13 | 1 | 2 |
| 3 | C | 341 | PX4 | C25-C24-C23 | 2.41 | 104.86 | 113.69 | 13 | 2 |
| 3 | B | 361 | PX4 | O5-C9-O6 | 2.41 | 129.66 | 123.63 | 15 | 1 |
| 3 | B | 390 | PX4 | O7-C23-C24 | 2.41 | 106.27 | 111.48 | 10 | 1 |
| 3 | C | 304 | PX4 | C13-C12-C11 | 2.41 | 102.19 | 114.37 | 5 | 1 |
| 3 | C | 306 | PX4 | O5-C9-C10 | 2.41 | 104.48 | 111.83 | 4 | 1 |
| 3 | C | 319 | PX4 | C8-O5-C9 | 2.41 | 108.31 | 117.12 | 14 | 1 |
| 3 | C | 351 | PX4 | C8-C7-C6 | 2.41 | 106.16 | 111.78 | 11 | 1 |
| 3 | B | 311 | PX4 | O3-P1-O2 | 2.41 | 99.38 | 108.94 | 5 | 1 |
| 3 | B | 342 | PX4 | O7-C7-C6 | 2.41 | 116.99 | 108.34 | 12 | 2 |
| 3 | B | 391 | PX4 | O5-C8-C7 | 2.41 | 115.34 | 108.40 | 12 | 3 |
| 3 | C | 320 | PX4 | C1-C2-N1 | 2.41 | 123.56 | 115.82 | 6 | 1 |
| 3 | A | 606 | PX4 | C5-N1-C4 | 2.41 | 115.30 | 108.98 | 5 | 1 |
| 3 | A | 624 | PX4 | C27-C26-C25 | 2.41 | 102.20 | 114.37 | 11 | 1 |
| 3 | B | 315 | PX4 | C26-C25-C24 | 2.41 | 104.28 | 113.13 | 10 | 1 |
| 3 | B | 338 | PX4 | O7-C23-O8 | 2.41 | 129.33 | 123.70 | 7 | 5 |
| 3 | B | 357 | PX4 | C8-C7-C6 | 2.41 | 106.17 | 111.78 | 8 | 2 |
| 3 | B | 373 | PX4 | C8-O5-C9 | 2.41 | 108.32 | 117.12 | 2 | 1 |
| 3 | C | 314 | PX4 | C1-C2-N1 | 2.41 | 123.55 | 115.82 | 13 | 2 |
| 3 | B | 382 | PX4 | C8-C7-C6 | 2.41 | 117.40 | 111.78 | 6 | 2 |
| 3 | B | 395 | PX4 | C5-N1-C3 | 2.41 | 102.65 | 108.98 | 7 | 1 |
| 3 | C | 356 | PX4 | P1-O3-C1 | 2.41 | 132.72 | 121.26 | 4 | 2 |
| 3 | B | 360 | PX4 | C26-C25-C24 | 2.41 | 104.29 | 113.13 | 7 | 1 |
| 3 | C | 336 | PX4 | O5-C9-O6 | 2.41 | 129.64 | 123.63 | 4 | 2 |
| 3 | C | 351 | PX4 | C12-C11-C10 | 2.41 | 104.29 | 113.13 | 13 | 2 |
| 3 | B | 313 | PX4 | C1-C2-N1 | 2.40 | 123.54 | 115.82 | 11 | 3 |
| 3 | B | 374 | PX4 | C26-C25-C24 | 2.40 | 104.30 | 113.13 | 2 | 1 |
| 3 | B | 385 | PX4 | C1-C2-N1 | 2.40 | 123.54 | 115.82 | 15 | 3 |
| 3 | C | 354 | PX4 | O7-C7-C8 | 2.40 | 116.97 | 108.34 | 4 | 1 |
| 3 | A | 622 | PX4 | O5-C9-C10 | 2.40 | 104.51 | 111.83 | 6 | 1 |
| 3 | A | 636 | PX4 | C26-C25-C24 | 2.40 | 121.96 | 113.13 | 11 | 1 |
| 3 | B | 303 | PX4 | O7-C23-O8 | 2.40 | 129.32 | 123.70 | 7 | 2 |
| 3 | B | 347 | PX4 | O1-P1-O2 | 2.40 | 123.62 | 112.44 | 14 | 3 |
| 3 | B | 349 | PX4 | O7-C7-C8 | 2.40 | 116.96 | 108.34 | 7 | 1 |
| 3 | A | 608 | PX4 | P1-O4-C6 | 2.40 | 107.59 | 121.35 | 14 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | A | 619 | PX4 | O1-P1-O2 | 2.40 | 123.61 | 112.44 | 11 | 1 |
| 3 | A | 654 | PX4 | O5-C9-C10 | 2.40 | 104.51 | 111.83 | 6 | 3 |
| 3 | A | 654 | PX4 | C20-C19-C18 | 2.40 | 102.23 | 114.37 | 3 | 1 |
| 3 | B | 390 | PX4 | C12-C11-C10 | 2.40 | 121.95 | 113.13 | 4 | 1 |
| 3 | C | 308 | PX4 | C5-N1-C2 | 2.40 | 119.46 | 109.91 | 10 | 1 |
| 3 | B | 306 | PX4 | C1-C2-N1 | 2.40 | 123.53 | 115.82 | 6 | 1 |
| 3 | B | 322 | PX4 | O5-C9-C10 | 2.40 | 104.51 | 111.83 | 1 | 1 |
| 3 | B | 358 | PX4 | C5-N1-C4 | 2.40 | 115.28 | 108.98 | 14 | 1 |
| 3 | A | 639 | PX4 | O7-C7-C8 | 2.40 | 116.95 | 108.34 | 5 | 4 |
| 3 | B | 314 | PX4 | C4-N1-C3 | 2.40 | 102.67 | 108.98 | 15 | 2 |
| 3 | B | 378 | PX4 | C26-C25-C24 | 2.40 | 104.31 | 113.13 | 3 | 1 |
| 3 | B | 333 | PX4 | C25-C24-C23 | 2.40 | 104.91 | 113.69 | 7 | 1 |
| 3 | C | 345 | PX4 | O7-C23-O8 | 2.40 | 129.31 | 123.70 | 12 | 1 |
| 3 | B | 377 | PX4 | C25-C24-C23 | 2.40 | 104.91 | 113.69 | 10 | 1 |
| 3 | A | 638 | PX4 | C5-N1-C2 | 2.40 | 119.43 | 109.91 | 12 | 1 |
| 3 | C | 332 | PX4 | C11-C10-C9 | 2.40 | 104.91 | 113.69 | 2 | 1 |
| 3 | A | 630 | PX4 | C1-C2-N1 | 2.39 | 123.51 | 115.82 | 10 | 1 |
| 3 | B | 324 | PX4 | C27-C26-C25 | 2.39 | 102.27 | 114.37 | 12 | 1 |
| 3 | B | 313 | PX4 | C19-C18-C17 | 2.39 | 102.28 | 114.37 | 12 | 1 |
| 3 | B | 325 | PX4 | C8-C7-C6 | 2.39 | 106.20 | 111.78 | 12 | 2 |
| 3 | C | 308 | PX4 | C12-C11-C10 | 2.39 | 121.92 | 113.13 | 7 | 2 |
| 3 | C | 351 | PX4 | C16-C15-C14 | 2.39 | 102.27 | 114.37 | 11 | 1 |
| 3 | A | 609 | PX4 | O7-C23-C24 | 2.39 | 106.31 | 111.48 | 12 | 1 |
| 3 | A | 627 | PX4 | O7-C7-C8 | 2.39 | 116.92 | 108.34 | 10 | 2 |
| 3 | A | 645 | PX4 | C34-C33-C32 | 2.39 | 102.29 | 114.37 | 15 | 1 |
| 3 | B | 315 | PX4 | O7-C7-C8 | 2.39 | 116.92 | 108.34 | 3 | 2 |
| 3 | B | 321 | PX4 | O7-C7-C6 | 2.39 | 116.92 | 108.34 | 1 | 1 |
| 3 | B | 385 | PX4 | C8-O5-C9 | 2.39 | 108.38 | 117.12 | 8 | 1 |
| 3 | C | 311 | PX4 | C5-N1-C3 | 2.39 | 102.70 | 108.98 | 5 | 2 |
| 3 | C | 318 | PX4 | O7-C7-C8 | 2.39 | 116.92 | 108.34 | 15 | 1 |
| 3 | C | 337 | PX4 | O7-C23-O8 | 2.39 | 129.29 | 123.70 | 10 | 2 |
| 3 | A | 611 | PX4 | O7-C23-O8 | 2.39 | 129.29 | 123.70 | 2 | 1 |
| 3 | A | 654 | PX4 | C25-C24-C23 | 2.39 | 104.94 | 113.69 | 8 | 1 |
| 3 | B | 352 | PX4 | O7-C7-C6 | 2.39 | 99.78 | 108.34 | 6 | 1 |
| 3 | B | 367 | PX4 | O5-C9-C10 | 2.39 | 104.56 | 111.83 | 14 | 2 |
| 3 | B | 382 | PX4 | C11-C10-C9 | 2.39 | 122.44 | 113.69 | 6 | 1 |
| 3 | C | 321 | PX4 | C15-C14-C13 | 2.39 | 102.30 | 114.37 | 14 | 1 |
| 3 | A | 618 | PX4 | O8-C23-C24 | 2.39 | 133.11 | 123.78 | 4 | 2 |
| 3 | A | 638 | PX4 | O3-C1-C2 | 2.39 | 121.13 | 109.65 | 13 | 2 |
| 3 | B | 326 | PX4 | C8-O5-C9 | 2.39 | 108.40 | 117.12 | 3 | 3 |
| 3 | C | 328 | PX4 | O7-C23-O8 | 2.39 | 129.28 | 123.70 | 1 | 2 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | A | 645 | PX4 | O7-C7-C6 | 2.38 | 116.90 | 108.34 | 8 | 1 |
| 3 | B | 350 | PX4 | O7-C23-O8 | 2.39 | 129.28 | 123.70 | 2 | 2 |
| 3 | B | 378 | PX4 | O5-C9-O6 | 2.39 | 129.59 | 123.63 | 1 | 2 |
| 3 | C | 333 | PX4 | O1-P1-O2 | 2.38 | 123.54 | 112.44 | 1 | 1 |
| 3 | C | 338 | PX4 | C8-C7-C6 | 2.39 | 106.22 | 111.78 | 9 | 2 |
| 3 | B | 342 | PX4 | C5-N1-C4 | 2.38 | 102.71 | 108.98 | 10 | 3 |
| 3 | C | 347 | PX4 | O7-C7-C8 | 2.38 | 116.90 | 108.34 | 1 | 1 |
| 3 | C | 356 | PX4 | C25-C24-C23 | 2.38 | 104.95 | 113.69 | 8 | 1 |
| 3 | B | 349 | PX4 | C1-C2-N1 | 2.38 | 123.47 | 115.82 | 8 | 2 |
| 3 | B | 351 | PX4 | O7-C7-C8 | 2.38 | 116.89 | 108.34 | 10 | 1 |
| 3 | B | 370 | PX4 | O1-P1-O2 | 2.38 | 123.53 | 112.44 | 11 | 1 |
| 3 | A | 617 | PX4 | O5-C9-O6 | 2.38 | 129.59 | 123.63 | 1 | 2 |
| 3 | B | 383 | PX4 | O3-C1-C2 | 2.38 | 121.11 | 109.65 | 1 | 1 |
| 3 | B | 385 | PX4 | O8-C23-C24 | 2.38 | 133.10 | 123.78 | 5 | 1 |
| 3 | C | 316 | PX4 | O7-C7-C6 | 2.38 | 116.89 | 108.34 | 8 | 1 |
| 3 | C | 349 | PX4 | C25-C24-C23 | 2.38 | 104.97 | 113.69 | 13 | 1 |
| 3 | A | 627 | PX4 | C11-C10-C9 | 2.38 | 122.42 | 113.69 | 6 | 1 |
| 3 | A | 649 | PX4 | C20-C19-C18 | 2.38 | 102.33 | 114.37 | 8 | 1 |
| 3 | A | 650 | PX4 | C4-N1-C3 | 2.38 | 115.23 | 108.98 | 1 | 4 |
| 3 | B | 313 | PX4 | C14-C13-C12 | 2.38 | 102.34 | 114.37 | 14 | 1 |
| 3 | B | 325 | PX4 | C8-O5-C9 | 2.38 | 108.42 | 117.12 | 8 | 1 |
| 3 | B | 397 | PX4 | O5-C9-O6 | 2.38 | 129.58 | 123.63 | 5 | 2 |
| 3 | C | 361 | PX4 | C4-N1-C2 | 2.38 | 119.37 | 109.91 | 4 | 1 |
| 3 | A | 617 | PX4 | C4-N1-C3 | 2.38 | 102.73 | 108.98 | 2 | 3 |
| 3 | B | 326 | PX4 | O1-P1-O2 | 2.38 | 123.50 | 112.44 | 2 | 1 |
| 3 | B | 332 | PX4 | C25-C24-C23 | 2.38 | 104.98 | 113.69 | 15 | 1 |
| 3 | C | 362 | PX4 | C26-C25-C24 | 2.38 | 121.87 | 113.13 | 11 | 2 |
| 3 | A | 602 | PX4 | O7-C23-O8 | 2.38 | 129.26 | 123.70 | 9 | 2 |
| 3 | B | 349 | PX4 | O5-C9-C10 | 2.38 | 104.59 | 111.83 | 4 | 3 |
| 3 | B | 370 | PX4 | C4-N1-C3 | 2.38 | 115.22 | 108.98 | 13 | 1 |
| 3 | B | 386 | PX4 | O7-C23-O8 | 2.38 | 129.26 | 123.70 | 7 | 1 |
| 3 | B | 397 | PX4 | O5-C9-C10 | 2.38 | 104.59 | 111.83 | 14 | 1 |
| 3 | C | 333 | PX4 | C5-N1-C3 | 2.38 | 102.73 | 108.98 | 9 | 1 |
| 3 | B | 352 | PX4 | O1-P1-O2 | 2.37 | 123.49 | 112.44 | 1 | 2 |
| 3 | A | 624 | PX4 | C5-N1-C4 | 2.37 | 102.74 | 108.98 | 1 | 1 |
| 3 | A | 641 | PX4 | O7-C7-C8 | 2.37 | 116.86 | 108.34 | 6 | 3 |
| 3 | A | 644 | PX4 | O5-C9-C10 | 2.37 | 104.60 | 111.83 | 13 | 1 |
| 3 | C | 331 | PX4 | C34-C33-C32 | 2.37 | 102.36 | 114.37 | 15 | 2 |
| 3 | A | 650 | PX4 | C5-N1-C4 | 2.37 | 102.74 | 108.98 | 1 | 2 |
| 3 | B | 307 | PX4 | O5-C9-C10 | 2.37 | 104.60 | 111.83 | 11 | 3 |
| 3 | B | 384 | PX4 | C32-C31-C30 | 2.37 | 102.37 | 114.37 | 9 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | C | 327 | PX4 | O5-C9-C10 | 2.37 | 104.60 | 111.83 | 14 | 2 |
| 3 | C | 363 | PX4 | O6-C9-C10 | 2.37 | 133.06 | 123.78 | 15 | 1 |
| 3 | A | 603 | PX4 | C15-C14-C13 | 2.37 | 102.38 | 114.37 | 2 | 1 |
| 3 | B | 303 | PX4 | O5-C8-C7 | 2.37 | 115.23 | 108.40 | 9 | 3 |
| 3 | B | 312 | PX4 | O7-C23-O8 | 2.37 | 129.25 | 123.70 | 10 | 3 |
| 3 | B | 325 | PX4 | C4-N1-C3 | 2.37 | 115.21 | 108.98 | 12 | 1 |
| 3 | C | 353 | PX4 | C8-C7-C6 | 2.37 | 106.26 | 111.78 | 12 | 2 |
| 3 | C | 315 | PX4 | C5-N1-C2 | 2.37 | 100.49 | 109.91 | 1 | 1 |
| 3 | C | 339 | PX4 | C25-C24-C23 | 2.37 | 122.38 | 113.69 | 9 | 1 |
| 3 | C | 364 | PX4 | C1-C2-N1 | 2.37 | 123.43 | 115.82 | 15 | 1 |
| 3 | A | 628 | PX4 | O7-C7-C8 | 2.37 | 116.83 | 108.34 | 11 | 1 |
| 3 | B | 385 | PX4 | C28-C27-C26 | 2.37 | 102.40 | 114.37 | 11 | 1 |
| 3 | B | 314 | PX4 | O5-C9-O6 | 2.37 | 129.55 | 123.63 | 8 | 1 |
| 3 | B | 320 | PX4 | C4-N1-C3 | 2.37 | 115.19 | 108.98 | 4 | 2 |
| 3 | B | 332 | PX4 | C8-O5-C9 | 2.37 | 108.47 | 117.12 | 11 | 1 |
| 3 | B | 399 | PX4 | C4-N1-C3 | 2.37 | 102.76 | 108.98 | 11 | 1 |
| 3 | C | 317 | PX4 | O5-C9-C10 | 2.37 | 119.05 | 111.83 | 4 | 3 |
| 3 | C | 329 | PX4 | C5-N1-C2 | 2.37 | 119.32 | 109.91 | 5 | 1 |
| 3 | B | 364 | PX4 | O3-P1-O2 | 2.36 | 118.31 | 108.94 | 4 | 1 |
| 3 | C | 341 | PX4 | C26-C25-C24 | 2.37 | 104.44 | 113.13 | 15 | 1 |
| 3 | C | 355 | PX4 | O6-C9-C10 | 2.37 | 133.03 | 123.78 | 11 | 1 |
| 3 | B | 392 | PX4 | O7-C7-C8 | 2.36 | 116.83 | 108.34 | 7 | 1 |
| 3 | B | 365 | PX4 | O5-C9-O6 | 2.36 | 129.54 | 123.63 | 4 | 1 |
| 3 | B | 394 | PX4 | C3-N1-C2 | 2.36 | 119.31 | 109.91 | 12 | 2 |
| 3 | A | 628 | PX4 | C8-C7-C6 | 2.36 | 117.29 | 111.78 | 10 | 3 |
| 3 | B | 308 | PX4 | C1-C2-N1 | 2.36 | 123.40 | 115.82 | 11 | 2 |
| 3 | C | 346 | PX4 | O7-C7-C8 | 2.36 | 116.82 | 108.34 | 7 | 3 |
| 3 | B | 320 | PX4 | O6-C9-C10 | 2.36 | 133.02 | 123.78 | 1 | 1 |
| 3 | C | 332 | PX4 | C4-N1-C3 | 2.36 | 115.18 | 108.98 | 9 | 2 |
| 3 | B | 308 | PX4 | C5-N1-C3 | 2.36 | 102.78 | 108.98 | 3 | 1 |
| 3 | C | 309 | PX4 | C26-C25-C24 | 2.36 | 104.46 | 113.13 | 15 | 1 |
| 3 | C | 315 | PX4 | O7-C7-C8 | 2.36 | 116.80 | 108.34 | 13 | 2 |
| 3 | A | 621 | PX4 | O5-C9-C10 | 2.35 | 104.66 | 111.83 | 14 | 1 |
| 3 | A | 623 | PX4 | O5-C9-C10 | 2.35 | 104.66 | 111.83 | 6 | 3 |
| 3 | A | 645 | PX4 | O1-P1-O2 | 2.35 | 123.40 | 112.44 | 10 | 1 |
| 3 | C | 319 | PX4 | C1-C2-N1 | 2.36 | 123.38 | 115.82 | 1 | 2 |
| 3 | B | 331 | PX4 | O7-C23-O8 | 2.35 | 129.21 | 123.70 | 5 | 2 |
| 3 | B | 379 | PX4 | C4-N1-C3 | 2.35 | 115.16 | 108.98 | 5 | 2 |
| 3 | C | 321 | PX4 | O5-C9-O6 | 2.35 | 129.52 | 123.63 | 8 | 2 |
| 3 | C | 359 | PX4 | O7-C23-O8 | 2.35 | 129.21 | 123.70 | 15 | 2 |
| 3 | C | 359 | PX4 | C11-C10-C9 | 2.35 | 122.32 | 113.69 | 9 | 2 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 347 | PX4 | C5-N1-C4 | 2.35 | 102.80 | 108.98 | 9 | 1 |
| 3 | B | 381 | PX4 | C5-N1-C4 | 2.35 | 115.15 | 108.98 | 7 | 1 |
| 3 | A | 639 | PX4 | C26-C25-C24 | 2.35 | 121.76 | 113.13 | 5 | 2 |
| 3 | B | 361 | PX4 | C5-N1-C3 | 2.35 | 102.80 | 108.98 | 4 | 3 |
| 3 | B | 379 | PX4 | C12-C11-C10 | 2.35 | 104.49 | 113.13 | 8 | 1 |
| 3 | B | 360 | PX4 | C4-N1-C3 | 2.35 | 115.15 | 108.98 | 6 | 3 |
| 3 | B | 371 | PX4 | O5-C9-O6 | 2.35 | 129.51 | 123.63 | 14 | 2 |
| 3 | B | 371 | PX4 | C25-C24-C23 | 2.35 | 122.30 | 113.69 | 9 | 1 |
| 3 | C | 311 | PX4 | C31-C30-C29 | 2.35 | 102.49 | 114.37 | 5 | 2 |
| 3 | A | 614 | PX4 | O5-C9-C10 | 2.35 | 104.68 | 111.83 | 4 | 3 |
| 3 | A | 617 | PX4 | O7-C23-O8 | 2.35 | 129.19 | 123.70 | 14 | 2 |
| 3 | A | 625 | PX4 | O5-C9-O6 | 2.35 | 129.50 | 123.63 | 4 | 2 |
| 3 | B | 327 | PX4 | C4-N1-C2 | 2.35 | 119.24 | 109.91 | 14 | 1 |
| 3 | B | 351 | PX4 | C1-C2-N1 | 2.35 | 123.36 | 115.82 | 7 | 2 |
| 3 | B | 397 | PX4 | C19-C18-C17 | 2.35 | 102.50 | 114.37 | 6 | 1 |
| 3 | C | 314 | PX4 | O7-C23-O8 | 2.35 | 129.20 | 123.70 | 12 | 2 |
| 3 | C | 326 | PX4 | O7-C7-C8 | 2.35 | 116.77 | 108.34 | 5 | 2 |
| 3 | B | 391 | PX4 | O3-P1-O2 | 2.35 | 99.64 | 108.94 | 5 | 1 |
| 3 | C | 310 | PX4 | C8-O5-C9 | 2.35 | 108.54 | 117.12 | 10 | 1 |
| 3 | C | 347 | PX4 | O5-C9-O6 | 2.35 | 129.50 | 123.63 | 13 | 3 |
| 3 | A | 628 | PX4 | C5-N1-C4 | 2.35 | 102.81 | 108.98 | 14 | 2 |
| 3 | C | 332 | PX4 | C32-C31-C30 | 2.35 | 102.51 | 114.37 | 8 | 1 |
| 3 | A | 651 | PX4 | C5-N1-C4 | 2.34 | 102.82 | 108.98 | 14 | 4 |
| 3 | B | 343 | PX4 | C8-C7-C6 | 2.34 | 106.32 | 111.78 | 11 | 1 |
| 3 | C | 349 | PX4 | C1-C2-N1 | 2.34 | 123.35 | 115.82 | 15 | 1 |
| 3 | C | 355 | PX4 | O7-C23-O8 | 2.34 | 129.19 | 123.70 | 4 | 1 |
| 3 | B | 304 | PX4 | C11-C10-C9 | 2.34 | 122.28 | 113.69 | 9 | 2 |
| 3 | B | 318 | PX4 | C5-N1-C4 | 2.34 | 115.13 | 108.98 | 15 | 3 |
| 3 | B | 320 | PX4 | O8-C23-C24 | 2.34 | 132.94 | 123.78 | 6 | 1 |
| 3 | B | 376 | PX4 | C8-C7-C6 | 2.34 | 117.25 | 111.78 | 13 | 1 |
| 3 | B | 377 | PX4 | O7-C7-C8 | 2.34 | 116.74 | 108.34 | 8 | 1 |
| 3 | C | 310 | PX4 | C4-N1-C3 | 2.34 | 115.13 | 108.98 | 15 | 3 |
| 3 | C | 328 | PX4 | O5-C9-C10 | 2.34 | 104.69 | 111.83 | 11 | 3 |
| 3 | C | 330 | PX4 | C25-C24-C23 | 2.34 | 122.28 | 113.69 | 3 | 1 |
| 3 | C | 331 | PX4 | C4-N1-C2 | 2.34 | 119.22 | 109.91 | 3 | 1 |
| 3 | B | 324 | PX4 | C8-C7-C6 | 2.34 | 117.25 | 111.78 | 15 | 3 |
| 3 | C | 338 | PX4 | O5-C9-O6 | 2.34 | 129.49 | 123.63 | 4 | 3 |
| 3 | B | 318 | PX4 | C11-C10-C9 | 2.34 | 122.27 | 113.69 | 4 | 1 |
| 3 | C | 338 | PX4 | O3-C1-C2 | 2.34 | 120.91 | 109.65 | 14 | 2 |
| 3 | A | 620 | PX4 | C8-C7-C6 | 2.34 | 106.33 | 111.78 | 13 | 1 |
| 3 | B | 368 | PX4 | O7-C7-C6 | 2.34 | 99.96 | 108.34 | 14 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 399 | PX4 | O7-C7-C6 | 2.34 | 99.96 | 108.34 | 6 | 2 |
| 3 | C | 326 | PX4 | C19-C18-C17 | 2.34 | 126.19 | 114.37 | 12 | 1 |
| 3 | A | 601 | PX4 | C4-N1-C3 | 2.34 | 115.11 | 108.98 | 2 | 1 |
| 3 | A | 604 | PX4 | C4-N1-C2 | 2.34 | 119.20 | 109.91 | 15 | 1 |
| 3 | B | 316 | PX4 | C5-N1-C4 | 2.34 | 115.11 | 108.98 | 6 | 2 |
| 3 | B | 346 | PX4 | O5-C9-O6 | 2.34 | 129.47 | 123.63 | 12 | 2 |
| 3 | C | 301 | PX4 | C5-N1-C3 | 2.34 | 102.84 | 108.98 | 13 | 1 |
| 3 | C | 313 | PX4 | C12-C11-C10 | 2.34 | 121.72 | 113.13 | 8 | 2 |
| 3 | C | 352 | PX4 | C18-C17-C16 | 2.34 | 102.55 | 114.37 | 13 | 1 |
| 3 | C | 353 | PX4 | C5-N1-C2 | 2.34 | 119.20 | 109.91 | 9 | 1 |
| 3 | A | 622 | PX4 | O7-C7-C6 | 2.33 | 116.72 | 108.34 | 6 | 1 |
| 3 | A | 627 | PX4 | P1-O3-C1 | 2.34 | 110.14 | 121.26 | 13 | 1 |
| 3 | A | 629 | PX4 | O5-C9-C10 | 2.34 | 104.71 | 111.83 | 2 | 1 |
| 3 | A | 638 | PX4 | C8-C7-C6 | 2.33 | 117.23 | 111.78 | 13 | 2 |
| 3 | B | 348 | PX4 | O7-C23-O8 | 2.34 | 129.16 | 123.70 | 12 | 3 |
| 3 | B | 360 | PX4 | C25-C24-C23 | 2.34 | 105.14 | 113.69 | 14 | 1 |
| 3 | C | 318 | PX4 | O1-P1-O2 | 2.34 | 123.31 | 112.44 | 4 | 2 |
| 3 | B | 395 | PX4 | C11-C10-C9 | 2.34 | 105.14 | 113.69 | 11 | 1 |
| 3 | C | 319 | PX4 | P1-O3-C1 | 2.33 | 132.38 | 121.26 | 9 | 1 |
| 3 | A | 639 | PX4 | C4-N1-C3 | 2.33 | 102.85 | 108.98 | 1 | 1 |
| 3 | B | 302 | PX4 | C8-C7-C6 | 2.33 | 106.34 | 111.78 | 10 | 3 |
| 3 | B | 321 | PX4 | O7-C7-C8 | 2.33 | 116.71 | 108.34 | 3 | 3 |
| 3 | B | 371 | PX4 | C5-N1-C4 | 2.33 | 102.85 | 108.98 | 11 | 2 |
| 3 | C | 312 | PX4 | P1-O3-C1 | 2.33 | 132.37 | 121.26 | 12 | 1 |
| 3 | C | 321 | PX4 | C5-N1-C3 | 2.33 | 115.11 | 108.98 | 11 | 2 |
| 3 | C | 349 | PX4 | O4-P1-O2 | 2.33 | 99.68 | 108.94 | 7 | 1 |
| 3 | A | 629 | PX4 | C4-N1-C2 | 2.33 | 119.18 | 109.91 | 12 | 1 |
| 3 | A | 647 | PX4 | O7-C7-C8 | 2.33 | 116.71 | 108.34 | 7 | 2 |
| 3 | B | 355 | PX4 | O5-C9-C10 | 2.33 | 104.72 | 111.83 | 5 | 1 |
| 3 | B | 356 | PX4 | C25-C24-C23 | 2.33 | 122.24 | 113.69 | 5 | 2 |
| 3 | B | 358 | PX4 | C8-C7-C6 | 2.33 | 106.35 | 111.78 | 11 | 3 |
| 3 | C | 343 | PX4 | O7-C23-C24 | 2.33 | 106.44 | 111.48 | 10 | 2 |
| 3 | A | 631 | PX4 | C8-O5-C9 | 2.33 | 108.60 | 117.12 | 3 | 1 |
| 3 | A | 635 | PX4 | O7-C7-C6 | 2.33 | 99.98 | 108.34 | 3 | 2 |
| 3 | B | 319 | PX4 | C12-C11-C10 | 2.33 | 121.69 | 113.13 | 4 | 1 |
| 3 | B | 337 | PX4 | C26-C25-C24 | 2.33 | 104.56 | 113.13 | 8 | 1 |
| 3 | C | 346 | PX4 | C4-N1-C3 | 2.33 | 115.10 | 108.98 | 12 | 2 |
| 3 | C | 309 | PX4 | O1-P1-O2 | 2.33 | 123.28 | 112.44 | 12 | 1 |
| 3 | C | 348 | PX4 | C8-C7-C6 | 2.33 | 106.35 | 111.78 | 15 | 2 |
| 3 | A | 621 | PX4 | O3-C1-C2 | 2.33 | 120.85 | 109.65 | 14 | 1 |
| 3 | B | 307 | PX4 | C5-N1-C3 | 2.33 | 115.09 | 108.98 | 5 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | A | 627 | PX4 | C28-C27-C26 | 2.33 | 102.61 | 114.37 | 3 | 1 |
| 3 | A | 643 | PX4 | O5-C9-C10 | 2.33 | 104.74 | 111.83 | 1 | 2 |
| 3 | B | 371 | PX4 | O1-P1-O4 | 2.33 | 118.11 | 107.57 | 9 | 1 |
| 3 | C | 324 | PX4 | C26-C25-C24 | 2.33 | 104.58 | 113.13 | 15 | 1 |
| 3 | C | 328 | PX4 | C29-C28-C27 | 2.33 | 102.60 | 114.37 | 7 | 1 |
| 3 | B | 302 | PX4 | O1-P1-O2 | 2.33 | 123.26 | 112.44 | 13 | 1 |
| 3 | B | 381 | PX4 | C26-C25-C24 | 2.33 | 104.58 | 113.13 | 8 | 1 |
| 3 | B | 391 | PX4 | O6-C9-C10 | 2.33 | 132.88 | 123.78 | 7 | 1 |
| 3 | A | 628 | PX4 | C12-C11-C10 | 2.32 | 121.66 | 113.13 | 1 | 1 |
| 3 | B | 315 | PX4 | C1-C2-N1 | 2.32 | 123.28 | 115.82 | 1 | 2 |
| 3 | C | 358 | PX4 | C4-N1-C3 | 2.32 | 115.08 | 108.98 | 8 | 1 |
| 3 | B | 355 | PX4 | O7-C23-O8 | 2.32 | 129.14 | 123.70 | 4 | 2 |
| 3 | A | 644 | PX4 | O7-C7-C6 | 2.32 | 116.67 | 108.34 | 5 | 1 |
| 3 | A | 646 | PX4 | C13-C12-C11 | 2.32 | 102.63 | 114.37 | 8 | 1 |
| 3 | B | 376 | PX4 | O7-C7-C6 | 2.32 | 116.68 | 108.34 | 2 | 2 |
| 3 | B | 390 | PX4 | C5-N1-C4 | 2.32 | 102.87 | 108.98 | 11 | 2 |
| 3 | C | 317 | PX4 | C4-N1-C3 | 2.32 | 102.87 | 108.98 | 14 | 1 |
| 3 | A | 653 | PX4 | C5-N1-C3 | 2.32 | 102.88 | 108.98 | 6 | 1 |
| 3 | B | 315 | PX4 | O5-C9-O6 | 2.32 | 129.44 | 123.63 | 10 | 1 |
| 3 | C | 320 | PX4 | C12-C11-C10 | 2.32 | 104.60 | 113.13 | 5 | 1 |
| 3 | C | 322 | PX4 | O1-P1-O3 | 2.32 | 118.09 | 107.57 | 10 | 1 |
| 3 | A | 602 | PX4 | O7-C7-C8 | 2.32 | 116.67 | 108.34 | 8 | 1 |
| 3 | C | 356 | PX4 | P1-O4-C6 | 2.32 | 134.65 | 121.35 | 2 | 2 |
| 3 | A | 620 | PX4 | O7-C7-C6 | 2.32 | 116.66 | 108.34 | 9 | 2 |
| 3 | A | 628 | PX4 | C5-N1-C3 | 2.32 | 115.07 | 108.98 | 6 | 2 |
| 3 | B | 357 | PX4 | O5-C9-C10 | 2.32 | 104.76 | 111.83 | 11 | 2 |
| 3 | A | 623 | PX4 | O5-C9-O6 | 2.32 | 129.43 | 123.63 | 14 | 1 |
| 3 | B | 319 | PX4 | O4-P1-O2 | 2.32 | 118.12 | 108.94 | 10 | 2 |
| 3 | B | 317 | PX4 | C5-N1-C3 | 2.32 | 115.06 | 108.98 | 13 | 1 |
| 3 | C | 316 | PX4 | O5-C9-O6 | 2.32 | 129.43 | 123.63 | 3 | 2 |
| 3 | C | 329 | PX4 | C5-N1-C4 | 2.32 | 102.89 | 108.98 | 14 | 1 |
| 3 | C | 353 | PX4 | O5-C9-C10 | 2.32 | 104.77 | 111.83 | 4 | 1 |
| 3 | A | 632 | PX4 | O7-C23-C24 | 2.32 | 106.47 | 111.48 | 5 | 2 |
| 3 | B | 363 | PX4 | C26-C25-C24 | 2.32 | 121.64 | 113.13 | 7 | 2 |
| 3 | B | 395 | PX4 | C12-C11-C10 | 2.31 | 104.62 | 113.13 | 15 | 1 |
| 3 | C | 324 | PX4 | C11-C10-C9 | 2.32 | 105.21 | 113.69 | 7 | 1 |
| 3 | C | 337 | PX4 | C1-C2-N1 | 2.32 | 123.25 | 115.82 | 7 | 2 |
| 3 | B | 302 | PX4 | C5-N1-C4 | 2.31 | 102.90 | 108.98 | 7 | 1 |
| 3 | B | 360 | PX4 | C4-N1-C2 | 2.31 | 119.11 | 109.91 | 7 | 1 |
| 3 | B | 376 | PX4 | O5-C9-O6 | 2.31 | 129.41 | 123.63 | 15 | 2 |
| 3 | B | 380 | PX4 | C5-N1-C4 | 2.31 | 102.90 | 108.98 | 13 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 396 | PX4 | C11-C10-C9 | 2.31 | 105.22 | 113.69 | 7 | 1 |
| 3 | A | 620 | PX4 | C7-O7-C23 | 2.31 | 112.26 | 117.80 | 7 | 3 |
| 3 | B | 301 | PX4 | C12-C11-C10 | 2.31 | 104.63 | 113.13 | 4 | 1 |
| 3 | B | 326 | PX4 | O8-C23-C24 | 2.31 | 132.82 | 123.78 | 14 | 1 |
| 3 | B | 347 | PX4 | C8-C7-C6 | 2.31 | 106.39 | 111.78 | 4 | 1 |
| 3 | C | 331 | PX4 | O7-C7-C6 | 2.31 | 116.64 | 108.34 | 5 | 2 |
| 3 | B | 337 | PX4 | C4-N1-C3 | 2.31 | 115.04 | 108.98 | 4 | 1 |
| 3 | B | 351 | PX4 | C31-C30-C29 | 2.31 | 126.05 | 114.37 | 11 | 1 |
| 3 | B | 396 | PX4 | O4-P1-O2 | 2.31 | 118.09 | 108.94 | 5 | 1 |
| 3 | C | 317 | PX4 | C12-C11-C10 | 2.31 | 104.64 | 113.13 | 3 | 1 |
| 3 | C | 320 | PX4 | O8-C23-C24 | 2.31 | 132.82 | 123.78 | 14 | 1 |
| 3 | C | 336 | PX4 | C12-C11-C10 | 2.31 | 104.64 | 113.13 | 4 | 1 |
| 3 | A | 630 | PX4 | C13-C12-C11 | 2.31 | 102.70 | 114.37 | 12 | 1 |
| 3 | B | 361 | PX4 | C4-N1-C3 | 2.31 | 102.91 | 108.98 | 5 | 1 |
| 3 | B | 367 | PX4 | C11-C10-C9 | 2.31 | 122.15 | 113.69 | 10 | 2 |
| 3 | B | 376 | PX4 | C1-C2-N1 | 2.31 | 123.23 | 115.82 | 4 | 2 |
| 3 | B | 384 | PX4 | O3-C1-C2 | 2.31 | 120.76 | 109.65 | 4 | 1 |
| 3 | C | 343 | PX4 | O7-C23-O8 | 2.31 | 129.10 | 123.70 | 3 | 3 |
| 3 | A | 625 | PX4 | O7-C7-C8 | 2.31 | 116.62 | 108.34 | 6 | 2 |
| 3 | A | 639 | PX4 | O5-C9-C10 | 2.31 | 104.80 | 111.83 | 12 | 1 |
| 3 | C | 325 | PX4 | O7-C7-C6 | 2.31 | 116.62 | 108.34 | 14 | 1 |
| 3 | C | 336 | PX4 | C8-O5-C9 | 2.31 | 108.68 | 117.12 | 9 | 1 |
| 3 | A | 609 | PX4 | C12-C11-C10 | 2.31 | 104.65 | 113.13 | 3 | 1 |
| 3 | B | 320 | PX4 | C12-C11-C10 | 2.31 | 121.60 | 113.13 | 9 | 1 |
| 3 | B | 333 | PX4 | C3-N1-C2 | 2.31 | 119.08 | 109.91 | 4 | 1 |
| 3 | B | 379 | PX4 | O5-C9-O6 | 2.31 | 129.40 | 123.63 | 8 | 1 |
| 3 | C | 338 | PX4 | C1-C2-N1 | 2.31 | 123.23 | 115.82 | 9 | 1 |
| 3 | C | 321 | PX4 | O7-C23-O8 | 2.31 | 129.09 | 123.70 | 5 | 2 |
| 3 | C | 333 | PX4 | O8-C23-C24 | 2.31 | 132.80 | 123.78 | 14 | 1 |
| 3 | C | 345 | PX4 | C12-C11-C10 | 2.31 | 104.66 | 113.13 | 2 | 1 |
| 3 | C | 349 | PX4 | C12-C11-C10 | 2.30 | 121.59 | 113.13 | 11 | 1 |
| 3 | B | 381 | PX4 | C8-C7-C6 | 2.30 | 106.41 | 111.78 | 14 | 1 |
| 3 | B | 369 | PX4 | O1-P1-O4 | 2.30 | 97.13 | 107.57 | 9 | 2 |
| 3 | C | 342 | PX4 | C11-C10-C9 | 2.30 | 105.25 | 113.69 | 15 | 1 |
| 3 | B | 324 | PX4 | O3-C1-C2 | 2.30 | 120.73 | 109.65 | 8 | 1 |
| 3 | A | 631 | PX4 | C4-N1-C3 | 2.30 | 115.02 | 108.98 | 3 | 1 |
| 3 | A | 646 | PX4 | C8-C7-C6 | 2.30 | 117.15 | 111.78 | 8 | 2 |
| 3 | A | 648 | PX4 | O7-C23-C24 | 2.30 | 106.50 | 111.48 | 6 | 2 |
| 3 | B | 400 | PX4 | C1-C2-N1 | 2.30 | 123.21 | 115.82 | 3 | 1 |
| 3 | C | 326 | PX4 | C33-C32-C31 | 2.30 | 126.00 | 114.37 | 3 | 1 |
| 3 | C | 361 | PX4 | O7-C7-C6 | 2.30 | 116.60 | 108.34 | 2 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | A | 653 | PX4 | C1-C2-N1 | 2.30 | 123.20 | 115.82 | 4 | 2 |
| 3 | B | 331 | PX4 | P1-O4-C6 | 2.30 | 134.53 | 121.35 | 11 | 1 |
| 3 | C | 304 | PX4 | O1-P1-O3 | 2.30 | 118.00 | 107.57 | 13 | 2 |
| 3 | B | 326 | PX4 | C34-C33-C32 | 2.30 | 125.99 | 114.37 | 11 | 1 |
| 3 | C | 315 | PX4 | O1-P1-O3 | 2.30 | 117.99 | 107.57 | 1 | 1 |
| 3 | C | 342 | PX4 | C8-O5-C9 | 2.30 | 108.71 | 117.12 | 9 | 1 |
| 3 | B | 380 | PX4 | C20-C19-C18 | 2.30 | 102.75 | 114.37 | 8 | 1 |
| 3 | B | 303 | PX4 | C12-C11-C10 | 2.30 | 121.57 | 113.13 | 12 | 1 |
| 3 | B | 400 | PX4 | C25-C24-C23 | 2.30 | 105.27 | 113.69 | 13 | 1 |
| 3 | B | 343 | PX4 | C4-N1-C3 | 2.30 | 115.01 | 108.98 | 12 | 2 |
| 3 | B | 352 | PX4 | C26-C25-C24 | 2.30 | 104.69 | 113.13 | 3 | 1 |
| 3 | B | 389 | PX4 | C4-N1-C3 | 2.30 | 102.94 | 108.98 | 15 | 2 |
| 3 | C | 342 | PX4 | C8-C7-C6 | 2.30 | 106.43 | 111.78 | 11 | 1 |
| 3 | C | 344 | PX4 | C4-N1-C2 | 2.30 | 119.03 | 109.91 | 12 | 1 |
| 3 | C | 357 | PX4 | C8-C7-C6 | 2.30 | 117.14 | 111.78 | 9 | 2 |
| 3 | A | 626 | PX4 | C1-C2-N1 | 2.30 | 123.19 | 115.82 | 13 | 1 |
| 3 | B | 376 | PX4 | O5-C8-C7 | 2.29 | 115.01 | 108.40 | 11 | 3 |
| 3 | B | 377 | PX4 | C4-N1-C3 | 2.29 | 102.95 | 108.98 | 11 | 3 |
| 3 | C | 307 | PX4 | O5-C9-C10 | 2.29 | 104.84 | 111.83 | 15 | 1 |
| 3 | C | 319 | PX4 | O7-C7-C6 | 2.29 | 116.58 | 108.34 | 1 | 1 |
| 3 | C | 325 | PX4 | C8-O5-C9 | 2.29 | 108.73 | 117.12 | 7 | 2 |
| 3 | C | 355 | PX4 | O7-C7-C6 | 2.29 | 116.58 | 108.34 | 4 | 1 |
| 3 | A | 624 | PX4 | O5-C8-C7 | 2.29 | 115.01 | 108.40 | 10 | 2 |
| 3 | A | 640 | PX4 | O1-P1-O2 | 2.29 | 123.11 | 112.44 | 2 | 1 |
| 3 | B | 346 | PX4 | O1-P1-O4 | 2.29 | 117.96 | 107.57 | 8 | 1 |
| 3 | C | 306 | PX4 | C17-C16-C15 | 2.29 | 102.78 | 114.37 | 11 | 1 |
| 3 | C | 319 | PX4 | O7-C23-C24 | 2.29 | 106.53 | 111.48 | 4 | 2 |
| 3 | C | 331 | PX4 | C3-N1-C2 | 2.29 | 119.02 | 109.91 | 4 | 1 |
| 3 | C | 334 | PX4 | C5-N1-C2 | 2.29 | 119.02 | 109.91 | 3 | 1 |
| 3 | C | 345 | PX4 | O5-C9-C10 | 2.29 | 104.85 | 111.83 | 9 | 1 |
| 3 | B | 325 | PX4 | O7-C7-C8 | 2.29 | 116.56 | 108.34 | 9 | 1 |
| 3 | B | 339 | PX4 | C5-N1-C4 | 2.29 | 102.96 | 108.98 | 11 | 1 |
| 3 | B | 342 | PX4 | C30-C29-C28 | 2.29 | 102.79 | 114.37 | 7 | 1 |
| 3 | B | 344 | PX4 | C25-C24-C23 | 2.29 | 122.09 | 113.69 | 5 | 1 |
| 3 | B | 362 | PX4 | O5-C9-O6 | 2.29 | 129.36 | 123.63 | 7 | 2 |
| 3 | B | 381 | PX4 | C5-N1-C3 | 2.29 | 102.96 | 108.98 | 2 | 2 |
| 3 | B | 393 | PX4 | C4-N1-C3 | 2.29 | 102.96 | 108.98 | 2 | 2 |
| 3 | C | 333 | PX4 | C26-C25-C24 | 2.29 | 121.54 | 113.13 | 7 | 2 |
| 3 | C | 356 | PX4 | C4-N1-C3 | 2.29 | 114.99 | 108.98 | 12 | 1 |
| 3 | A | 612 | PX4 | O5-C9-C10 | 2.29 | 104.86 | 111.83 | 11 | 2 |
| 3 | A | 652 | PX4 | C19-C18-C17 | 2.29 | 102.80 | 114.37 | 8 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | C | 355 | PX4 | C26-C25-C24 | 2.29 | 121.53 | 113.13 | 14 | 1 |
| 3 | C | 357 | PX4 | O5-C9-C10 | 2.29 | 104.86 | 111.83 | 4 | 2 |
| 3 | A | 634 | PX4 | O1-P1-O2 | 2.29 | 123.09 | 112.44 | 14 | 1 |
| 3 | B | 380 | PX4 | O5-C9-O6 | 2.29 | 129.35 | 123.63 | 5 | 3 |
| 3 | A | 613 | PX4 | O5-C9-O6 | 2.29 | 129.35 | 123.63 | 7 | 1 |
| 3 | A | 617 | PX4 | C33-C32-C31 | 2.29 | 102.81 | 114.37 | 13 | 1 |
| 3 | A | 644 | PX4 | C8-O5-C9 | 2.29 | 125.47 | 117.12 | 10 | 1 |
| 3 | B | 303 | PX4 | C5-N1-C3 | 2.29 | 102.97 | 108.98 | 6 | 2 |
| 3 | B | 392 | PX4 | O5-C9-O6 | 2.29 | 129.34 | 123.63 | 15 | 1 |
| 3 | C | 310 | PX4 | O3-C1-C2 | 2.29 | 120.65 | 109.65 | 7 | 1 |
| 3 | C | 342 | PX4 | C5-N1-C3 | 2.29 | 102.97 | 108.98 | 5 | 4 |
| 3 | B | 325 | PX4 | C5-N1-C3 | 2.28 | 102.98 | 108.98 | 8 | 2 |
| 3 | B | 340 | PX4 | C11-C10-C9 | 2.28 | 122.06 | 113.69 | 4 | 1 |
| 3 | C | 331 | PX4 | C26-C25-C24 | 2.28 | 104.73 | 113.13 | 12 | 1 |
| 3 | C | 315 | PX4 | P1-O3-C1 | 2.28 | 132.13 | 121.26 | 6 | 1 |
| 3 | C | 364 | PX4 | C5-N1-C4 | 2.28 | 102.98 | 108.98 | 3 | 1 |
| 3 | A | 640 | PX4 | C16-C15-C14 | 2.28 | 102.84 | 114.37 | 4 | 1 |
| 3 | B | 315 | PX4 | C11-C10-C9 | 2.28 | 122.05 | 113.69 | 2 | 1 |
| 3 | B | 368 | PX4 | O1-P1-O2 | 2.28 | 123.06 | 112.44 | 1 | 1 |
| 3 | B | 376 | PX4 | C5-N1-C2 | 2.28 | 118.98 | 109.91 | 7 | 1 |
| 3 | C | 316 | PX4 | P1-O3-C1 | 2.28 | 110.40 | 121.26 | 4 | 2 |
| 3 | A | 632 | PX4 | C5-N1-C3 | 2.28 | 114.96 | 108.98 | 11 | 1 |
| 3 | A | 634 | PX4 | C26-C25-C24 | 2.28 | 104.75 | 113.13 | 1 | 1 |
| 3 | A | 644 | PX4 | O6-C9-C10 | 2.28 | 132.70 | 123.78 | 13 | 1 |
| 3 | A | 645 | PX4 | O5-C9-O6 | 2.28 | 129.33 | 123.63 | 11 | 2 |
| 3 | B | 331 | PX4 | C8-C7-C6 | 2.28 | 106.47 | 111.78 | 1 | 1 |
| 3 | B | 357 | PX4 | O7-C23-O8 | 2.28 | 129.04 | 123.70 | 11 | 3 |
| 3 | B | 338 | PX4 | O5-C9-C10 | 2.28 | 118.78 | 111.83 | 1 | 1 |
| 3 | B | 338 | PX4 | C7-O7-C23 | 2.28 | 112.34 | 117.80 | 12 | 3 |
| 3 | B | 366 | PX4 | O5-C9-C10 | 2.28 | 104.89 | 111.83 | 11 | 1 |
| 3 | B | 372 | PX4 | C8-C7-C6 | 2.28 | 106.47 | 111.78 | 4 | 3 |
| 3 | C | 331 | PX4 | C12-C11-C10 | 2.28 | 104.75 | 113.13 | 7 | 1 |
| 3 | B | 301 | PX4 | C25-C24-C23 | 2.28 | 122.04 | 113.69 | 2 | 1 |
| 3 | B | 363 | PX4 | O3-C1-C2 | 2.28 | 120.61 | 109.65 | 10 | 1 |
| 3 | C | 314 | PX4 | C26-C25-C24 | 2.28 | 104.76 | 113.13 | 2 | 1 |
| 3 | C | 314 | PX4 | C25-C24-C23 | 2.28 | 122.04 | 113.69 | 13 | 1 |
| 3 | B | 322 | PX4 | C12-C11-C10 | 2.28 | 104.76 | 113.13 | 13 | 1 |
| 3 | A | 623 | PX4 | P1-O4-C6 | 2.28 | 108.31 | 121.35 | 15 | 1 |
| 3 | B | 334 | PX4 | C4-N1-C3 | 2.28 | 103.00 | 108.98 | 2 | 1 |
| 3 | C | 361 | PX4 | C12-C11-C10 | 2.28 | 121.49 | 113.13 | 5 | 1 |
| 3 | A | 631 | PX4 | C3-N1-C2 | 2.27 | 100.87 | 109.91 | 8 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | A | 633 | PX4 | O7-C7-C8 | 2.27 | 116.50 | 108.34 | 2 | 2 |
| 3 | A | 633 | PX4 | O7-C23-O8 | 2.28 | 129.02 | 123.70 | 10 | 2 |
| 3 | B | 350 | PX4 | C29-C28-C27 | 2.27 | 102.87 | 114.37 | 8 | 1 |
| 3 | C | 302 | PX4 | C5-N1-C4 | 2.27 | 103.00 | 108.98 | 13 | 2 |
| 3 | C | 322 | PX4 | C4-N1-C3 | 2.27 | 114.95 | 108.98 | 13 | 2 |
| 3 | C | 327 | PX4 | C4-N1-C2 | 2.28 | 118.95 | 109.91 | 10 | 1 |
| 3 | C | 339 | PX4 | C11-C10-C9 | 2.28 | 105.36 | 113.69 | 1 | 1 |
| 3 | A | 619 | PX4 | O4-P1-O2 | 2.27 | 117.94 | 108.94 | 15 | 1 |
| 3 | A | 642 | PX4 | C1-C2-N1 | 2.27 | 123.12 | 115.82 | 1 | 1 |
| 3 | B | 309 | PX4 | O5-C8-C7 | 2.27 | 114.95 | 108.40 | 10 | 2 |
| 3 | C | 333 | PX4 | O5-C9-C10 | 2.27 | 104.90 | 111.83 | 4 | 1 |
| 3 | B | 384 | PX4 | C5-N1-C4 | 2.27 | 114.95 | 108.98 | 3 | 2 |
| 3 | C | 326 | PX4 | P1-O4-C6 | 2.27 | 108.33 | 121.35 | 3 | 1 |
| 3 | A | 633 | PX4 | C8-O5-C9 | 2.27 | 108.82 | 117.12 | 3 | 1 |
| 3 | B | 397 | PX4 | C4-N1-C3 | 2.27 | 114.94 | 108.98 | 10 | 1 |
| 3 | C | 340 | PX4 | P1-O3-C1 | 2.27 | 110.44 | 121.26 | 12 | 2 |
| 3 | A | 606 | PX4 | C25-C24-C23 | 2.27 | 122.01 | 113.69 | 11 | 1 |
| 3 | B | 324 | PX4 | C5-N1-C4 | 2.27 | 103.01 | 108.98 | 15 | 2 |
| 3 | A | 646 | PX4 | C25-C24-C23 | 2.27 | 105.38 | 113.69 | 5 | 2 |
| 3 | A | 649 | PX4 | C5-N1-C4 | 2.27 | 114.94 | 108.98 | 1 | 1 |
| 3 | B | 308 | PX4 | C29-C28-C27 | 2.27 | 102.90 | 114.37 | 2 | 1 |
| 3 | B | 316 | PX4 | C4-N1-C3 | 2.27 | 103.01 | 108.98 | 6 | 2 |
| 3 | B | 317 | PX4 | C8-O5-C9 | 2.27 | 108.82 | 117.12 | 11 | 2 |
| 3 | A | 651 | PX4 | C29-C28-C27 | 2.27 | 102.91 | 114.37 | 2 | 1 |
| 3 | B | 307 | PX4 | C4-N1-C3 | 2.27 | 103.02 | 108.98 | 9 | 1 |
| 3 | C | 326 | PX4 | P1-O3-C1 | 2.27 | 132.06 | 121.26 | 14 | 1 |
| 3 | B | 314 | PX4 | C32-C31-C30 | 2.27 | 102.91 | 114.37 | 5 | 1 |
| 3 | B | 350 | PX4 | C12-C11-C10 | 2.27 | 104.80 | 113.13 | 5 | 2 |
| 3 | B | 379 | PX4 | C5-N1-C4 | 2.27 | 103.02 | 108.98 | 7 | 1 |
| 3 | C | 344 | PX4 | O5-C9-C10 | 2.27 | 104.92 | 111.83 | 7 | 3 |
| 3 | A | 642 | PX4 | C4-N1-C2 | 2.27 | 118.91 | 109.91 | 3 | 1 |
| 3 | C | 316 | PX4 | O6-C9-C10 | 2.27 | 132.64 | 123.78 | 1 | 1 |
| 3 | B | 307 | PX4 | O1-P1-O2 | 2.26 | 122.97 | 112.44 | 10 | 2 |
| 3 | B | 331 | PX4 | C5-N1-C2 | 2.26 | 118.91 | 109.91 | 6 | 1 |
| 3 | C | 332 | PX4 | C31-C30-C29 | 2.26 | 102.92 | 114.37 | 7 | 1 |
| 3 | C | 337 | PX4 | C13-C12-C11 | 2.26 | 102.92 | 114.37 | 11 | 1 |
| 3 | A | 627 | PX4 | C33-C32-C31 | 2.26 | 102.93 | 114.37 | 14 | 1 |
| 3 | A | 640 | PX4 | C25-C24-C23 | 2.26 | 105.40 | 113.69 | 11 | 1 |
| 3 | B | 382 | PX4 | C1-C2-N1 | 2.26 | 123.08 | 115.82 | 8 | 3 |
| 3 | B | 392 | PX4 | C5-N1-C3 | 2.26 | 103.03 | 108.98 | 5 | 1 |
| 3 | B | 313 | PX4 | C12-C11-C10 | 2.26 | 104.82 | 113.13 | 3 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 391 | PX4 | O7-C7-C6 | 2.26 | 116.46 | 108.34 | 2 | 1 |
| 3 | B | 399 | PX4 | C32-C31-C30 | 2.26 | 102.93 | 114.37 | 3 | 1 |
| 3 | C | 334 | PX4 | C7-O7-C23 | 2.26 | 112.38 | 117.80 | 9 | 2 |
| 3 | C | 346 | PX4 | C26-C25-C24 | 2.26 | 121.44 | 113.13 | 15 | 1 |
| 3 | C | 360 | PX4 | C25-C24-C23 | 2.26 | 105.41 | 113.69 | 2 | 1 |
| 3 | A | 617 | PX4 | C11-C10-C9 | 2.26 | 105.42 | 113.69 | 11 | 2 |
| 3 | A | 647 | PX4 | C4-N1-C3 | 2.26 | 103.04 | 108.98 | 6 | 1 |
| 3 | A | 624 | PX4 | O3-P1-O2 | 2.26 | 99.98 | 108.94 | 5 | 1 |
| 3 | B | 308 | PX4 | C11-C10-C9 | 2.26 | 121.97 | 113.69 | 8 | 1 |
| 3 | B | 362 | PX4 | O7-C7-C8 | 2.26 | 116.45 | 108.34 | 12 | 1 |
| 3 | B | 389 | PX4 | C5-N1-C3 | 2.26 | 103.04 | 108.98 | 2 | 2 |
| 3 | B | 361 | PX4 | O3-P1-O2 | 2.26 | 117.88 | 108.94 | 8 | 1 |
| 3 | C | 317 | PX4 | C25-C24-C23 | 2.26 | 105.42 | 113.69 | 11 | 2 |
| 3 | C | 322 | PX4 | O7-C7-C8 | 2.26 | 116.45 | 108.34 | 3 | 1 |
| 3 | C | 351 | PX4 | O7-C7-C8 | 2.26 | 116.45 | 108.34 | 4 | 3 |
| 3 | A | 641 | PX4 | C8-C7-C6 | 2.26 | 106.52 | 111.78 | 14 | 1 |
| 3 | C | 330 | PX4 | C12-C11-C10 | 2.26 | 104.83 | 113.13 | 14 | 1 |
| 3 | C | 358 | PX4 | O6-C9-C10 | 2.26 | 132.62 | 123.78 | 4 | 1 |
| 3 | B | 396 | PX4 | C1-C2-N1 | 2.26 | 123.07 | 115.82 | 5 | 1 |
| 3 | C | 361 | PX4 | C33-C32-C31 | 2.26 | 102.95 | 114.37 | 4 | 1 |
| 3 | C | 335 | PX4 | O1-P1-O2 | 2.26 | 122.94 | 112.44 | 2 | 3 |
| 3 | C | 347 | PX4 | C1-C2-N1 | 2.26 | 123.06 | 115.82 | 3 | 2 |
| 3 | B | 319 | PX4 | C3-N1-C2 | 2.26 | 118.88 | 109.91 | 7 | 1 |
| 3 | B | 366 | PX4 | O7-C23-C24 | 2.25 | 106.60 | 111.48 | 1 | 2 |
| 3 | B | 378 | PX4 | O1-P1-O2 | 2.25 | 122.93 | 112.44 | 15 | 1 |
| 3 | C | 339 | PX4 | O5-C9-O6 | 2.25 | 117.99 | 123.63 | 6 | 1 |
| 3 | C | 350 | PX4 | O8-C23-C24 | 2.26 | 114.96 | 123.78 | 7 | 1 |
| 3 | A | 610 | PX4 | C8-C7-C6 | 2.25 | 106.53 | 111.78 | 12 | 1 |
| 3 | A | 613 | PX4 | O1-P1-O2 | 2.25 | 122.92 | 112.44 | 5 | 1 |
| 3 | A | 614 | PX4 | C8-O5-C9 | 2.25 | 108.88 | 117.12 | 10 | 1 |
| 3 | A | 627 | PX4 | C5-N1-C3 | 2.25 | 103.06 | 108.98 | 13 | 1 |
| 3 | A | 631 | PX4 | C12-C11-C10 | 2.25 | 104.85 | 113.13 | 14 | 1 |
| 3 | A | 648 | PX4 | C26-C25-C24 | 2.25 | 104.85 | 113.13 | 3 | 1 |
| 3 | B | 332 | PX4 | O3-C1-C2 | 2.25 | 120.49 | 109.65 | 5 | 2 |
| 3 | B | 343 | PX4 | C19-C18-C17 | 2.25 | 102.97 | 114.37 | 5 | 1 |
| 3 | C | 308 | PX4 | C5-N1-C4 | 2.25 | 103.05 | 108.98 | 10 | 4 |
| 3 | B | 383 | PX4 | C5-N1-C3 | 2.25 | 103.06 | 108.98 | 9 | 2 |
| 3 | B | 341 | PX4 | P1-O3-C1 | 2.25 | 131.98 | 121.26 | 13 | 1 |
| 3 | C | 315 | PX4 | C8-C7-C6 | 2.25 | 106.53 | 111.78 | 12 | 1 |
| 3 | C | 321 | PX4 | C12-C11-C10 | 2.25 | 121.40 | 113.13 | 9 | 1 |
| 3 | C | 331 | PX4 | O7-C23-O8 | 2.25 | 128.97 | 123.70 | 14 | 2 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 372 | PX4 | C13-C12-C11 | 2.25 | 102.99 | 114.37 | 1 | 1 |
| 3 | C | 345 | PX4 | C8-O5-C9 | 2.25 | 108.89 | 117.12 | 9 | 1 |
| 3 | A | 605 | PX4 | O5-C9-O6 | 2.25 | 129.26 | 123.63 | 5 | 2 |
| 3 | A | 653 | PX4 | C5-N1-C4 | 2.25 | 103.06 | 108.98 | 13 | 1 |
| 3 | B | 379 | PX4 | C1-C2-N1 | 2.25 | 123.05 | 115.82 | 9 | 2 |
| 3 | C | 319 | PX4 | C25-C24-C23 | 2.25 | 105.45 | 113.69 | 5 | 1 |
| 3 | C | 361 | PX4 | C18-C17-C16 | 2.25 | 102.99 | 114.37 | 6 | 1 |
| 3 | A | 623 | PX4 | O1-P1-O2 | 2.25 | 122.91 | 112.44 | 13 | 1 |
| 3 | A | 640 | PX4 | O5-C9-O6 | 2.25 | 129.25 | 123.63 | 8 | 1 |
| 3 | B | 359 | PX4 | O1-P1-O2 | 2.25 | 122.91 | 112.44 | 3 | 1 |
| 3 | A | 643 | PX4 | C11-C10-C9 | 2.25 | 105.46 | 113.69 | 14 | 1 |
| 3 | B | 375 | PX4 | O7-C23-O8 | 2.25 | 128.96 | 123.70 | 1 | 1 |
| 3 | B | 375 | PX4 | O8-C23-C24 | 2.25 | 132.57 | 123.78 | 7 | 1 |
| 3 | B | 383 | PX4 | O7-C7-C8 | 2.25 | 116.41 | 108.34 | 9 | 1 |
| 3 | C | 349 | PX4 | C11-C10-C9 | 2.25 | 121.93 | 113.69 | 4 | 2 |
| 3 | A | 602 | PX4 | C8-O5-C9 | 2.25 | 108.91 | 117.12 | 13 | 1 |
| 3 | B | 324 | PX4 | C5-N1-C3 | 2.25 | 103.07 | 108.98 | 1 | 3 |
| 3 | B | 337 | PX4 | C5-N1-C4 | 2.25 | 114.88 | 108.98 | 1 | 1 |
| 3 | A | 604 | PX4 | O1-P1-O2 | 2.25 | 122.89 | 112.44 | 15 | 1 |
| 3 | B | 329 | PX4 | C1-C2-N1 | 2.25 | 123.03 | 115.82 | 5 | 1 |
| 3 | B | 340 | PX4 | C1-C2-N1 | 2.25 | 123.03 | 115.82 | 2 | 1 |
| 3 | A | 602 | PX4 | O1-P1-O2 | 2.24 | 122.88 | 112.44 | 9 | 1 |
| 3 | A | 612 | PX4 | C4-N1-C3 | 2.24 | 103.08 | 108.98 | 6 | 1 |
| 3 | A | 619 | PX4 | C12-C11-C10 | 2.25 | 104.88 | 113.13 | 4 | 1 |
| 3 | A | 636 | PX4 | C5-N1-C3 | 2.25 | 103.08 | 108.98 | 2 | 2 |
| 3 | C | 332 | PX4 | O1-P1-O3 | 2.25 | 117.75 | 107.57 | 6 | 1 |
| 3 | C | 333 | PX4 | C5-N1-C2 | 2.25 | 118.84 | 109.91 | 7 | 1 |
| 3 | C | 338 | PX4 | C4-N1-C3 | 2.25 | 103.08 | 108.98 | 12 | 2 |
| 3 | B | 340 | PX4 | P1-O3-C1 | 2.24 | 131.94 | 121.26 | 4 | 1 |
| 3 | B | 303 | PX4 | O7-C7-C8 | 2.24 | 116.39 | 108.34 | 12 | 1 |
| 3 | A | 601 | PX4 | O5-C9-C10 | 2.24 | 105.00 | 111.83 | 8 | 1 |
| 3 | A | 610 | PX4 | C5-N1-C3 | 2.24 | 103.09 | 108.98 | 9 | 1 |
| 3 | A | 627 | PX4 | C17-C16-C15 | 2.24 | 103.04 | 114.37 | 14 | 1 |
| 3 | A | 630 | PX4 | C29-C28-C27 | 2.24 | 103.04 | 114.37 | 14 | 1 |
| 3 | B | 302 | PX4 | O5-C9-O6 | 2.24 | 129.23 | 123.63 | 6 | 1 |
| 3 | B | 338 | PX4 | O7-C7-C6 | 2.24 | 116.38 | 108.34 | 5 | 1 |
| 3 | B | 350 | PX4 | C16-C15-C14 | 2.24 | 103.04 | 114.37 | 6 | 1 |
| 3 | B | 369 | PX4 | C8-C7-C6 | 2.24 | 106.56 | 111.78 | 11 | 1 |
| 3 | C | 318 | PX4 | C11-C10-C9 | 2.24 | 105.48 | 113.69 | 9 | 1 |
| 3 | C | 329 | PX4 | O5-C9-C10 | 2.24 | 105.00 | 111.83 | 3 | 1 |
| 3 | B | 370 | PX4 | O7-C23-O8 | 2.24 | 128.94 | 123.70 | 10 | 2 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 385 | PX4 | C33-C32-C31 | 2.24 | 103.05 | 114.37 | 2 | 1 |
| 3 | C | 311 | PX4 | C5-N1-C4 | 2.24 | 103.09 | 108.98 | 13 | 2 |
| 3 | A | 650 | PX4 | C5-N1-C2 | 2.24 | 118.80 | 109.91 | 1 | 1 |
| 3 | B | 323 | PX4 | O5-C9-C10 | 2.24 | 105.01 | 111.83 | 3 | 1 |
| 3 | B | 373 | PX4 | O5-C9-O6 | 2.24 | 129.22 | 123.63 | 4 | 1 |
| 3 | C | 316 | PX4 | C5-N1-C4 | 2.24 | 103.10 | 108.98 | 3 | 1 |
| 3 | C | 330 | PX4 | C11-C10-C9 | 2.24 | 105.49 | 113.69 | 15 | 1 |
| 3 | A | 650 | PX4 | C1-C2-N1 | 2.24 | 123.00 | 115.82 | 10 | 1 |
| 3 | B | 305 | PX4 | O1-P1-O2 | 2.24 | 122.84 | 112.44 | 8 | 2 |
| 3 | B | 310 | PX4 | P1-O3-C1 | 2.24 | 131.90 | 121.26 | 5 | 1 |
| 3 | B | 332 | PX4 | C4-N1-C3 | 2.24 | 114.85 | 108.98 | 11 | 2 |
| 3 | A | 641 | PX4 | O5-C9-O6 | 2.23 | 129.22 | 123.63 | 7 | 2 |
| 3 | B | 344 | PX4 | C1-C2-N1 | 2.23 | 122.99 | 115.82 | 12 | 2 |
| 3 | B | 357 | PX4 | C12-C11-C10 | 2.24 | 121.34 | 113.13 | 10 | 1 |
| 3 | B | 371 | PX4 | C1-C2-N1 | 2.24 | 123.00 | 115.82 | 7 | 2 |
| 3 | C | 339 | PX4 | O5-C8-C7 | 2.24 | 114.84 | 108.40 | 3 | 1 |
| 3 | B | 380 | PX4 | O4-P1-O2 | 2.23 | 100.08 | 108.94 | 13 | 1 |
| 3 | C | 350 | PX4 | C4-N1-C3 | 2.24 | 114.85 | 108.98 | 5 | 2 |
| 3 | B | 342 | PX4 | O5-C9-O6 | 2.23 | 129.22 | 123.63 | 12 | 1 |
| 3 | B | 344 | PX4 | C34-C33-C32 | 2.23 | 103.08 | 114.37 | 3 | 1 |
| 3 | B | 376 | PX4 | C19-C18-C17 | 2.23 | 103.08 | 114.37 | 14 | 1 |
| 3 | C | 316 | PX4 | C25-C24-C23 | 2.23 | 121.88 | 113.69 | 12 | 1 |
| 3 | C | 321 | PX4 | C5-N1-C4 | 2.23 | 114.84 | 108.98 | 15 | 1 |
| 3 | C | 335 | PX4 | C3-N1-C2 | 2.23 | 118.79 | 109.91 | 15 | 1 |
| 3 | B | 385 | PX4 | C26-C25-C24 | 2.23 | 121.33 | 113.13 | 14 | 1 |
| 3 | B | 397 | PX4 | C1-C2-N1 | 2.23 | 122.98 | 115.82 | 3 | 2 |
| 3 | C | 333 | PX4 | C4-N1-C2 | 2.23 | 118.78 | 109.91 | 5 | 1 |
| 3 | B | 337 | PX4 | C22-C21-C20 | 2.23 | 128.42 | 113.36 | 8 | 1 |
| 3 | B | 356 | PX4 | C5-N1-C4 | 2.23 | 103.12 | 108.98 | 15 | 1 |
| 3 | A | 642 | PX4 | C8-C7-C6 | 2.23 | 106.59 | 111.78 | 6 | 2 |
| 3 | B | 340 | PX4 | O7-C23-O8 | 2.23 | 128.92 | 123.70 | 12 | 2 |
| 3 | B | 372 | PX4 | C26-C25-C24 | 2.23 | 104.94 | 113.13 | 13 | 2 |
| 3 | A | 626 | PX4 | C5-N1-C4 | 2.23 | 114.83 | 108.98 | 7 | 4 |
| 3 | B | 304 | PX4 | O5-C9-O6 | 2.23 | 129.20 | 123.63 | 8 | 1 |
| 3 | B | 307 | PX4 | C26-C25-C24 | 2.23 | 121.31 | 113.13 | 6 | 1 |
| 3 | B | 381 | PX4 | C25-C24-C23 | 2.23 | 105.53 | 113.69 | 4 | 3 |
| 3 | C | 318 | PX4 | O7-C7-C6 | 2.23 | 100.35 | 108.34 | 15 | 2 |
| 3 | C | 336 | PX4 | C17-C16-C15 | 2.23 | 103.11 | 114.37 | 14 | 1 |
| 3 | C | 339 | PX4 | C4-N1-C3 | 2.23 | 103.12 | 108.98 | 13 | 1 |
| 3 | C | 341 | PX4 | P1-O3-C1 | 2.23 | 131.87 | 121.26 | 13 | 1 |
| 3 | A | 632 | PX4 | C3-N1-C2 | 2.23 | 101.06 | 109.91 | 9 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 314 | PX4 | O5-C9-C10 | 2.23 | 105.05 | 111.83 | 4 | 1 |
| 3 | C | 343 | PX4 | C20-C19-C18 | 2.23 | 125.62 | 114.37 | 13 | 2 |
| 3 | A | 632 | PX4 | O1-P1-O2 | 2.22 | 122.79 | 112.44 | 6 | 1 |
| 3 | A | 614 | PX4 | C4-N1-C3 | 2.22 | 103.14 | 108.98 | 3 | 3 |
| 3 | A | 652 | PX4 | C5-N1-C3 | 2.22 | 114.82 | 108.98 | 1 | 1 |
| 3 | A | 623 | PX4 | C26-C25-C24 | 2.22 | 104.96 | 113.13 | 8 | 1 |
| 3 | A | 646 | PX4 | O5-C8-C7 | 2.22 | 114.80 | 108.40 | 12 | 2 |
| 3 | B | 311 | PX4 | C31-C30-C29 | 2.22 | 125.61 | 114.37 | 3 | 1 |
| 3 | B | 344 | PX4 | C4-N1-C3 | 2.22 | 103.14 | 108.98 | 2 | 1 |
| 3 | B | 364 | PX4 | C26-C25-C24 | 2.22 | 121.29 | 113.13 | 11 | 1 |
| 3 | B | 396 | PX4 | C5-N1-C4 | 2.22 | 103.14 | 108.98 | 11 | 1 |
| 3 | C | 308 | PX4 | O5-C8-C7 | 2.22 | 114.80 | 108.40 | 13 | 1 |
| 3 | B | 373 | PX4 | P1-O3-C1 | 2.22 | 131.84 | 121.26 | 7 | 1 |
| 3 | C | 325 | PX4 | O4-P1-O2 | 2.22 | 117.74 | 108.94 | 8 | 1 |
| 3 | C | 328 | PX4 | C1-C2-N1 | 2.22 | 122.95 | 115.82 | 11 | 1 |
| 3 | A | 650 | PX4 | C26-C25-C24 | 2.22 | 104.97 | 113.13 | 10 | 1 |
| 3 | A | 635 | PX4 | C5-N1-C4 | 2.22 | 103.14 | 108.98 | 15 | 3 |
| 3 | B | 344 | PX4 | O4-P1-O2 | 2.22 | 117.73 | 108.94 | 1 | 2 |
| 3 | C | 354 | PX4 | O1-P1-O2 | 2.22 | 122.78 | 112.44 | 12 | 2 |
| 3 | A | 620 | PX4 | C12-C11-C10 | 2.22 | 104.98 | 113.13 | 10 | 2 |
| 3 | A | 644 | PX4 | C12-C11-C10 | 2.22 | 104.98 | 113.13 | 8 | 1 |
| 3 | B | 303 | PX4 | C26-C25-C24 | 2.22 | 104.97 | 113.13 | 6 | 1 |
| 3 | B | 353 | PX4 | C1-C2-N1 | 2.22 | 122.95 | 115.82 | 5 | 1 |
| 3 | B | 366 | PX4 | C4-N1-C3 | 2.22 | 114.81 | 108.98 | 2 | 2 |
| 3 | C | 328 | PX4 | O8-C23-C24 | 2.22 | 132.46 | 123.78 | 10 | 1 |
| 3 | B | 341 | PX4 | C3-N1-C2 | 2.22 | 118.72 | 109.91 | 4 | 1 |
| 3 | B | 367 | PX4 | C5-N1-C4 | 2.22 | 103.15 | 108.98 | 12 | 2 |
| 3 | B | 394 | PX4 | O1-P1-O2 | 2.22 | 122.76 | 112.44 | 12 | 1 |
| 3 | C | 306 | PX4 | C29-C28-C27 | 2.22 | 103.16 | 114.37 | 12 | 1 |
| 3 | B | 312 | PX4 | C34-C33-C32 | 2.22 | 103.17 | 114.37 | 10 | 1 |
| 3 | B | 340 | PX4 | O5-C8-C7 | 2.22 | 114.78 | 108.40 | 3 | 4 |
| 3 | B | 343 | PX4 | O7-C23-O8 | 2.22 | 128.88 | 123.70 | 12 | 2 |
| 3 | C | 334 | PX4 | C1-C2-N1 | 2.22 | 122.93 | 115.82 | 7 | 2 |
| 3 | C | 355 | PX4 | C16-C15-C14 | 2.22 | 103.16 | 114.37 | 4 | 1 |
| 3 | C | 359 | PX4 | C25-C24-C23 | 2.22 | 105.57 | 113.69 | 10 | 2 |
| 3 | B | 394 | PX4 | C4-N1-C3 | 2.21 | 114.79 | 108.98 | 12 | 1 |
| 3 | C | 304 | PX4 | C4-N1-C2 | 2.21 | 118.71 | 109.91 | 8 | 1 |
| 3 | A | 602 | PX4 | C3-N1-C2 | 2.21 | 118.70 | 109.91 | 9 | 1 |
| 3 | A | 609 | PX4 | C8-O5-C9 | 2.21 | 109.03 | 117.12 | 1 | 2 |
| 3 | A | 623 | PX4 | C5-N1-C4 | 2.21 | 114.79 | 108.98 | 6 | 1 |
| 3 | A | 632 | PX4 | C4-N1-C3 | 2.21 | 103.17 | 108.98 | 3 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | A | 634 | PX4 | O3-P1-O2 | 2.21 | 117.70 | 108.94 | 3 | 1 |
| 3 | A | 637 | PX4 | O7-C23-O8 | 2.21 | 128.88 | 123.70 | 11 | 2 |
| 3 | B | 315 | PX4 | C3-N1-C2 | 2.21 | 118.70 | 109.91 | 13 | 1 |
| 3 | B | 378 | PX4 | O7-C23-O8 | 2.21 | 128.88 | 123.70 | 6 | 1 |
| 3 | B | 343 | PX4 | O4-P1-O2 | 2.21 | 100.17 | 108.94 | 15 | 1 |
| 3 | B | 335 | PX4 | O6-C9-C10 | 2.21 | 132.42 | 123.78 | 12 | 1 |
| 3 | B | 369 | PX4 | C26-C25-C24 | 2.21 | 121.25 | 113.13 | 14 | 2 |
| 3 | C | 346 | PX4 | C31-C30-C29 | 2.21 | 103.20 | 114.37 | 1 | 1 |
| 3 | C | 347 | PX4 | C25-C24-C23 | 2.21 | 105.60 | 113.69 | 3 | 2 |
| 3 | B | 315 | PX4 | O1-P1-O2 | 2.21 | 122.72 | 112.44 | 10 | 1 |
| 3 | C | 356 | PX4 | C11-C10-C9 | 2.21 | 105.60 | 113.69 | 8 | 1 |
| 3 | B | 332 | PX4 | C14-C13-C12 | 2.21 | 103.21 | 114.37 | 5 | 1 |
| 3 | B | 360 | PX4 | C12-C11-C10 | 2.21 | 105.01 | 113.13 | 7 | 1 |
| 3 | B | 390 | PX4 | O5-C9-C10 | 2.21 | 105.10 | 111.83 | 4 | 2 |
| 3 | C | 328 | PX4 | O7-C7-C6 | 2.21 | 116.27 | 108.34 | 2 | 1 |
| 3 | A | 631 | PX4 | C8-C7-C6 | 2.21 | 106.64 | 111.78 | 6 | 1 |
| 3 | A | 637 | PX4 | O5-C9-C10 | 2.21 | 105.11 | 111.83 | 4 | 1 |
| 3 | B | 384 | PX4 | C20-C19-C18 | 2.21 | 103.22 | 114.37 | 5 | 1 |
| 3 | B | 384 | PX4 | O5-C9-O6 | 2.21 | 129.15 | 123.63 | 6 | 1 |
| 3 | C | 307 | PX4 | C8-C7-C6 | 2.21 | 116.93 | 111.78 | 1 | 2 |
| 3 | C | 352 | PX4 | C8-C7-C6 | 2.21 | 116.93 | 111.78 | 3 | 1 |
| 3 | A | 607 | PX4 | O7-C7-C8 | 2.21 | 116.25 | 108.34 | 11 | 1 |
| 3 | A | 623 | PX4 | C29-C28-C27 | 2.21 | 103.22 | 114.37 | 1 | 1 |
| 3 | A | 640 | PX4 | C5-N1-C2 | 2.21 | 118.68 | 109.91 | 15 | 1 |
| 3 | C | 301 | PX4 | C11-C10-C9 | 2.21 | 105.61 | 113.69 | 5 | 1 |
| 3 | B | 365 | PX4 | O3-C1-C2 | 2.20 | 120.26 | 109.65 | 7 | 1 |
| 3 | C | 307 | PX4 | O6-C9-C10 | 2.20 | 132.40 | 123.78 | 8 | 1 |
| 3 | C | 325 | PX4 | O1-P1-O3 | 2.21 | 117.56 | 107.57 | 6 | 1 |
| 3 | A | 603 | PX4 | C31-C30-C29 | 2.20 | 103.23 | 114.37 | 1 | 1 |
| 3 | A | 618 | PX4 | O7-C7-C8 | 2.20 | 116.25 | 108.34 | 15 | 1 |
| 3 | A | 636 | PX4 | O7-C7-C6 | 2.20 | 116.24 | 108.34 | 6 | 2 |
| 3 | B | 331 | PX4 | O1-P1-O2 | 2.20 | 122.69 | 112.44 | 8 | 1 |
| 3 | B | 346 | PX4 | O3-P1-O2 | 2.20 | 117.67 | 108.94 | 1 | 1 |
| 3 | B | 349 | PX4 | C12-C11-C10 | 2.20 | 121.22 | 113.13 | 12 | 1 |
| 3 | B | 354 | PX4 | C1-C2-N1 | 2.20 | 122.89 | 115.82 | 10 | 2 |
| 3 | C | 333 | PX4 | C25-C24-C23 | 2.20 | 121.77 | 113.69 | 9 | 1 |
| 3 | C | 344 | PX4 | O3-C1-C2 | 2.20 | 120.25 | 109.65 | 10 | 1 |
| 3 | A | 603 | PX4 | C8-O5-C9 | 2.20 | 109.08 | 117.12 | 15 | 1 |
| 3 | A | 644 | PX4 | C1-C2-N1 | 2.20 | 122.88 | 115.82 | 7 | 1 |
| 3 | A | 647 | PX4 | C25-C24-C23 | 2.20 | 105.63 | 113.69 | 12 | 3 |
| 3 | B | 308 | PX4 | O7-C7-C8 | 2.20 | 116.24 | 108.34 | 7 | 2 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 332 | PX4 | C11-C10-C9 | 2.20 | 105.63 | 113.69 | 6 | 3 |
| 3 | B | 391 | PX4 | O8-C23-C24 | 2.20 | 115.17 | 123.78 | 13 | 1 |
| 3 | C | 302 | PX4 | C26-C25-C24 | 2.20 | 105.04 | 113.13 | 1 | 1 |
| 3 | C | 313 | PX4 | C8-C7-C6 | 2.20 | 106.65 | 111.78 | 2 | 2 |
| 3 | A | 622 | PX4 | O3-C1-C2 | 2.20 | 120.23 | 109.65 | 1 | 1 |
| 3 | A | 622 | PX4 | C32-C31-C30 | 2.20 | 103.25 | 114.37 | 5 | 1 |
| 3 | A | 649 | PX4 | C12-C11-C10 | 2.20 | 121.21 | 113.13 | 3 | 1 |
| 3 | B | 325 | PX4 | C12-C11-C10 | 2.20 | 105.05 | 113.13 | 13 | 2 |
| 3 | B | 392 | PX4 | O7-C7-C6 | 2.20 | 116.23 | 108.34 | 13 | 1 |
| 3 | C | 323 | PX4 | O7-C7-C8 | 2.20 | 116.24 | 108.34 | 2 | 1 |
| 3 | C | 335 | PX4 | C31-C30-C29 | 2.20 | 103.25 | 114.37 | 9 | 1 |
| 3 | C | 340 | PX4 | O1-P1-O2 | 2.20 | 122.68 | 112.44 | 11 | 1 |
| 3 | A | 612 | PX4 | C12-C11-C10 | 2.20 | 105.05 | 113.13 | 5 | 1 |
| 3 | B | 358 | PX4 | C13-C12-C11 | 2.20 | 125.48 | 114.37 | 15 | 1 |
| 3 | B | 364 | PX4 | O1-P1-O4 | 2.20 | 117.53 | 107.57 | 12 | 1 |
| 3 | C | 312 | PX4 | C5-N1-C3 | 2.20 | 103.20 | 108.98 | 7 | 1 |
| 3 | C | 332 | PX4 | C13-C12-C11 | 2.20 | 103.26 | 114.37 | 9 | 1 |
| 3 | C | 359 | PX4 | O7-C23-C24 | 2.20 | 106.72 | 111.48 | 15 | 1 |
| 3 | C | 307 | PX4 | C26-C25-C24 | 2.20 | 121.20 | 113.13 | 8 | 1 |
| 3 | C | 327 | PX4 | O5-C9-O6 | 2.20 | 129.12 | 123.63 | 5 | 1 |
| 3 | C | 336 | PX4 | O7-C7-C8 | 2.20 | 116.23 | 108.34 | 3 | 1 |
| 3 | A | 638 | PX4 | O5-C9-C10 | 2.20 | 105.14 | 111.83 | 9 | 1 |
| 3 | B | 325 | PX4 | O5-C9-O6 | 2.20 | 129.12 | 123.63 | 2 | 1 |
| 3 | C | 312 | PX4 | C1-C2-N1 | 2.20 | 122.87 | 115.82 | 12 | 1 |
| 3 | B | 357 | PX4 | C26-C25-C24 | 2.19 | 105.06 | 113.13 | 13 | 1 |
| 3 | B | 369 | PX4 | C5-N1-C4 | 2.19 | 103.21 | 108.98 | 3 | 1 |
| 3 | B | 374 | PX4 | C15-C14-C13 | 2.19 | 103.28 | 114.37 | 12 | 1 |
| 3 | C | 303 | PX4 | C8-O5-C9 | 2.19 | 109.10 | 117.12 | 5 | 1 |
| 3 | C | 354 | PX4 | O5-C9-O6 | 2.19 | 129.12 | 123.63 | 13 | 2 |
| 3 | A | 652 | PX4 | O7-C23-O8 | 2.19 | 128.83 | 123.70 | 7 | 3 |
| 3 | A | 612 | PX4 | O8-C23-C24 | 2.19 | 132.35 | 123.78 | 4 | 1 |
| 3 | B | 382 | PX4 | O1-P1-O2 | 2.19 | 122.64 | 112.44 | 15 | 1 |
| 3 | B | 387 | PX4 | O6-C9-C10 | 2.19 | 132.35 | 123.78 | 7 | 1 |
| 3 | C | 352 | PX4 | C1-C2-N1 | 2.19 | 122.86 | 115.82 | 5 | 1 |
| 3 | B | 319 | PX4 | C5-N1-C3 | 2.19 | 114.73 | 108.98 | 14 | 2 |
| 3 | B | 334 | PX4 | O5-C9-O6 | 2.19 | 129.10 | 123.63 | 11 | 1 |
| 3 | B | 338 | PX4 | C8-O5-C9 | 2.19 | 109.12 | 117.12 | 1 | 3 |
| 3 | B | 387 | PX4 | C5-N1-C3 | 2.19 | 114.73 | 108.98 | 4 | 1 |
| 3 | C | 317 | PX4 | C18-C17-C16 | 2.19 | 103.30 | 114.37 | 1 | 1 |
| 3 | A | 604 | PX4 | O5-C9-O6 | 2.19 | 129.10 | 123.63 | 5 | 1 |
| 3 | B | 324 | PX4 | O5-C9-C10 | 2.19 | 105.17 | 111.83 | 11 | 2 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | C | 320 | PX4 | O7-C23-O8 | 2.19 | 128.82 | 123.70 | 9 | 2 |
| 3 | A | 628 | PX4 | C33-C32-C31 | 2.19 | 103.32 | 114.37 | 7 | 1 |
| 3 | C | 329 | PX4 | O1-P1-O4 | 2.19 | 117.47 | 107.57 | 6 | 1 |
| 3 | C | 352 | PX4 | C11-C10-C9 | 2.19 | 105.68 | 113.69 | 12 | 3 |
| 3 | A | 629 | PX4 | O7-C23-O8 | 2.19 | 128.81 | 123.70 | 6 | 1 |
| 3 | A | 617 | PX4 | C1-C2-N1 | 2.18 | 122.83 | 115.82 | 4 | 2 |
| 3 | A | 618 | PX4 | C19-C18-C17 | 2.18 | 103.33 | 114.37 | 12 | 1 |
| 3 | B | 320 | PX4 | O7-C7-C6 | 2.18 | 116.18 | 108.34 | 5 | 2 |
| 3 | C | 313 | PX4 | C8-O5-C9 | 2.19 | 125.11 | 117.12 | 4 | 1 |
| 3 | C | 340 | PX4 | C26-C25-C24 | 2.19 | 121.16 | 113.13 | 10 | 1 |
| 3 | A | 646 | PX4 | C1-C2-N1 | 2.18 | 122.83 | 115.82 | 9 | 1 |
| 3 | A | 654 | PX4 | C5-N1-C4 | 2.18 | 114.71 | 108.98 | 10 | 1 |
| 3 | B | 336 | PX4 | C8-C7-C6 | 2.18 | 106.69 | 111.78 | 7 | 1 |
| 3 | B | 363 | PX4 | O4-P1-O2 | 2.18 | 117.59 | 108.94 | 9 | 1 |
| 3 | C | 337 | PX4 | O5-C9-O6 | 2.18 | 129.09 | 123.63 | 3 | 1 |
| 3 | C | 350 | PX4 | C5-N1-C2 | 2.18 | 118.59 | 109.91 | 7 | 1 |
| 3 | B | 336 | PX4 | C5-N1-C3 | 2.18 | 114.71 | 108.98 | 13 | 1 |
| 3 | A | 625 | PX4 | O5-C9-C10 | 2.18 | 105.18 | 111.83 | 13 | 2 |
| 3 | A | 628 | PX4 | C11-C10-C9 | 2.18 | 105.70 | 113.69 | 2 | 2 |
| 3 | B | 386 | PX4 | O8-C23-C24 | 2.18 | 132.32 | 123.78 | 14 | 1 |
| 3 | B | 388 | PX4 | O7-C7-C6 | 2.18 | 116.17 | 108.34 | 3 | 2 |
| 3 | B | 369 | PX4 | O4-P1-O2 | 2.18 | 100.29 | 108.94 | 3 | 1 |
| 3 | B | 377 | PX4 | C12-C11-C10 | 2.18 | 121.14 | 113.13 | 12 | 1 |
| 3 | C | 325 | PX4 | C15-C14-C13 | 2.18 | 103.34 | 114.37 | 15 | 1 |
| 3 | C | 340 | PX4 | C5-N1-C3 | 2.18 | 103.24 | 108.98 | 2 | 2 |
| 3 | B | 347 | PX4 | C31-C30-C29 | 2.18 | 103.34 | 114.37 | 7 | 1 |
| 3 | A | 606 | PX4 | C4-N1-C2 | 2.18 | 118.57 | 109.91 | 6 | 1 |
| 3 | A | 619 | PX4 | O5-C9-O6 | 2.18 | 129.08 | 123.63 | 9 | 3 |
| 3 | B | 308 | PX4 | C17-C16-C15 | 2.18 | 103.35 | 114.37 | 11 | 1 |
| 3 | B | 318 | PX4 | O7-C23-O8 | 2.18 | 128.80 | 123.70 | 1 | 1 |
| 3 | B | 329 | PX4 | C5-N1-C2 | 2.18 | 101.25 | 109.91 | 9 | 1 |
| 3 | B | 336 | PX4 | C5-N1-C4 | 2.18 | 103.25 | 108.98 | 4 | 2 |
| 3 | B | 375 | PX4 | C5-N1-C4 | 2.18 | 114.70 | 108.98 | 11 | 2 |
| 3 | B | 382 | PX4 | C4-N1-C3 | 2.18 | 103.25 | 108.98 | 1 | 3 |
| 3 | B | 397 | PX4 | C33-C32-C31 | 2.18 | 103.35 | 114.37 | 3 | 1 |
| 3 | C | 308 | PX4 | C1-C2-N1 | 2.18 | 122.82 | 115.82 | 2 | 1 |
| 3 | C | 310 | PX4 | O7-C7-C8 | 2.18 | 116.16 | 108.34 | 9 | 1 |
| 3 | C | 311 | PX4 | C25-C24-C23 | 2.18 | 105.70 | 113.69 | 5 | 2 |
| 3 | B | 302 | PX4 | C4-N1-C2 | 2.18 | 118.56 | 109.91 | 7 | 1 |
| 3 | B | 364 | PX4 | C4-N1-C2 | 2.18 | 118.56 | 109.91 | 3 | 1 |
| 3 | B | 392 | PX4 | C3-N1-C2 | 2.18 | 101.25 | 109.91 | 10 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | A | 626 | PX4 | O7-C7-C8 | 2.18 | 116.15 | 108.34 | 14 | 2 |
| 3 | A | 626 | PX4 | C4-N1-C3 | 2.18 | 103.26 | 108.98 | 3 | 1 |
| 3 | B | 303 | PX4 | O7-C7-C6 | 2.18 | 116.15 | 108.34 | 1 | 1 |
| 3 | B | 382 | PX4 | O7-C23-O8 | 2.18 | 118.62 | 123.70 | 6 | 1 |
| 3 | C | 351 | PX4 | O8-C23-C24 | 2.18 | 132.29 | 123.78 | 4 | 1 |
| 3 | C | 352 | PX4 | C4-N1-C3 | 2.18 | 114.69 | 108.98 | 14 | 1 |
| 3 | A | 648 | PX4 | C5-N1-C4 | 2.17 | 103.27 | 108.98 | 6 | 1 |
| 3 | B | 331 | PX4 | C32-C31-C30 | 2.18 | 103.37 | 114.37 | 1 | 1 |
| 3 | B | 315 | PX4 | C25-C24-C23 | 2.17 | 121.66 | 113.69 | 4 | 2 |
| 3 | B | 320 | PX4 | C28-C27-C26 | 2.17 | 103.37 | 114.37 | 12 | 2 |
| 3 | B | 374 | PX4 | C11-C10-C9 | 2.17 | 121.66 | 113.69 | 14 | 1 |
| 3 | C | 358 | PX4 | P1-O3-C1 | 2.18 | 131.62 | 121.26 | 1 | 1 |
| 3 | B | 310 | PX4 | O1-P1-O2 | 2.17 | 122.55 | 112.44 | 15 | 1 |
| 3 | A | 602 | PX4 | O7-C23-C24 | 2.17 | 106.78 | 111.48 | 11 | 1 |
| 3 | A | 602 | PX4 | O3-P1-O2 | 2.17 | 117.54 | 108.94 | 13 | 1 |
| 3 | B | 327 | PX4 | C28-C27-C26 | 2.17 | 125.35 | 114.37 | 3 | 1 |
| 3 | B | 359 | PX4 | O7-C7-C8 | 2.17 | 116.14 | 108.34 | 3 | 3 |
| 3 | B | 381 | PX4 | P1-O3-C1 | 2.17 | 131.60 | 121.26 | 13 | 1 |
| 3 | C | 314 | PX4 | C8-O5-C9 | 2.17 | 109.18 | 117.12 | 15 | 1 |
| 3 | A | 643 | PX4 | O7-C23-C24 | 2.17 | 106.78 | 111.48 | 12 | 1 |
| 3 | A | 646 | PX4 | O1-P1-O2 | 2.17 | 122.55 | 112.44 | 2 | 2 |
| 3 | A | 644 | PX4 | C5-N1-C3 | 2.17 | 103.28 | 108.98 | 4 | 2 |
| 3 | B | 340 | PX4 | O8-C23-C24 | 2.17 | 132.27 | 123.78 | 9 | 1 |
| 3 | C | 347 | PX4 | O8-C23-C24 | 2.17 | 132.27 | 123.78 | 11 | 1 |
| 3 | B | 370 | PX4 | C19-C18-C17 | 2.17 | 125.33 | 114.37 | 15 | 1 |
| 3 | C | 356 | PX4 | C14-C13-C12 | 2.17 | 103.40 | 114.37 | 13 | 1 |
| 3 | A | 610 | PX4 | C26-C25-C24 | 2.17 | 105.16 | 113.13 | 10 | 1 |
| 3 | C | 358 | PX4 | C5-N1-C4 | 2.17 | 114.67 | 108.98 | 13 | 1 |
| 3 | C | 361 | PX4 | C5-N1-C2 | 2.17 | 118.53 | 109.91 | 9 | 1 |
| 3 | B | 304 | PX4 | C5-N1-C4 | 2.17 | 114.67 | 108.98 | 13 | 1 |
| 3 | B | 364 | PX4 | C32-C31-C30 | 2.17 | 103.42 | 114.37 | 10 | 1 |
| 3 | B | 386 | PX4 | O4-P1-O2 | 2.17 | 100.35 | 108.94 | 13 | 1 |
| 3 | C | 322 | PX4 | C8-O5-C9 | 2.17 | 109.20 | 117.12 | 8 | 1 |
| 3 | A | 601 | PX4 | C33-C32-C31 | 2.16 | 103.43 | 114.37 | 11 | 1 |
| 3 | B | 309 | PX4 | C27-C26-C25 | 2.16 | 103.42 | 114.37 | 10 | 1 |
| 3 | B | 310 | PX4 | O7-C7-C6 | 2.16 | 116.11 | 108.34 | 4 | 1 |
| 3 | B | 340 | PX4 | C4-N1-C2 | 2.17 | 118.52 | 109.91 | 13 | 1 |
| 3 | B | 393 | PX4 | O5-C9-O6 | 2.17 | 129.05 | 123.63 | 4 | 4 |
| 3 | B | 393 | PX4 | C5-N1-C4 | 2.17 | 114.66 | 108.98 | 13 | 1 |
| 3 | C | 334 | PX4 | C25-C24-C23 | 2.16 | 105.77 | 113.69 | 7 | 1 |
| 3 | C | 346 | PX4 | C5-N1-C4 | 2.16 | 103.30 | 108.98 | 6 | 2 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | C | 348 | PX4 | O5-C9-O6 | 2.16 | 129.04 | 123.63 | 9 | 1 |
| 3 | A | 605 | PX4 | O7-C7-C8 | 2.16 | 100.59 | 108.34 | 1 | 1 |
| 3 | A | 627 | PX4 | C1-C2-N1 | 2.16 | 122.76 | 115.82 | 13 | 2 |
| 3 | B | 375 | PX4 | C33-C32-C31 | 2.16 | 103.44 | 114.37 | 4 | 1 |
| 3 | C | 306 | PX4 | C34-C33-C32 | 2.16 | 125.30 | 114.37 | 15 | 1 |
| 3 | B | 334 | PX4 | C11-C10-C9 | 2.16 | 105.78 | 113.69 | 4 | 1 |
| 3 | B | 374 | PX4 | O7-C7-C6 | 2.16 | 116.09 | 108.34 | 1 | 1 |
| 3 | B | 388 | PX4 | C34-C33-C32 | 2.16 | 103.45 | 114.37 | 13 | 1 |
| 3 | C | 303 | PX4 | C32-C31-C30 | 2.16 | 103.45 | 114.37 | 2 | 1 |
| 3 | C | 344 | PX4 | C4-N1-C3 | 2.16 | 103.30 | 108.98 | 4 | 1 |
| 3 | B | 334 | PX4 | C1-C2-N1 | 2.16 | 122.75 | 115.82 | 15 | 1 |
| 3 | C | 351 | PX4 | C11-C10-C9 | 2.16 | 121.61 | 113.69 | 10 | 1 |
| 3 | A | 604 | PX4 | C30-C29-C28 | 2.16 | 103.46 | 114.37 | 13 | 1 |
| 3 | B | 342 | PX4 | C5-N1-C3 | 2.16 | 114.65 | 108.98 | 5 | 1 |
| 3 | B | 346 | PX4 | P1-O4-C6 | 2.16 | 133.72 | 121.35 | 4 | 1 |
| 3 | B | 347 | PX4 | O3-C1-C2 | 2.16 | 120.04 | 109.65 | 2 | 1 |
| 3 | B | 323 | PX4 | C8-O5-C9 | 2.16 | 125.00 | 117.12 | 8 | 1 |
| 3 | B | 393 | PX4 | C14-C13-C12 | 2.16 | 125.28 | 114.37 | 12 | 1 |
| 3 | B | 394 | PX4 | C18-C17-C16 | 2.16 | 103.46 | 114.37 | 7 | 1 |
| 3 | C | 322 | PX4 | O5-C9-C10 | 2.16 | 105.25 | 111.83 | 12 | 1 |
| 3 | B | 355 | PX4 | O5-C9-O6 | 2.16 | 129.03 | 123.63 | 6 | 1 |
| 3 | C | 330 | PX4 | C5-N1-C2 | 2.16 | 118.49 | 109.91 | 5 | 1 |
| 3 | B | 385 | PX4 | O6-C9-C10 | 2.16 | 132.22 | 123.78 | 5 | 1 |
| 3 | B | 398 | PX4 | C12-C11-C10 | 2.16 | 121.05 | 113.13 | 10 | 1 |
| 3 | C | 343 | PX4 | P1-O3-C1 | 2.16 | 131.53 | 121.26 | 6 | 1 |
| 3 | A | 622 | PX4 | C5-N1-C2 | 2.16 | 118.48 | 109.91 | 4 | 1 |
| 3 | A | 636 | PX4 | C27-C26-C25 | 2.16 | 103.47 | 114.37 | 7 | 1 |
| 3 | B | 341 | PX4 | C29-C28-C27 | 2.16 | 125.27 | 114.37 | 5 | 1 |
| 3 | B | 356 | PX4 | C20-C19-C18 | 2.16 | 103.47 | 114.37 | 3 | 1 |
| 3 | B | 363 | PX4 | O7-C7-C8 | 2.15 | 116.07 | 108.34 | 2 | 1 |
| 3 | C | 309 | PX4 | C4-N1-C2 | 2.16 | 118.48 | 109.91 | 11 | 1 |
| 3 | C | 312 | PX4 | C4-N1-C3 | 2.16 | 103.31 | 108.98 | 9 | 4 |
| 3 | C | 349 | PX4 | O1-P1-O2 | 2.16 | 122.48 | 112.44 | 4 | 1 |
| 3 | B | 356 | PX4 | C8-O5-C9 | 2.15 | 109.24 | 117.12 | 13 | 1 |
| 3 | B | 372 | PX4 | C5-N1-C2 | 2.15 | 118.47 | 109.91 | 15 | 1 |
| 3 | B | 389 | PX4 | O7-C23-O8 | 2.15 | 128.74 | 123.70 | 3 | 1 |
| 3 | B | 399 | PX4 | O4-P1-O2 | 2.15 | 117.47 | 108.94 | 11 | 1 |
| 3 | C | 335 | PX4 | C28-C27-C26 | 2.15 | 125.26 | 114.37 | 7 | 1 |
| 3 | C | 347 | PX4 | O5-C8-C7 | 2.15 | 114.61 | 108.40 | 10 | 2 |
| 3 | C | 349 | PX4 | O7-C7-C8 | 2.15 | 116.07 | 108.34 | 6 | 3 |
| 3 | B | 357 | PX4 | C34-C33-C32 | 2.15 | 103.48 | 114.37 | 14 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | C | 332 | PX4 | C16-C15-C14 | 2.15 | 103.48 | 114.37 | 4 | 1 |
| 3 | C | 344 | PX4 | O8-C23-C24 | 2.15 | 132.20 | 123.78 | 9 | 1 |
| 3 | C | 358 | PX4 | C31-C30-C29 | 2.15 | 103.48 | 114.37 | 15 | 1 |
| 3 | A | 615 | PX4 | C11-C10-C9 | 2.15 | 105.81 | 113.69 | 6 | 1 |
| 3 | A | 621 | PX4 | C4-N1-C2 | 2.15 | 118.46 | 109.91 | 12 | 1 |
| 3 | B | 312 | PX4 | O3-C1-C2 | 2.15 | 120.00 | 109.65 | 7 | 1 |
| 3 | B | 340 | PX4 | C14-C13-C12 | 2.15 | 103.50 | 114.37 | 1 | 1 |
| 3 | B | 354 | PX4 | O5-C9-C10 | 2.15 | 105.27 | 111.83 | 3 | 2 |
| 3 | C | 354 | PX4 | C4-N1-C3 | 2.15 | 103.32 | 108.98 | 5 | 1 |
| 3 | B | 384 | PX4 | C1-C2-N1 | 2.15 | 122.72 | 115.82 | 6 | 1 |
| 3 | C | 303 | PX4 | C4-N1-C2 | 2.15 | 118.46 | 109.91 | 3 | 1 |
| 3 | A | 632 | PX4 | C26-C25-C24 | 2.15 | 105.23 | 113.13 | 3 | 1 |
| 3 | B | 314 | PX4 | C25-C24-C23 | 2.15 | 105.82 | 113.69 | 6 | 1 |
| 3 | C | 347 | PX4 | C8-O5-C9 | 2.15 | 124.97 | 117.12 | 9 | 1 |
| 3 | C | 348 | PX4 | O7-C7-C8 | 2.15 | 116.06 | 108.34 | 4 | 1 |
| 3 | C | 358 | PX4 | C12-C11-C10 | 2.15 | 105.23 | 113.13 | 14 | 1 |
| 3 | B | 341 | PX4 | C28-C27-C26 | 2.15 | 103.51 | 114.37 | 7 | 1 |
| 3 | B | 396 | PX4 | P1-O4-C6 | 2.15 | 109.04 | 121.35 | 6 | 1 |
| 3 | C | 301 | PX4 | C5-N1-C4 | 2.15 | 114.62 | 108.98 | 8 | 1 |
| 3 | C | 304 | PX4 | C8-O5-C9 | 2.15 | 109.26 | 117.12 | 6 | 2 |
| 3 | C | 310 | PX4 | O5-C9-O6 | 2.15 | 129.00 | 123.63 | 7 | 1 |
| 3 | C | 316 | PX4 | C17-C16-C15 | 2.15 | 103.51 | 114.37 | 2 | 1 |
| 3 | C | 343 | PX4 | O7-C7-C6 | 2.15 | 116.05 | 108.34 | 2 | 2 |
| 3 | C | 358 | PX4 | O8-C23-C24 | 2.15 | 132.19 | 123.78 | 1 | 1 |
| 3 | A | 605 | PX4 | C5-N1-C4 | 2.15 | 103.34 | 108.98 | 13 | 1 |
| 3 | B | 366 | PX4 | O7-C23-O8 | 2.15 | 128.72 | 123.70 | 8 | 1 |
| 3 | A | 609 | PX4 | O4-P1-O2 | 2.14 | 100.44 | 108.94 | 15 | 1 |
| 3 | A | 642 | PX4 | O7-C7-C6 | 2.15 | 116.04 | 108.34 | 10 | 1 |
| 3 | C | 302 | PX4 | P1-O4-C6 | 2.15 | 133.65 | 121.35 | 9 | 2 |
| 3 | C | 355 | PX4 | C5-N1-C3 | 2.15 | 103.34 | 108.98 | 2 | 3 |
| 3 | A | 623 | PX4 | O7-C7-C8 | 2.14 | 116.03 | 108.34 | 11 | 1 |
| 3 | B | 309 | PX4 | O1-P1-O2 | 2.14 | 122.42 | 112.44 | 15 | 1 |
| 3 | B | 342 | PX4 | O1-P1-O2 | 2.14 | 122.42 | 112.44 | 13 | 1 |
| 3 | B | 357 | PX4 | C5-N1-C2 | 2.14 | 118.43 | 109.91 | 8 | 1 |
| 3 | B | 371 | PX4 | C13-C12-C11 | 2.14 | 103.53 | 114.37 | 3 | 1 |
| 3 | A | 609 | PX4 | C4-N1-C3 | 2.14 | 114.60 | 108.98 | 3 | 1 |
| 3 | A | 616 | PX4 | C20-C19-C18 | 2.14 | 103.54 | 114.37 | 2 | 1 |
| 3 | A | 638 | PX4 | O1-P1-O2 | 2.14 | 122.41 | 112.44 | 2 | 1 |
| 3 | B | 383 | PX4 | O6-C9-C10 | 2.14 | 132.17 | 123.78 | 1 | 2 |
| 3 | C | 321 | PX4 | C1-C2-N1 | 2.14 | 122.70 | 115.82 | 9 | 2 |
| 3 | C | 325 | PX4 | C11-C10-C9 | 2.14 | 121.55 | 113.69 | 4 | 2 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | A | 636 | PX4 | C25-C24-C23 | 2.14 | 105.85 | 113.69 | 10 | 1 |
| 3 | A | 644 | PX4 | C32-C31-C30 | 2.14 | 103.54 | 114.37 | 14 | 1 |
| 3 | B | 309 | PX4 | C5-N1-C2 | 2.14 | 118.42 | 109.91 | 2 | 1 |
| 3 | B | 327 | PX4 | C8-C7-C6 | 2.14 | 106.79 | 111.78 | 3 | 1 |
| 3 | B | 357 | PX4 | O7-C7-C6 | 2.14 | 116.03 | 108.34 | 11 | 1 |
| 3 | C | 328 | PX4 | C19-C18-C17 | 2.14 | 103.53 | 114.37 | 13 | 1 |
| 3 | C | 310 | PX4 | C12-C11-C10 | 2.14 | 105.26 | 113.13 | 12 | 1 |
| 3 | C | 337 | PX4 | C8-C7-C6 | 2.14 | 106.79 | 111.78 | 2 | 1 |
| 3 | C | 352 | PX4 | O1-P1-O2 | 2.14 | 122.41 | 112.44 | 7 | 2 |
| 3 | A | 629 | PX4 | O7-C7-C6 | 2.14 | 116.02 | 108.34 | 9 | 2 |
| 3 | A | 642 | PX4 | C15-C14-C13 | 2.14 | 125.18 | 114.37 | 5 | 1 |
| 3 | B | 324 | PX4 | C26-C25-C24 | 2.14 | 120.99 | 113.13 | 12 | 1 |
| 3 | B | 348 | PX4 | O1-P1-O2 | 2.14 | 122.40 | 112.44 | 1 | 1 |
| 3 | B | 359 | PX4 | C7-O7-C23 | 2.14 | 112.67 | 117.80 | 2 | 2 |
| 3 | B | 360 | PX4 | O1-P1-O2 | 2.14 | 122.40 | 112.44 | 14 | 1 |
| 3 | B | 384 | PX4 | C19-C18-C17 | 2.14 | 103.55 | 114.37 | 14 | 1 |
| 3 | B | 386 | PX4 | C33-C32-C31 | 2.14 | 103.55 | 114.37 | 4 | 1 |
| 3 | C | 310 | PX4 | O1-P1-O3 | 2.14 | 117.27 | 107.57 | 12 | 1 |
| 3 | B | 305 | PX4 | C8-C7-C6 | 2.14 | 106.80 | 111.78 | 4 | 1 |
| 3 | C | 323 | PX4 | C4-N1-C2 | 2.14 | 101.41 | 109.91 | 2 | 1 |
| 3 | B | 391 | PX4 | C12-C11-C10 | 2.14 | 105.28 | 113.13 | 13 | 1 |
| 3 | C | 310 | PX4 | C28-C27-C26 | 2.14 | 103.56 | 114.37 | 8 | 1 |
| 3 | C | 327 | PX4 | C25-C24-C23 | 2.14 | 105.87 | 113.69 | 1 | 1 |
| 3 | C | 333 | PX4 | C8-O5-C9 | 2.14 | 124.93 | 117.12 | 12 | 1 |
| 3 | A | 604 | PX4 | C33-C32-C31 | 2.14 | 103.57 | 114.37 | 8 | 1 |
| 3 | A | 605 | PX4 | C28-C27-C26 | 2.14 | 125.16 | 114.37 | 6 | 1 |
| 3 | A | 622 | PX4 | O7-C7-C8 | 2.13 | 116.00 | 108.34 | 13 | 1 |
| 3 | B | 307 | PX4 | O3-C1-C2 | 2.14 | 119.92 | 109.65 | 11 | 2 |
| 3 | B | 351 | PX4 | C8-C7-C6 | 2.14 | 106.81 | 111.78 | 4 | 3 |
| 3 | B | 374 | PX4 | O7-C23-O8 | 2.14 | 128.70 | 123.70 | 9 | 2 |
| 3 | A | 634 | PX4 | P1-O4-C6 | 2.13 | 109.12 | 121.35 | 2 | 1 |
| 3 | C | 311 | PX4 | C26-C25-C24 | 2.13 | 120.97 | 113.13 | 2 | 1 |
| 3 | C | 313 | PX4 | O5-C9-C10 | 2.13 | 105.33 | 111.83 | 10 | 1 |
| 3 | C | 328 | PX4 | O3-C1-C2 | 2.13 | 119.92 | 109.65 | 9 | 1 |
| 3 | A | 614 | PX4 | C5-N1-C3 | 2.13 | 103.38 | 108.98 | 3 | 1 |
| 3 | A | 625 | PX4 | O7-C23-O8 | 2.13 | 118.72 | 123.70 | 8 | 2 |
| 3 | A | 635 | PX4 | C26-C25-C24 | 2.13 | 120.96 | 113.13 | 12 | 1 |
| 3 | A | 653 | PX4 | C11-C10-C9 | 2.13 | 105.89 | 113.69 | 2 | 1 |
| 3 | B | 319 | PX4 | O1-P1-O2 | 2.13 | 122.36 | 112.44 | 14 | 1 |
| 3 | B | 341 | PX4 | C8-O5-C9 | 2.13 | 109.33 | 117.12 | 12 | 1 |
| 3 | B | 349 | PX4 | O3-C1-C2 | 2.13 | 119.90 | 109.65 | 14 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 371 | PX4 | C8-O5-C9 | 2.13 | 109.33 | 117.12 | 7 | 1 |
| 3 | C | 312 | PX4 | C26-C25-C24 | 2.13 | 105.30 | 113.13 | 13 | 1 |
| 3 | A | 603 | PX4 | C5-N1-C3 | 2.13 | 103.38 | 108.98 | 2 | 1 |
| 3 | B | 356 | PX4 | P1-O3-C1 | 2.13 | 131.40 | 121.26 | 2 | 1 |
| 3 | A | 609 | PX4 | C11-C10-C9 | 2.13 | 105.90 | 113.69 | 6 | 2 |
| 3 | A | 611 | PX4 | C5-N1-C4 | 2.13 | 114.56 | 108.98 | 15 | 2 |
| 3 | A | 622 | PX4 | O5-C9-O6 | 2.13 | 128.95 | 123.63 | 5 | 2 |
| 3 | B | 322 | PX4 | C11-C10-C9 | 2.13 | 105.90 | 113.69 | 1 | 1 |
| 3 | B | 323 | PX4 | C4-N1-C3 | 2.13 | 103.39 | 108.98 | 6 | 1 |
| 3 | B | 352 | PX4 | O6-C9-C10 | 2.13 | 132.11 | 123.78 | 1 | 1 |
| 3 | B | 354 | PX4 | O1-P1-O4 | 2.13 | 117.21 | 107.57 | 9 | 1 |
| 3 | B | 381 | PX4 | C7-O7-C23 | 2.13 | 122.89 | 117.80 | 14 | 3 |
| 3 | B | 388 | PX4 | C18-C17-C16 | 2.13 | 103.62 | 114.37 | 2 | 1 |
| 3 | C | 346 | PX4 | O5-C9-C10 | 2.13 | 105.35 | 111.83 | 9 | 1 |
| 3 | C | 353 | PX4 | C33-C32-C31 | 2.13 | 103.62 | 114.37 | 13 | 1 |
| 3 | C | 360 | PX4 | C11-C10-C9 | 2.13 | 105.90 | 113.69 | 12 | 1 |
| 3 | A | 643 | PX4 | C33-C32-C31 | 2.13 | 103.62 | 114.37 | 2 | 1 |
| 3 | A | 652 | PX4 | C14-C13-C12 | 2.13 | 103.62 | 114.37 | 8 | 1 |
| 3 | B | 309 | PX4 | C4-N1-C3 | 2.13 | 114.56 | 108.98 | 11 | 2 |
| 3 | A | 635 | PX4 | O7-C23-C24 | 2.12 | 106.89 | 111.48 | 6 | 1 |
| 3 | B | 321 | PX4 | O1-P1-O2 | 2.13 | 122.33 | 112.44 | 6 | 1 |
| 3 | B | 368 | PX4 | O6-C9-C10 | 2.13 | 132.10 | 123.78 | 4 | 1 |
| 3 | B | 378 | PX4 | C36-C35-C34 | 2.13 | 127.72 | 113.36 | 9 | 1 |
| 3 | B | 378 | PX4 | C30-C29-C28 | 2.13 | 103.62 | 114.37 | 13 | 1 |
| 3 | C | 324 | PX4 | O7-C7-C6 | 2.13 | 100.72 | 108.34 | 11 | 1 |
| 3 | C | 331 | PX4 | O3-C1-C2 | 2.13 | 119.88 | 109.65 | 13 | 2 |
| 3 | C | 336 | PX4 | O7-C7-C6 | 2.13 | 100.72 | 108.34 | 11 | 1 |
| 3 | C | 340 | PX4 | O6-C9-C10 | 2.13 | 132.10 | 123.78 | 12 | 1 |
| 3 | C | 356 | PX4 | O7-C7-C8 | 2.13 | 115.97 | 108.34 | 14 | 1 |
| 3 | A | 606 | PX4 | C1-C2-N1 | 2.12 | 122.64 | 115.82 | 5 | 1 |
| 3 | A | 650 | PX4 | C8-C7-C6 | 2.12 | 106.83 | 111.78 | 11 | 1 |
| 3 | B | 307 | PX4 | O7-C7-C8 | 2.12 | 100.72 | 108.34 | 8 | 2 |
| 3 | B | 338 | PX4 | C1-C2-N1 | 2.12 | 122.64 | 115.82 | 13 | 1 |
| 3 | B | 353 | PX4 | C26-C25-C24 | 2.12 | 120.93 | 113.13 | 6 | 1 |
| 3 | C | 305 | PX4 | C19-C18-C17 | 2.12 | 125.11 | 114.37 | 7 | 1 |
| 3 | C | 311 | PX4 | C12-C11-C10 | 2.12 | 105.32 | 113.13 | 10 | 1 |
| 3 | C | 323 | PX4 | O1-P1-O2 | 2.12 | 122.33 | 112.44 | 15 | 1 |
| 3 | C | 340 | PX4 | C5-N1-C2 | 2.12 | 118.35 | 109.91 | 11 | 1 |
| 3 | C | 343 | PX4 | C11-C10-C9 | 2.12 | 105.92 | 113.69 | 12 | 1 |
| 3 | C | 354 | PX4 | C8-O5-C9 | 2.12 | 124.88 | 117.12 | 8 | 2 |
| 3 | A | 629 | PX4 | O5-C9-O6 | 2.12 | 128.94 | 123.63 | 9 | 2 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 341 | PX4 | C31-C30-C29 | 2.12 | 103.64 | 114.37 | 11 | 2 |
| 3 | B | 347 | PX4 | C29-C28-C27 | 2.12 | 103.64 | 114.37 | 11 | 1 |
| 3 | B | 349 | PX4 | C27-C26-C25 | 2.12 | 103.64 | 114.37 | 12 | 1 |
| 3 | B | 352 | PX4 | C27-C26-C25 | 2.12 | 125.09 | 114.37 | 15 | 1 |
| 3 | B | 397 | PX4 | C5-N1-C2 | 2.12 | 118.35 | 109.91 | 15 | 1 |
| 3 | B | 374 | PX4 | C5-N1-C3 | 2.12 | 103.40 | 108.98 | 3 | 1 |
| 3 | B | 375 | PX4 | C8-C7-C6 | 2.12 | 106.84 | 111.78 | 15 | 1 |
| 3 | A | 618 | PX4 | C27-C26-C25 | 2.12 | 103.65 | 114.37 | 12 | 1 |
| 3 | C | 361 | PX4 | C5-N1-C4 | 2.12 | 103.41 | 108.98 | 4 | 1 |
| 3 | A | 606 | PX4 | C8-O5-C9 | 2.12 | 109.37 | 117.12 | 14 | 1 |
| 3 | A | 643 | PX4 | O1-P1-O2 | 2.12 | 122.30 | 112.44 | 14 | 1 |
| 3 | B | 363 | PX4 | C5-N1-C3 | 2.12 | 103.41 | 108.98 | 15 | 1 |
| 3 | B | 386 | PX4 | C12-C11-C10 | 2.12 | 120.92 | 113.13 | 4 | 1 |
| 3 | C | 361 | PX4 | O1-P1-O2 | 2.12 | 122.31 | 112.44 | 2 | 1 |
| 3 | A | 649 | PX4 | P1-O3-C1 | 2.12 | 131.34 | 121.26 | 4 | 1 |
| 3 | B | 319 | PX4 | C4-N1-C3 | 2.12 | 114.54 | 108.98 | 3 | 1 |
| 3 | B | 383 | PX4 | O7-C7-C6 | 2.12 | 115.94 | 108.34 | 9 | 2 |
| 3 | B | 395 | PX4 | C4-N1-C3 | 2.12 | 114.54 | 108.98 | 2 | 1 |
| 3 | B | 333 | PX4 | O7-C7-C8 | 2.12 | 100.75 | 108.34 | 13 | 2 |
| 3 | A | 613 | PX4 | C28-C27-C26 | 2.12 | 103.67 | 114.37 | 14 | 1 |
| 3 | A | 616 | PX4 | O7-C7-C6 | 2.12 | 115.94 | 108.34 | 3 | 1 |
| 3 | A | 624 | PX4 | C28-C27-C26 | 2.12 | 103.67 | 114.37 | 13 | 1 |
| 3 | A | 631 | PX4 | P1-O3-C1 | 2.12 | 131.33 | 121.26 | 12 | 1 |
| 3 | A | 651 | PX4 | C32-C31-C30 | 2.12 | 103.67 | 114.37 | 3 | 1 |
| 3 | B | 301 | PX4 | P1-O4-C6 | 2.12 | 133.48 | 121.35 | 15 | 1 |
| 3 | C | 301 | PX4 | C15-C14-C13 | 2.12 | 103.67 | 114.37 | 11 | 1 |
| 3 | C | 328 | PX4 | C25-C24-C23 | 2.12 | 105.94 | 113.69 | 13 | 1 |
| 3 | C | 353 | PX4 | C26-C25-C24 | 2.12 | 105.35 | 113.13 | 13 | 1 |
| 3 | B | 352 | PX4 | O7-C23-O8 | 2.12 | 128.65 | 123.70 | 7 | 1 |
| 3 | C | 341 | PX4 | C5-N1-C4 | 2.12 | 114.53 | 108.98 | 7 | 1 |
| 3 | B | 304 | PX4 | O4-P1-O2 | 2.11 | 100.56 | 108.94 | 2 | 1 |
| 3 | B | 317 | PX4 | O7-C23-O8 | 2.11 | 128.65 | 123.70 | 12 | 2 |
| 3 | B | 343 | PX4 | O5-C9-C10 | 2.11 | 105.39 | 111.83 | 11 | 1 |
| 3 | C | 347 | PX4 | C5-N1-C2 | 2.12 | 101.50 | 109.91 | 5 | 1 |
| 3 | C | 348 | PX4 | C15-C14-C13 | 2.12 | 103.68 | 114.37 | 4 | 1 |
| 3 | C | 348 | PX4 | C26-C25-C24 | 2.11 | 105.36 | 113.13 | 14 | 1 |
| 3 | C | 361 | PX4 | C14-C13-C12 | 2.12 | 103.67 | 114.37 | 10 | 1 |
| 3 | B | 385 | PX4 | C5-N1-C3 | 2.11 | 103.42 | 108.98 | 2 | 2 |
| 3 | C | 324 | PX4 | O5-C9-O6 | 2.11 | 128.92 | 123.63 | 8 | 2 |
| 3 | A | 616 | PX4 | C8-C7-C6 | 2.11 | 116.71 | 111.78 | 5 | 1 |
| 3 | C | 335 | PX4 | C5-N1-C4 | 2.11 | 114.53 | 108.98 | 3 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | A | 636 | PX4 | C15-C14-C13 | 2.11 | 103.69 | 114.37 | 8 | 1 |
| 3 | B | 363 | PX4 | C4-N1-C3 | 2.11 | 114.52 | 108.98 | 1 | 1 |
| 3 | B | 366 | PX4 | O1-P1-O3 | 2.11 | 117.14 | 107.57 | 15 | 1 |
| 3 | B | 386 | PX4 | C11-C10-C9 | 2.11 | 105.96 | 113.69 | 8 | 1 |
| 3 | C | 312 | PX4 | O3-C1-C2 | 2.11 | 119.81 | 109.65 | 13 | 1 |
| 3 | C | 323 | PX4 | O6-C9-C10 | 2.11 | 132.04 | 123.78 | 3 | 1 |
| 3 | C | 344 | PX4 | O7-C7-C8 | 2.11 | 115.92 | 108.34 | 4 | 1 |
| 3 | A | 628 | PX4 | C1-C2-N1 | 2.11 | 122.60 | 115.82 | 3 | 1 |
| 3 | B | 342 | PX4 | O3-C1-C2 | 2.11 | 119.81 | 109.65 | 15 | 1 |
| 3 | C | 355 | PX4 | O1-P1-O2 | 2.11 | 122.27 | 112.44 | 8 | 1 |
| 3 | C | 363 | PX4 | O3-P1-O2 | 2.11 | 117.31 | 108.94 | 6 | 1 |
| 3 | B | 319 | PX4 | C8-O5-C9 | 2.11 | 109.41 | 117.12 | 5 | 1 |
| 3 | B | 330 | PX4 | O1-P1-O2 | 2.11 | 122.27 | 112.44 | 11 | 1 |
| 3 | B | 352 | PX4 | O3-C1-C2 | 2.11 | 119.80 | 109.65 | 3 | 1 |
| 3 | C | 318 | PX4 | O7-C23-O8 | 2.11 | 128.64 | 123.70 | 6 | 3 |
| 3 | C | 362 | PX4 | O7-C7-C8 | 2.11 | 115.91 | 108.34 | 7 | 1 |
| 3 | C | 362 | PX4 | O5-C9-O6 | 2.11 | 128.91 | 123.63 | 14 | 1 |
| 3 | B | 352 | PX4 | C14-C13-C12 | 2.11 | 125.03 | 114.37 | 7 | 1 |
| 3 | B | 363 | PX4 | O1-P1-O2 | 2.11 | 122.25 | 112.44 | 11 | 1 |
| 3 | B | 380 | PX4 | C36-C35-C34 | 2.11 | 127.60 | 113.36 | 2 | 1 |
| 3 | B | 395 | PX4 | P1-O3-C1 | 2.11 | 131.29 | 121.26 | 3 | 1 |
| 3 | C | 304 | PX4 | C5-N1-C3 | 2.11 | 103.44 | 108.98 | 2 | 2 |
| 3 | C | 357 | PX4 | O7-C7-C8 | 2.11 | 115.91 | 108.34 | 2 | 1 |
| 3 | A | 605 | PX4 | C5-N1-C3 | 2.11 | 103.44 | 108.98 | 5 | 1 |
| 3 | A | 624 | PX4 | C25-C24-C23 | 2.11 | 121.41 | 113.69 | 15 | 1 |
| 3 | A | 628 | PX4 | C17-C16-C15 | 2.11 | 103.72 | 114.37 | 7 | 1 |
| 3 | A | 633 | PX4 | O7-C7-C6 | 2.11 | 115.90 | 108.34 | 6 | 1 |
| 3 | B | 319 | PX4 | C5-N1-C4 | 2.11 | 103.44 | 108.98 | 13 | 1 |
| 3 | B | 341 | PX4 | C15-C14-C13 | 2.11 | 125.01 | 114.37 | 15 | 1 |
| 3 | B | 382 | PX4 | C16-C15-C14 | 2.11 | 103.72 | 114.37 | 1 | 1 |
| 3 | B | 395 | PX4 | C17-C16-C15 | 2.11 | 125.02 | 114.37 | 6 | 1 |
| 3 | C | 321 | PX4 | O5-C9-C10 | 2.11 | 105.41 | 111.83 | 8 | 1 |
| 3 | C | 326 | PX4 | O1-P1-O2 | 2.11 | 122.24 | 112.44 | 10 | 1 |
| 3 | C | 338 | PX4 | C5-N1-C3 | 2.11 | 114.51 | 108.98 | 13 | 1 |
| 3 | C | 344 | PX4 | C3-N1-C2 | 2.11 | 118.28 | 109.91 | 4 | 1 |
| 3 | A | 637 | PX4 | C1-C2-N1 | 2.10 | 122.58 | 115.82 | 2 | 1 |
| 3 | B | 317 | PX4 | O7-C23-C24 | 2.11 | 106.93 | 111.48 | 13 | 1 |
| 3 | C | 359 | PX4 | O5-C9-O6 | 2.11 | 128.89 | 123.63 | 6 | 1 |
| 3 | A | 605 | PX4 | C20-C19-C18 | 2.10 | 103.73 | 114.37 | 2 | 1 |
| 3 | A | 611 | PX4 | C12-C11-C10 | 2.10 | 120.86 | 113.13 | 12 | 1 |
| 3 | B | 318 | PX4 | C4-N1-C3 | 2.10 | 103.45 | 108.98 | 14 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 396 | PX4 | O1-P1-O4 | 2.10 | 117.10 | 107.57 | 10 | 1 |
| 3 | C | 313 | PX4 | C32-C31-C30 | 2.10 | 125.00 | 114.37 | 2 | 1 |
| 3 | C | 344 | PX4 | O1-P1-O2 | 2.10 | 122.23 | 112.44 | 15 | 1 |
| 3 | C | 348 | PX4 | C29-C28-C27 | 2.10 | 103.74 | 114.37 | 3 | 1 |
| 3 | A | 626 | PX4 | O3-C1-C2 | 2.10 | 119.76 | 109.65 | 8 | 2 |
| 3 | A | 640 | PX4 | C8-O5-C9 | 2.10 | 109.44 | 117.12 | 8 | 1 |
| 3 | A | 644 | PX4 | O3-C1-C2 | 2.10 | 119.76 | 109.65 | 12 | 1 |
| 3 | B | 302 | PX4 | C12-C11-C10 | 2.10 | 105.41 | 113.13 | 7 | 1 |
| 3 | B | 312 | PX4 | C8-O5-C9 | 2.10 | 109.44 | 117.12 | 15 | 1 |
| 3 | B | 359 | PX4 | C26-C25-C24 | 2.10 | 105.41 | 113.13 | 12 | 1 |
| 3 | B | 384 | PX4 | C29-C28-C27 | 2.10 | 124.99 | 114.37 | 12 | 1 |
| 3 | B | 389 | PX4 | O1-P1-O4 | 2.10 | 117.09 | 107.57 | 3 | 1 |
| 3 | A | 651 | PX4 | C26-C25-C24 | 2.10 | 120.84 | 113.13 | 12 | 1 |
| 3 | C | 327 | PX4 | C8-O5-C9 | 2.10 | 124.79 | 117.12 | 10 | 1 |
| 3 | C | 330 | PX4 | O7-C7-C8 | 2.10 | 115.88 | 108.34 | 4 | 1 |
| 3 | C | 359 | PX4 | C7-O7-C23 | 2.10 | 112.77 | 117.80 | 8 | 1 |
| 3 | C | 306 | PX4 | O3-C1-C2 | 2.10 | 119.75 | 109.65 | 11 | 1 |
| 3 | A | 632 | PX4 | O5-C9-O6 | 2.10 | 128.88 | 123.63 | 6 | 1 |
| 3 | B | 312 | PX4 | C31-C30-C29 | 2.10 | 103.76 | 114.37 | 1 | 1 |
| 3 | B | 368 | PX4 | O3-C1-C2 | 2.10 | 119.74 | 109.65 | 6 | 1 |
| 3 | C | 363 | PX4 | C5-N1-C4 | 2.10 | 103.46 | 108.98 | 3 | 1 |
| 3 | A | 644 | PX4 | O4-P1-O2 | 2.10 | 100.62 | 108.94 | 2 | 1 |
| 3 | B | 393 | PX4 | O7-C7-C6 | 2.10 | 115.87 | 108.34 | 8 | 1 |
| 3 | B | 394 | PX4 | C26-C25-C24 | 2.10 | 120.83 | 113.13 | 13 | 1 |
| 3 | B | 321 | PX4 | C1-C2-N1 | 2.10 | 122.55 | 115.82 | 11 | 1 |
| 3 | C | 350 | PX4 | O6-C9-C10 | 2.10 | 131.98 | 123.78 | 8 | 1 |
| 3 | A | 603 | PX4 | O1-P1-O2 | 2.09 | 122.19 | 112.44 | 14 | 1 |
| 3 | A | 629 | PX4 | C25-C24-C23 | 2.10 | 121.37 | 113.69 | 5 | 1 |
| 3 | B | 314 | PX4 | C36-C35-C34 | 2.09 | 99.22 | 113.36 | 10 | 1 |
| 3 | B | 329 | PX4 | O7-C7-C8 | 2.10 | 115.86 | 108.34 | 15 | 2 |
| 3 | B | 387 | PX4 | C5-N1-C4 | 2.10 | 114.48 | 108.98 | 15 | 1 |
| 3 | C | 351 | PX4 | C30-C29-C28 | 2.10 | 103.78 | 114.37 | 1 | 1 |
| 3 | C | 352 | PX4 | C25-C24-C23 | 2.10 | 106.02 | 113.69 | 12 | 1 |
| 3 | A | 620 | PX4 | C8-O5-C9 | 2.09 | 124.77 | 117.12 | 10 | 1 |
| 3 | B | 333 | PX4 | O7-C7-C6 | 2.09 | 100.83 | 108.34 | 7 | 1 |
| 3 | B | 338 | PX4 | C11-C10-C9 | 2.09 | 121.37 | 113.69 | 11 | 1 |
| 3 | C | 353 | PX4 | C4-N1-C3 | 2.09 | 114.48 | 108.98 | 6 | 1 |
| 3 | A | 651 | PX4 | O7-C7-C6 | 2.09 | 115.85 | 108.34 | 3 | 1 |
| 3 | A | 652 | PX4 | O7-C7-C8 | 2.09 | 115.85 | 108.34 | 8 | 1 |
| 3 | B | 306 | PX4 | O7-C7-C8 | 2.09 | 115.85 | 108.34 | 13 | 2 |
| 3 | B | 329 | PX4 | O5-C9-C10 | 2.09 | 105.45 | 111.83 | 8 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | C | 301 | PX4 | P1-O4-C6 | 2.09 | 133.34 | 121.35 | 6 | 1 |
| 3 | C | 313 | PX4 | O1-P1-O2 | 2.09 | 122.18 | 112.44 | 2 | 1 |
| 3 | C | 313 | PX4 | C19-C18-C17 | 2.09 | 103.79 | 114.37 | 10 | 1 |
| 3 | C | 355 | PX4 | P1-O3-C1 | 2.09 | 131.22 | 121.26 | 2 | 1 |
| 3 | A | 643 | PX4 | O3-C1-C2 | 2.09 | 119.71 | 109.65 | 13 | 1 |
| 3 | A | 645 | PX4 | O5-C9-C10 | 2.09 | 105.46 | 111.83 | 8 | 1 |
| 3 | C | 350 | PX4 | C25-C24-C23 | 2.09 | 106.03 | 113.69 | 12 | 1 |
| 3 | A | 601 | PX4 | C19-C18-C17 | 2.09 | 103.81 | 114.37 | 3 | 1 |
| 3 | B | 343 | PX4 | C14-C13-C12 | 2.09 | 103.80 | 114.37 | 5 | 1 |
| 3 | B | 382 | PX4 | C5-N1-C3 | 2.09 | 103.49 | 108.98 | 8 | 1 |
| 3 | A | 627 | PX4 | O5-C9-O6 | 2.09 | 128.85 | 123.63 | 7 | 1 |
| 3 | A | 647 | PX4 | C15-C14-C13 | 2.09 | 103.81 | 114.37 | 14 | 1 |
| 3 | B | 307 | PX4 | C8-O5-C9 | 2.09 | 109.48 | 117.12 | 14 | 1 |
| 3 | B | 339 | PX4 | C4-N1-C3 | 2.09 | 114.46 | 108.98 | 10 | 1 |
| 3 | A | 630 | PX4 | C12-C11-C10 | 2.09 | 105.46 | 113.13 | 11 | 1 |
| 3 | B | 335 | PX4 | C25-C24-C23 | 2.09 | 106.05 | 113.69 | 4 | 1 |
| 3 | A | 604 | PX4 | C19-C18-C17 | 2.09 | 103.82 | 114.37 | 11 | 1 |
| 3 | A | 642 | PX4 | C26-C25-C24 | 2.09 | 105.46 | 113.13 | 15 | 1 |
| 3 | B | 337 | PX4 | P1-O3-C1 | 2.09 | 111.33 | 121.26 | 3 | 1 |
| 3 | B | 337 | PX4 | O1-P1-O2 | 2.09 | 122.15 | 112.44 | 12 | 1 |
| 3 | B | 341 | PX4 | O7-C7-C6 | 2.09 | 115.83 | 108.34 | 13 | 1 |
| 3 | B | 380 | PX4 | O7-C7-C8 | 2.09 | 115.83 | 108.34 | 9 | 1 |
| 3 | B | 343 | PX4 | O5-C9-O6 | 2.09 | 128.85 | 123.63 | 1 | 2 |
| 3 | B | 399 | PX4 | C5-N1-C3 | 2.09 | 114.46 | 108.98 | 6 | 1 |
| 3 | B | 333 | PX4 | C27-C26-C25 | 2.09 | 103.83 | 114.37 | 15 | 1 |
| 3 | B | 359 | PX4 | O3-C1-C2 | 2.09 | 119.68 | 109.65 | 4 | 1 |
| 3 | C | 309 | PX4 | O7-C7-C6 | 2.09 | 100.86 | 108.34 | 3 | 1 |
| 3 | C | 342 | PX4 | O1-P1-O2 | 2.09 | 122.15 | 112.44 | 7 | 1 |
| 3 | B | 365 | PX4 | O7-C7-C8 | 2.08 | 115.82 | 108.34 | 13 | 1 |
| 3 | C | 342 | PX4 | O4-P1-O2 | 2.09 | 100.67 | 108.94 | 12 | 1 |
| 3 | A | 603 | PX4 | C8-C7-C6 | 2.08 | 106.93 | 111.78 | 8 | 1 |
| 3 | A | 619 | PX4 | O7-C7-C8 | 2.08 | 115.82 | 108.34 | 4 | 1 |
| 3 | B | 395 | PX4 | C1-C2-N1 | 2.08 | 122.51 | 115.82 | 13 | 1 |
| 3 | C | 348 | PX4 | C12-C11-C10 | 2.08 | 120.79 | 113.13 | 7 | 1 |
| 3 | A | 619 | PX4 | C5-N1-C2 | 2.08 | 118.19 | 109.91 | 5 | 1 |
| 3 | B | 334 | PX4 | C26-C25-C24 | 2.08 | 105.47 | 113.13 | 2 | 1 |
| 3 | B | 353 | PX4 | O7-C7-C6 | 2.08 | 115.81 | 108.34 | 11 | 1 |
| 3 | B | 356 | PX4 | O5-C9-O6 | 2.08 | 128.84 | 123.63 | 8 | 1 |
| 3 | B | 400 | PX4 | C11-C10-C9 | 2.08 | 121.33 | 113.69 | 15 | 1 |
| 3 | C | 309 | PX4 | C4-N1-C3 | 2.08 | 103.50 | 108.98 | 11 | 1 |
| 3 | C | 356 | PX4 | C8-O5-C9 | 2.08 | 109.50 | 117.12 | 1 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | A | 604 | PX4 | O8-C23-C24 | 2.08 | 131.92 | 123.78 | 3 | 1 |
| 3 | A | 620 | PX4 | O8-C23-C24 | 2.08 | 131.92 | 123.78 | 13 | 1 |
| 3 | B | 306 | PX4 | C26-C25-C24 | 2.08 | 120.77 | 113.13 | 1 | 1 |
| 3 | B | 307 | PX4 | C3-N1-C2 | 2.08 | 118.18 | 109.91 | 9 | 1 |
| 3 | B | 352 | PX4 | O5-C9-O6 | 2.08 | 128.83 | 123.63 | 2 | 1 |
| 3 | B | 388 | PX4 | O8-C23-C24 | 2.08 | 131.93 | 123.78 | 3 | 1 |
| 3 | B | 362 | PX4 | C5-N1-C3 | 2.08 | 103.51 | 108.98 | 10 | 1 |
| 3 | A | 628 | PX4 | C4-N1-C3 | 2.08 | 114.44 | 108.98 | 11 | 2 |
| 3 | B | 380 | PX4 | C18-C17-C16 | 2.08 | 103.85 | 114.37 | 2 | 1 |
| 3 | C | 320 | PX4 | O4-P1-O2 | 2.08 | 100.69 | 108.94 | 3 | 1 |
| 3 | C | 332 | PX4 | C25-C24-C23 | 2.08 | 106.07 | 113.69 | 15 | 1 |
| 3 | C | 340 | PX4 | O4-P1-O2 | 2.08 | 100.69 | 108.94 | 6 | 1 |
| 3 | C | 358 | PX4 | P1-O4-C6 | 2.08 | 109.43 | 121.35 | 3 | 1 |
| 3 | A | 624 | PX4 | C11-C10-C9 | 2.08 | 106.08 | 113.69 | 1 | 1 |
| 3 | B | 301 | PX4 | O8-C23-C24 | 2.08 | 115.65 | 123.78 | 13 | 1 |
| 3 | A | 633 | PX4 | C13-C12-C11 | 2.08 | 103.86 | 114.37 | 7 | 1 |
| 3 | B | 305 | PX4 | C5-N1-C2 | 2.08 | 118.17 | 109.91 | 15 | 1 |
| 3 | B | 314 | PX4 | C5-N1-C2 | 2.08 | 118.17 | 109.91 | 12 | 1 |
| 3 | C | 311 | PX4 | C1-C2-N1 | 2.08 | 122.49 | 115.82 | 9 | 1 |
| 3 | C | 313 | PX4 | C30-C29-C28 | 2.08 | 103.87 | 114.37 | 3 | 1 |
| 3 | C | 321 | PX4 | C26-C25-C24 | 2.08 | 105.49 | 113.13 | 1 | 1 |
| 3 | C | 325 | PX4 | C25-C24-C23 | 2.08 | 106.08 | 113.69 | 2 | 2 |
| 3 | C | 343 | PX4 | C4-N1-C2 | 2.08 | 118.17 | 109.91 | 5 | 1 |
| 3 | A | 624 | PX4 | O7-C7-C8 | 2.08 | 115.79 | 108.34 | 10 | 1 |
| 3 | A | 628 | PX4 | C26-C25-C24 | 2.08 | 120.75 | 113.13 | 6 | 1 |
| 3 | B | 351 | PX4 | C4-N1-C3 | 2.08 | 103.52 | 108.98 | 7 | 1 |
| 3 | B | 356 | PX4 | O4-P1-O2 | 2.08 | 100.70 | 108.94 | 15 | 1 |
| 3 | C | 354 | PX4 | C16-C15-C14 | 2.08 | 103.87 | 114.37 | 15 | 1 |
| 3 | A | 608 | PX4 | O6-C9-C10 | 2.07 | 131.90 | 123.78 | 4 | 1 |
| 3 | A | 647 | PX4 | C8-O5-C9 | 2.08 | 109.53 | 117.12 | 6 | 1 |
| 3 | B | 369 | PX4 | C12-C11-C10 | 2.08 | 105.50 | 113.13 | 5 | 2 |
| 3 | B | 397 | PX4 | C12-C11-C10 | 2.08 | 105.50 | 113.13 | 15 | 1 |
| 3 | B | 304 | PX4 | O3-P1-O2 | 2.07 | 117.16 | 108.94 | 3 | 1 |
| 3 | B | 399 | PX4 | C14-C13-C12 | 2.07 | 103.88 | 114.37 | 10 | 1 |
| 3 | C | 336 | PX4 | C30-C29-C28 | 2.08 | 103.88 | 114.37 | 4 | 1 |
| 3 | C | 328 | PX4 | C8-O5-C9 | 2.07 | 109.54 | 117.12 | 7 | 1 |
| 3 | C | 338 | PX4 | C8-O5-C9 | 2.07 | 124.70 | 117.12 | 15 | 3 |
| 3 | C | 360 | PX4 | C5-N1-C4 | 2.08 | 103.53 | 108.98 | 3 | 1 |
| 3 | C | 362 | PX4 | C8-O5-C9 | 2.08 | 109.53 | 117.12 | 4 | 1 |
| 3 | A | 618 | PX4 | O1-P1-O2 | 2.07 | 122.09 | 112.44 | 11 | 1 |
| 3 | A | 629 | PX4 | C1-C2-N1 | 2.07 | 122.48 | 115.82 | 8 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 310 | PX4 | C4-N1-C2 | 2.07 | 118.15 | 109.91 | 3 | 1 |
| 3 | B | 318 | PX4 | C8-O5-C9 | 2.07 | 109.54 | 117.12 | 7 | 1 |
| 3 | A | 621 | PX4 | C32-C31-C30 | 2.07 | 124.84 | 114.37 | 9 | 1 |
| 3 | A | 631 | PX4 | O5-C9-C10 | 2.07 | 105.51 | 111.83 | 10 | 2 |
| 3 | C | 357 | PX4 | C8-O5-C9 | 2.07 | 109.54 | 117.12 | 6 | 1 |
| 3 | A | 634 | PX4 | O7-C7-C8 | 2.07 | 115.78 | 108.34 | 15 | 1 |
| 3 | A | 654 | PX4 | C11-C10-C9 | 2.07 | 121.29 | 113.69 | 11 | 1 |
| 3 | C | 302 | PX4 | C8-O5-C9 | 2.07 | 109.54 | 117.12 | 13 | 1 |
| 3 | A | 606 | PX4 | O5-C9-O6 | 2.07 | 128.81 | 123.63 | 14 | 1 |
| 3 | B | 341 | PX4 | O1-P1-O2 | 2.07 | 122.08 | 112.44 | 9 | 1 |
| 3 | B | 351 | PX4 | C3-N1-C2 | 2.07 | 101.68 | 109.91 | 1 | 1 |
| 3 | B | 366 | PX4 | O7-C7-C6 | 2.07 | 100.91 | 108.34 | 9 | 1 |
| 3 | B | 377 | PX4 | C27-C26-C25 | 2.07 | 103.89 | 114.37 | 11 | 1 |
| 3 | B | 356 | PX4 | C16-C15-C14 | 2.07 | 103.90 | 114.37 | 3 | 1 |
| 3 | B | 371 | PX4 | C4-N1-C2 | 2.07 | 118.14 | 109.91 | 1 | 1 |
| 3 | C | 312 | PX4 | C11-C10-C9 | 2.07 | 121.28 | 113.69 | 10 | 1 |
| 3 | C | 320 | PX4 | C26-C25-C24 | 2.07 | 120.74 | 113.13 | 6 | 1 |
| 3 | C | 334 | PX4 | O7-C23-C24 | 2.07 | 107.00 | 111.48 | 4 | 1 |
| 3 | A | 618 | PX4 | O5-C9-O6 | 2.07 | 128.80 | 123.63 | 1 | 1 |
| 3 | A | 619 | PX4 | C8-C7-C6 | 2.07 | 106.96 | 111.78 | 11 | 1 |
| 3 | A | 625 | PX4 | C4-N1-C2 | 2.07 | 118.14 | 109.91 | 2 | 1 |
| 3 | A | 629 | PX4 | O7-C23-C24 | 2.07 | 107.00 | 111.48 | 7 | 1 |
| 3 | A | 642 | PX4 | C31-C30-C29 | 2.07 | 103.91 | 114.37 | 9 | 1 |
| 3 | A | 638 | PX4 | C25-C24-C23 | 2.07 | 106.11 | 113.69 | 5 | 1 |
| 3 | B | 302 | PX4 | O7-C7-C8 | 2.07 | 115.77 | 108.34 | 14 | 1 |
| 3 | B | 317 | PX4 | O5-C8-C7 | 2.07 | 114.36 | 108.40 | 11 | 2 |
| 3 | B | 369 | PX4 | C19-C18-C17 | 2.07 | 124.83 | 114.37 | 1 | 1 |
| 3 | B | 369 | PX4 | O7-C7-C6 | 2.07 | 115.77 | 108.34 | 3 | 1 |
| 3 | B | 374 | PX4 | O7-C23-C24 | 2.07 | 107.00 | 111.48 | 8 | 2 |
| 3 | C | 307 | PX4 | C18-C17-C16 | 2.07 | 103.91 | 114.37 | 12 | 1 |
| 3 | C | 327 | PX4 | C16-C15-C14 | 2.07 | 103.91 | 114.37 | 15 | 1 |
| 3 | B | 325 | PX4 | C15-C14-C13 | 2.07 | 103.91 | 114.37 | 12 | 1 |
| 3 | B | 344 | PX4 | O7-C7-C6 | 2.07 | 115.77 | 108.34 | 14 | 1 |
| 3 | C | 320 | PX4 | C4-N1-C3 | 2.07 | 103.54 | 108.98 | 11 | 1 |
| 3 | C | 322 | PX4 | O4-P1-O2 | 2.07 | 100.73 | 108.94 | 2 | 1 |
| 3 | A | 606 | PX4 | C11-C10-C9 | 2.07 | 121.27 | 113.69 | 6 | 1 |
| 3 | B | 304 | PX4 | C3-N1-C2 | 2.07 | 118.13 | 109.91 | 10 | 1 |
| 3 | B | 308 | PX4 | C31-C30-C29 | 2.07 | 103.92 | 114.37 | 8 | 2 |
| 3 | A | 616 | PX4 | C8-O5-C9 | 2.07 | 109.56 | 117.12 | 15 | 1 |
| 3 | B | 301 | PX4 | C34-C33-C32 | 2.07 | 103.92 | 114.37 | 10 | 1 |
| 3 | A | 632 | PX4 | C8-O5-C9 | 2.07 | 124.67 | 117.12 | 15 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 302 | PX4 | C11-C10-C9 | 2.07 | 106.12 | 113.69 | 2 | 1 |
| 3 | B | 349 | PX4 | O6-C9-C10 | 2.07 | 131.87 | 123.78 | 3 | 1 |
| 3 | A | 610 | PX4 | P1-O3-C1 | 2.06 | 111.43 | 121.26 | 6 | 2 |
| 3 | A | 618 | PX4 | C13-C12-C11 | 2.06 | 103.93 | 114.37 | 11 | 1 |
| 3 | B | 308 | PX4 | C32-C31-C30 | 2.07 | 103.93 | 114.37 | 10 | 1 |
| 3 | B | 325 | PX4 | C5-N1-C4 | 2.07 | 103.55 | 108.98 | 11 | 1 |
| 3 | B | 382 | PX4 | C12-C11-C10 | 2.07 | 105.53 | 113.13 | 9 | 1 |
| 3 | C | 325 | PX4 | C5-N1-C4 | 2.07 | 103.55 | 108.98 | 11 | 1 |
| 3 | C | 337 | PX4 | C5-N1-C3 | 2.07 | 114.40 | 108.98 | 8 | 1 |
| 3 | C | 343 | PX4 | O5-C9-O6 | 2.07 | 128.80 | 123.63 | 13 | 1 |
| 3 | B | 390 | PX4 | C11-C10-C9 | 2.07 | 121.26 | 113.69 | 3 | 1 |
| 3 | B | 346 | PX4 | O7-C23-O8 | 2.06 | 128.53 | 123.70 | 15 | 1 |
| 3 | A | 601 | PX4 | C25-C24-C23 | 2.06 | 106.13 | 113.69 | 15 | 1 |
| 3 | A | 651 | PX4 | C16-C15-C14 | 2.06 | 103.93 | 114.37 | 11 | 1 |
| 3 | C | 326 | PX4 | C25-C24-C23 | 2.06 | 106.13 | 113.69 | 4 | 1 |
| 3 | B | 302 | PX4 | C26-C25-C24 | 2.06 | 105.55 | 113.13 | 15 | 1 |
| 3 | B | 313 | PX4 | O1-P1-O2 | 2.06 | 122.04 | 112.44 | 11 | 1 |
| 3 | B | 330 | PX4 | C5-N1-C2 | 2.06 | 118.11 | 109.91 | 4 | 1 |
| 3 | B | 372 | PX4 | C20-C19-C18 | 2.06 | 124.80 | 114.37 | 6 | 1 |
| 3 | C | 359 | PX4 | C1-C2-N1 | 2.06 | 122.45 | 115.82 | 15 | 1 |
| 3 | A | 613 | PX4 | C5-N1-C4 | 2.06 | 114.39 | 108.98 | 9 | 1 |
| 3 | A | 616 | PX4 | C3-N1-C2 | 2.06 | 118.10 | 109.91 | 3 | 1 |
| 3 | B | 324 | PX4 | O1-P1-O2 | 2.06 | 122.04 | 112.44 | 8 | 1 |
| 3 | B | 375 | PX4 | O5-C8-C7 | 2.06 | 114.34 | 108.40 | 14 | 1 |
| 3 | B | 376 | PX4 | C30-C29-C28 | 2.06 | 103.95 | 114.37 | 5 | 2 |
| 3 | C | 341 | PX4 | C4-N1-C3 | 2.06 | 114.39 | 108.98 | 5 | 1 |
| 3 | A | 605 | PX4 | C3-N1-C2 | 2.06 | 118.10 | 109.91 | 4 | 1 |
| 3 | A | 608 | PX4 | C4-N1-C3 | 2.06 | 103.57 | 108.98 | 15 | 1 |
| 3 | A | 653 | PX4 | P1-O4-C6 | 2.06 | 133.15 | 121.35 | 3 | 1 |
| 3 | B | 371 | PX4 | C12-C11-C10 | 2.06 | 105.56 | 113.13 | 4 | 1 |
| 3 | C | 304 | PX4 | O1-P1-O2 | 2.06 | 122.03 | 112.44 | 7 | 1 |
| 3 | C | 305 | PX4 | C5-N1-C4 | 2.06 | 103.56 | 108.98 | 1 | 2 |
| 3 | C | 354 | PX4 | C1-C2-N1 | 2.06 | 122.44 | 115.82 | 12 | 1 |
| 3 | A | 610 | PX4 | O8-C23-C24 | 2.06 | 131.83 | 123.78 | 5 | 1 |
| 3 | B | 379 | PX4 | O6-C9-C10 | 2.06 | 131.83 | 123.78 | 9 | 1 |
| 3 | C | 304 | PX4 | P1-O3-C1 | 2.06 | 111.46 | 121.26 | 8 | 1 |
| 3 | B | 386 | PX4 | C1-C2-N1 | 2.06 | 122.42 | 115.82 | 9 | 1 |
| 3 | C | 359 | PX4 | C4-N1-C3 | 2.06 | 103.57 | 108.98 | 6 | 1 |
| 3 | A | 607 | PX4 | O3-C1-C2 | 2.05 | 119.54 | 109.65 | 1 | 1 |
| 3 | A | 607 | PX4 | C33-C32-C31 | 2.05 | 103.98 | 114.37 | 1 | 1 |
| 3 | A | 629 | PX4 | C18-C17-C16 | 2.06 | 103.98 | 114.37 | 8 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | A | 627 | PX4 | C5-N1-C4 | 2.05 | 103.58 | 108.98 | 9 | 1 |
| 3 | A | 630 | PX4 | O1-P1-O2 | 2.05 | 122.00 | 112.44 | 12 | 1 |
| 3 | B | 318 | PX4 | C16-C15-C14 | 2.05 | 124.75 | 114.37 | 10 | 1 |
| 3 | B | 320 | PX4 | O7-C7-C8 | 2.05 | 115.71 | 108.34 | 3 | 1 |
| 3 | B | 323 | PX4 | P1-O3-C1 | 2.05 | 131.04 | 121.26 | 6 | 1 |
| 3 | B | 325 | PX4 | C5-N1-C2 | 2.05 | 118.07 | 109.91 | 8 | 1 |
| 3 | B | 332 | PX4 | O5-C9-C10 | 2.05 | 105.57 | 111.83 | 11 | 1 |
| 3 | B | 372 | PX4 | C25-C24-C23 | 2.05 | 106.17 | 113.69 | 2 | 2 |
| 3 | B | 376 | PX4 | C34-C33-C32 | 2.05 | 103.99 | 114.37 | 4 | 1 |
| 3 | B | 398 | PX4 | O7-C7-C8 | 2.05 | 115.71 | 108.34 | 14 | 2 |
| 3 | C | 302 | PX4 | O7-C7-C6 | 2.05 | 100.98 | 108.34 | 8 | 2 |
| 3 | A | 604 | PX4 | C5-N1-C4 | 2.05 | 114.37 | 108.98 | 14 | 2 |
| 3 | A | 637 | PX4 | C5-N1-C4 | 2.05 | 103.59 | 108.98 | 14 | 2 |
| 3 | A | 639 | PX4 | C11-C10-C9 | 2.05 | 106.17 | 113.69 | 8 | 1 |
| 3 | B | 305 | PX4 | C25-C24-C23 | 2.05 | 106.17 | 113.69 | 2 | 1 |
| 3 | B | 376 | PX4 | C5-N1-C3 | 2.05 | 103.58 | 108.98 | 11 | 1 |
| 3 | B | 378 | PX4 | C13-C12-C11 | 2.05 | 103.99 | 114.37 | 9 | 1 |
| 3 | C | 319 | PX4 | O7-C7-C8 | 2.05 | 115.71 | 108.34 | 6 | 1 |
| 3 | C | 320 | PX4 | C11-C10-C9 | 2.05 | 106.18 | 113.69 | 9 | 1 |
| 3 | B | 306 | PX4 | O1-P1-O2 | 2.05 | 121.98 | 112.44 | 4 | 1 |
| 3 | B | 375 | PX4 | P1-O3-C1 | 2.05 | 131.02 | 121.26 | 6 | 1 |
| 3 | B | 386 | PX4 | C15-C14-C13 | 2.05 | 124.73 | 114.37 | 15 | 1 |
| 3 | C | 310 | PX4 | O1-P1-O2 | 2.05 | 121.98 | 112.44 | 3 | 1 |
| 3 | C | 327 | PX4 | C1-C2-N1 | 2.05 | 122.40 | 115.82 | 5 | 1 |
| 3 | A | 615 | PX4 | C8-O5-C9 | 2.05 | 109.63 | 117.12 | 11 | 1 |
| 3 | A | 618 | PX4 | C1-C2-N1 | 2.05 | 122.39 | 115.82 | 7 | 1 |
| 3 | A | 636 | PX4 | O5-C9-O6 | 2.05 | 128.75 | 123.63 | 4 | 1 |
| 3 | C | 301 | PX4 | C30-C29-C28 | 2.05 | 104.01 | 114.37 | 4 | 1 |
| 3 | C | 305 | PX4 | C16-C15-C14 | 2.05 | 104.01 | 114.37 | 6 | 1 |
| 3 | C | 344 | PX4 | C25-C24-C23 | 2.05 | 106.19 | 113.69 | 11 | 1 |
| 3 | C | 352 | PX4 | O4-P1-O2 | 2.05 | 117.06 | 108.94 | 10 | 1 |
| 3 | A | 624 | PX4 | C20-C19-C18 | 2.05 | 104.02 | 114.37 | 11 | 1 |
| 3 | A | 638 | PX4 | O7-C23-O8 | 2.05 | 118.92 | 123.70 | 4 | 1 |
| 3 | B | 303 | PX4 | C31-C30-C29 | 2.05 | 104.02 | 114.37 | 11 | 1 |
| 3 | B | 310 | PX4 | C4-N1-C3 | 2.05 | 103.60 | 108.98 | 5 | 1 |
| 3 | B | 349 | PX4 | C3-N1-C2 | 2.05 | 118.05 | 109.91 | 5 | 1 |
| 3 | B | 362 | PX4 | C14-C13-C12 | 2.05 | 104.03 | 114.37 | 7 | 1 |
| 3 | B | 376 | PX4 | O1-P1-O2 | 2.05 | 121.97 | 112.44 | 6 | 1 |
| 3 | B | 386 | PX4 | C4-N1-C2 | 2.05 | 118.05 | 109.91 | 4 | 1 |
| 3 | C | 325 | PX4 | O1-P1-O2 | 2.05 | 121.97 | 112.44 | 11 | 1 |
| 3 | C | 351 | PX4 | C5-N1-C4 | 2.05 | 114.35 | 108.98 | 11 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | A | 604 | PX4 | C5-N1-C3 | 2.05 | 103.60 | 108.98 | 7 | 1 |
| 3 | A | 613 | PX4 | C29-C28-C27 | 2.05 | 104.03 | 114.37 | 7 | 1 |
| 3 | A | 615 | PX4 | O7-C7-C6 | 2.05 | 115.68 | 108.34 | 14 | 1 |
| 3 | C | 352 | PX4 | C4-N1-C2 | 2.05 | 118.04 | 109.91 | 11 | 1 |
| 3 | C | 359 | PX4 | O7-C7-C8 | 2.05 | 115.69 | 108.34 | 4 | 1 |
| 3 | B | 322 | PX4 | O5-C9-O6 | 2.05 | 128.75 | 123.63 | 1 | 1 |
| 3 | A | 642 | PX4 | P1-O4-C6 | 2.04 | 133.06 | 121.35 | 6 | 1 |
| 3 | A | 649 | PX4 | C8-O5-C9 | 2.04 | 109.64 | 117.12 | 13 | 1 |
| 3 | B | 317 | PX4 | C12-C11-C10 | 2.04 | 120.64 | 113.13 | 8 | 1 |
| 3 | B | 335 | PX4 | C19-C18-C17 | 2.05 | 104.03 | 114.37 | 8 | 1 |
| 3 | B | 369 | PX4 | O6-C9-C10 | 2.05 | 131.78 | 123.78 | 15 | 1 |
| 3 | C | 359 | PX4 | O3-P1-O2 | 2.05 | 117.04 | 108.94 | 8 | 1 |
| 3 | C | 363 | PX4 | P1-O3-C1 | 2.05 | 131.00 | 121.26 | 8 | 1 |
| 3 | C | 337 | PX4 | C3-N1-C2 | 2.05 | 101.78 | 109.91 | 6 | 2 |
| 3 | B | 327 | PX4 | C31-C30-C29 | 2.04 | 104.04 | 114.37 | 12 | 1 |
| 3 | B | 379 | PX4 | C20-C19-C18 | 2.04 | 124.70 | 114.37 | 13 | 1 |
| 3 | C | 330 | PX4 | C1-C2-N1 | 2.04 | 122.38 | 115.82 | 3 | 1 |
| 3 | C | 363 | PX4 | O1-P1-O4 | 2.04 | 116.83 | 107.57 | 9 | 1 |
| 3 | A | 609 | PX4 | C3-N1-C2 | 2.04 | 101.79 | 109.91 | 3 | 1 |
| 3 | B | 387 | PX4 | O5-C8-C7 | 2.04 | 114.28 | 108.40 | 9 | 2 |
| 3 | B | 395 | PX4 | C25-C24-C23 | 2.04 | 106.21 | 113.69 | 1 | 1 |
| 3 | C | 314 | PX4 | O8-C23-C24 | 2.04 | 131.77 | 123.78 | 13 | 1 |
| 3 | A | 629 | PX4 | C5-N1-C3 | 2.04 | 103.61 | 108.98 | 13 | 1 |
| 3 | B | 369 | PX4 | O5-C9-C10 | 2.04 | 105.61 | 111.83 | 1 | 2 |
| 3 | B | 374 | PX4 | C4-N1-C3 | 2.04 | 103.62 | 108.98 | 8 | 1 |
| 3 | B | 394 | PX4 | C8-O5-C9 | 2.04 | 109.66 | 117.12 | 6 | 1 |
| 3 | C | 312 | PX4 | C16-C15-C14 | 2.04 | 104.05 | 114.37 | 9 | 2 |
| 3 | C | 315 | PX4 | C4-N1-C3 | 2.04 | 114.34 | 108.98 | 1 | 1 |
| 3 | A | 626 | PX4 | C11-C10-C9 | 2.04 | 106.22 | 113.69 | 3 | 1 |
| 3 | A | 632 | PX4 | C17-C16-C15 | 2.04 | 104.06 | 114.37 | 12 | 1 |
| 3 | A | 639 | PX4 | C25-C24-C23 | 2.04 | 106.22 | 113.69 | 1 | 1 |
| 3 | C | 336 | PX4 | C5-N1-C4 | 2.04 | 103.62 | 108.98 | 12 | 1 |
| 3 | C | 351 | PX4 | C19-C18-C17 | 2.04 | 104.05 | 114.37 | 9 | 1 |
| 3 | C | 364 | PX4 | C18-C17-C16 | 2.04 | 104.05 | 114.37 | 7 | 1 |
| 3 | A | 607 | PX4 | O7-C23-O8 | 2.04 | 128.47 | 123.70 | 6 | 1 |
| 3 | A | 622 | PX4 | C1-C2-N1 | 2.04 | 122.36 | 115.82 | 14 | 1 |
| 3 | B | 313 | PX4 | O5-C9-C10 | 2.04 | 105.62 | 111.83 | 7 | 2 |
| 3 | B | 364 | PX4 | O4-P1-O2 | 2.04 | 100.85 | 108.94 | 7 | 1 |
| 3 | C | 310 | PX4 | C25-C24-C23 | 2.04 | 106.22 | 113.69 | 1 | 1 |
| 3 | B | 366 | PX4 | C8-O5-C9 | 2.04 | 109.67 | 117.12 | 6 | 1 |
| 3 | C | 327 | PX4 | C4-N1-C3 | 2.04 | 114.33 | 108.98 | 10 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | C | 338 | PX4 | O1-P1-O4 | 2.04 | 116.81 | 107.57 | 14 | 1 |
| 3 | A | 630 | PX4 | C5-N1-C3 | 2.04 | 103.63 | 108.98 | 11 | 1 |
| 3 | B | 307 | PX4 | O7-C23-O8 | 2.04 | 128.47 | 123.70 | 8 | 1 |
| 3 | B | 316 | PX4 | C25-C24-C23 | 2.04 | 121.15 | 113.69 | 9 | 1 |
| 3 | A | 608 | PX4 | C1-C2-N1 | 2.03 | 122.35 | 115.82 | 4 | 1 |
| 3 | A | 610 | PX4 | C5-N1-C2 | 2.03 | 101.82 | 109.91 | 13 | 1 |
| 3 | A | 622 | PX4 | P1-O3-C1 | 2.03 | 111.57 | 121.26 | 7 | 1 |
| 3 | A | 624 | PX4 | P1-O3-C1 | 2.03 | 130.94 | 121.26 | 15 | 1 |
| 3 | A | 653 | PX4 | C12-C11-C10 | 2.03 | 105.65 | 113.13 | 1 | 1 |
| 3 | B | 307 | PX4 | C16-C15-C14 | 2.03 | 104.08 | 114.37 | 6 | 1 |
| 3 | B | 331 | PX4 | O7-C7-C8 | 2.04 | 115.64 | 108.34 | 3 | 1 |
| 3 | B | 336 | PX4 | O7-C7-C6 | 2.04 | 115.65 | 108.34 | 2 | 1 |
| 3 | B | 338 | PX4 | C5-N1-C3 | 2.04 | 103.63 | 108.98 | 7 | 1 |
| 3 | B | 355 | PX4 | C11-C10-C9 | 2.04 | 121.15 | 113.69 | 9 | 1 |
| 3 | C | 323 | PX4 | C12-C11-C10 | 2.04 | 105.64 | 113.13 | 8 | 2 |
| 3 | C | 342 | PX4 | O8-C23-C24 | 2.04 | 131.74 | 123.78 | 3 | 1 |
| 3 | C | 348 | PX4 | O1-P1-O2 | 2.04 | 121.92 | 112.44 | 4 | 1 |
| 3 | C | 356 | PX4 | O5-C8-C7 | 2.04 | 114.27 | 108.40 | 7 | 1 |
| 3 | B | 332 | PX4 | P1-O3-C1 | 2.03 | 130.94 | 121.26 | 5 | 1 |
| 3 | B | 336 | PX4 | P1-O4-C6 | 2.03 | 133.00 | 121.35 | 8 | 1 |
| 3 | B | 380 | PX4 | C11-C10-C9 | 2.03 | 106.24 | 113.69 | 2 | 1 |
| 3 | C | 330 | PX4 | C14-C13-C12 | 2.03 | 104.09 | 114.37 | 7 | 1 |
| 3 | C | 333 | PX4 | O5-C8-C7 | 2.03 | 114.26 | 108.40 | 1 | 1 |
| 3 | C | 345 | PX4 | O1-P1-O2 | 2.03 | 121.91 | 112.44 | 7 | 1 |
| 3 | C | 356 | PX4 | C27-C26-C25 | 2.03 | 104.08 | 114.37 | 14 | 1 |
| 3 | B | 312 | PX4 | C33-C32-C31 | 2.03 | 104.09 | 114.37 | 12 | 1 |
| 3 | B | 323 | PX4 | O3-C1-C2 | 2.03 | 119.43 | 109.65 | 9 | 1 |
| 3 | B | 377 | PX4 | O7-C23-C24 | 2.03 | 107.08 | 111.48 | 14 | 2 |
| 3 | C | 364 | PX4 | O7-C7-C8 | 2.03 | 101.05 | 108.34 | 7 | 1 |
| 3 | B | 319 | PX4 | C28-C27-C26 | 2.03 | 104.10 | 114.37 | 1 | 1 |
| 3 | C | 311 | PX4 | C14-C13-C12 | 2.03 | 104.10 | 114.37 | 12 | 1 |
| 3 | C | 333 | PX4 | C3-N1-C2 | 2.03 | 117.98 | 109.91 | 14 | 1 |
| 3 | C | 336 | PX4 | C1-C2-N1 | 2.03 | 122.33 | 115.82 | 10 | 1 |
| 3 | C | 338 | PX4 | C3-N1-C2 | 2.03 | 117.98 | 109.91 | 12 | 1 |
| 3 | C | 339 | PX4 | O7-C7-C8 | 2.03 | 115.63 | 108.34 | 3 | 1 |
| 3 | A | 635 | PX4 | O1-P1-O4 | 2.03 | 116.76 | 107.57 | 7 | 1 |
| 3 | A | 648 | PX4 | C3-N1-C2 | 2.03 | 101.84 | 109.91 | 11 | 1 |
| 3 | A | 606 | PX4 | O1-P1-O2 | 2.03 | 121.88 | 112.44 | 5 | 1 |
| 3 | A | 645 | PX4 | C25-C24-C23 | 2.03 | 121.12 | 113.69 | 7 | 1 |
| 3 | B | 328 | PX4 | O1-P1-O4 | 2.03 | 116.76 | 107.57 | 15 | 1 |
| 3 | B | 371 | PX4 | C11-C10-C9 | 2.03 | 106.26 | 113.69 | 12 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 373 | PX4 | C5-N1-C2 | 2.03 | 117.97 | 109.91 | 8 | 1 |
| 3 | C | 339 | PX4 | C4-N1-C2 | 2.03 | 117.98 | 109.91 | 15 | 1 |
| 3 | C | 302 | PX4 | C13-C12-C11 | 2.03 | 104.11 | 114.37 | 12 | 1 |
| 3 | B | 377 | PX4 | C8-O5-C9 | 2.03 | 109.71 | 117.12 | 2 | 1 |
| 3 | B | 379 | PX4 | O8-C23-C24 | 2.03 | 131.71 | 123.78 | 1 | 1 |
| 3 | C | 304 | PX4 | O8-C23-C24 | 2.03 | 131.71 | 123.78 | 12 | 1 |
| 3 | C | 311 | PX4 | C4-N1-C3 | 2.03 | 103.65 | 108.98 | 4 | 1 |
| 3 | C | 327 | PX4 | C5-N1-C2 | 2.03 | 101.85 | 109.91 | 11 | 1 |
| 3 | C | 351 | PX4 | C27-C26-C25 | 2.03 | 104.12 | 114.37 | 6 | 1 |
| 3 | C | 360 | PX4 | C26-C25-C24 | 2.03 | 105.67 | 113.13 | 12 | 1 |
| 3 | A | 615 | PX4 | C4-N1-C3 | 2.03 | 103.65 | 108.98 | 11 | 1 |
| 3 | B | 379 | PX4 | O1-P1-O2 | 2.02 | 121.86 | 112.44 | 5 | 1 |
| 3 | B | 390 | PX4 | O7-C23-O8 | 2.03 | 128.44 | 123.70 | 6 | 2 |
| 3 | C | 314 | PX4 | O5-C9-O6 | 2.03 | 128.70 | 123.63 | 4 | 1 |
| 3 | C | 362 | PX4 | C20-C19-C18 | 2.03 | 104.12 | 114.37 | 3 | 1 |
| 3 | B | 306 | PX4 | O1-P1-O3 | 2.03 | 116.75 | 107.57 | 11 | 1 |
| 3 | A | 617 | PX4 | C13-C12-C11 | 2.02 | 104.14 | 114.37 | 11 | 1 |
| 3 | A | 644 | PX4 | O1-P1-O2 | 2.02 | 121.86 | 112.44 | 12 | 1 |
| 3 | A | 623 | PX4 | C20-C19-C18 | 2.02 | 104.14 | 114.37 | 14 | 1 |
| 3 | C | 316 | PX4 | O7-C7-C8 | 2.02 | 115.61 | 108.34 | 5 | 1 |
| 3 | B | 384 | PX4 | C26-C25-C24 | 2.02 | 105.69 | 113.13 | 3 | 1 |
| 3 | C | 322 | PX4 | C31-C30-C29 | 2.02 | 104.14 | 114.37 | 10 | 1 |
| 3 | A | 641 | PX4 | C5-N1-C3 | 2.02 | 114.29 | 108.98 | 5 | 1 |
| 3 | A | 632 | PX4 | C13-C12-C11 | 2.02 | 104.15 | 114.37 | 12 | 1 |
| 3 | B | 306 | PX4 | P1-O3-C1 | 2.02 | 130.88 | 121.26 | 14 | 1 |
| 3 | B | 321 | PX4 | C28-C27-C26 | 2.02 | 104.15 | 114.37 | 9 | 1 |
| 3 | B | 358 | PX4 | O7-C7-C8 | 2.02 | 101.09 | 108.34 | 9 | 1 |
| 3 | C | 305 | PX4 | O3-P1-O2 | 2.02 | 116.95 | 108.94 | 5 | 1 |
| 3 | C | 347 | PX4 | O3-C1-C2 | 2.02 | 119.38 | 109.65 | 9 | 1 |
| 3 | C | 362 | PX4 | C32-C31-C30 | 2.02 | 104.14 | 114.37 | 10 | 1 |
| 3 | B | 378 | PX4 | O7-C7-C6 | 2.02 | 101.09 | 108.34 | 3 | 1 |
| 3 | C | 364 | PX4 | C26-C25-C24 | 2.02 | 105.70 | 113.13 | 5 | 1 |
| 3 | A | 639 | PX4 | O3-C1-C2 | 2.02 | 119.37 | 109.65 | 6 | 1 |
| 3 | A | 618 | PX4 | O7-C7-C6 | 2.02 | 115.59 | 108.34 | 14 | 1 |
| 3 | B | 312 | PX4 | O1-P1-O2 | 2.02 | 121.84 | 112.44 | 2 | 1 |
| 3 | B | 358 | PX4 | O7-C7-C6 | 2.02 | 115.59 | 108.34 | 9 | 1 |
| 3 | B | 397 | PX4 | C11-C10-C9 | 2.02 | 121.09 | 113.69 | 12 | 1 |
| 3 | C | 305 | PX4 | O7-C7-C8 | 2.02 | 115.59 | 108.34 | 3 | 1 |
| 3 | C | 312 | PX4 | O7-C7-C8 | 2.02 | 115.59 | 108.34 | 8 | 1 |
| 3 | C | 312 | PX4 | C15-C14-C13 | 2.02 | 104.16 | 114.37 | 13 | 1 |
| 3 | C | 327 | PX4 | C20-C19-C18 | 2.02 | 104.16 | 114.37 | 8 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | C | 332 | PX4 | C33-C32-C31 | 2.02 | 104.16 | 114.37 | 9 | 1 |
| 3 | B | 306 | PX4 | O3-C1-C2 | 2.02 | 119.36 | 109.65 | 6 | 1 |
| 3 | B | 316 | PX4 | O1-P1-O2 | 2.02 | 121.83 | 112.44 | 14 | 1 |
| 3 | A | 603 | PX4 | C5-N1-C2 | 2.02 | 117.92 | 109.91 | 2 | 1 |
| 3 | A | 615 | PX4 | O1-P1-O2 | 2.02 | 121.82 | 112.44 | 12 | 1 |
| 3 | B | 308 | PX4 | C8-C7-C6 | 2.02 | 107.08 | 111.78 | 11 | 1 |
| 3 | B | 363 | PX4 | O8-C23-C24 | 2.02 | 131.67 | 123.78 | 7 | 1 |
| 3 | C | 305 | PX4 | O1-P1-O4 | 2.02 | 116.70 | 107.57 | 1 | 1 |
| 3 | C | 322 | PX4 | P1-O3-C1 | 2.02 | 111.67 | 121.26 | 3 | 1 |
| 3 | C | 337 | PX4 | C4-N1-C3 | 2.02 | 114.27 | 108.98 | 5 | 1 |
| 3 | C | 339 | PX4 | C26-C25-C24 | 2.02 | 105.72 | 113.13 | 12 | 1 |
| 3 | C | 361 | PX4 | C4-N1-C3 | 2.02 | 103.68 | 108.98 | 7 | 1 |
| 3 | A | 613 | PX4 | C25-C24-C23 | 2.01 | 121.07 | 113.69 | 8 | 1 |
| 3 | A | 622 | PX4 | C8-O5-C9 | 2.01 | 124.48 | 117.12 | 14 | 1 |
| 3 | A | 632 | PX4 | C19-C18-C17 | 2.01 | 104.19 | 114.37 | 6 | 1 |
| 3 | C | 314 | PX4 | C18-C17-C16 | 2.02 | 104.18 | 114.37 | 2 | 1 |
| 3 | A | 646 | PX4 | C27-C26-C25 | 2.01 | 104.19 | 114.37 | 6 | 1 |
| 3 | A | 652 | PX4 | O8-C23-C24 | 2.01 | 131.66 | 123.78 | 6 | 1 |
| 3 | B | 336 | PX4 | C12-C11-C10 | 2.01 | 105.73 | 113.13 | 2 | 1 |
| 3 | C | 343 | PX4 | O3-C1-C2 | 2.01 | 119.34 | 109.65 | 14 | 1 |
| 3 | B | 384 | PX4 | O1-P1-O4 | 2.01 | 116.69 | 107.57 | 8 | 1 |
| 3 | C | 321 | PX4 | C8-O5-C9 | 2.01 | 109.76 | 117.12 | 4 | 1 |
| 3 | C | 354 | PX4 | O3-C1-C2 | 2.01 | 119.33 | 109.65 | 1 | 1 |
| 3 | A | 620 | PX4 | C33-C32-C31 | 2.01 | 104.20 | 114.37 | 2 | 1 |
| 3 | A | 629 | PX4 | O3-C1-C2 | 2.01 | 99.97 | 109.65 | 3 | 1 |
| 3 | B | 334 | PX4 | C5-N1-C4 | 2.01 | 114.26 | 108.98 | 9 | 1 |
| 3 | B | 360 | PX4 | O7-C7-C8 | 2.01 | 115.56 | 108.34 | 7 | 1 |
| 3 | B | 362 | PX4 | O1-P1-O2 | 2.01 | 121.80 | 112.44 | 7 | 1 |
| 3 | B | 370 | PX4 | C12-C11-C10 | 2.01 | 105.74 | 113.13 | 10 | 1 |
| 3 | B | 385 | PX4 | O7-C7-C8 | 2.01 | 115.56 | 108.34 | 10 | 1 |
| 3 | C | 312 | PX4 | O5-C9-O6 | 2.01 | 128.66 | 123.63 | 5 | 1 |
| 3 | B | 372 | PX4 | C27-C26-C25 | 2.01 | 104.21 | 114.37 | 13 | 1 |
| 3 | C | 341 | PX4 | C19-C18-C17 | 2.01 | 104.20 | 114.37 | 9 | 1 |
| 3 | A | 608 | PX4 | C17-C16-C15 | 2.01 | 124.53 | 114.37 | 10 | 1 |
| 3 | A | 614 | PX4 | C27-C26-C25 | 2.01 | 104.22 | 114.37 | 10 | 1 |
| 3 | B | 305 | PX4 | C5-N1-C3 | 2.01 | 114.25 | 108.98 | 1 | 1 |
| 3 | B | 358 | PX4 | O5-C8-C7 | 2.01 | 114.19 | 108.40 | 15 | 1 |
| 3 | B | 322 | PX4 | C25-C24-C23 | 2.01 | 106.33 | 113.69 | 1 | 1 |
| 3 | B | 370 | PX4 | C25-C24-C23 | 2.01 | 106.33 | 113.69 | 9 | 1 |
| 3 | C | 332 | PX4 | C5-N1-C3 | 2.01 | 114.25 | 108.98 | 11 | 1 |
| 3 | C | 337 | PX4 | O3-P1-O2 | 2.01 | 116.89 | 108.94 | 10 | 1 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | C | 348 | PX4 | O4-P1-O2 | 2.01 | 100.97 | 108.94 | 14 | 1 |
| 3 | A | 610 | PX4 | O6-C9-C10 | 2.01 | 115.93 | 123.78 | 7 | 1 |
| 3 | A | 647 | PX4 | O1-P1-O2 | 2.01 | 121.78 | 112.44 | 12 | 1 |
| 3 | B | 350 | PX4 | O3-P1-O2 | 2.01 | 100.98 | 108.94 | 2 | 1 |
| 3 | B | 381 | PX4 | C14-C13-C12 | 2.01 | 104.22 | 114.37 | 12 | 1 |
| 3 | B | 358 | PX4 | P1-O3-C1 | 2.01 | 130.81 | 121.26 | 12 | 1 |
| 3 | C | 340 | PX4 | C5-N1-C4 | 2.01 | 103.70 | 108.98 | 9 | 1 |
| 3 | B | 350 | PX4 | C25-C24-C23 | 2.01 | 106.35 | 113.69 | 11 | 1 |
| 3 | A | 630 | PX4 | O5-C8-C7 | 2.00 | 114.17 | 108.40 | 12 | 1 |
| 3 | A | 643 | PX4 | C5-N1-C3 | 2.00 | 103.71 | 108.98 | 7 | 1 |
| 3 | A | 651 | PX4 | C11-C10-C9 | 2.01 | 121.04 | 113.69 | 9 | 1 |
| 3 | B | 390 | PX4 | O1-P1-O4 | 2.01 | 116.66 | 107.57 | 11 | 1 |
| 3 | A | 654 | PX4 | C15-C14-C13 | 2.00 | 104.24 | 114.37 | 9 | 1 |
| 3 | B | 301 | PX4 | C8-O5-C9 | 2.00 | 109.79 | 117.12 | 10 | 1 |
| 3 | C | 328 | PX4 | O4-P1-O2 | 2.00 | 100.99 | 108.94 | 8 | 1 |
| 3 | C | 333 | PX4 | C28-C27-C26 | 2.00 | 124.50 | 114.37 | 14 | 1 |
| 3 | B | 367 | PX4 | O1-P1-O2 | 2.00 | 121.77 | 112.44 | 8 | 1 |
| 3 | C | 335 | PX4 | O5-C9-C10 | 2.00 | 105.72 | 111.83 | 7 | 1 |
| 3 | C | 343 | PX4 | C25-C24-C23 | 2.00 | 121.04 | 113.69 | 14 | 1 |
| 3 | C | 355 | PX4 | C4-N1-C3 | 2.00 | 103.71 | 108.98 | 14 | 1 |
| 3 | C | 356 | PX4 | C26-C25-C24 | 2.00 | 105.76 | 113.13 | 15 | 1 |
| 3 | C | 361 | PX4 | C27-C26-C25 | 2.00 | 104.24 | 114.37 | 11 | 1 |
| 3 | A | 618 | PX4 | C26-C25-C24 | 2.00 | 105.77 | 113.13 | 11 | 1 |
| 3 | B | 320 | PX4 | C8-O5-C9 | 2.00 | 109.80 | 117.12 | 11 | 1 |
| 3 | B | 330 | PX4 | O5-C9-C10 | 2.00 | 105.73 | 111.83 | 13 | 1 |
| 3 | B | 342 | PX4 | C1-C2-N1 | 2.00 | 122.25 | 115.82 | 10 | 1 |
| 3 | A | 624 | PX4 | C8-O5-C9 | 2.00 | 109.80 | 117.12 | 5 | 1 |
| 3 | A | 647 | PX4 | O5-C9-O6 | 2.00 | 128.64 | 123.63 | 12 | 1 |
| 3 | B | 369 | PX4 | O1-P1-O3 | 2.00 | 116.64 | 107.57 | 3 | 1 |
| 3 | C | 311 | PX4 | O7-C7-C6 | 2.00 | 101.16 | 108.34 | 15 | 1 |
| 3 | C | 319 | PX4 | O1-P1-O2 | 2.00 | 121.76 | 112.44 | 11 | 1 |
| 3 | B | 301 | PX4 | O6-C9-C10 | 2.00 | 131.61 | 123.78 | 10 | 1 |
| 3 | A | 630 | PX4 | C5-N1-C4 | 2.00 | 103.72 | 108.98 | 15 | 1 |
| 3 | B | 302 | PX4 | C31-C30-C29 | 2.00 | 104.26 | 114.37 | 8 | 1 |
| 3 | B | 361 | PX4 | C30-C29-C28 | 2.00 | 124.48 | 114.37 | 12 | 1 |
| 3 | C | 326 | PX4 | O3-P1-O2 | 2.00 | 116.86 | 108.94 | 13 | 1 |

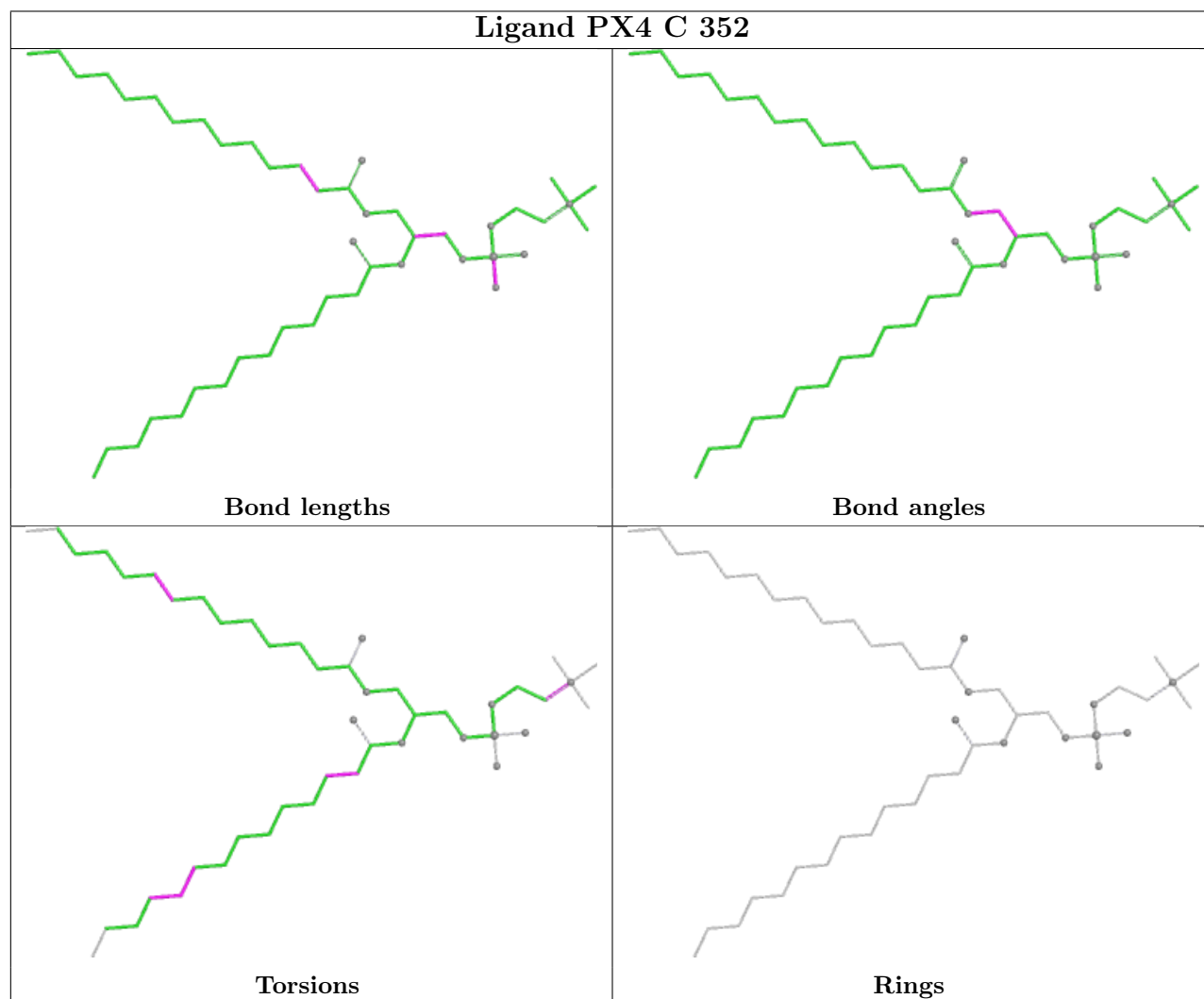
There are no chirality outliers.

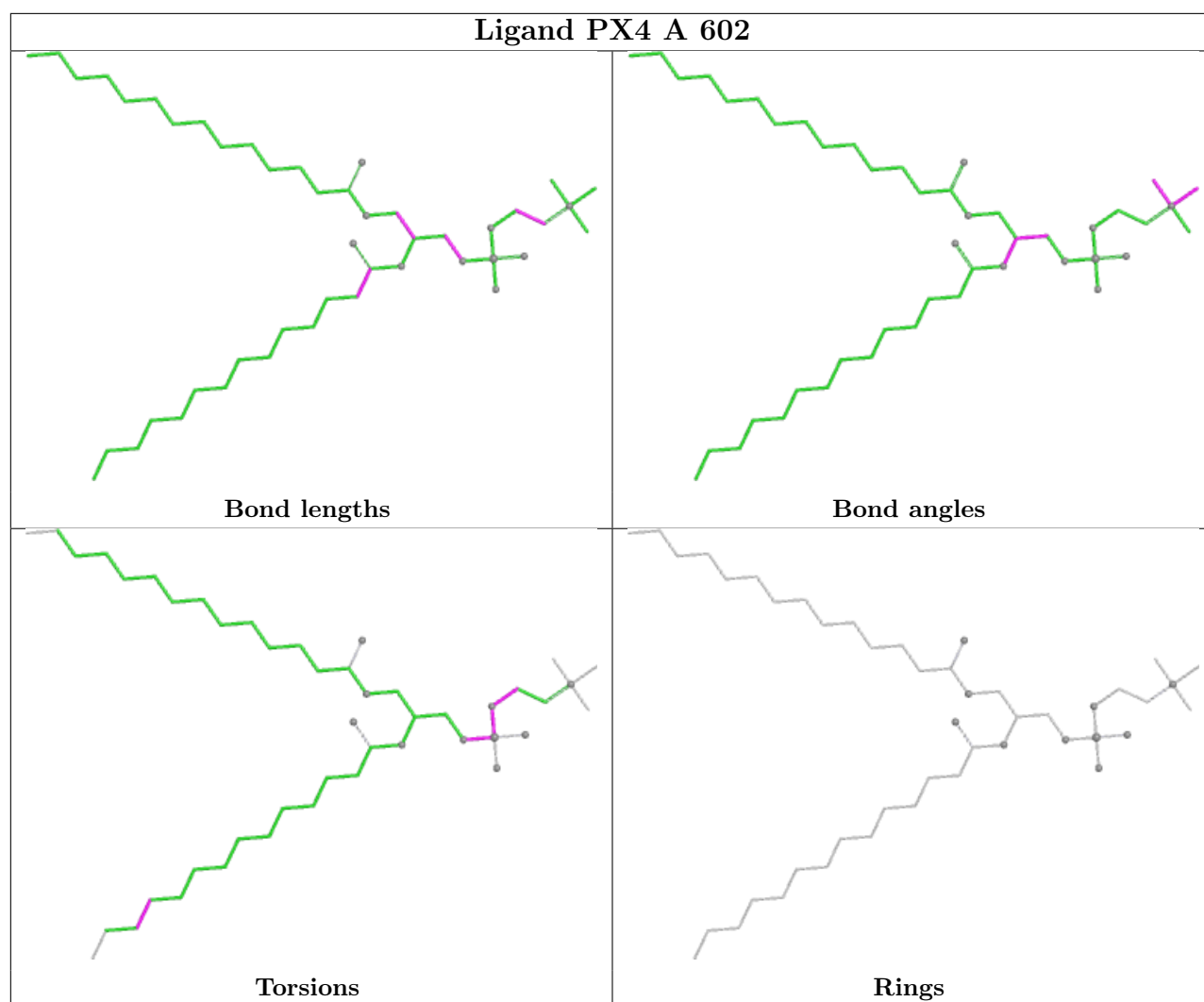
All unique torsion outliers are listed below.

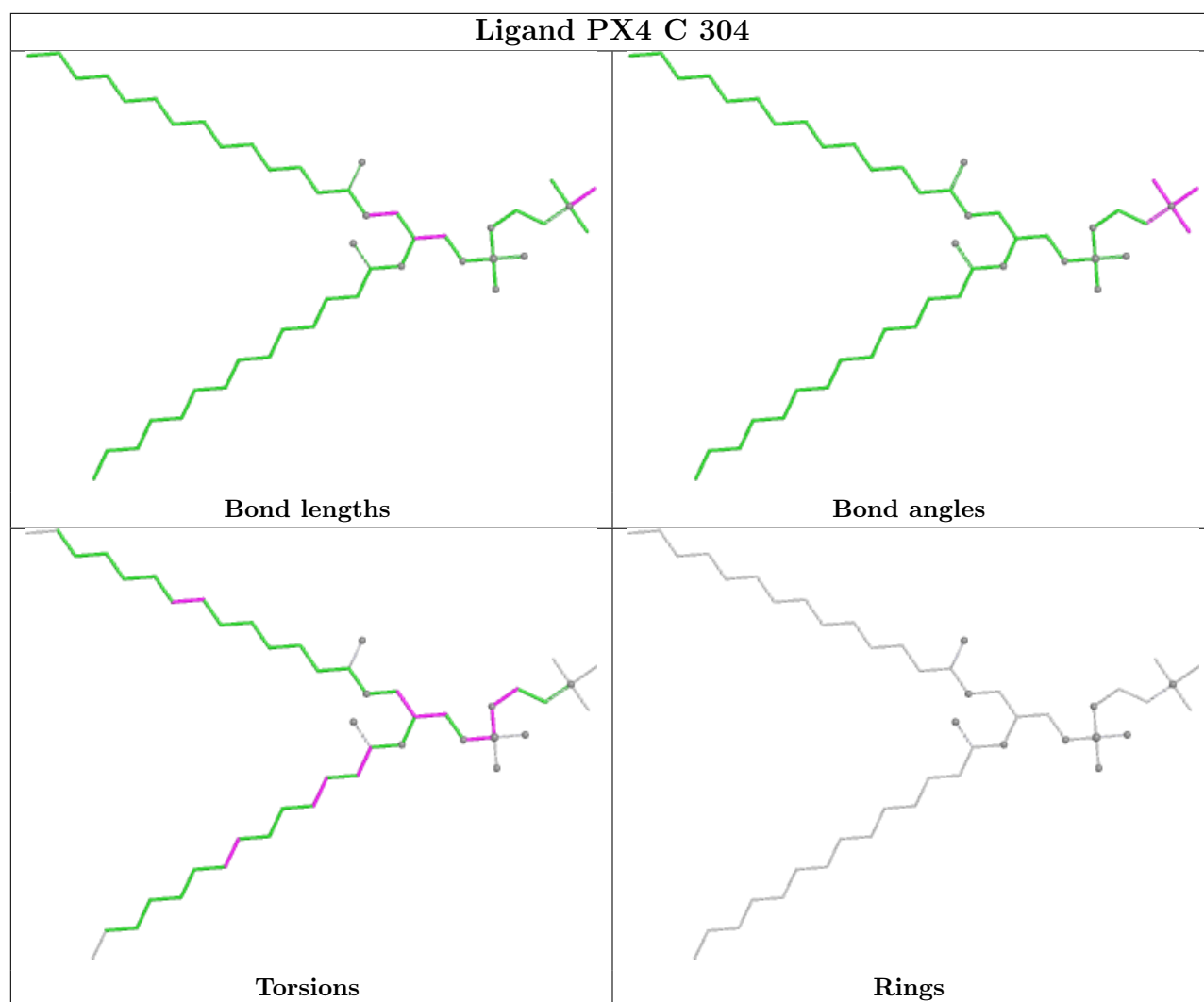
| Mol | Chain | Res | Type | Atoms | Models (Total) |
|-----|-------|-----|------|-------------|----------------|
| 3 | C | 320 | PX4 | C7-C6-O4-P1 | 1 |

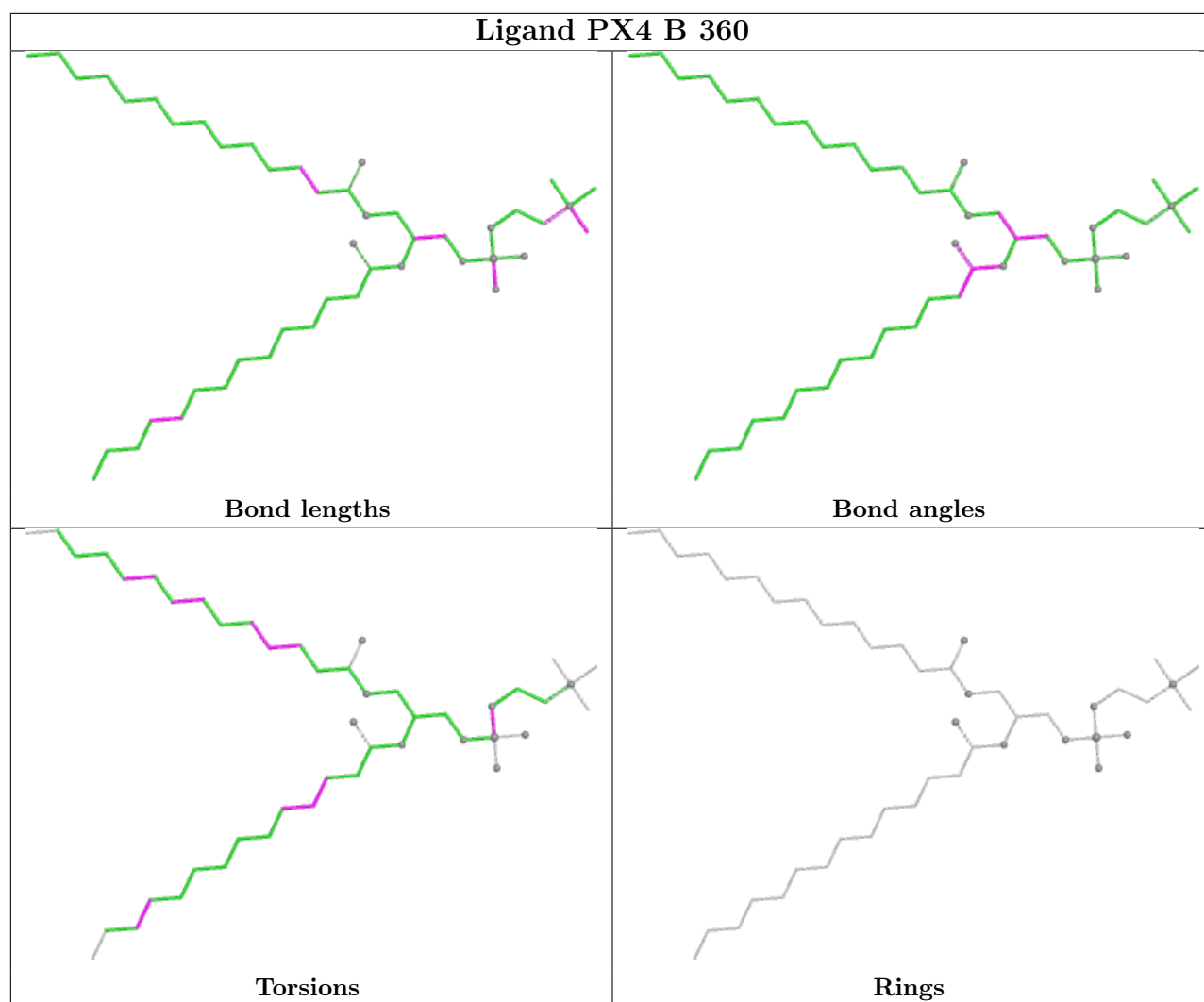
There are no ring outliers.

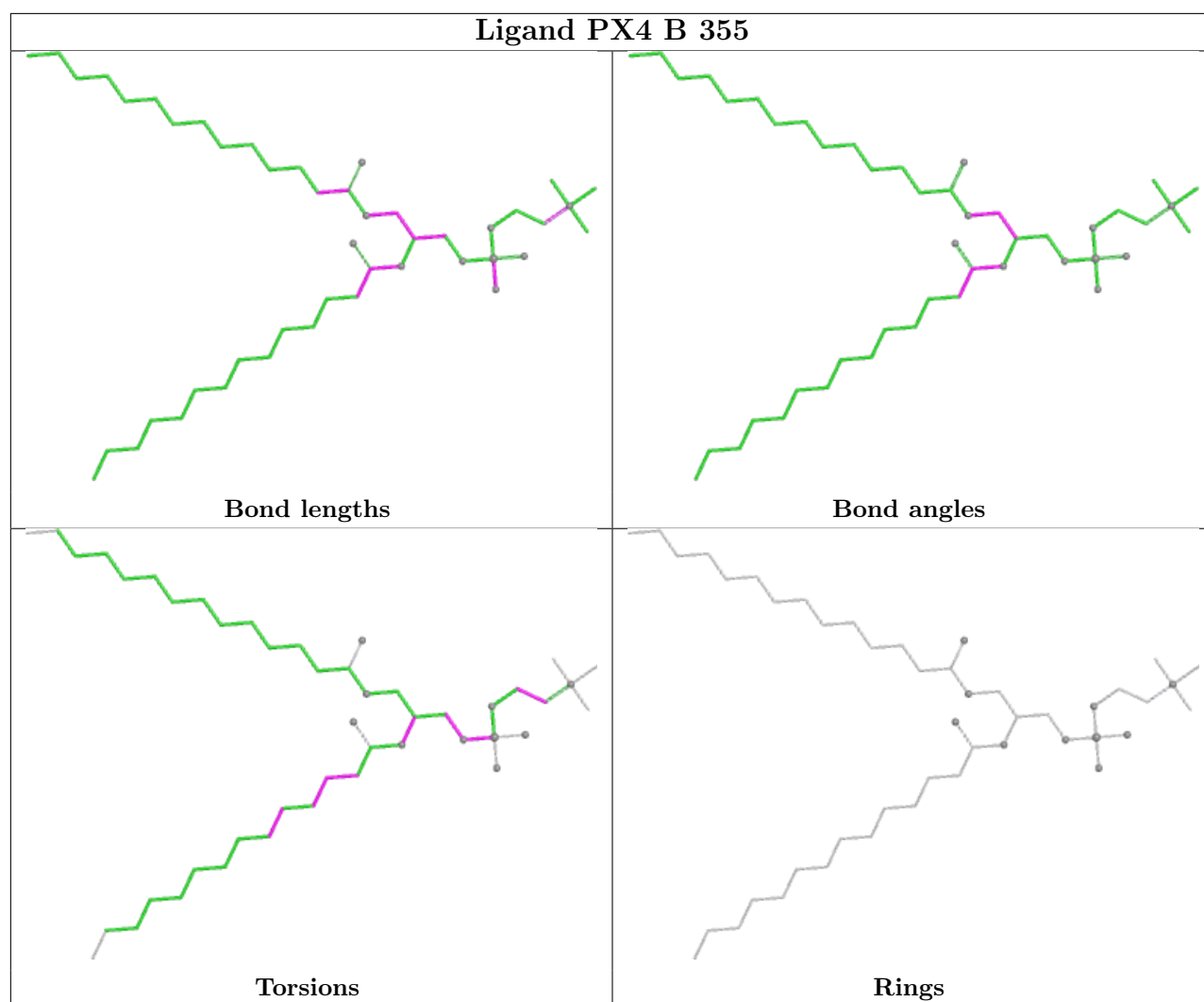
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

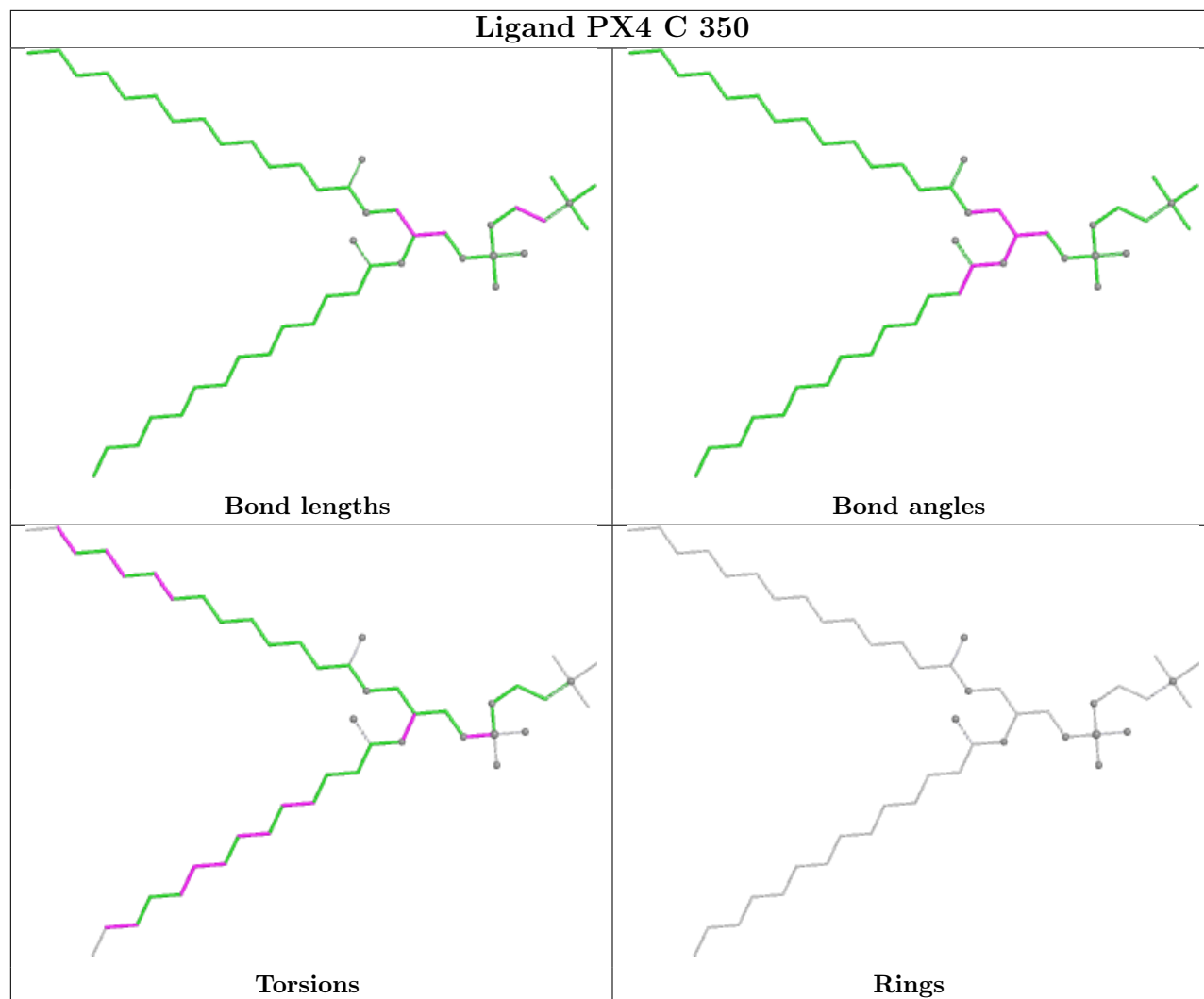


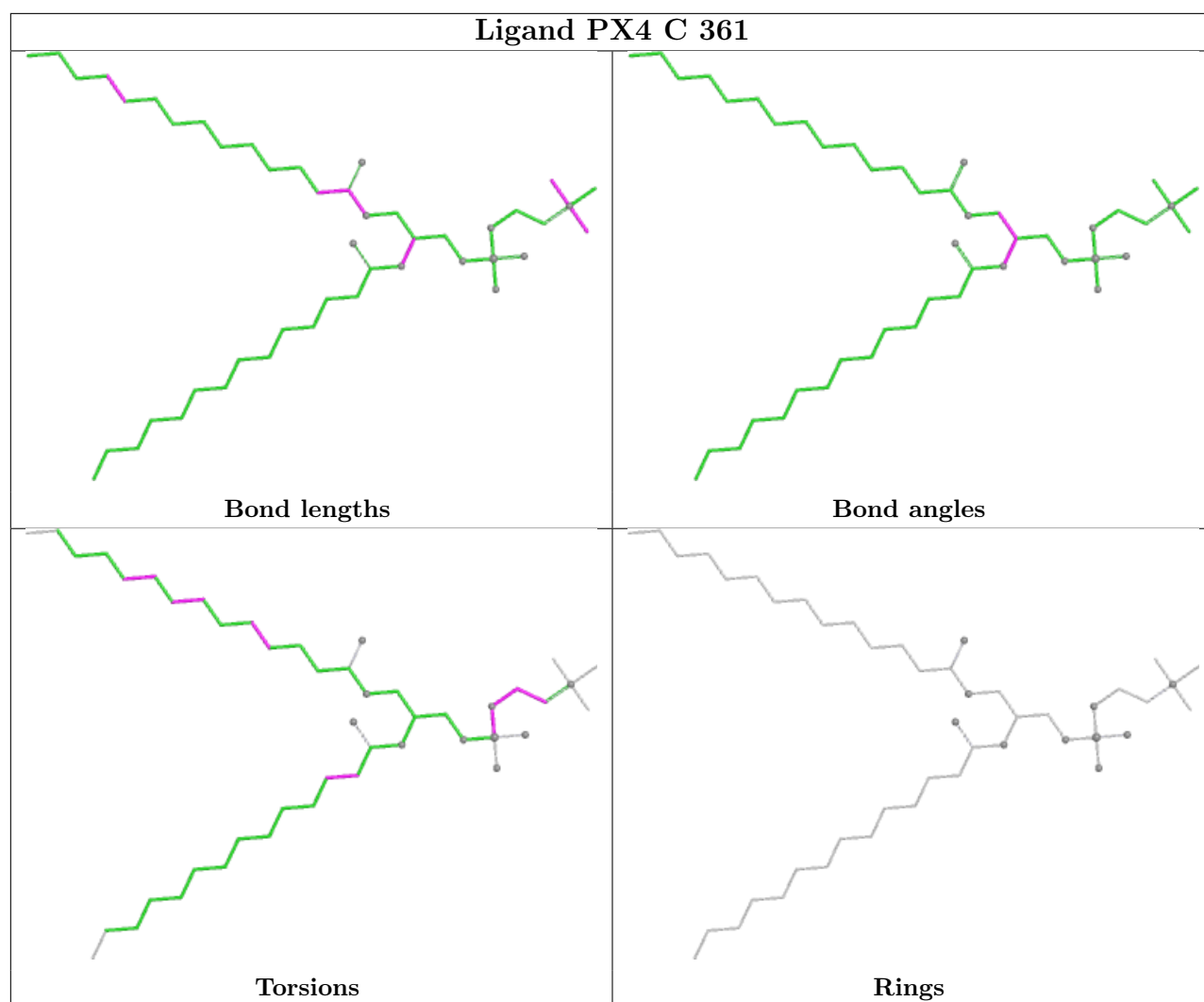


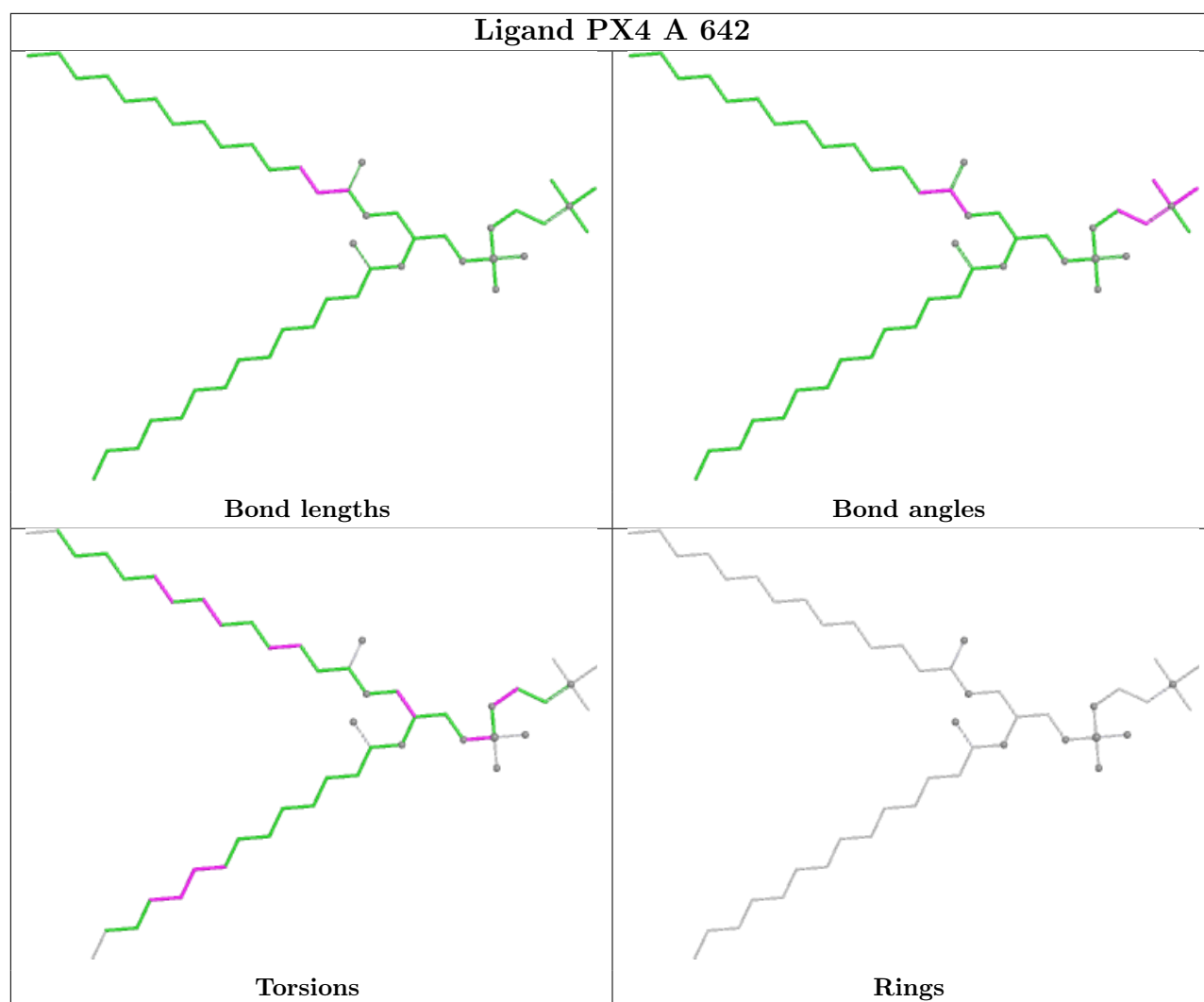


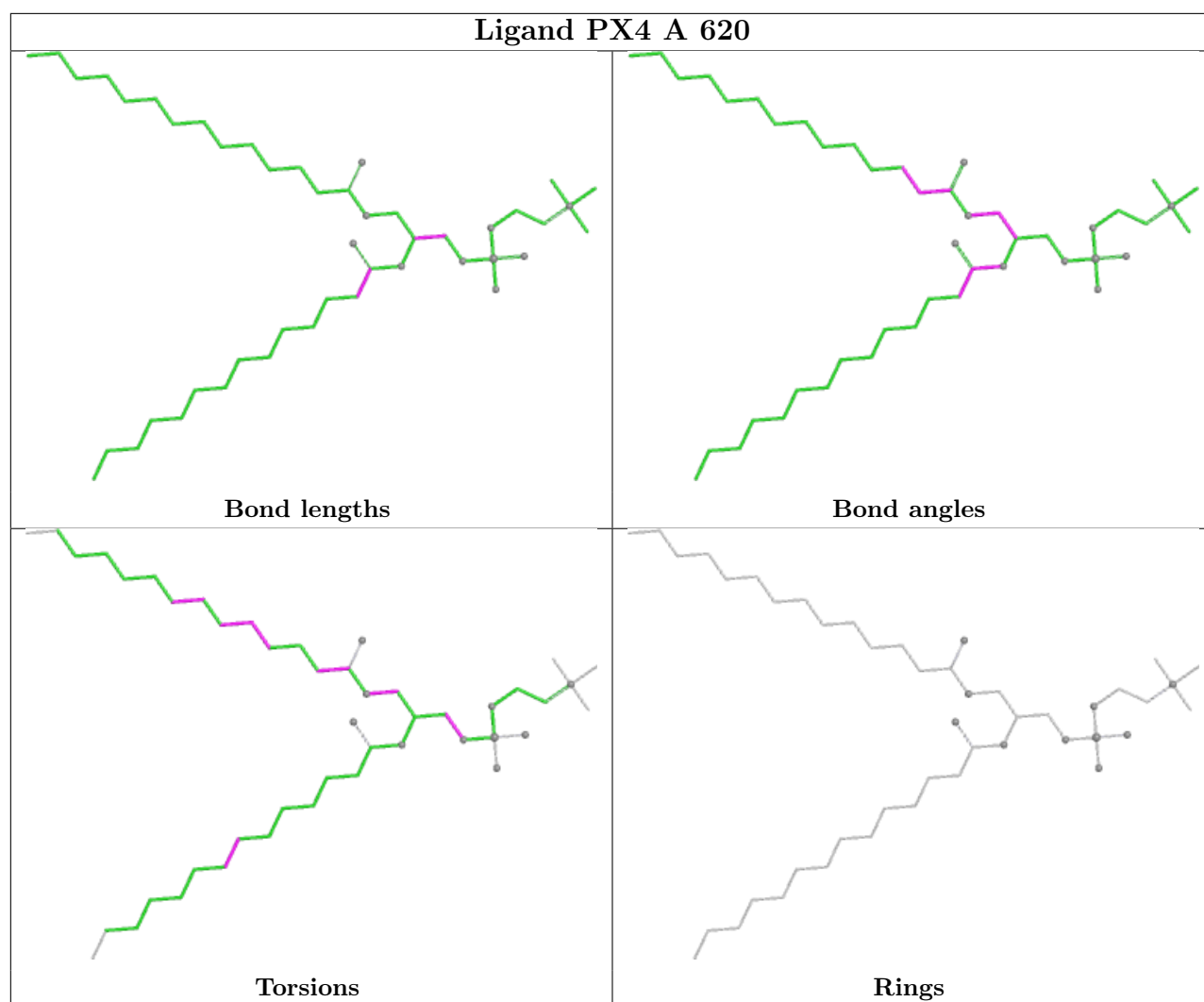


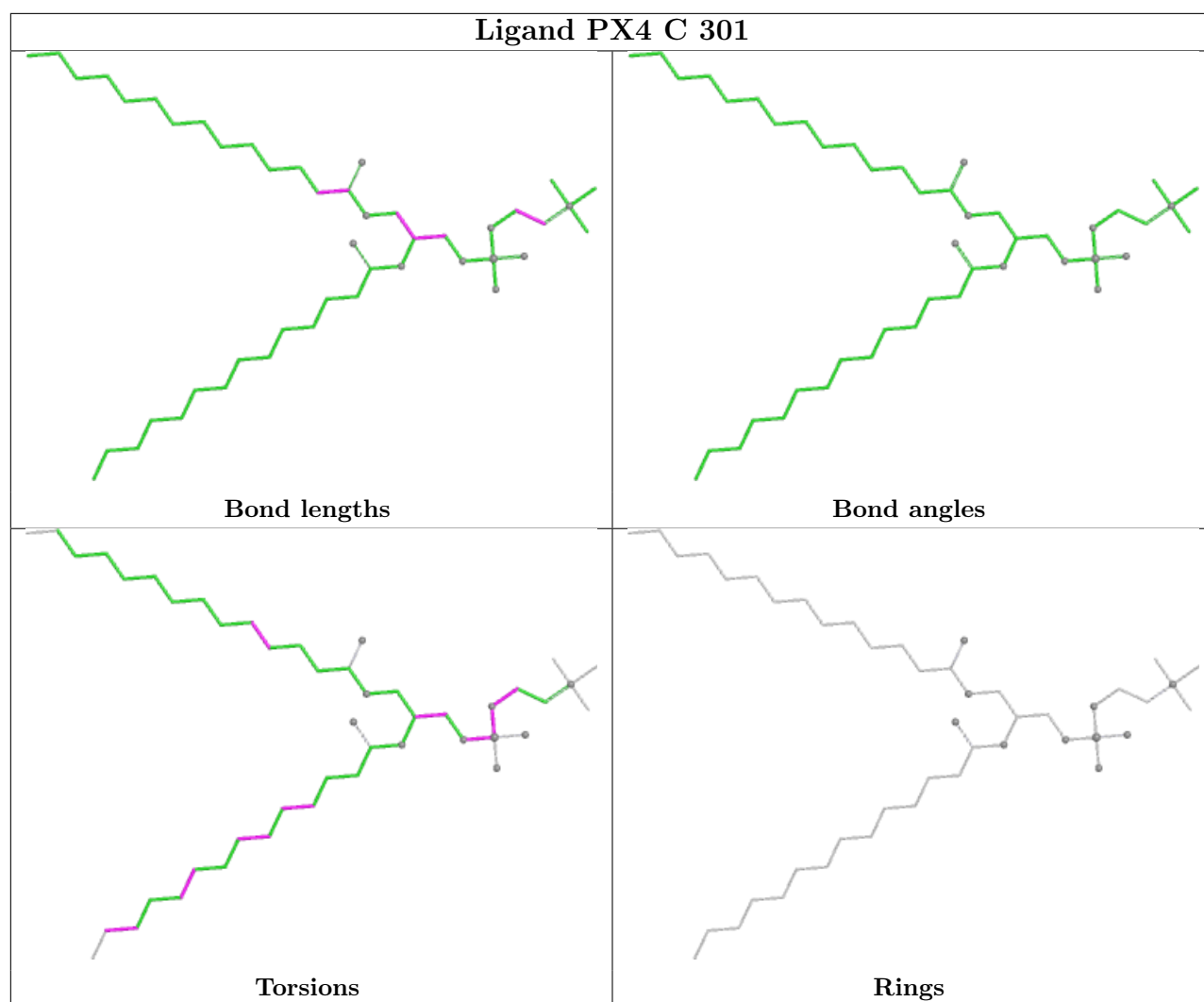


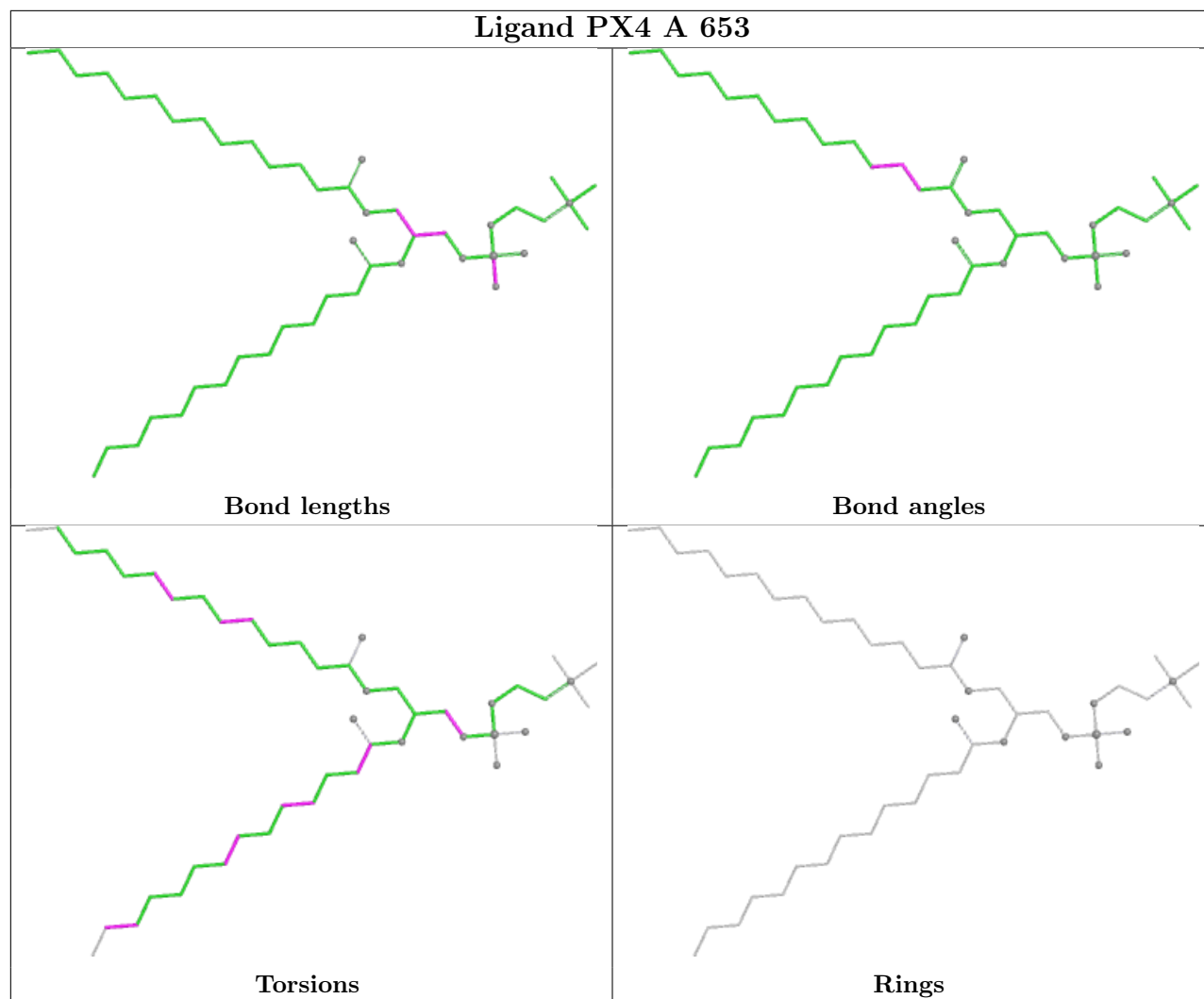


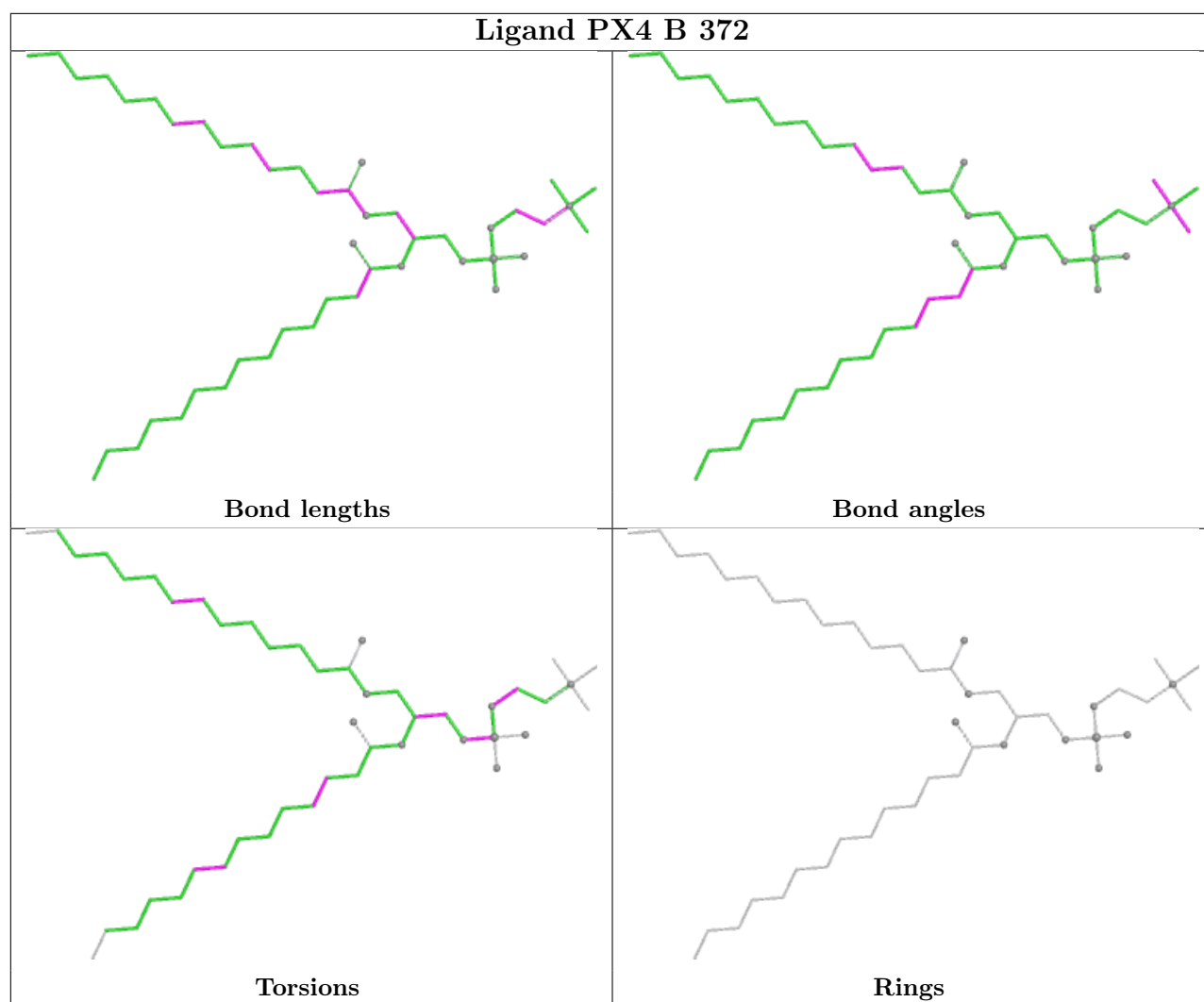


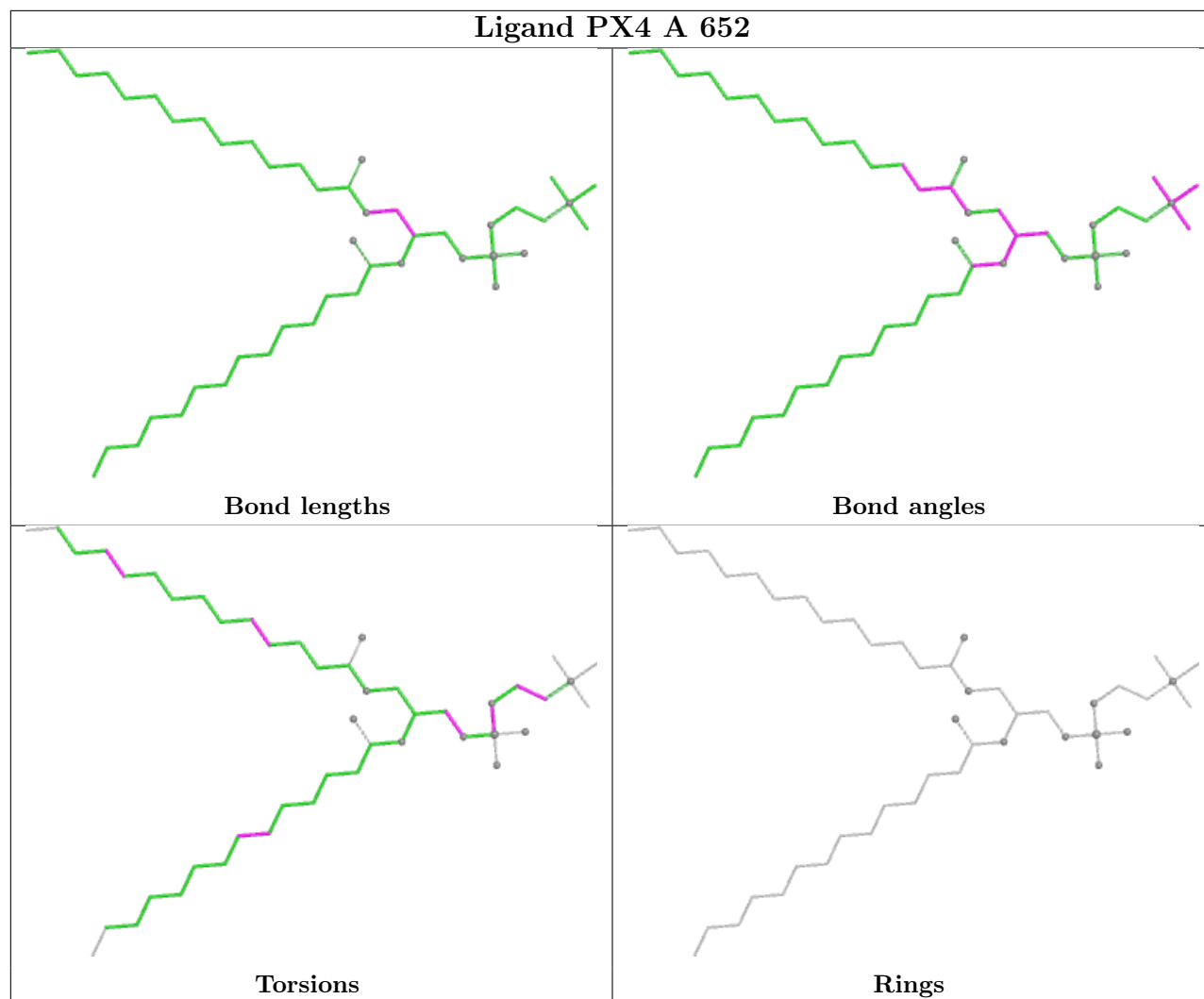


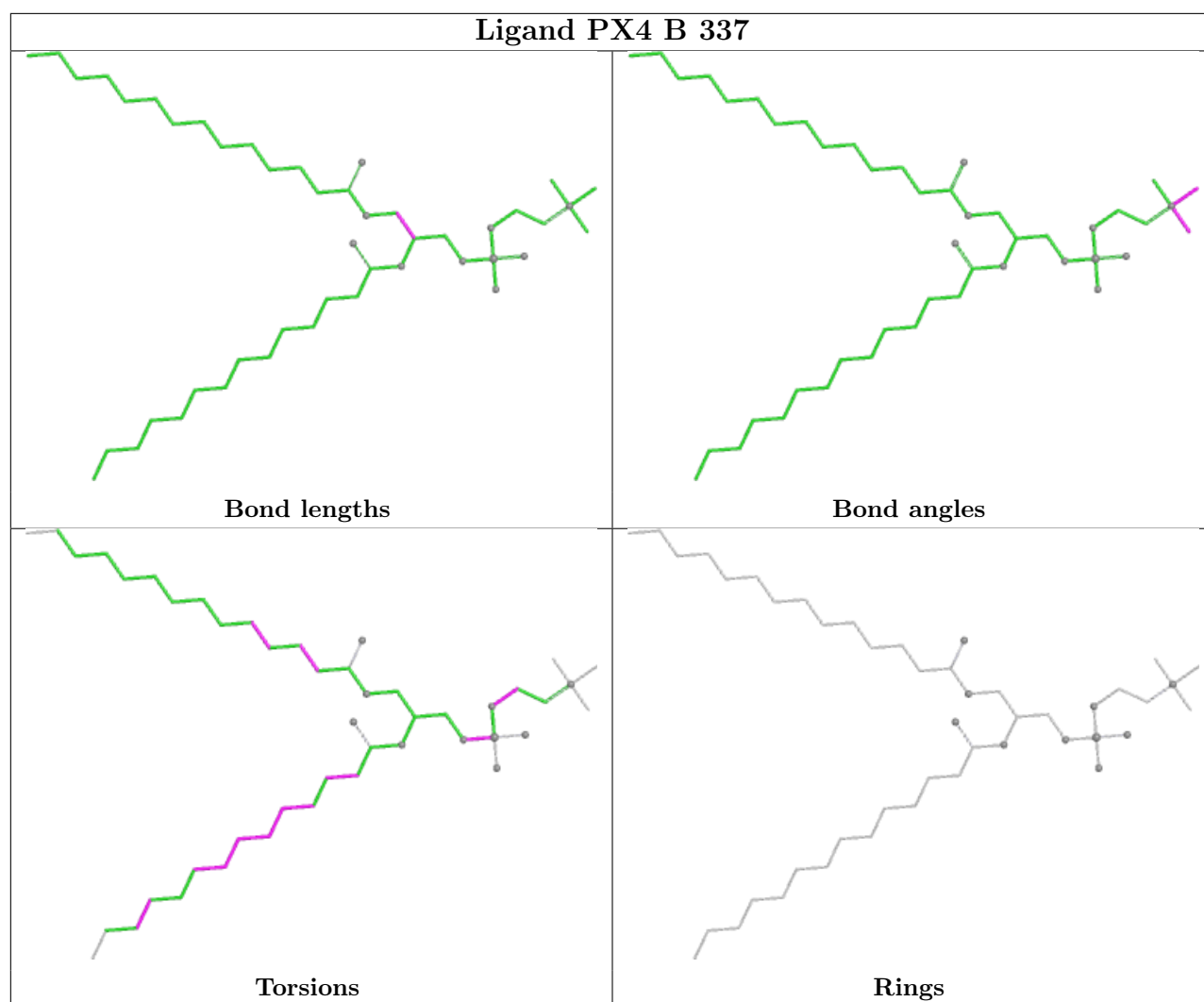


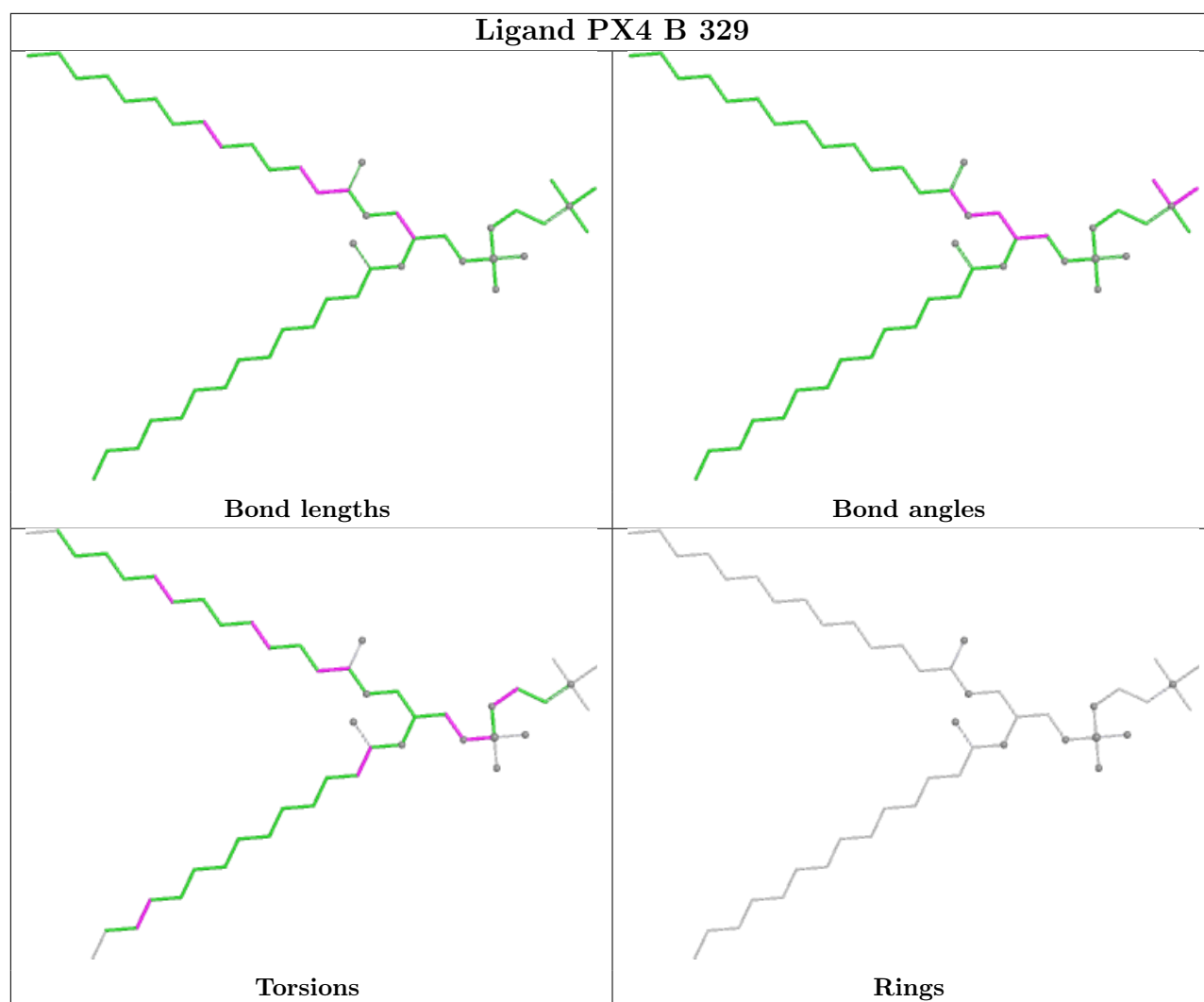


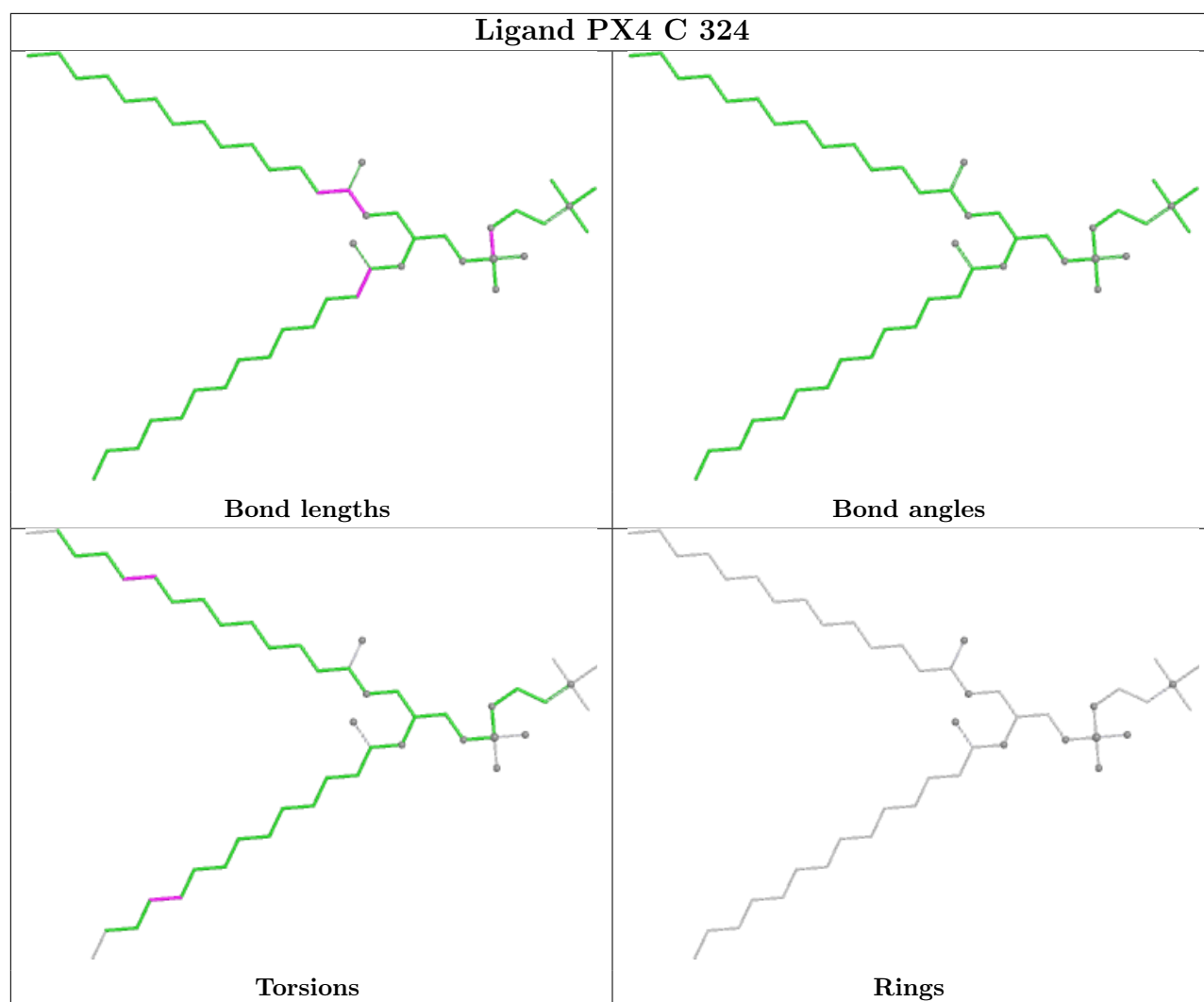


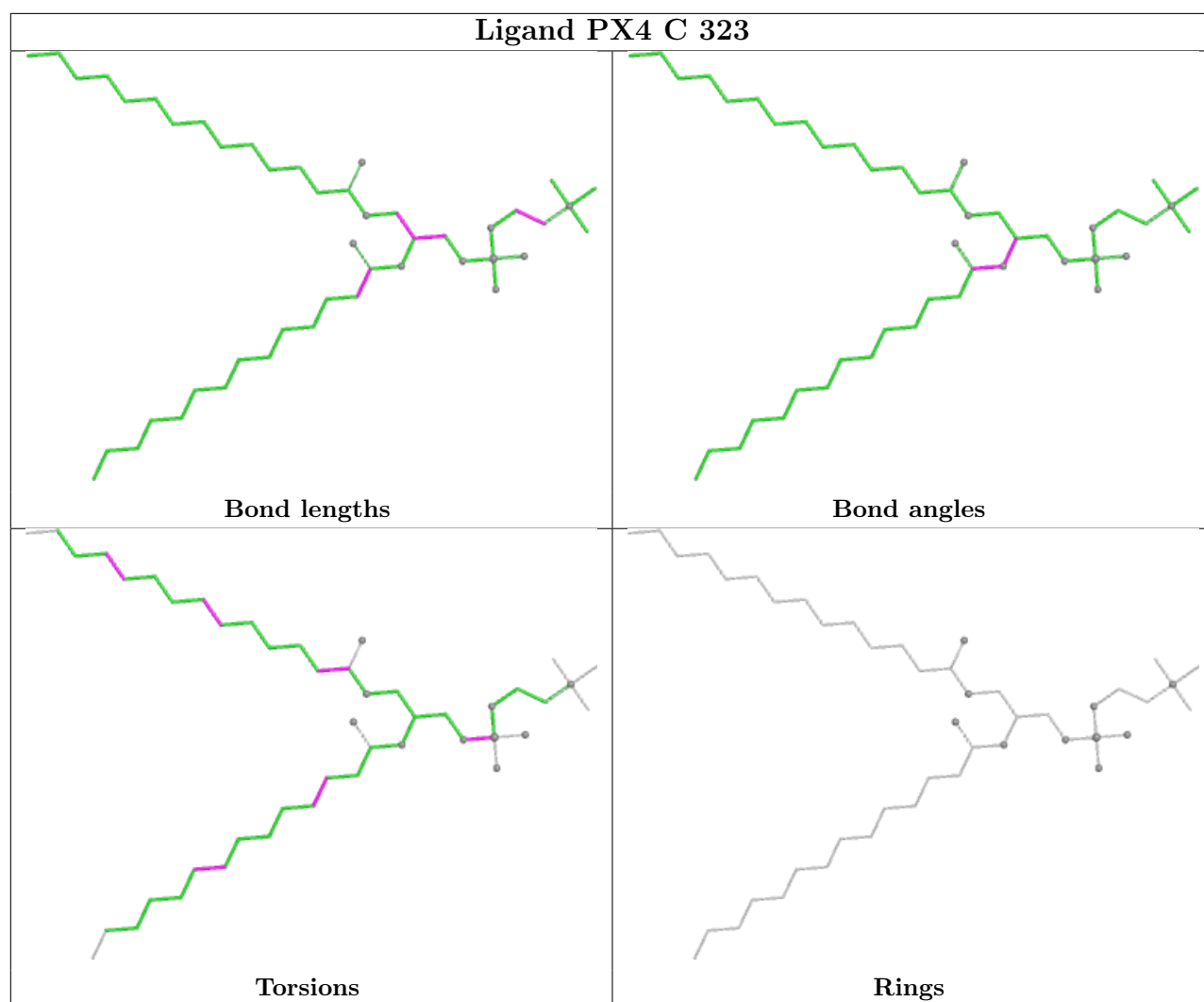


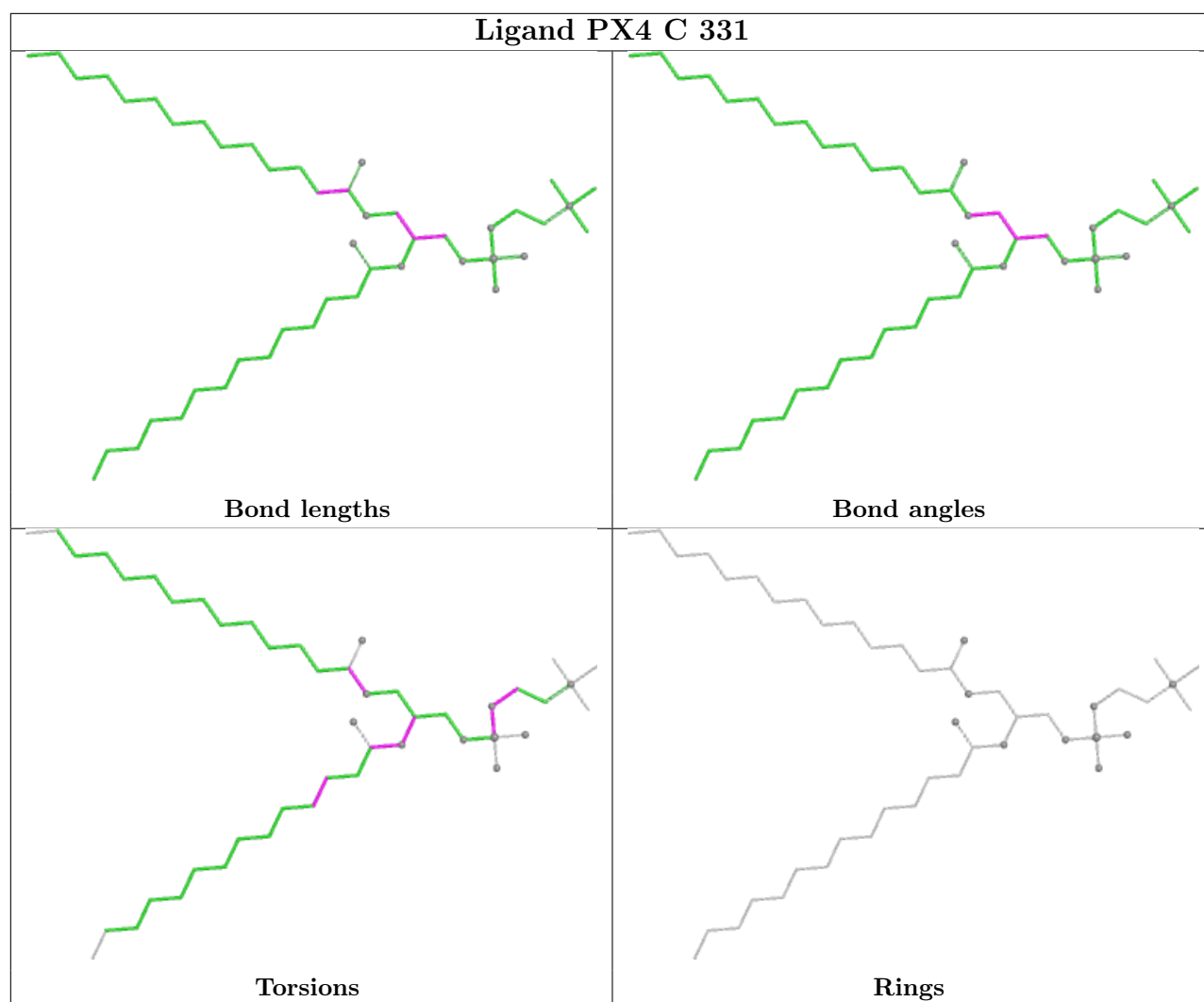


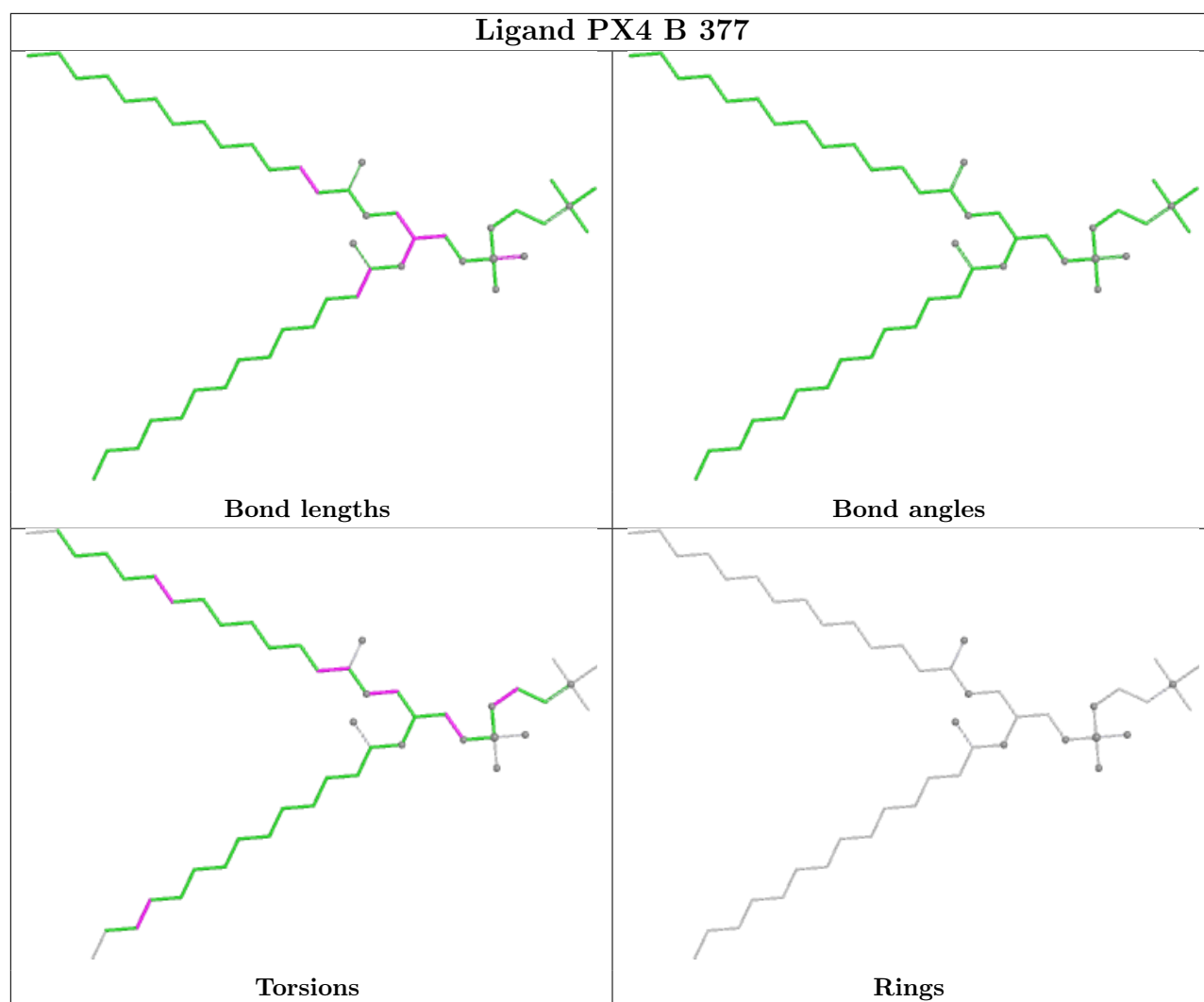


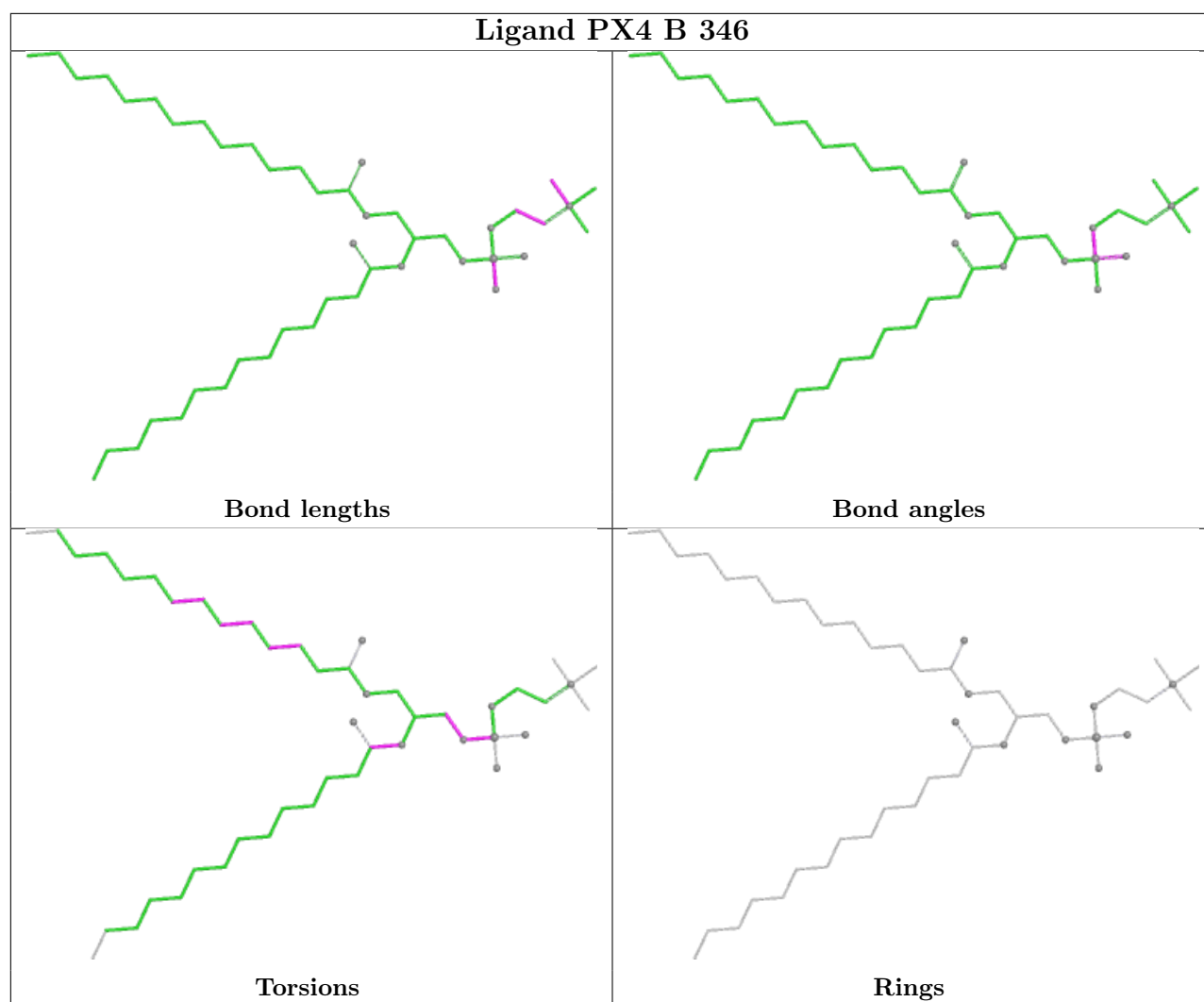


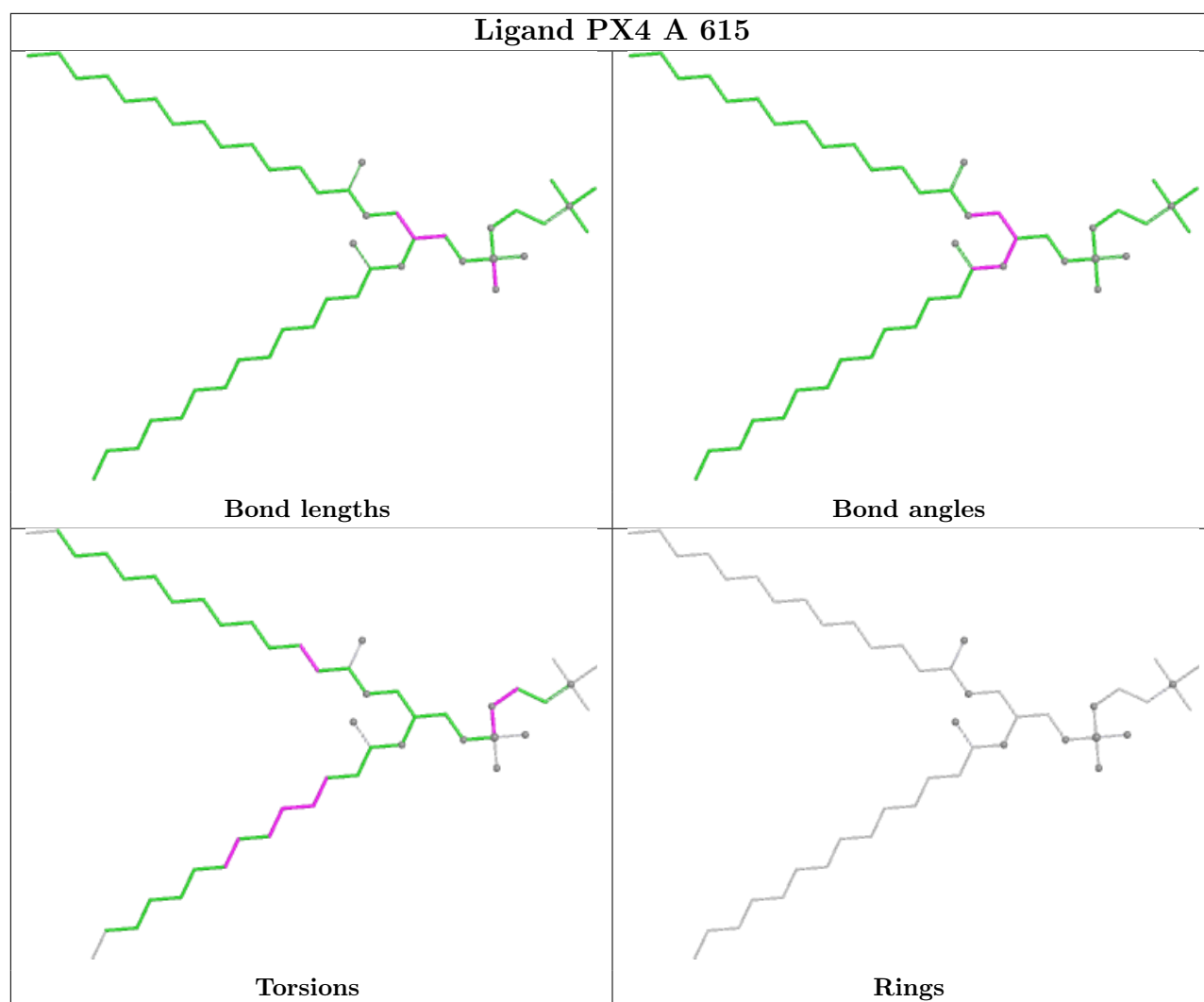


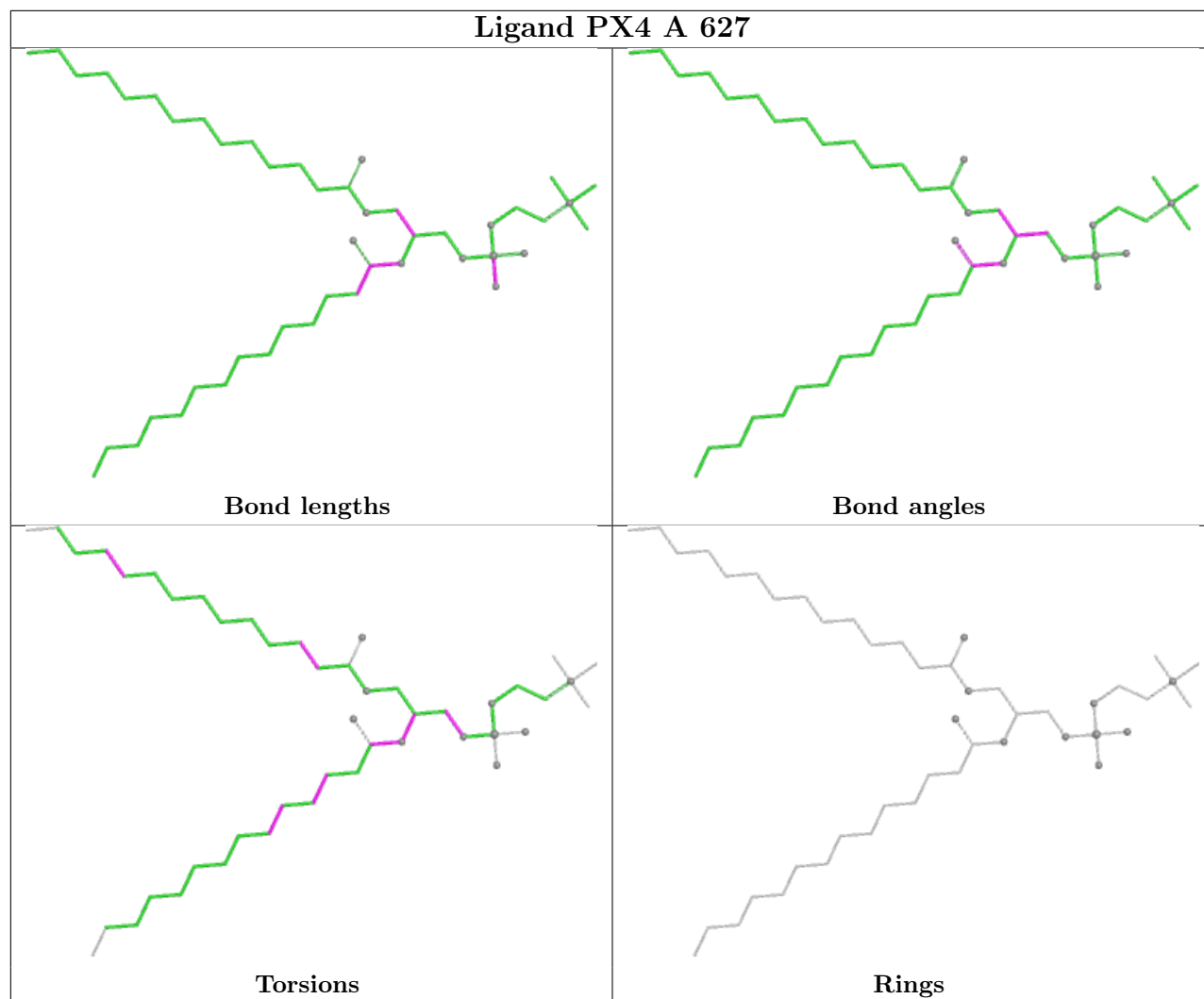


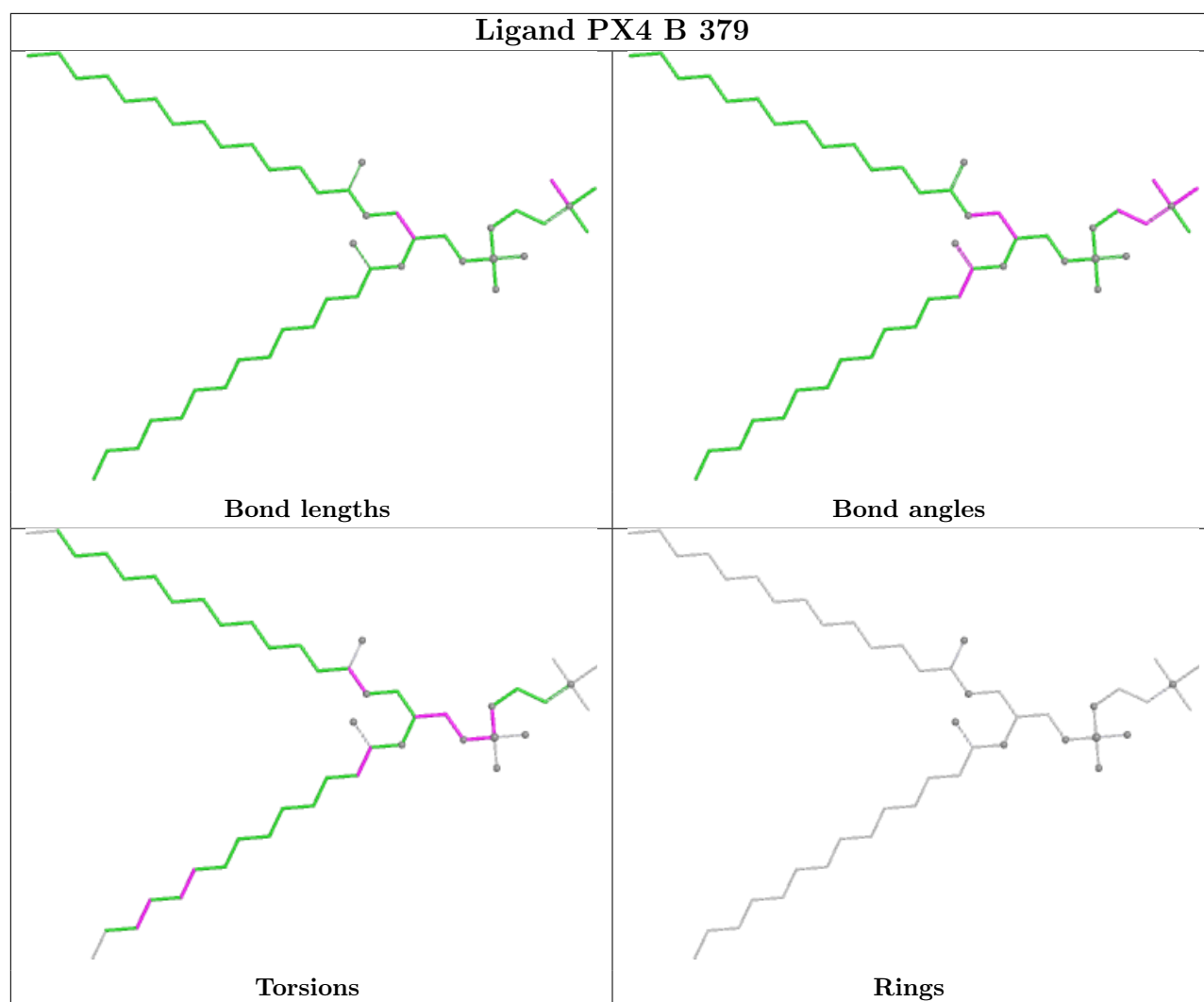


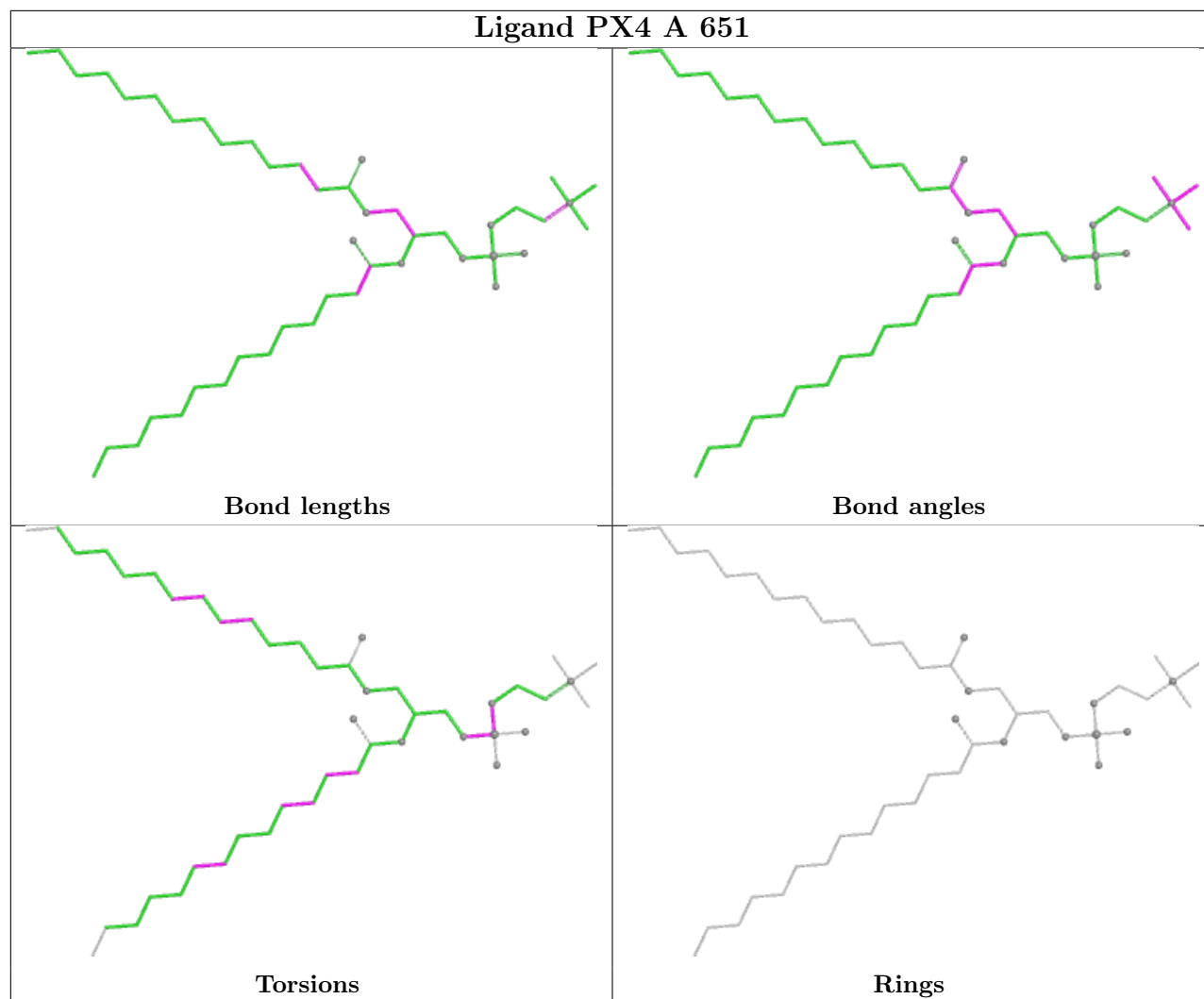


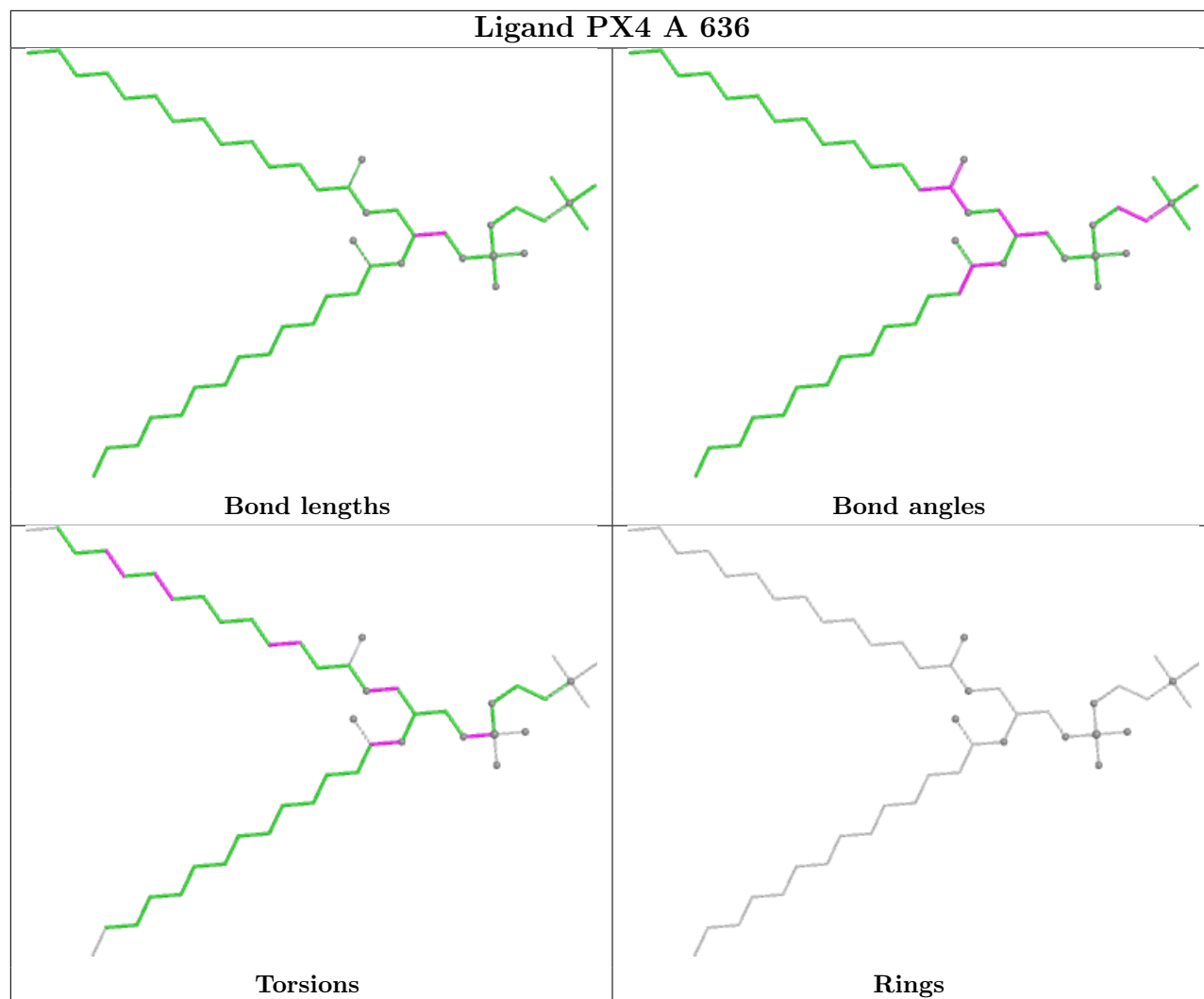


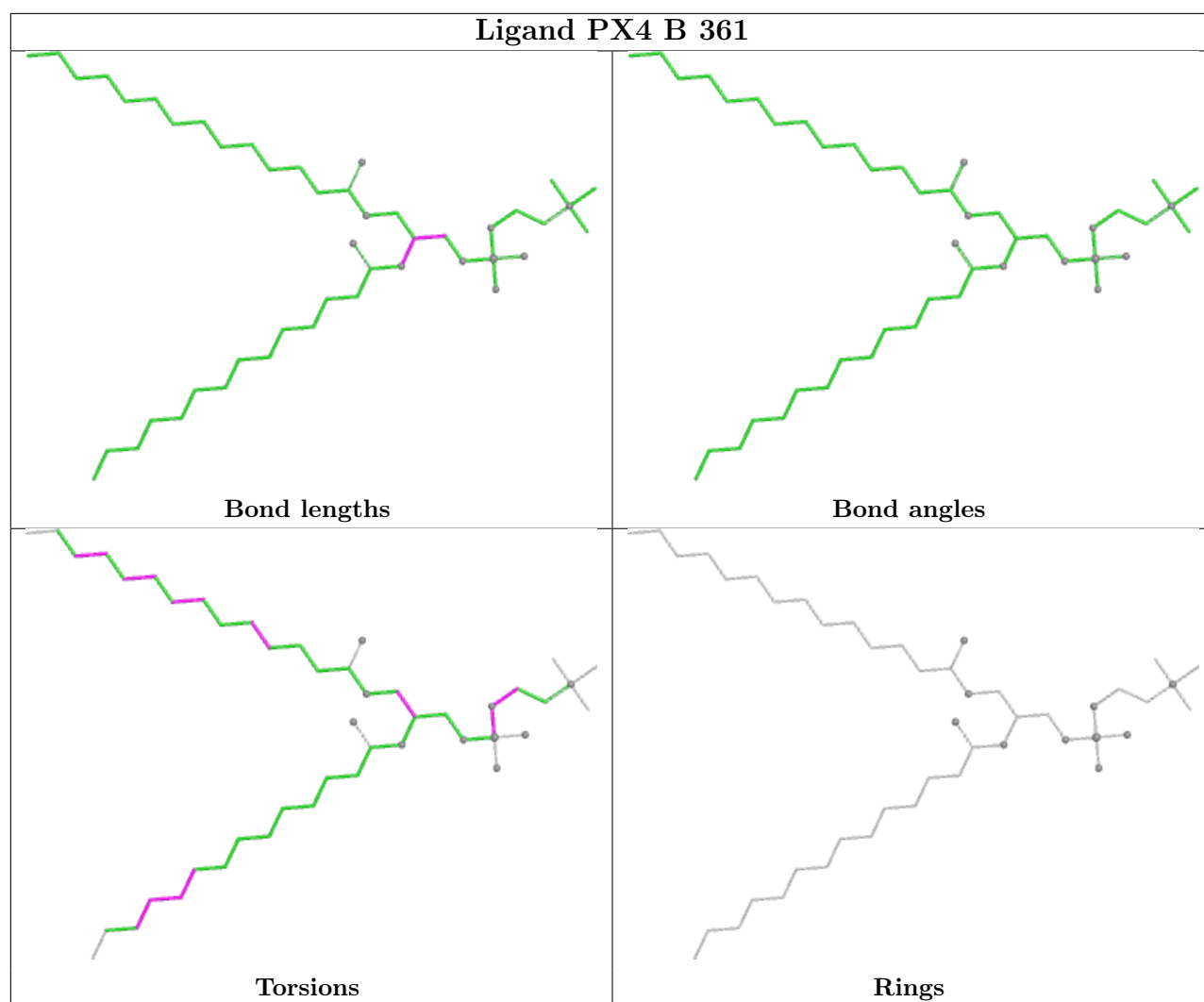


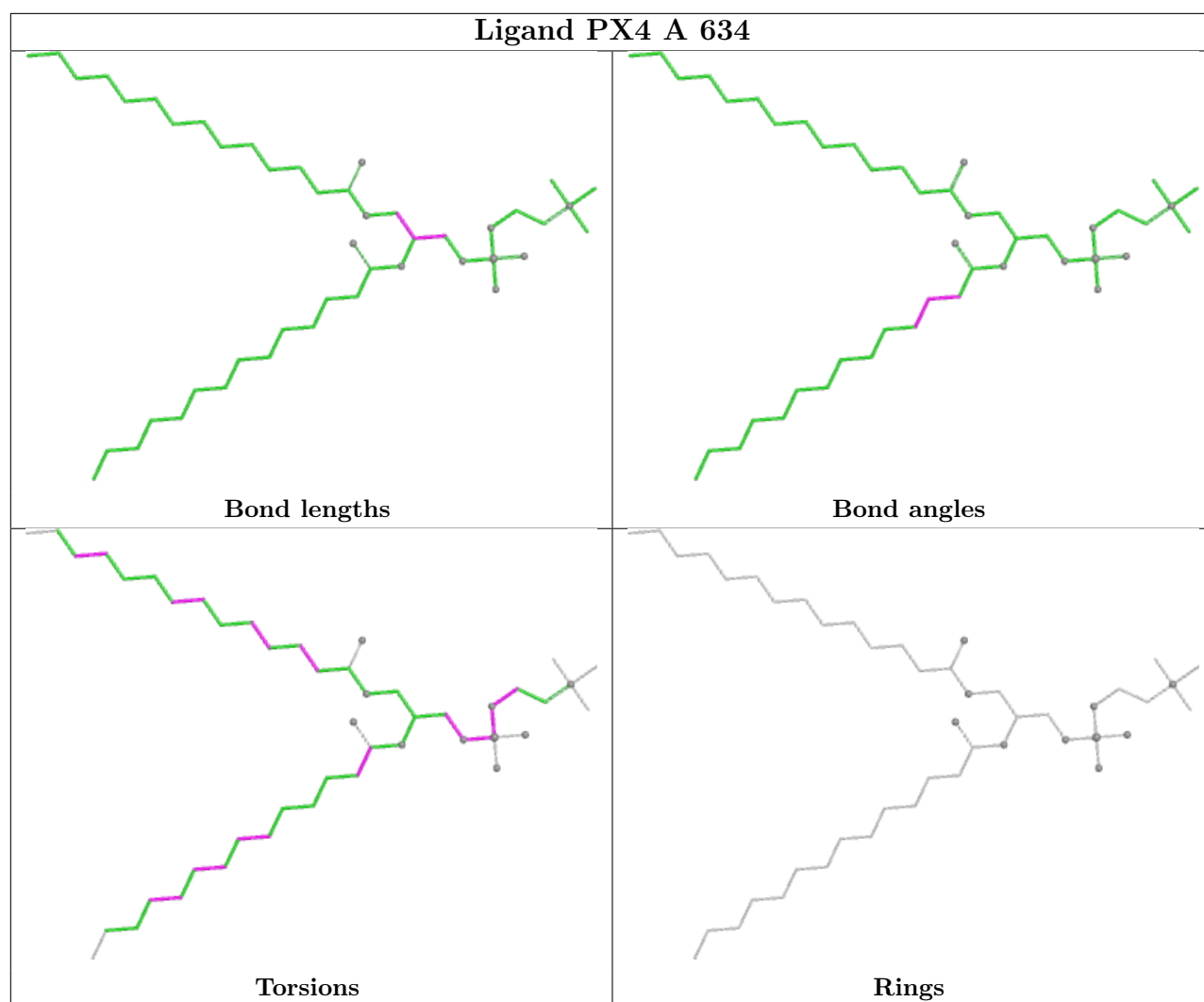


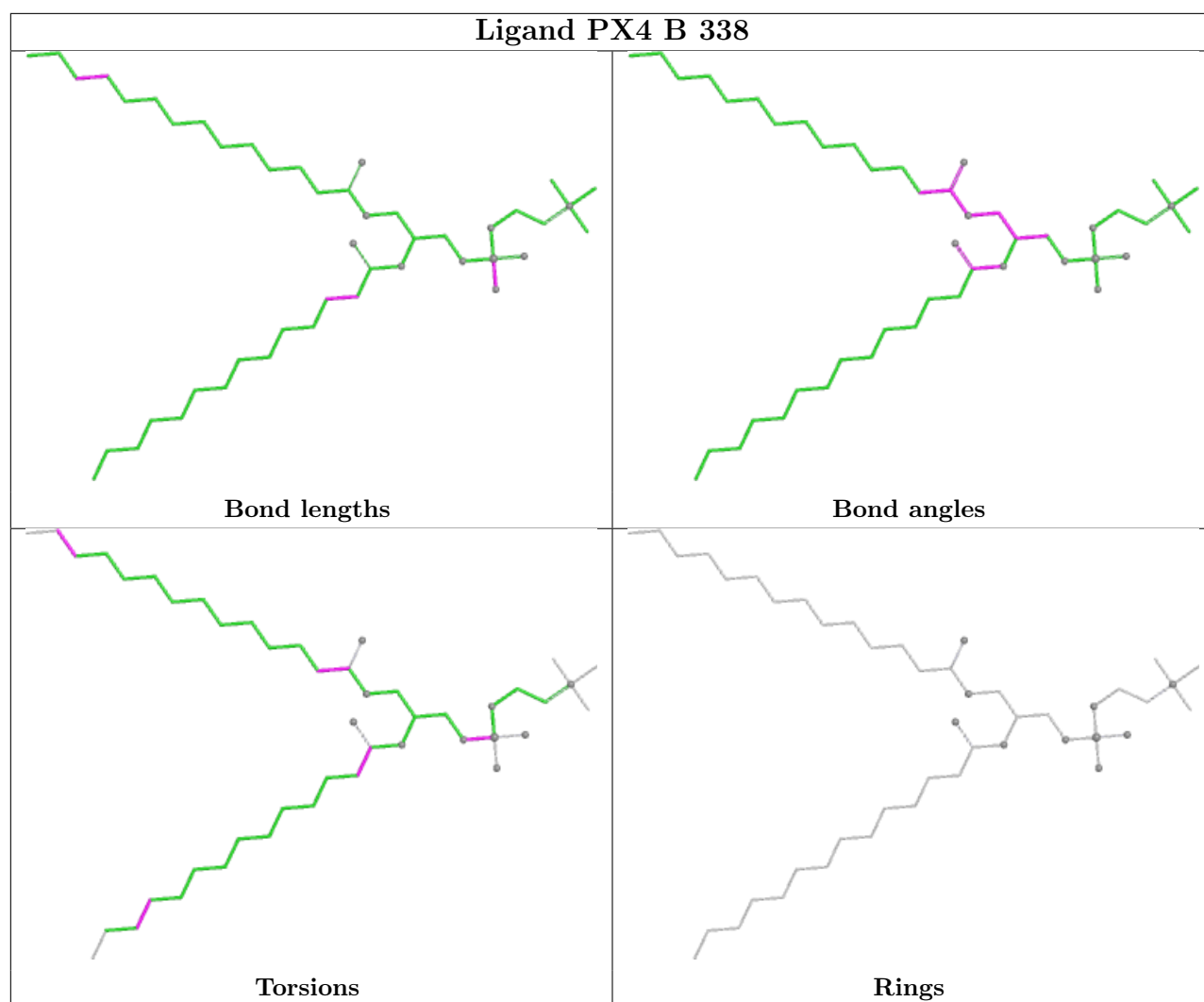


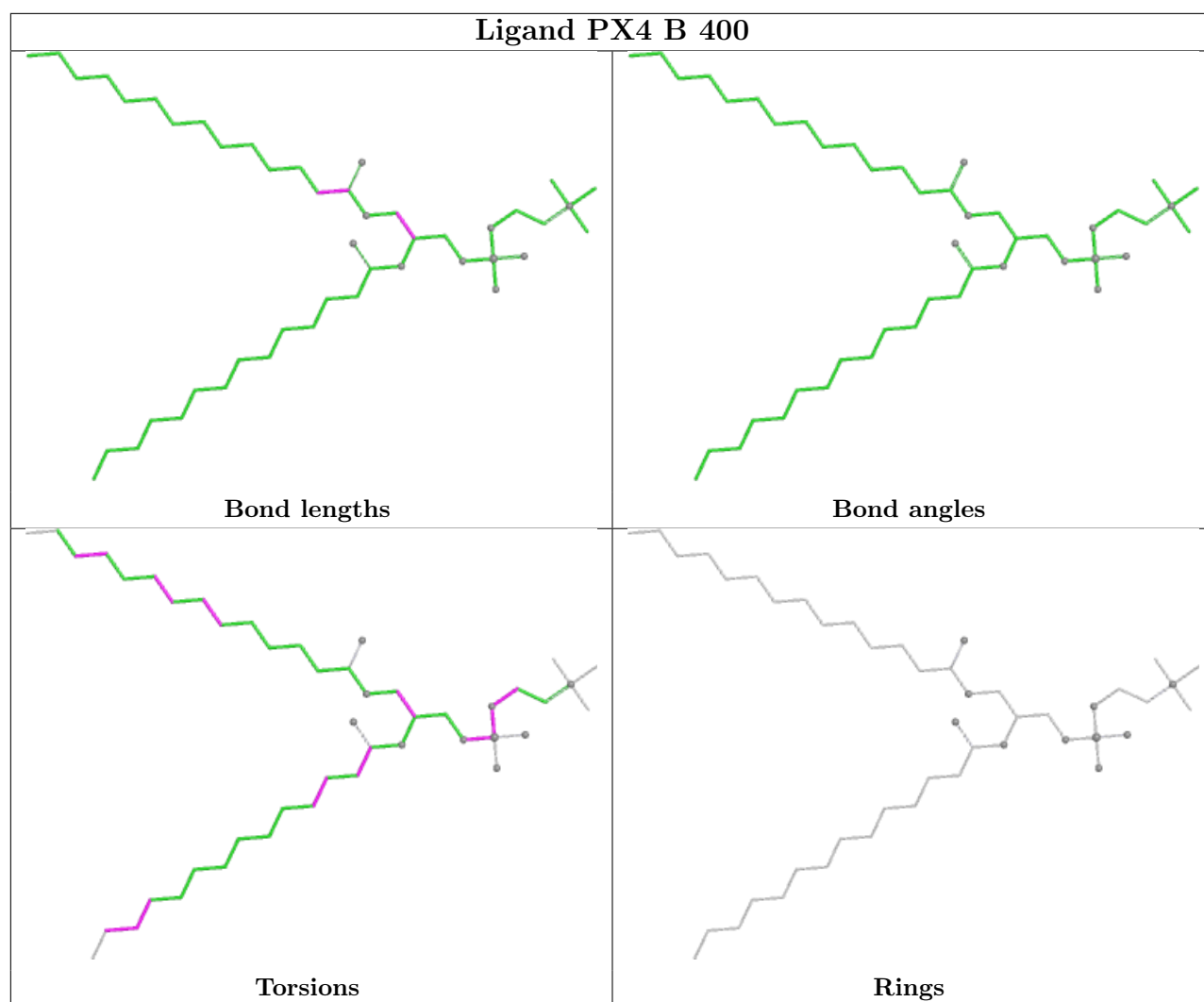


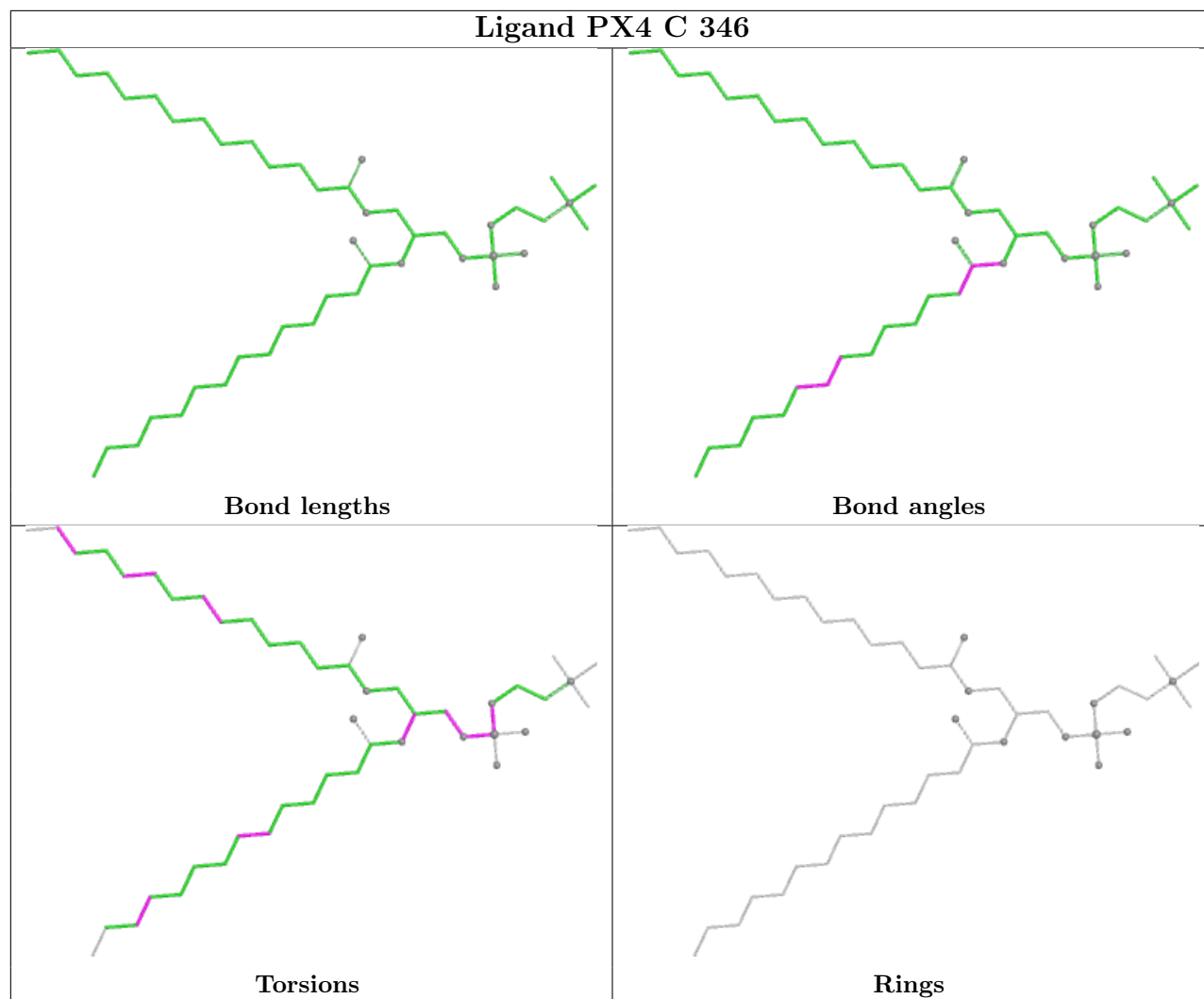


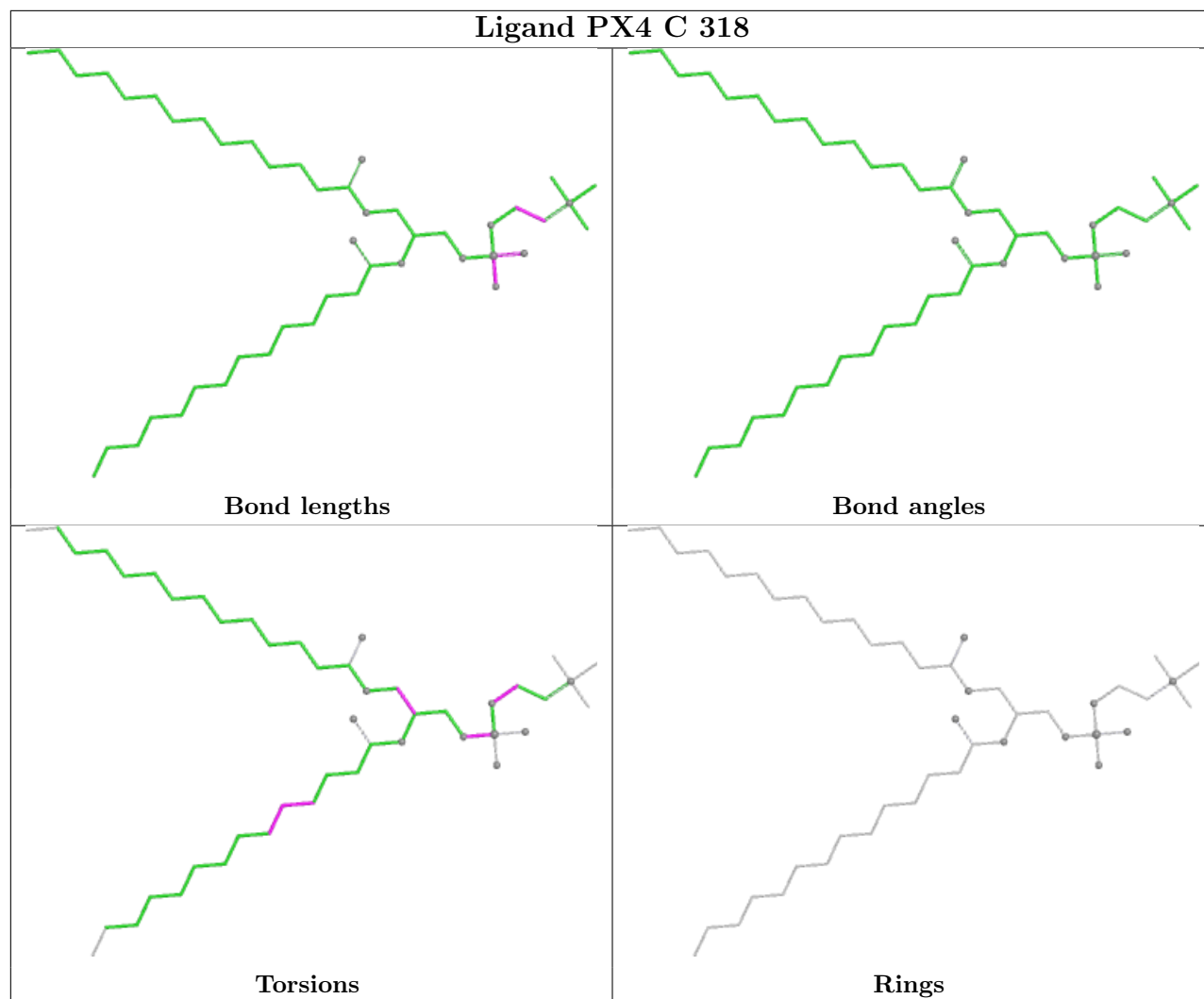


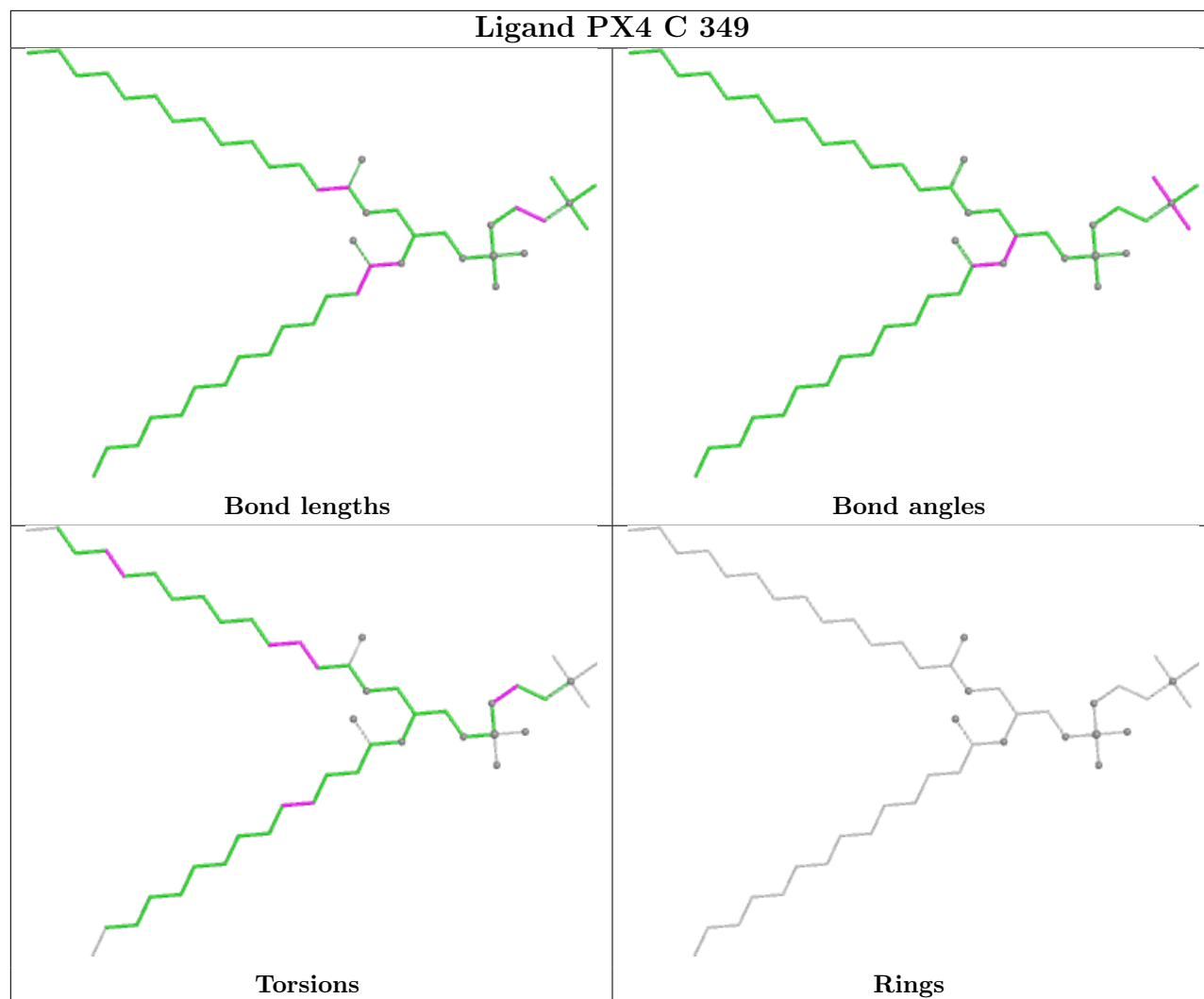


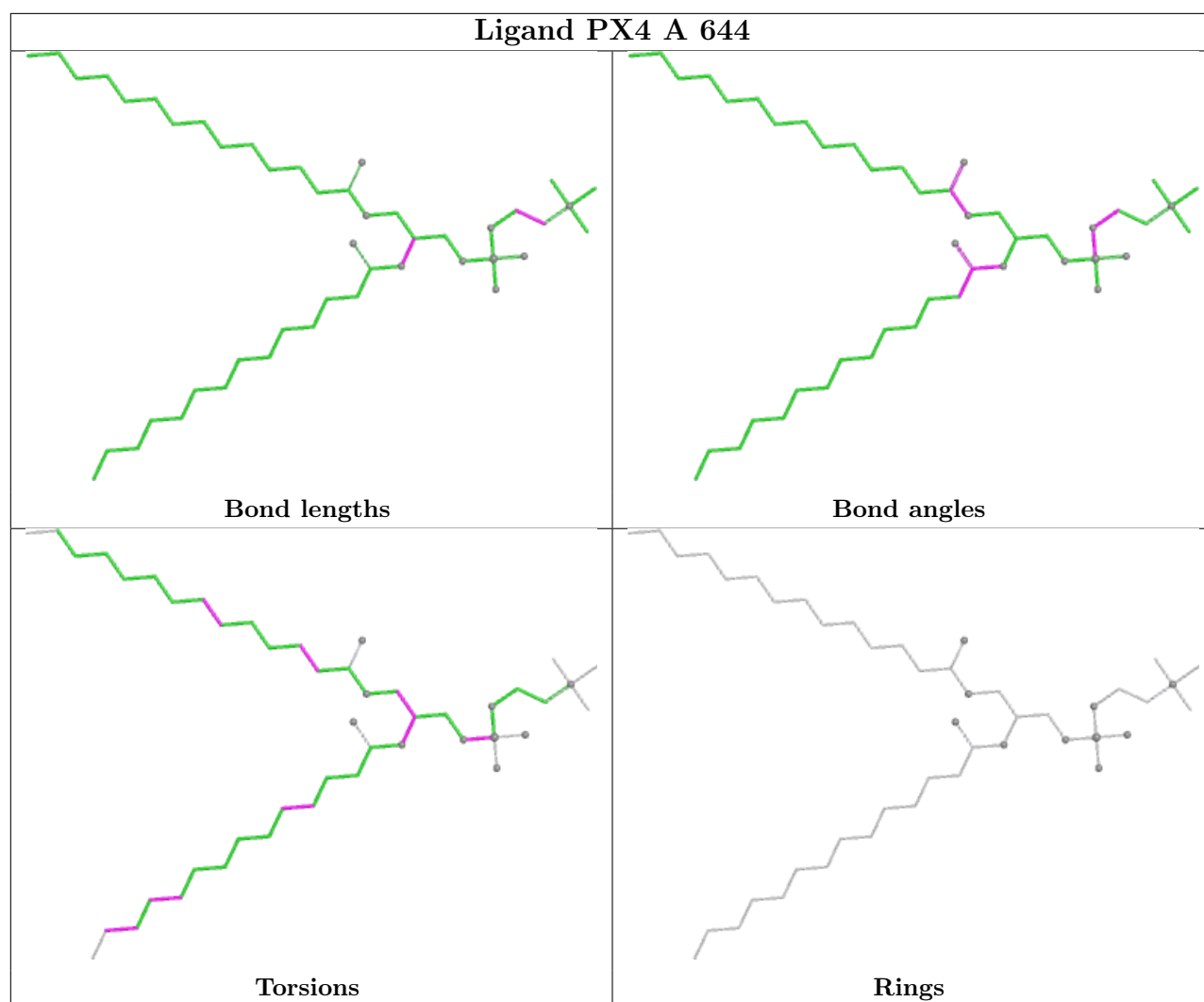


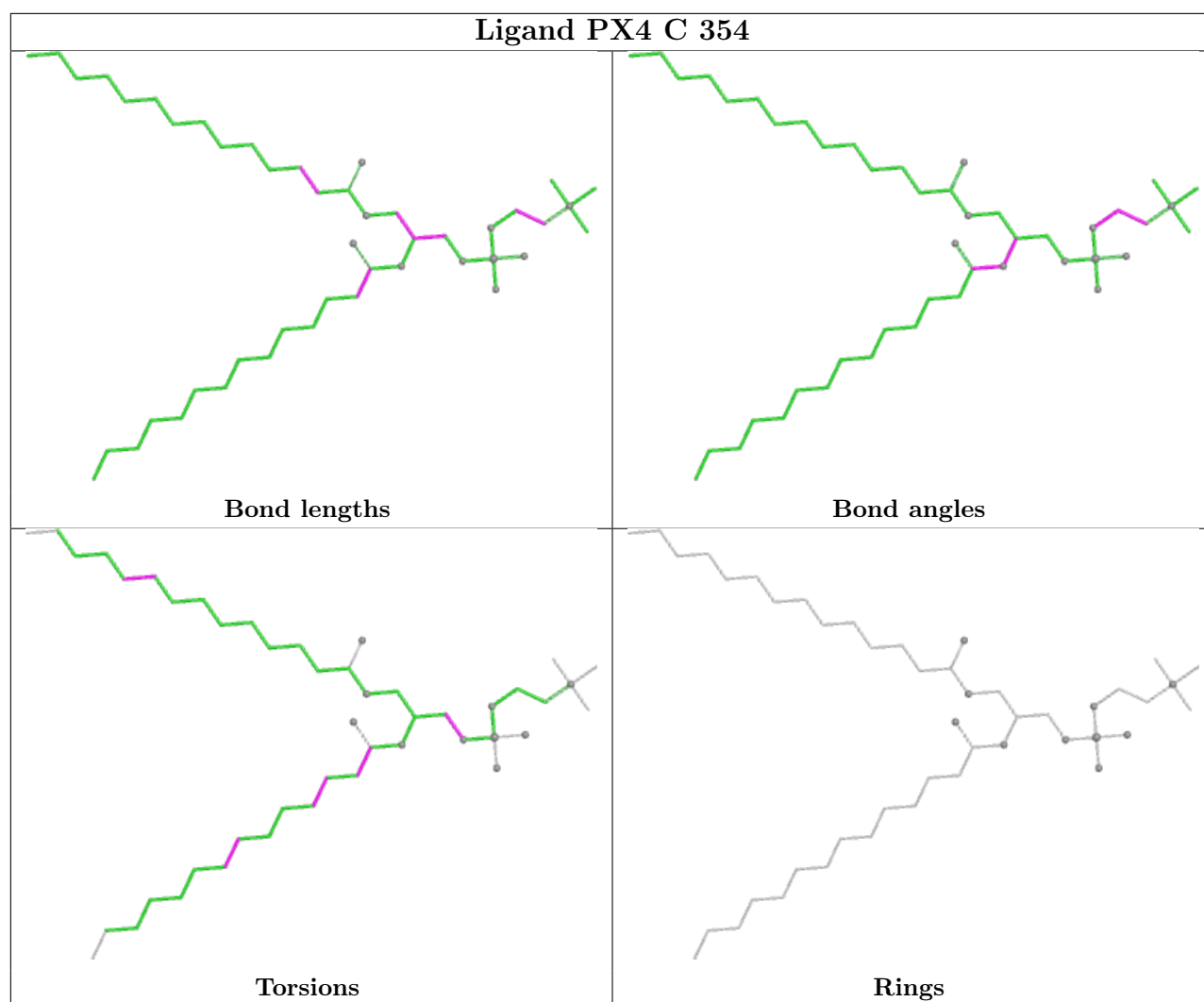


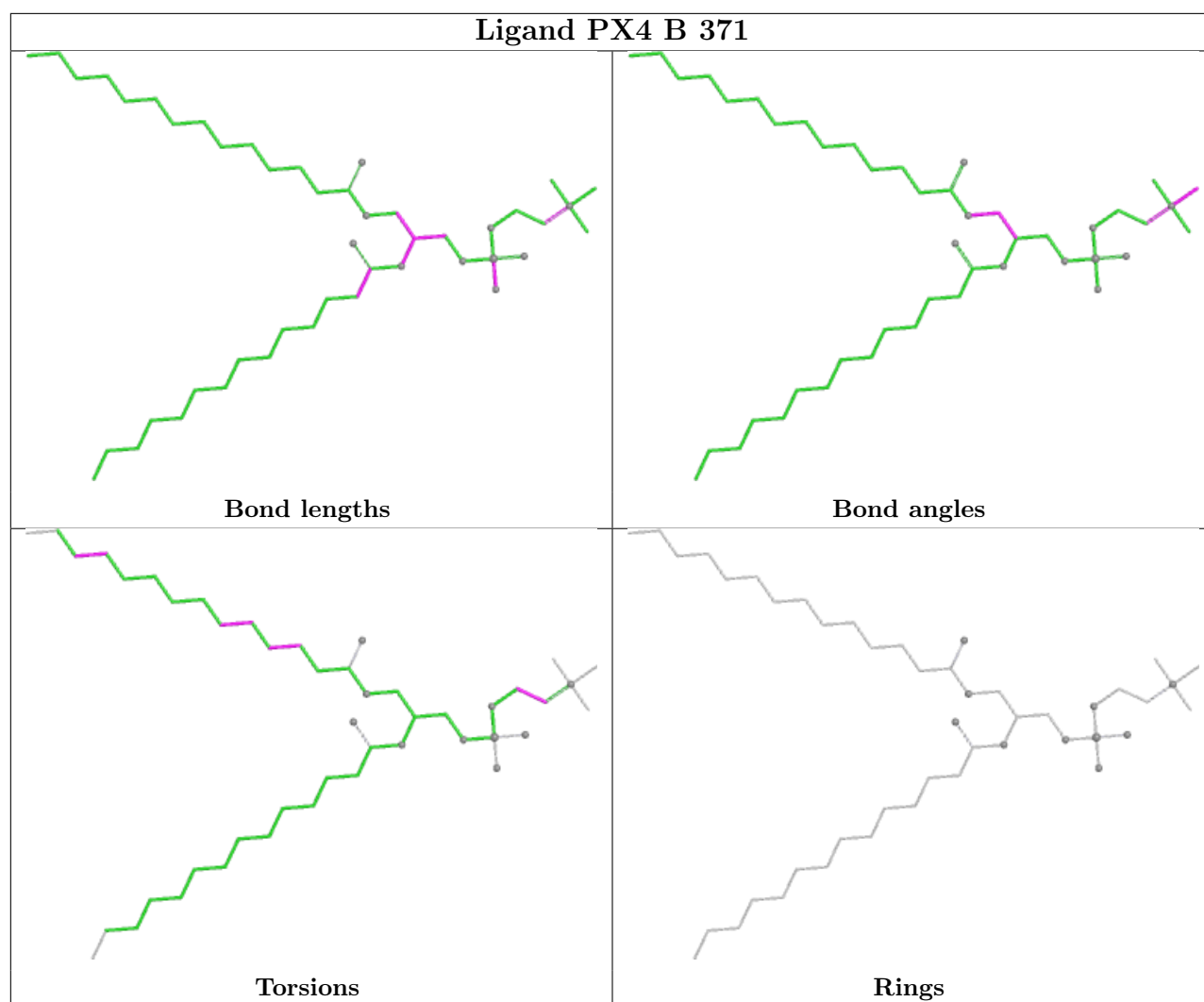


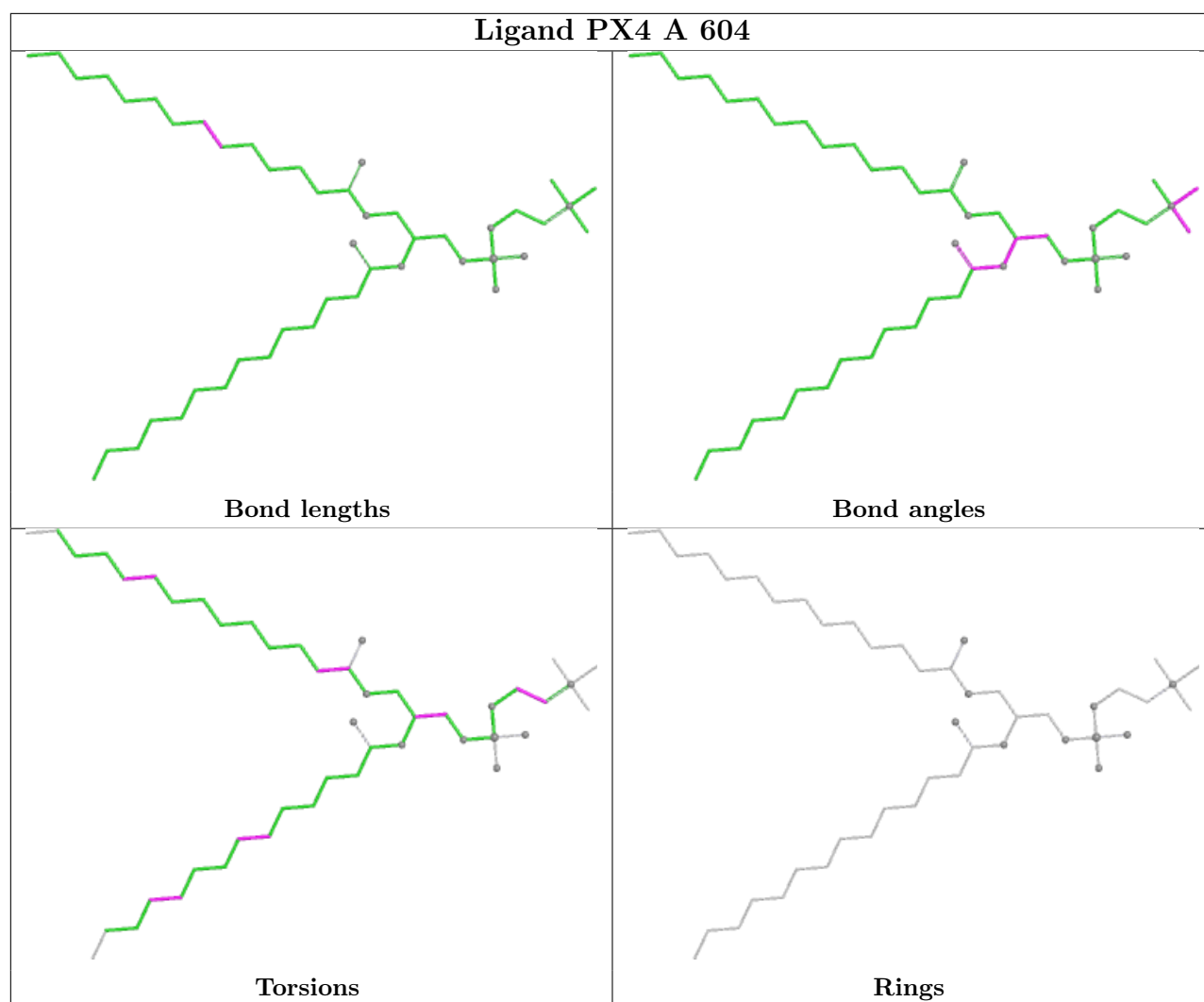


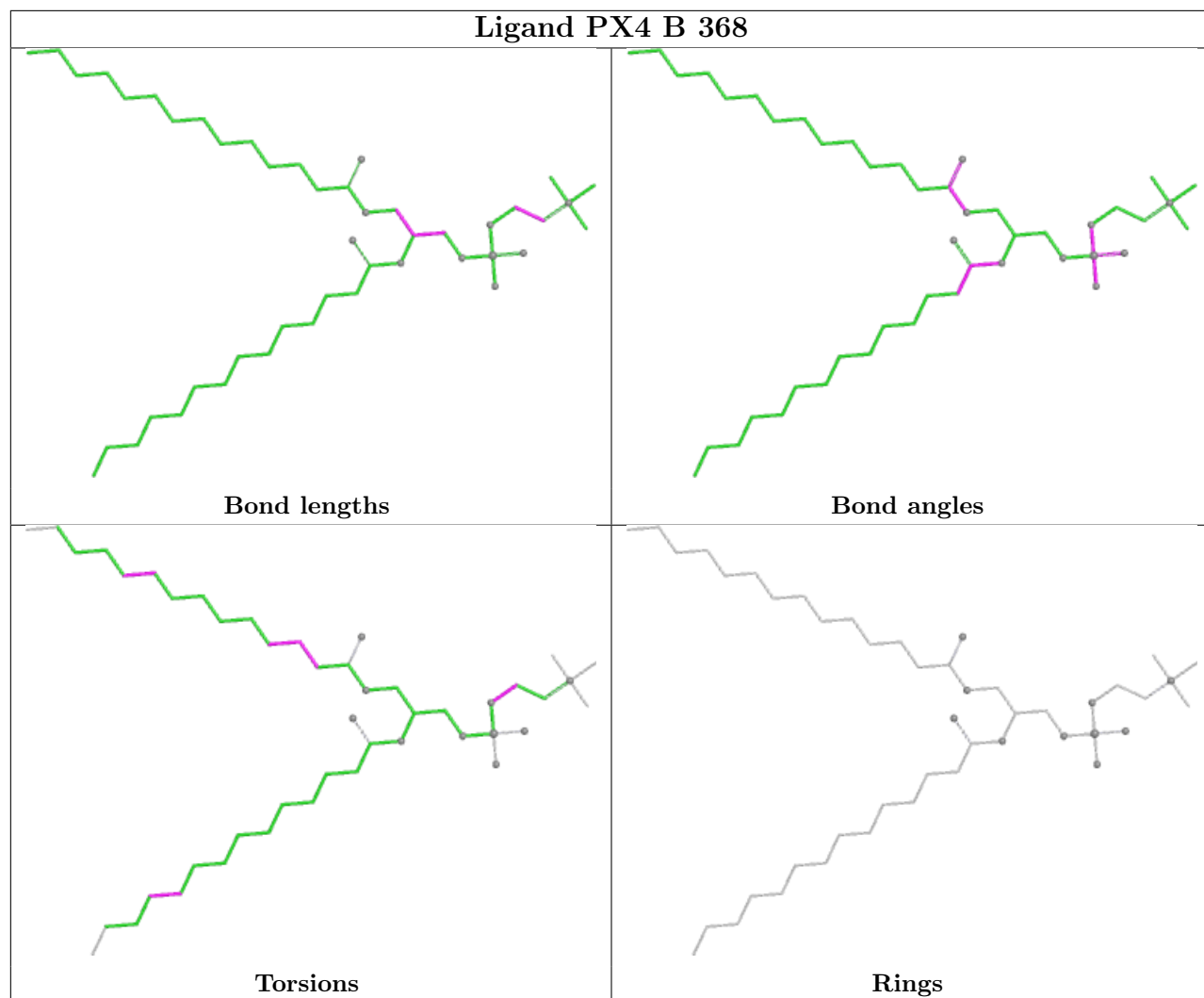


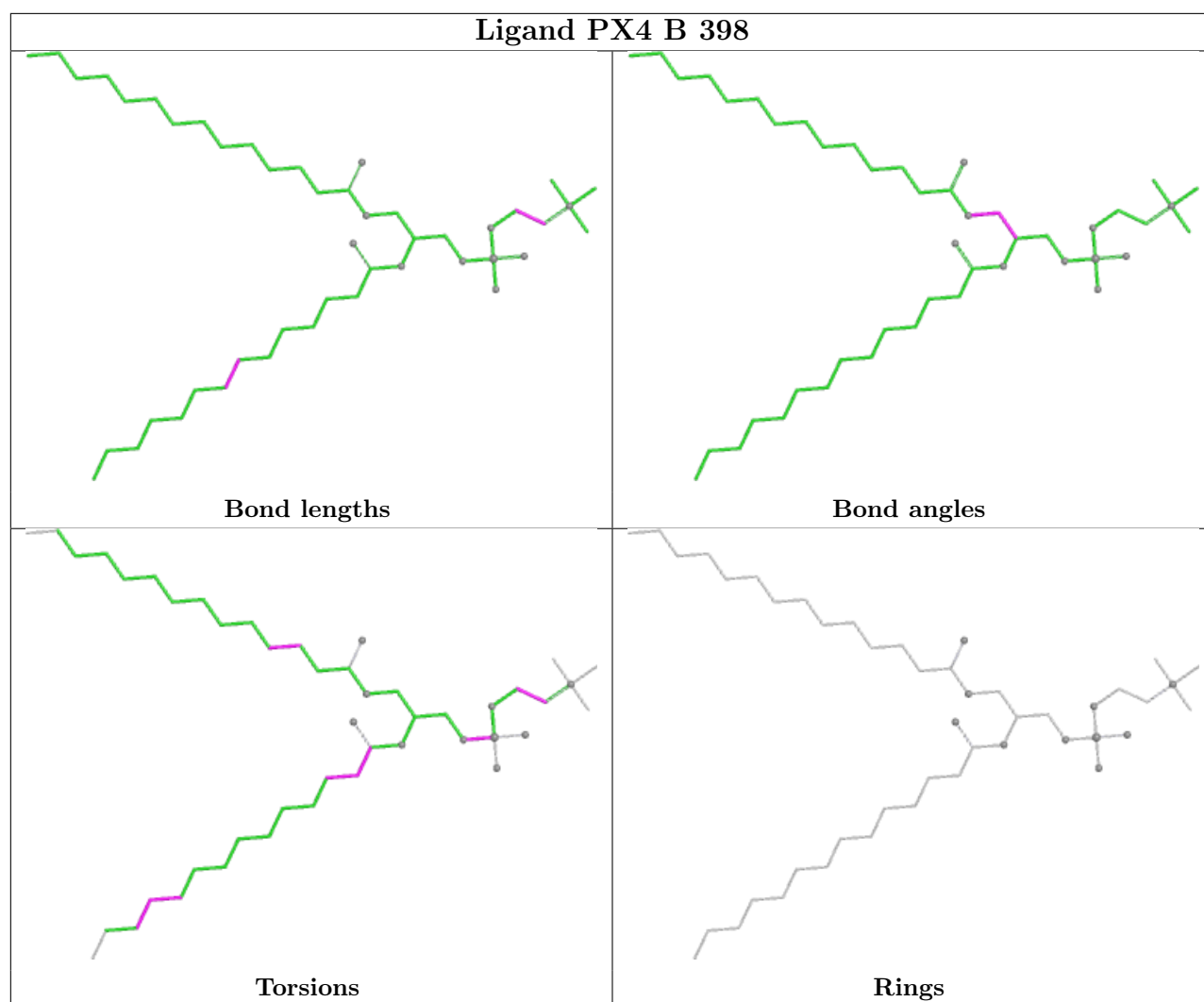


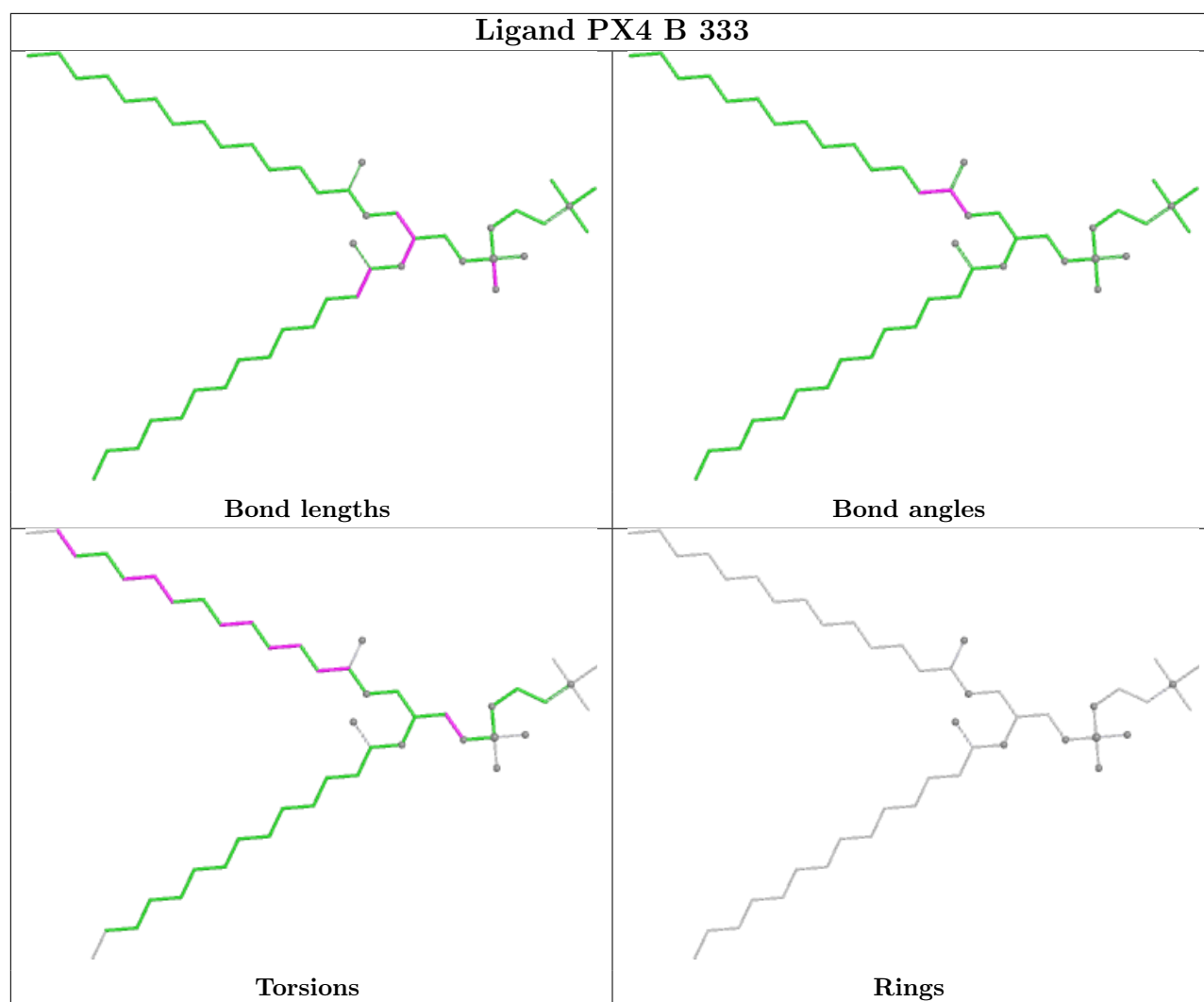


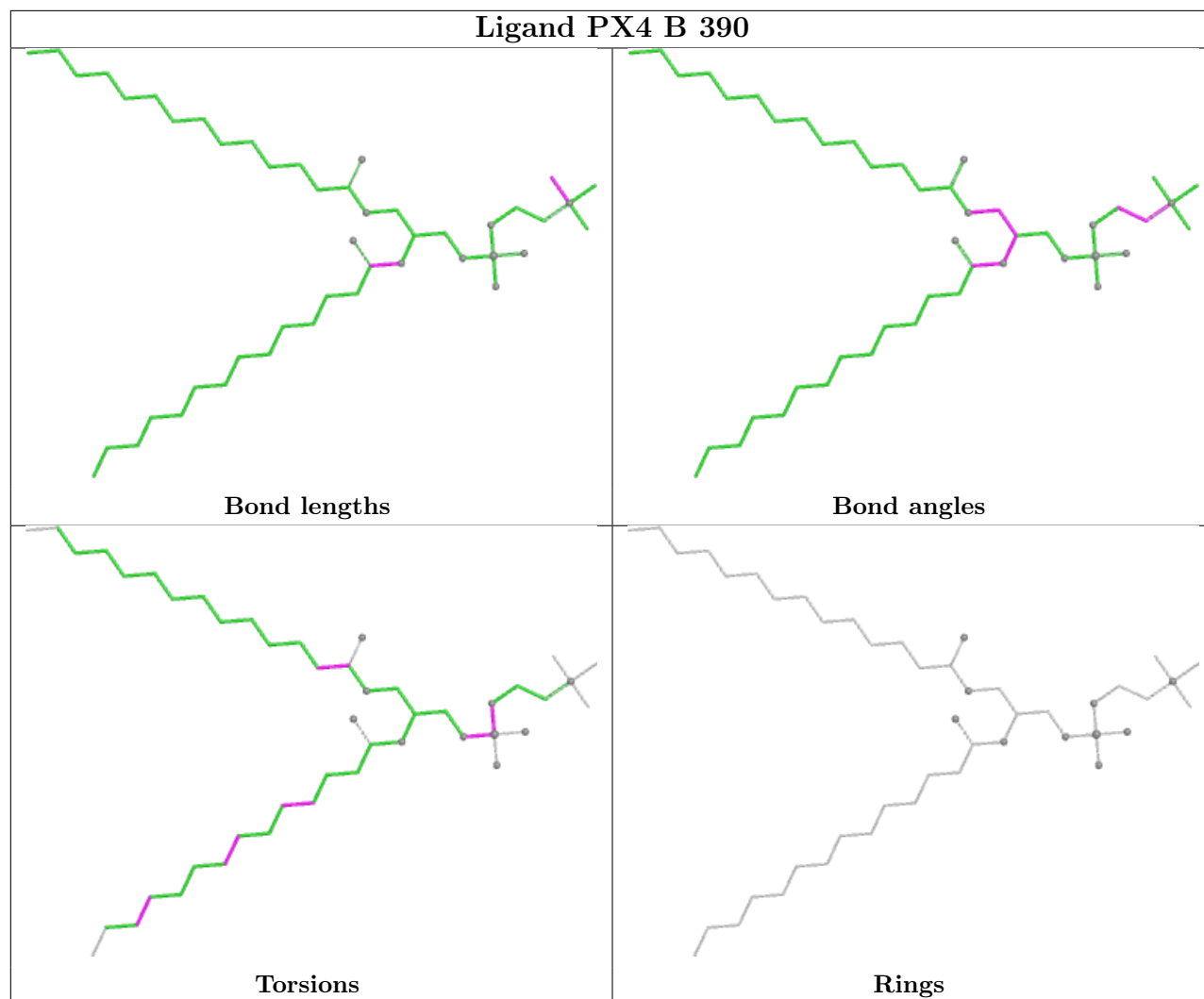


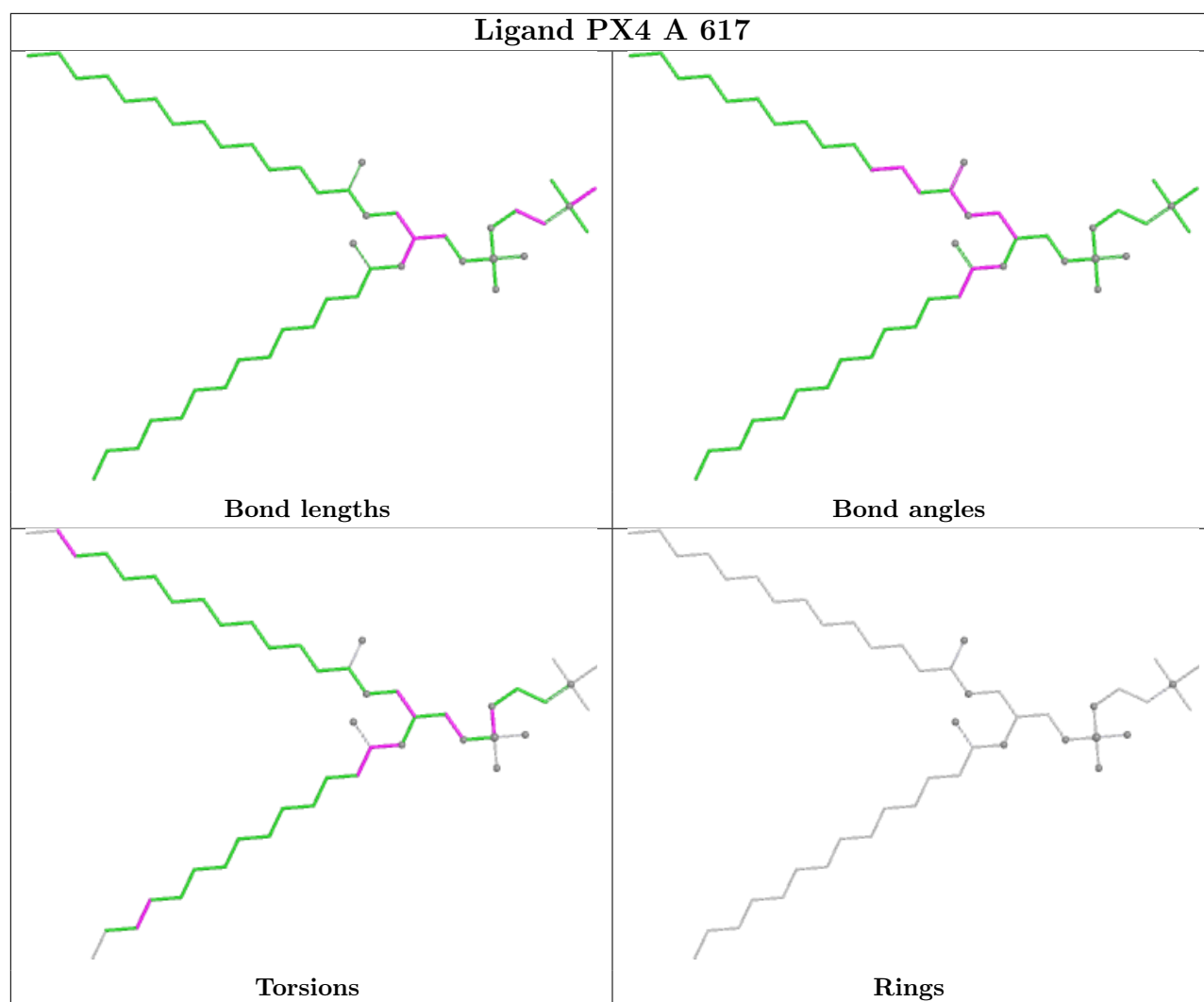


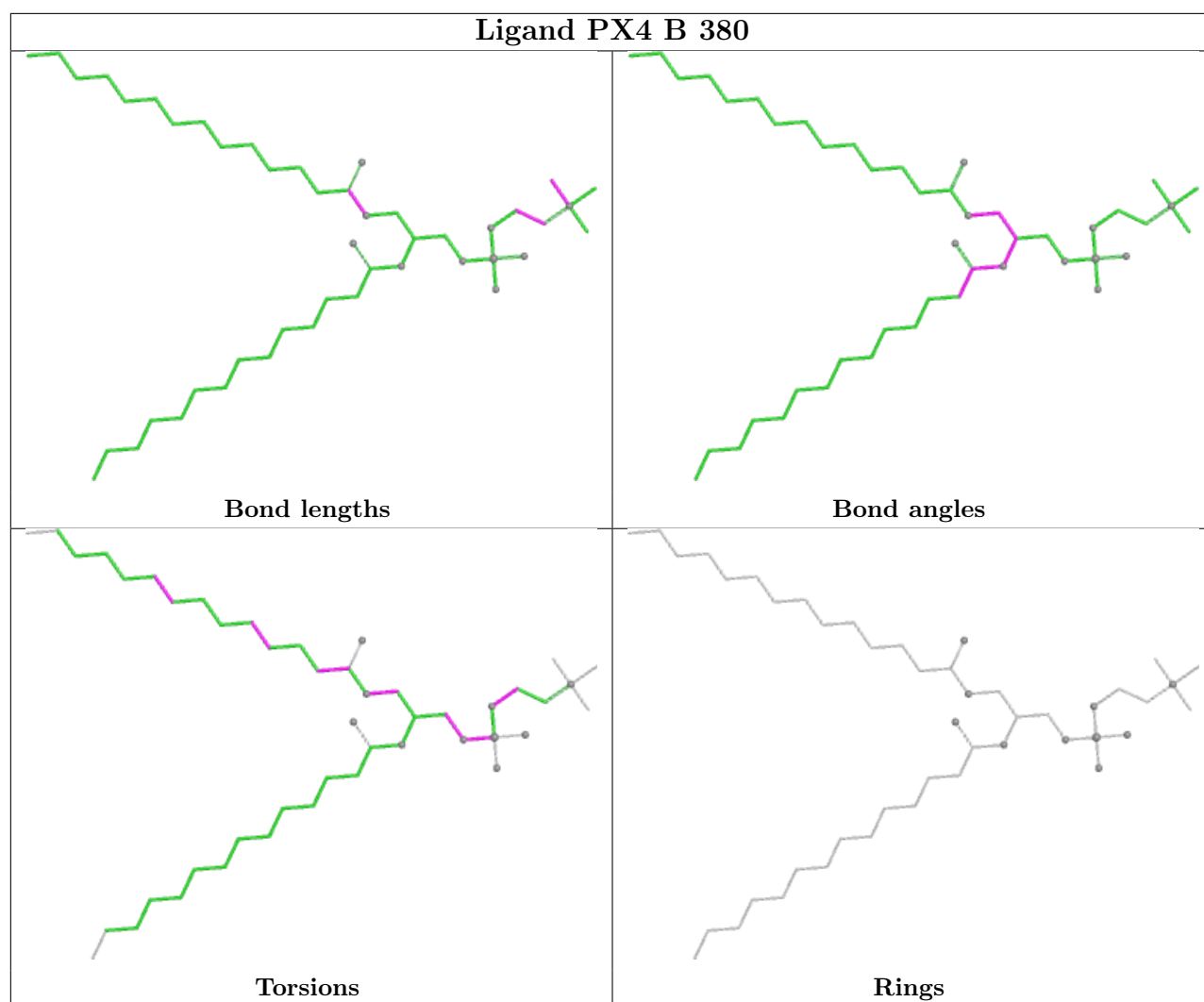


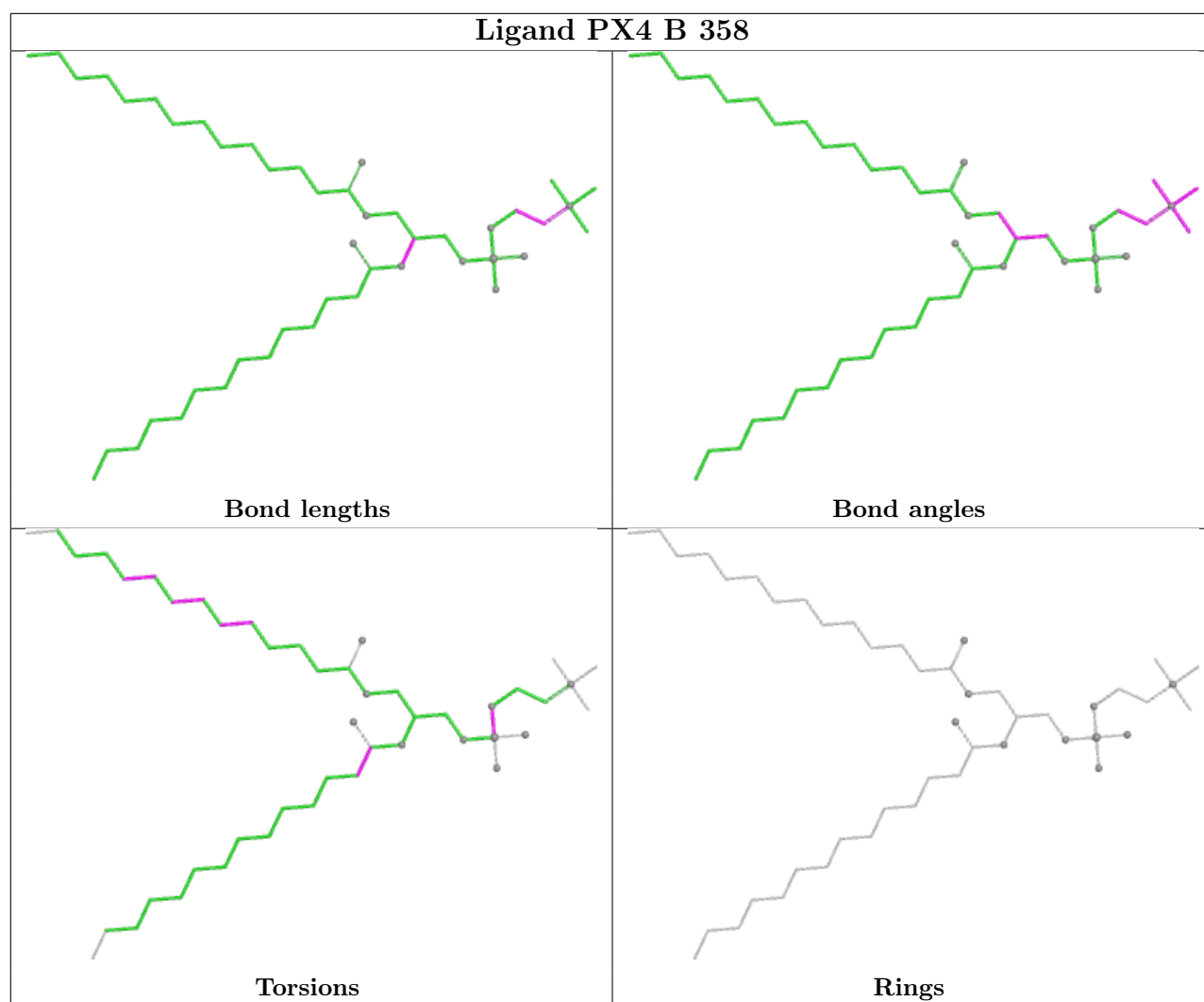


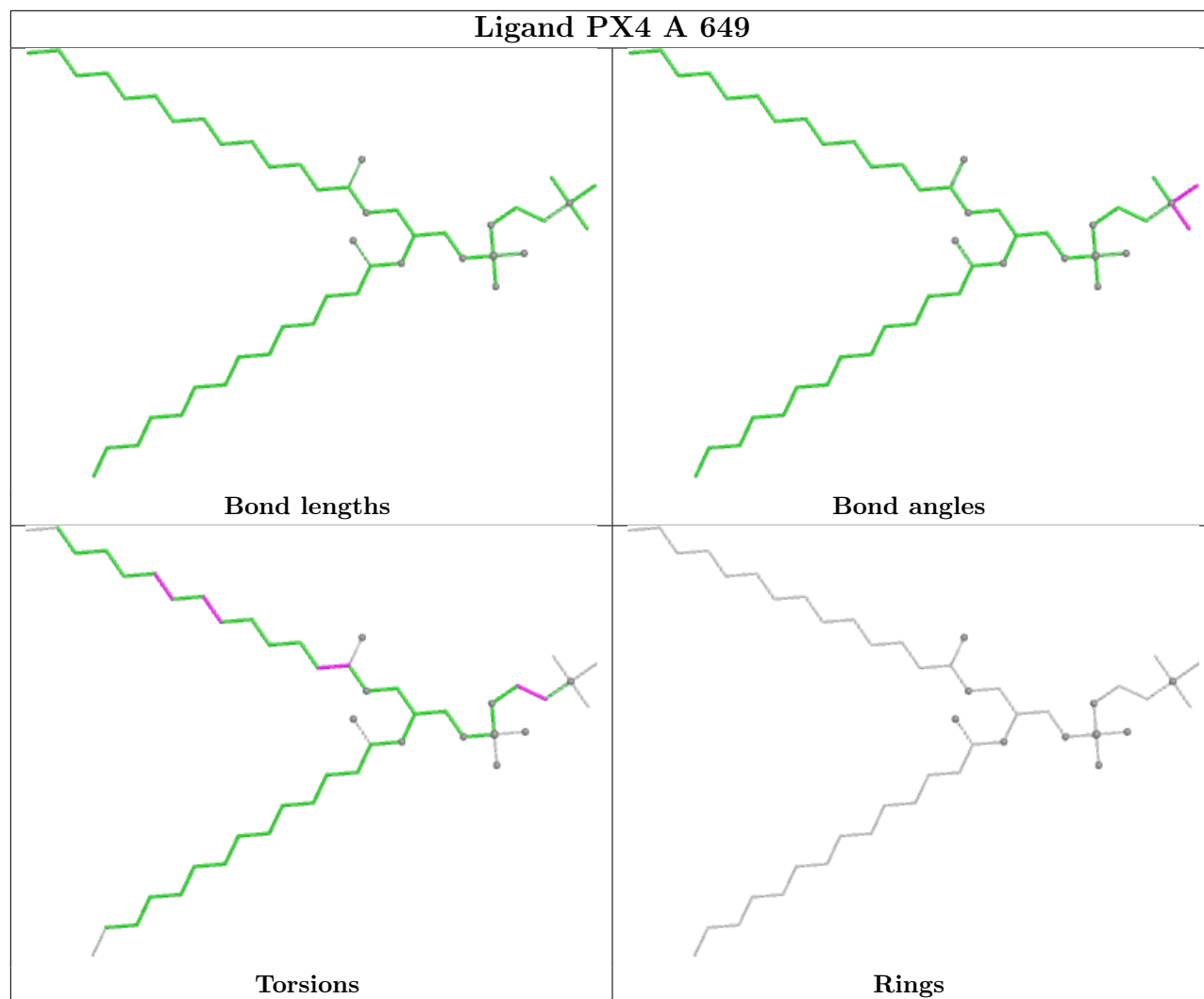


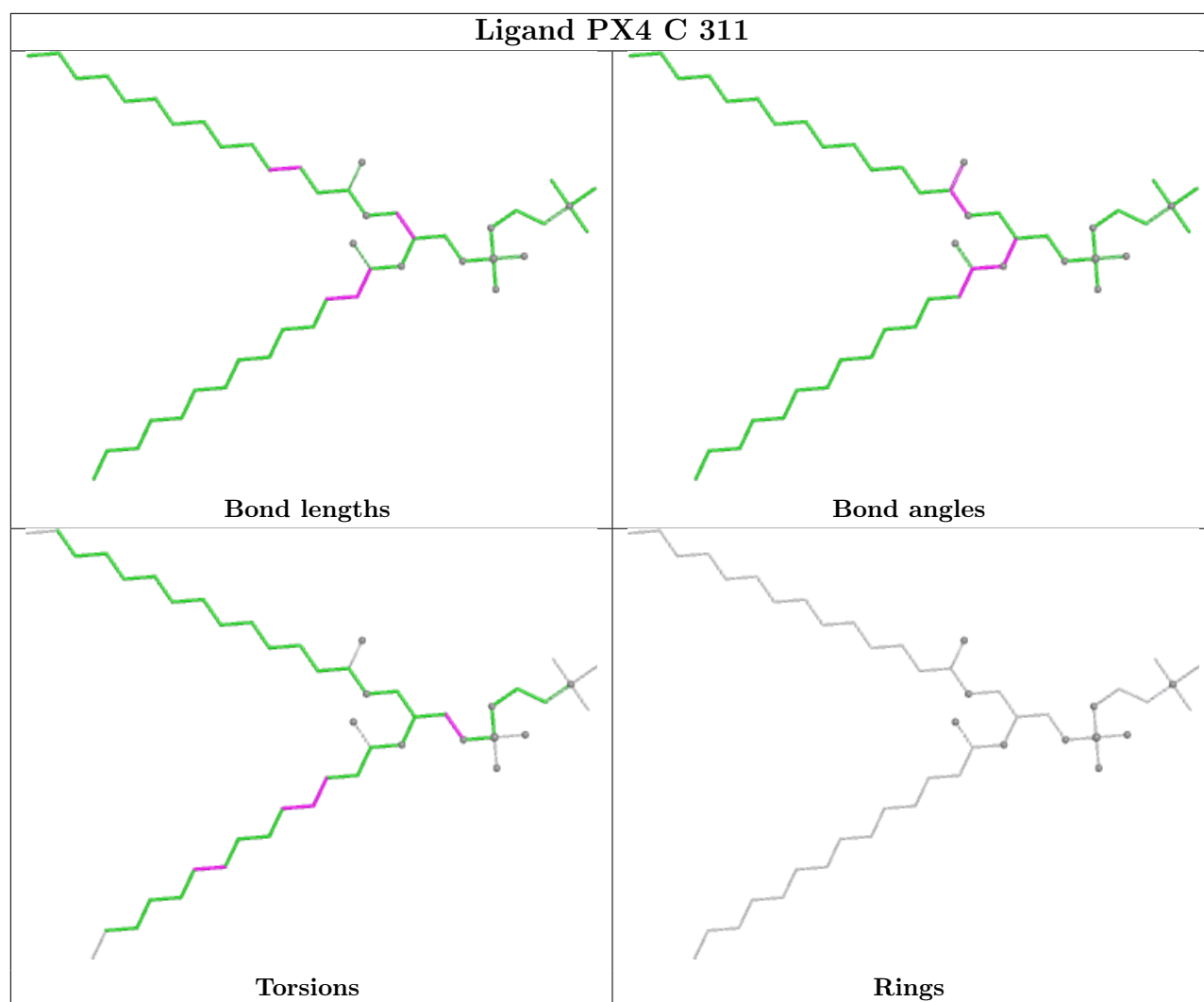


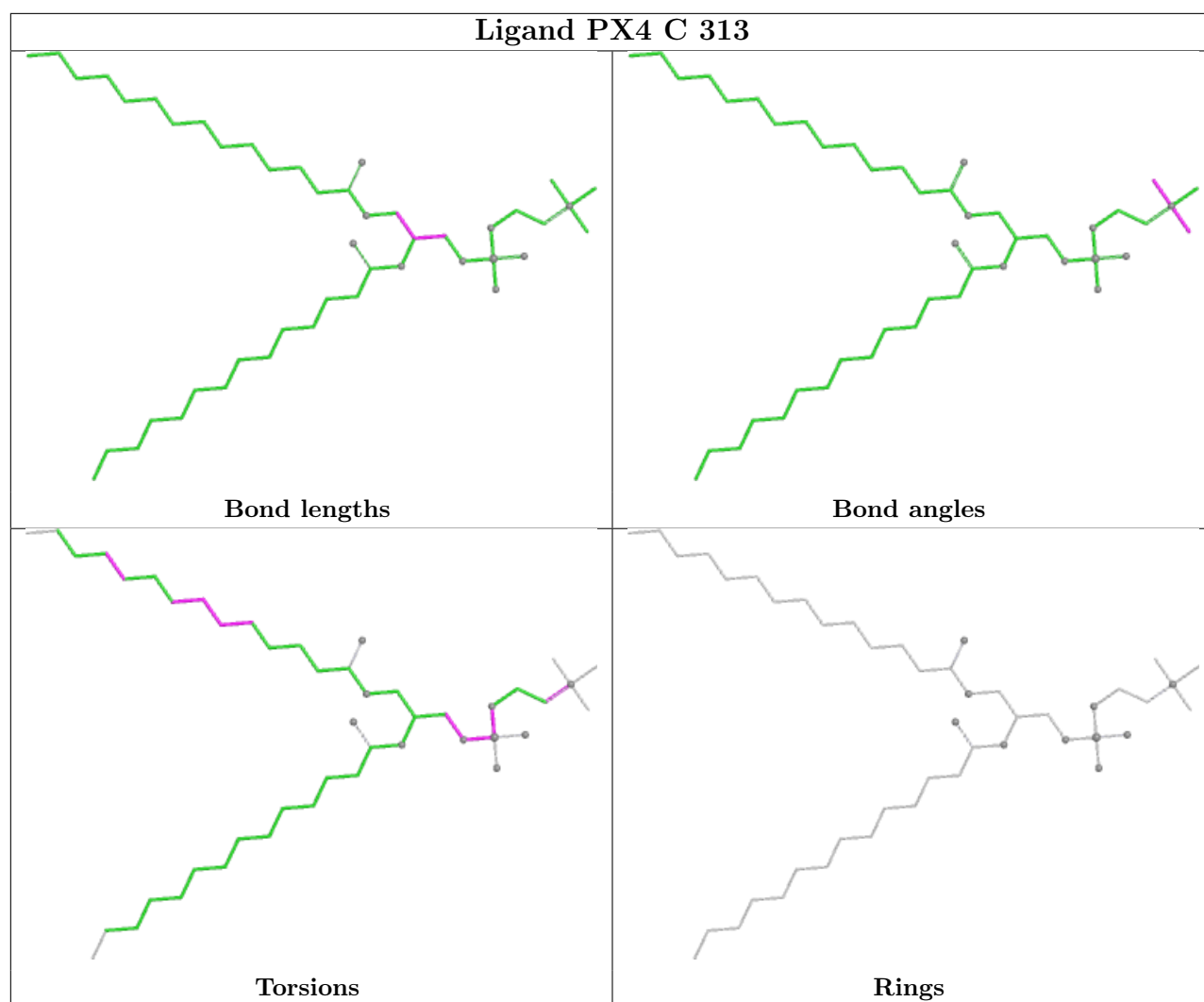


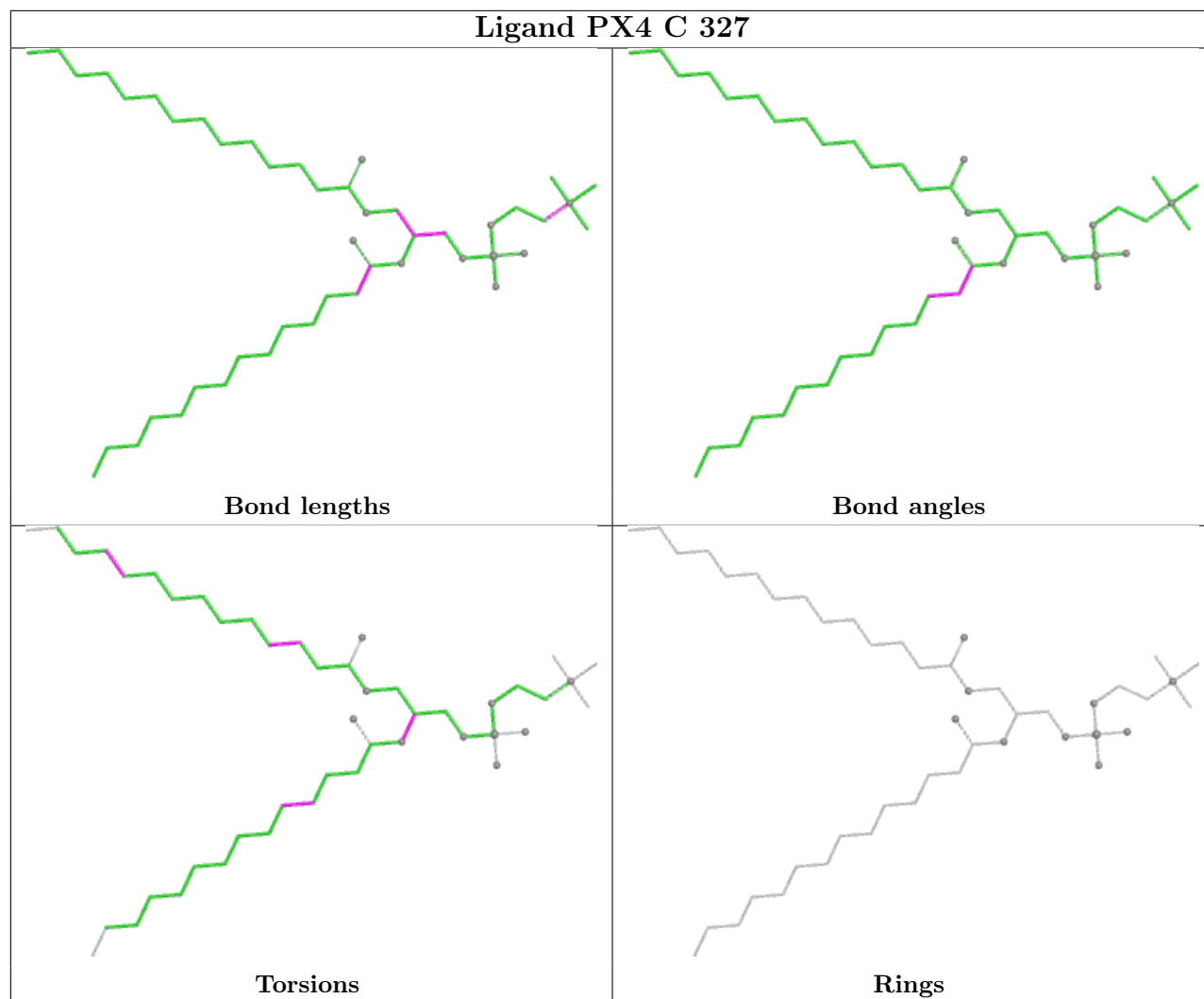


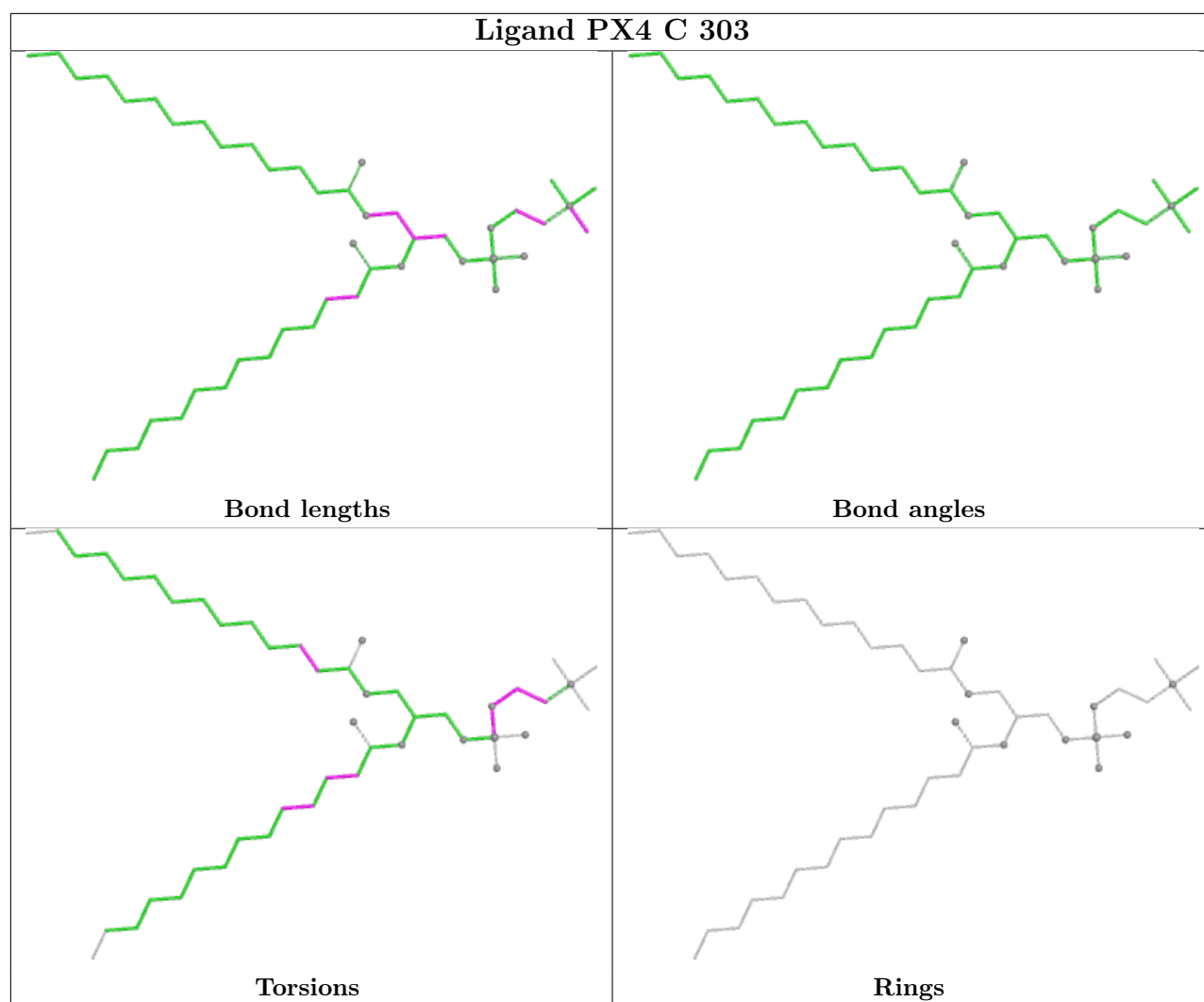


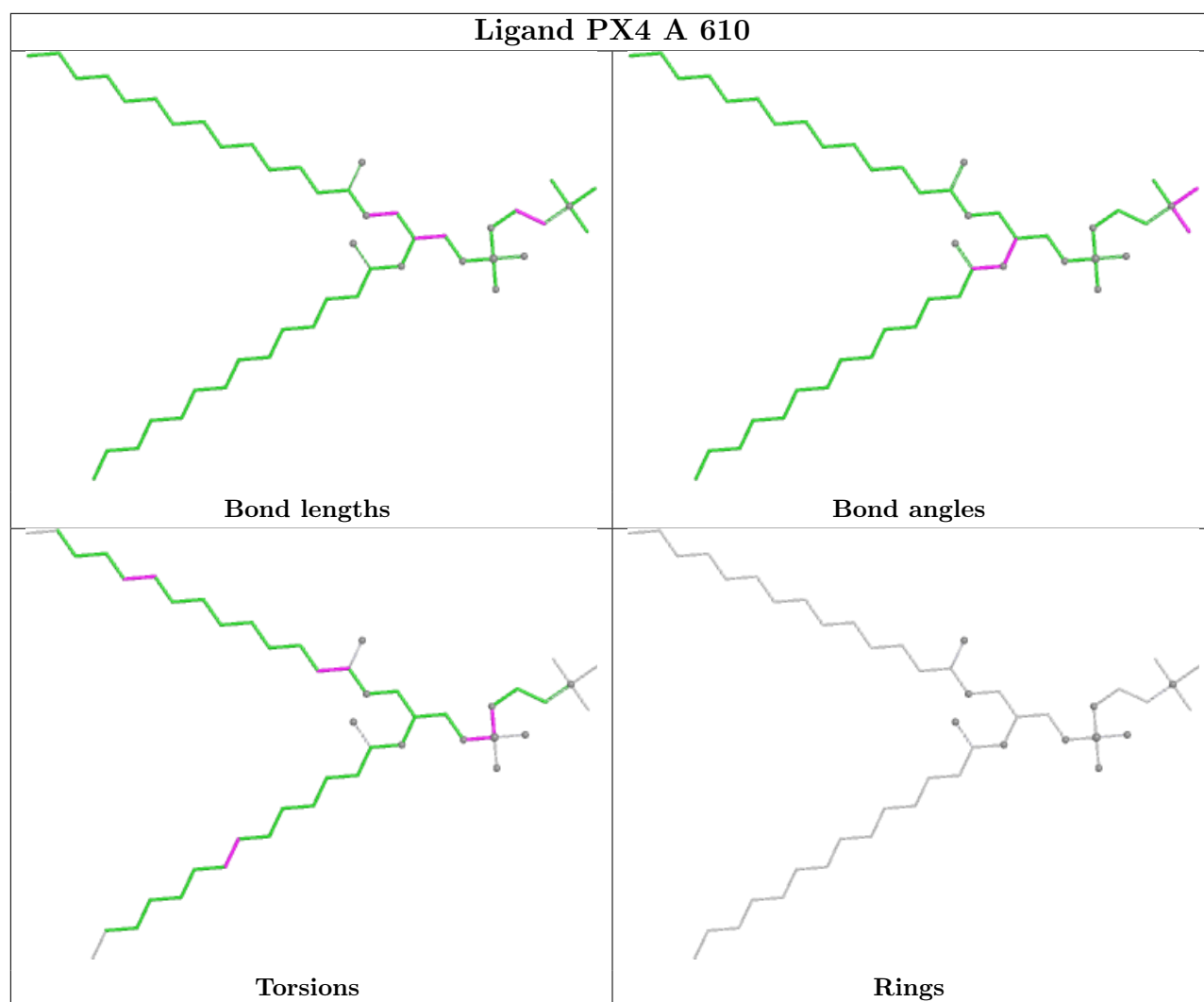


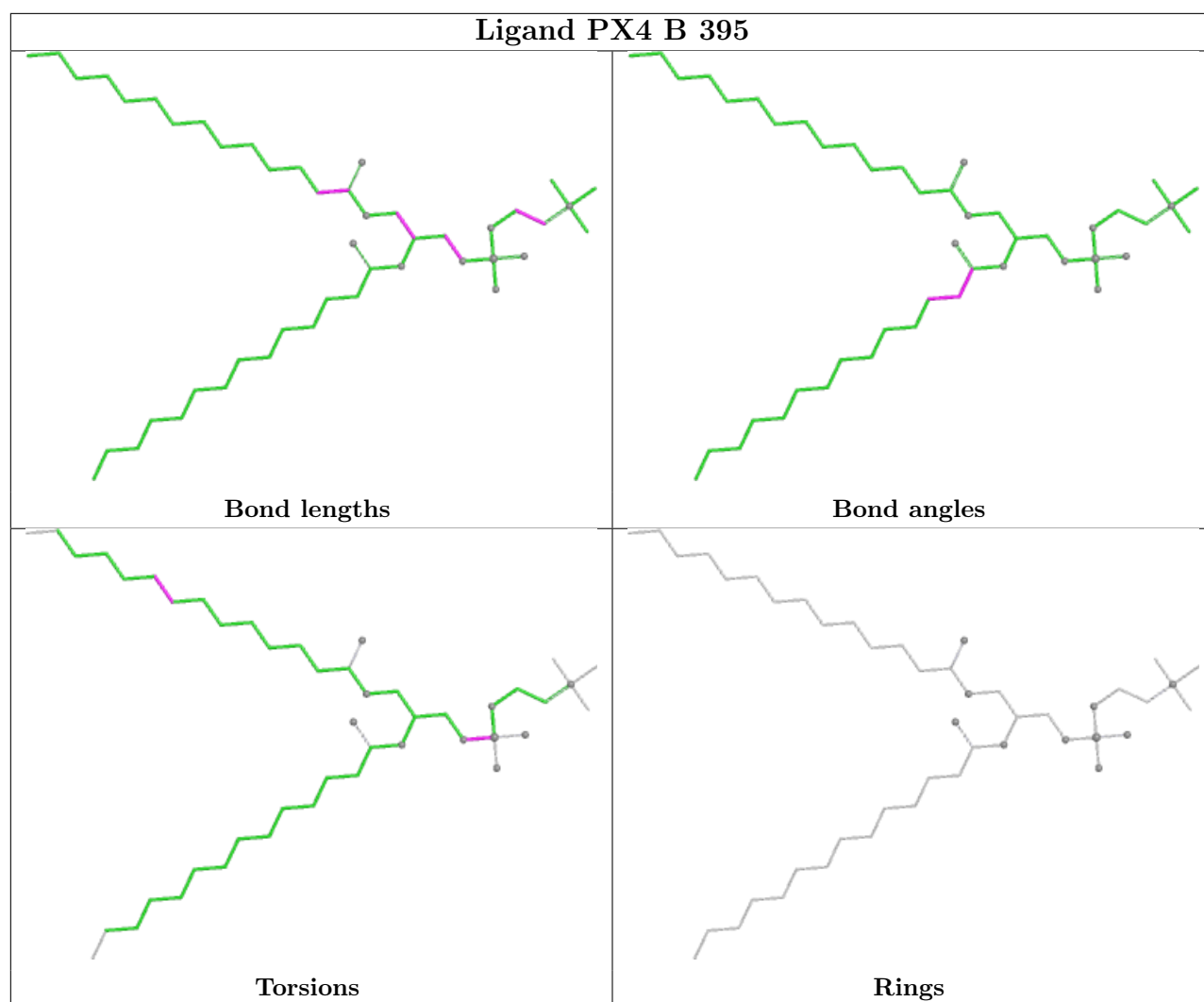


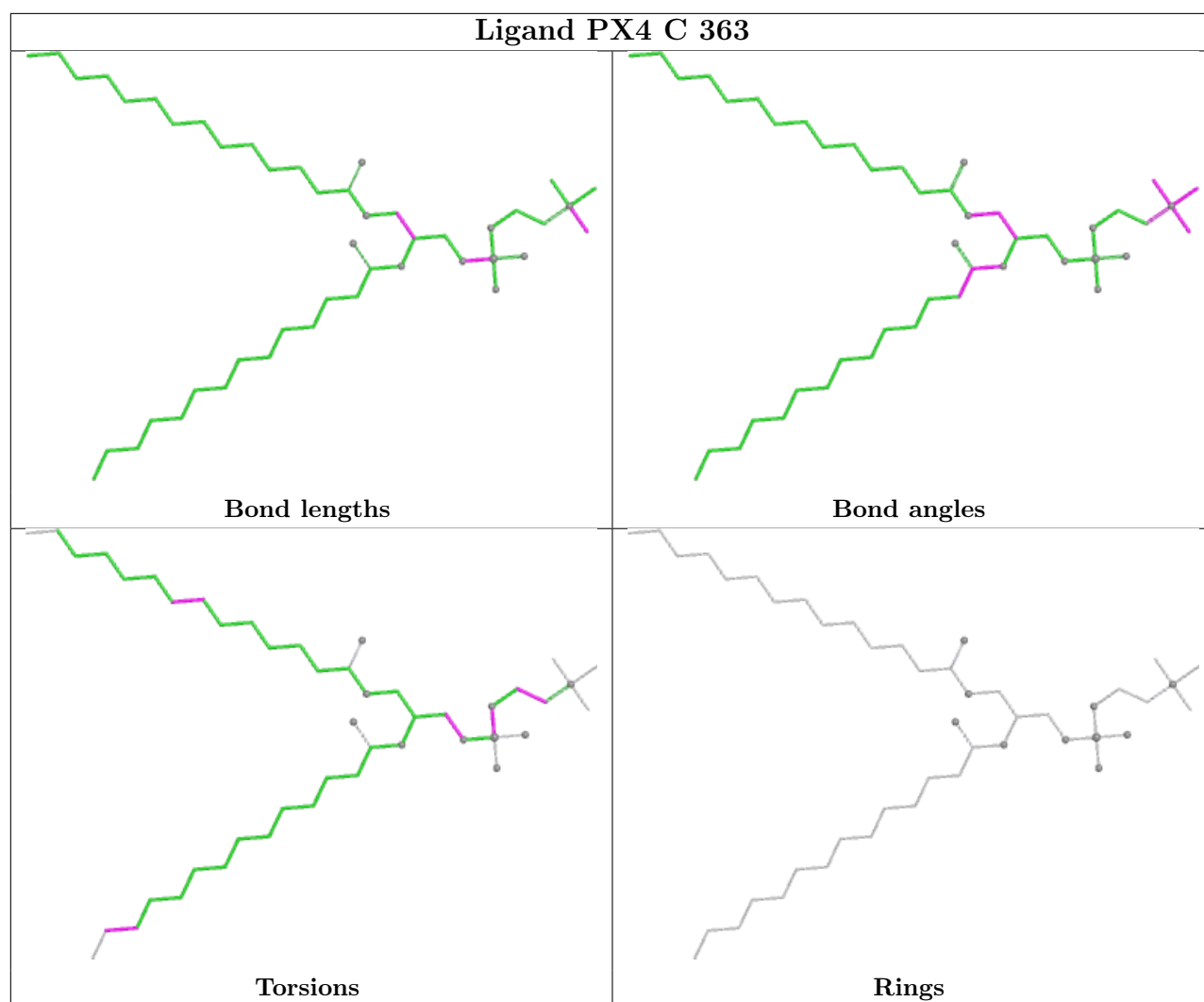


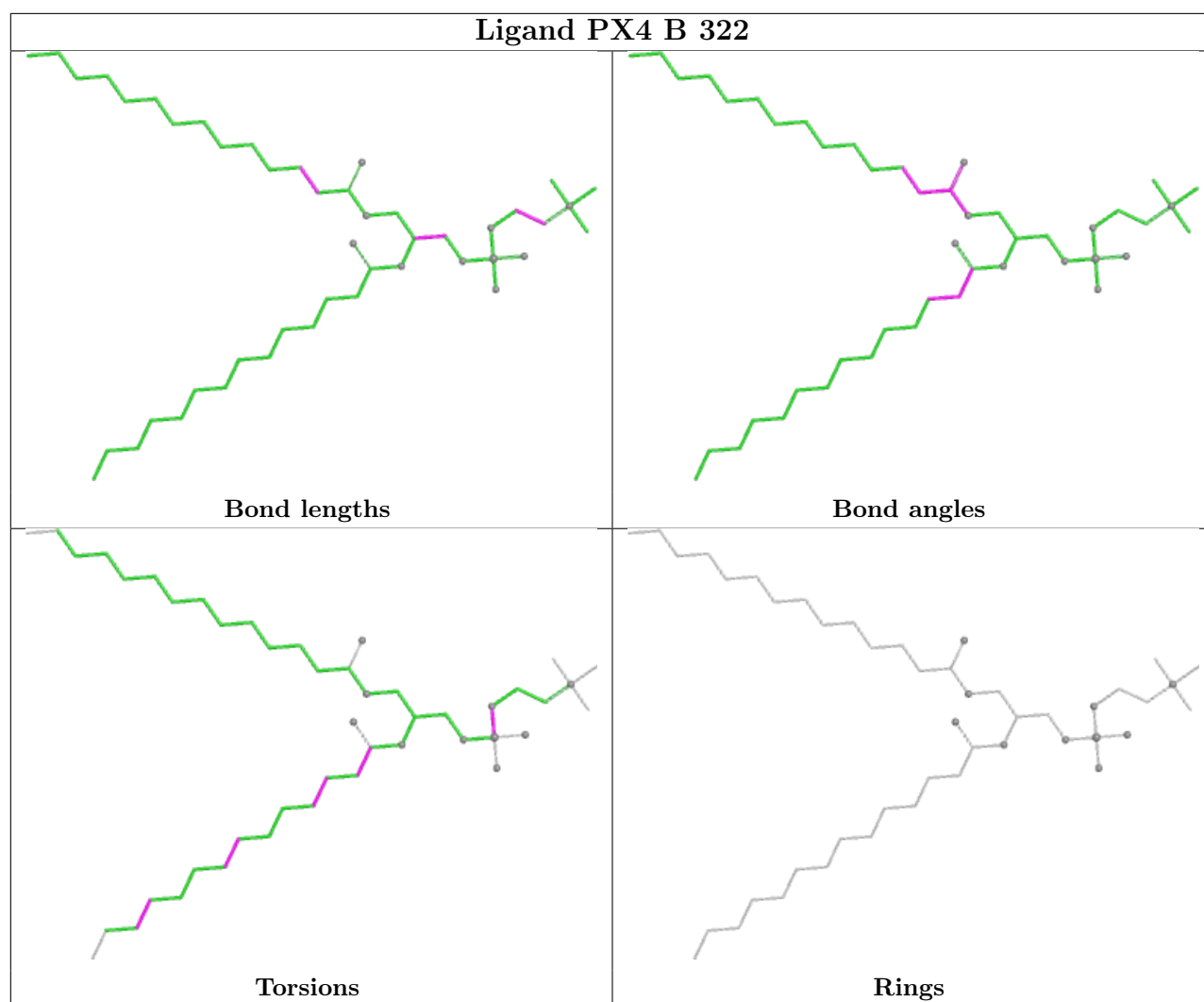


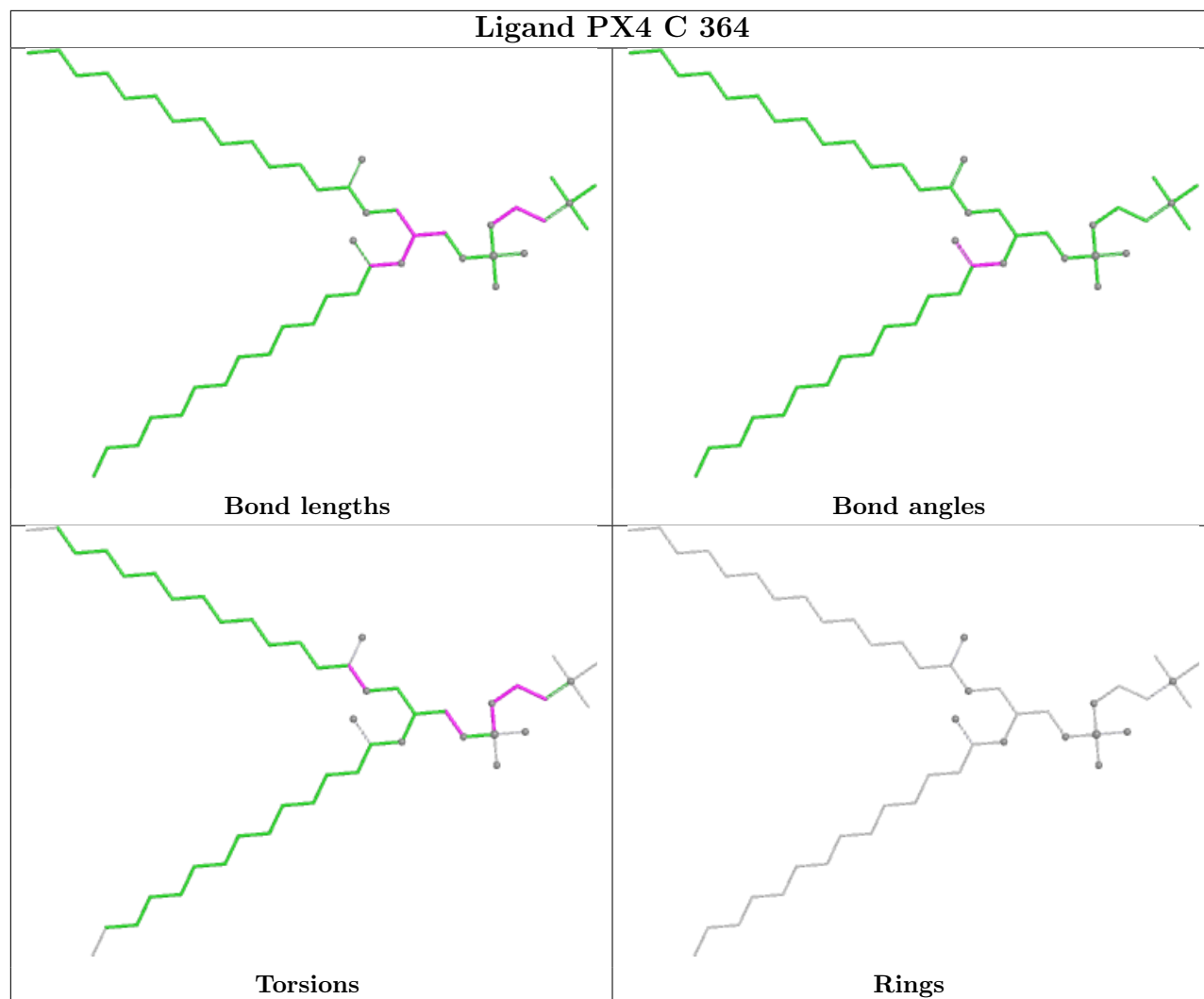


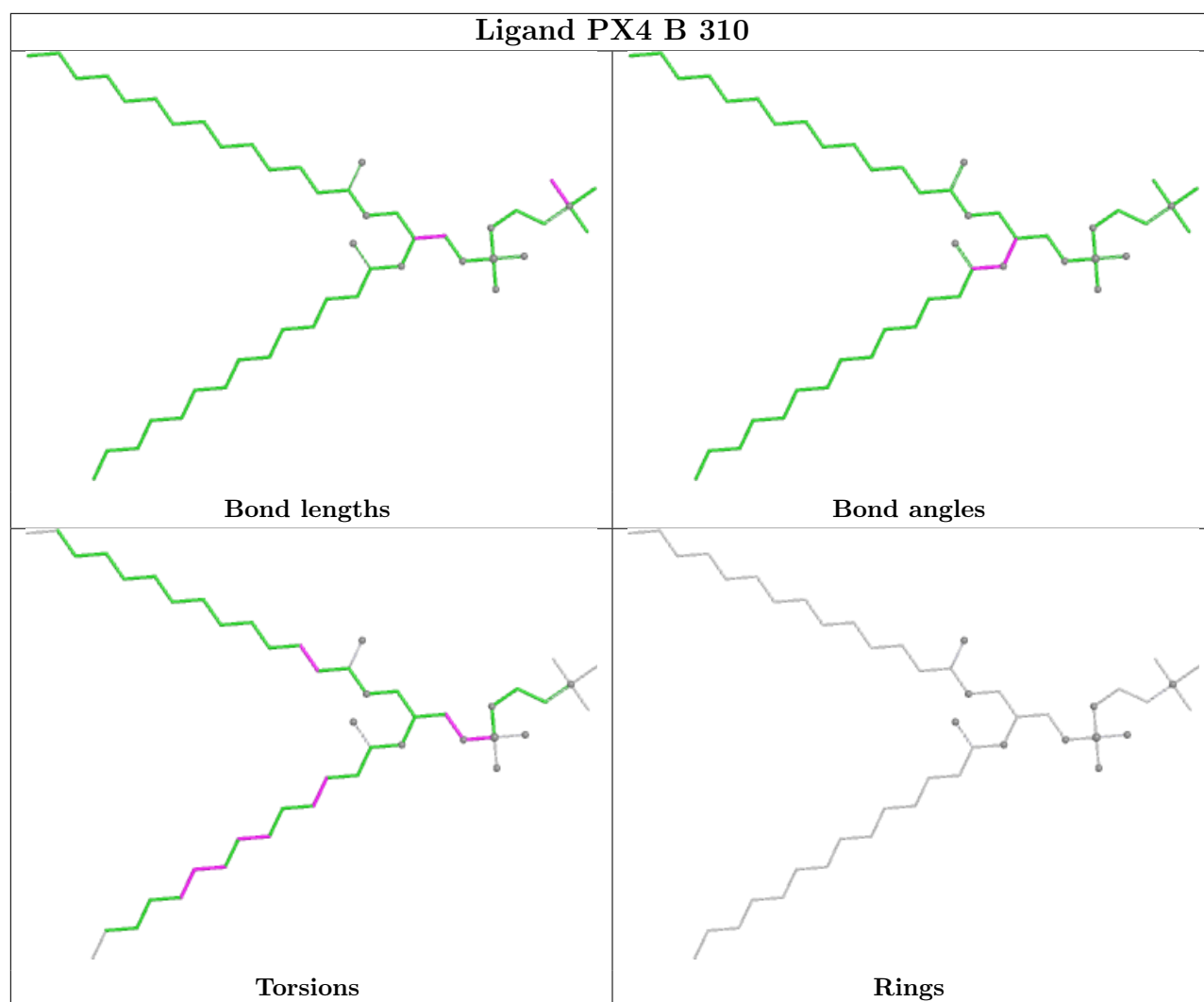


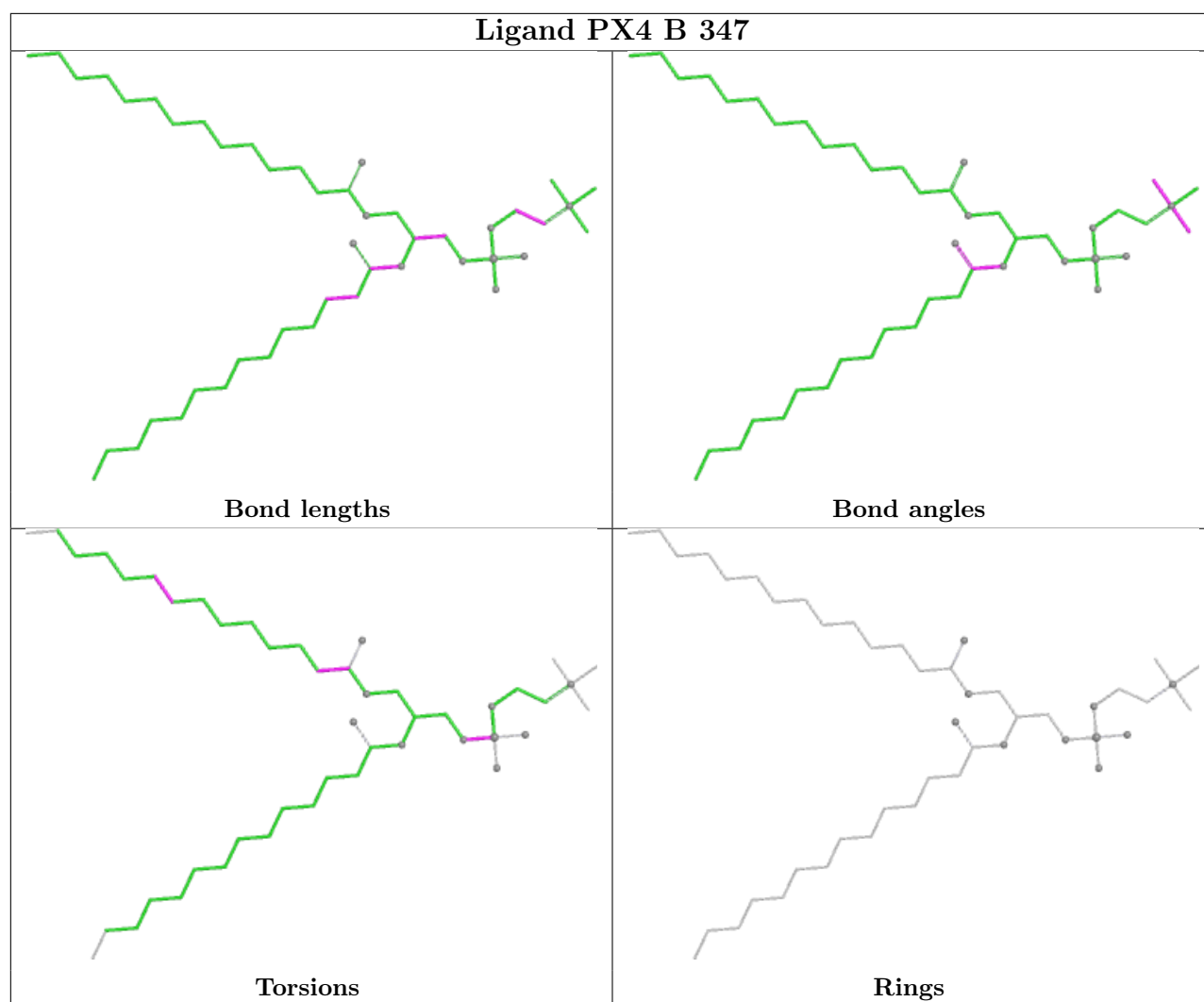


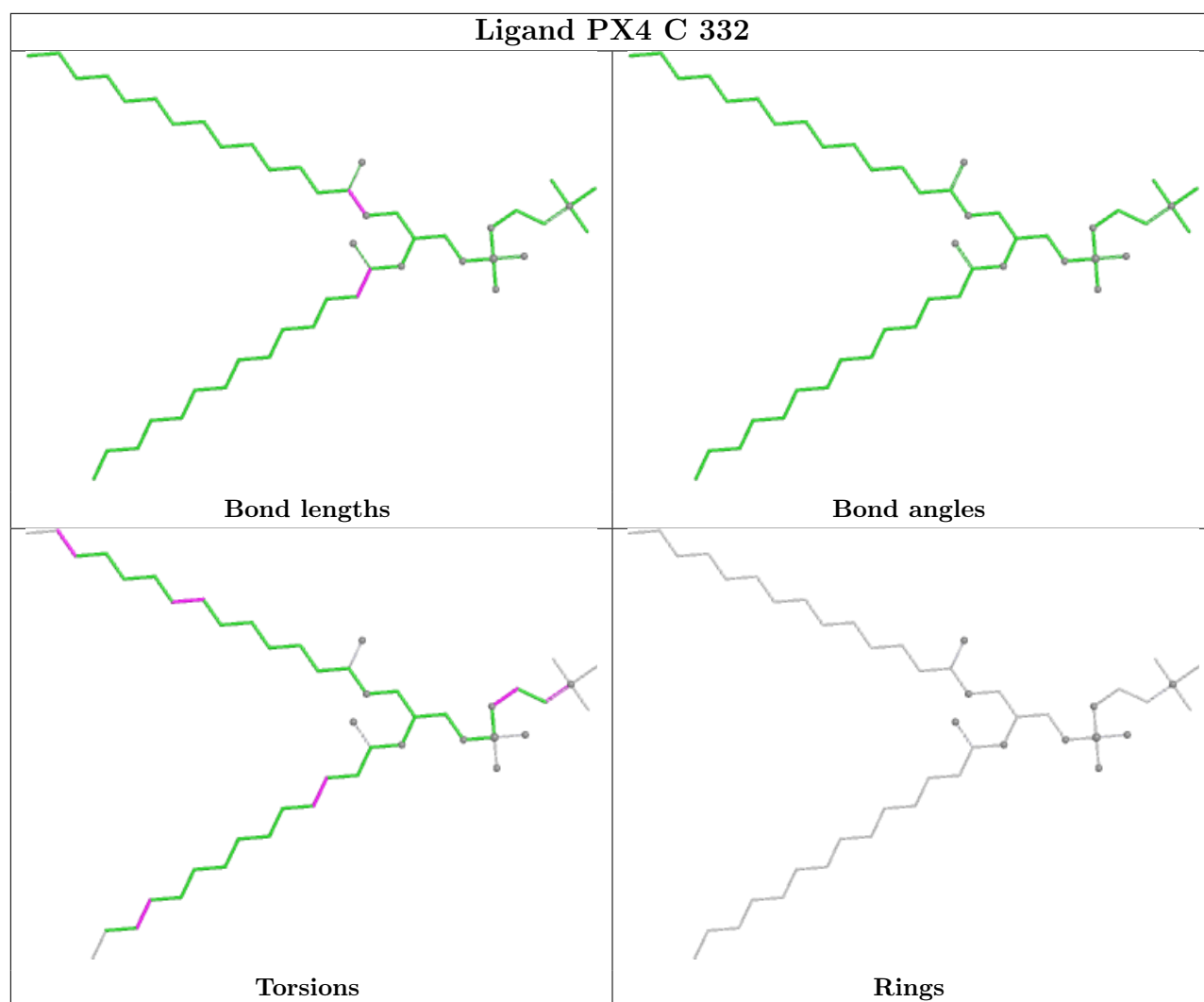


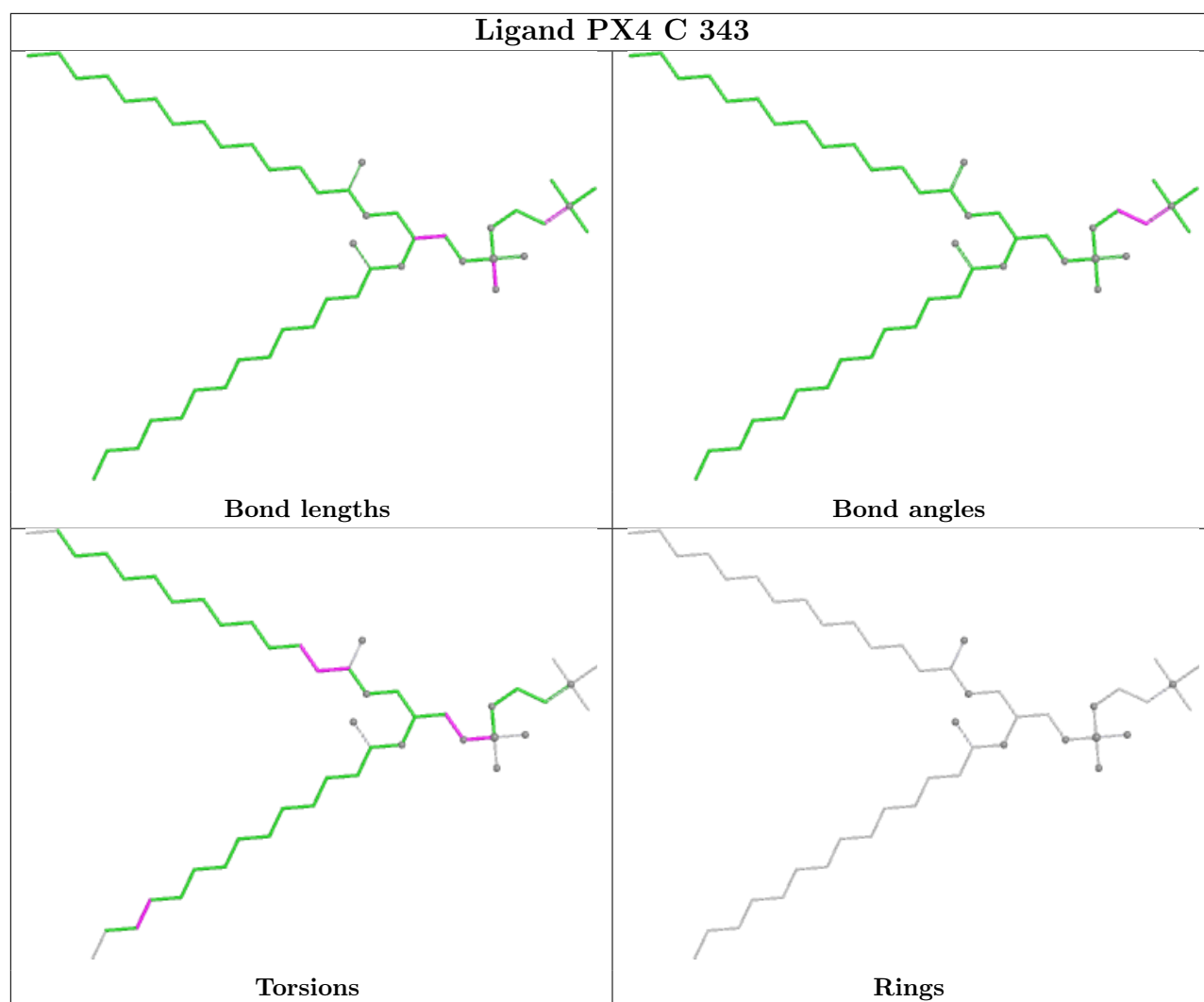


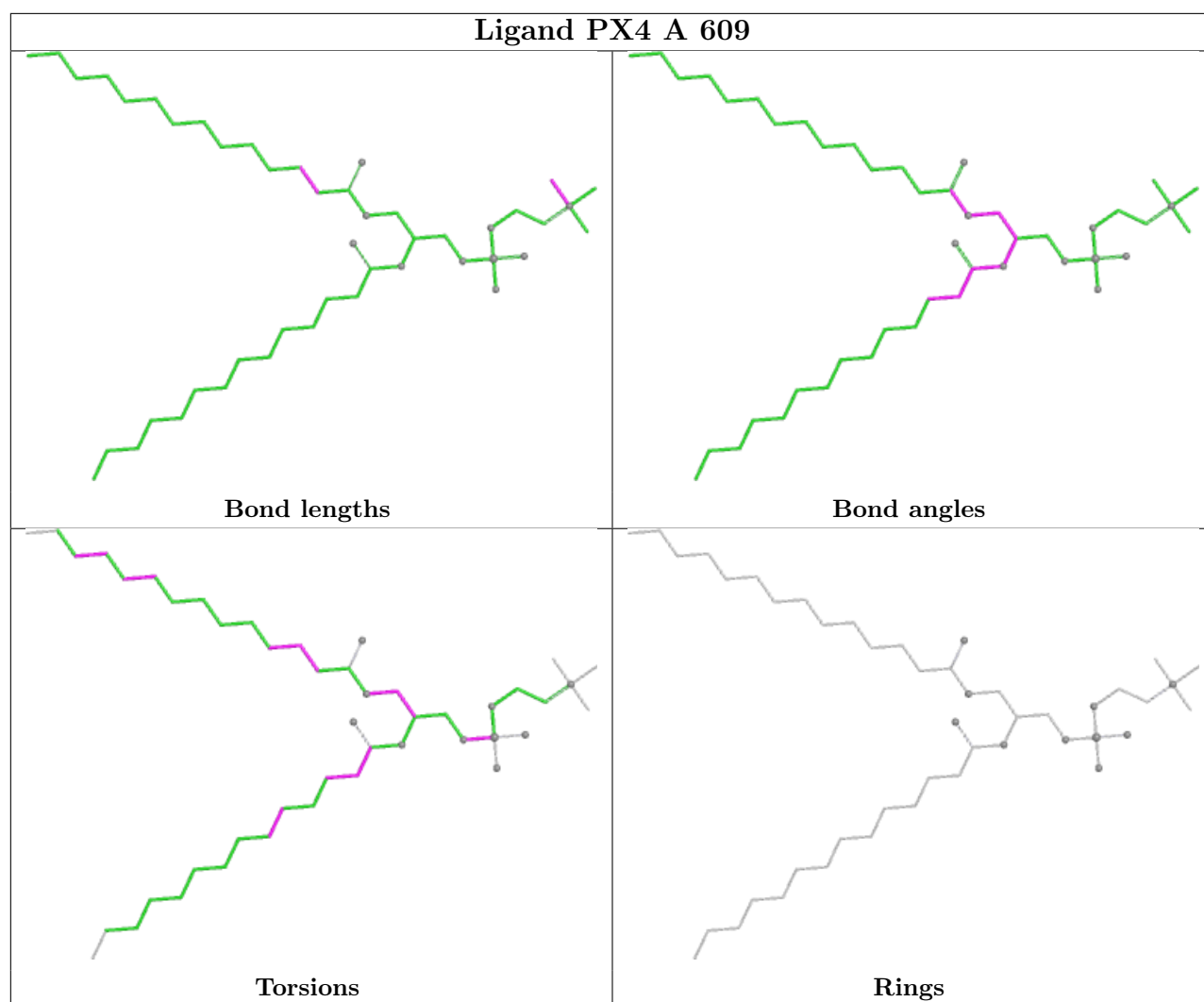


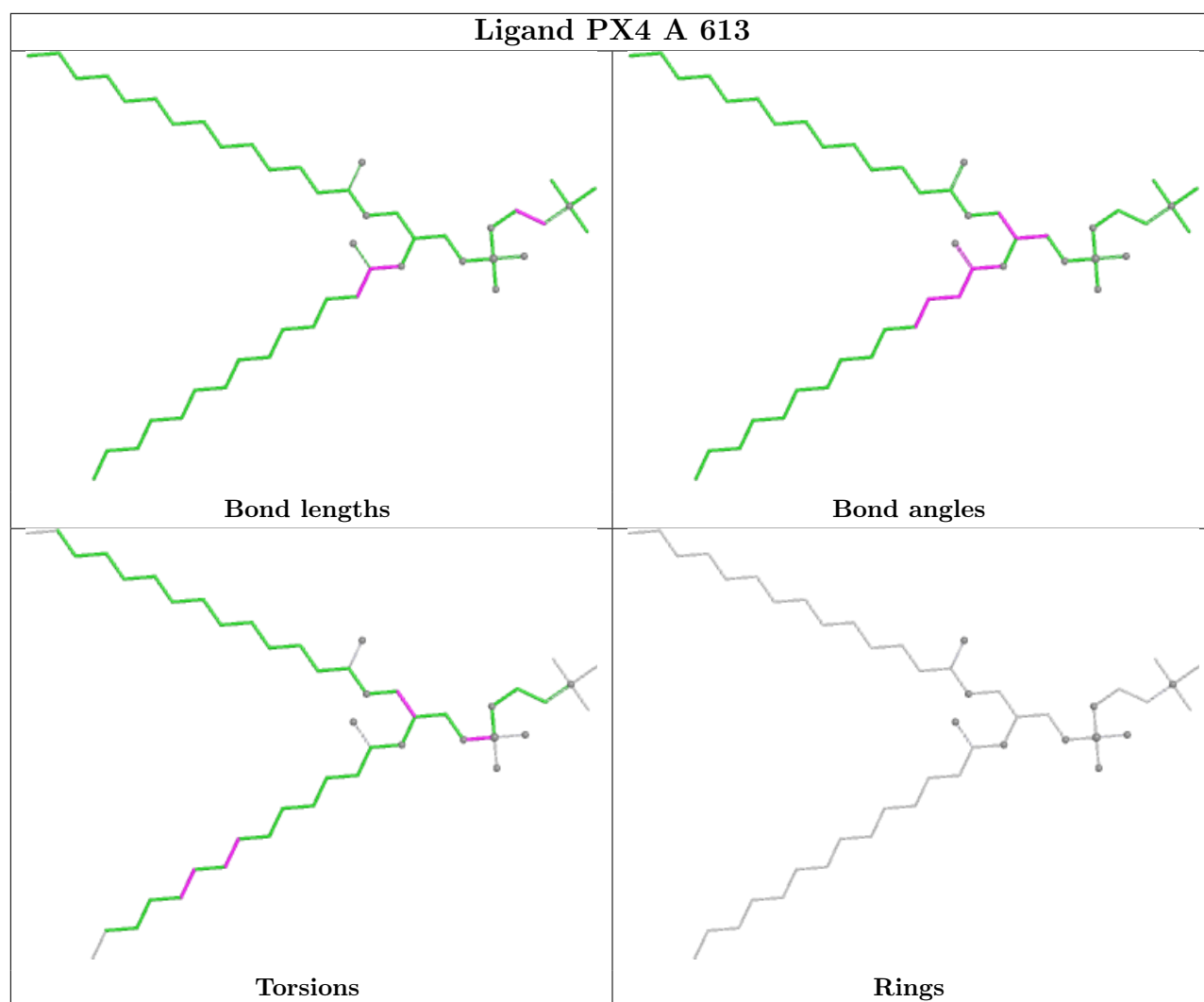


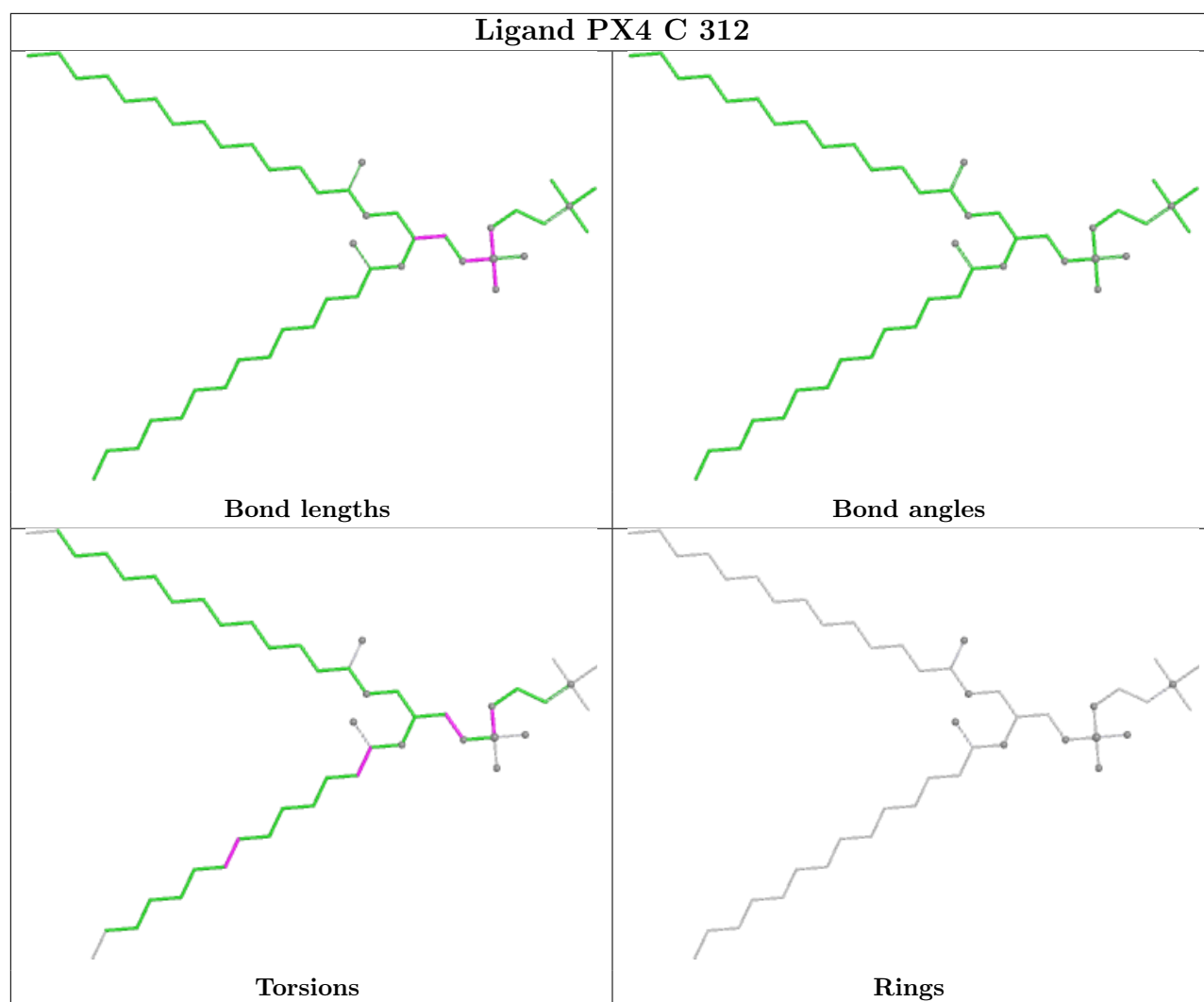


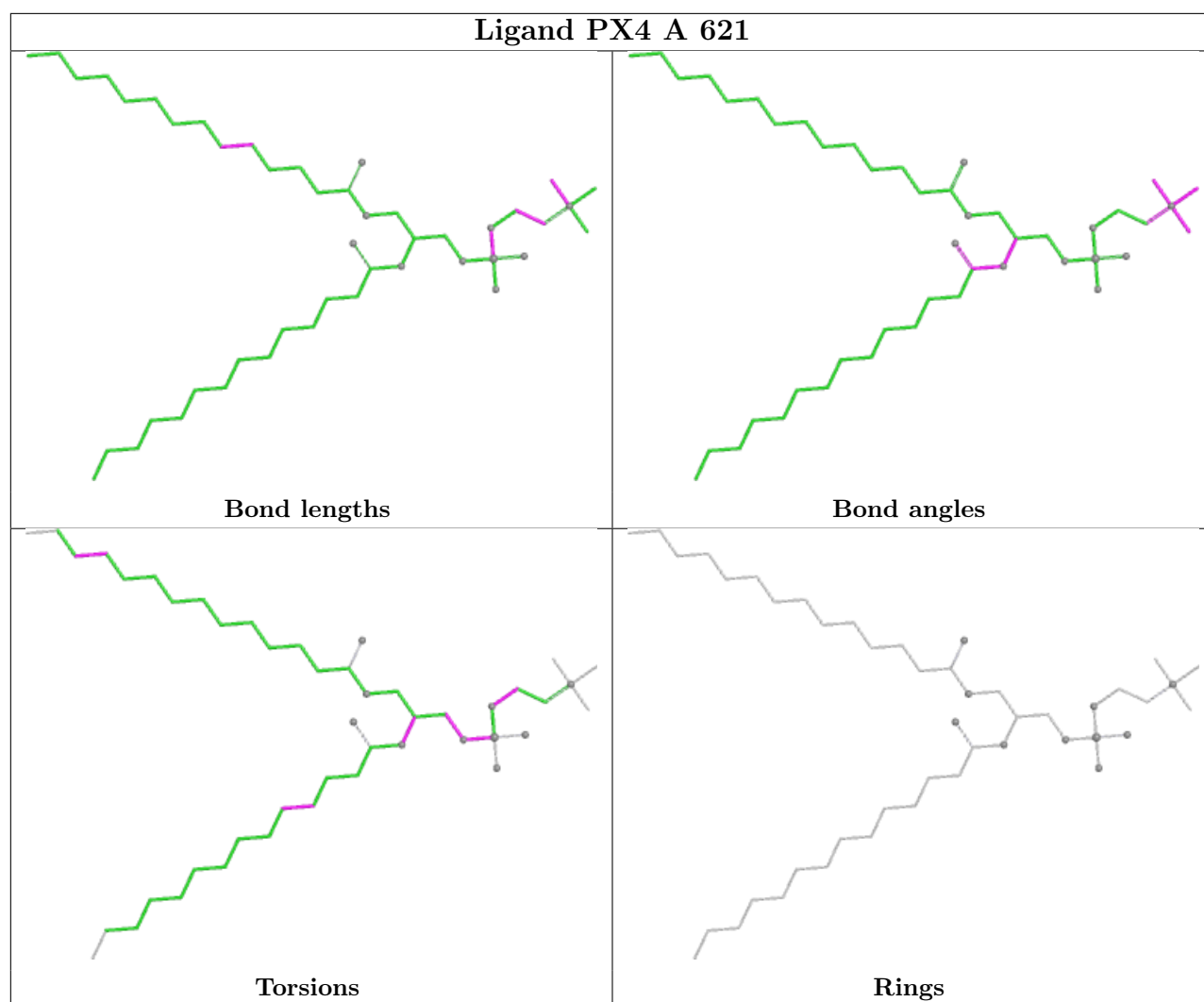


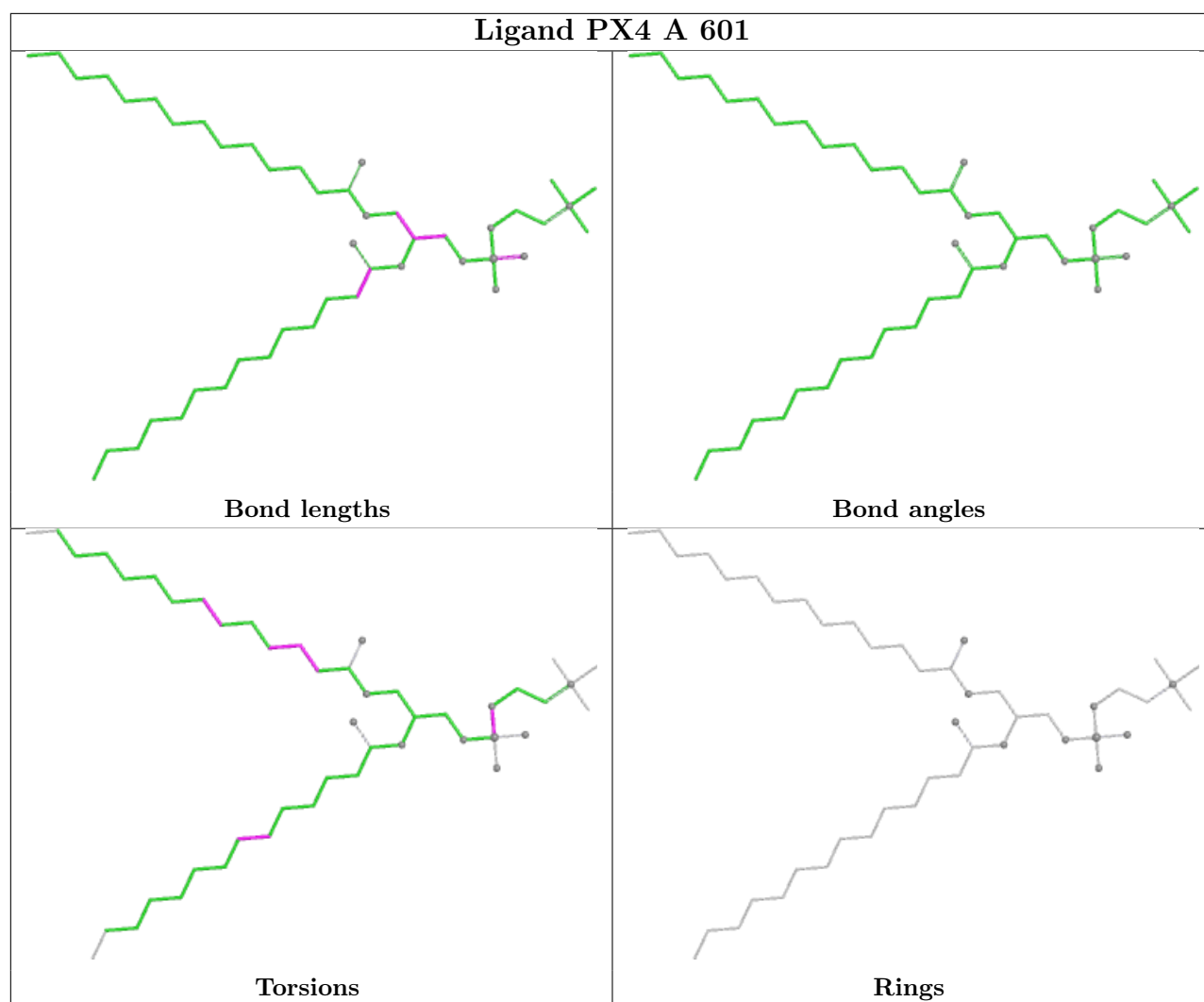


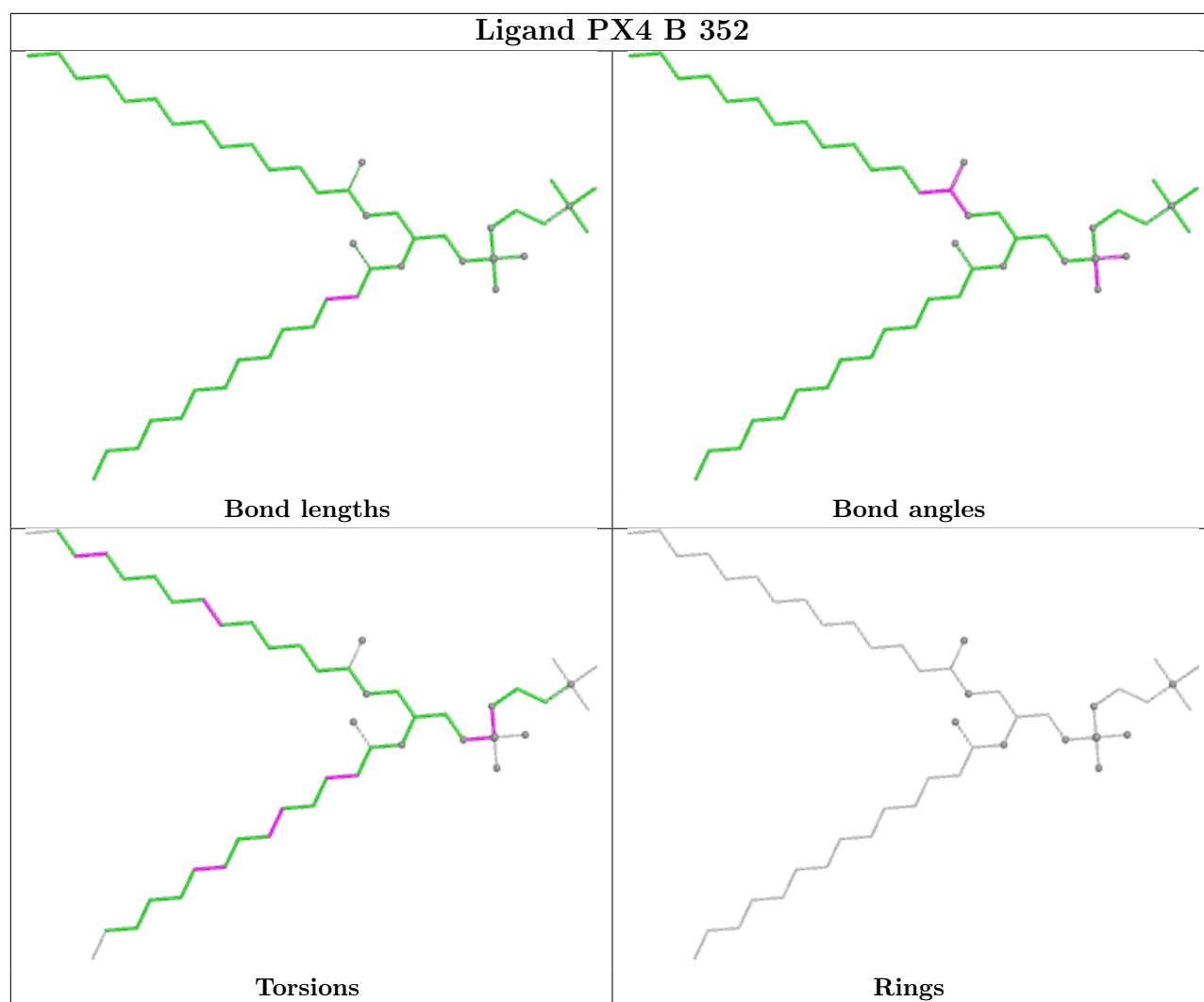


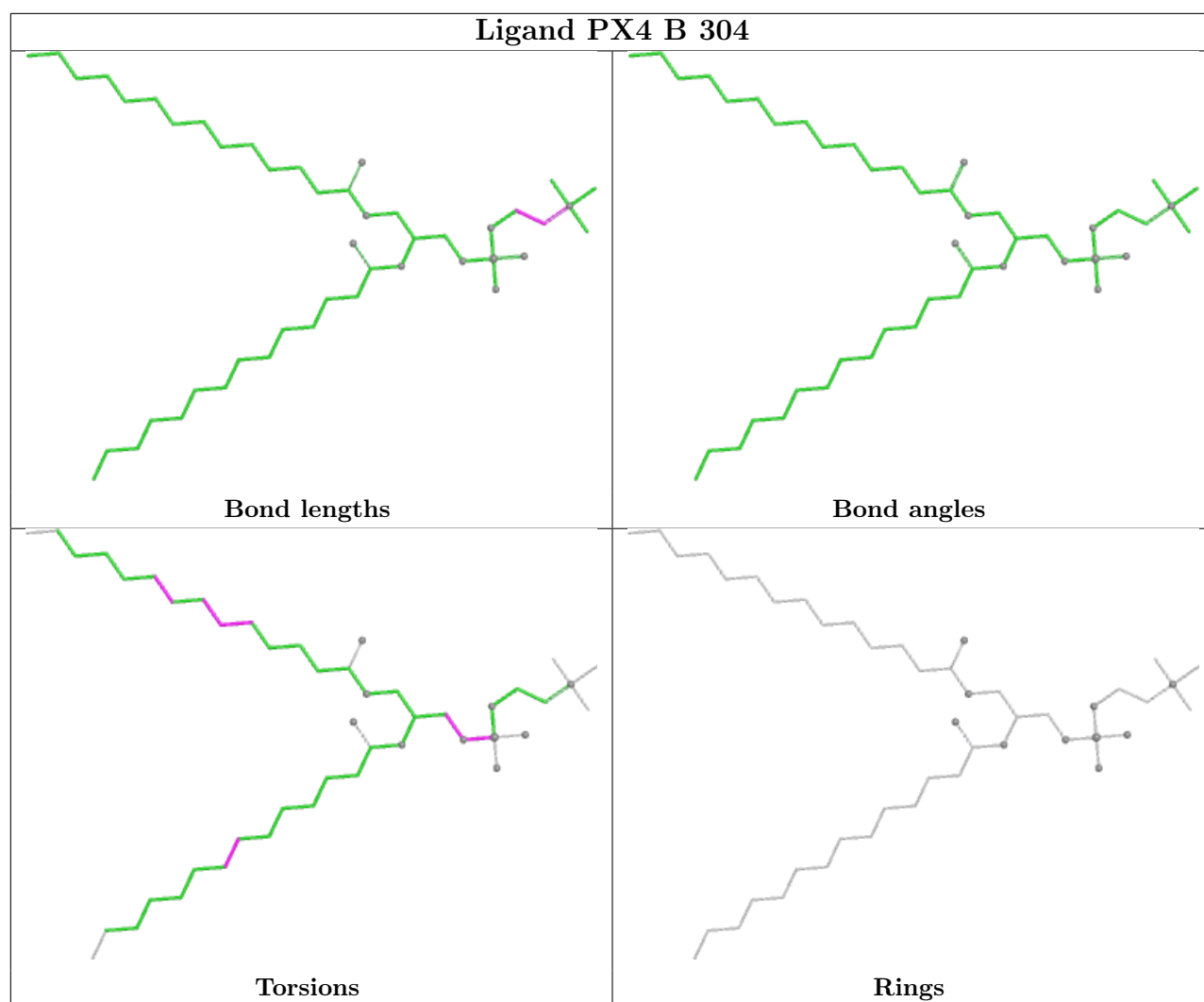


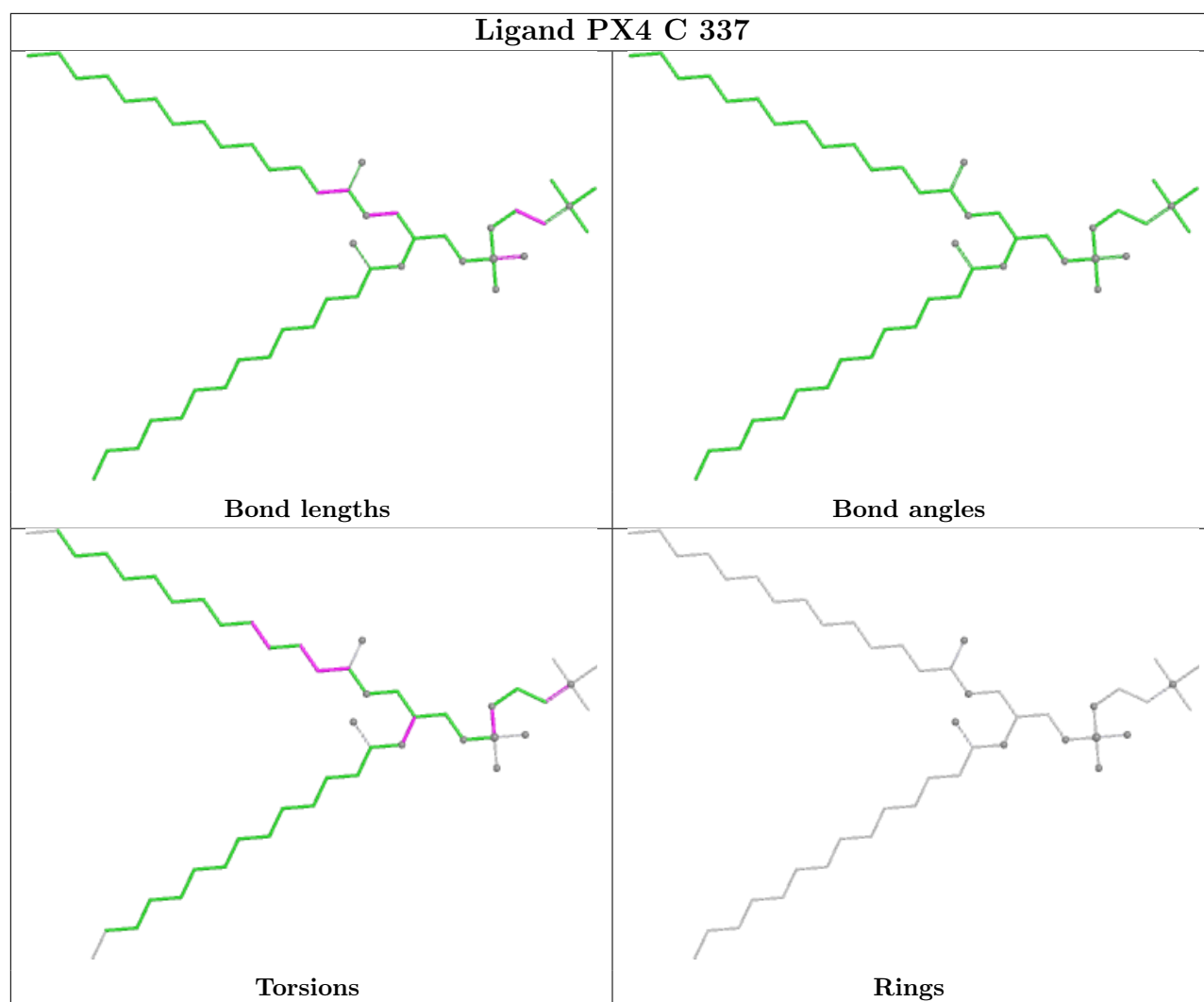


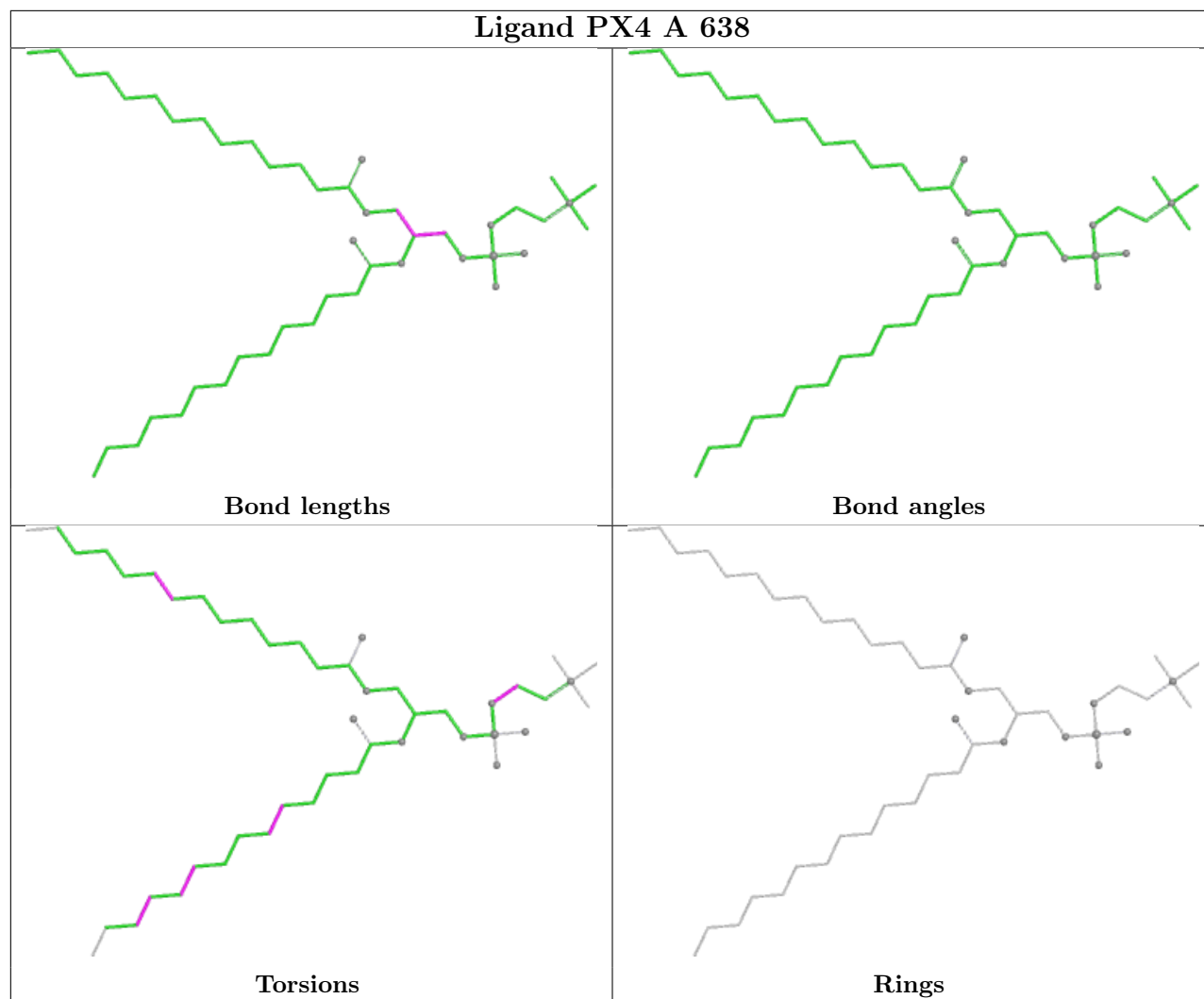


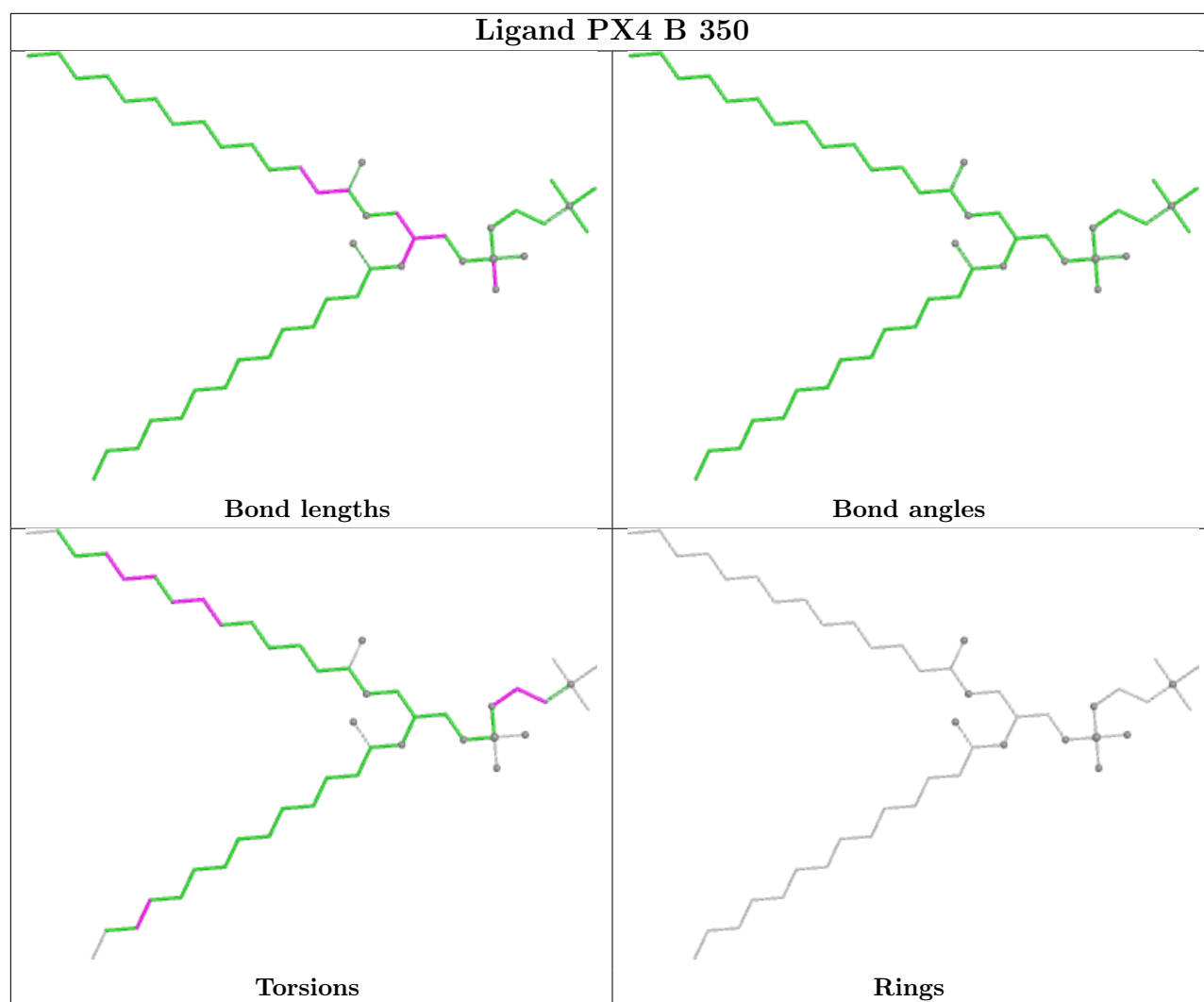


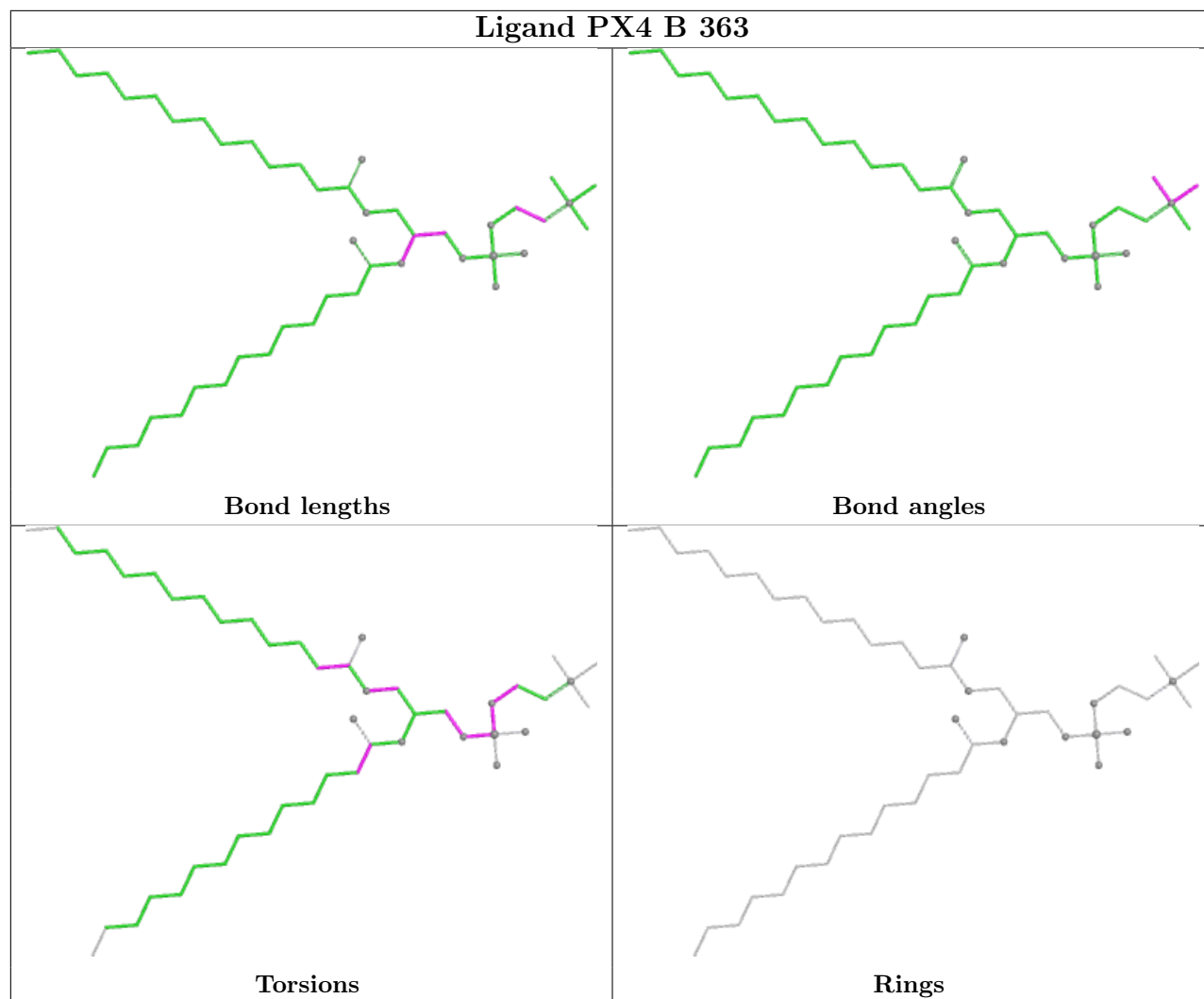


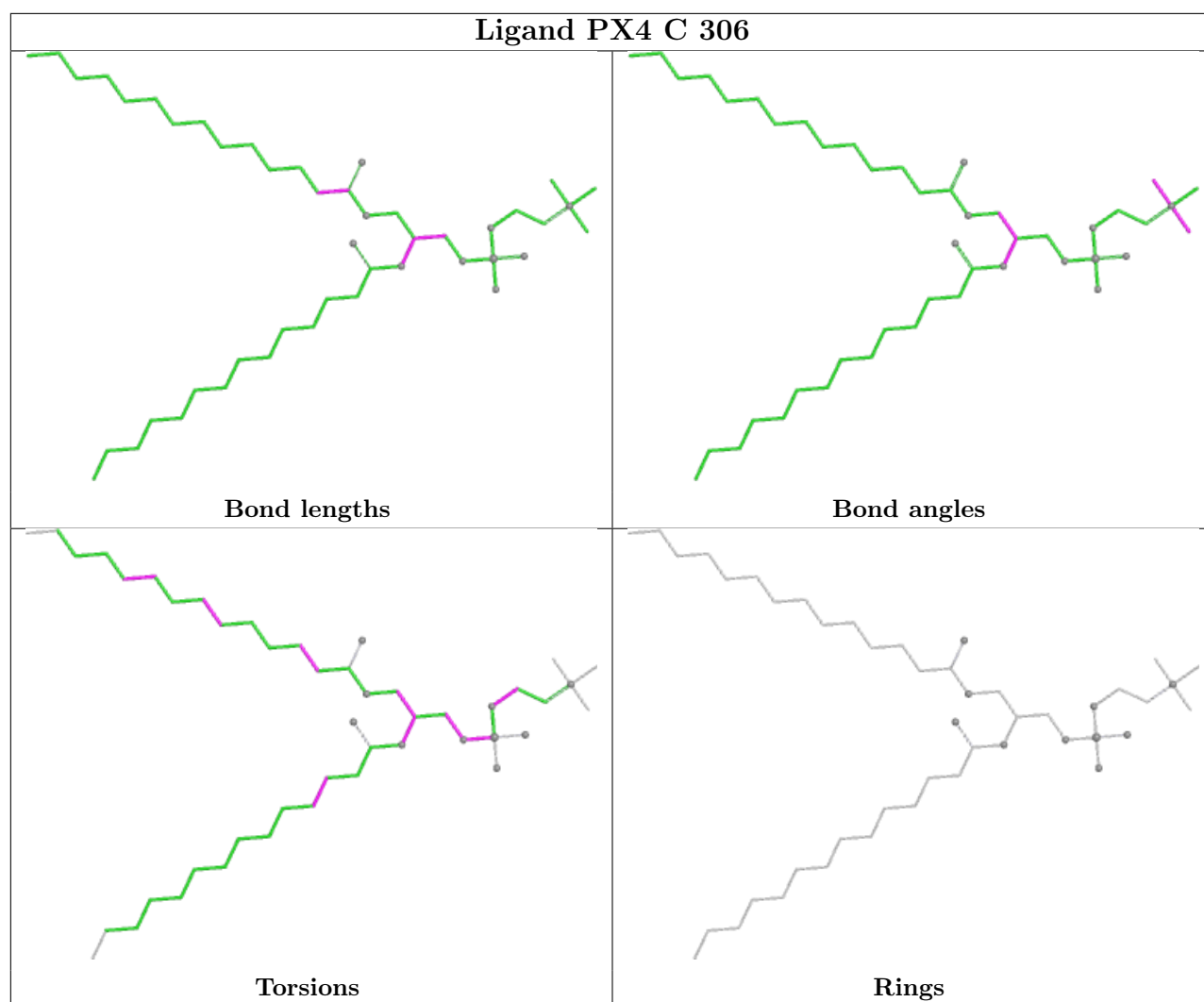


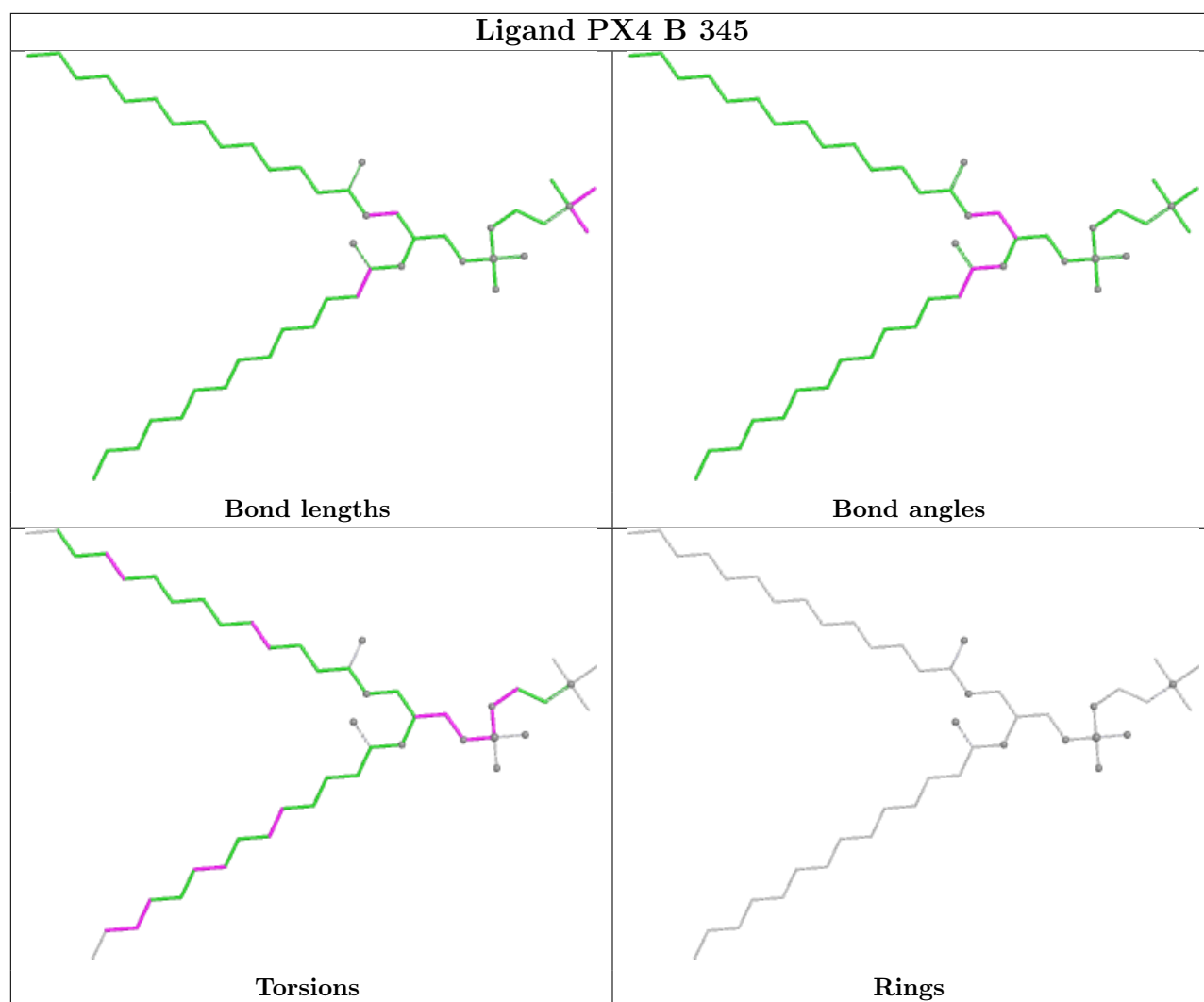


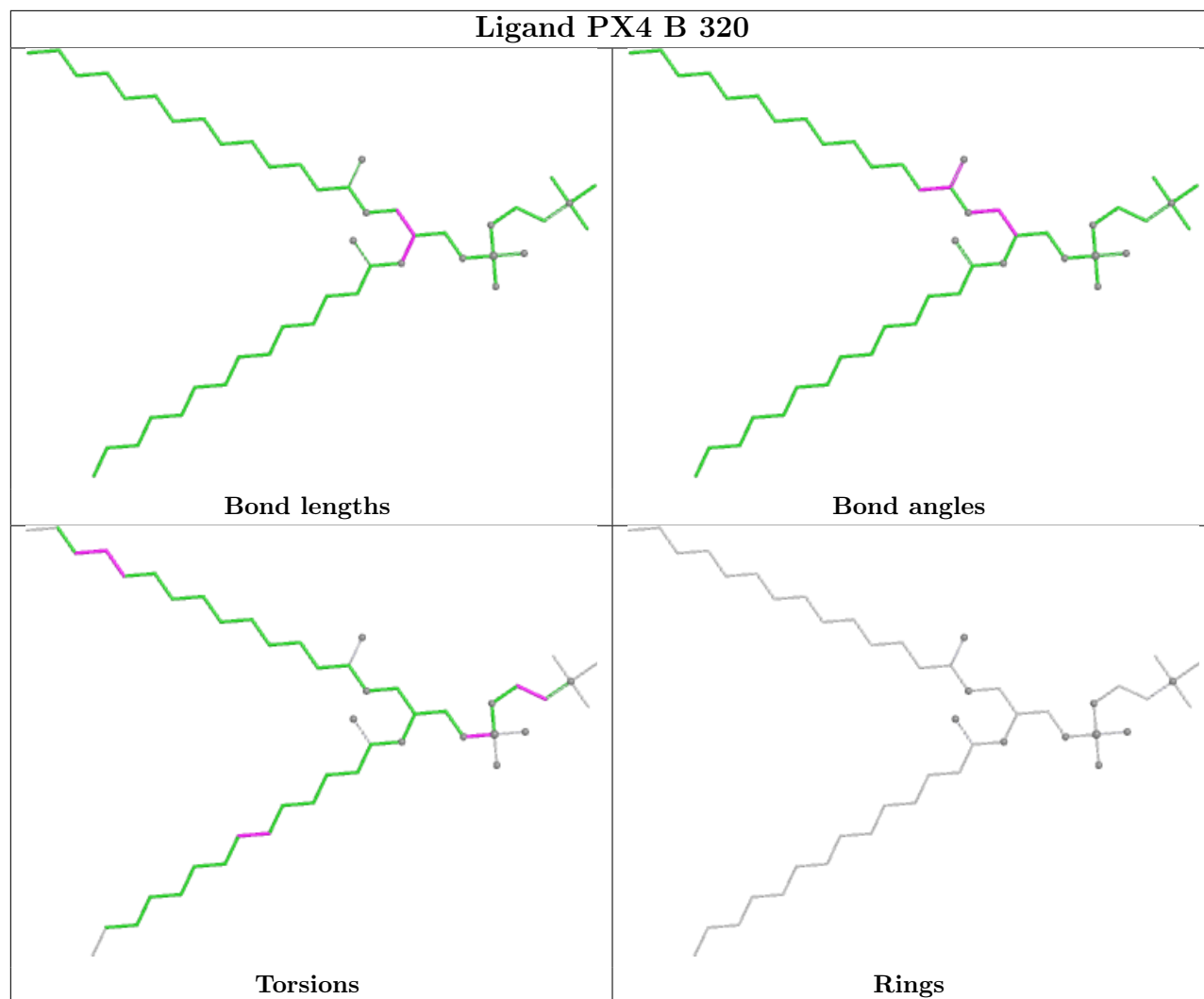


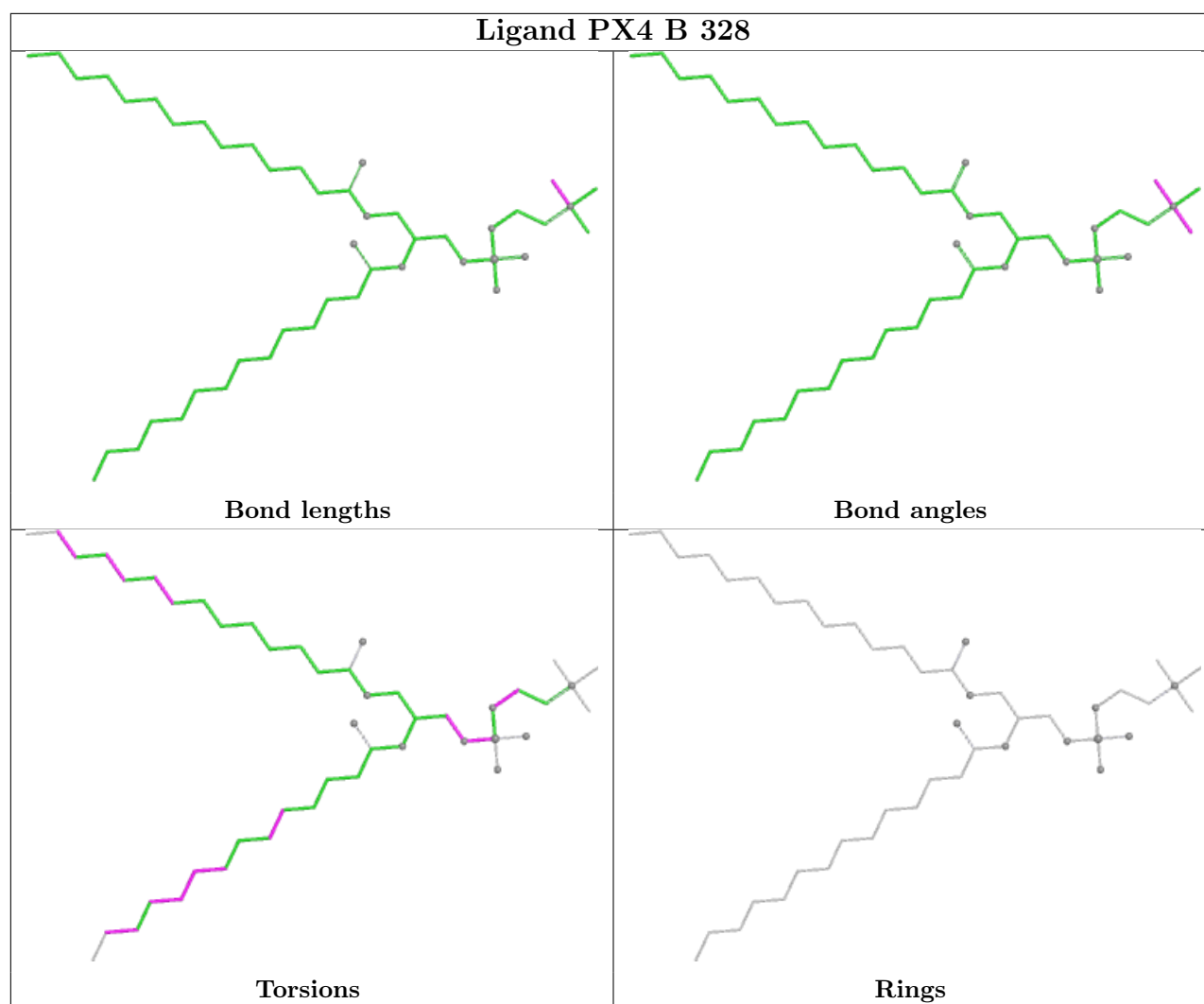


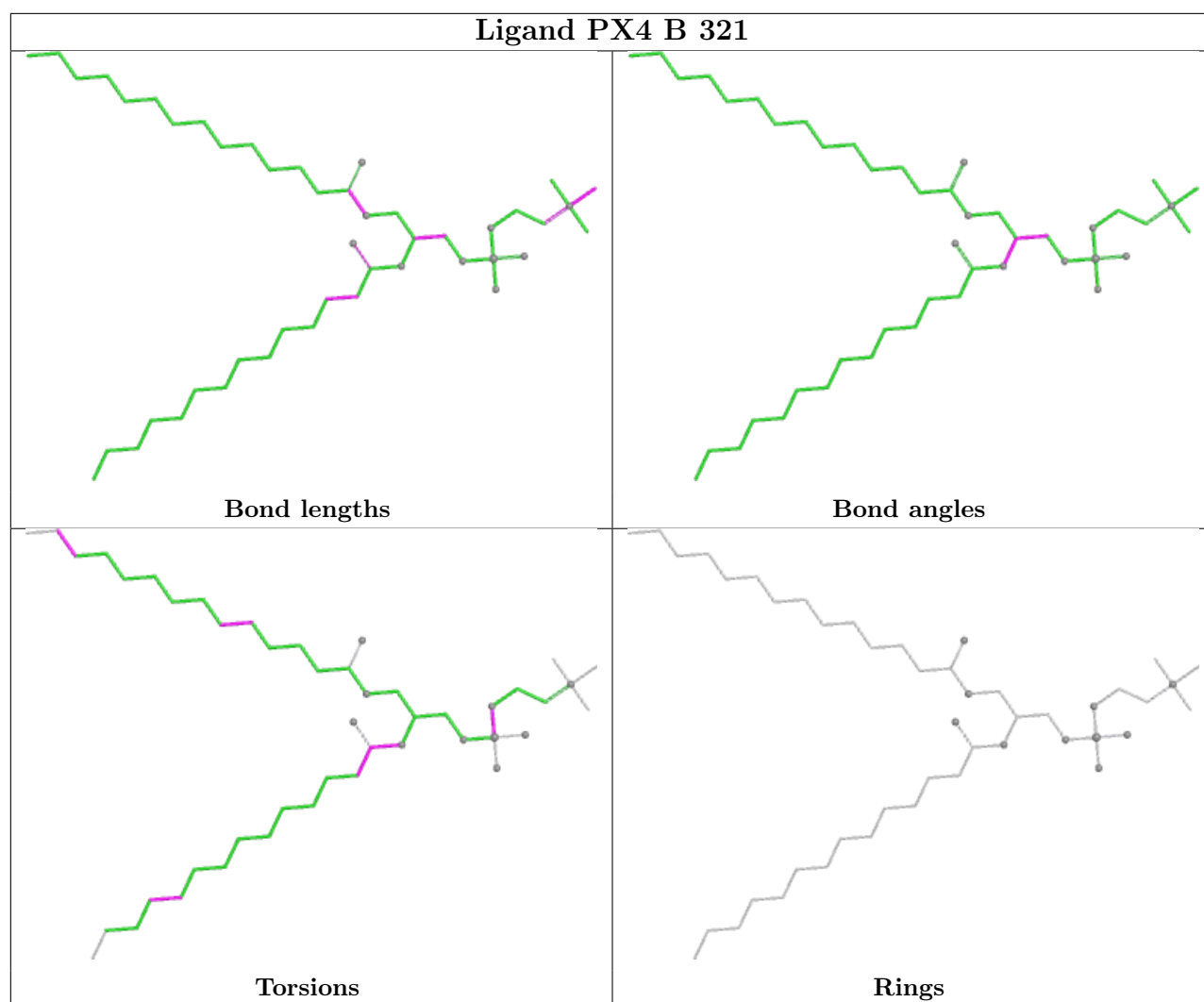


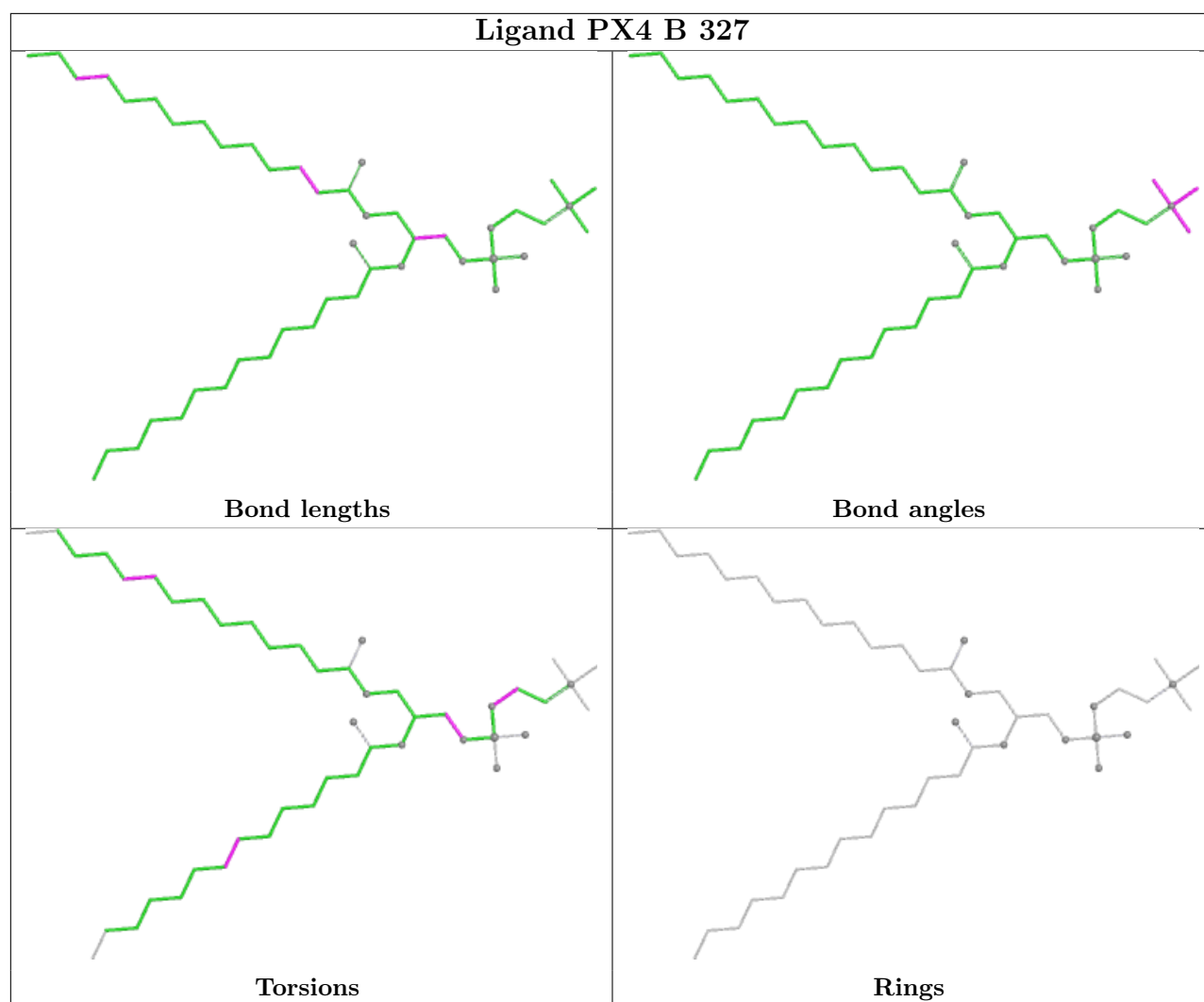


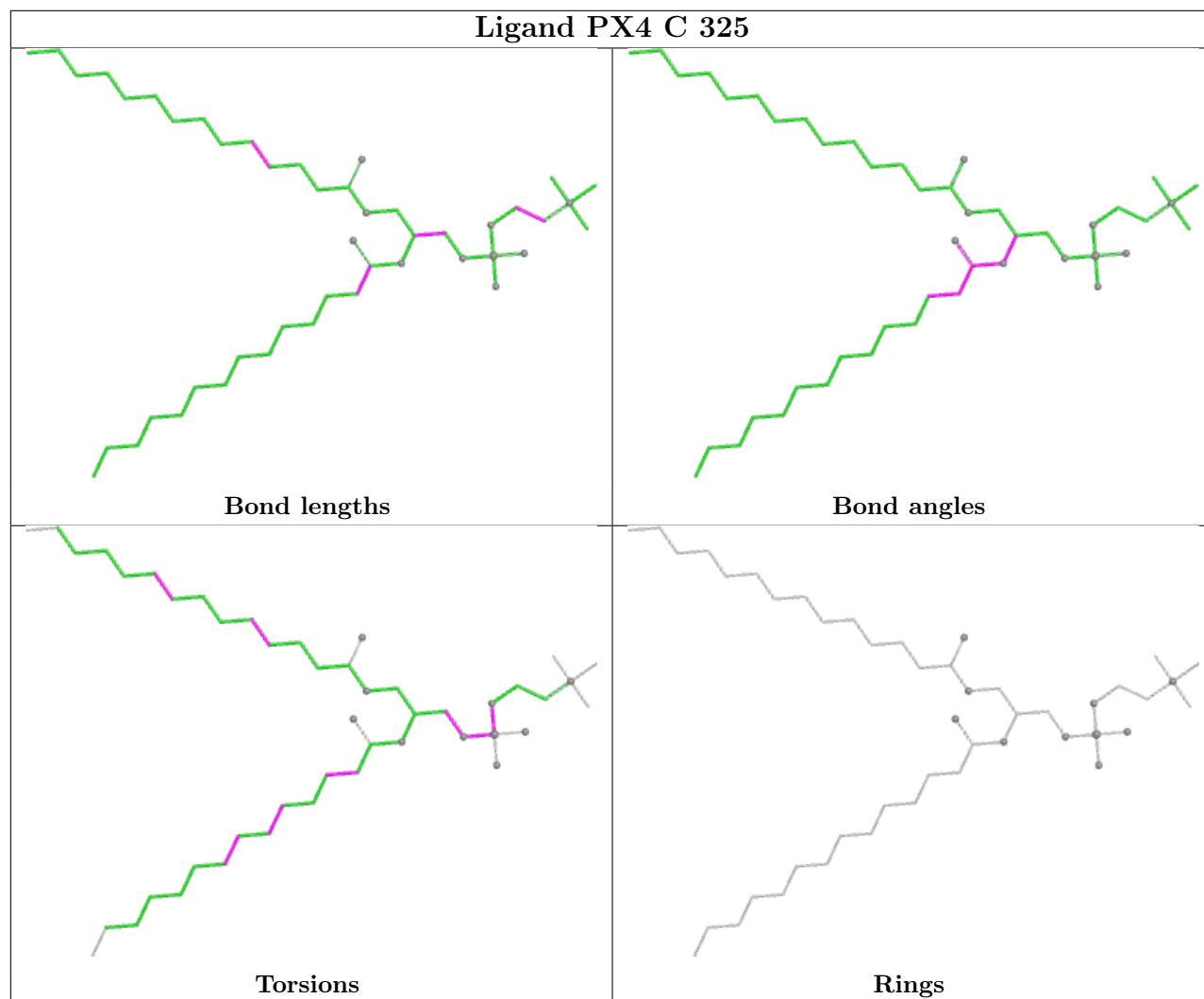


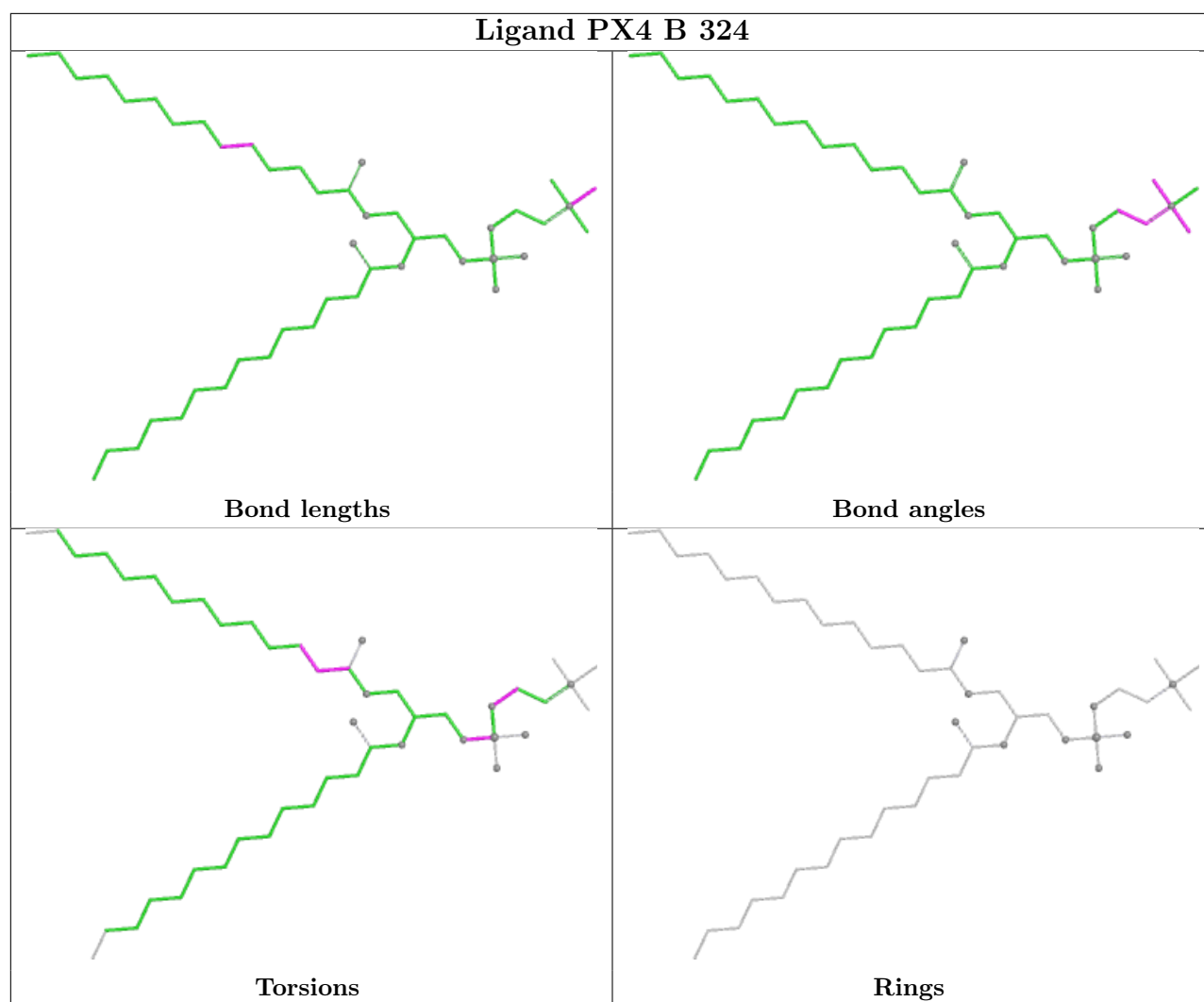


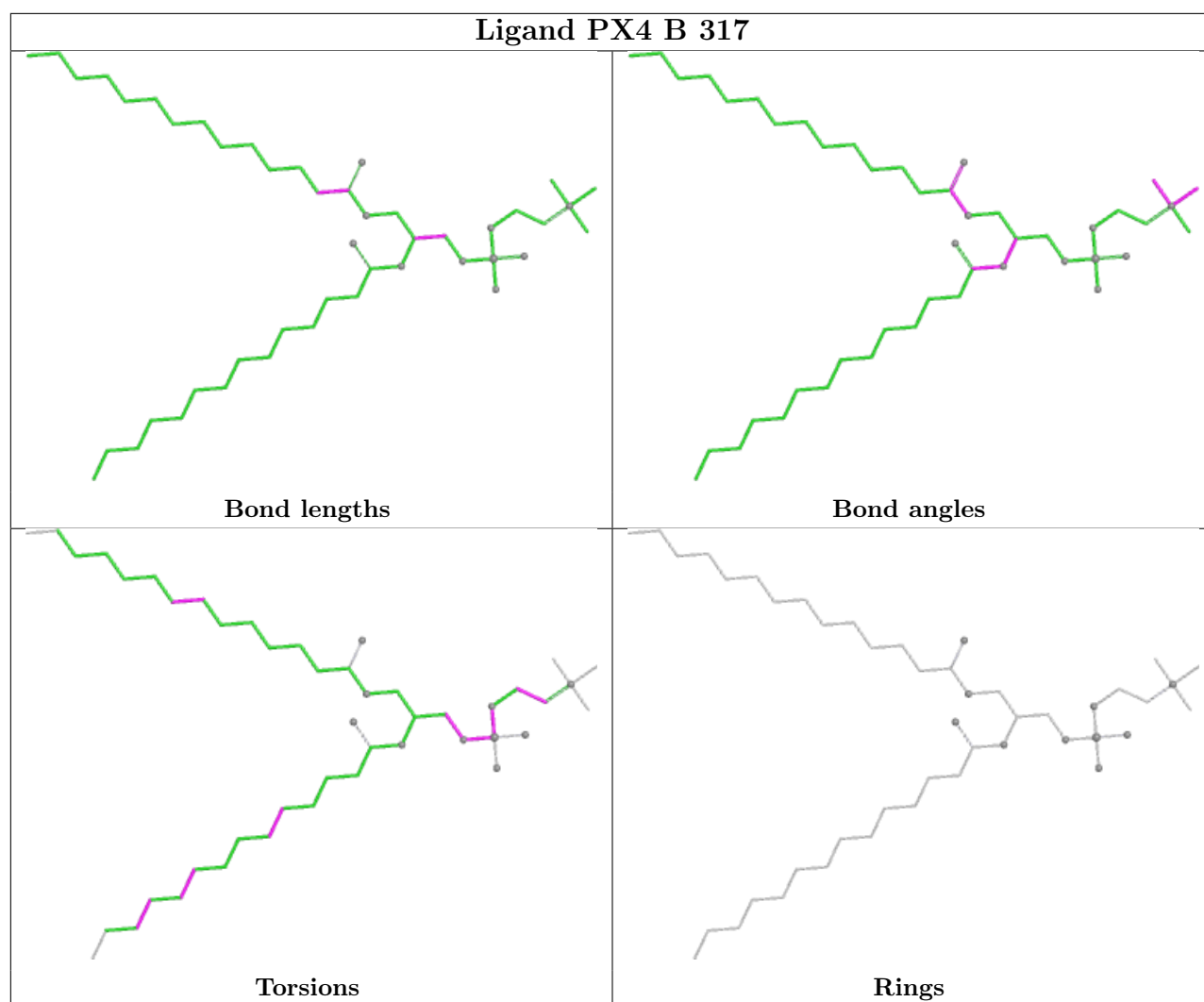


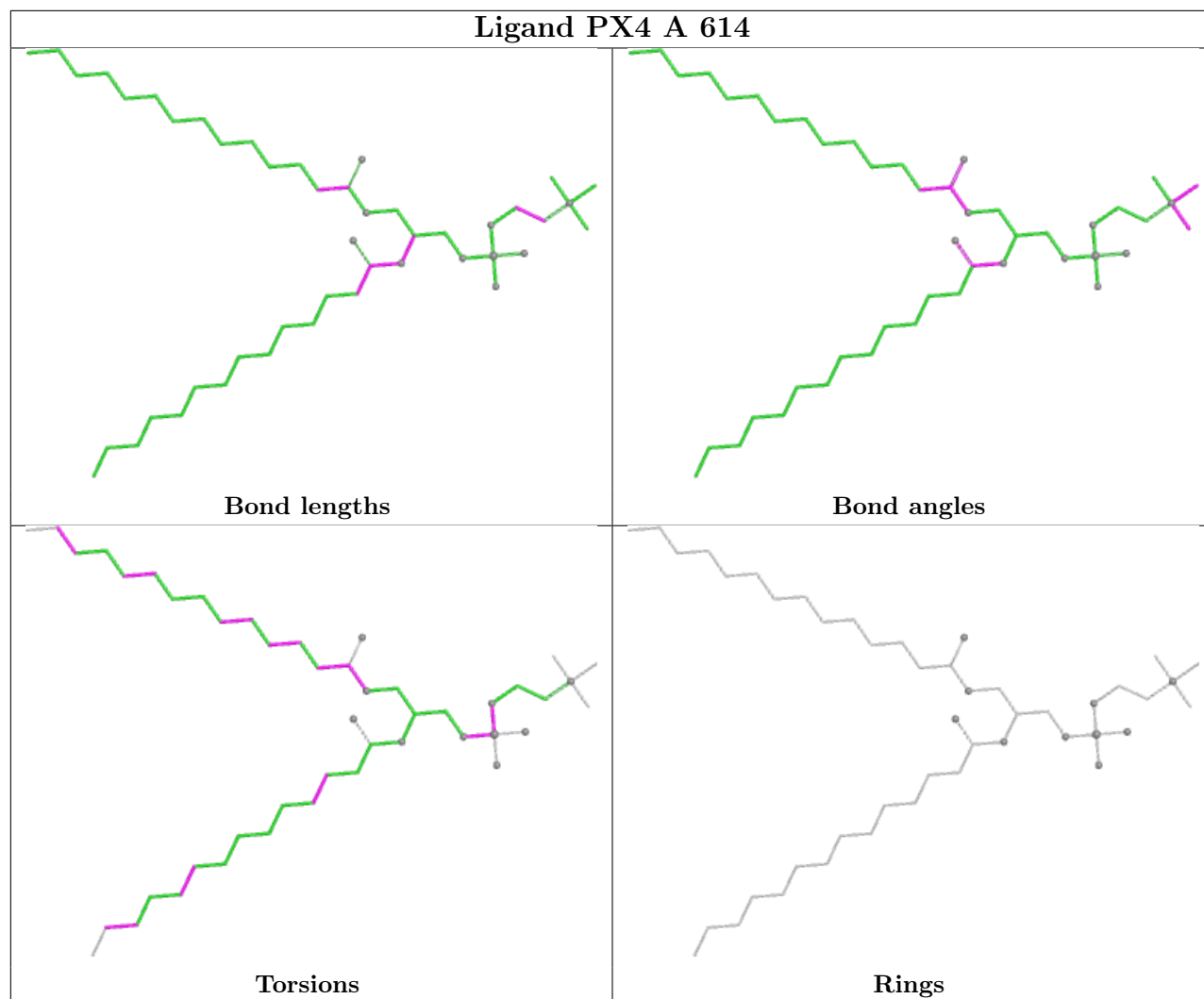


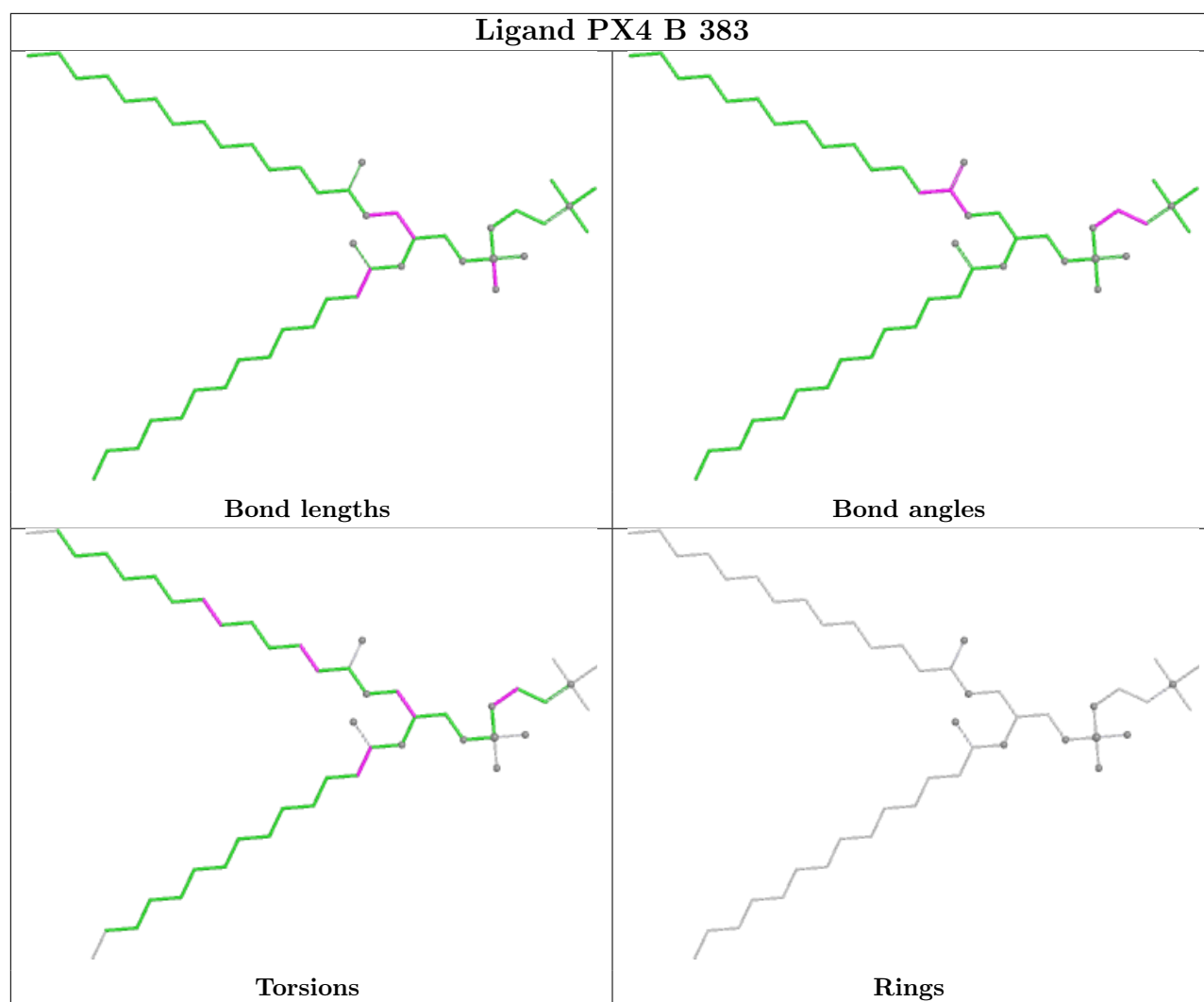


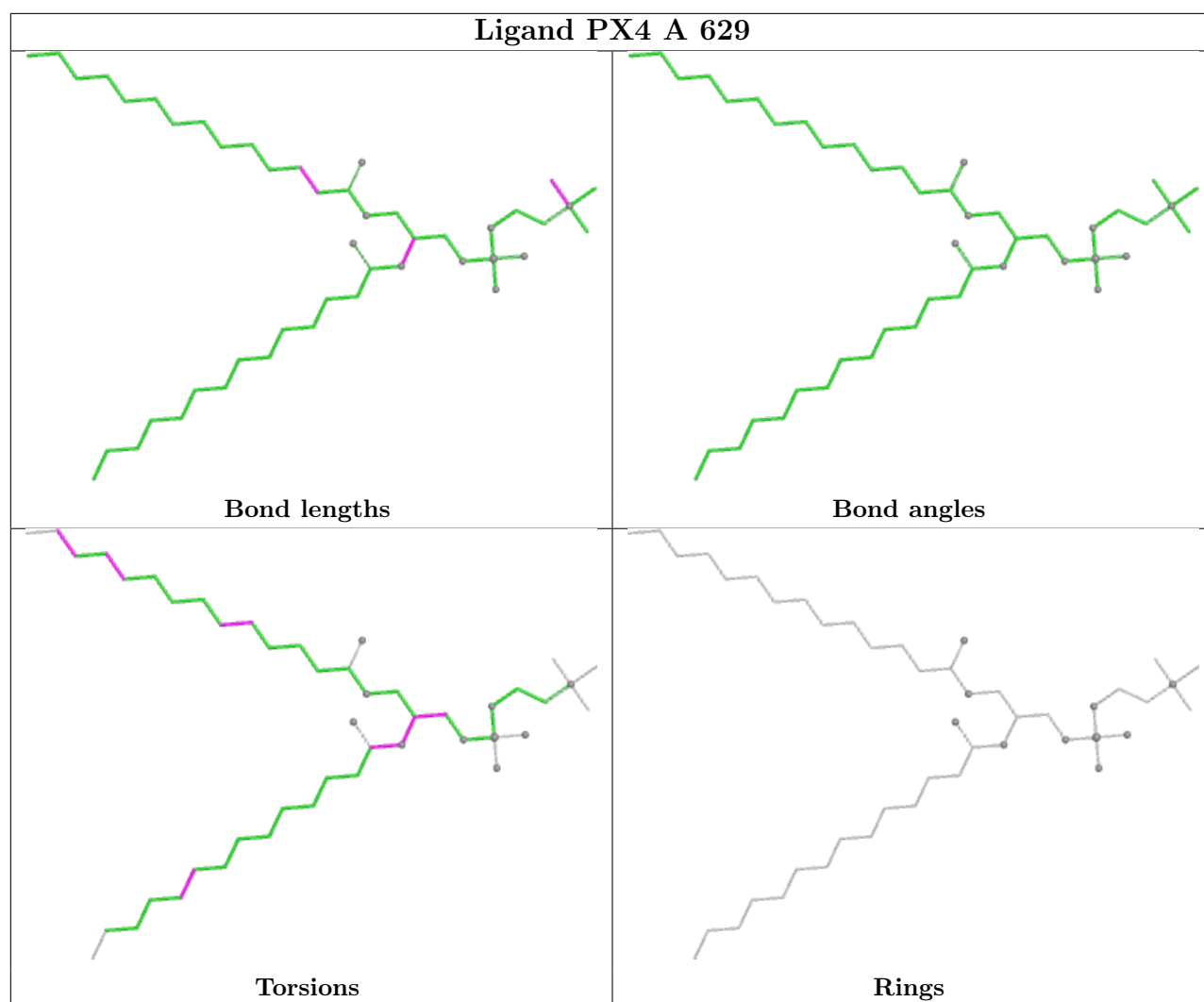


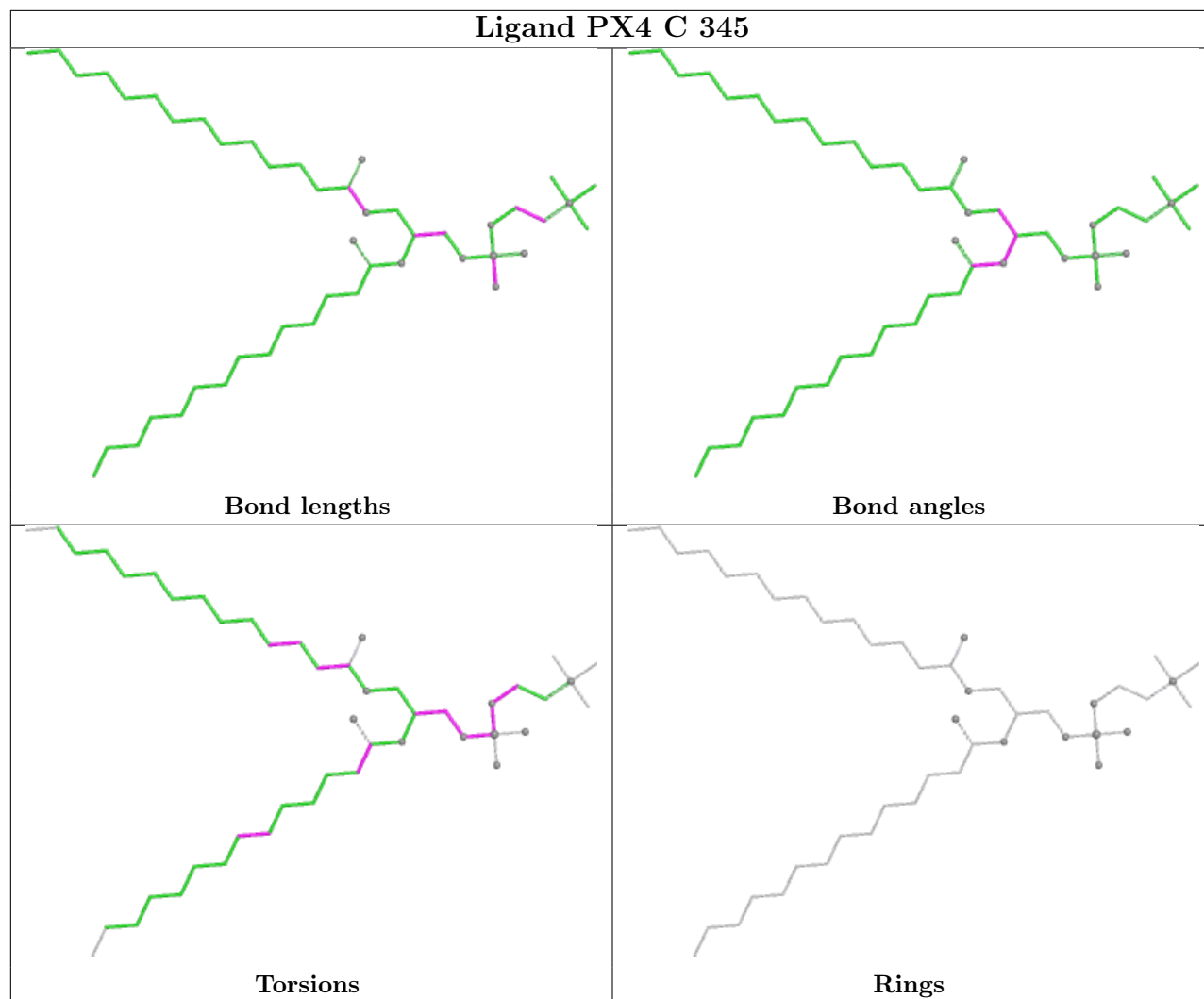


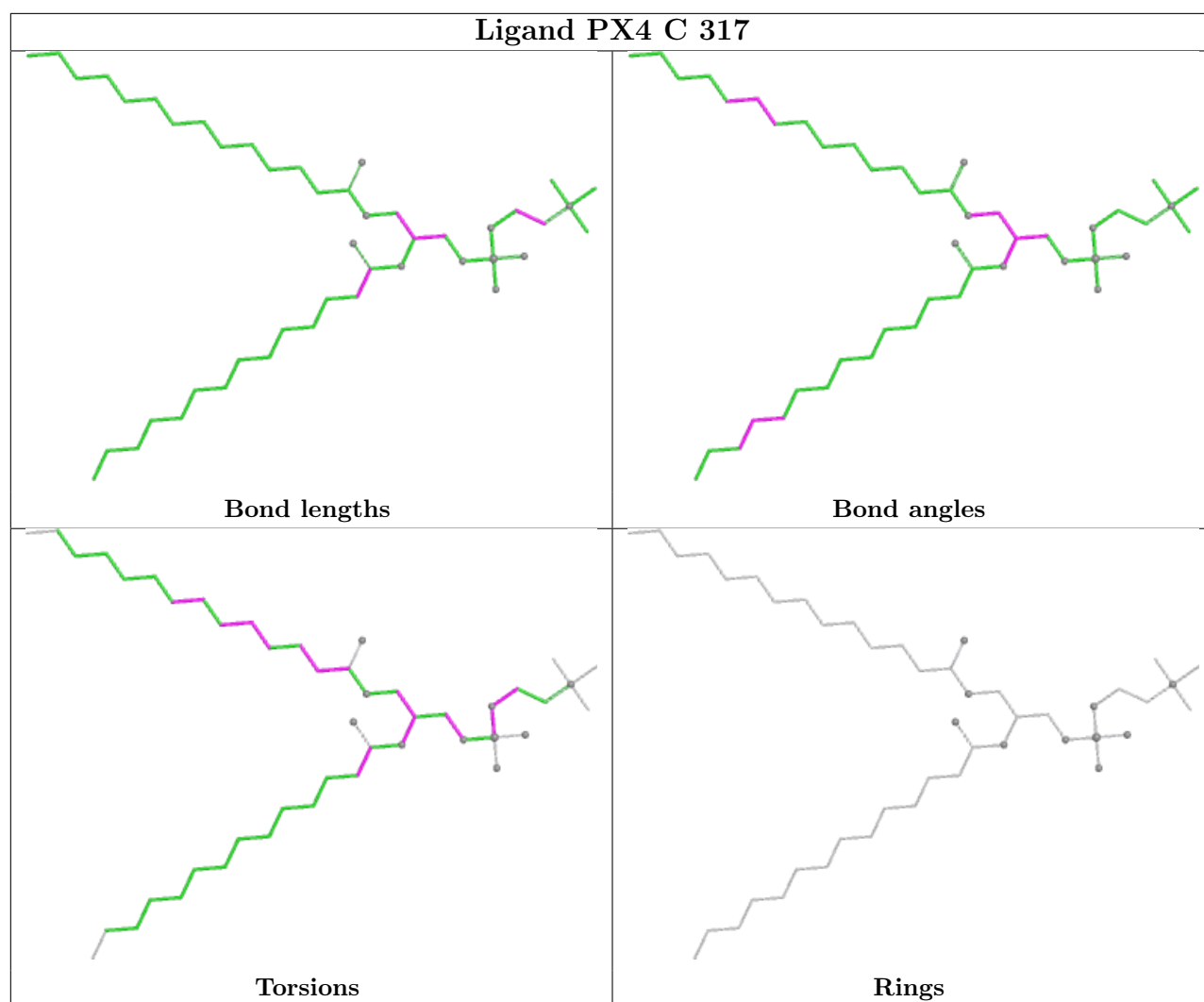


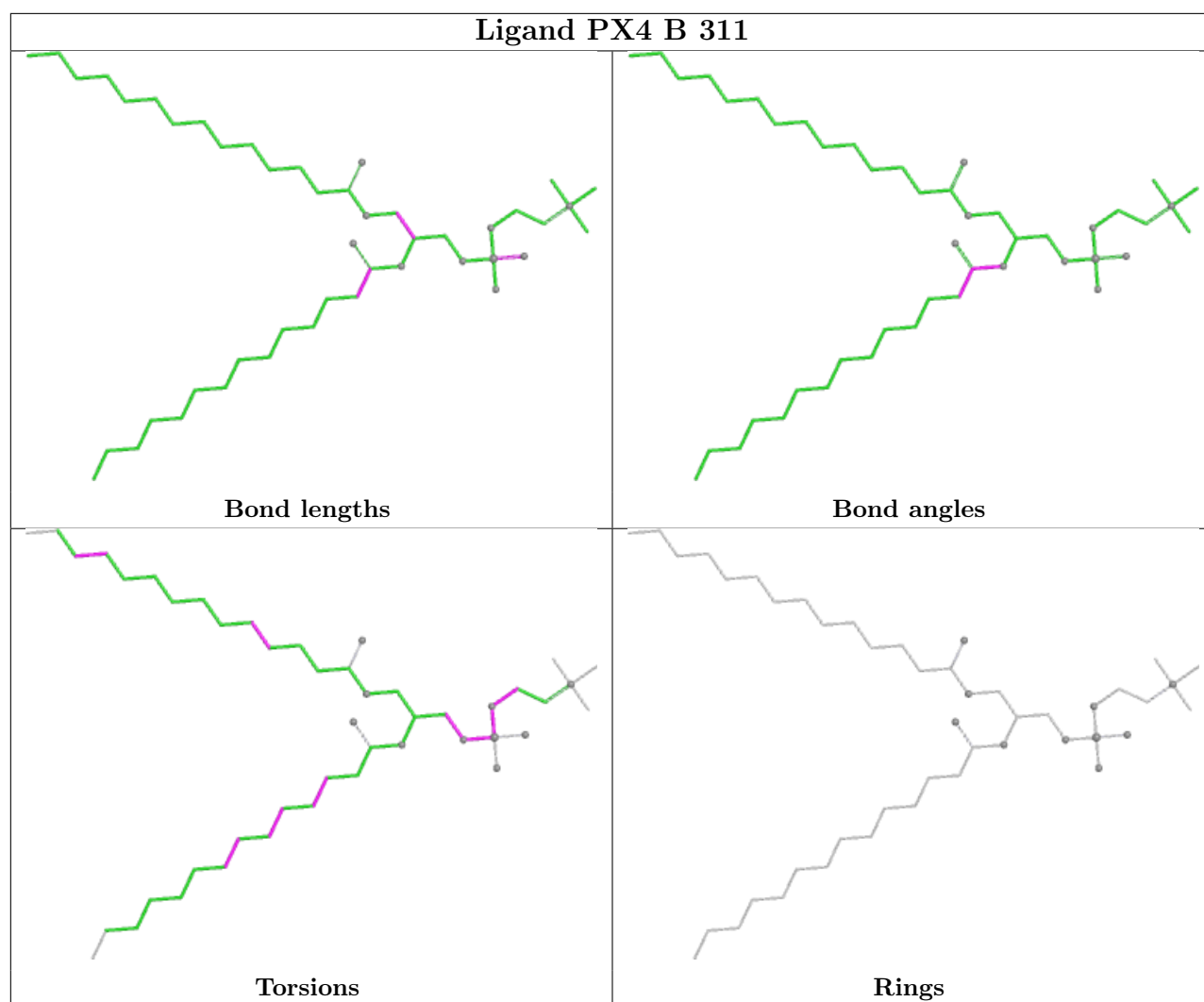


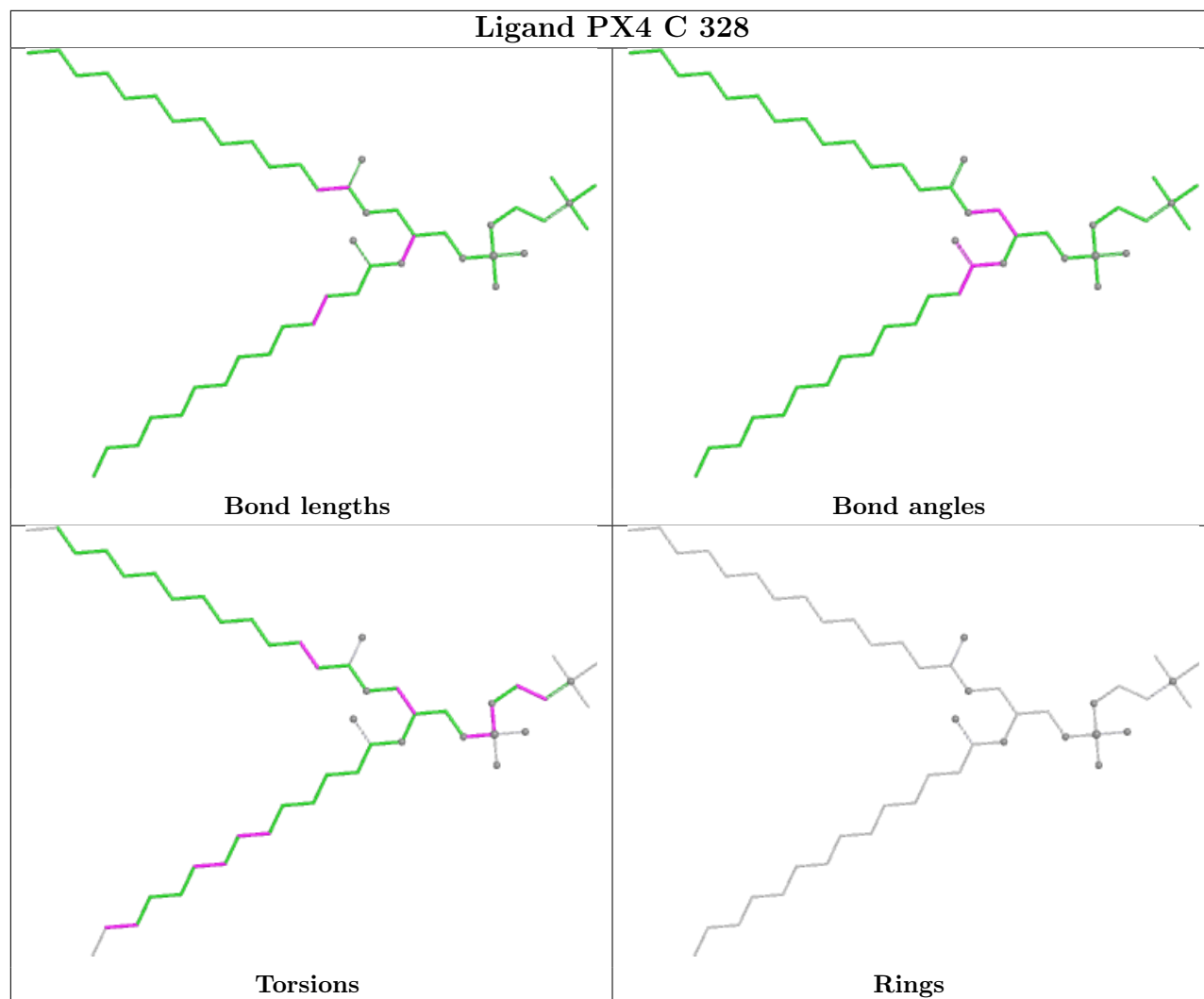


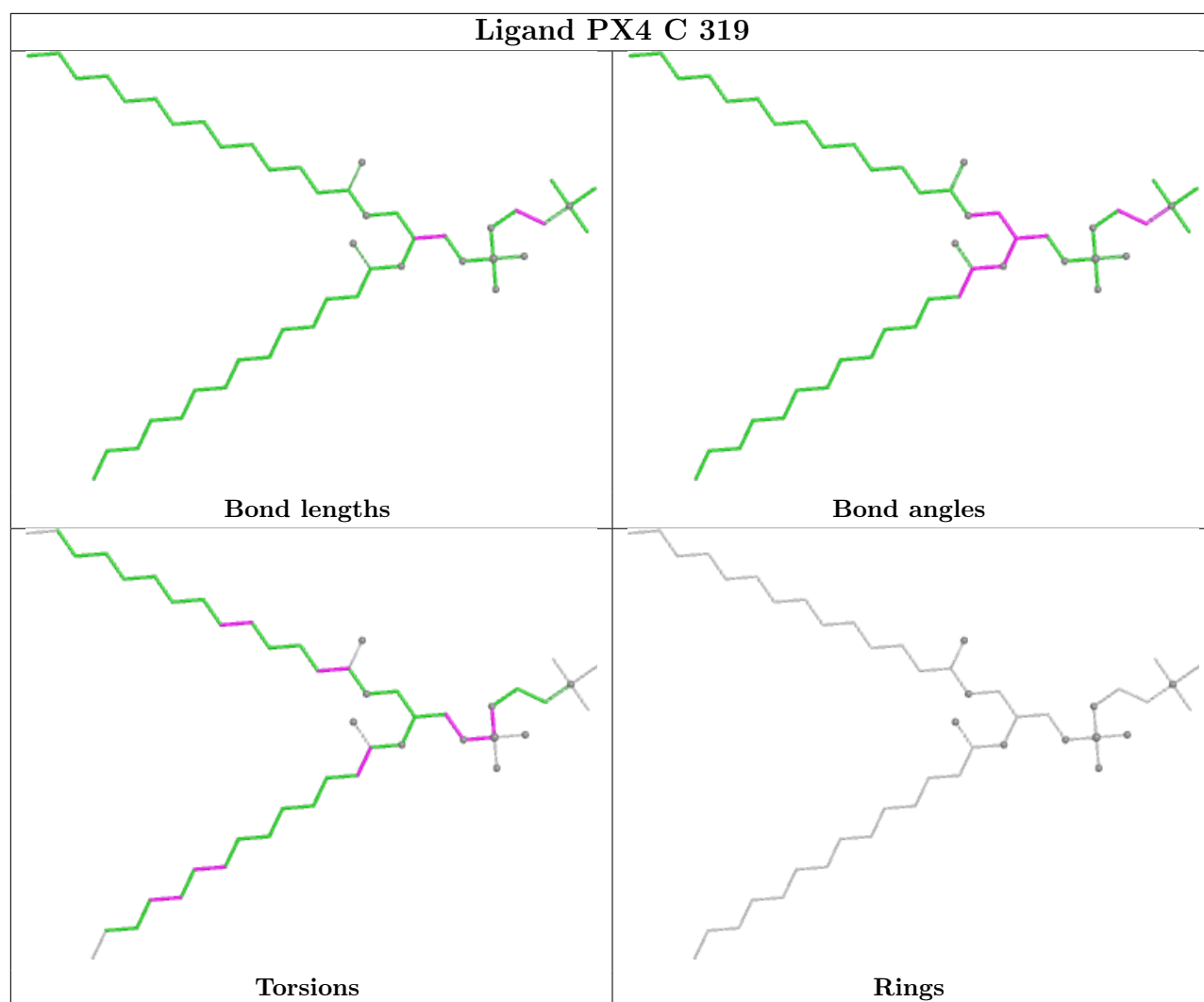


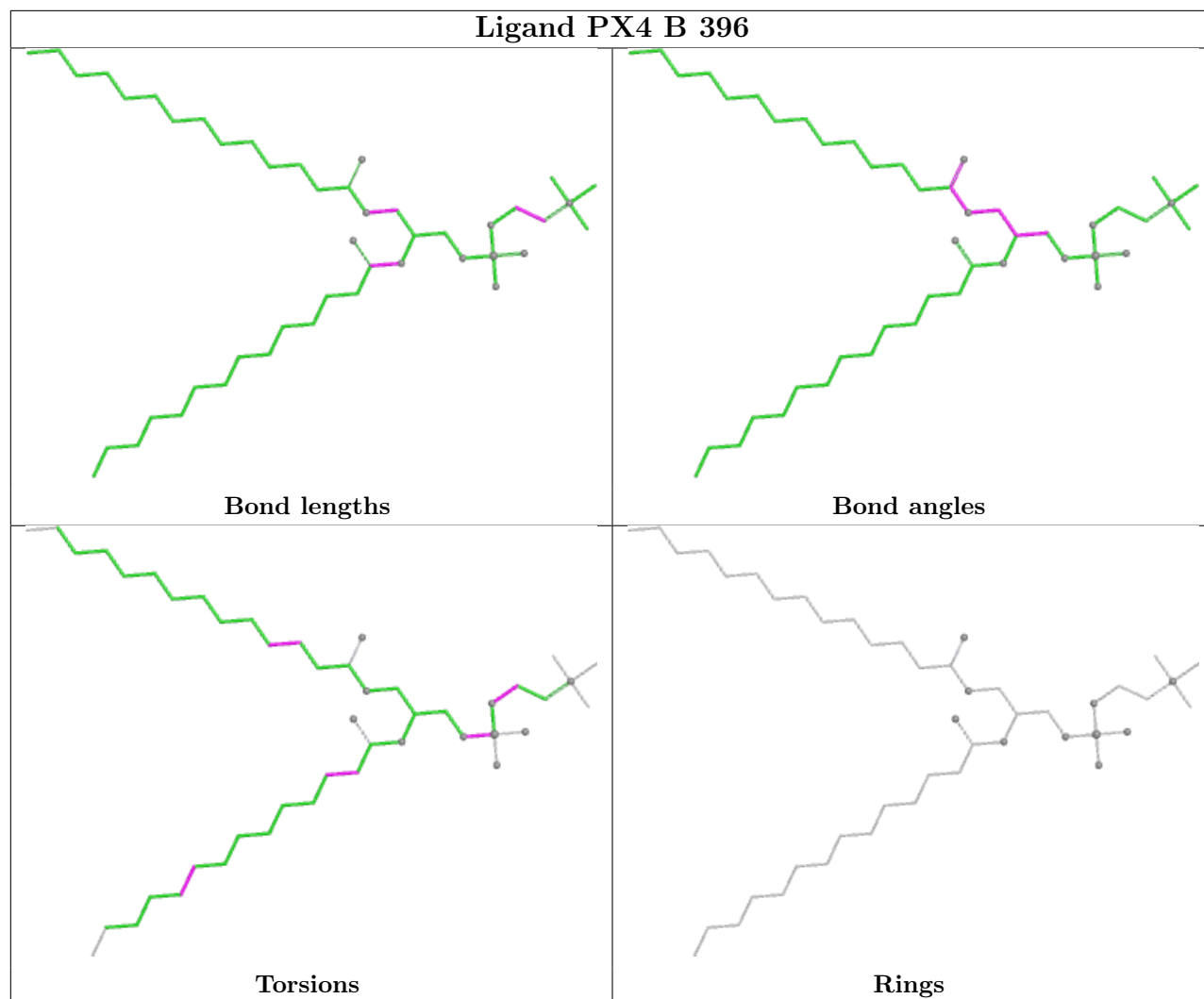


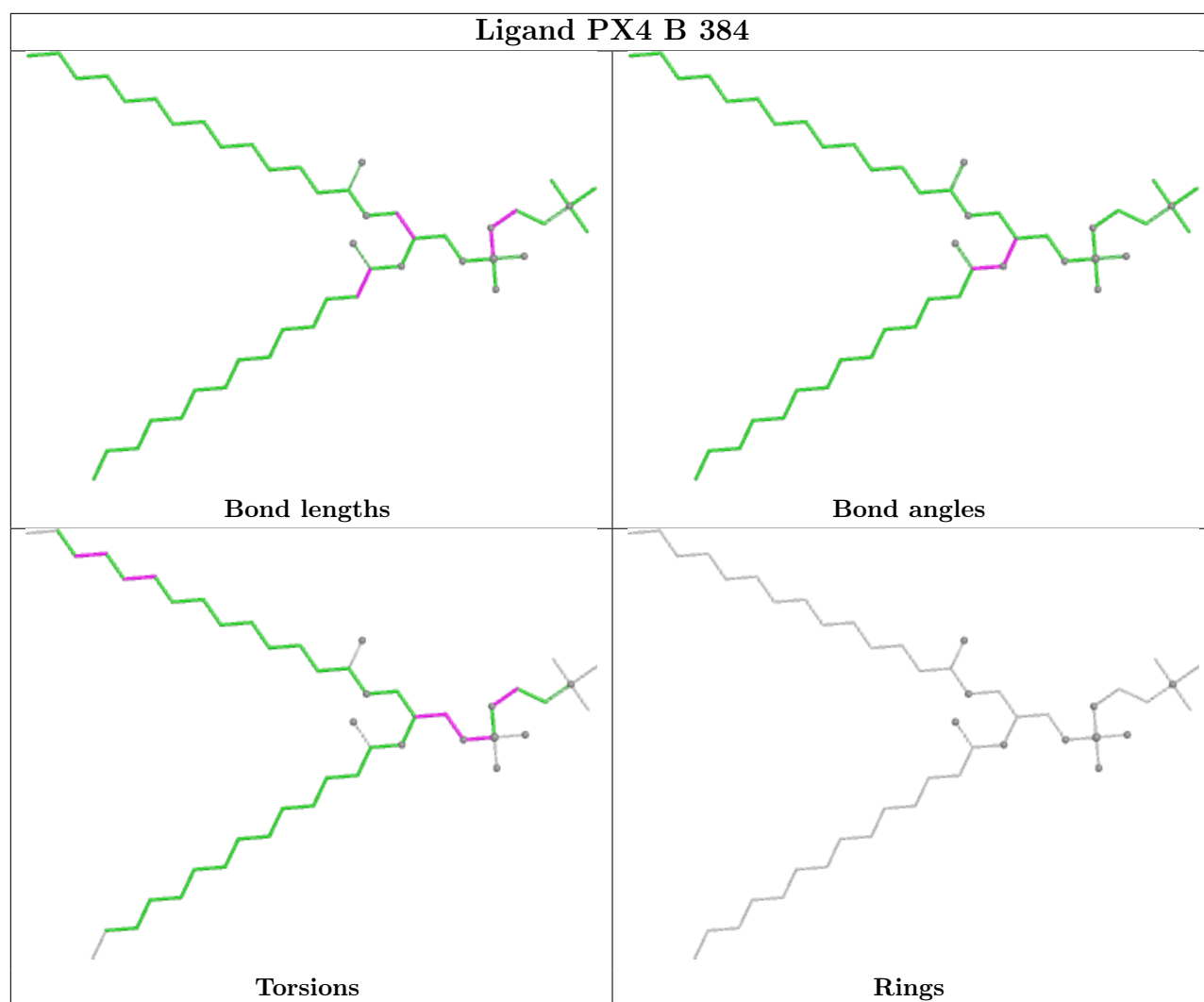


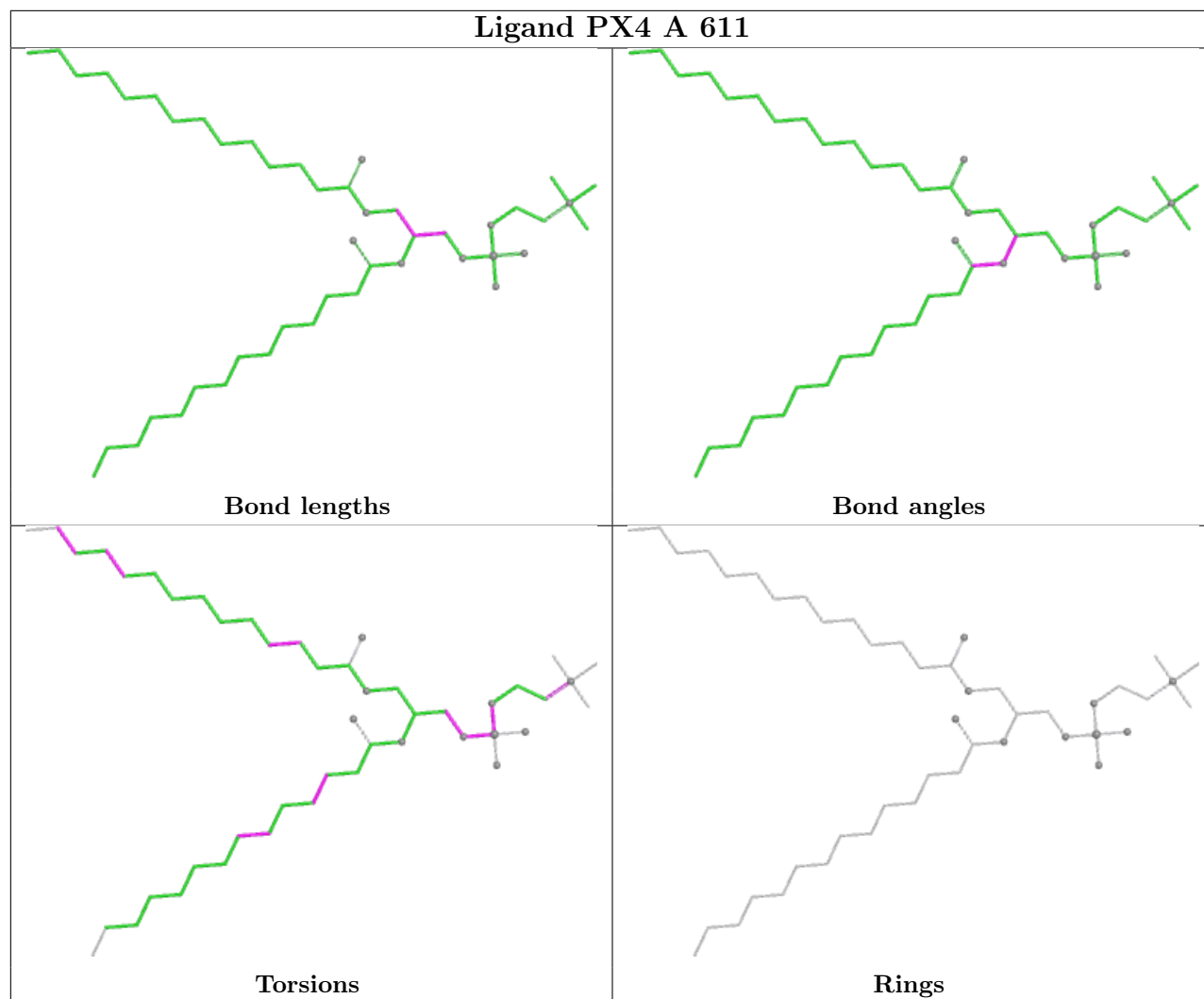


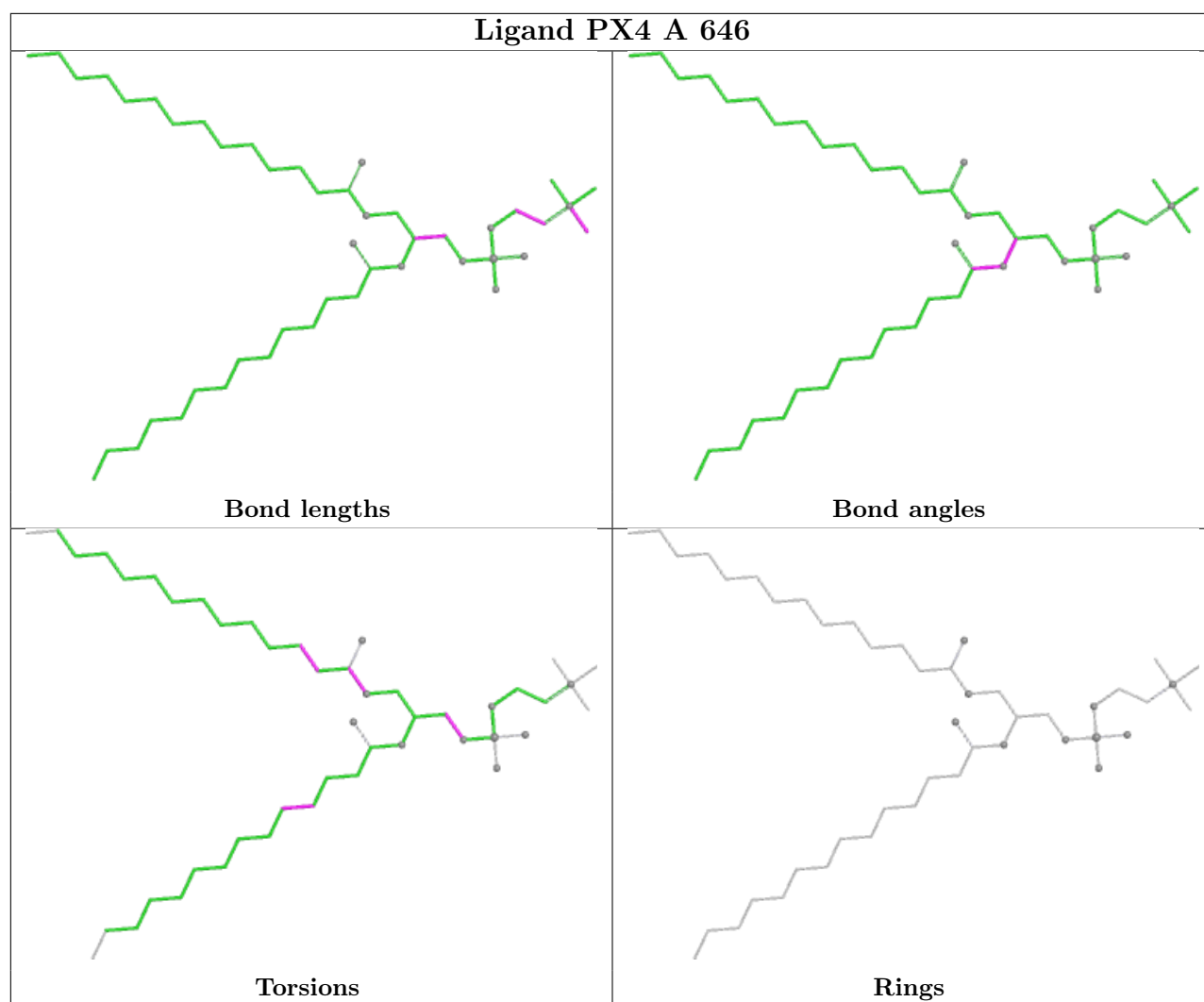


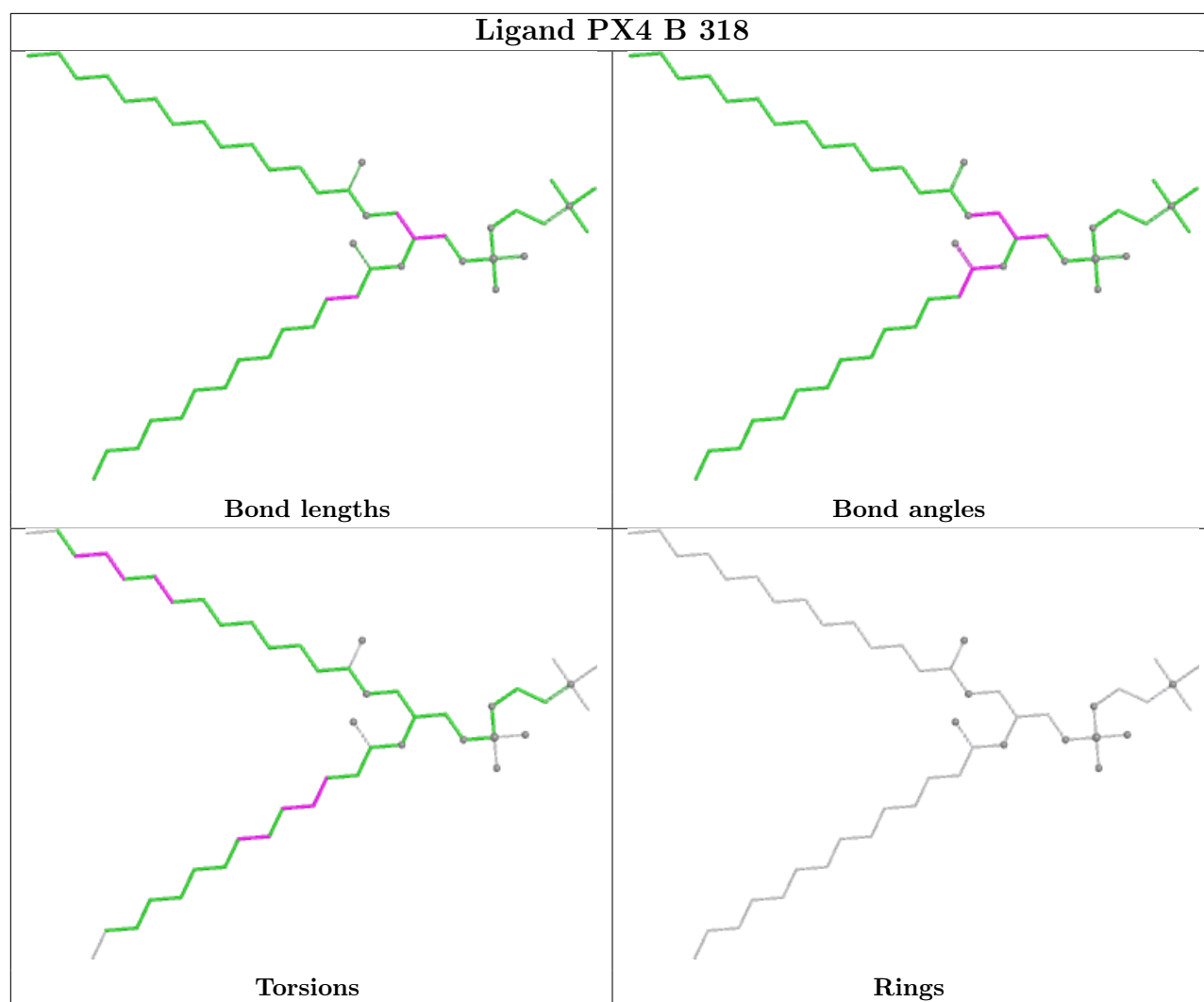


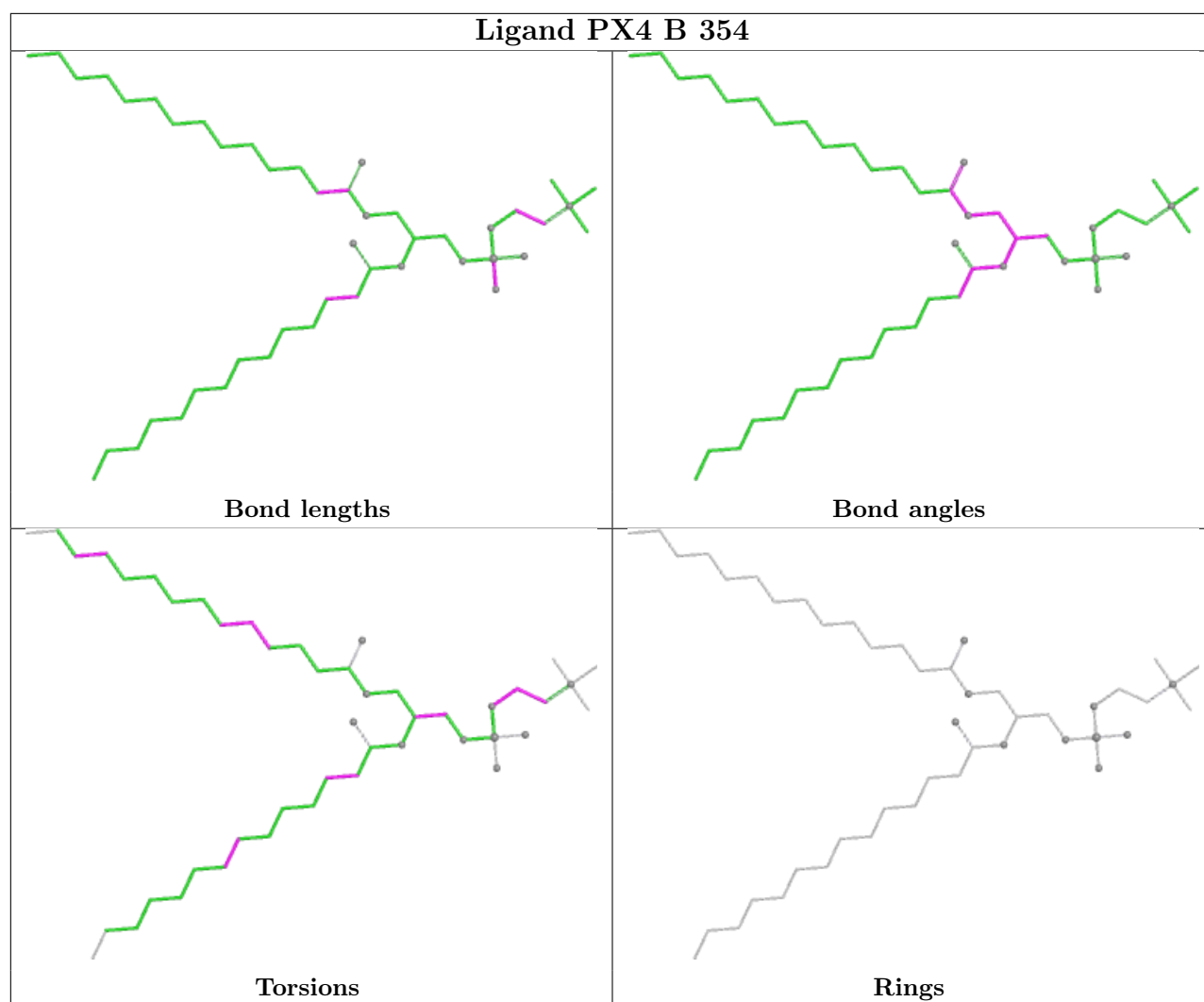


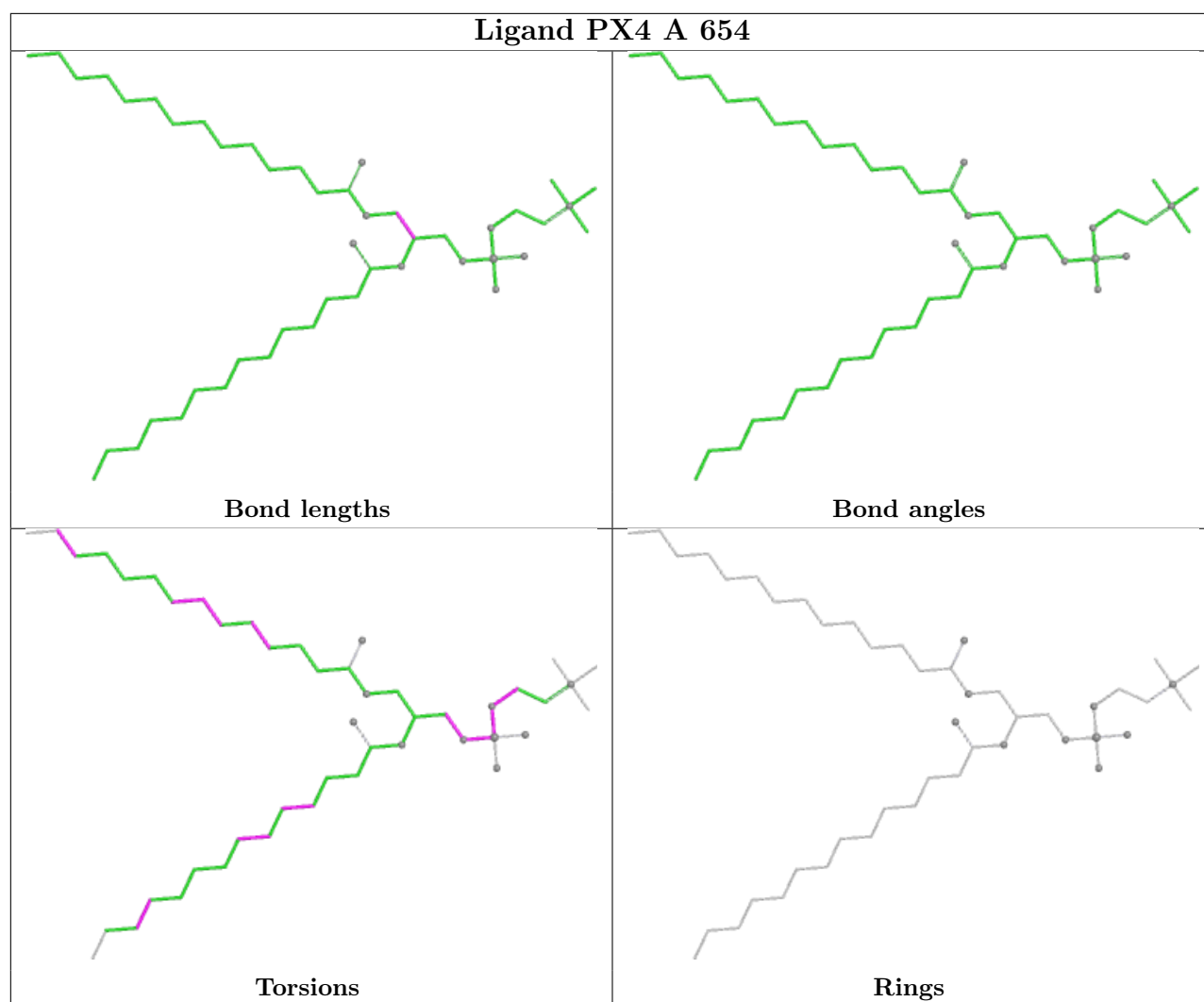


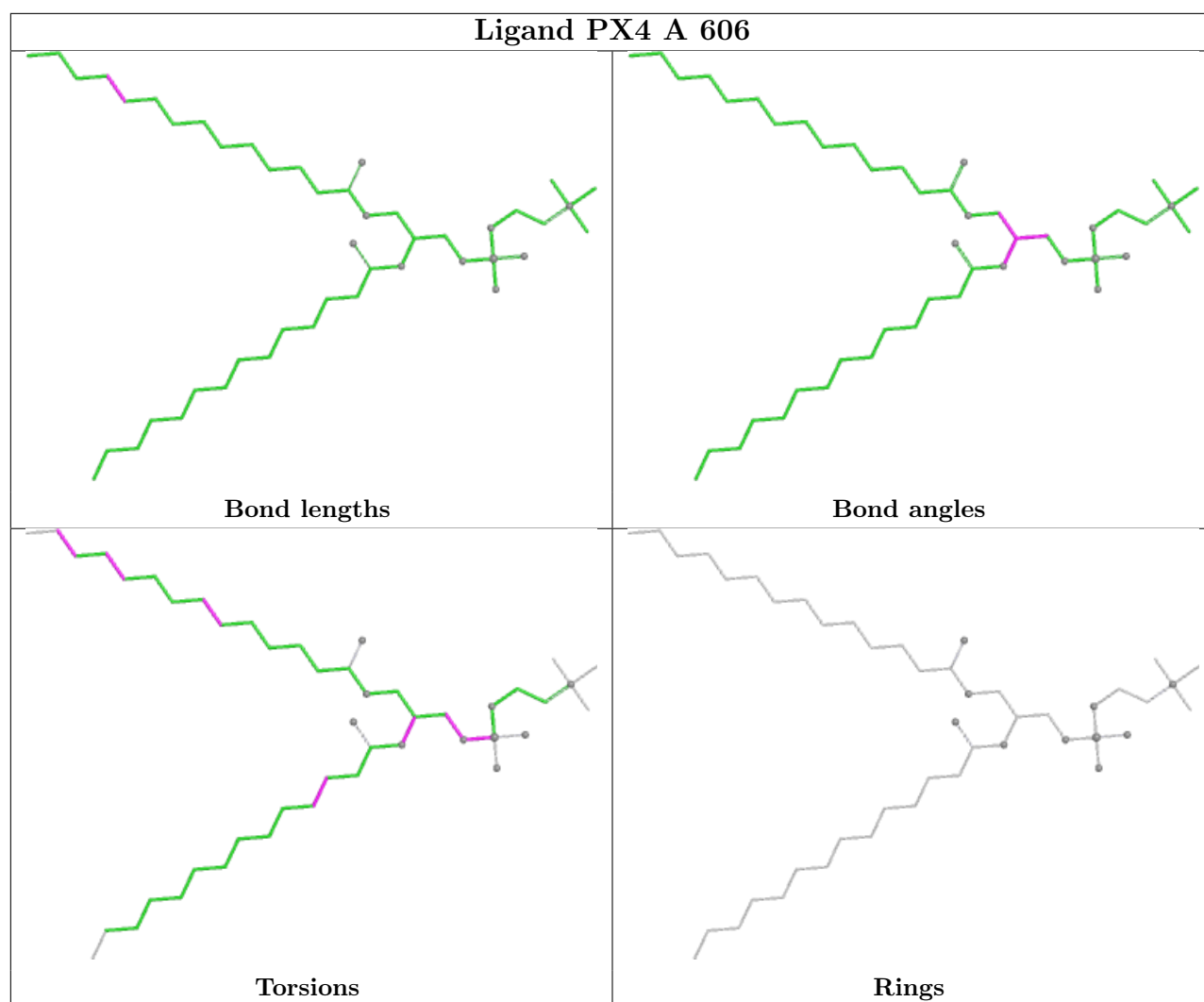


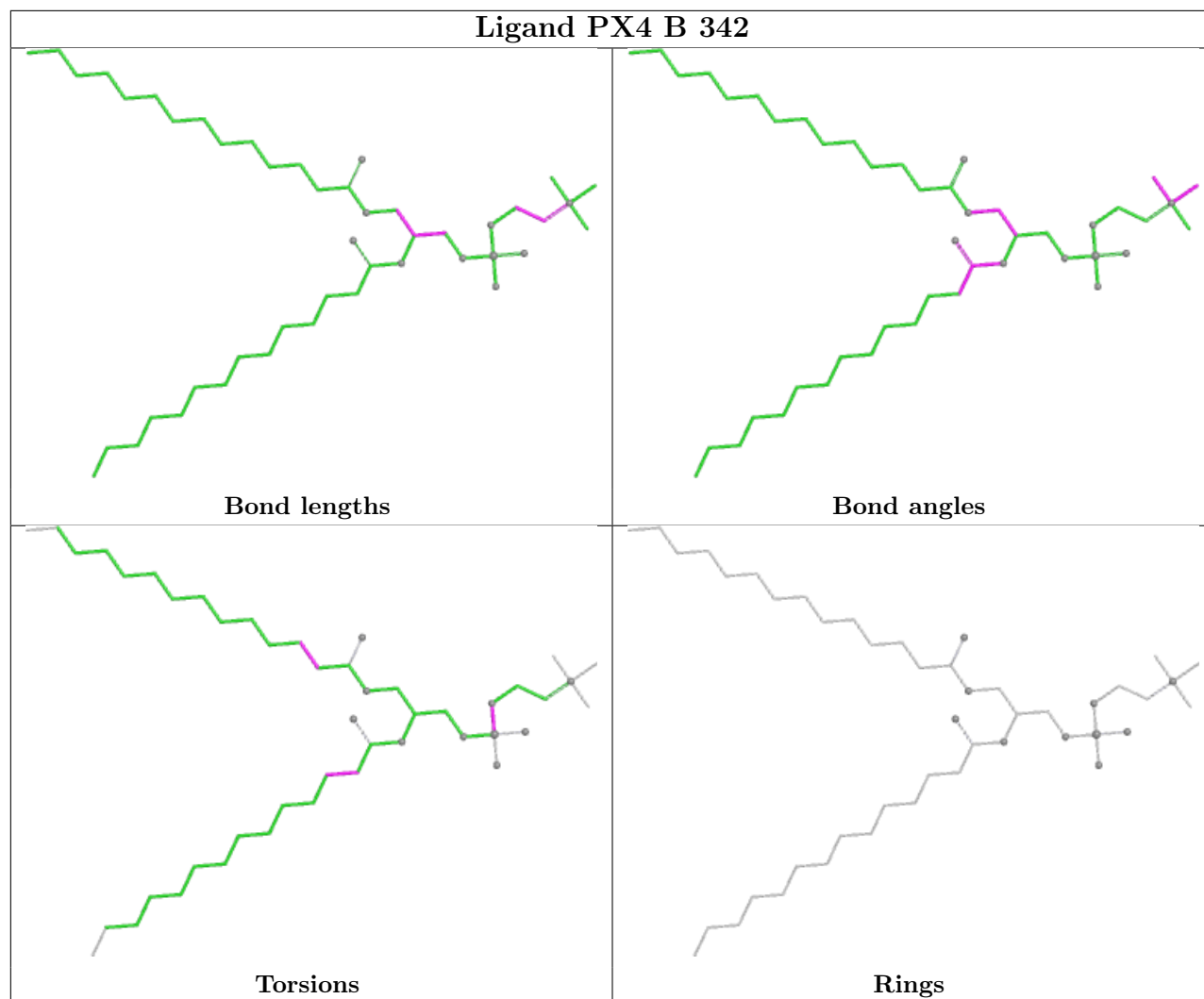


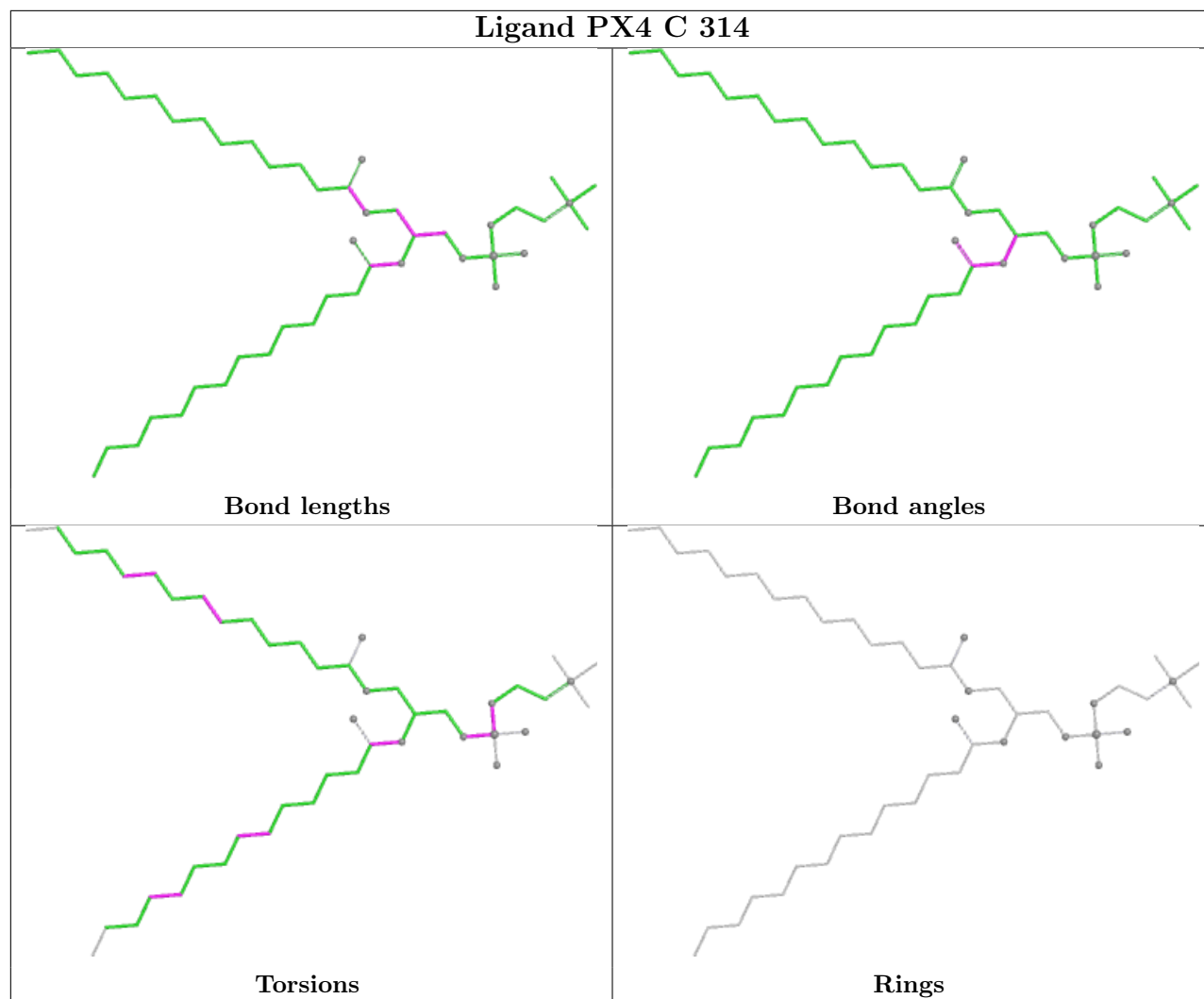


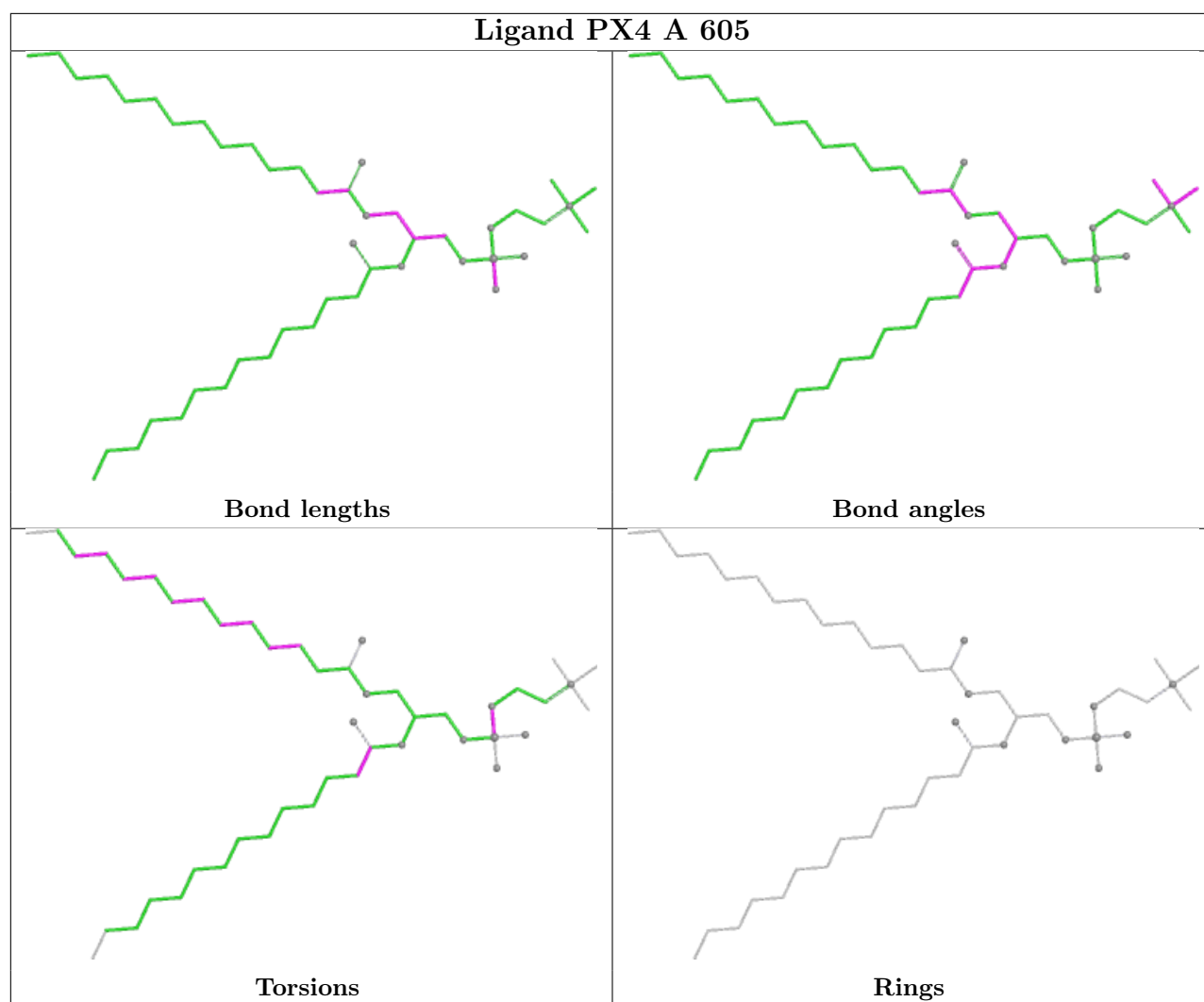


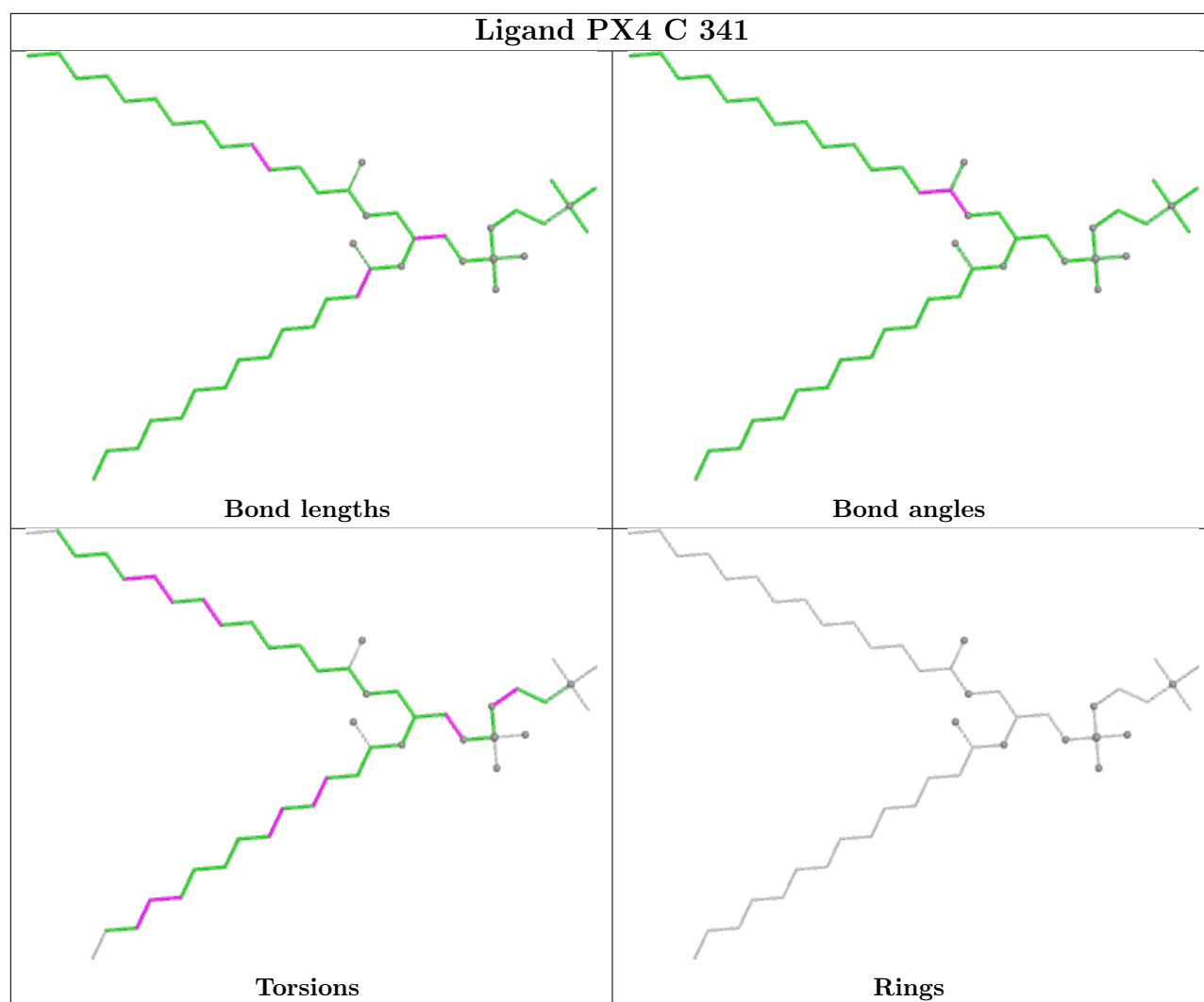


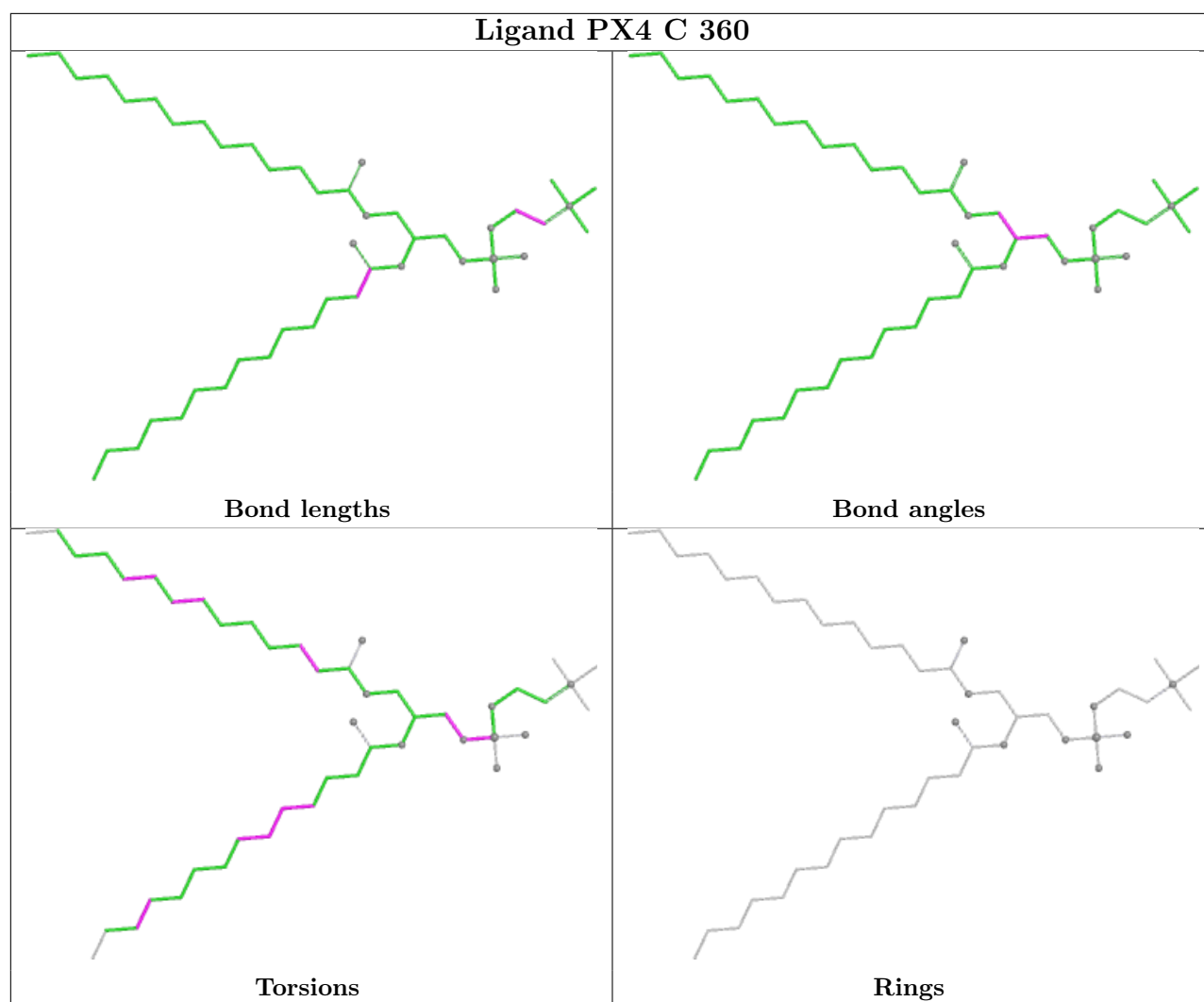


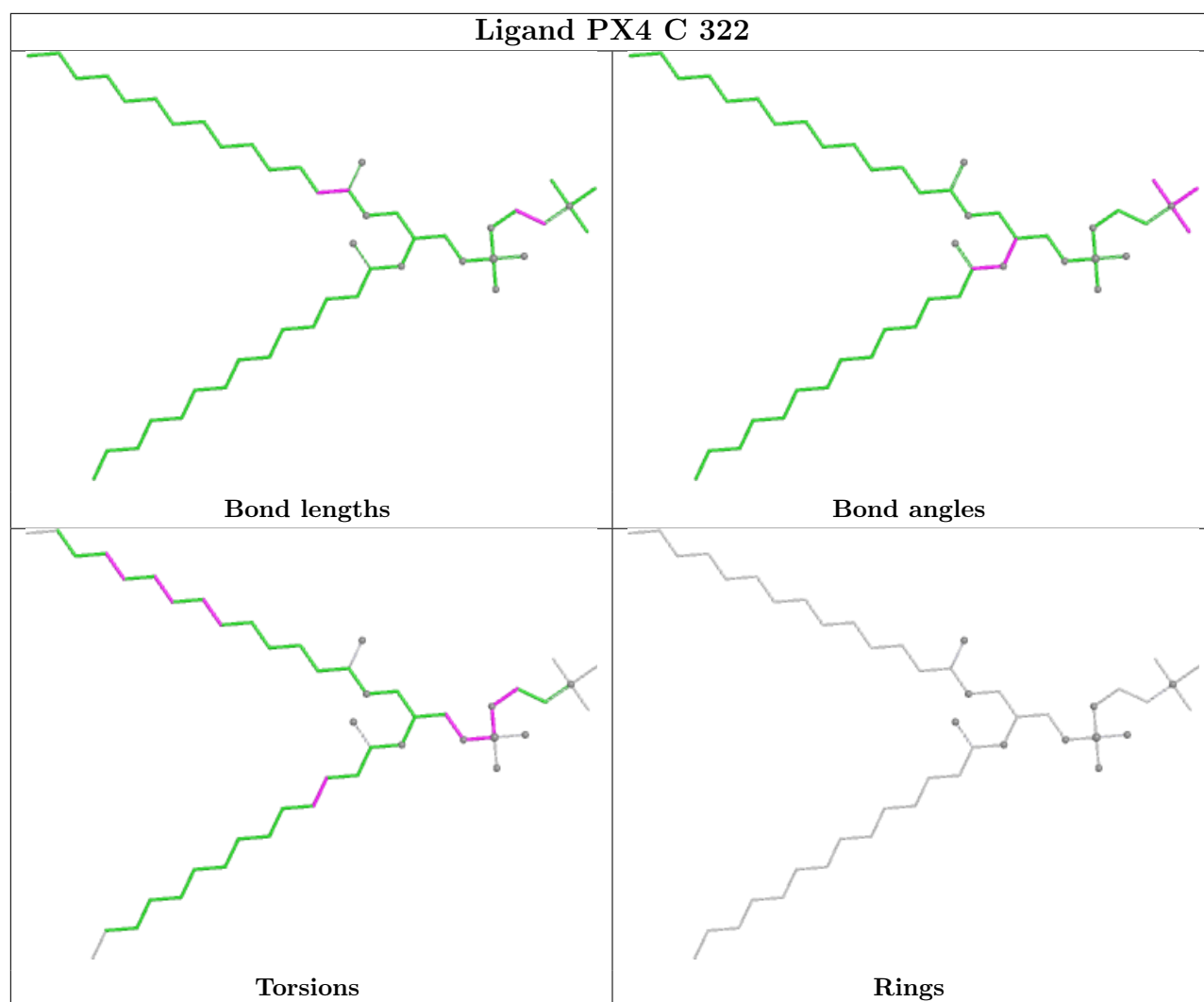




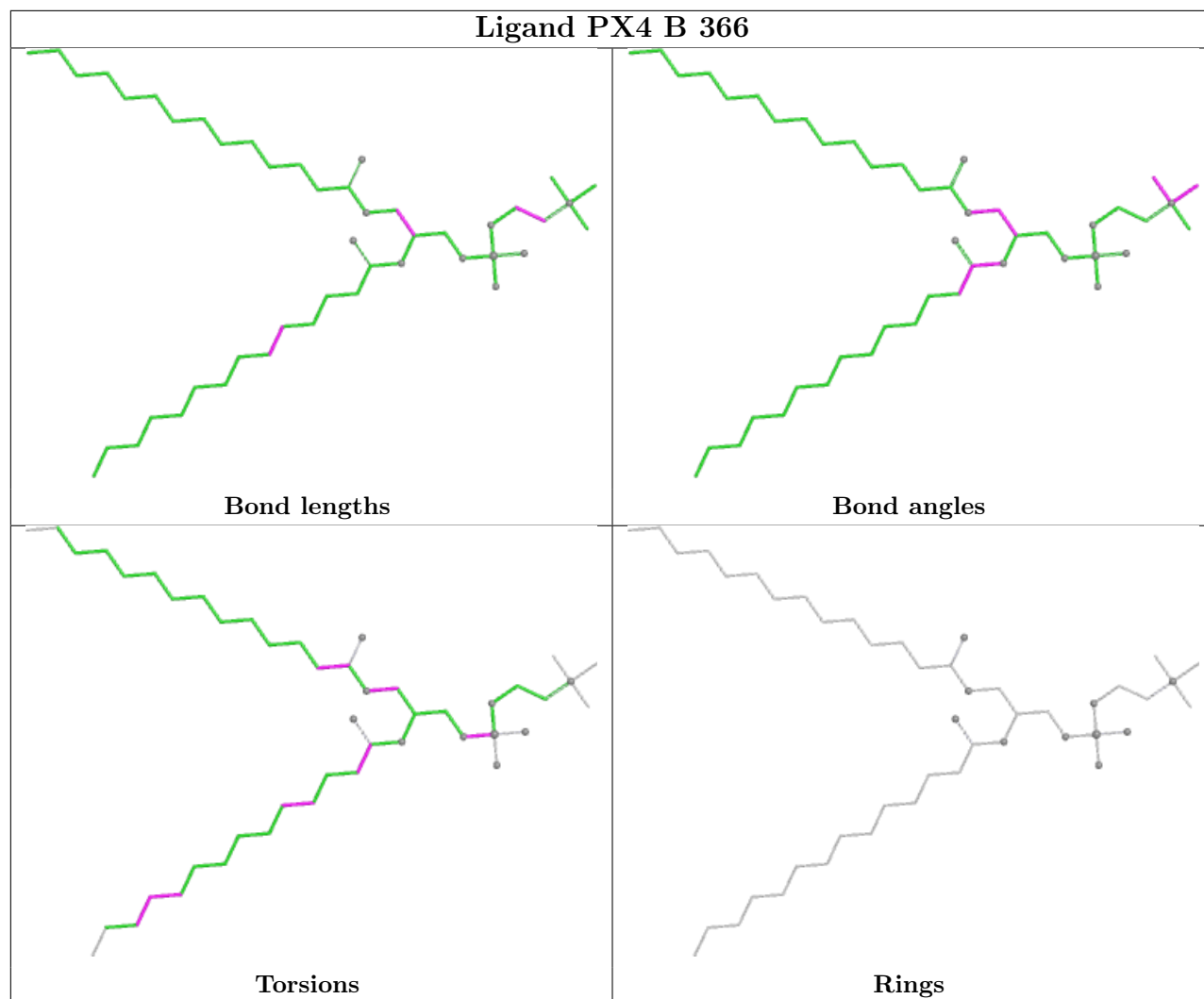


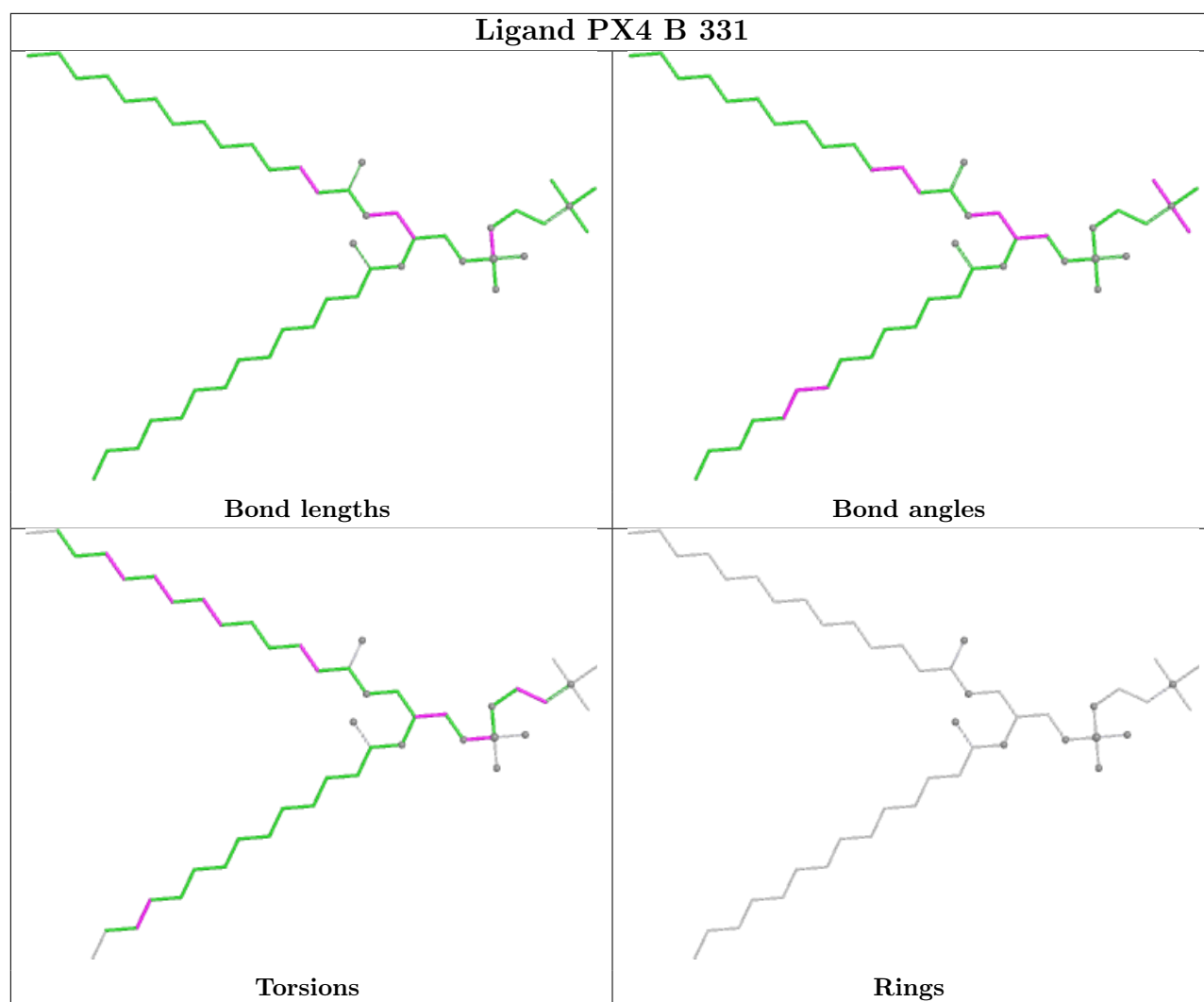


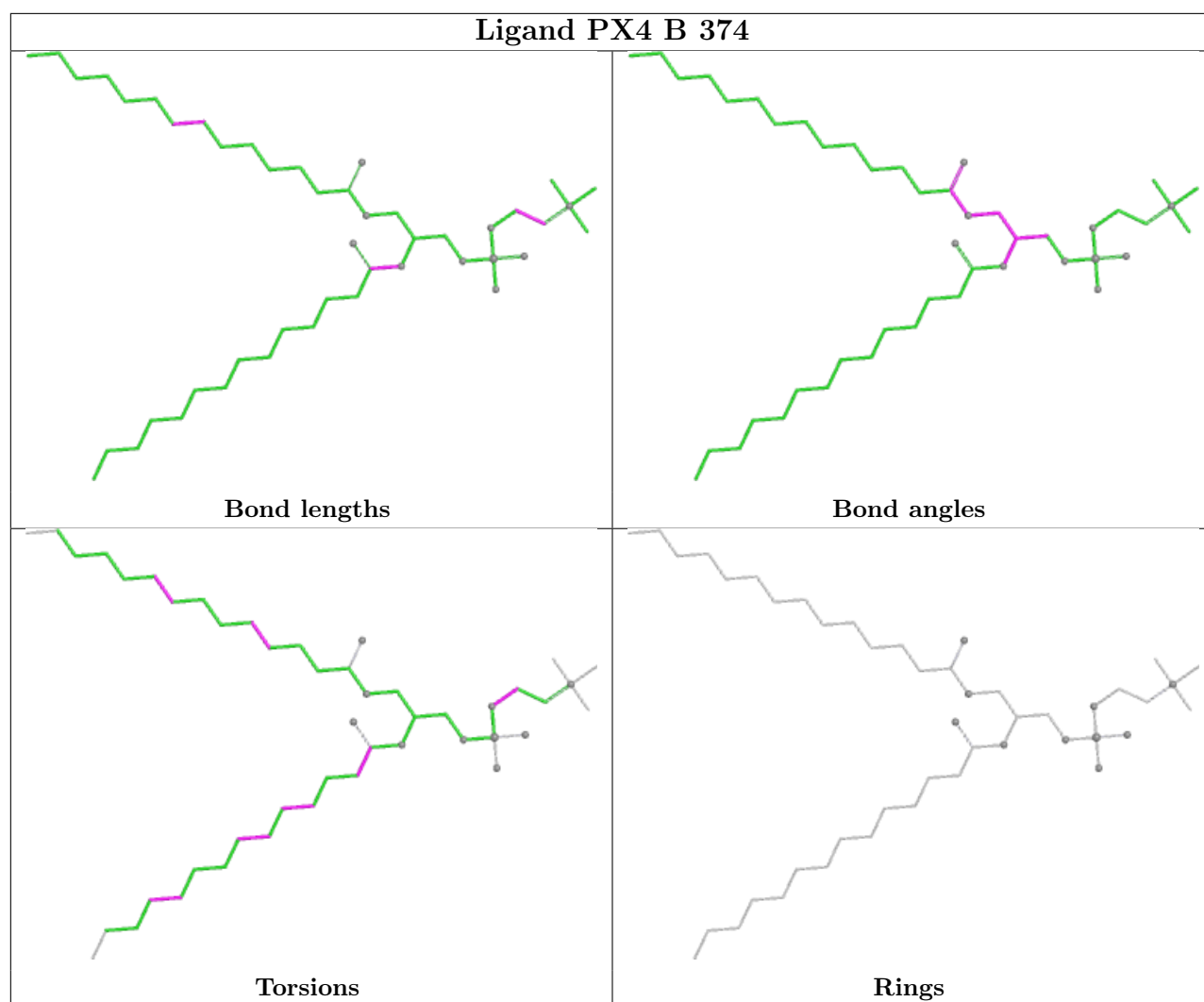


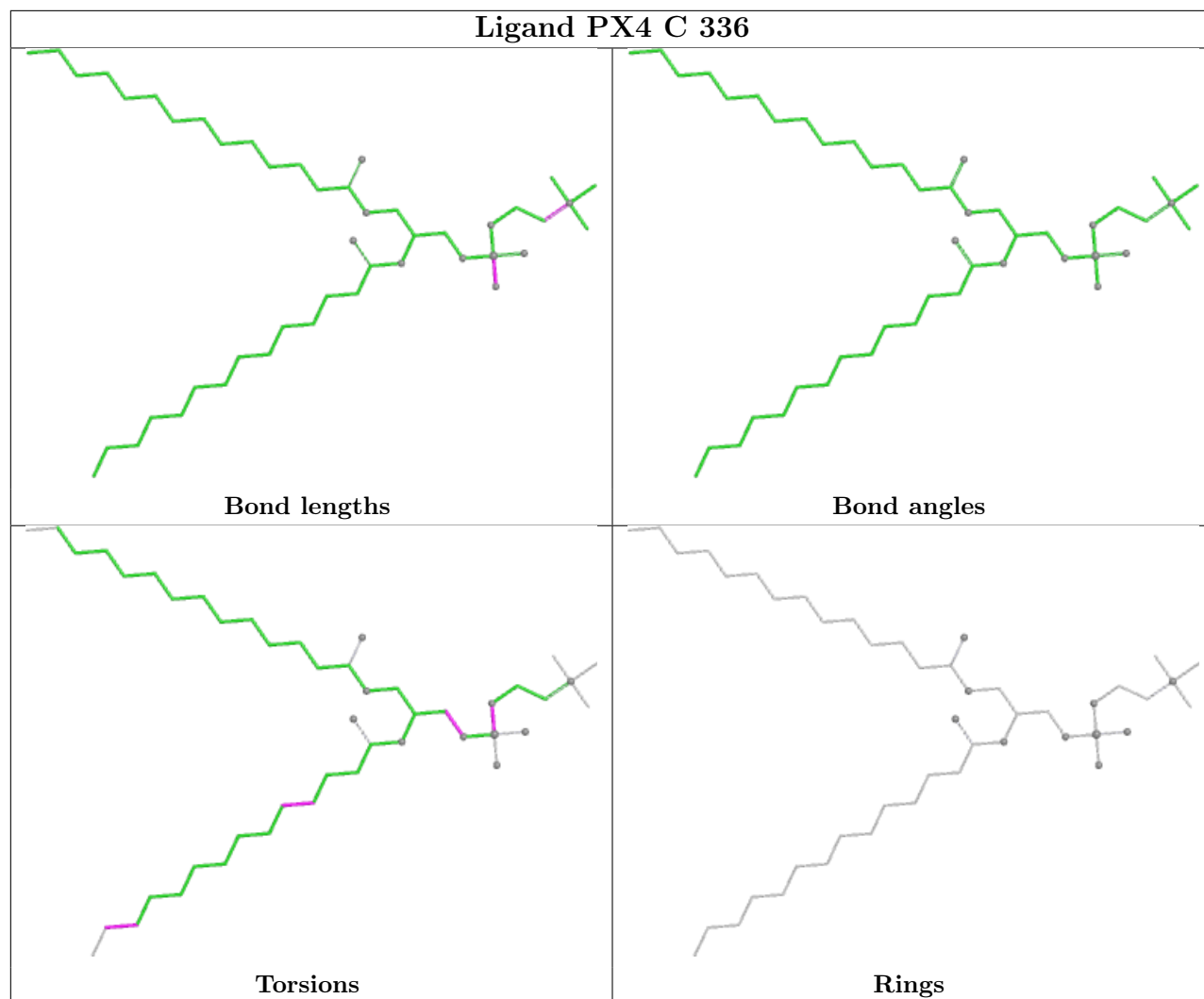


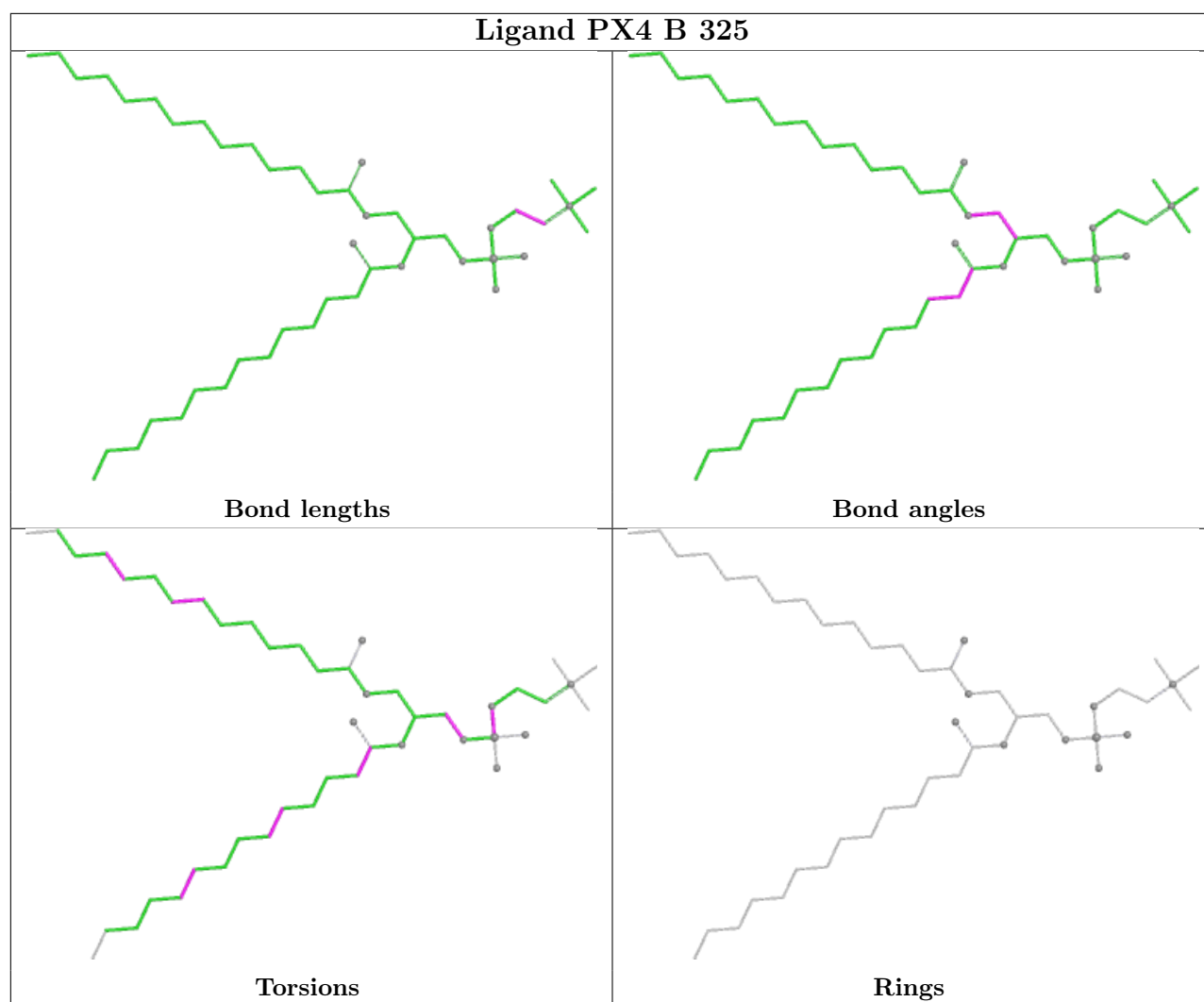
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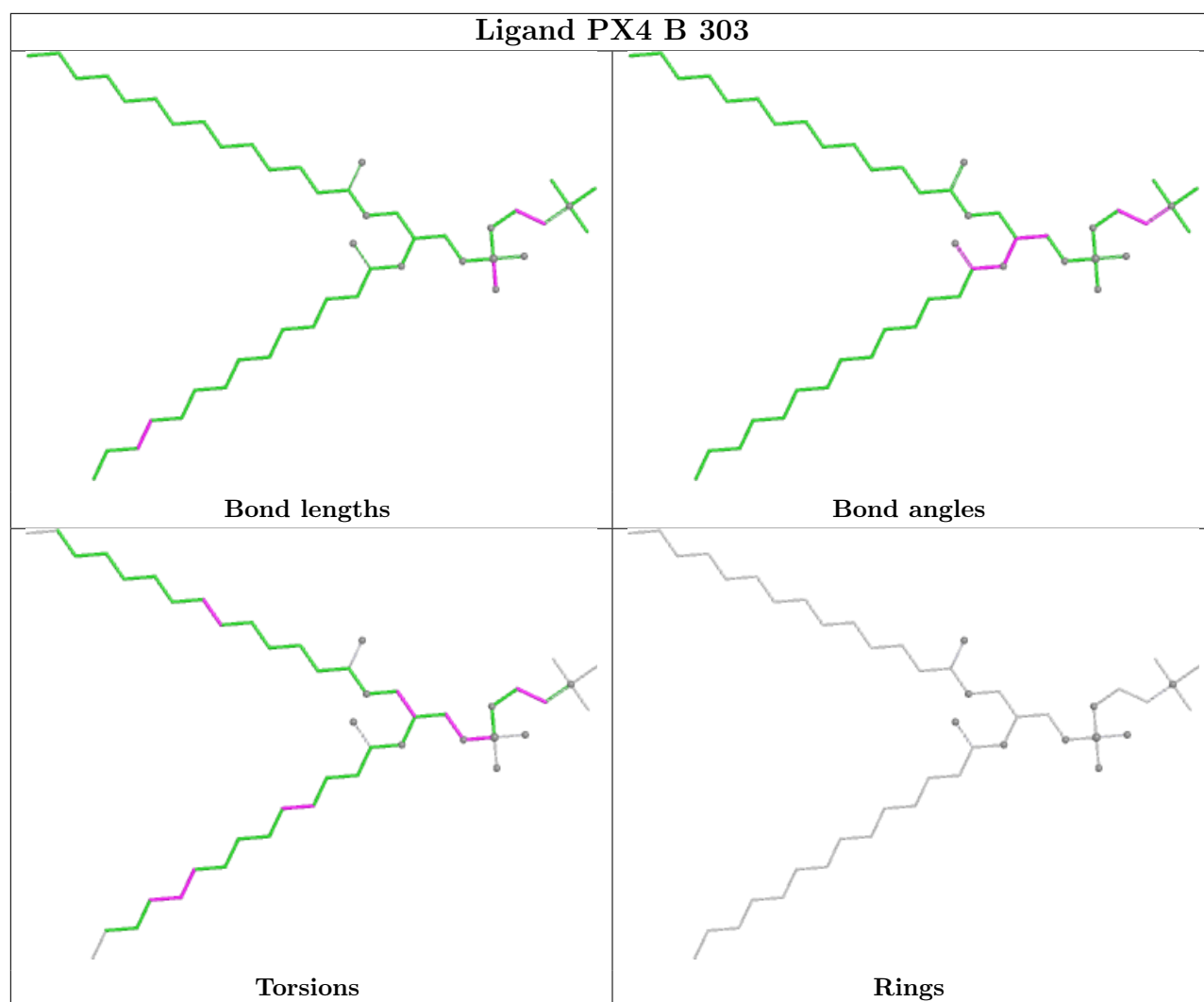


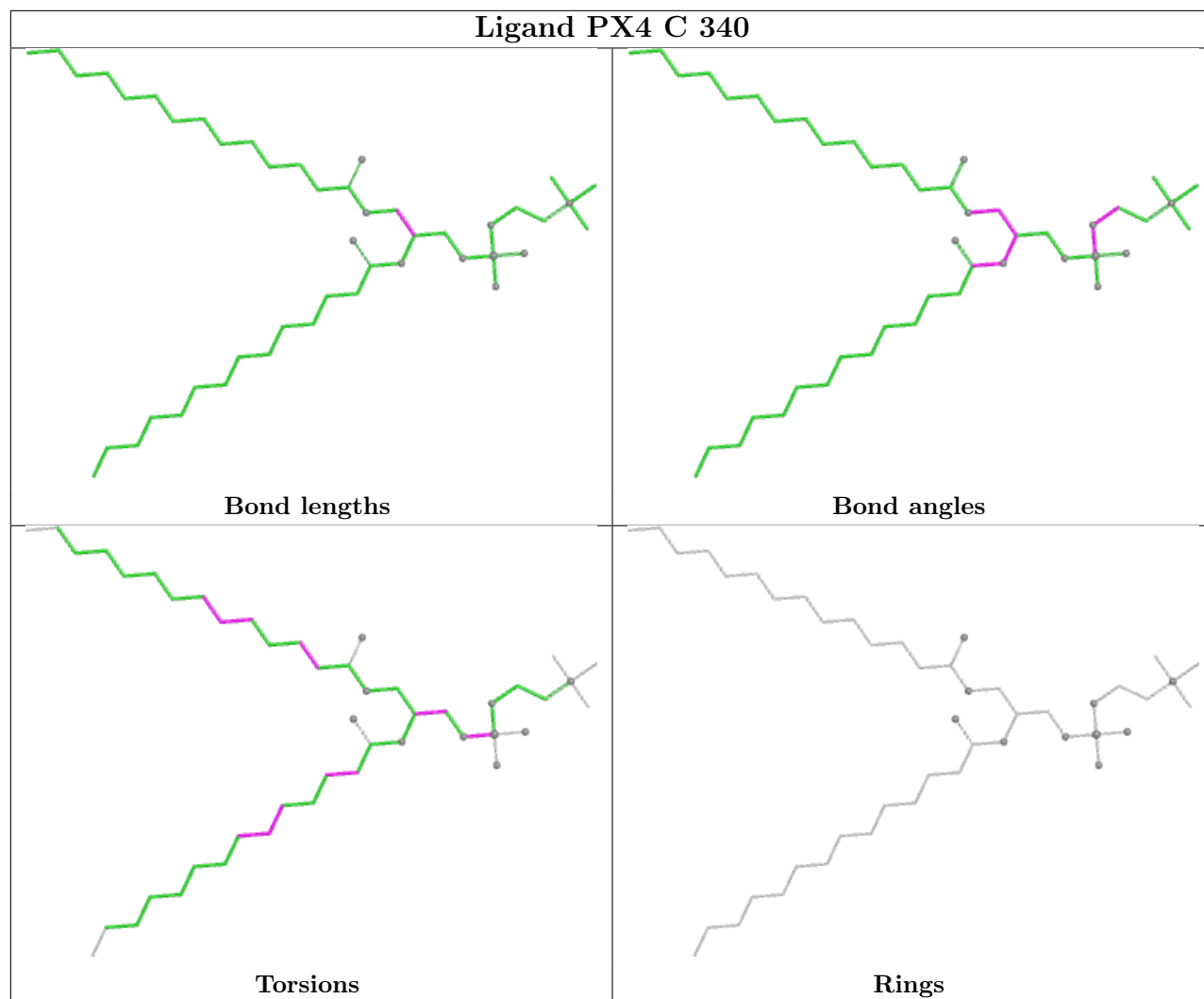


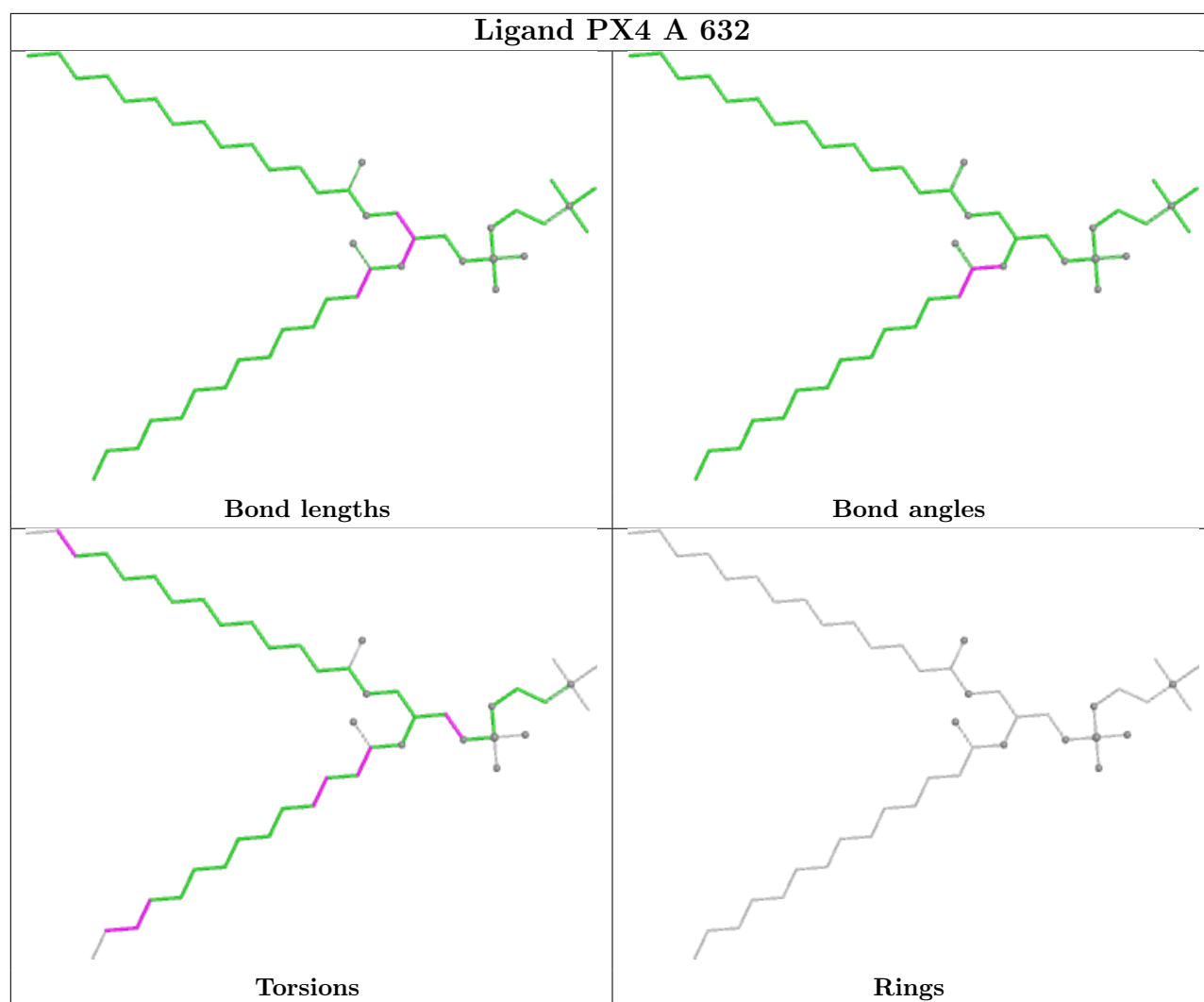


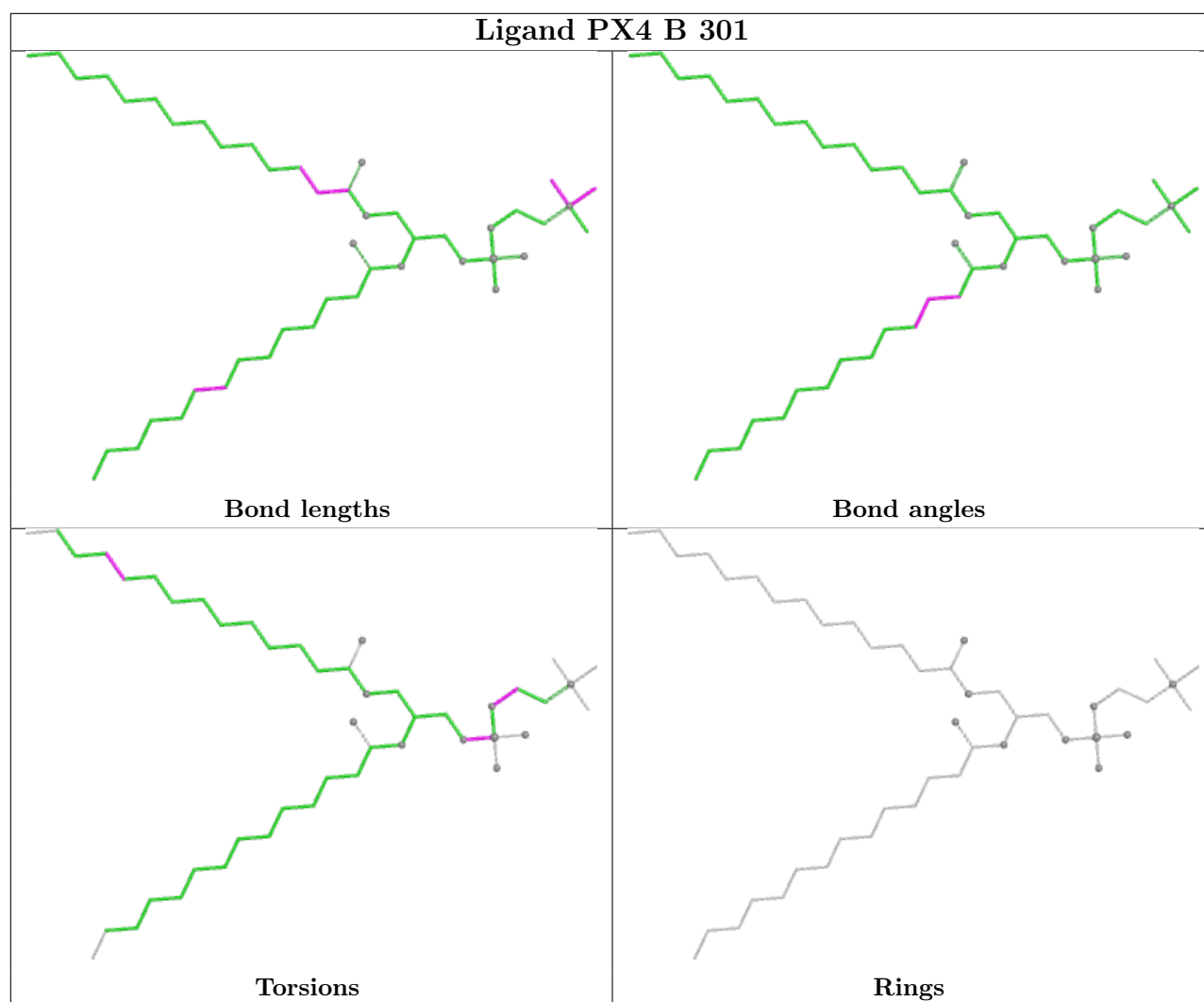


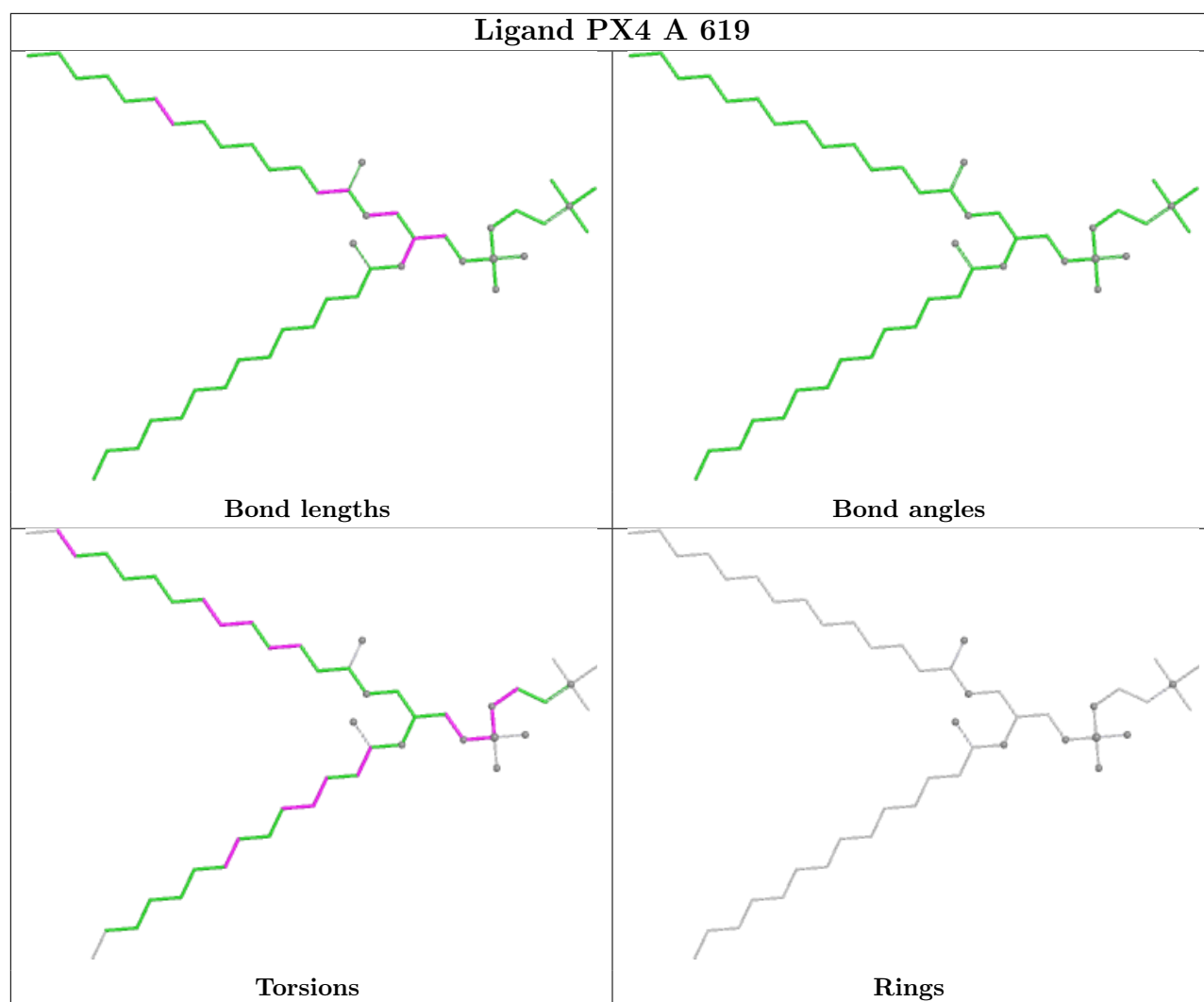


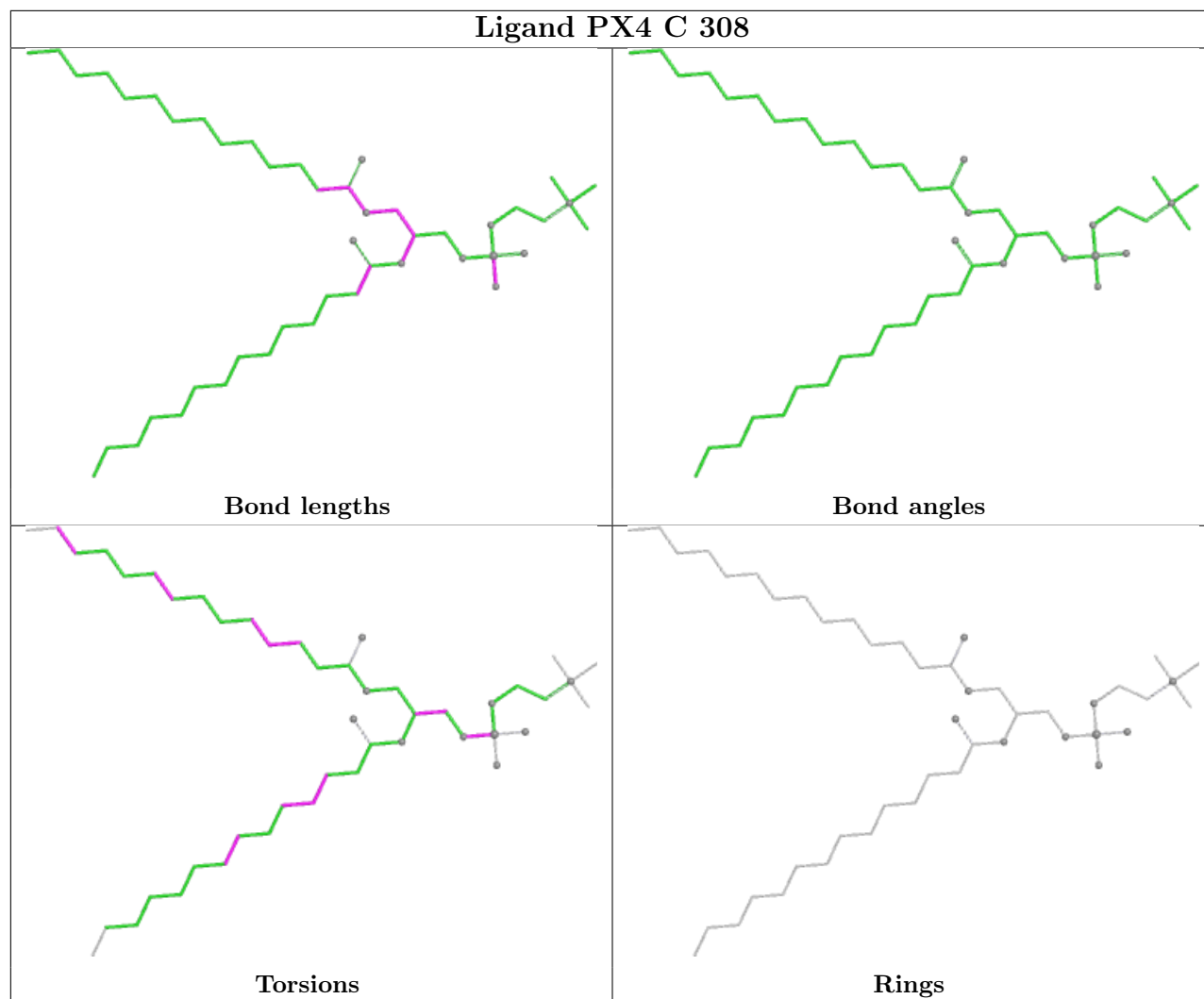


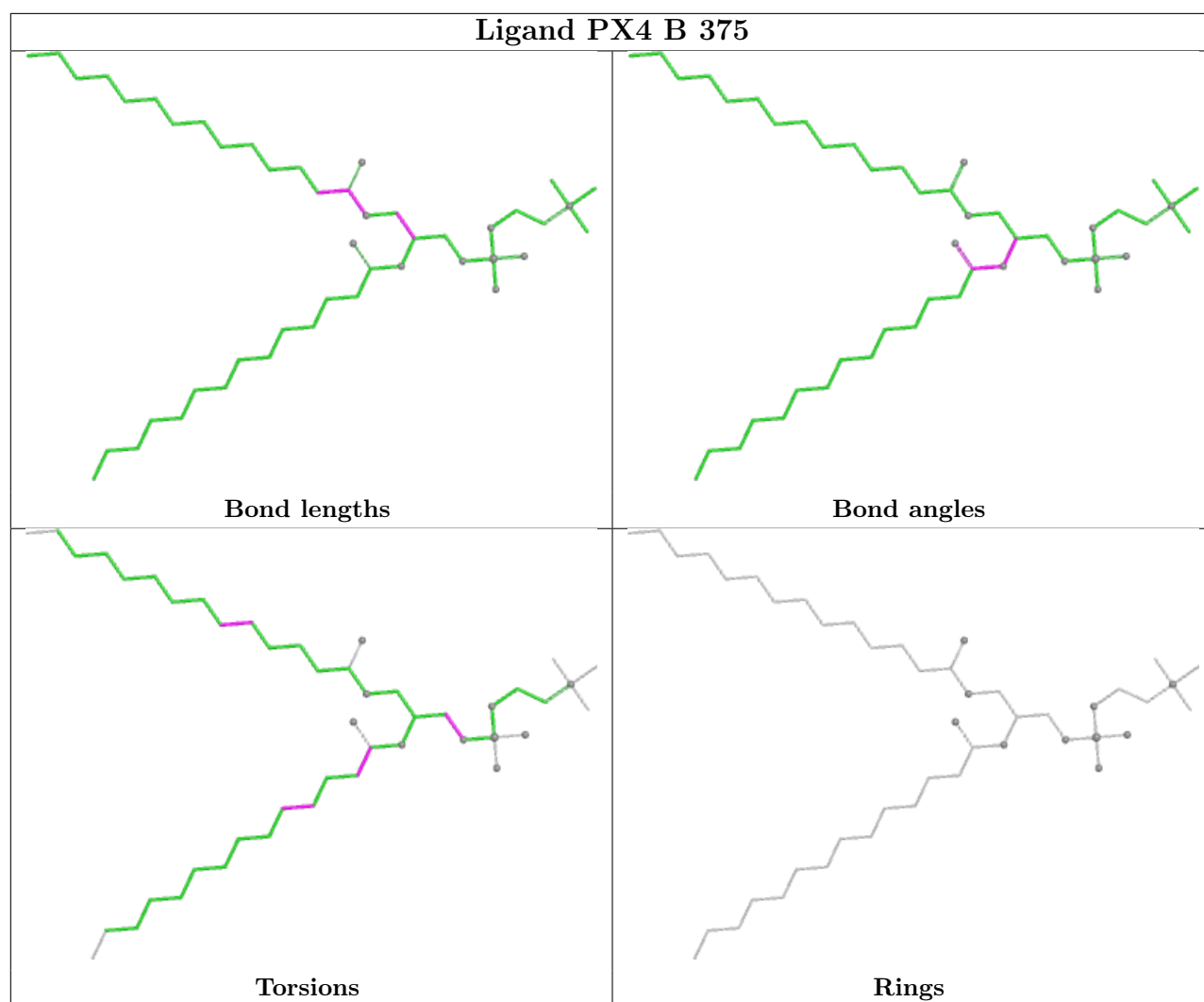


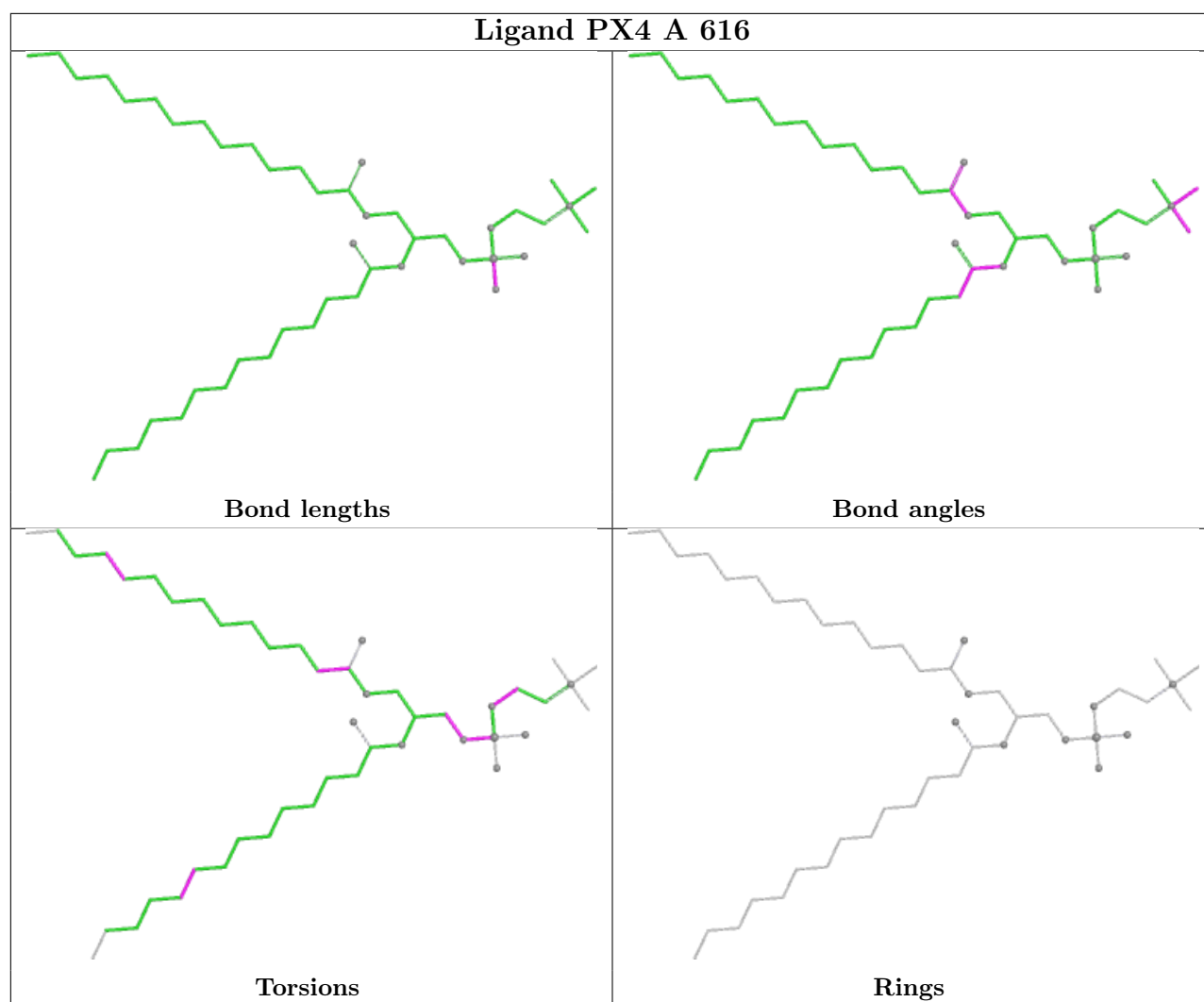


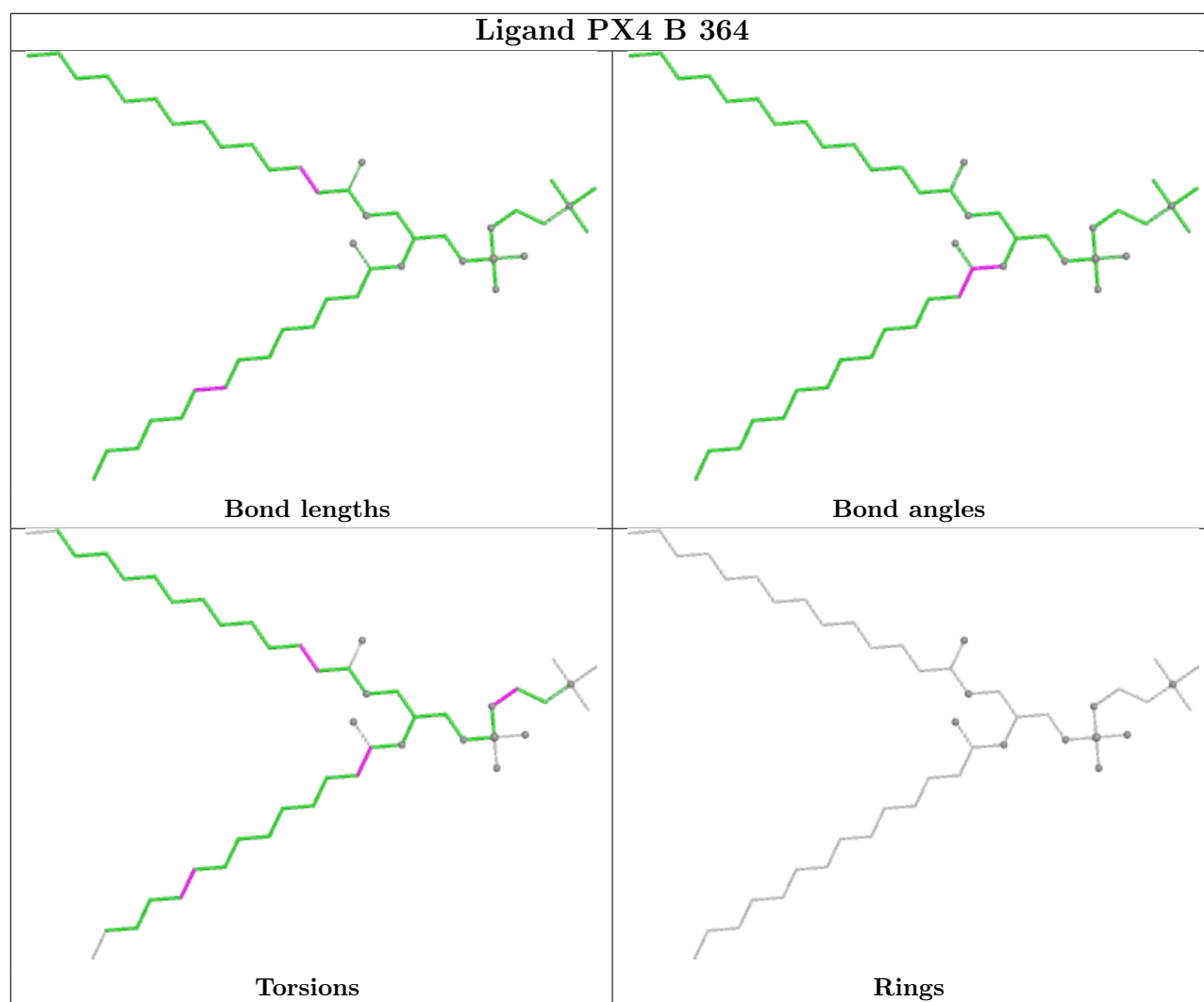


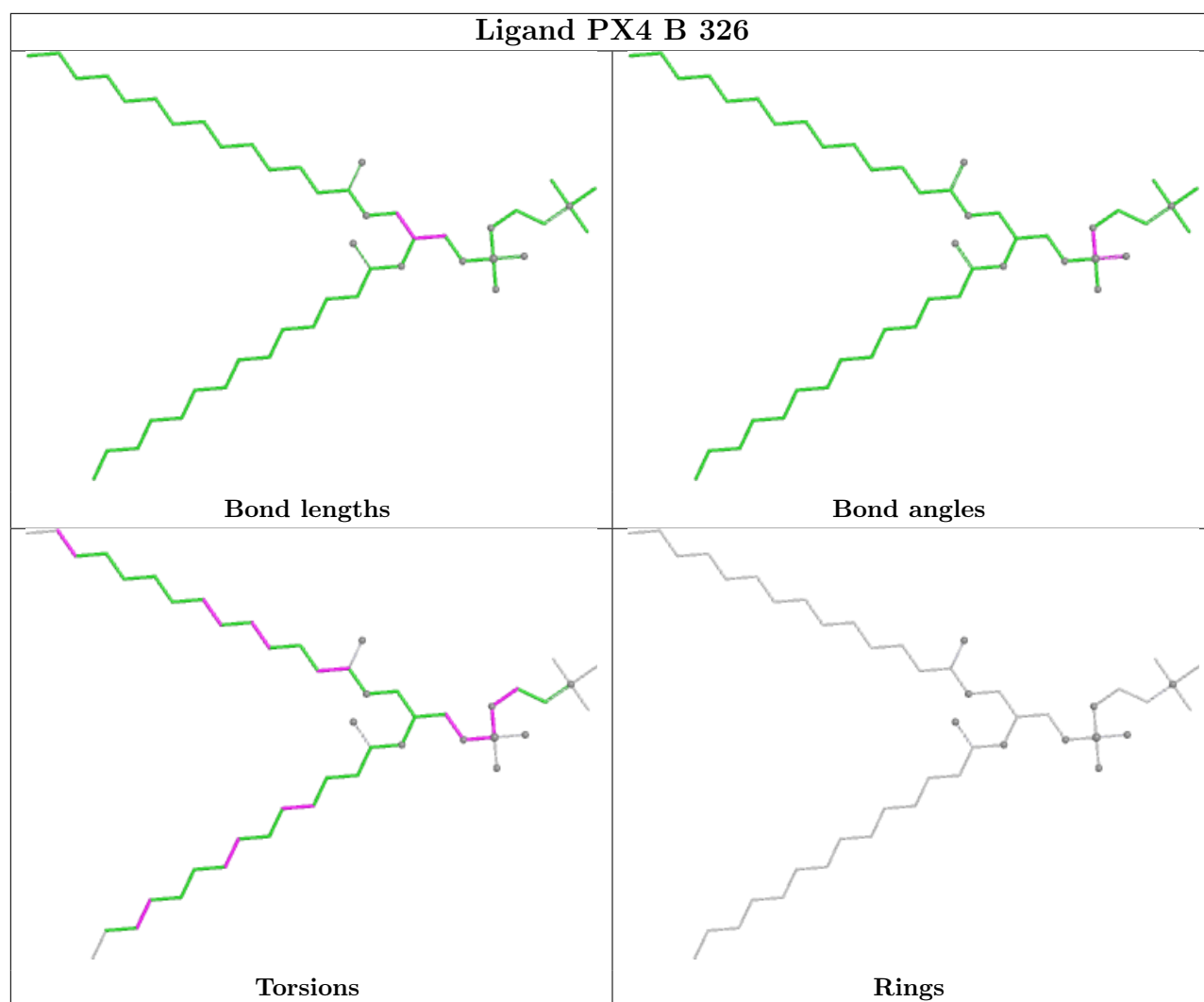


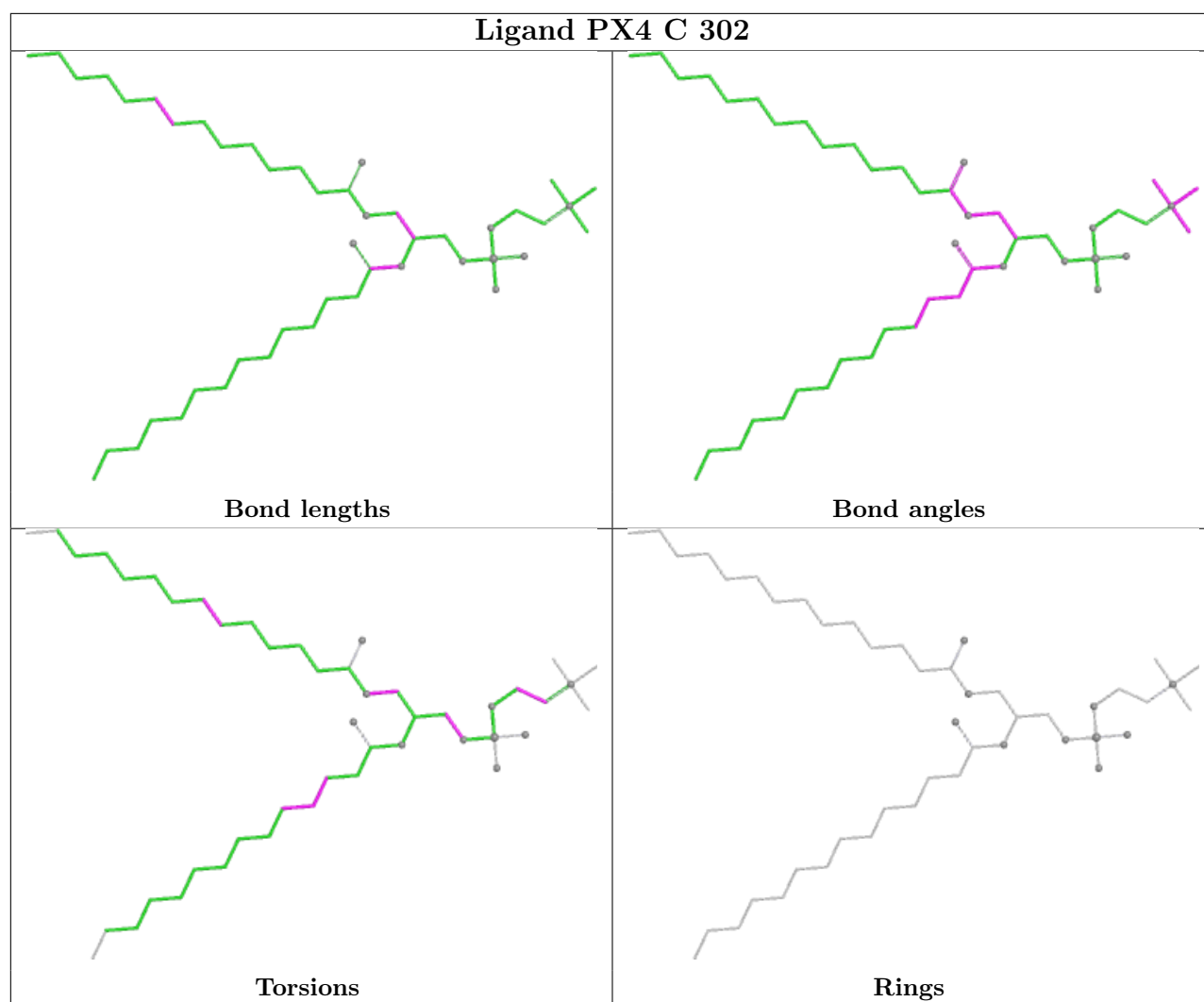


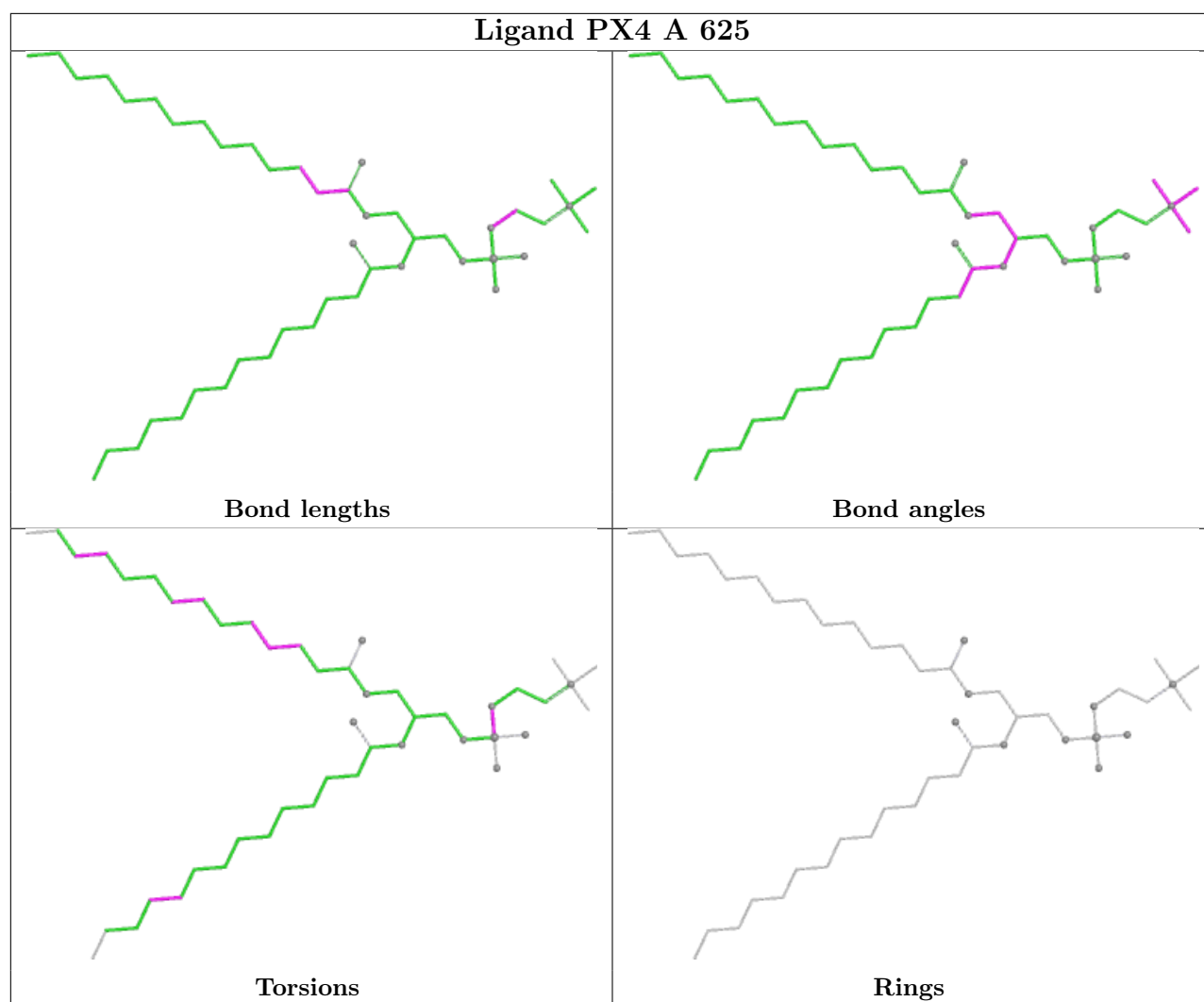


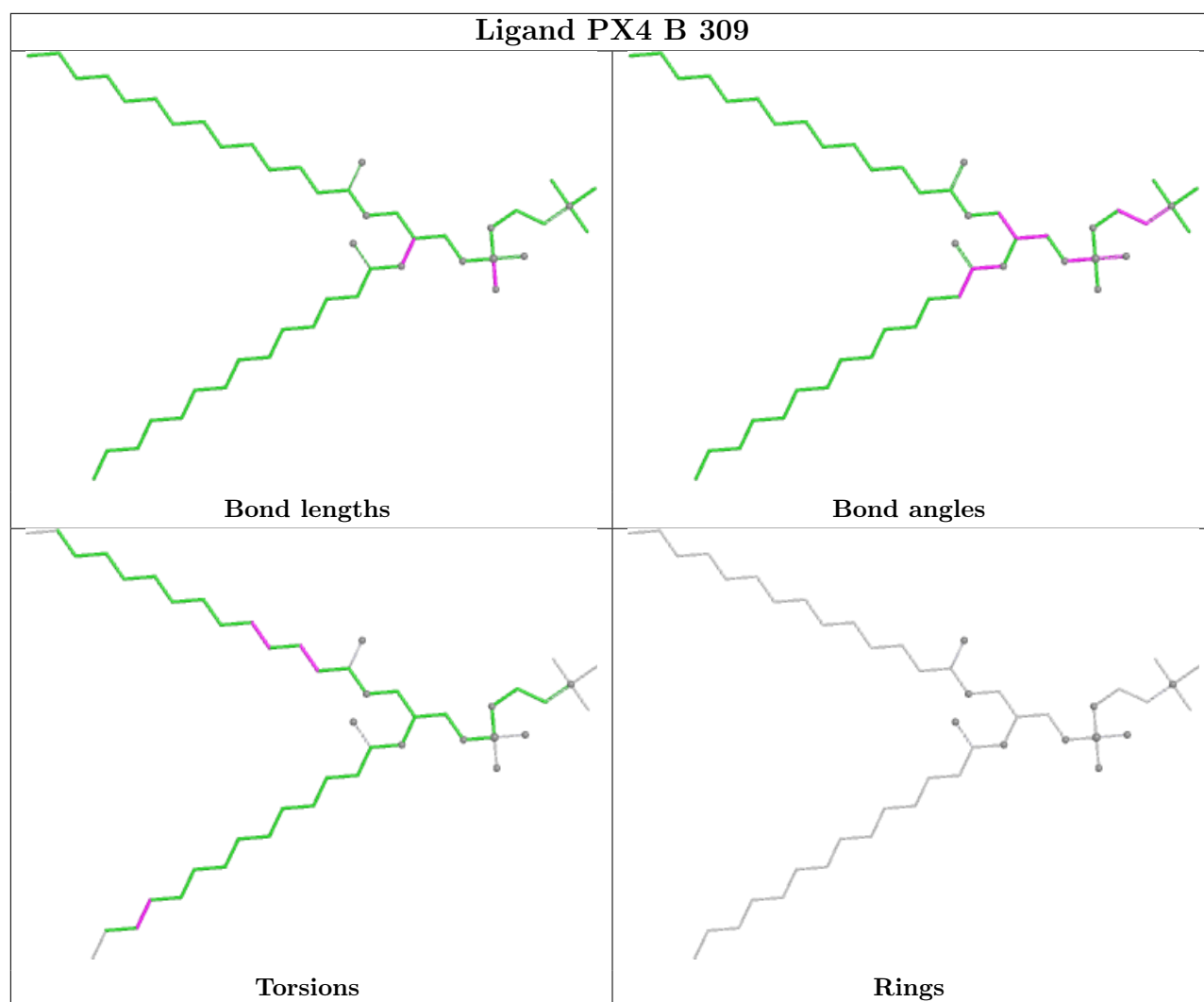


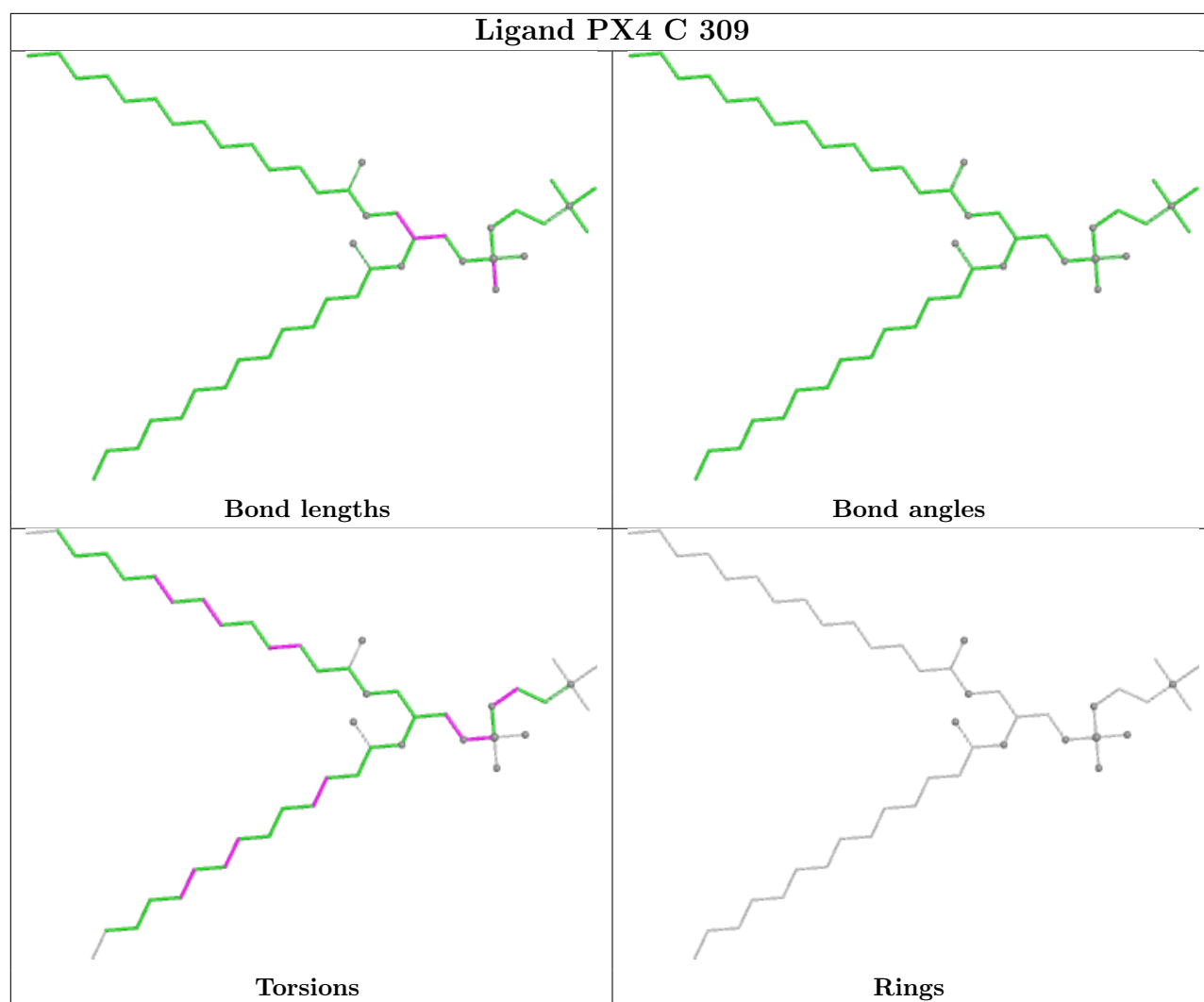


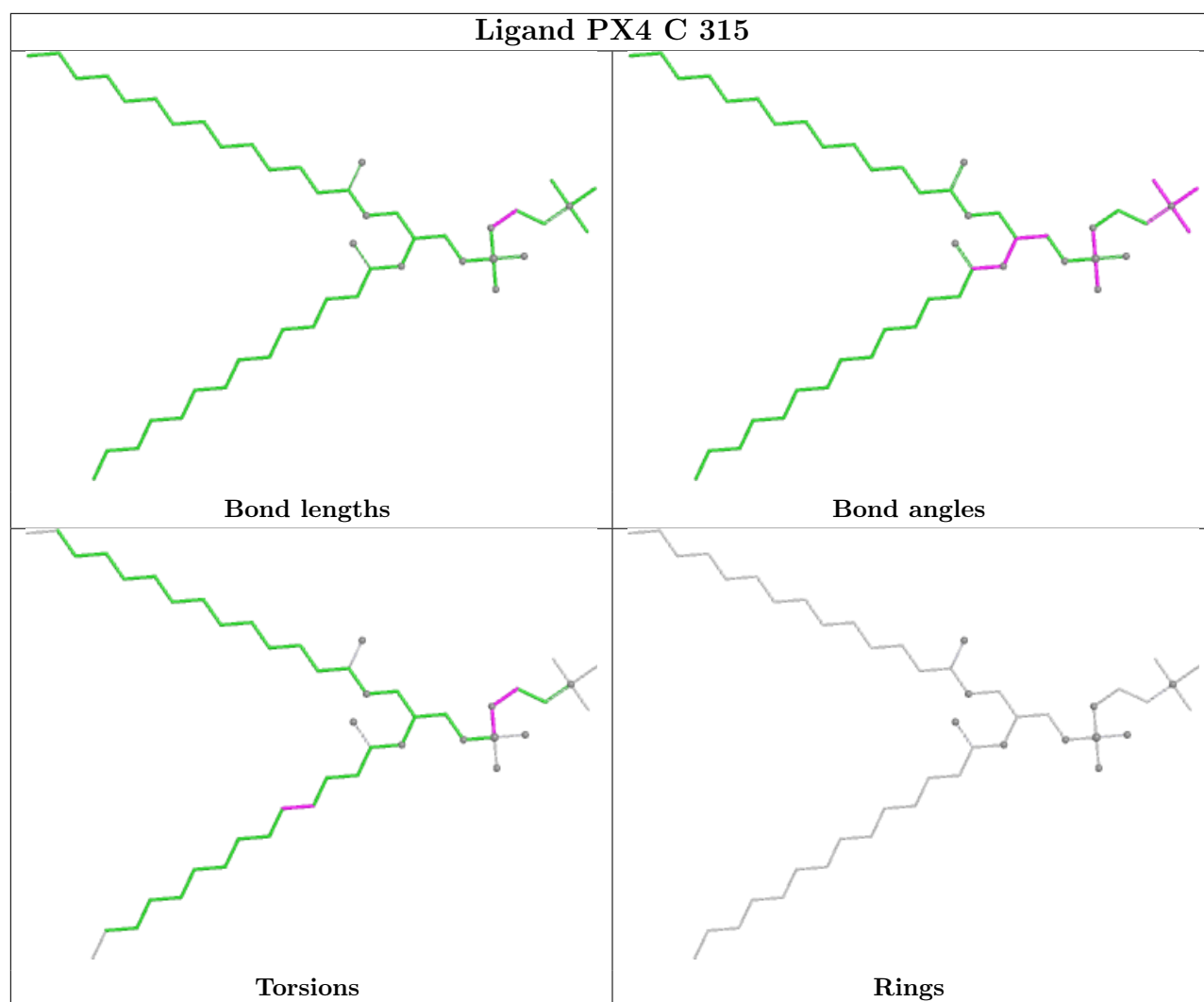


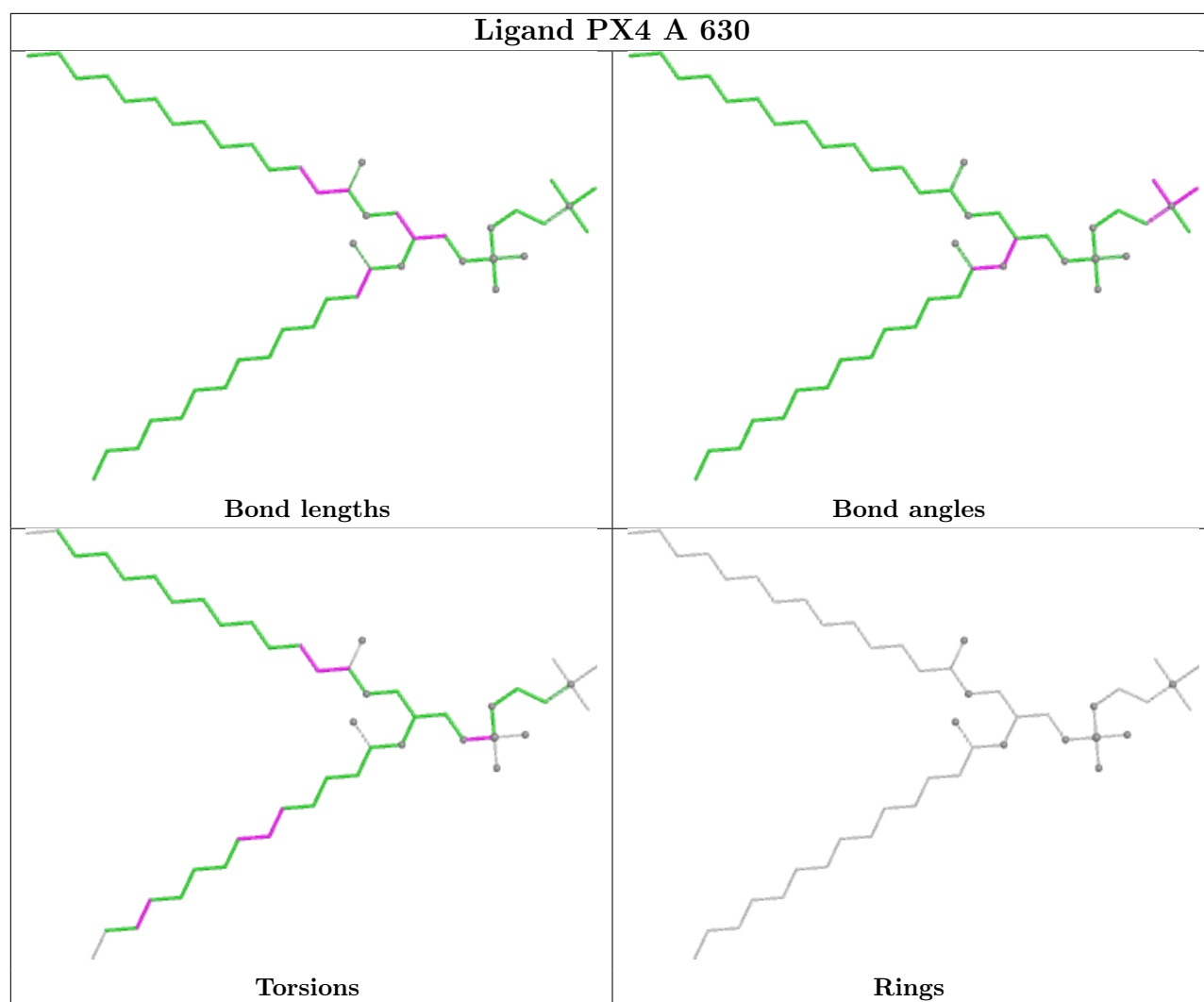


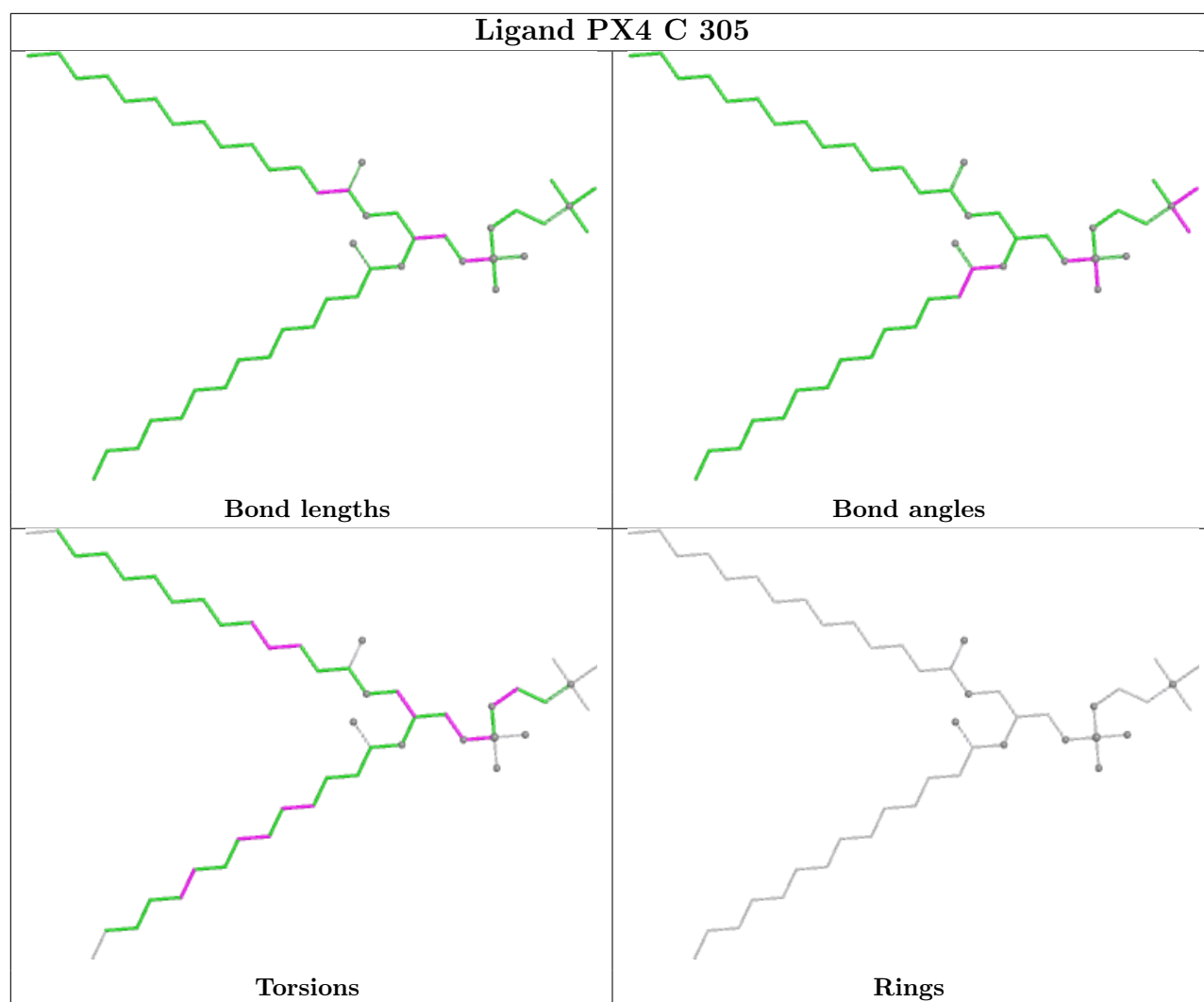


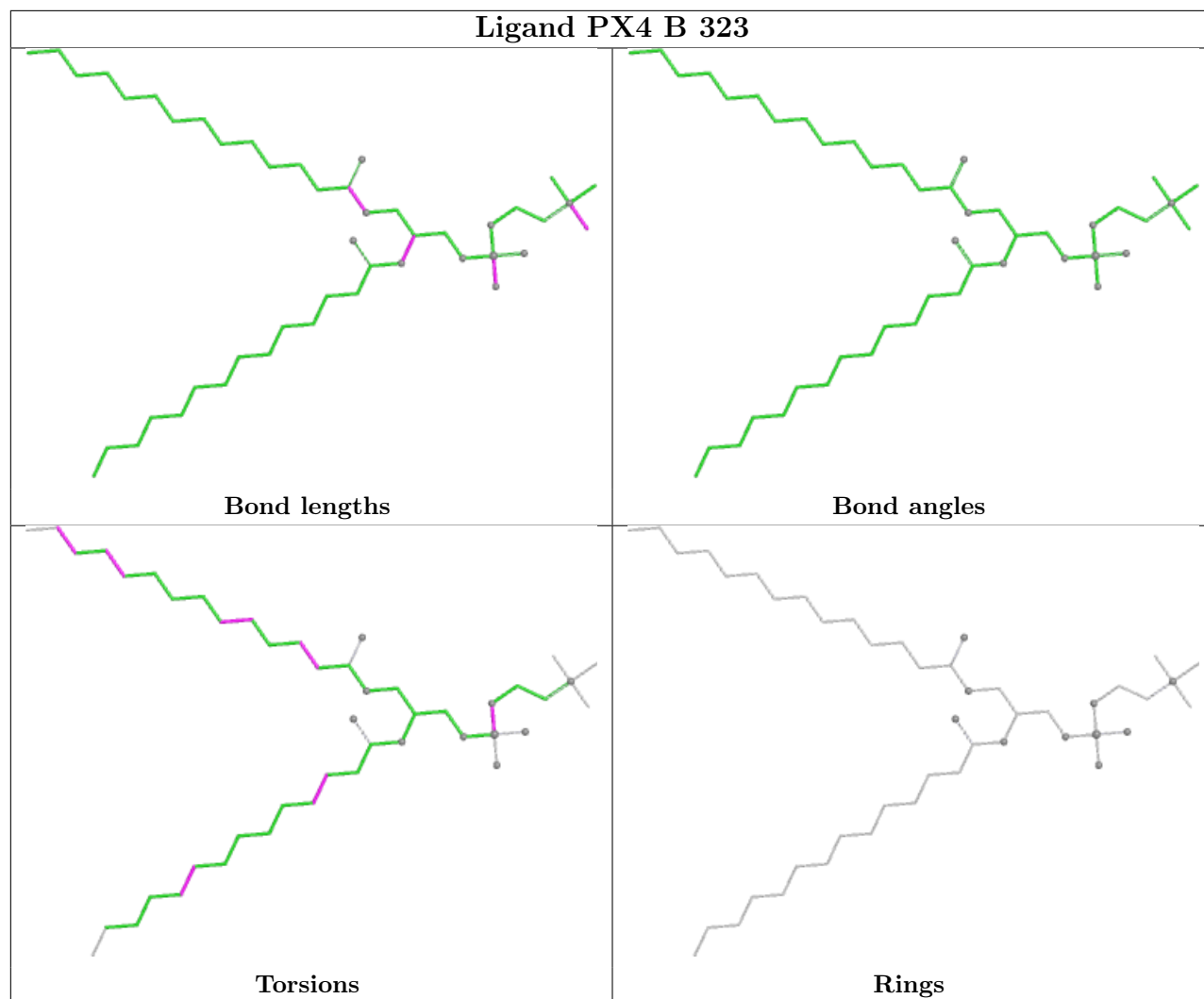


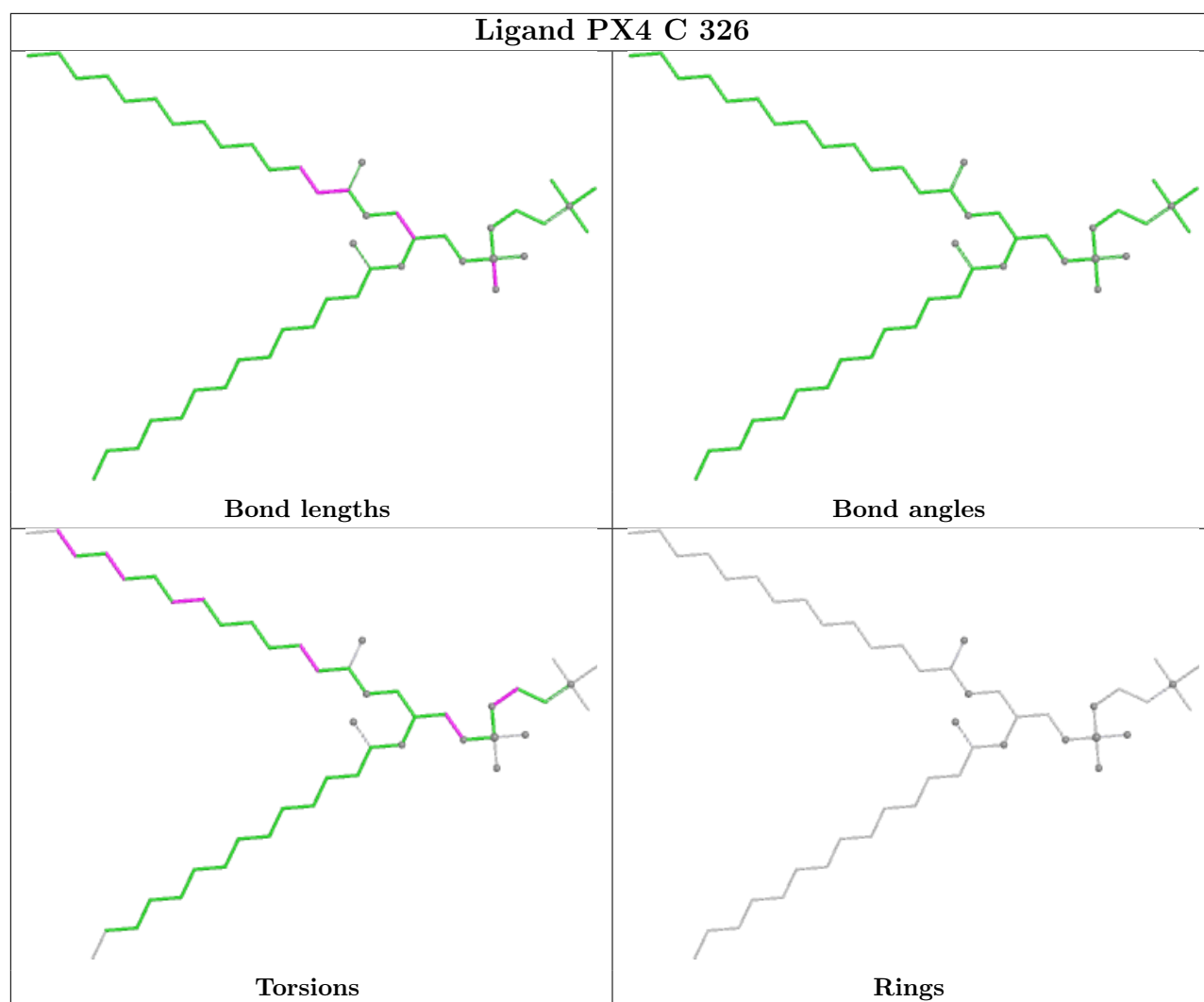


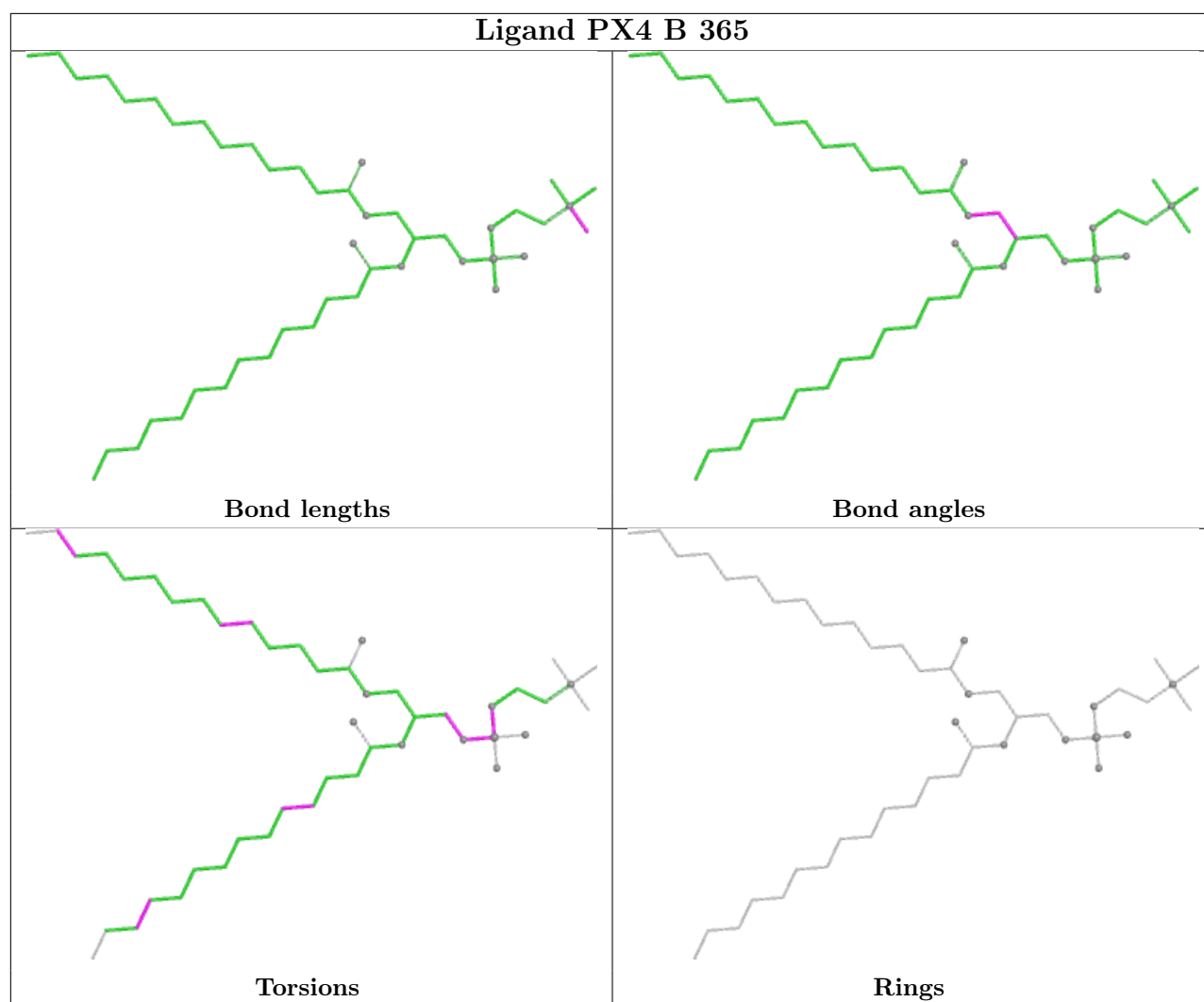


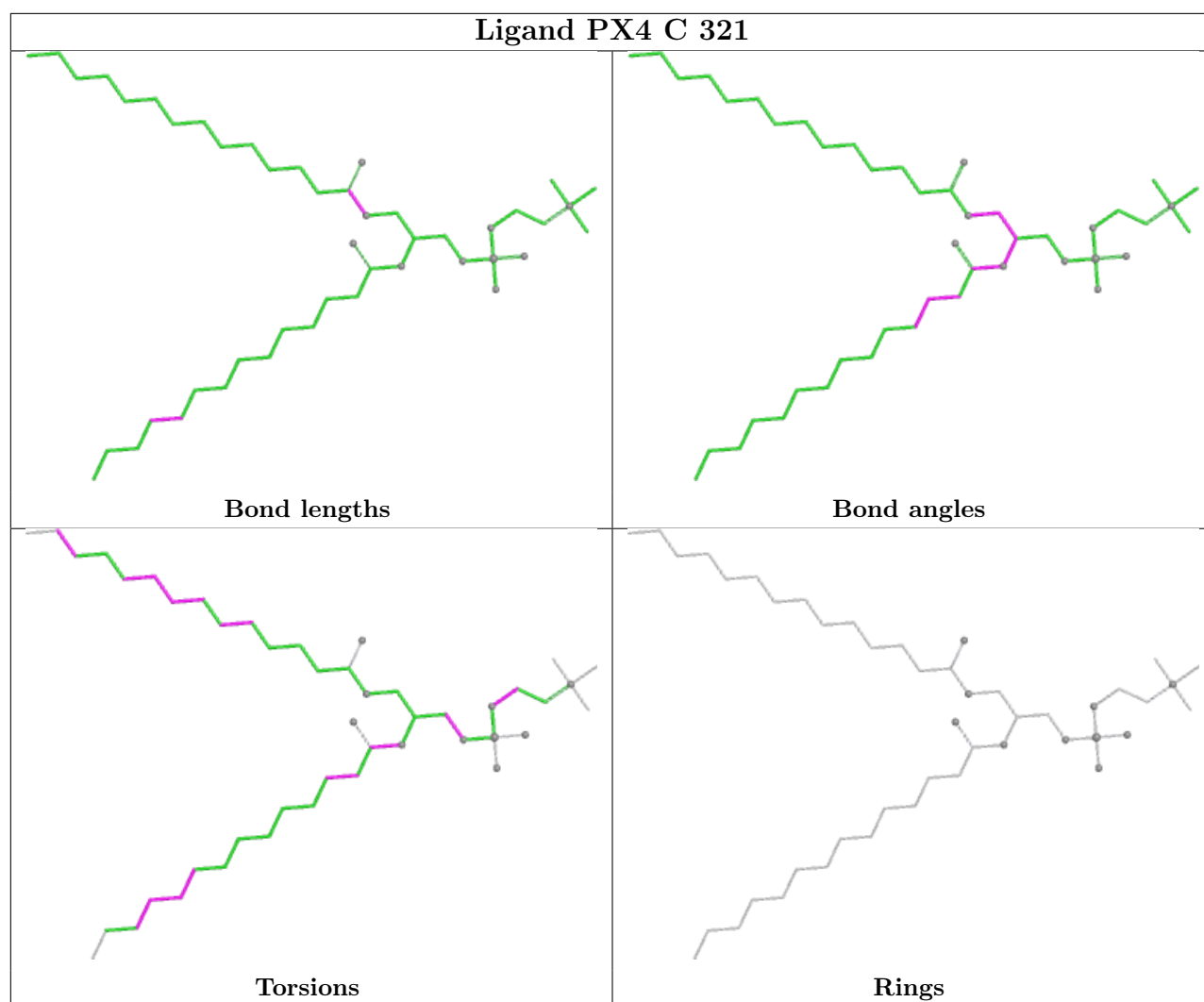


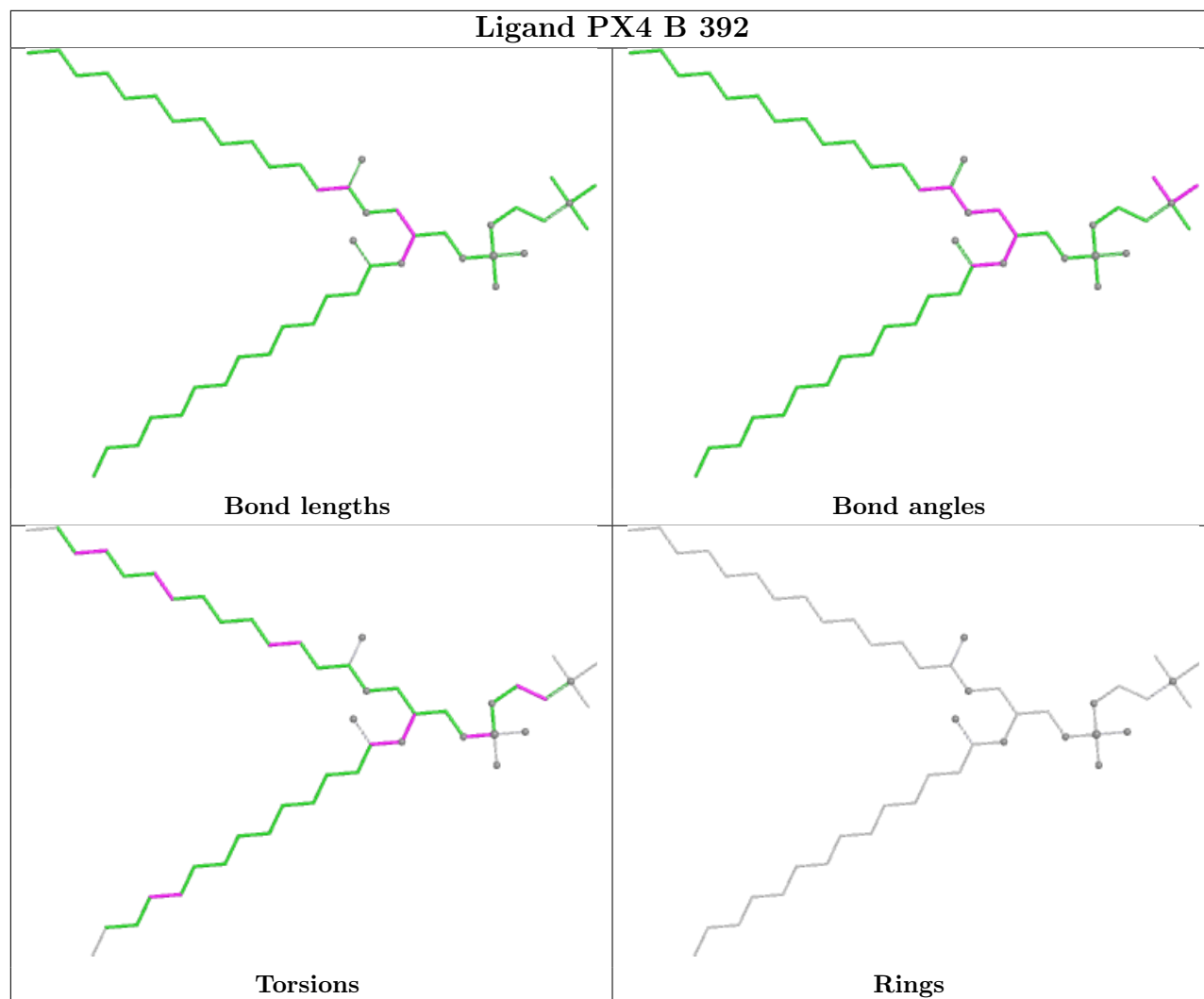


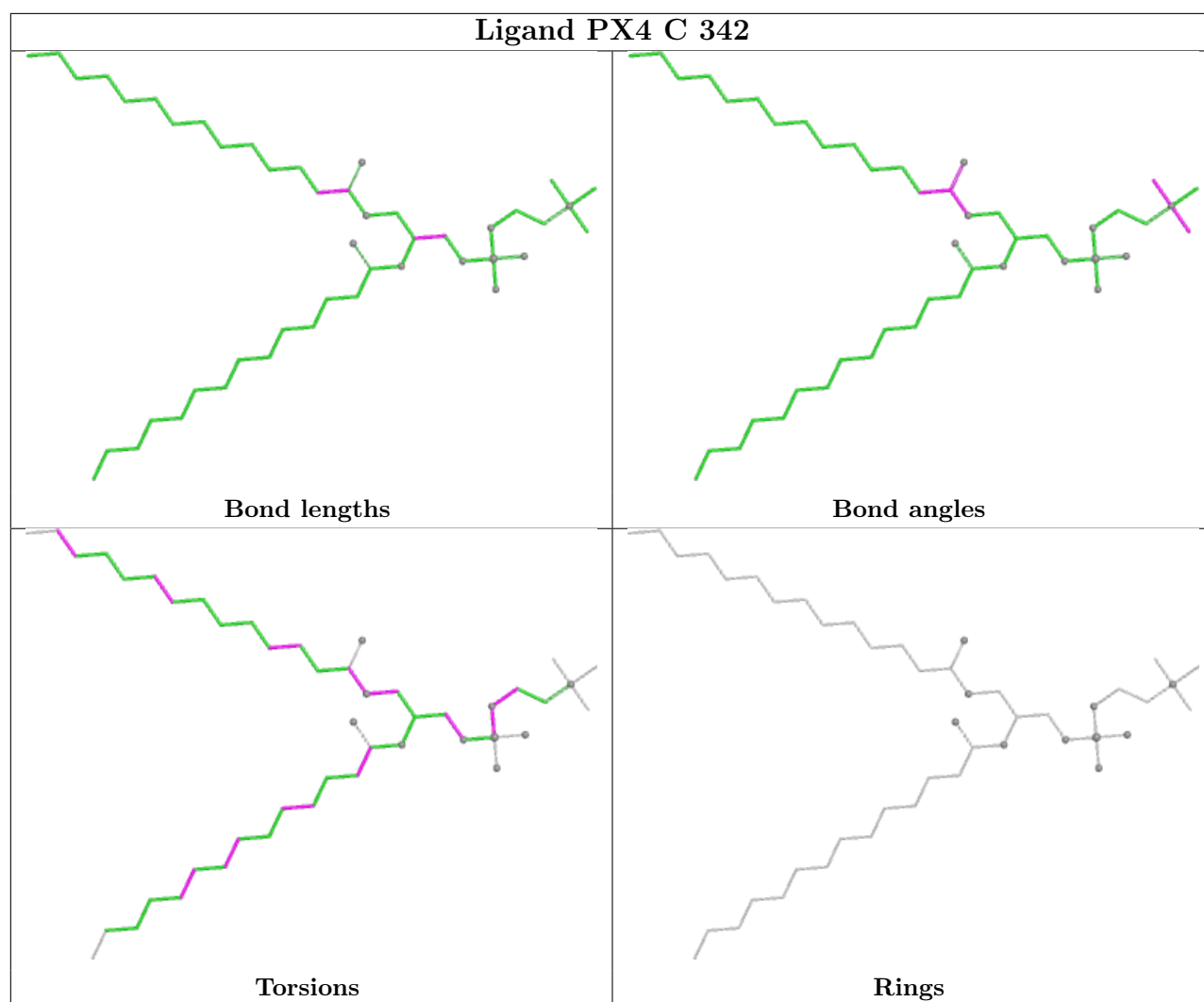


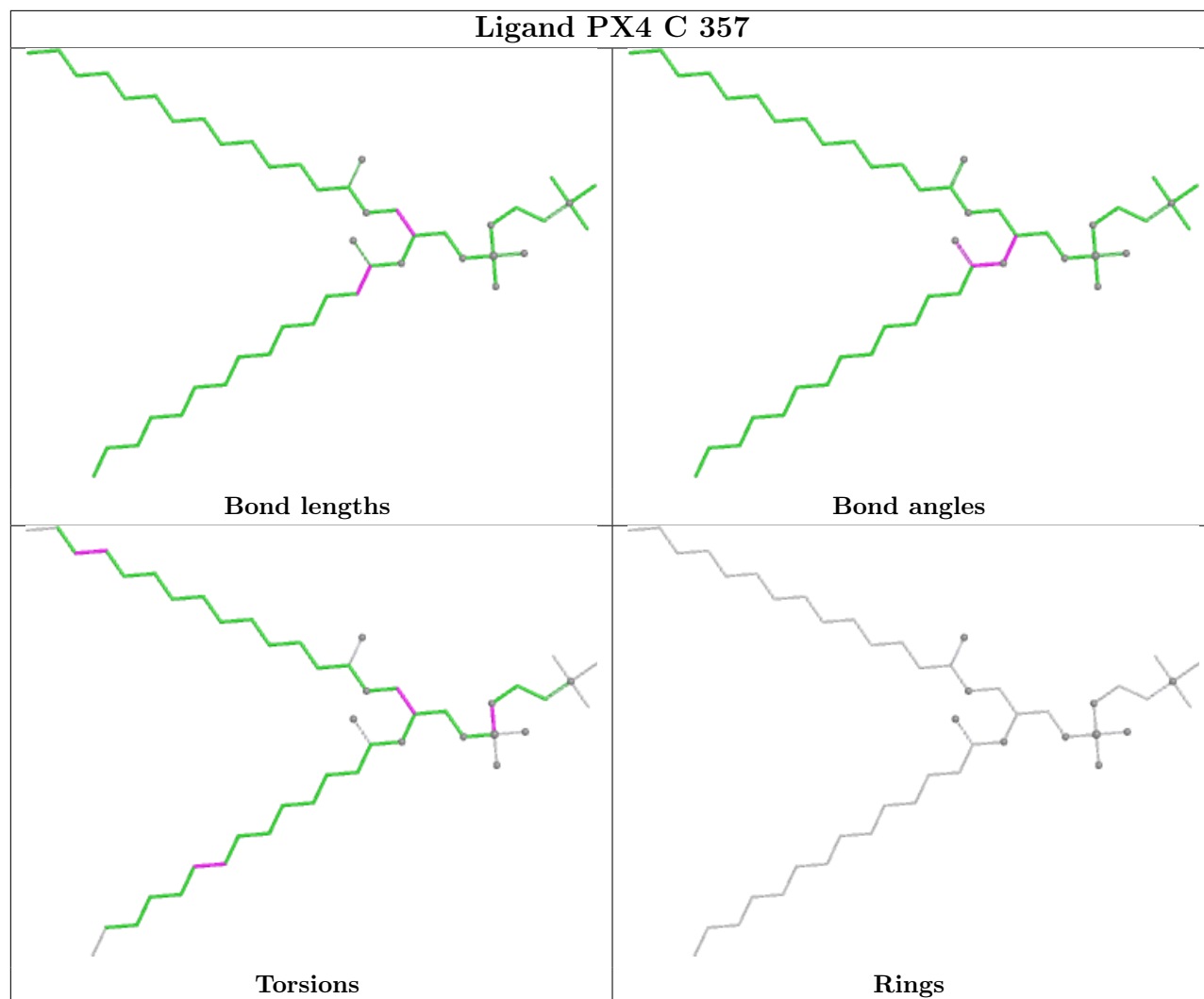


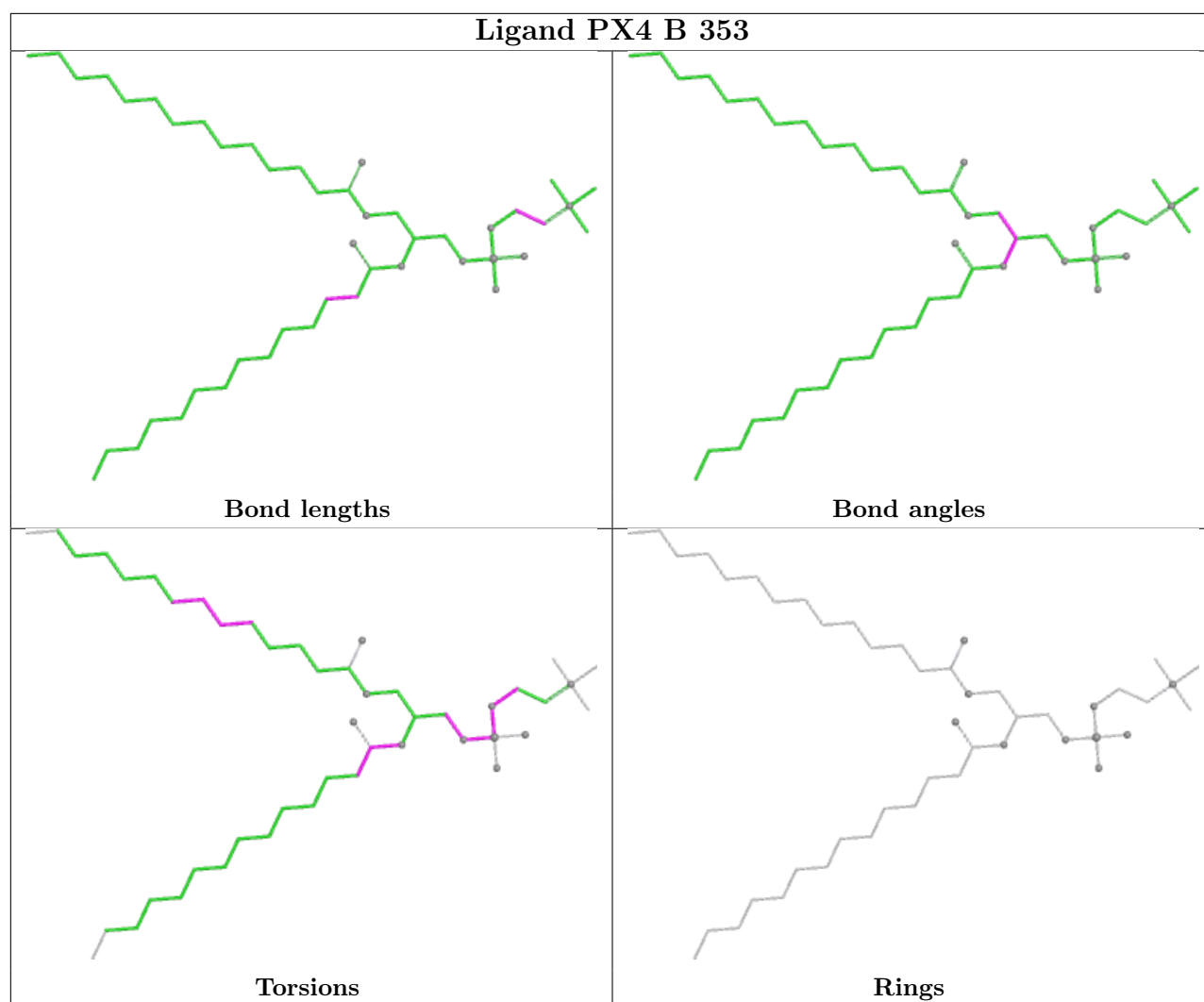


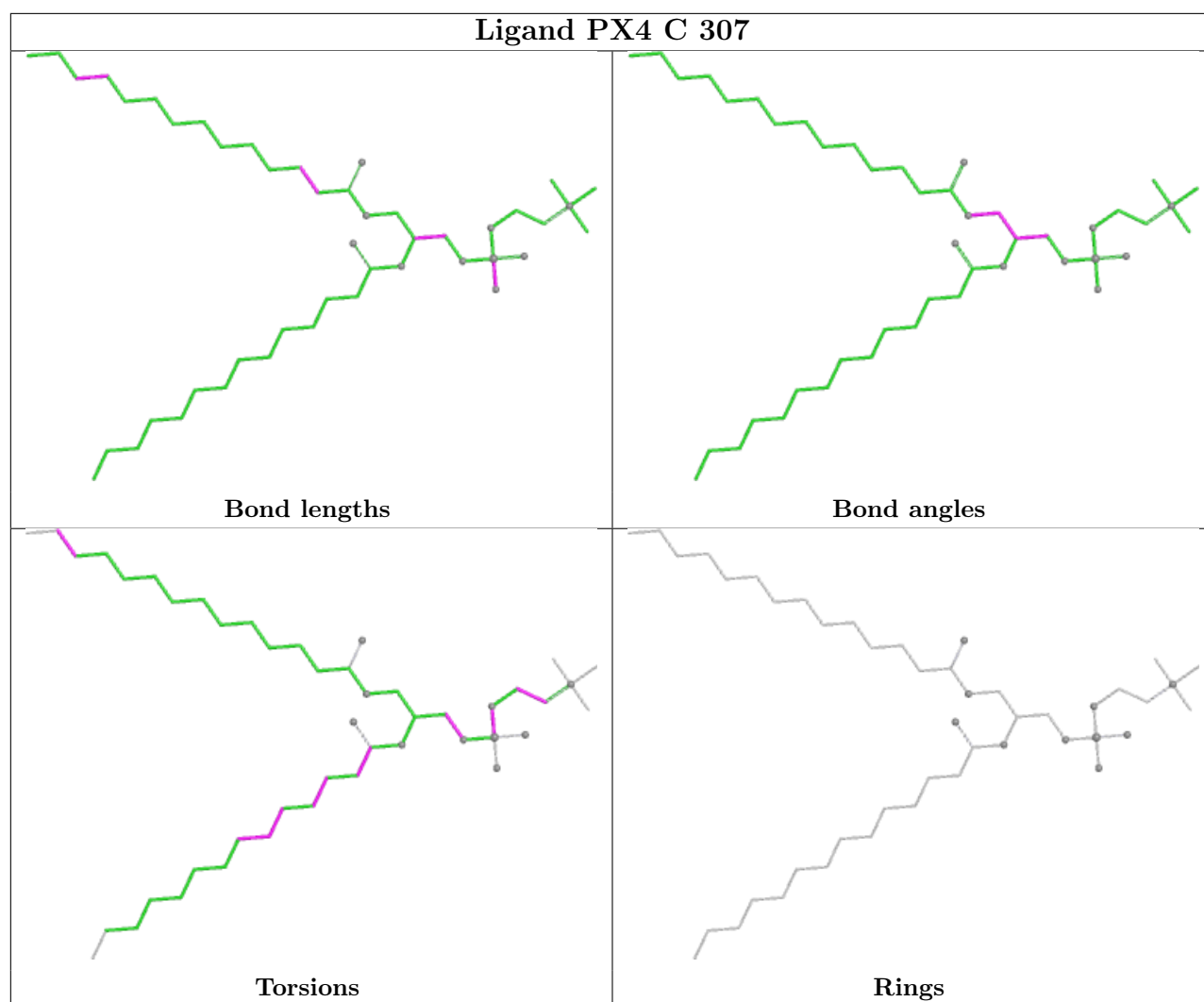


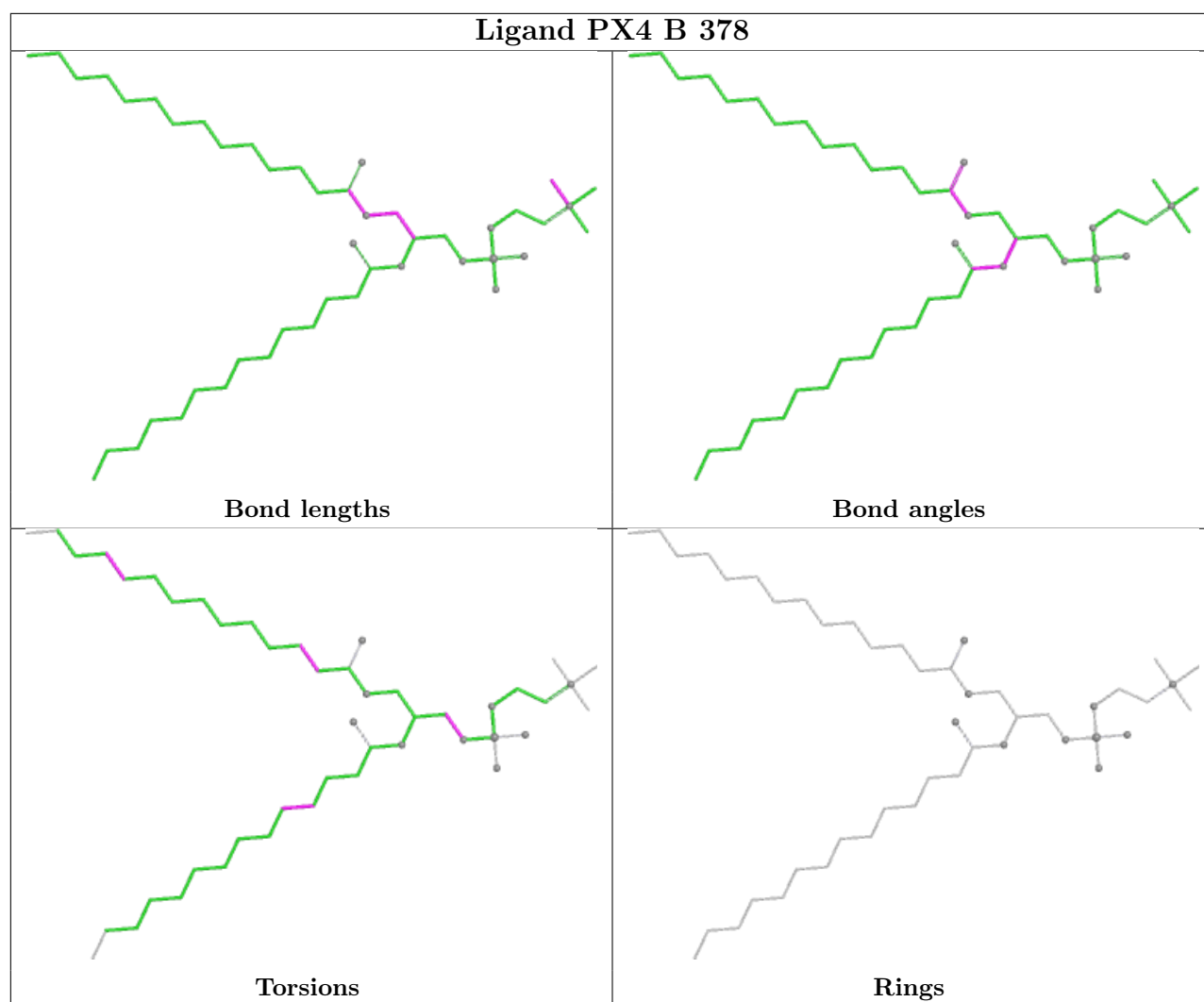


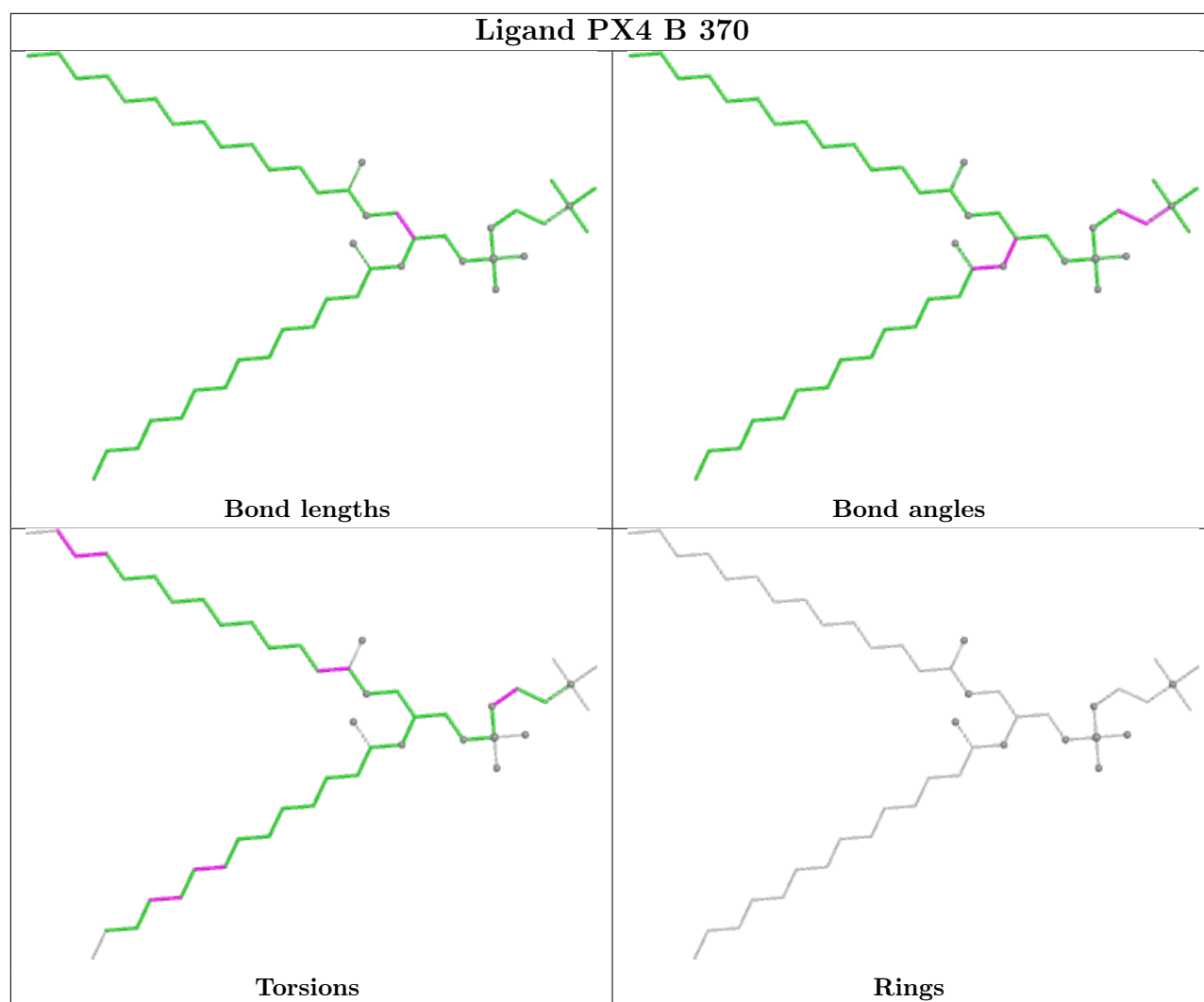


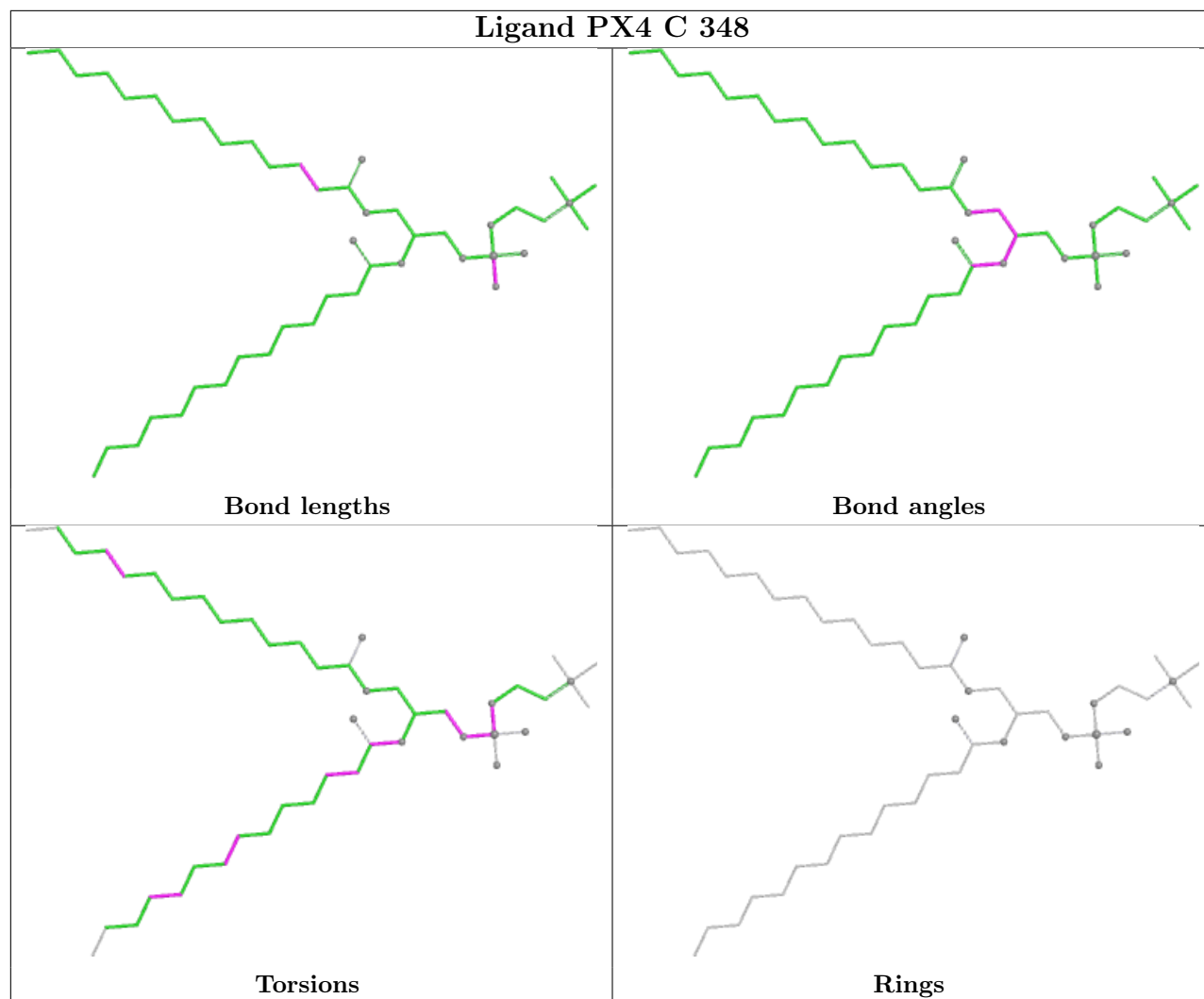


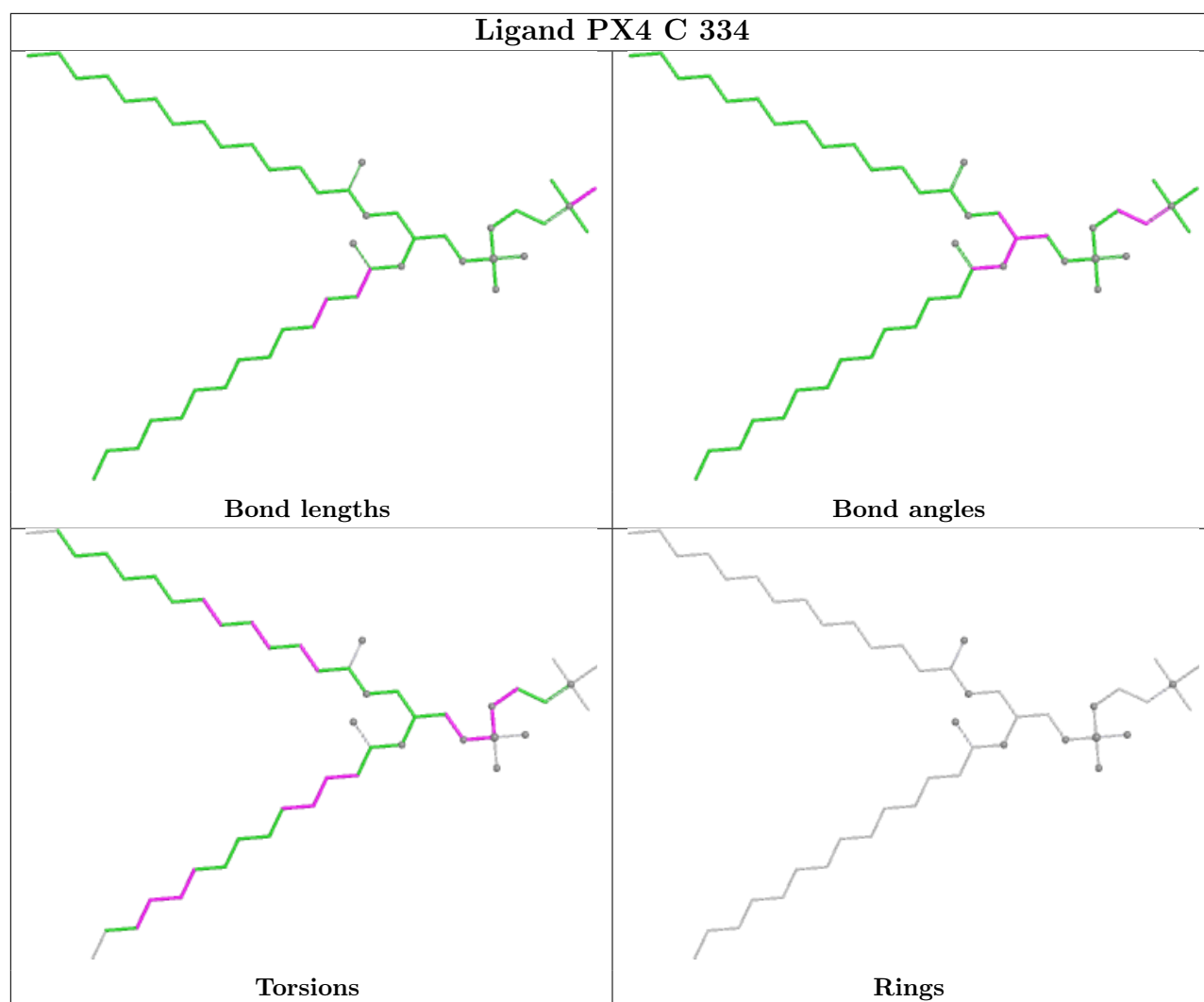


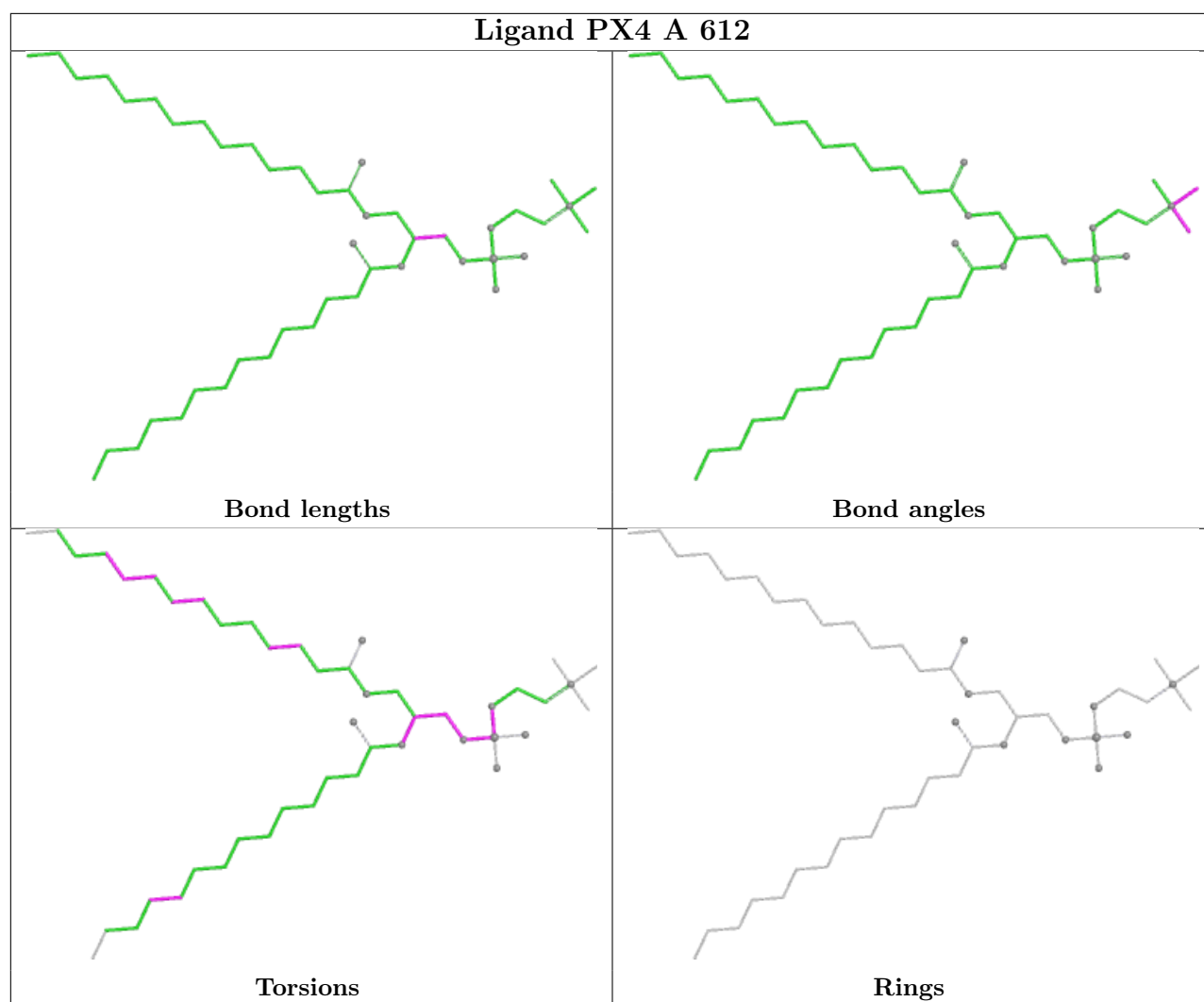


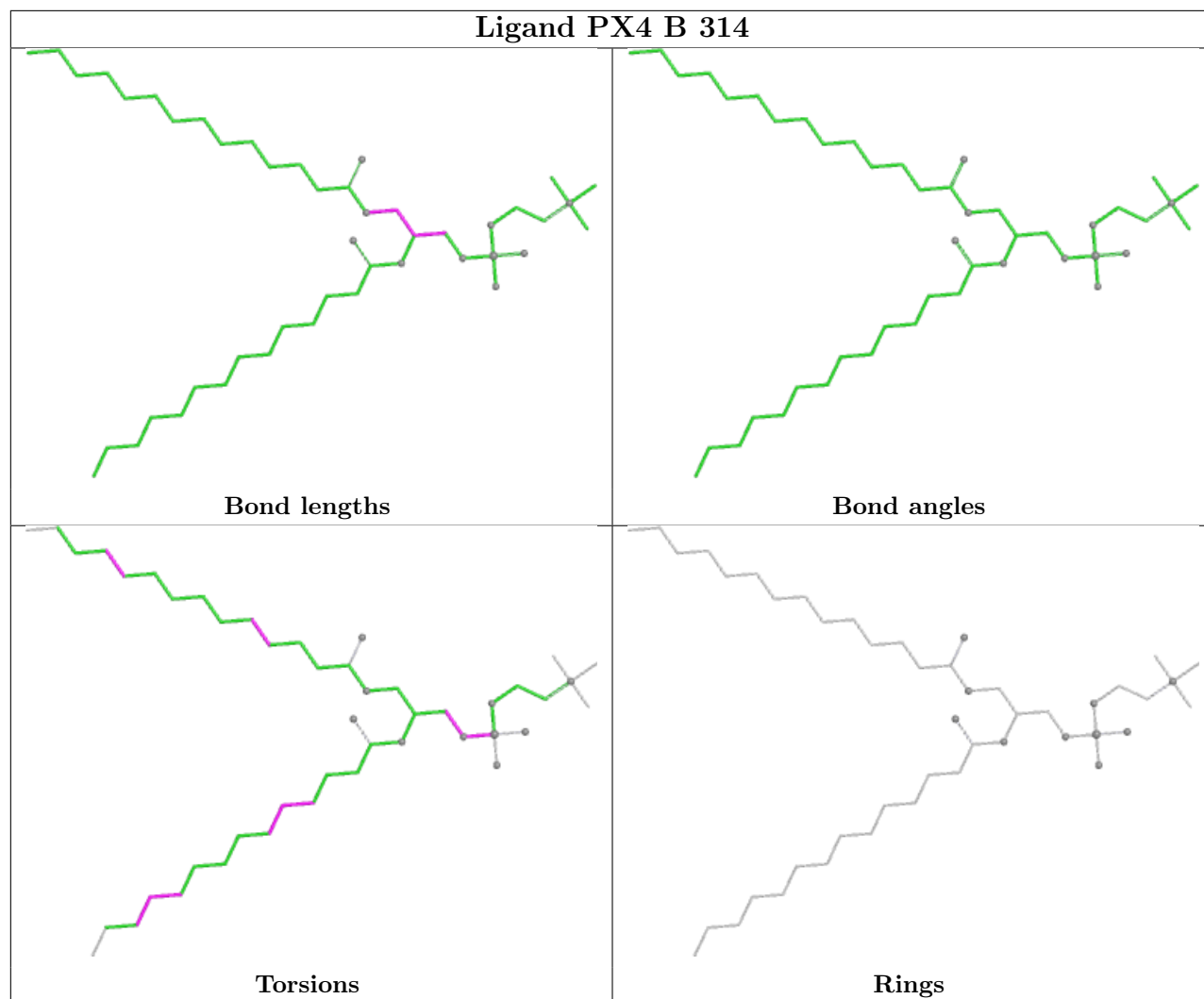


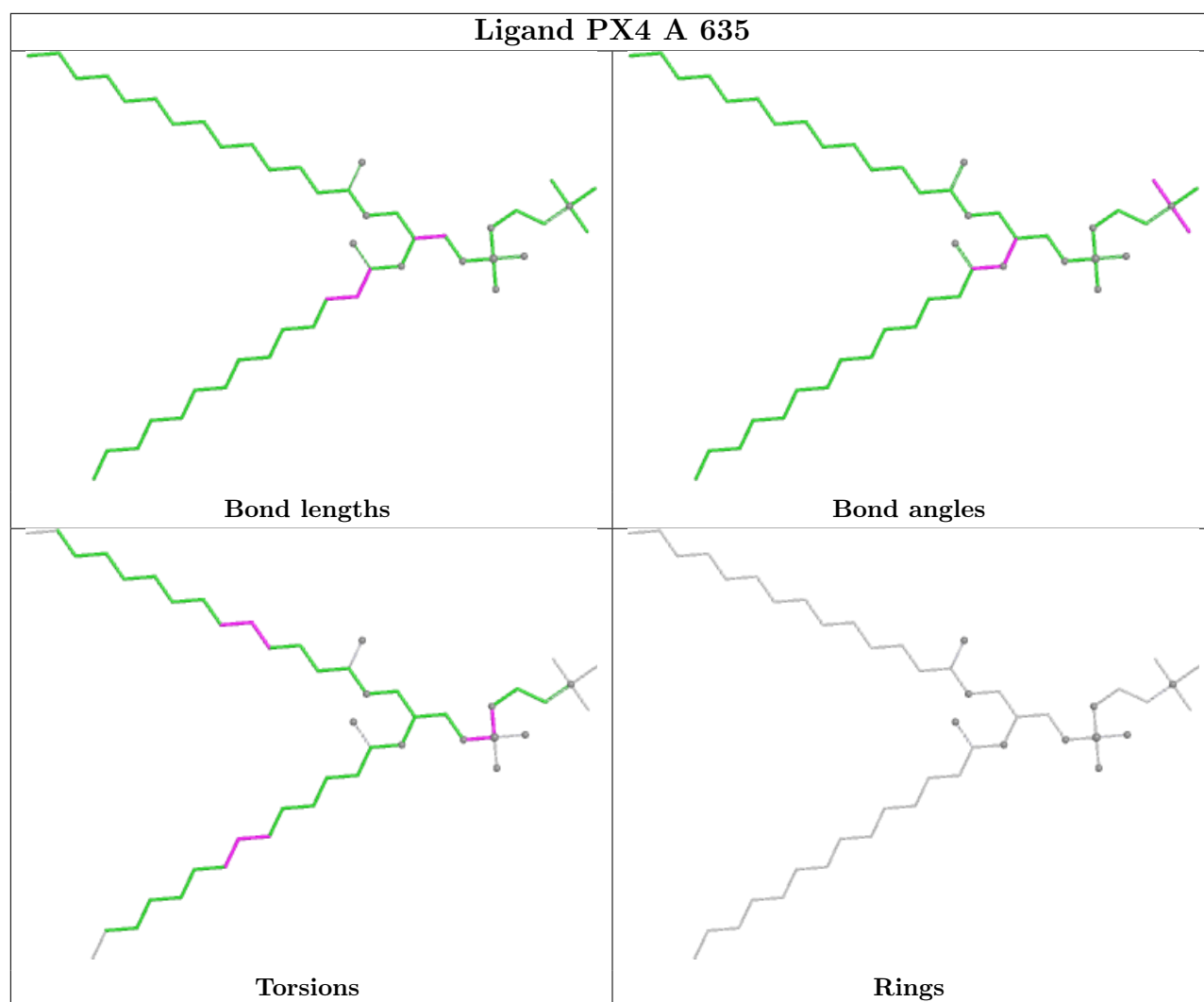


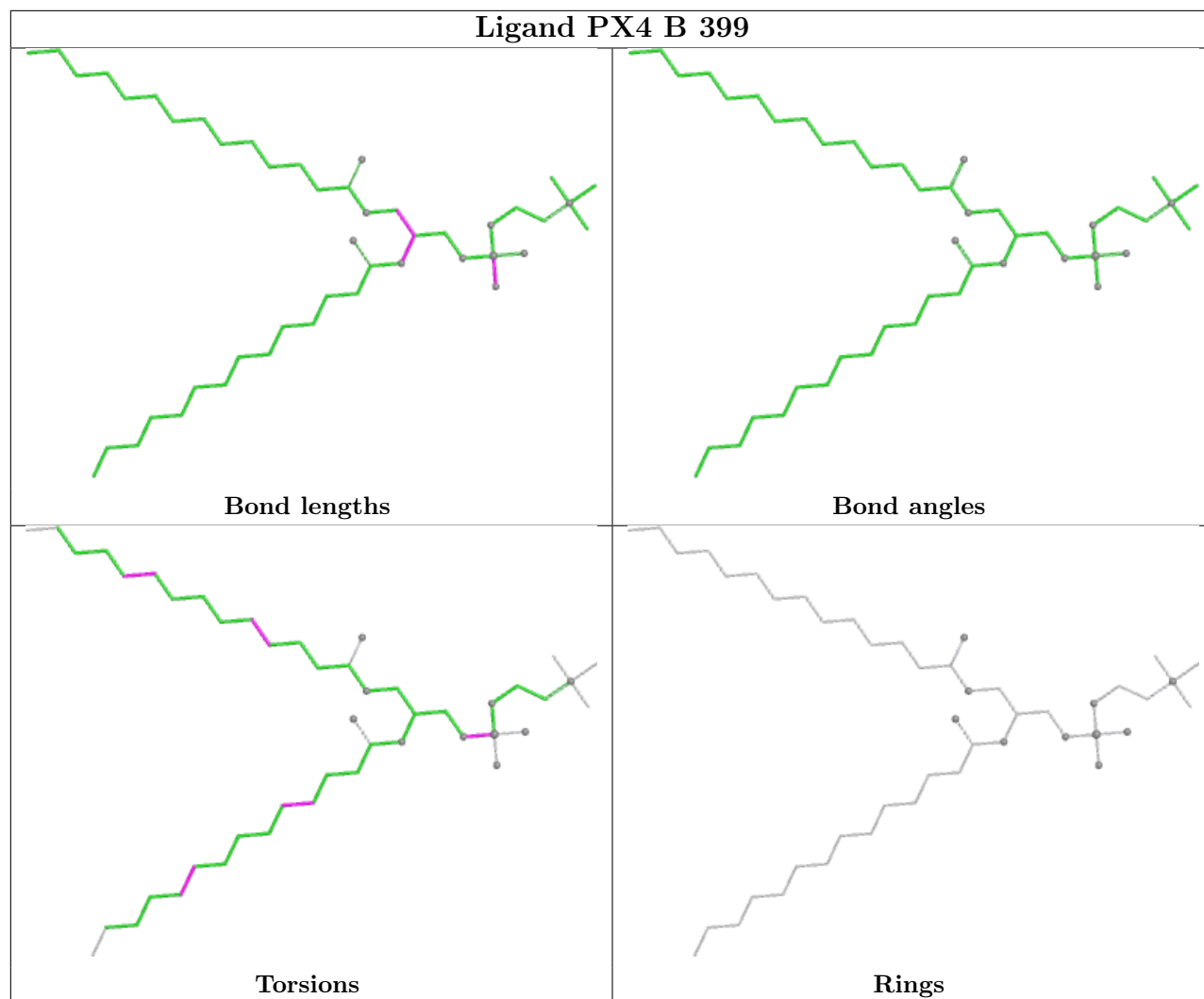


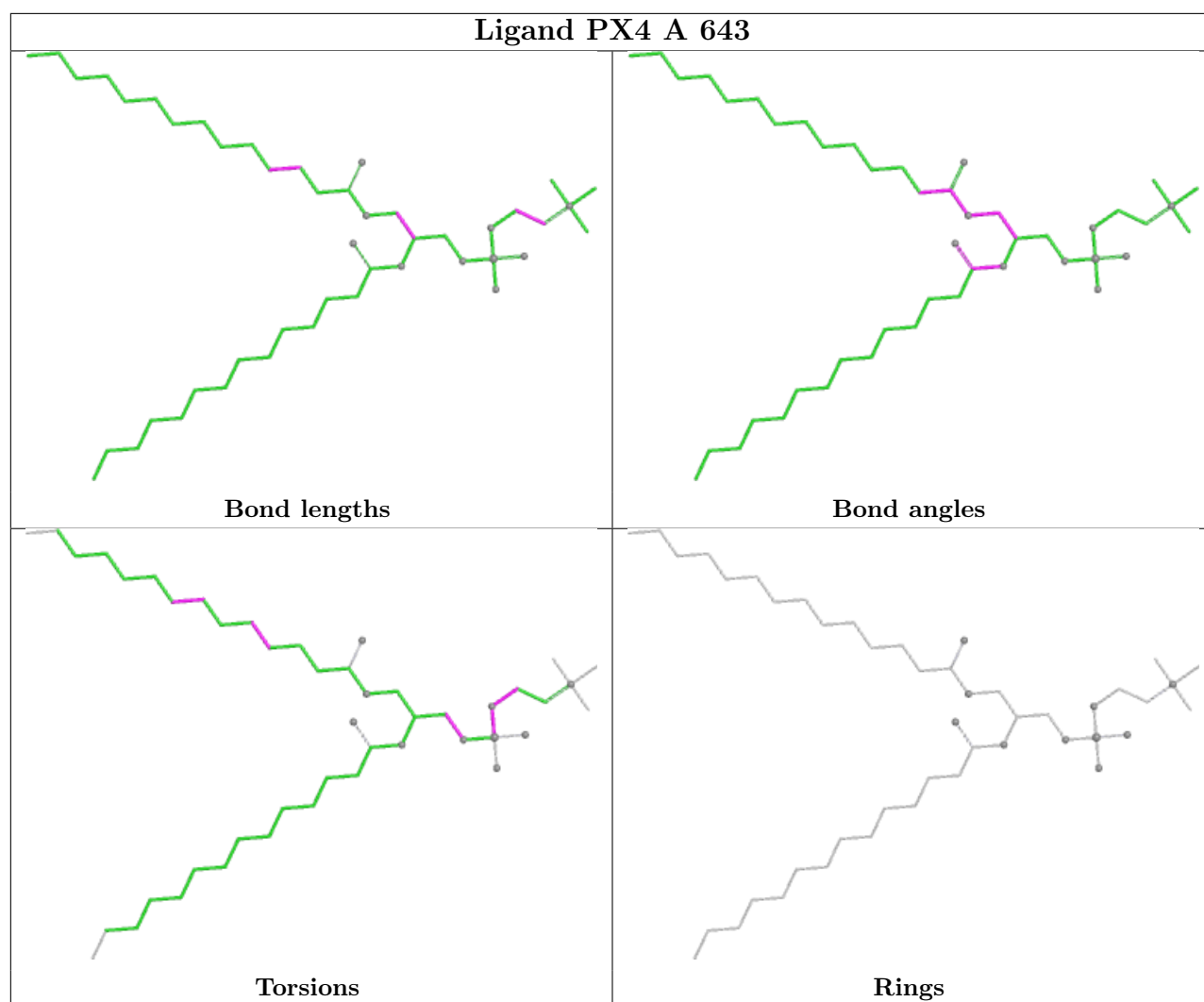


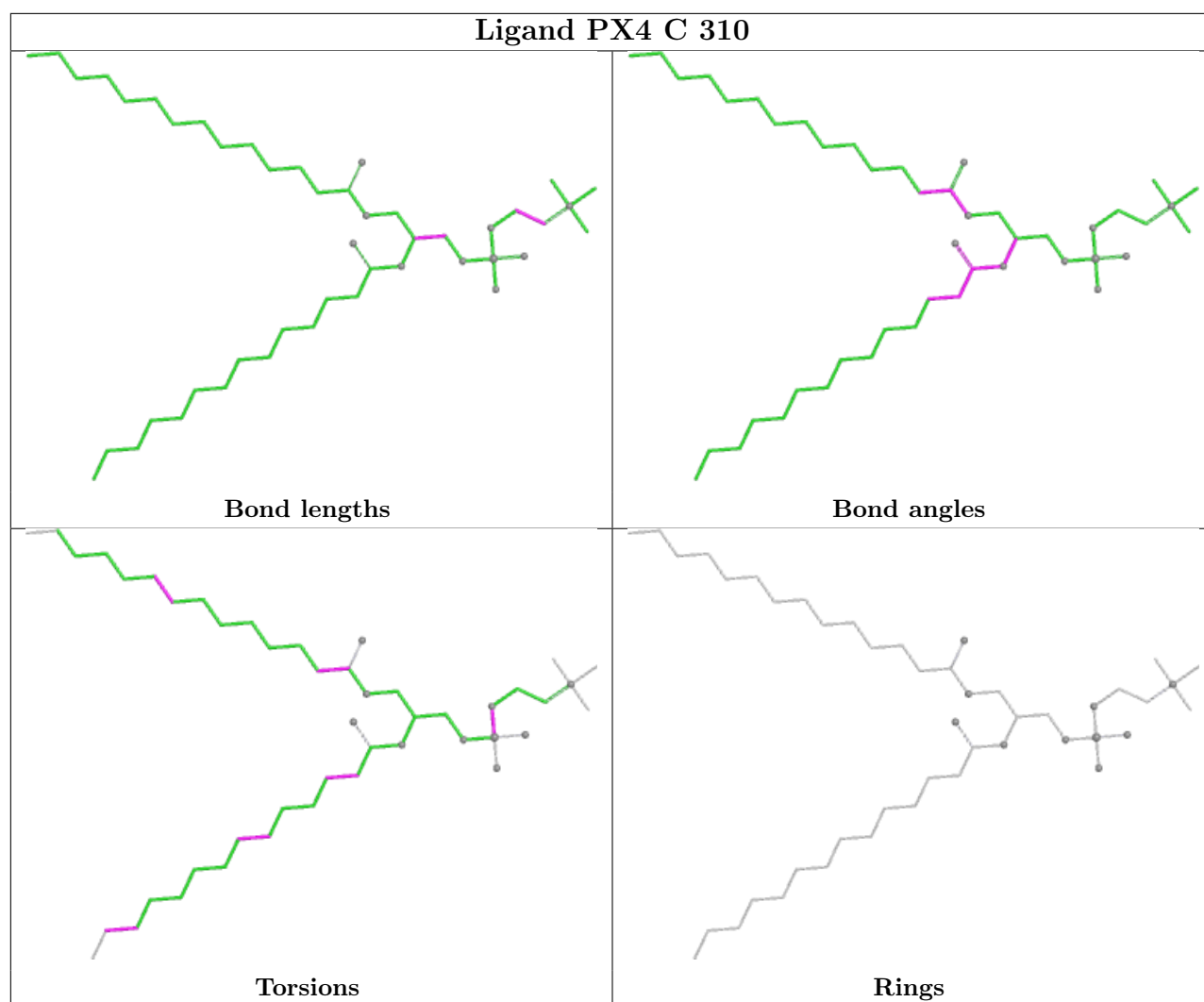


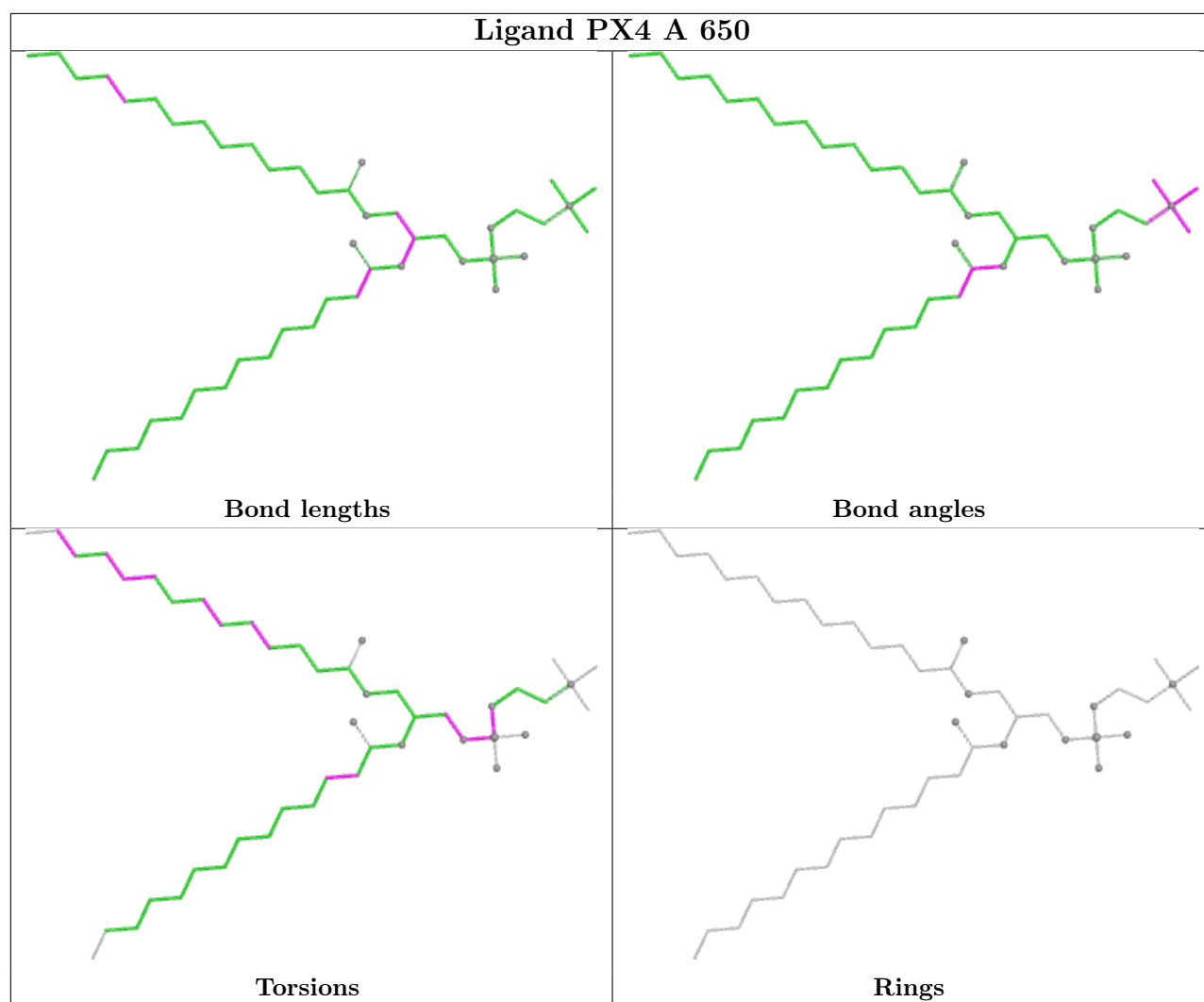


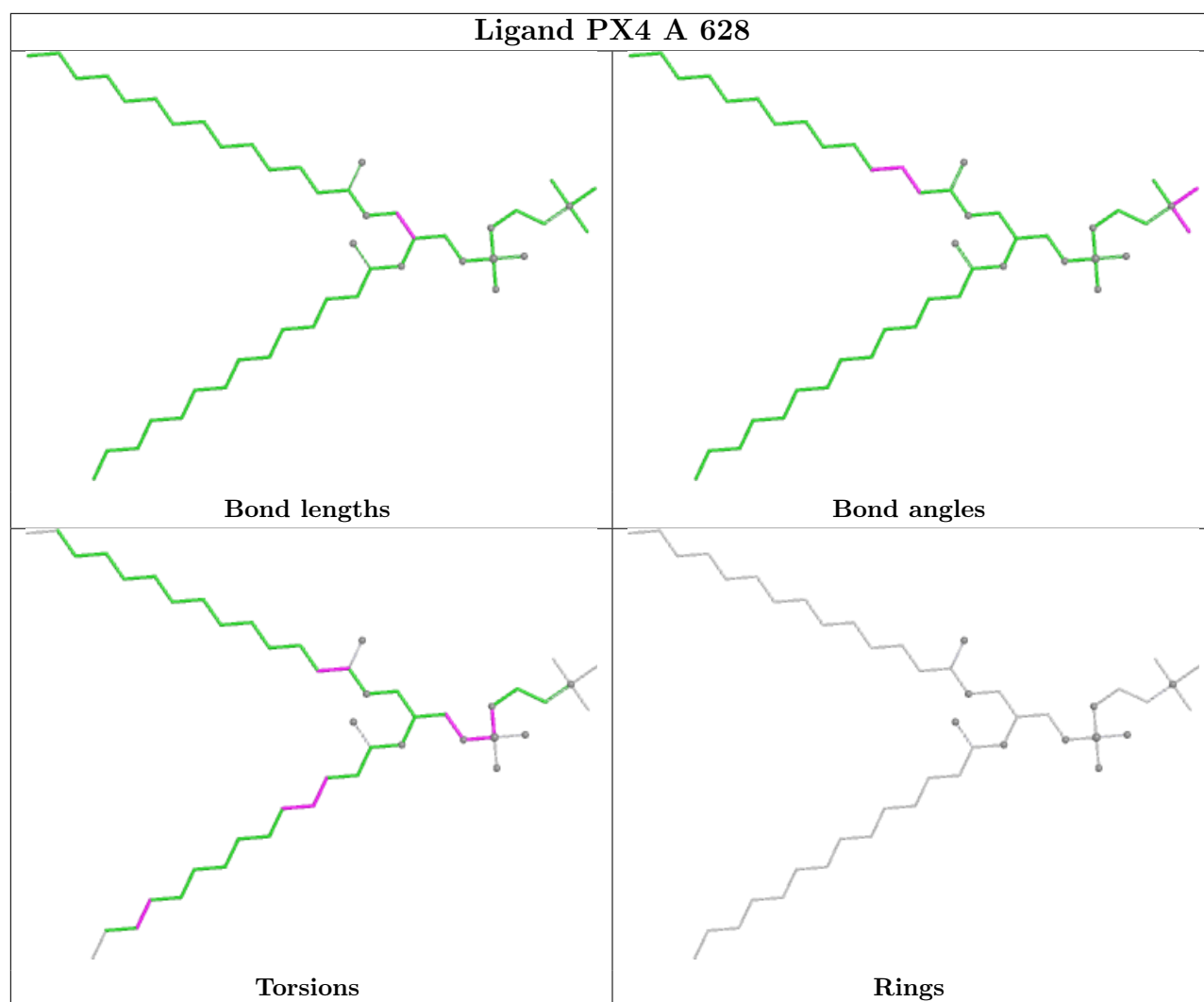


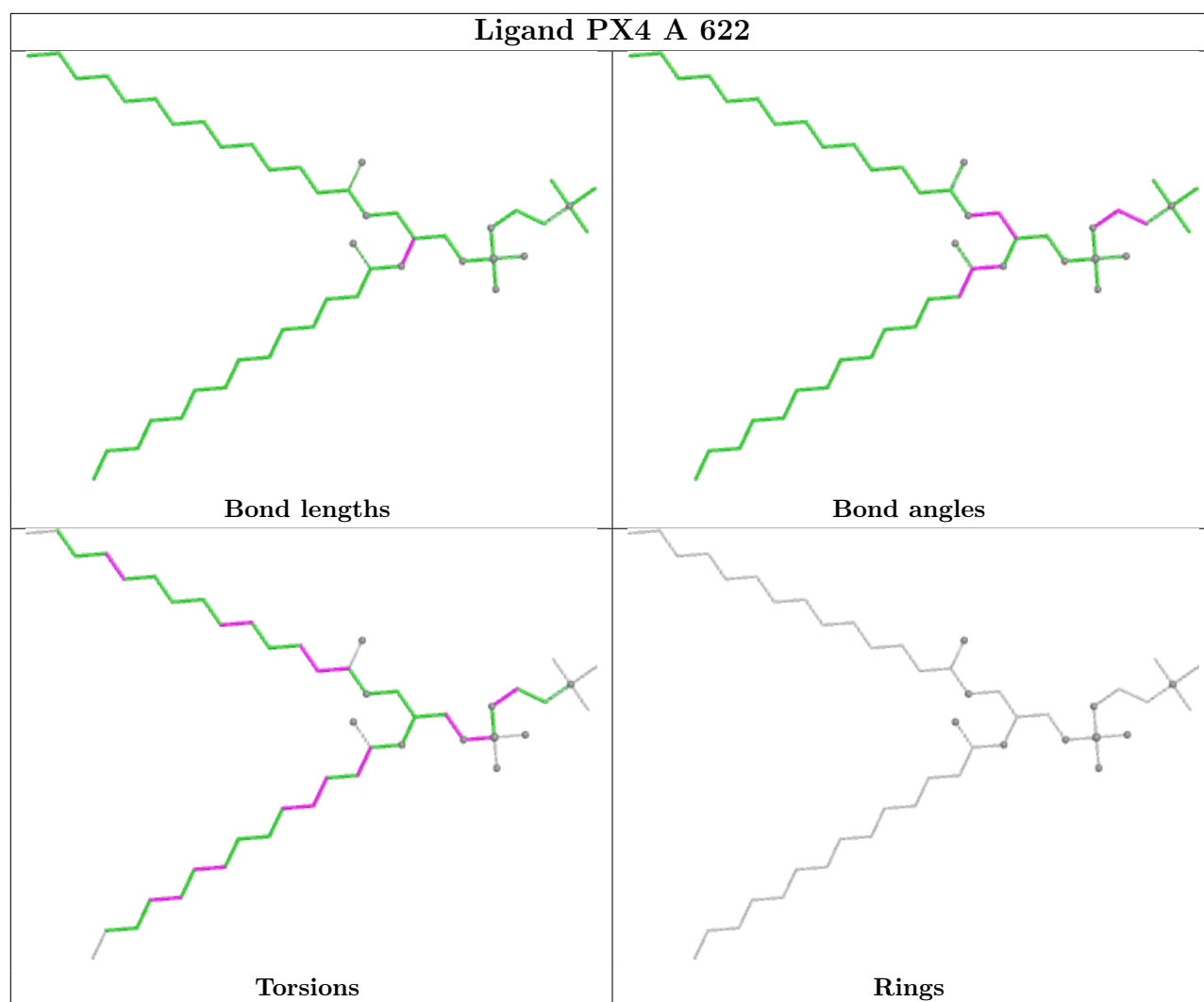


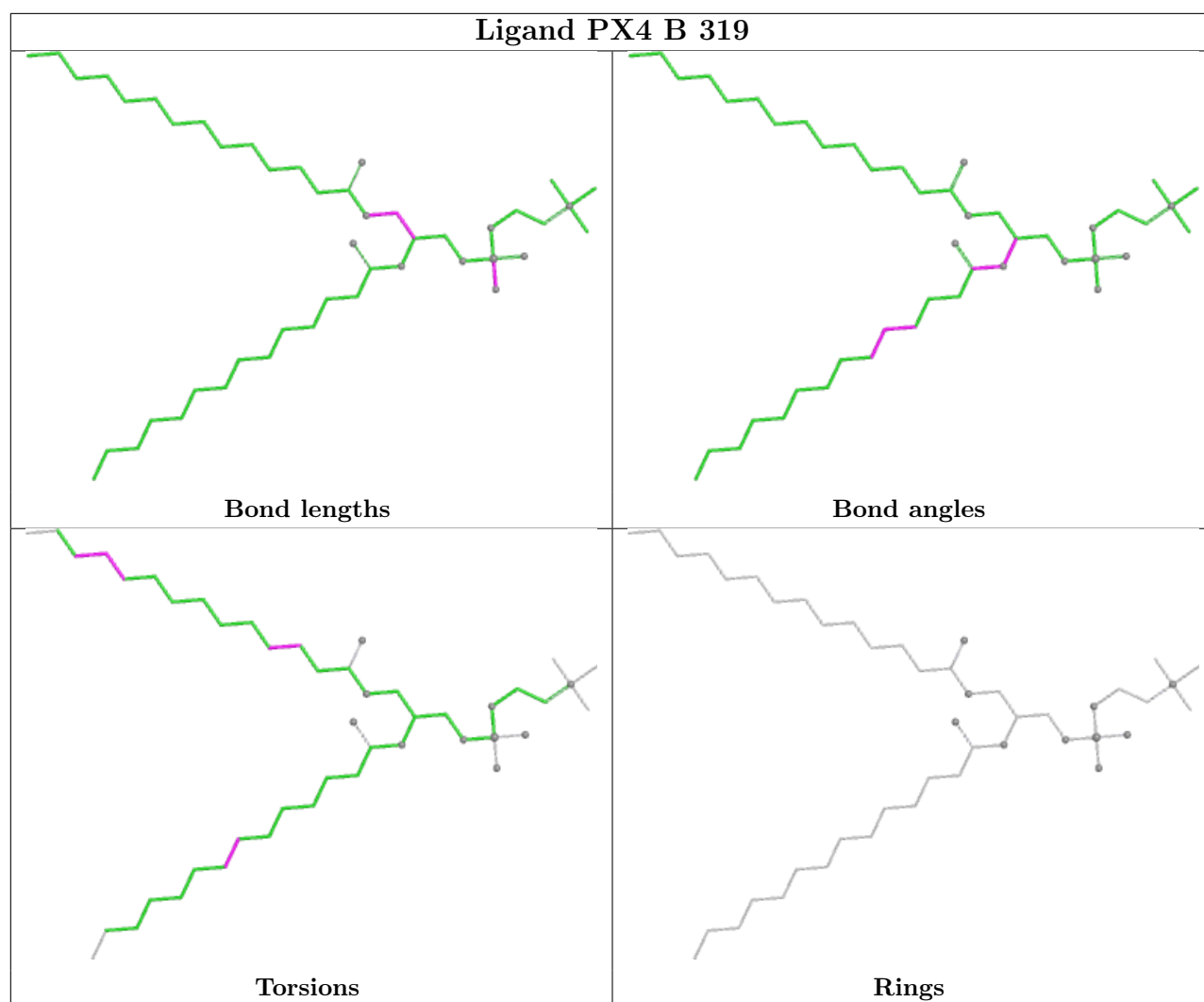


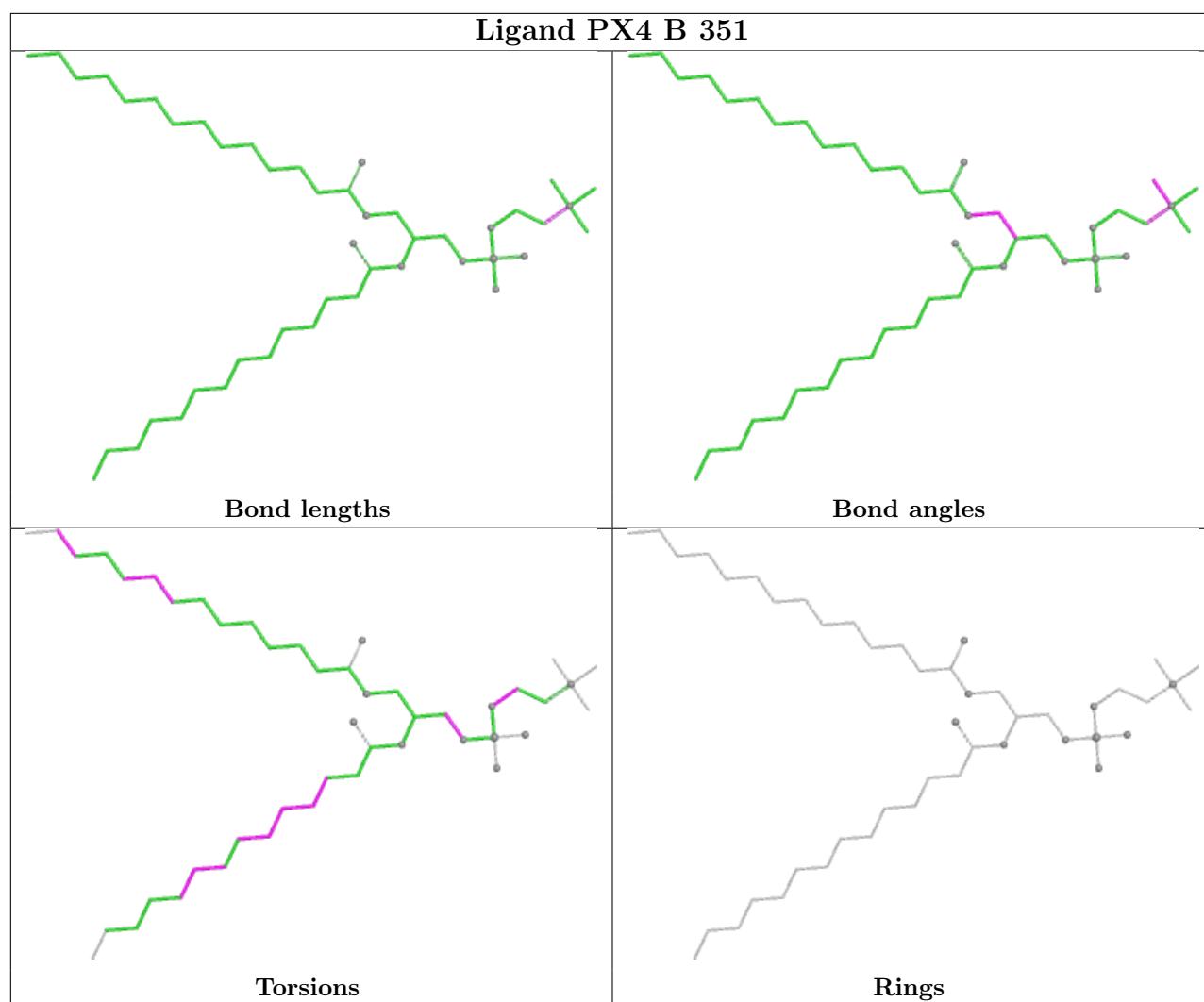


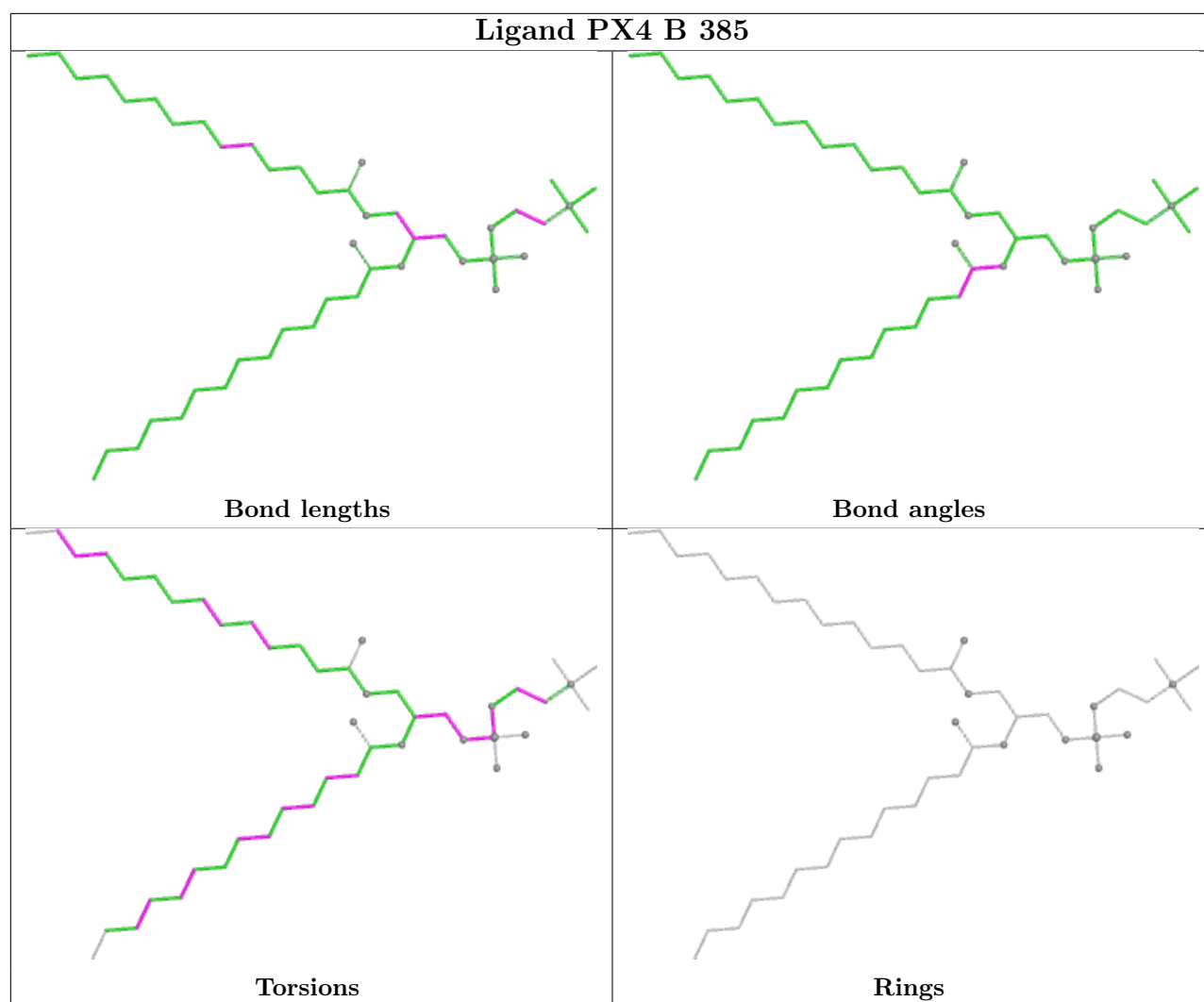


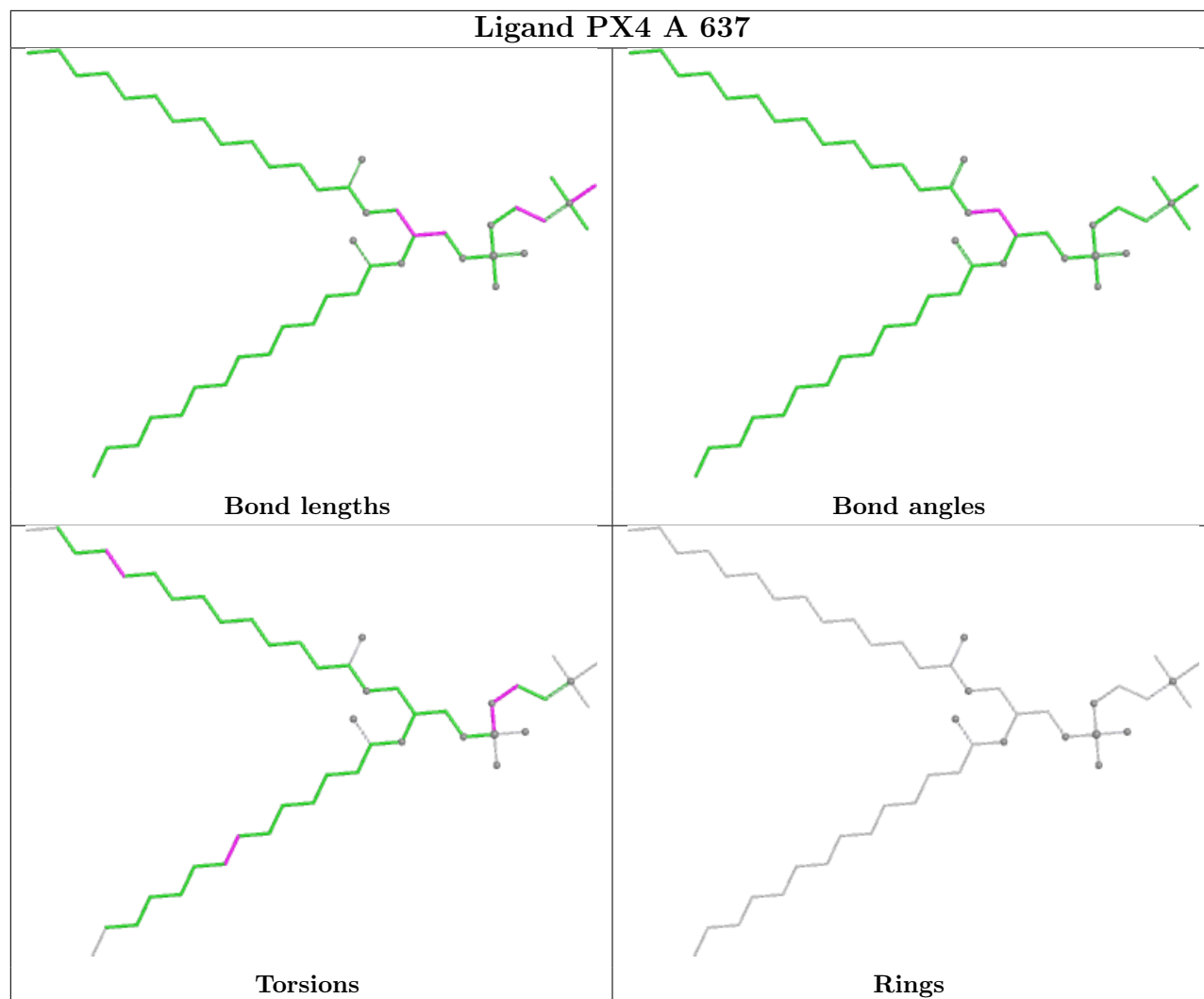


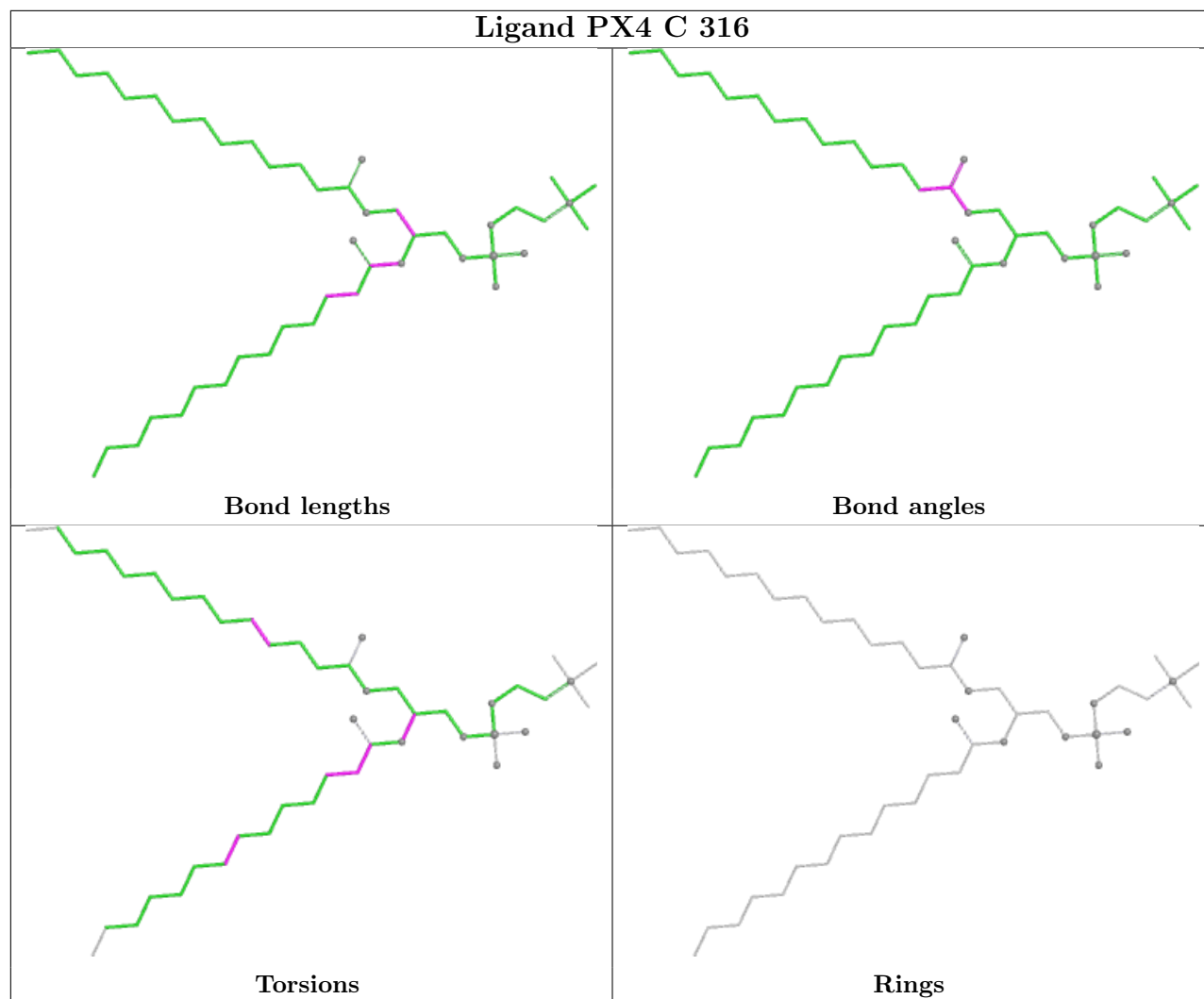


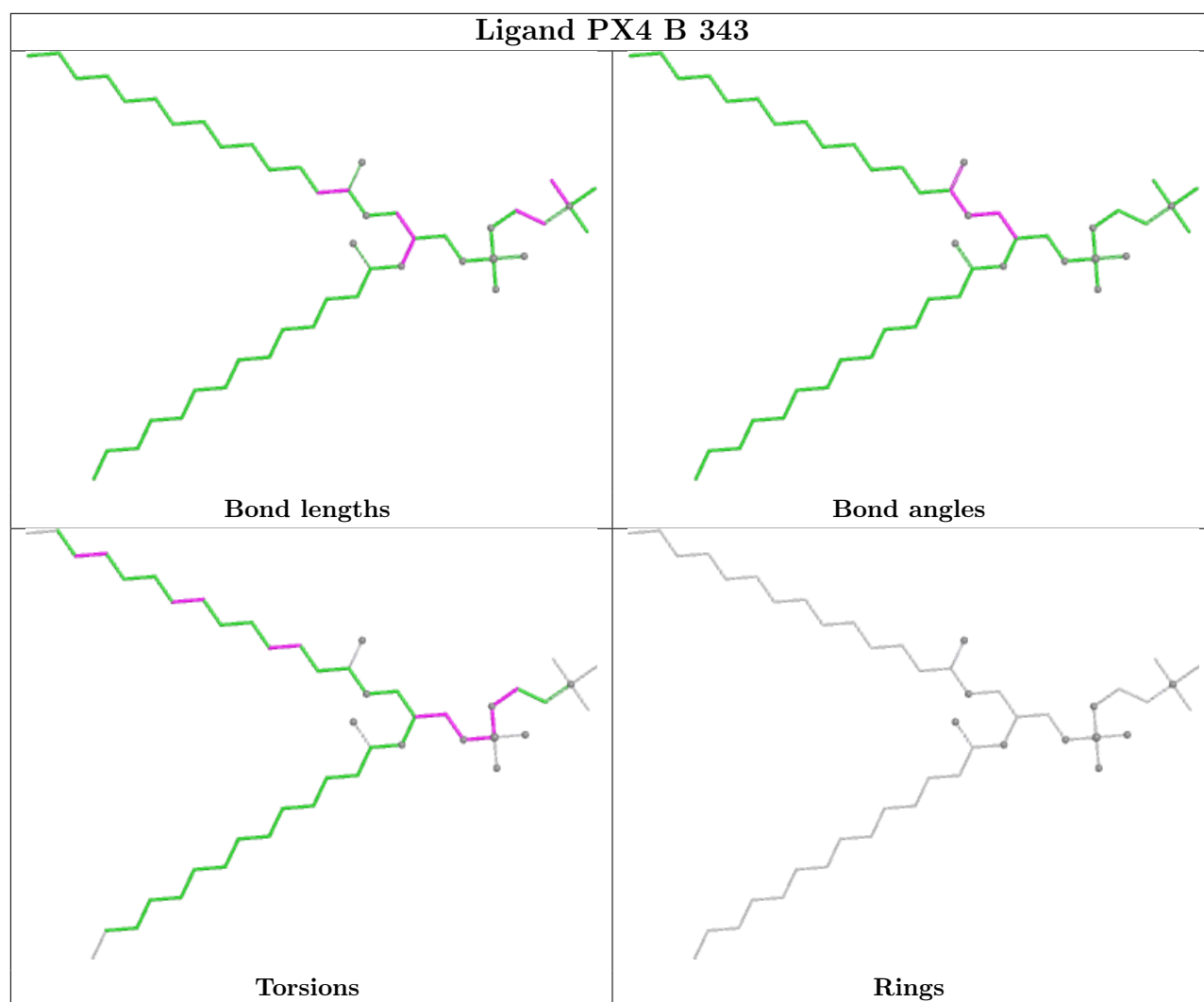


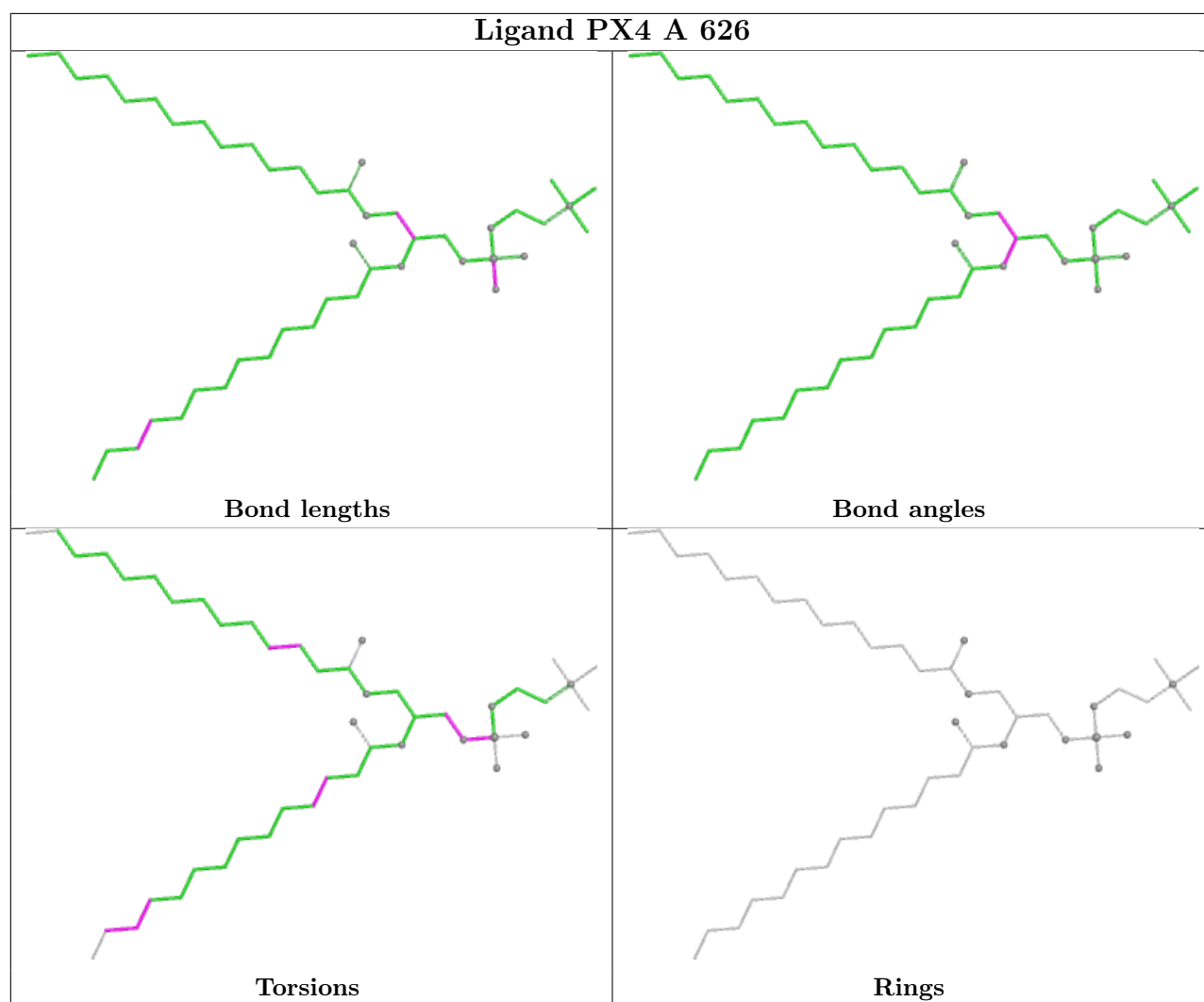


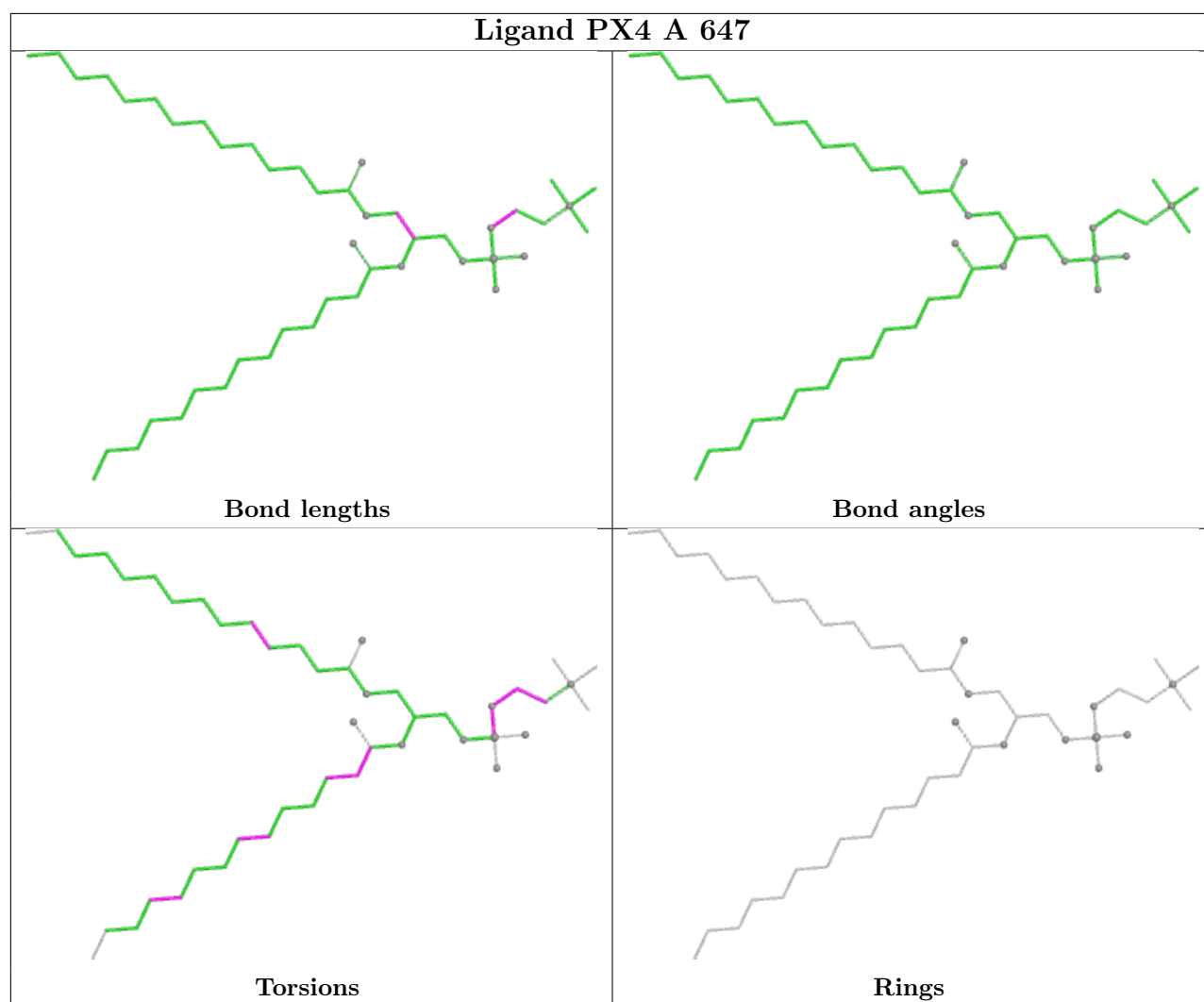


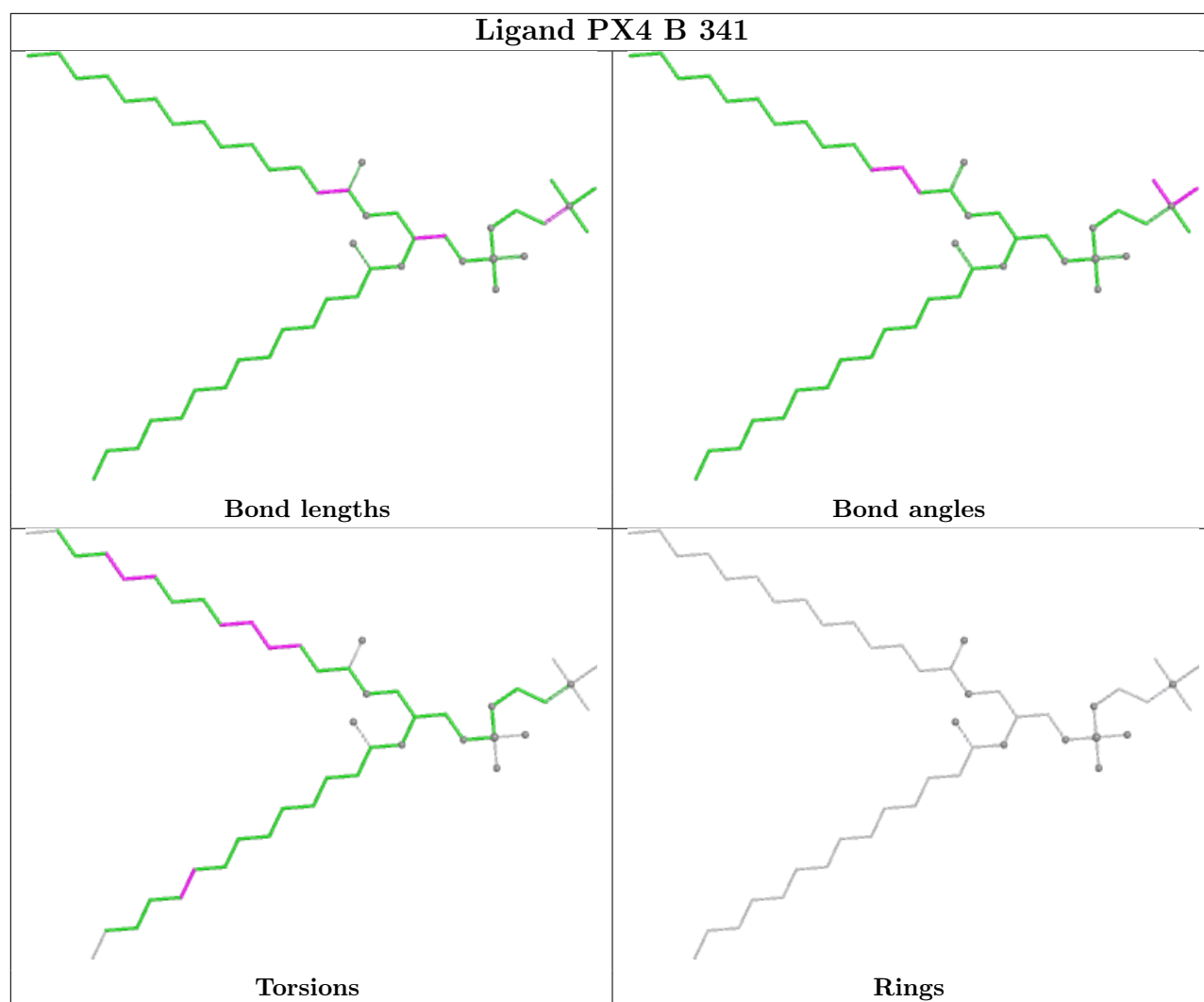


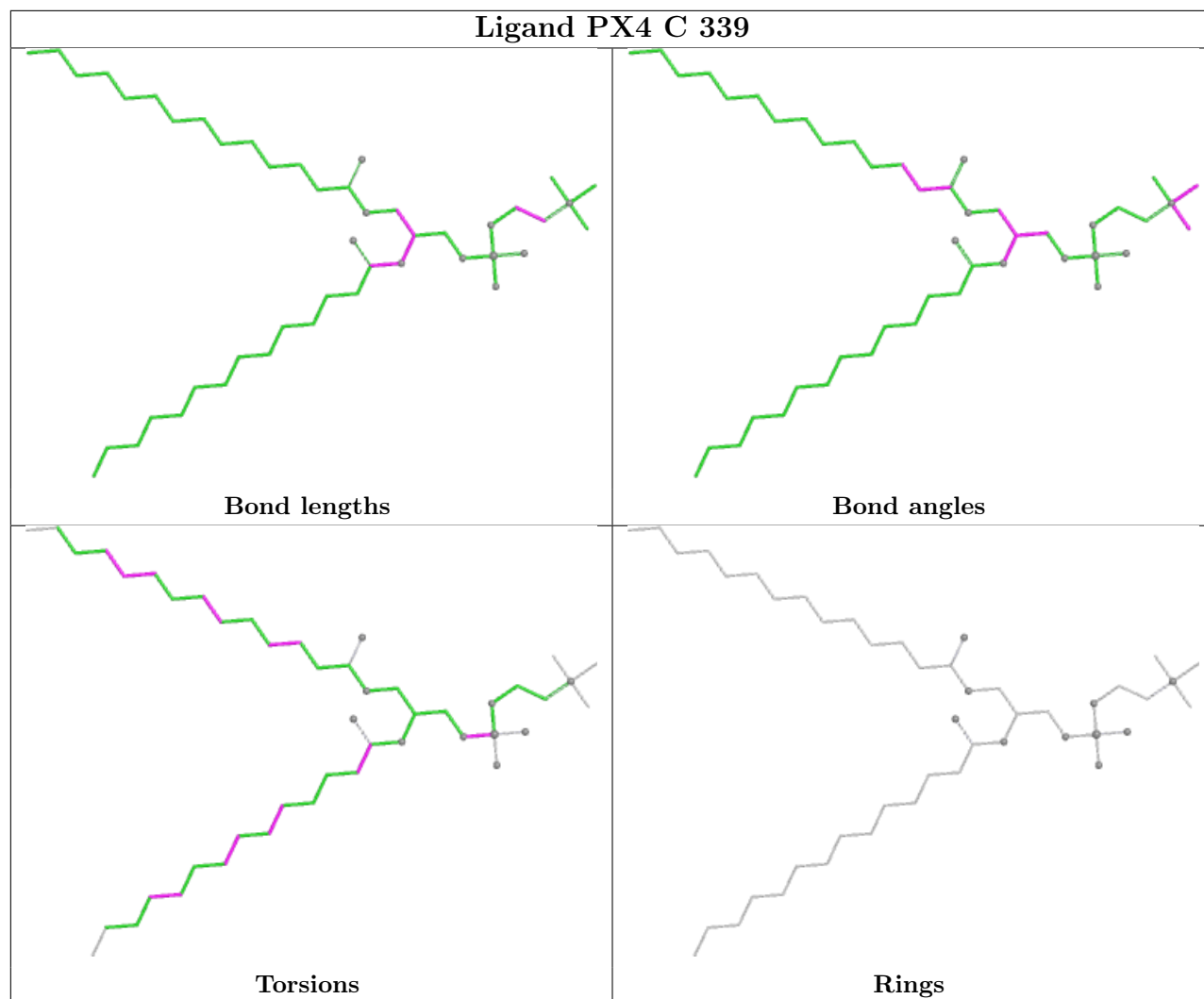


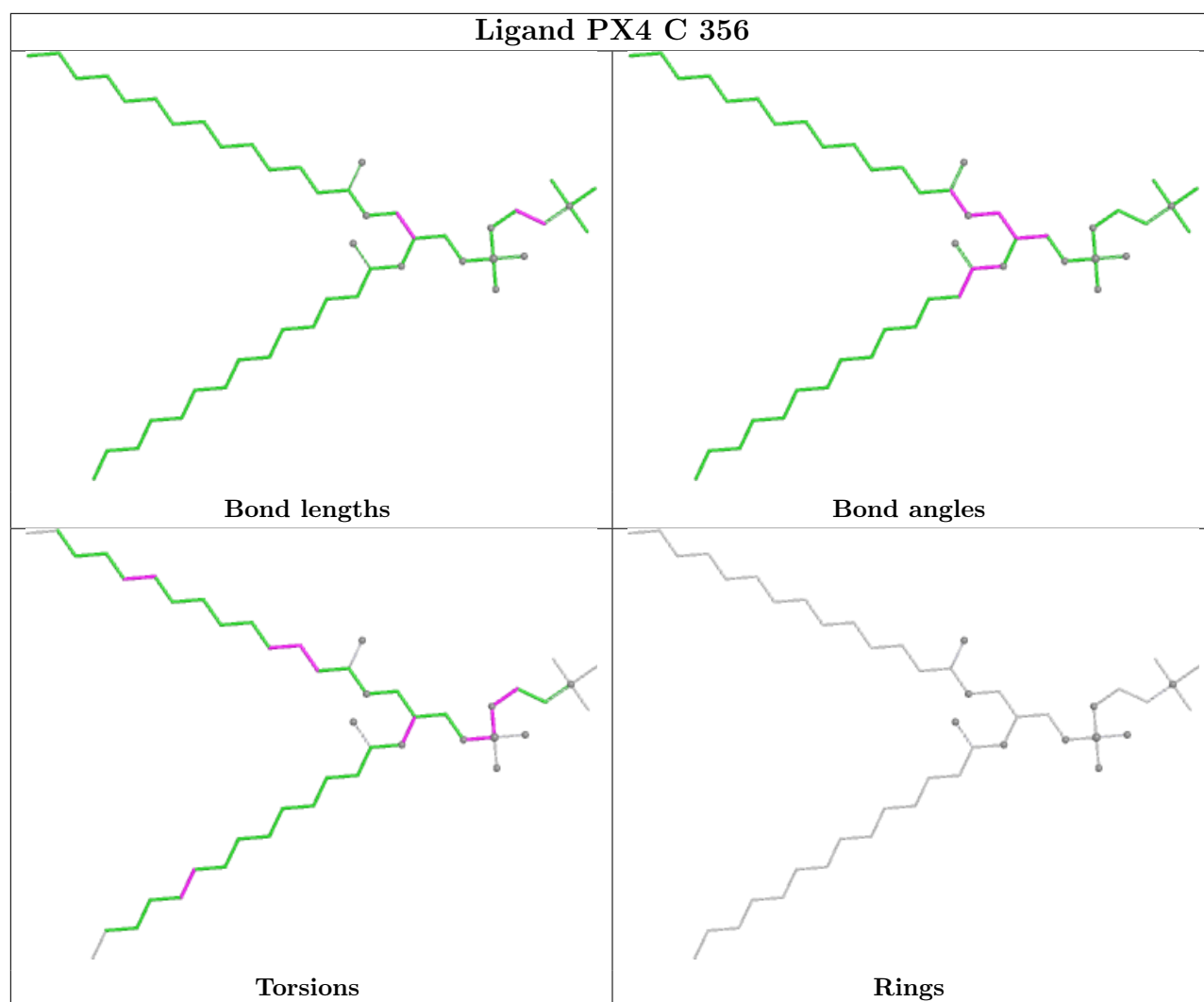


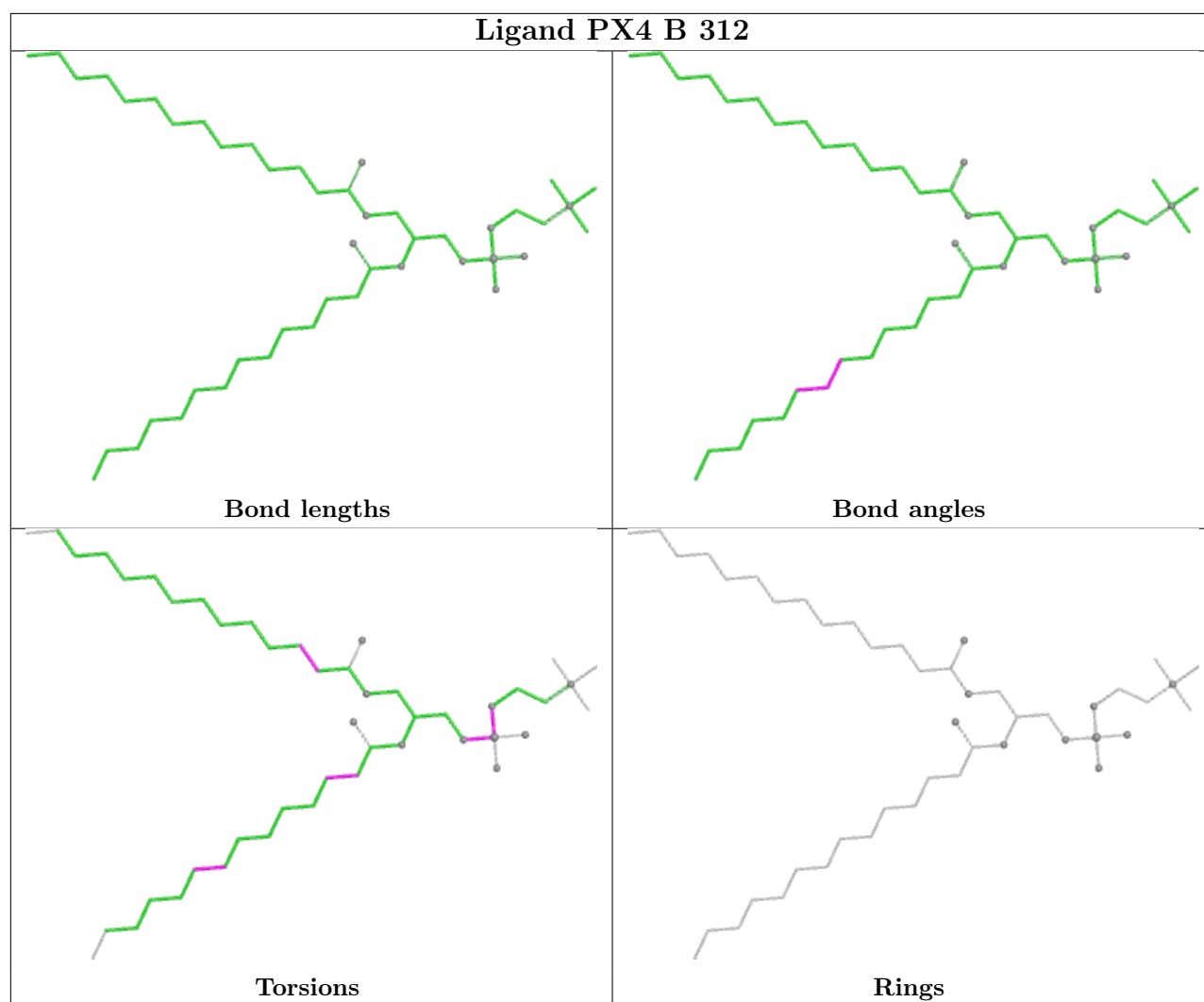


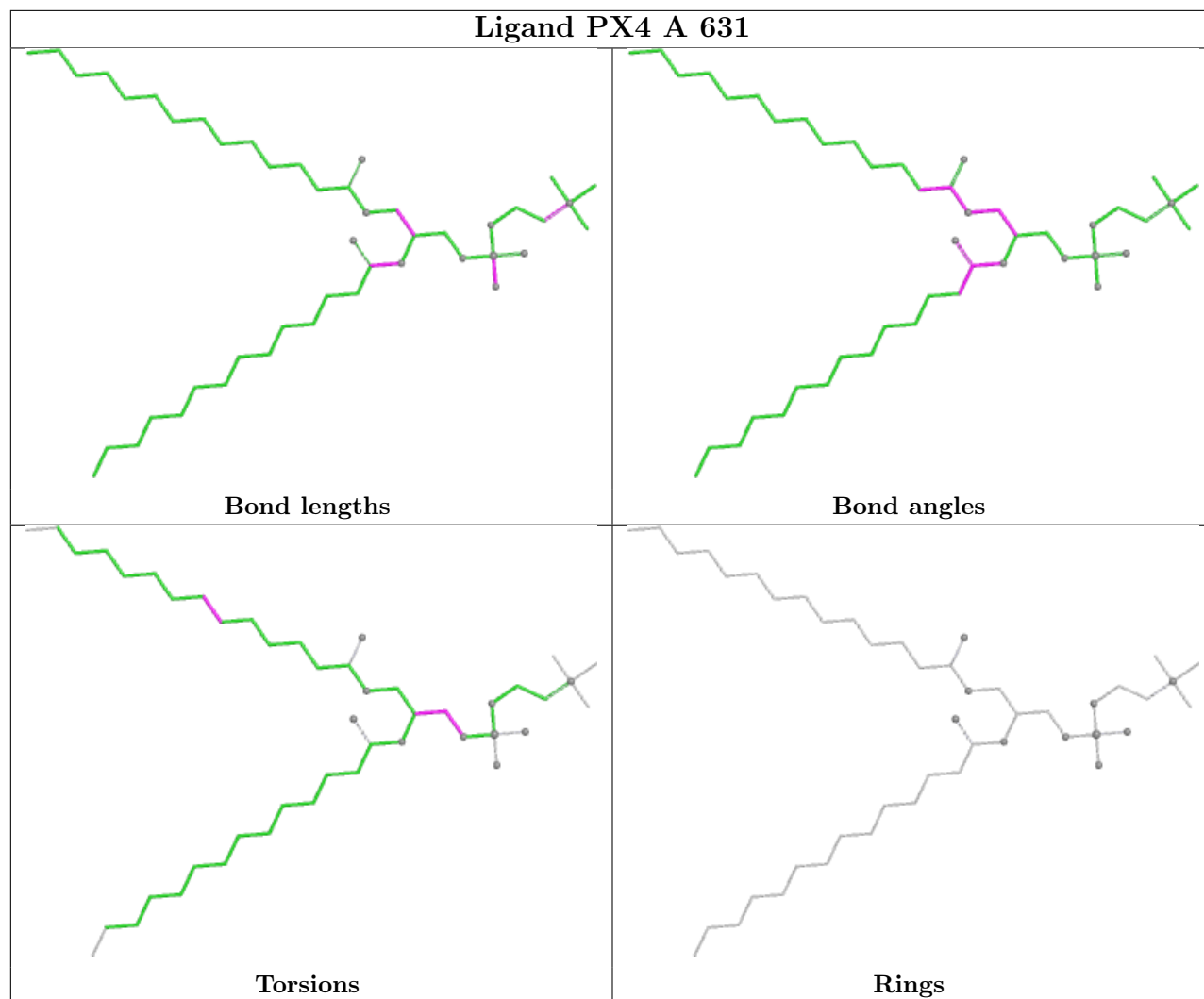


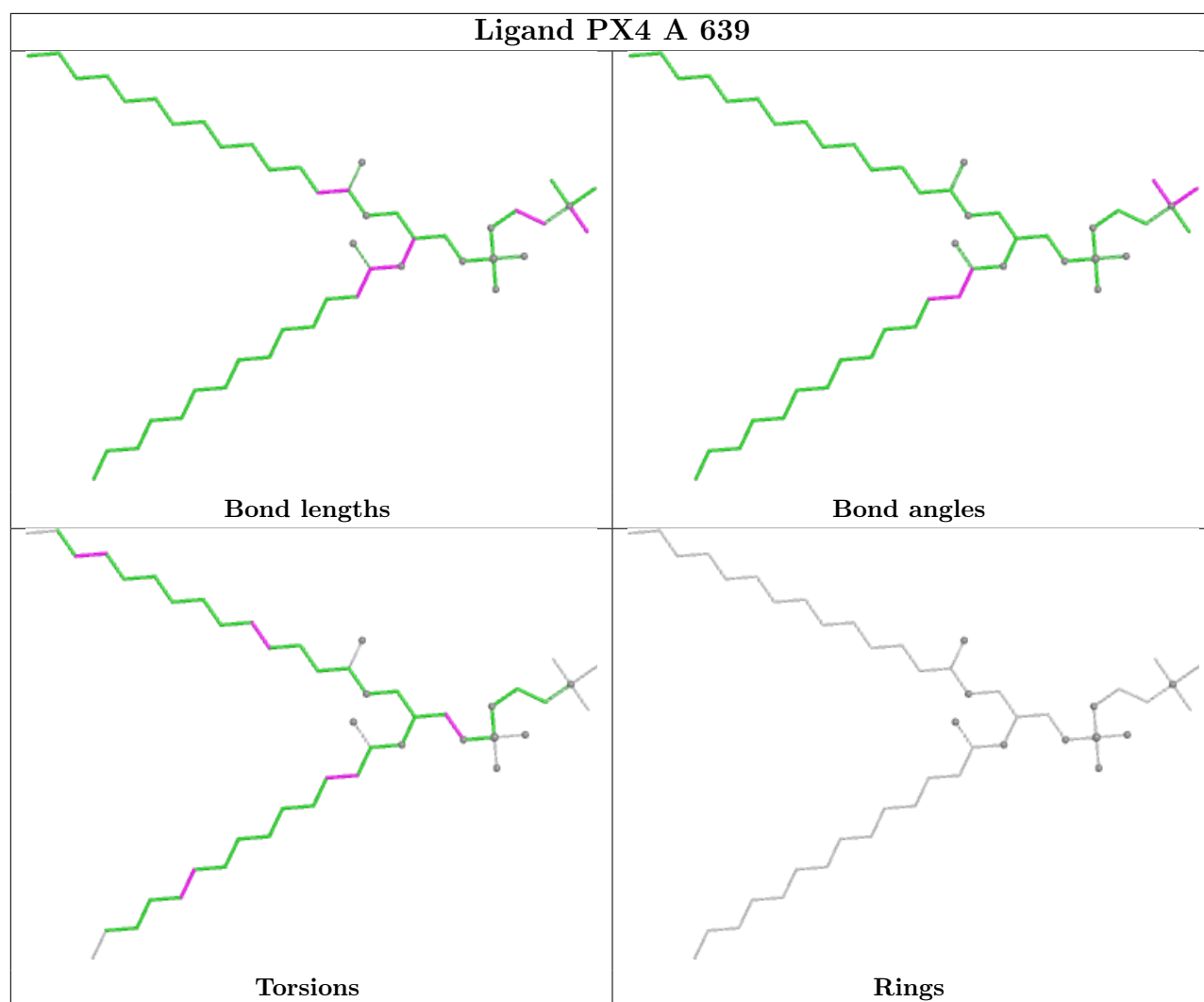


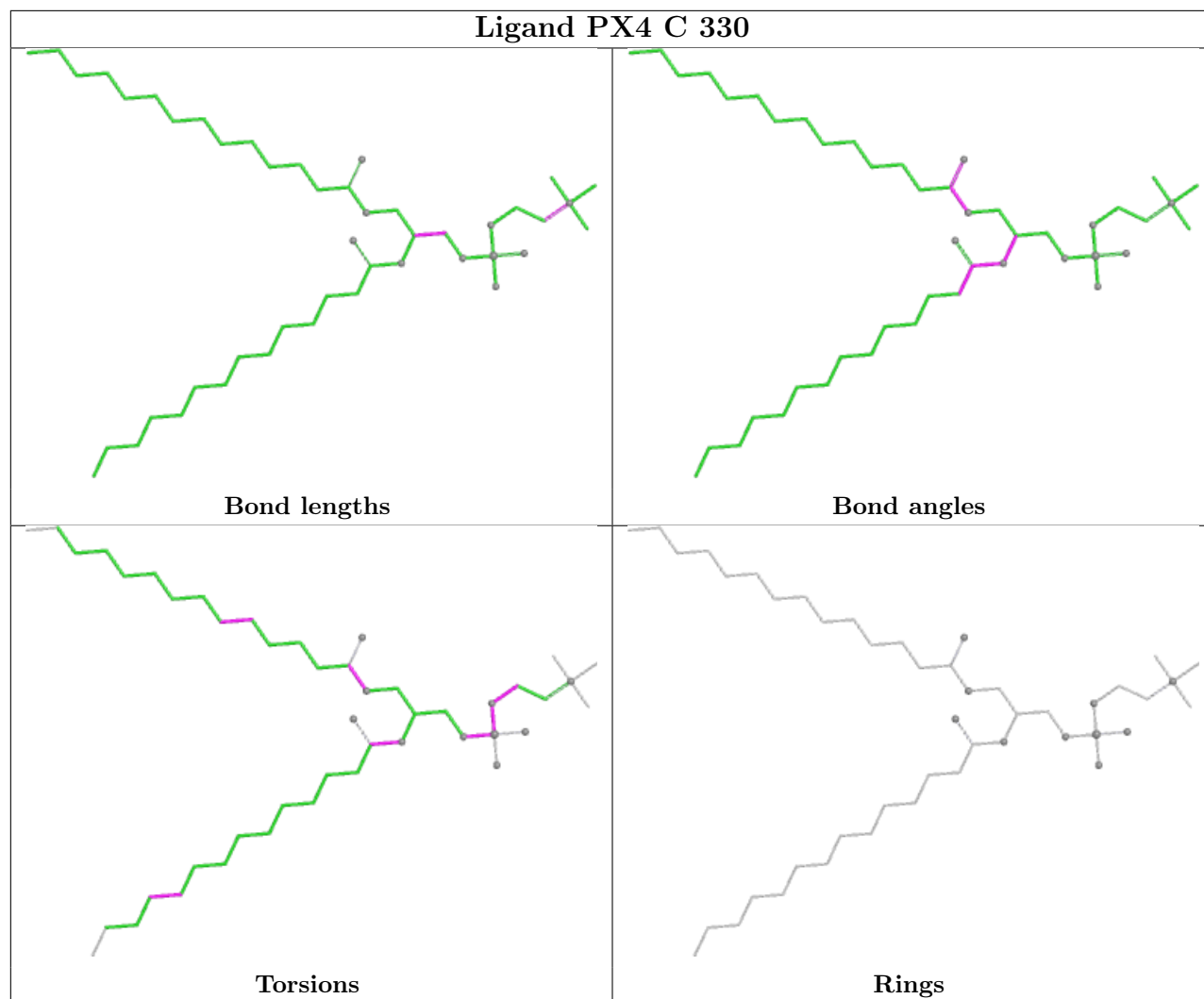


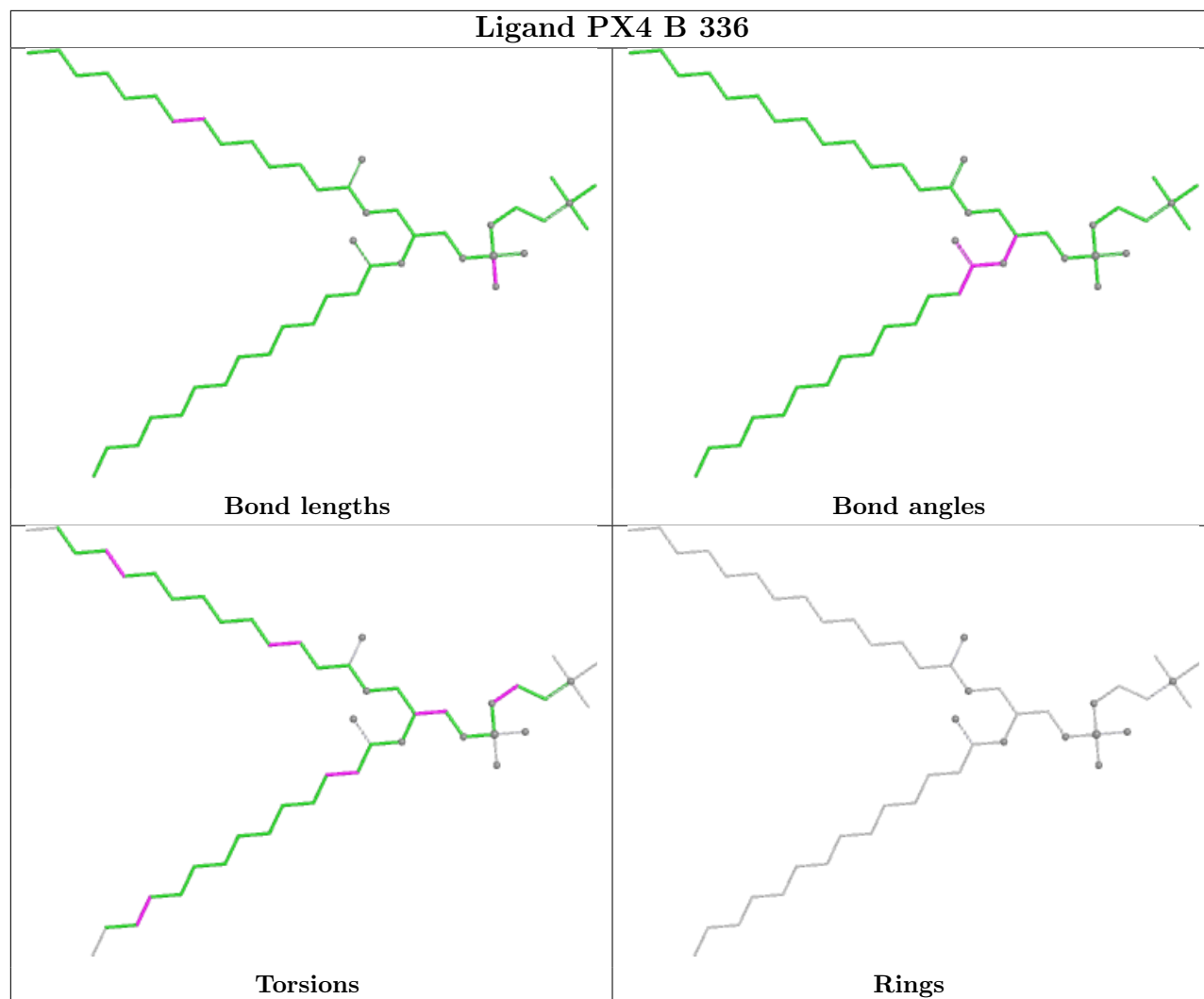


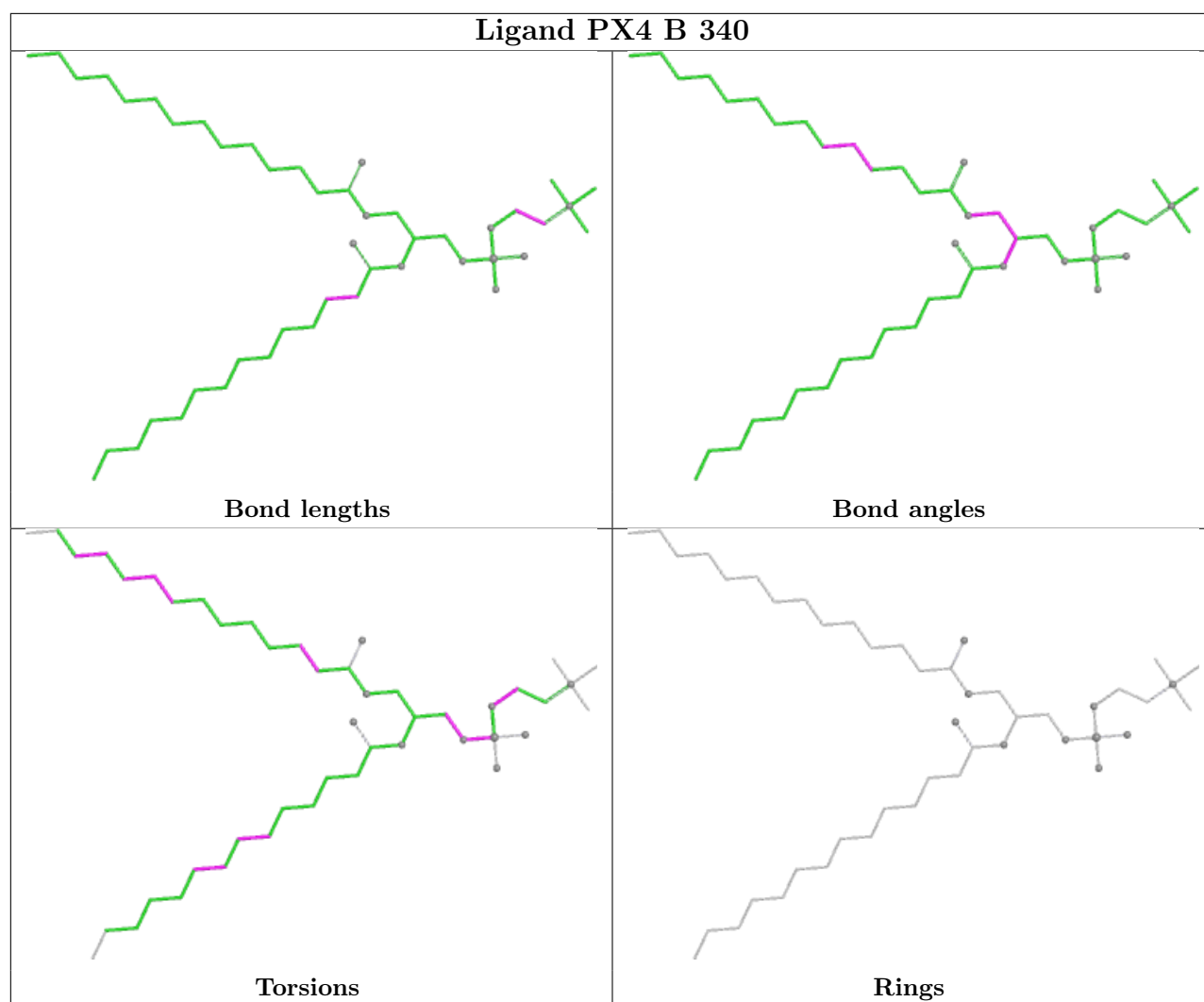


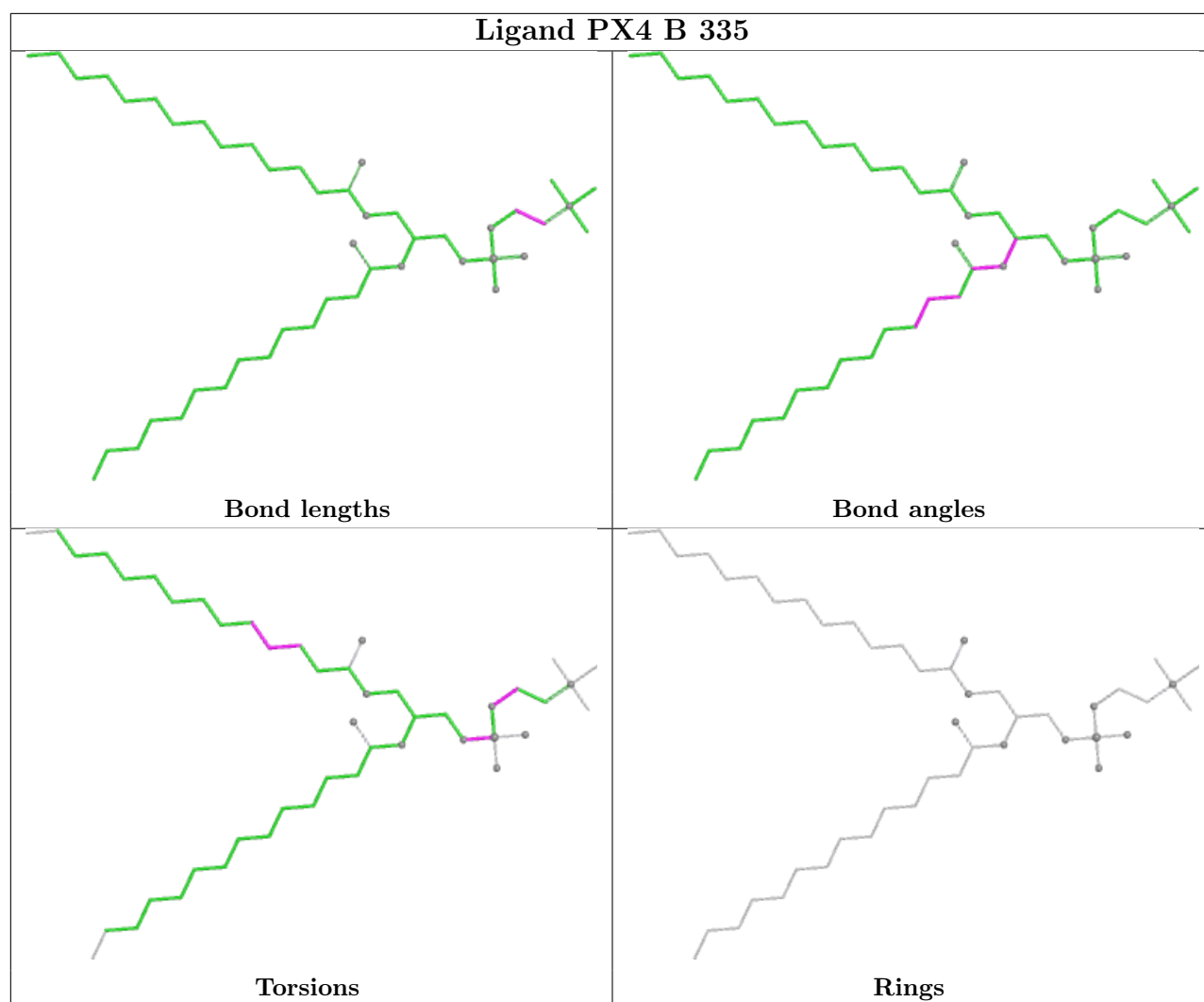


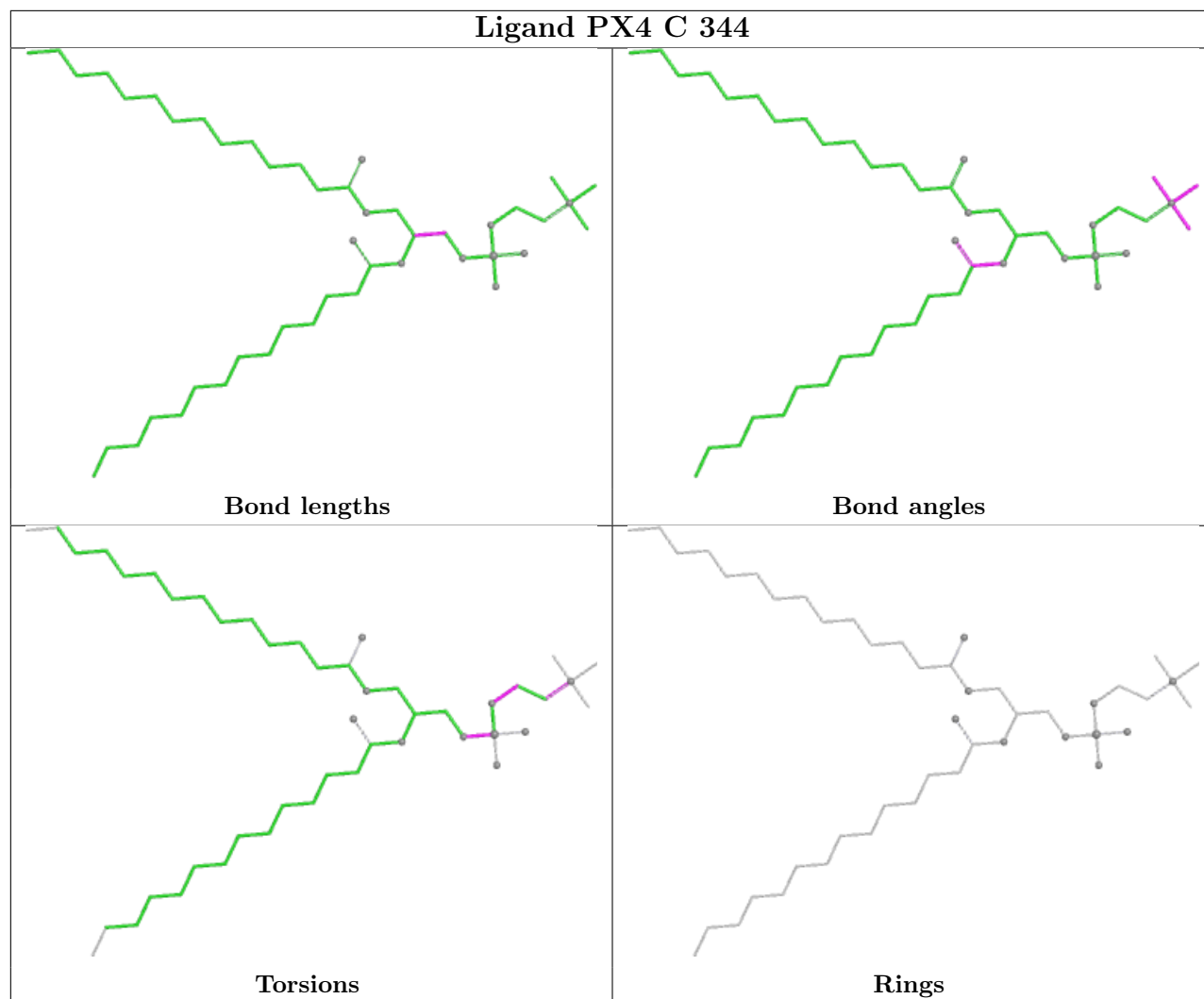


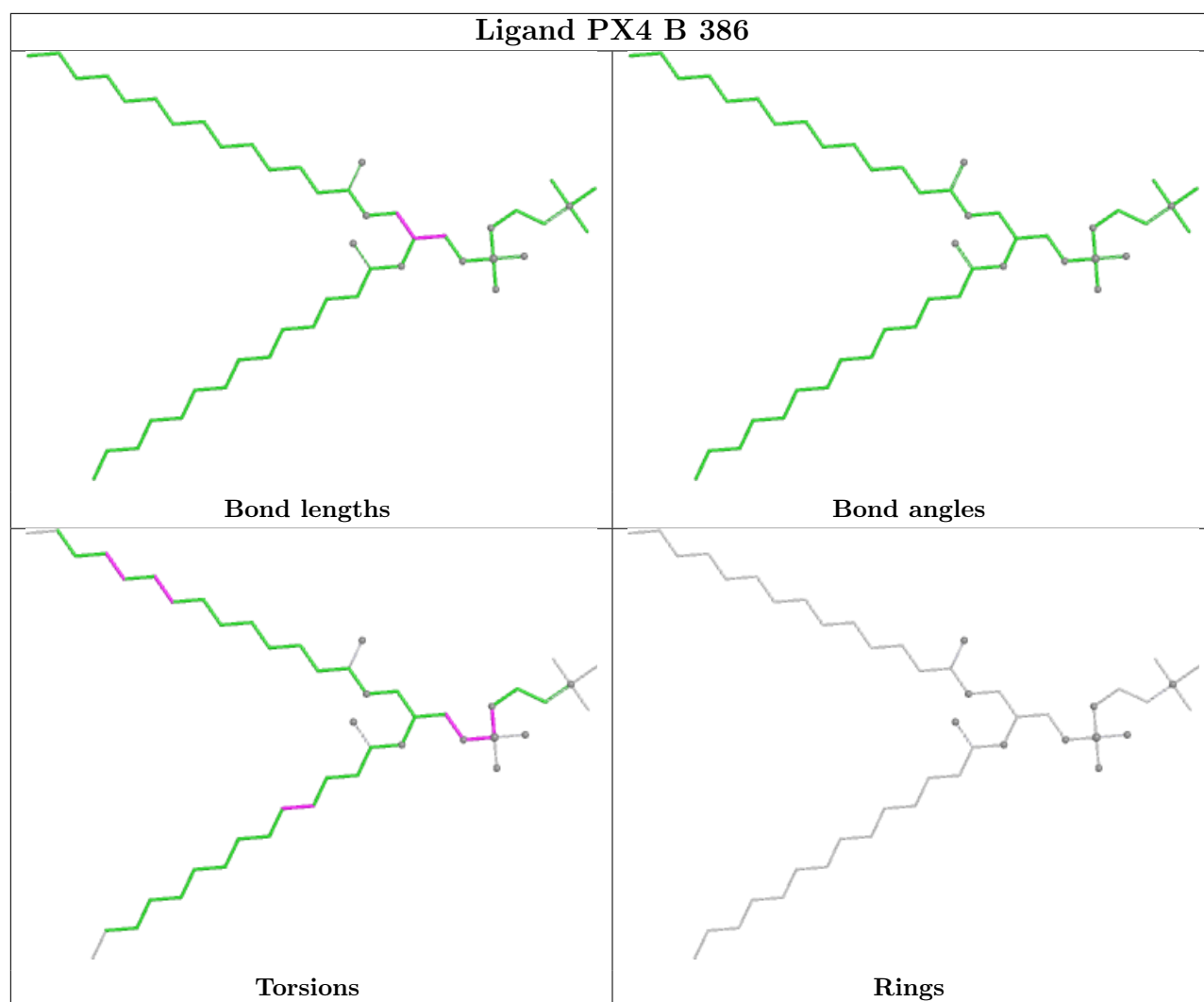


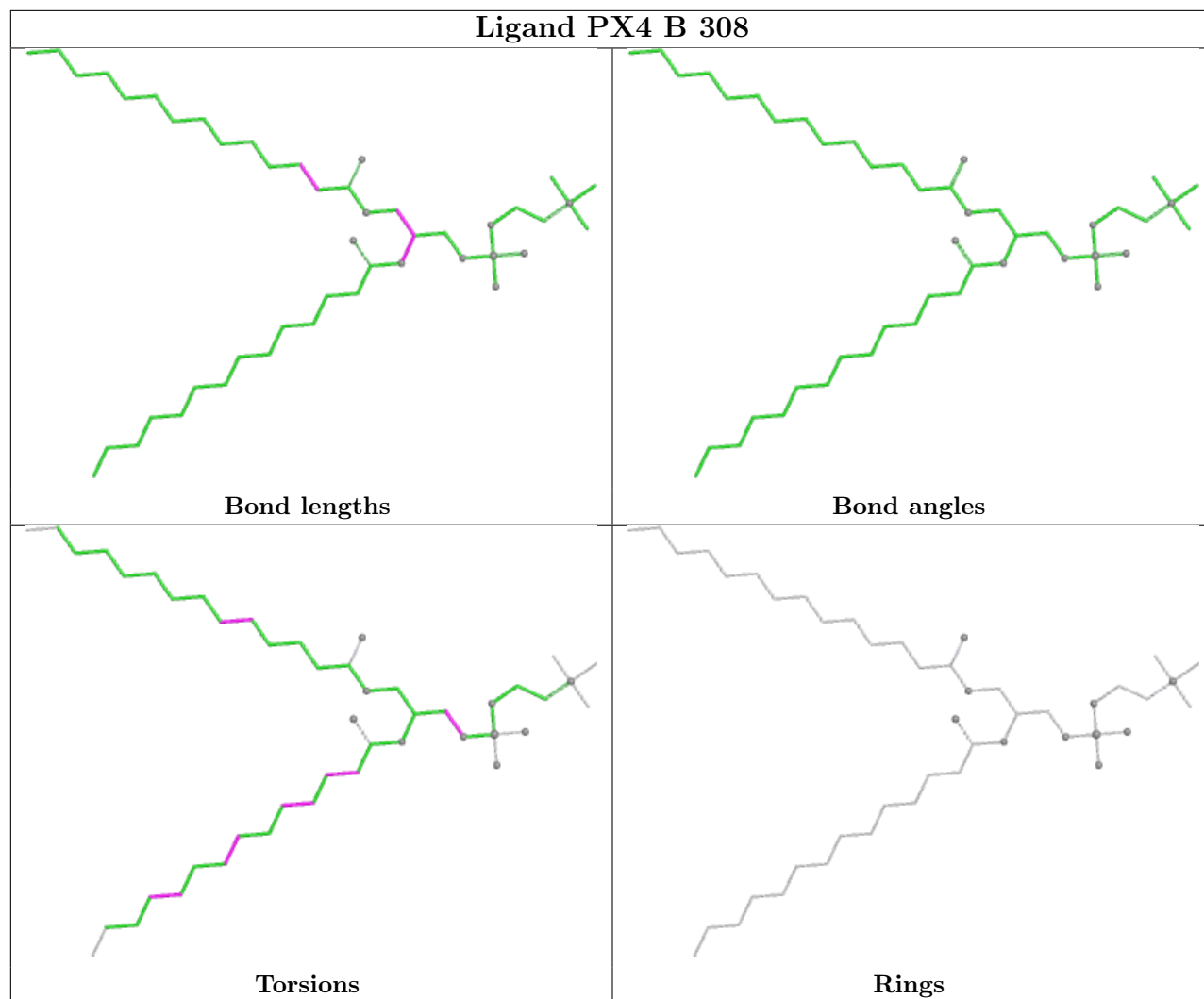


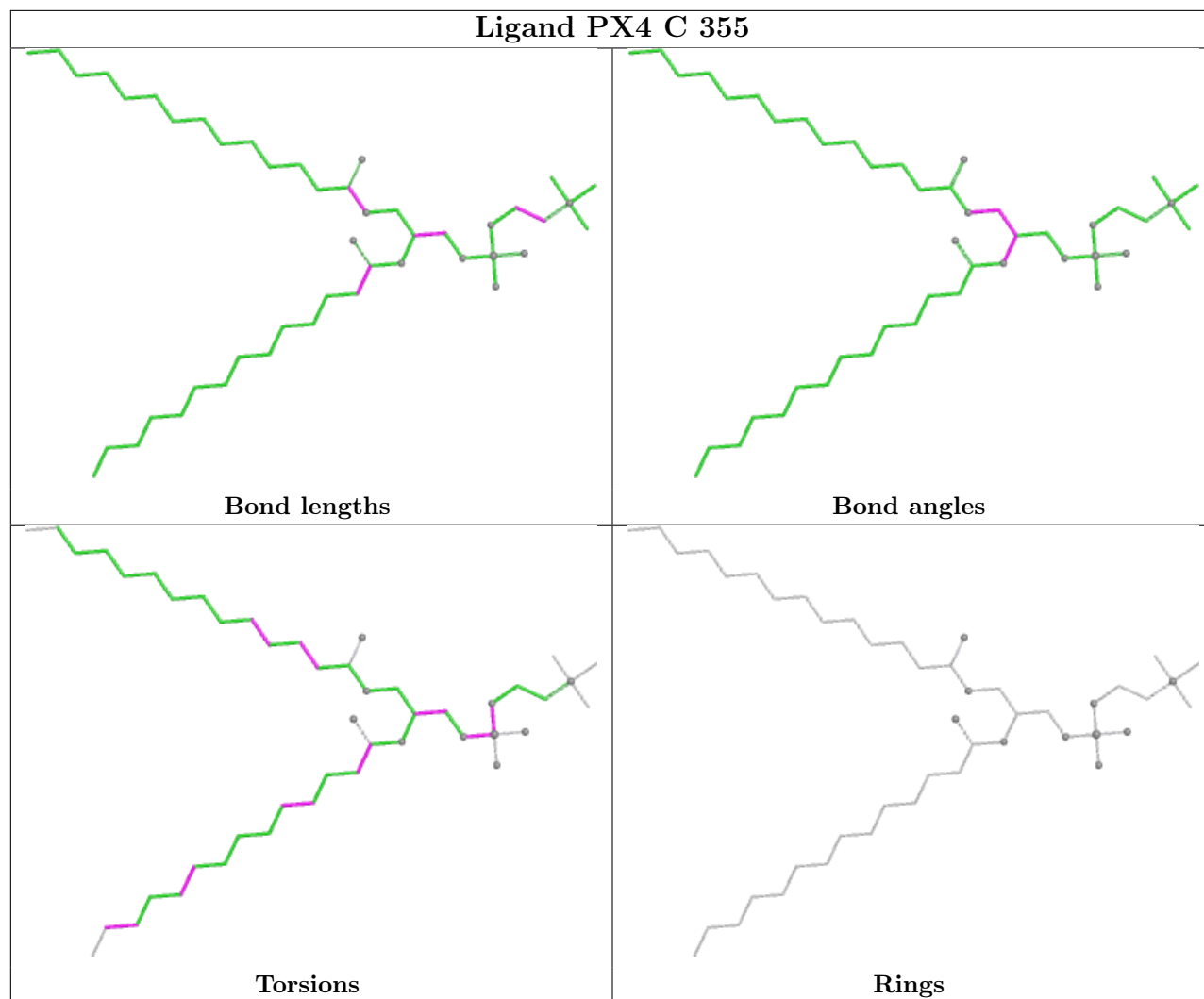


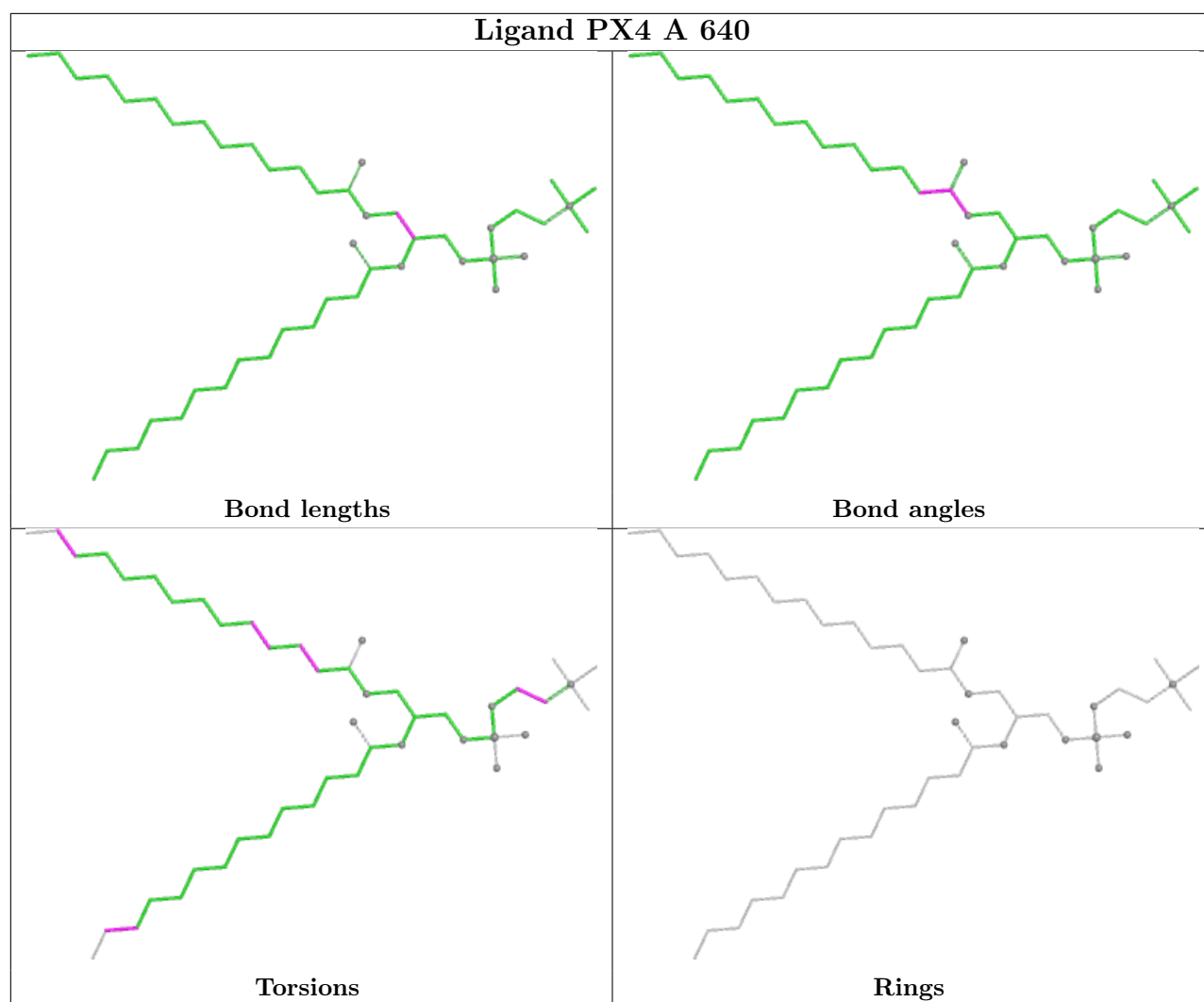


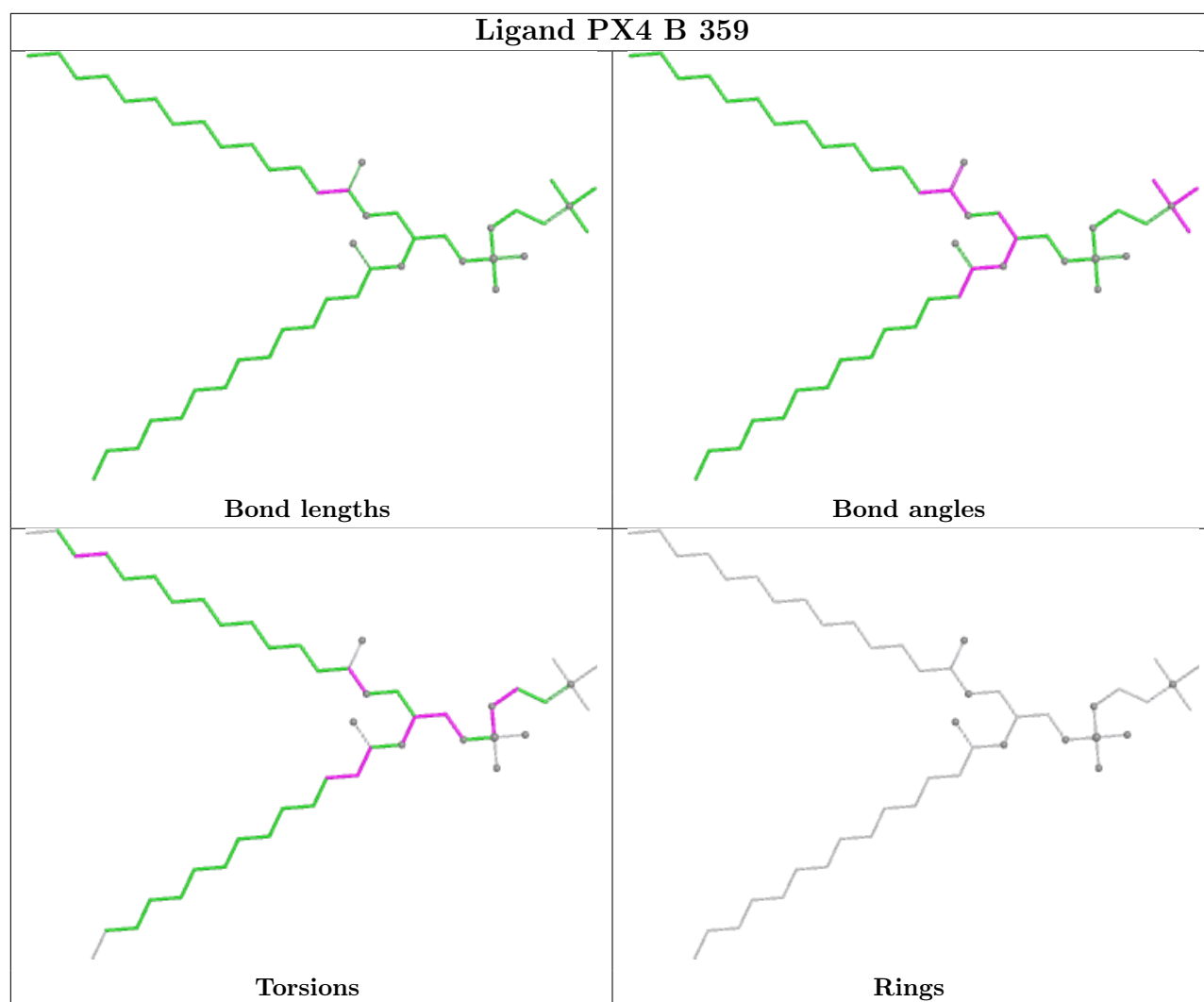


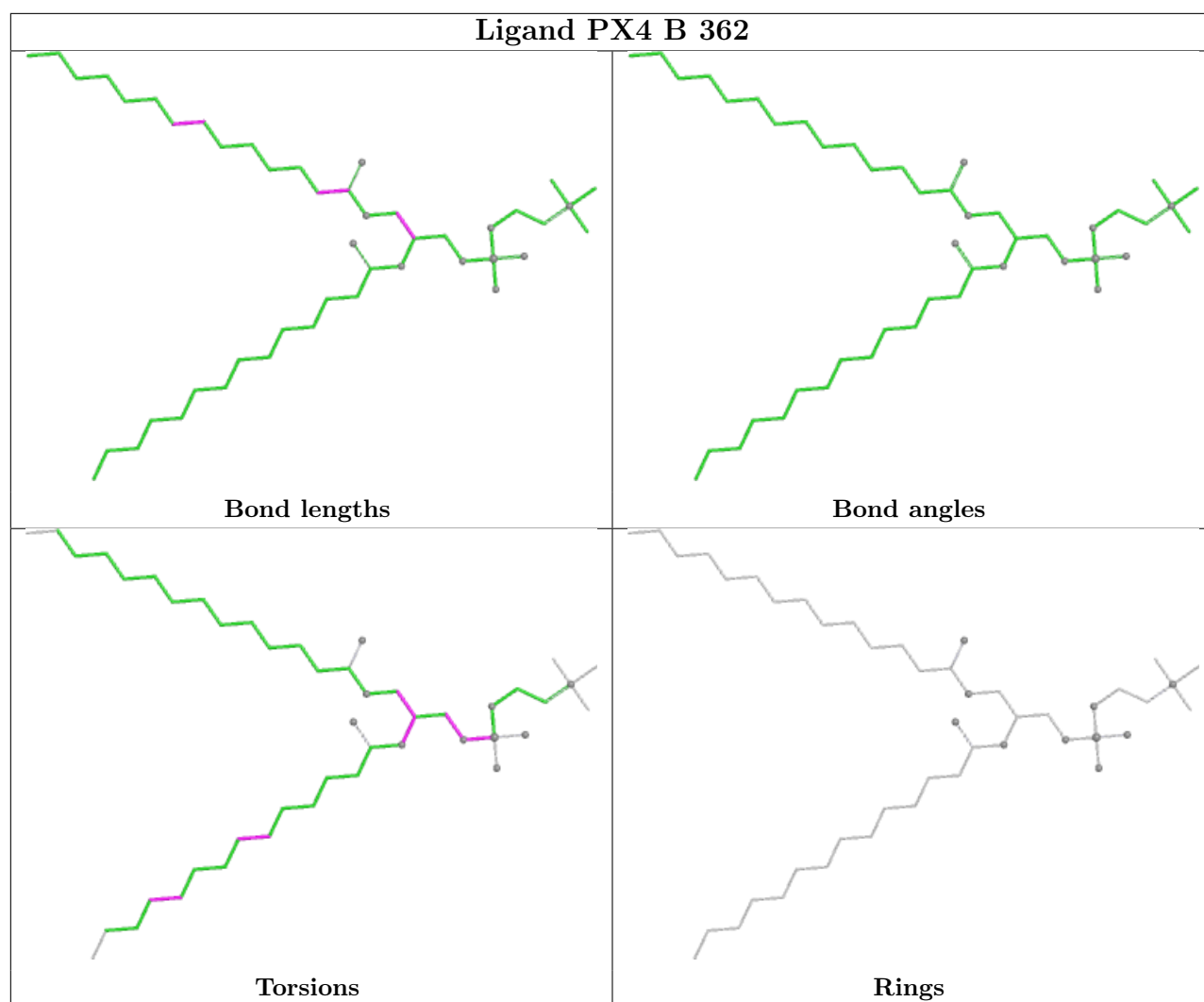


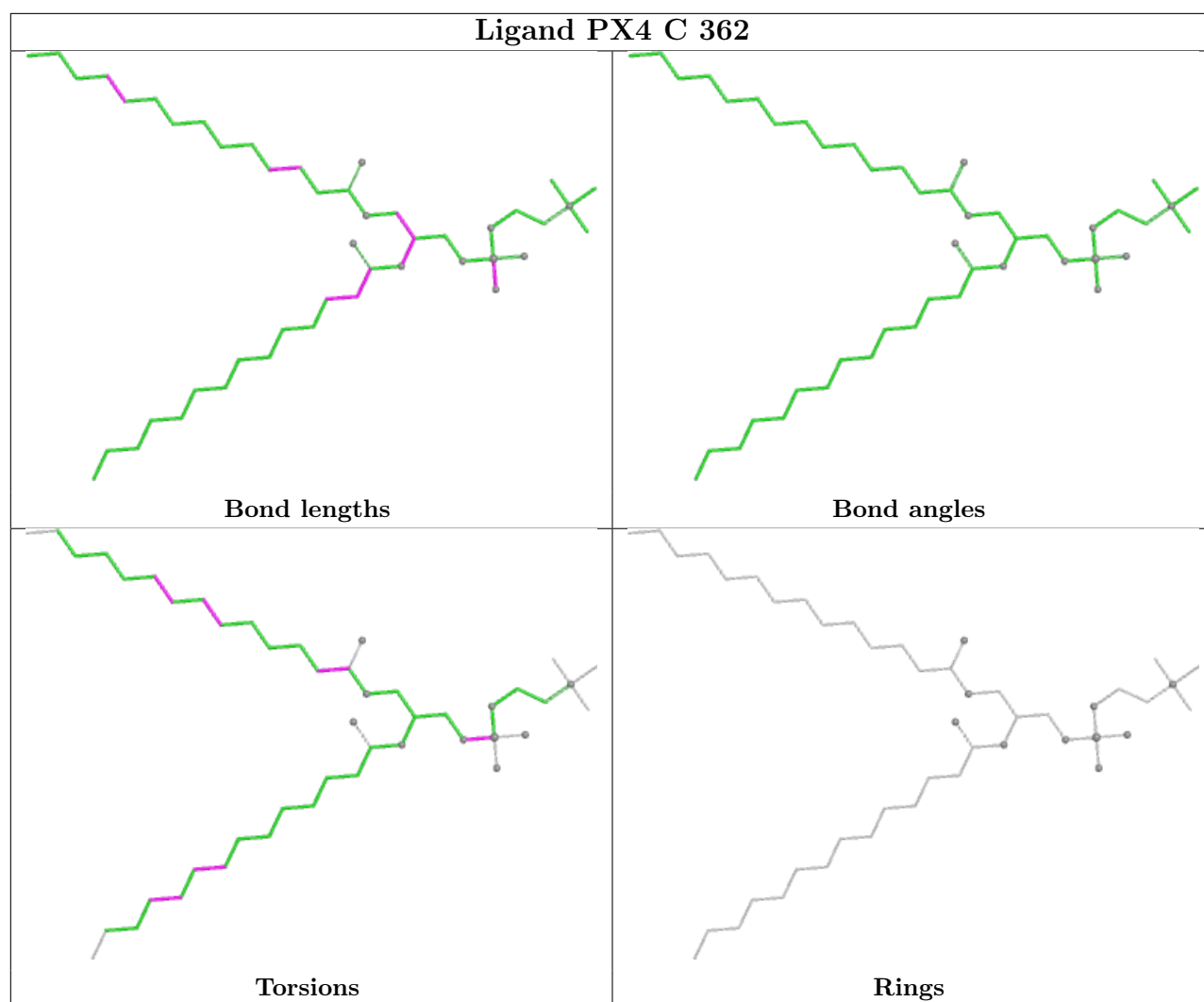


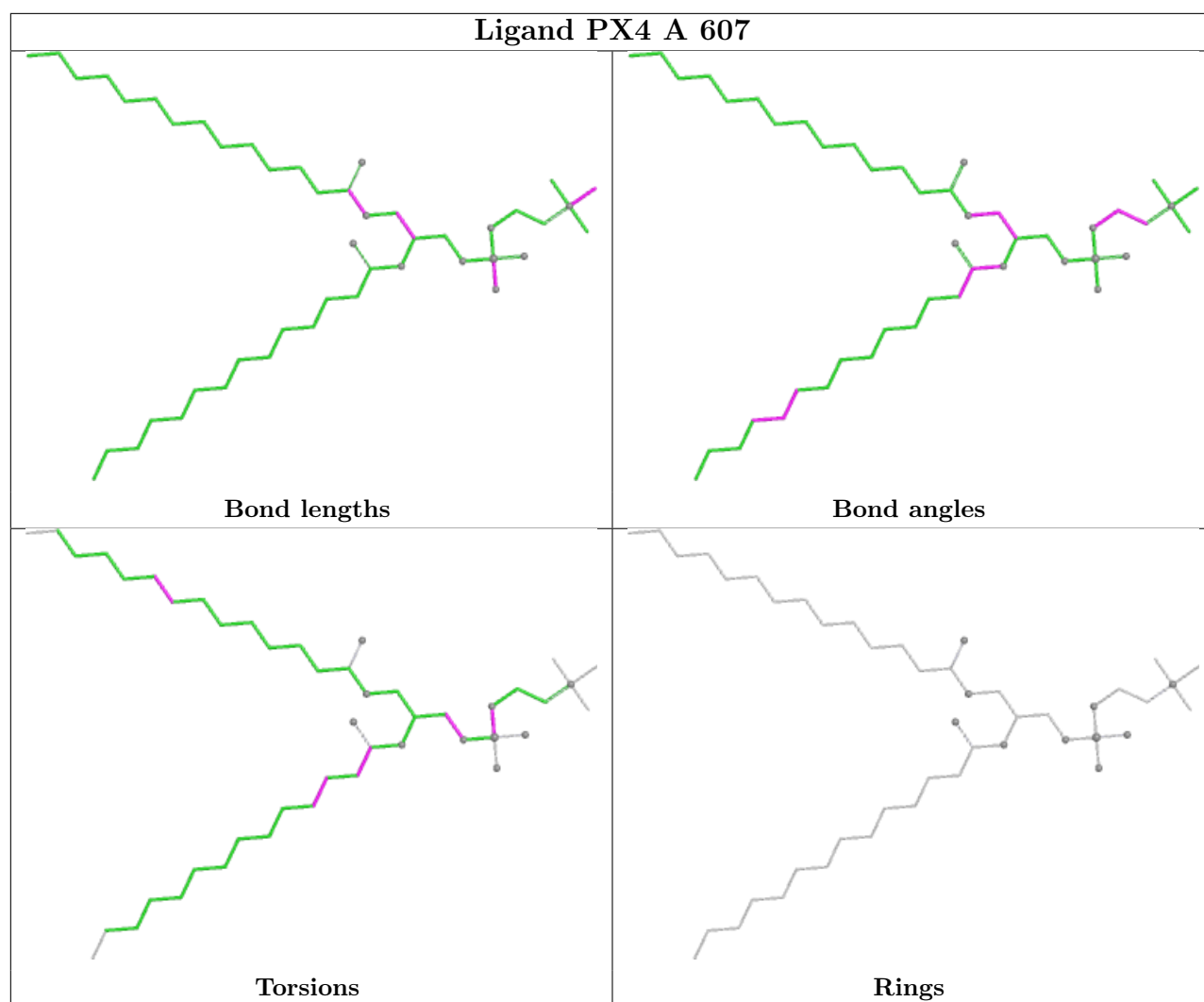


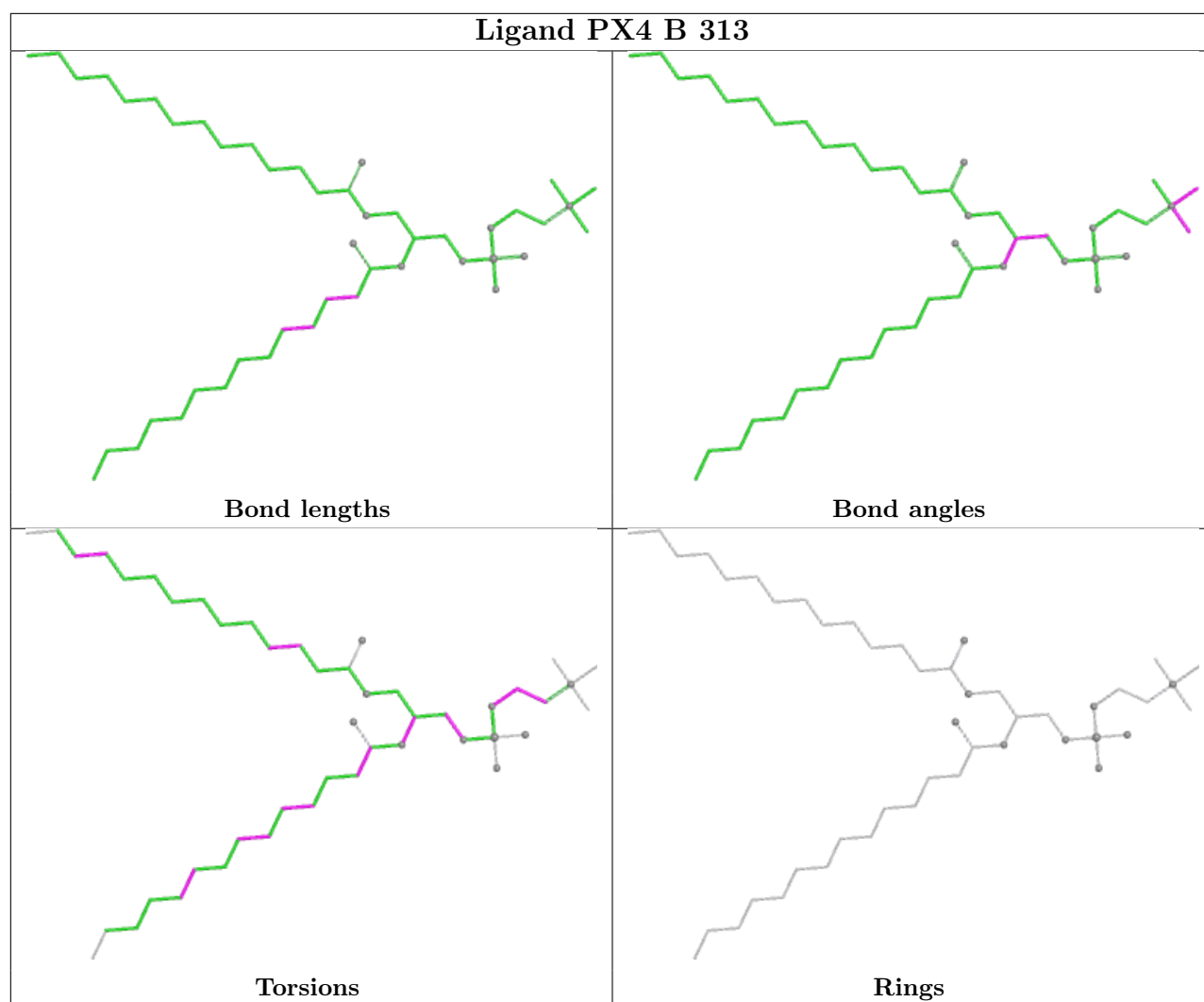


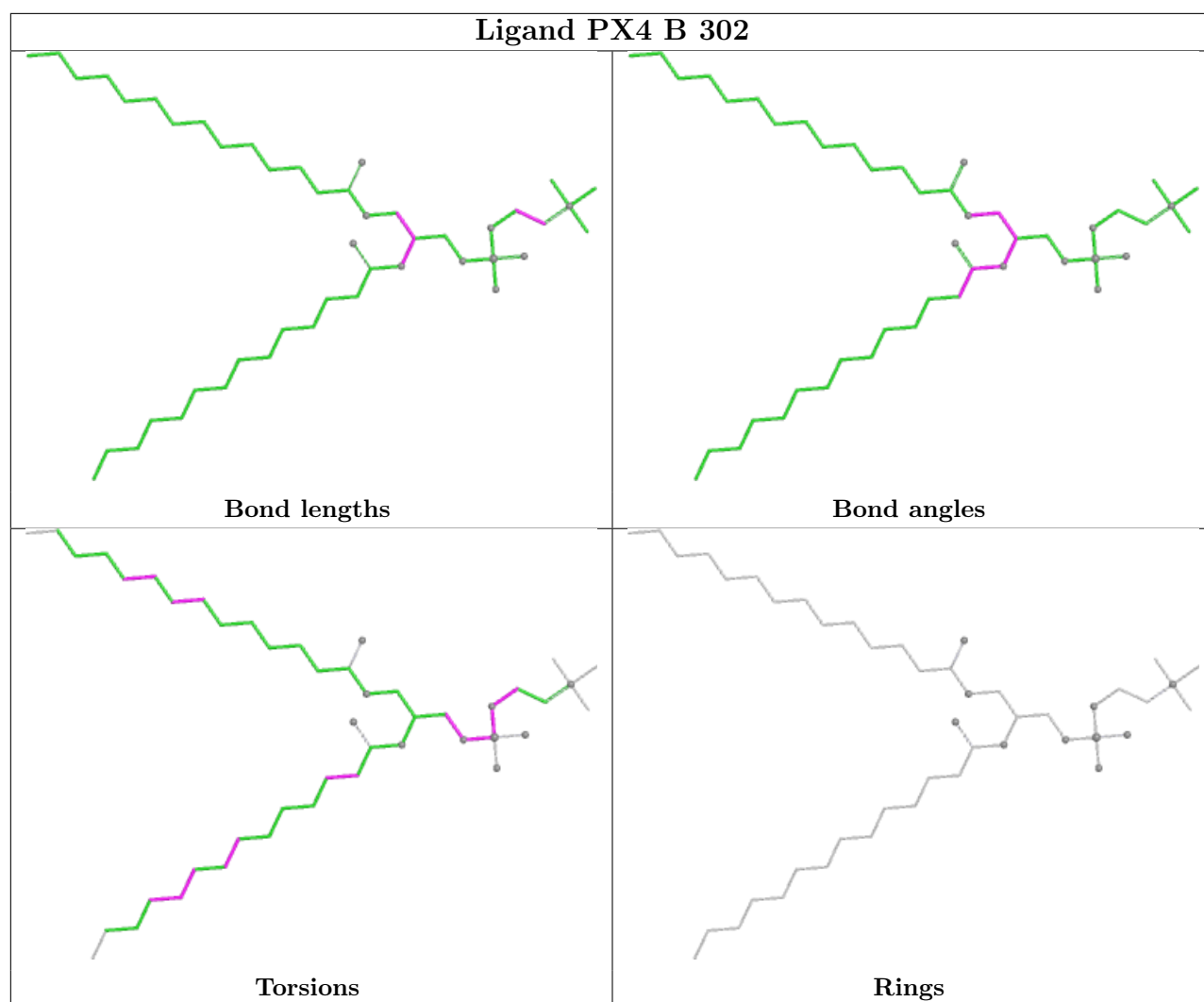


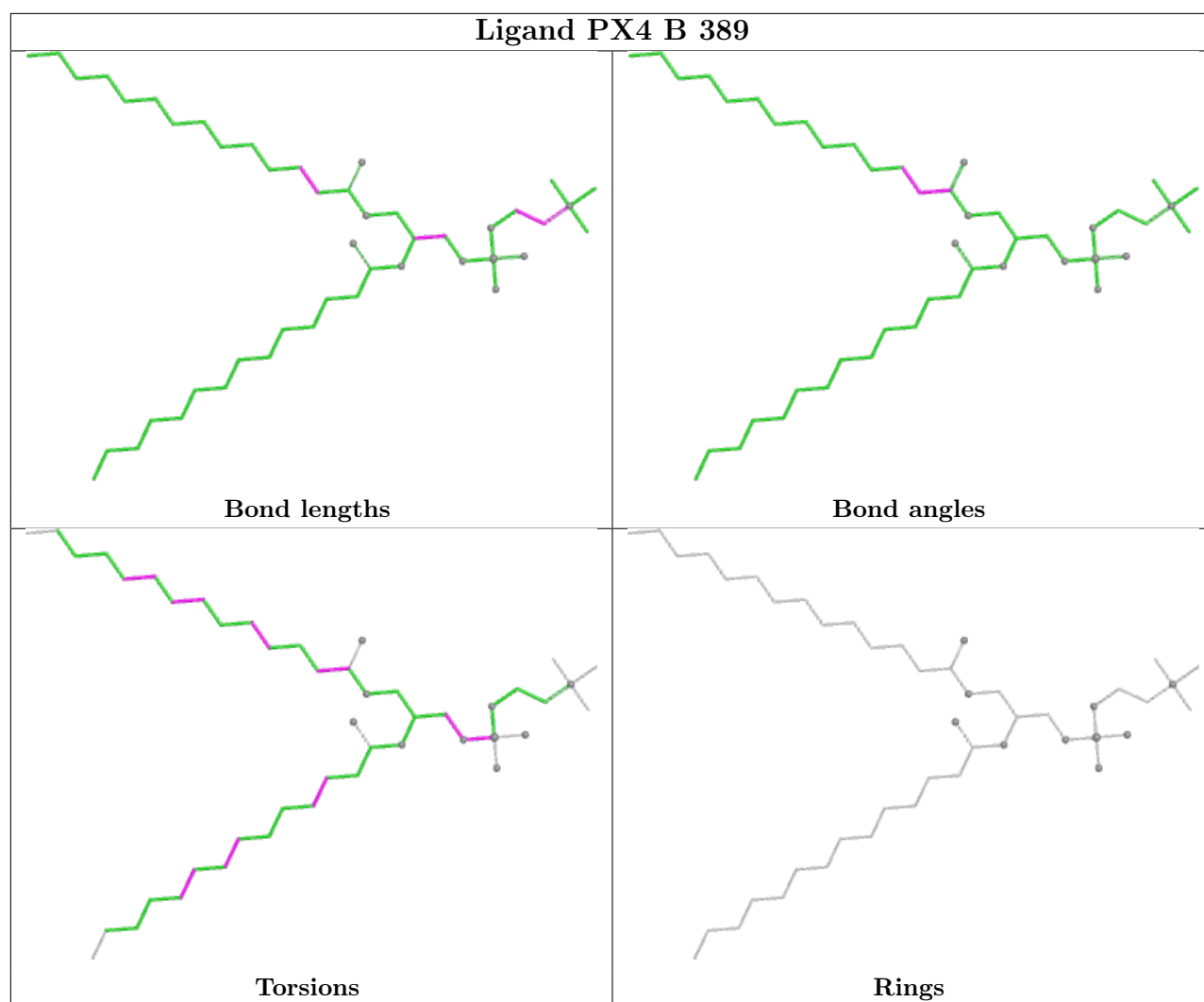


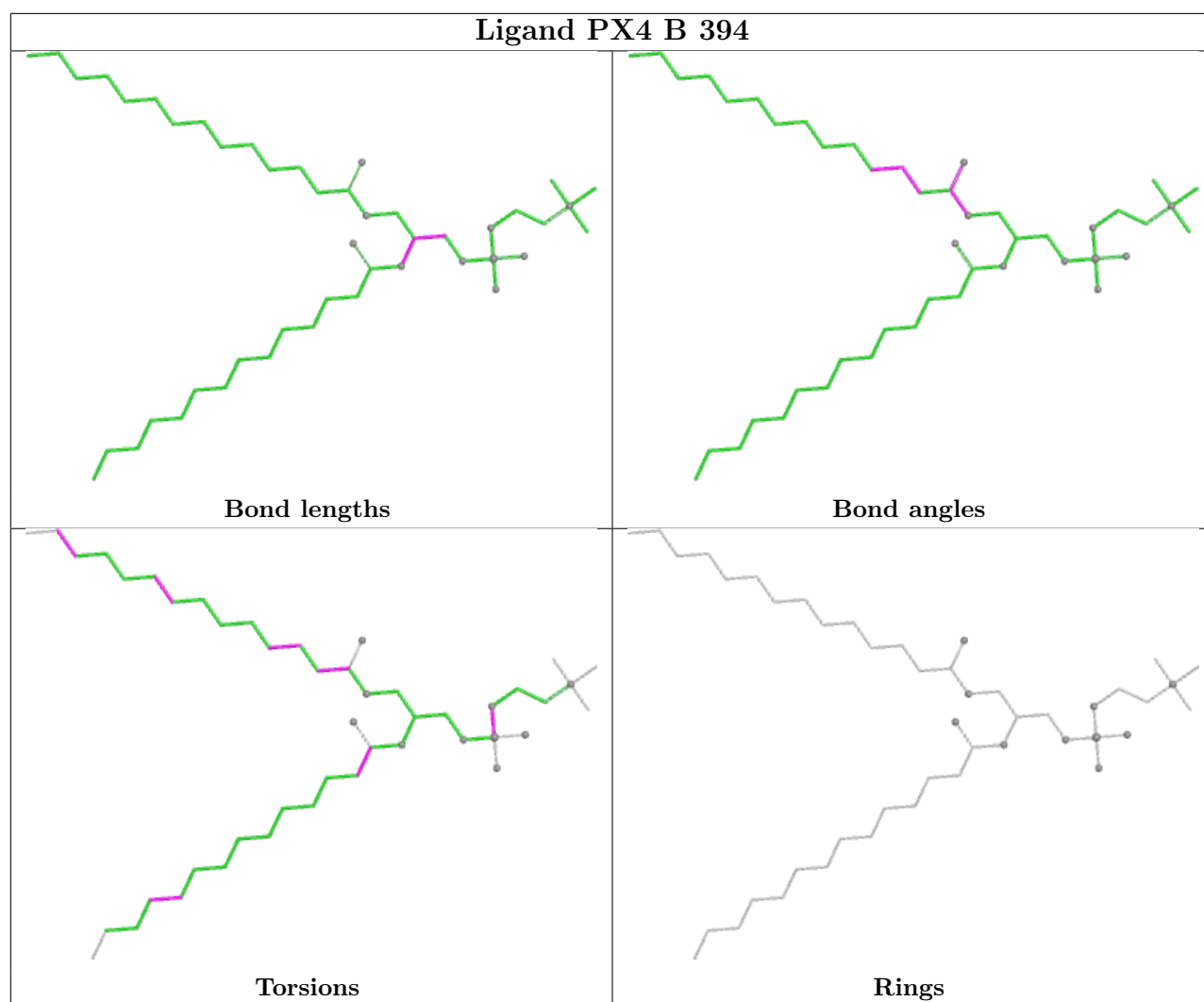


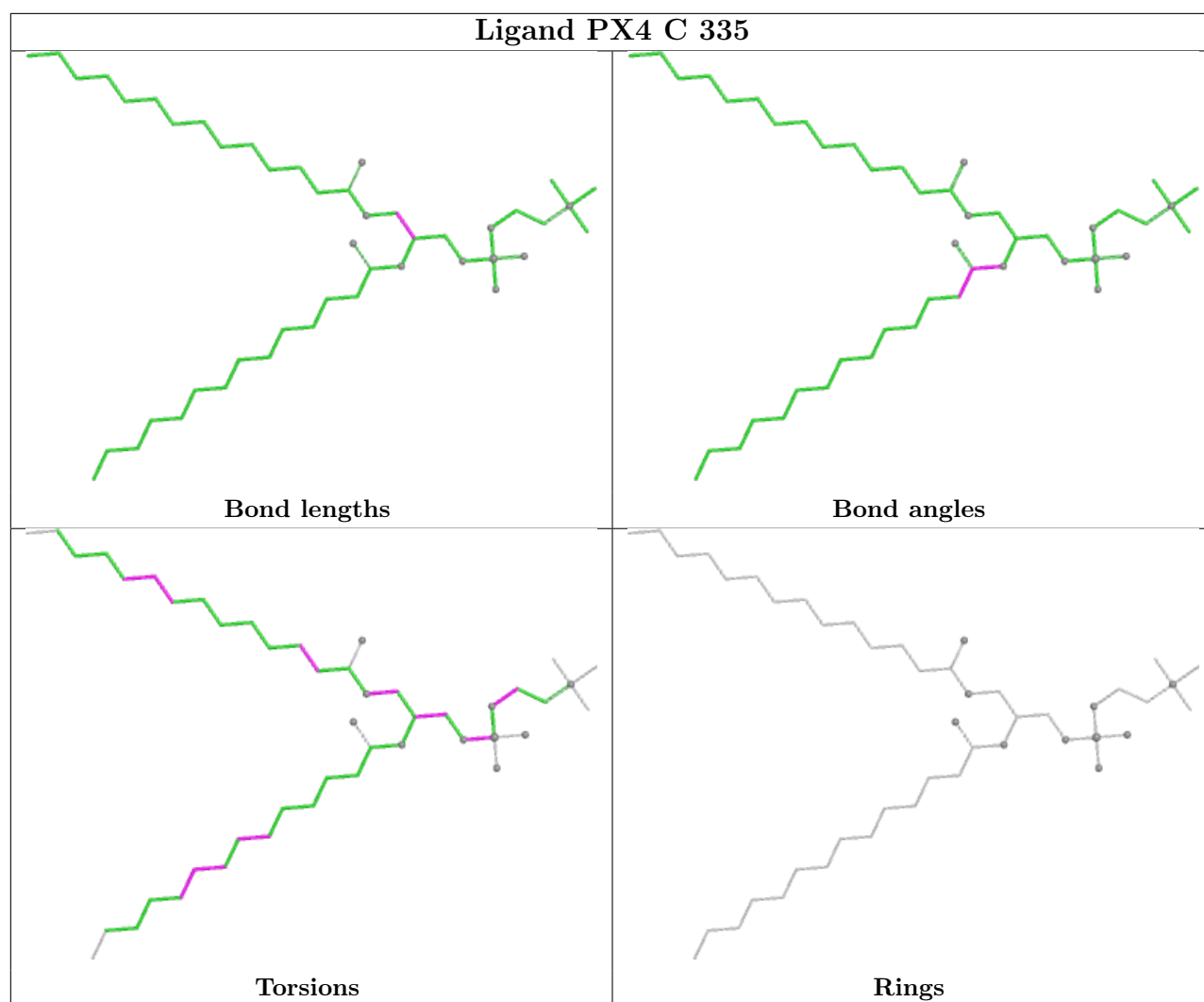


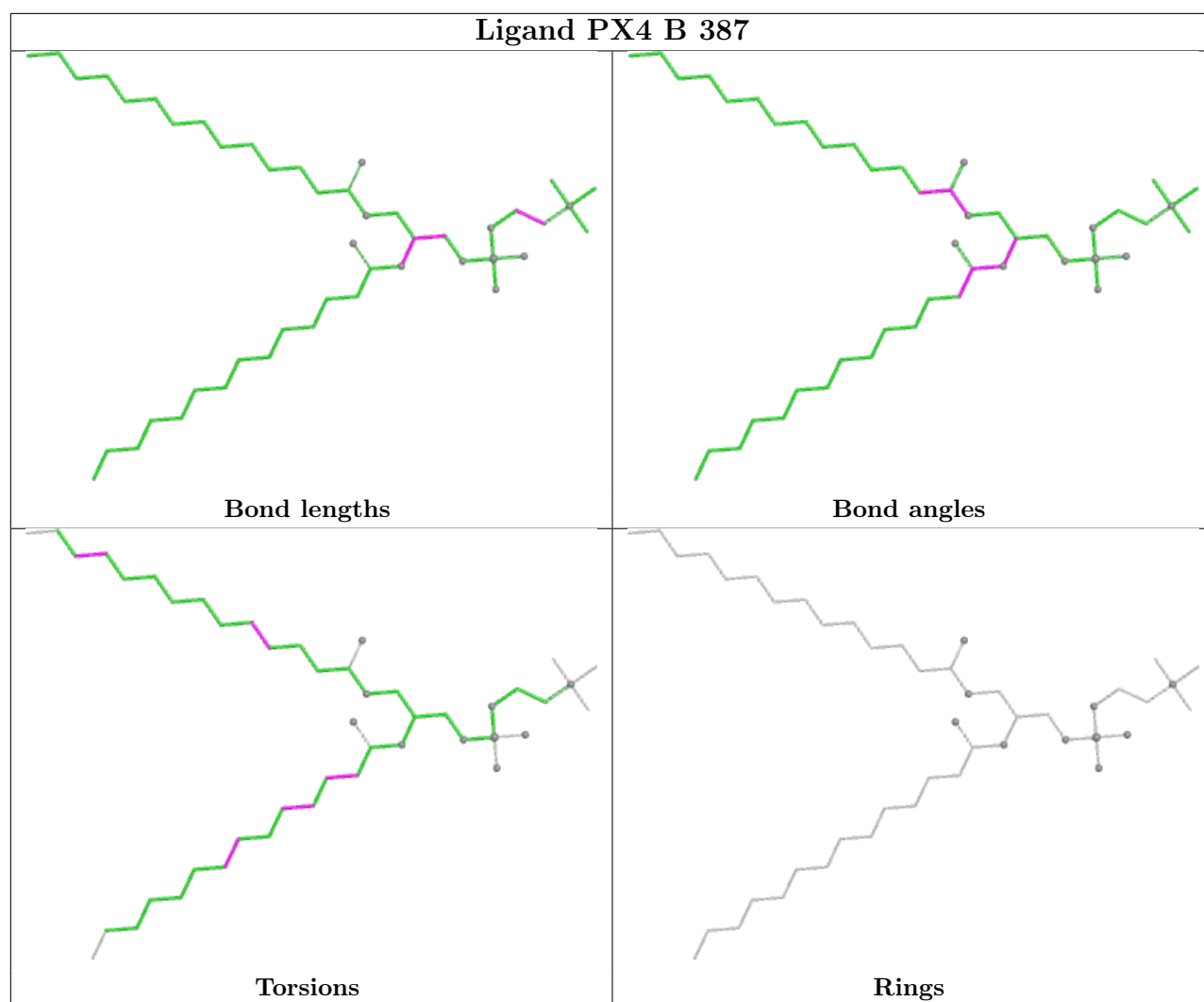


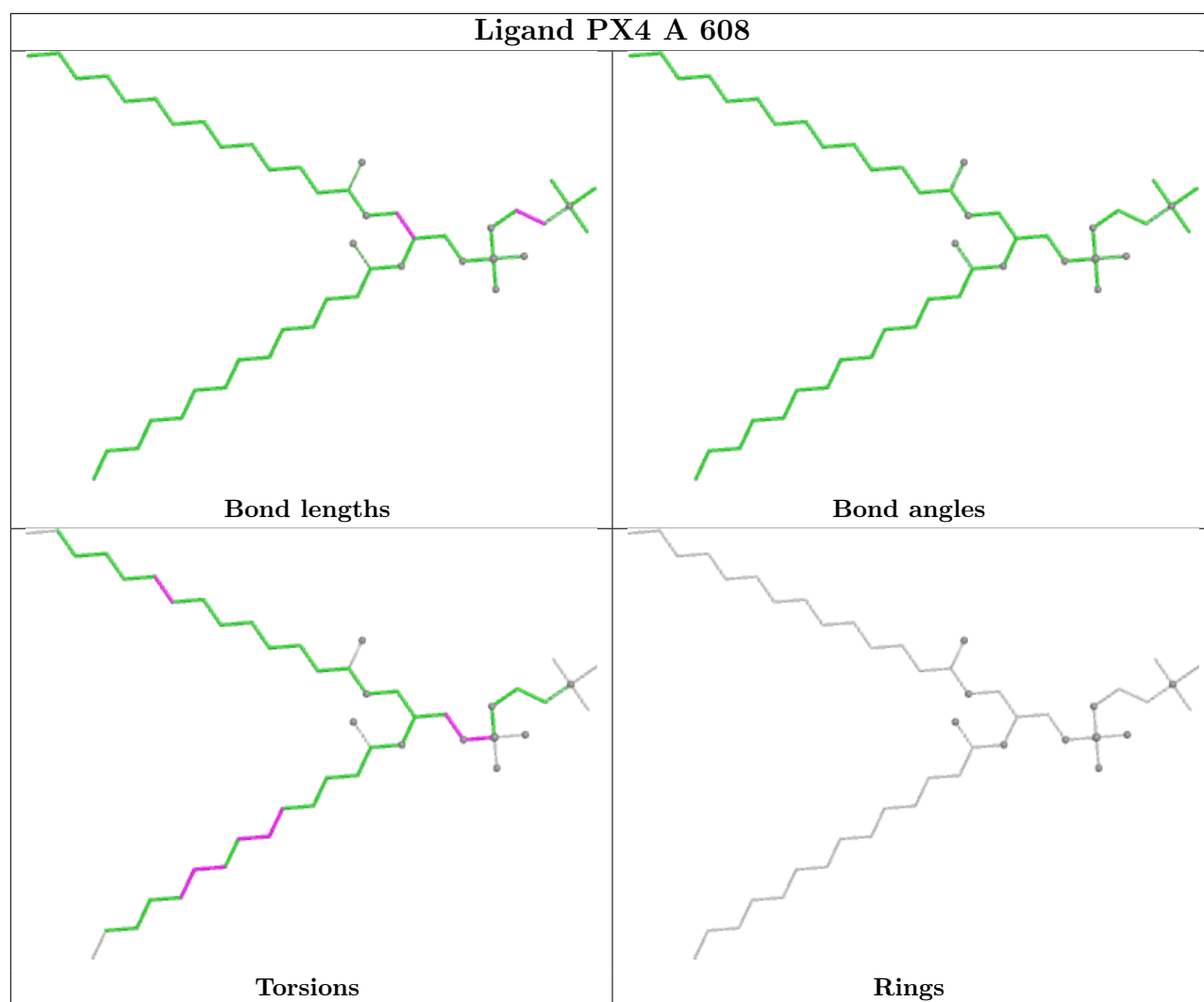


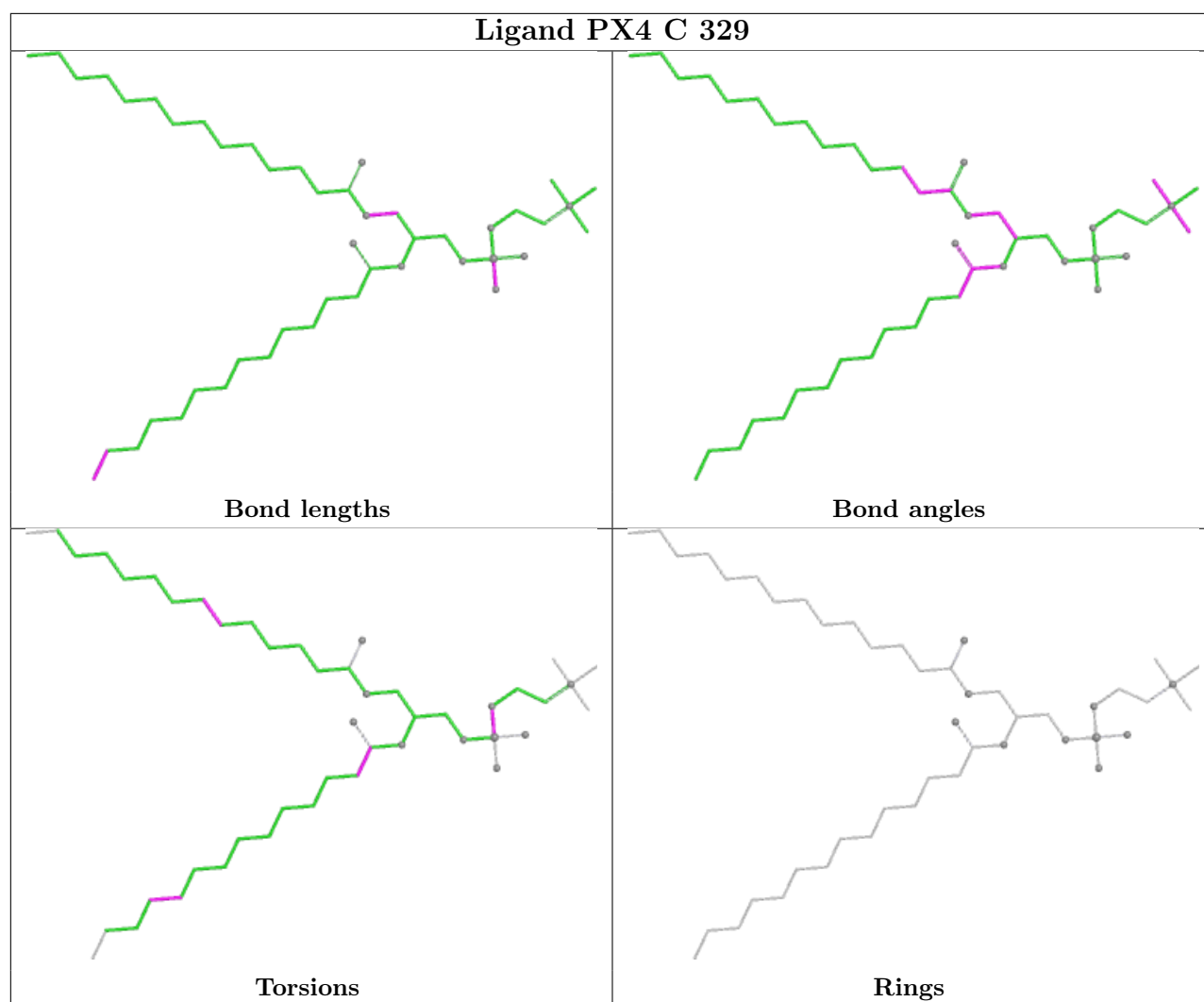


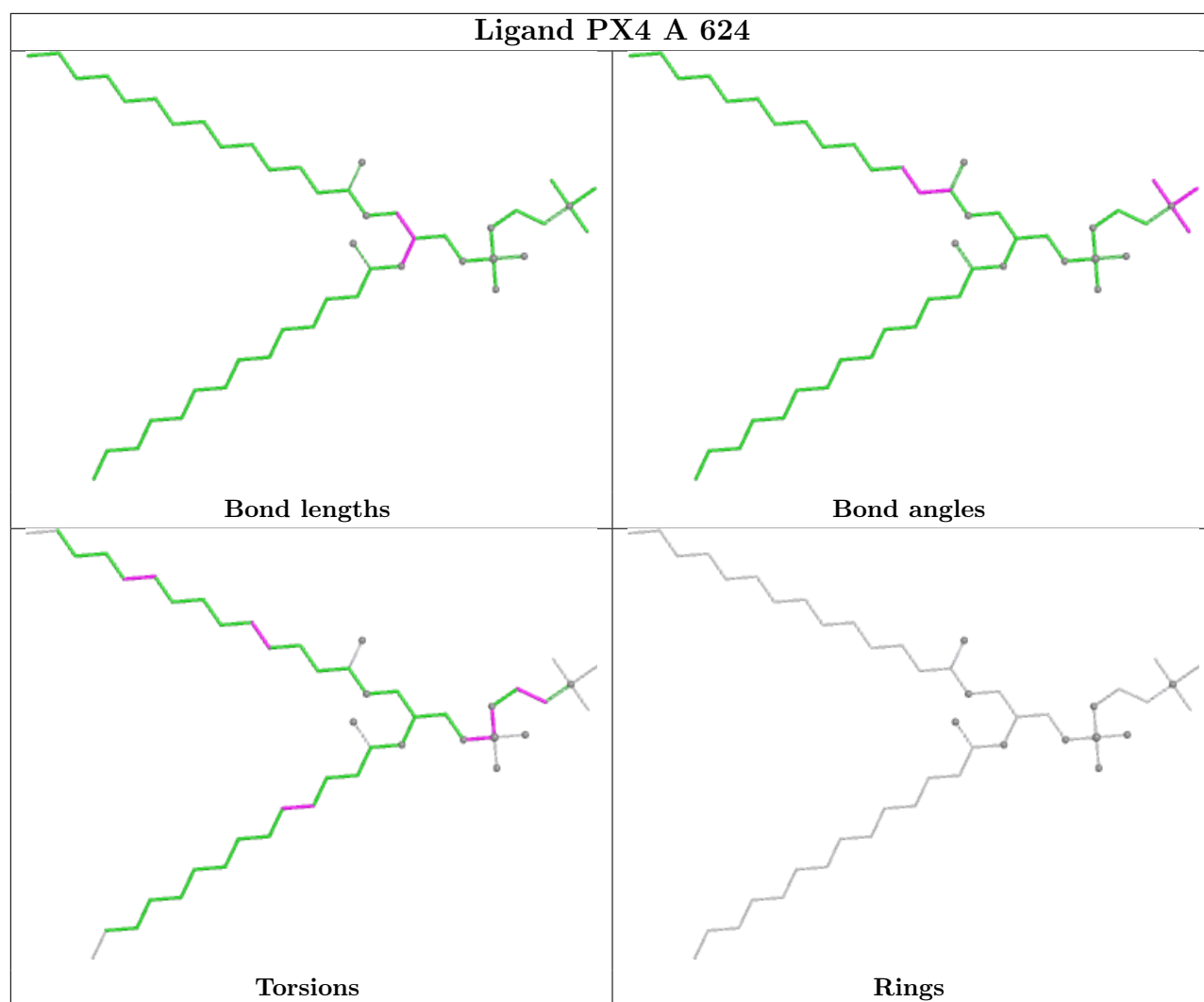


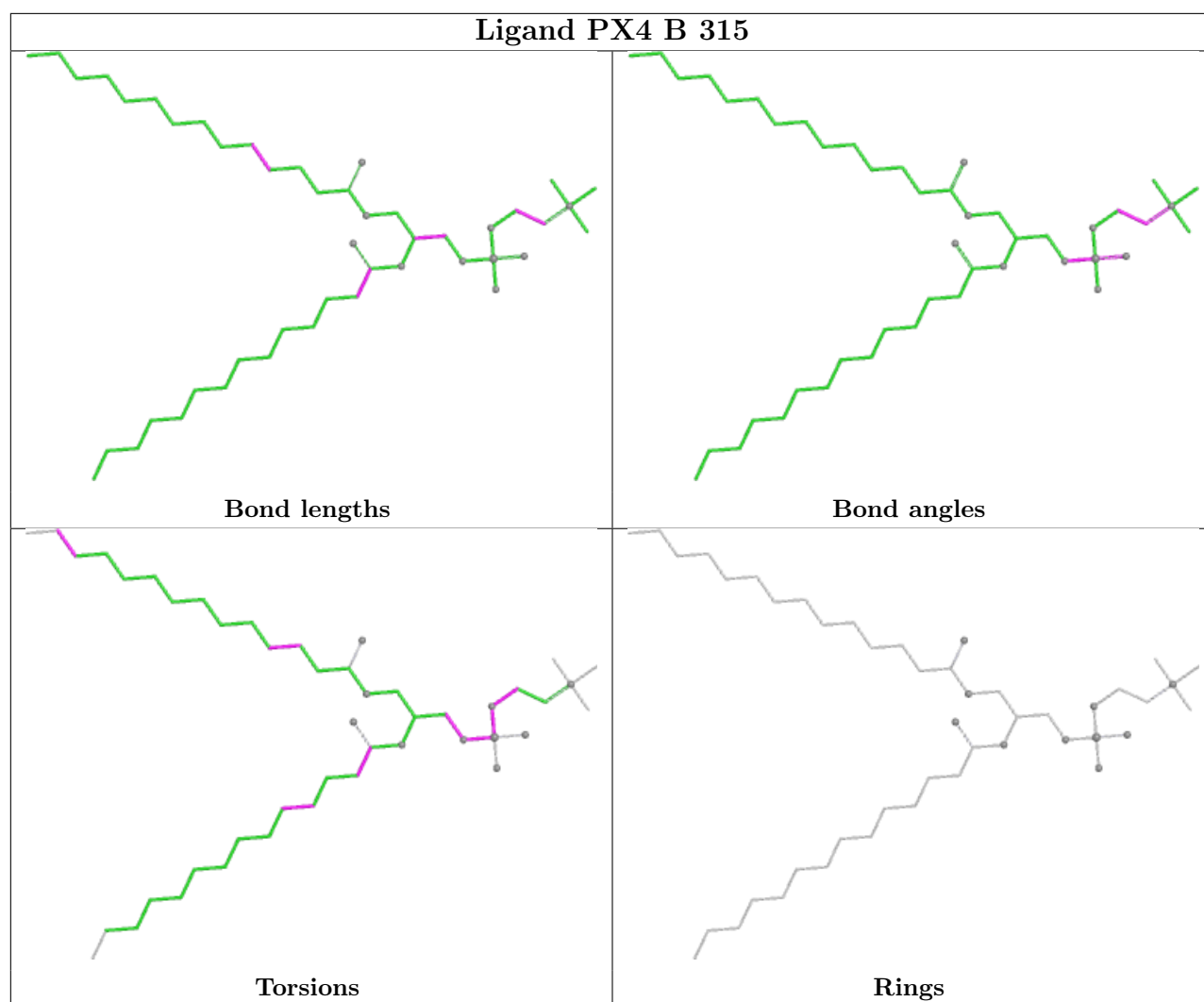


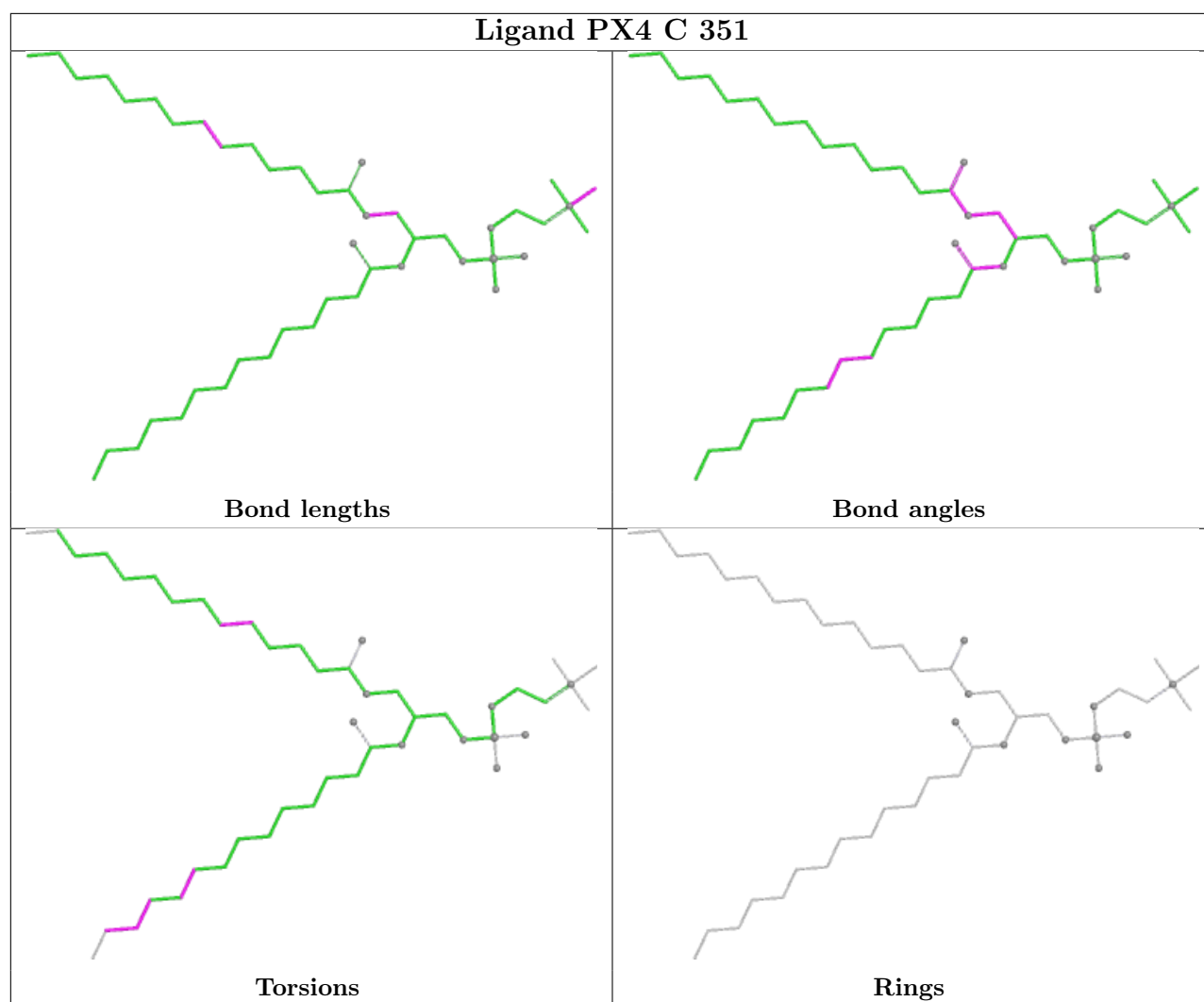


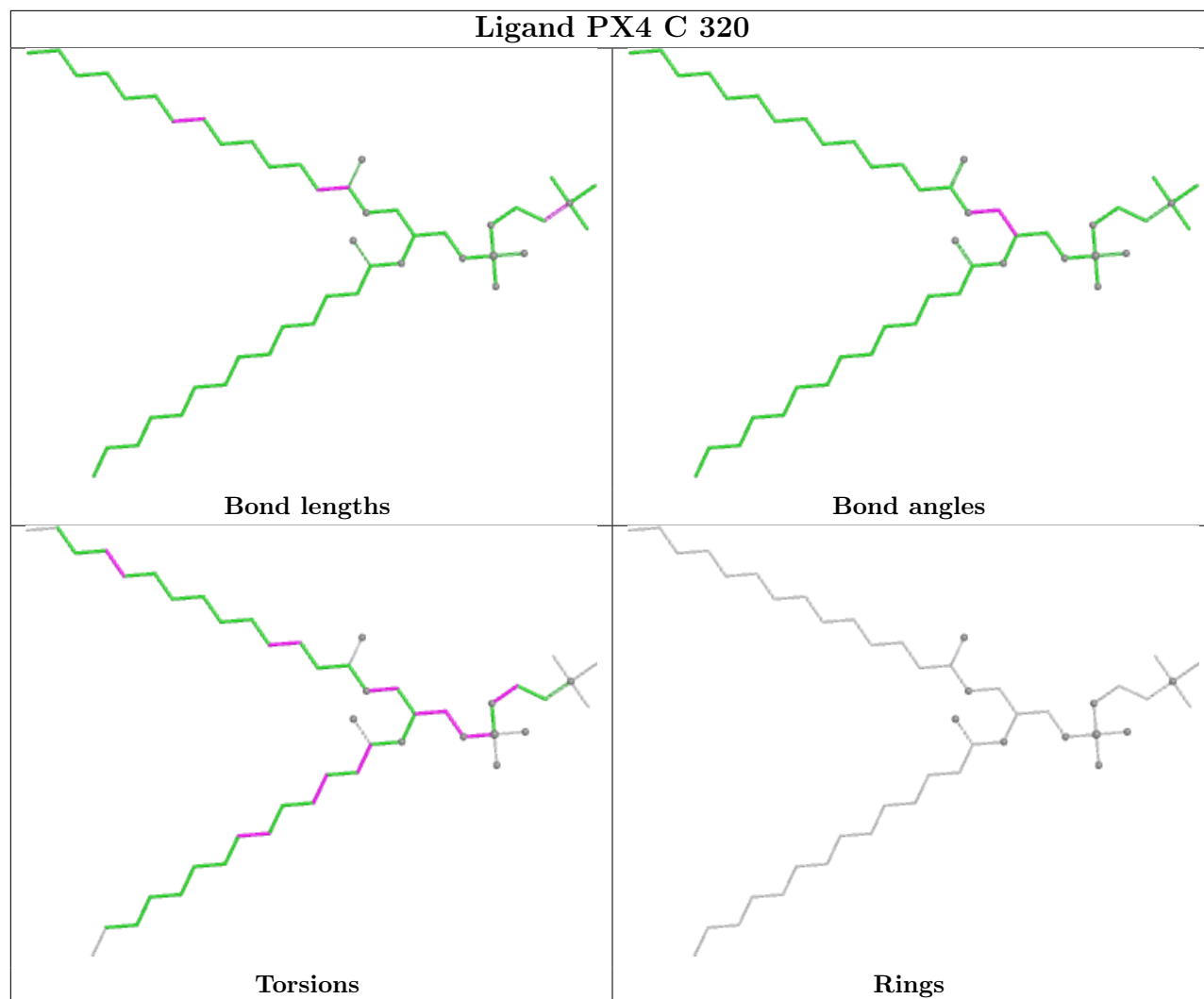


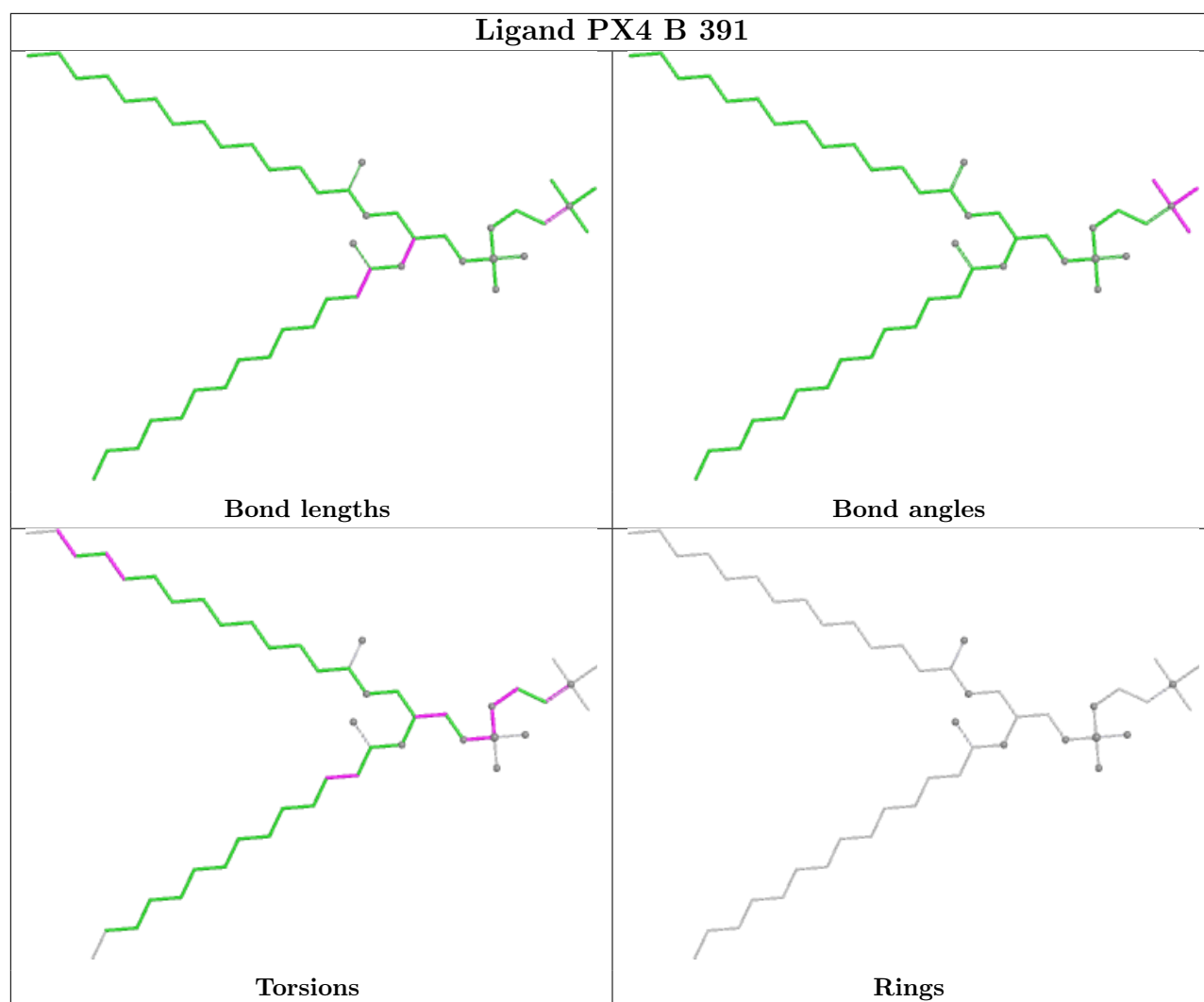


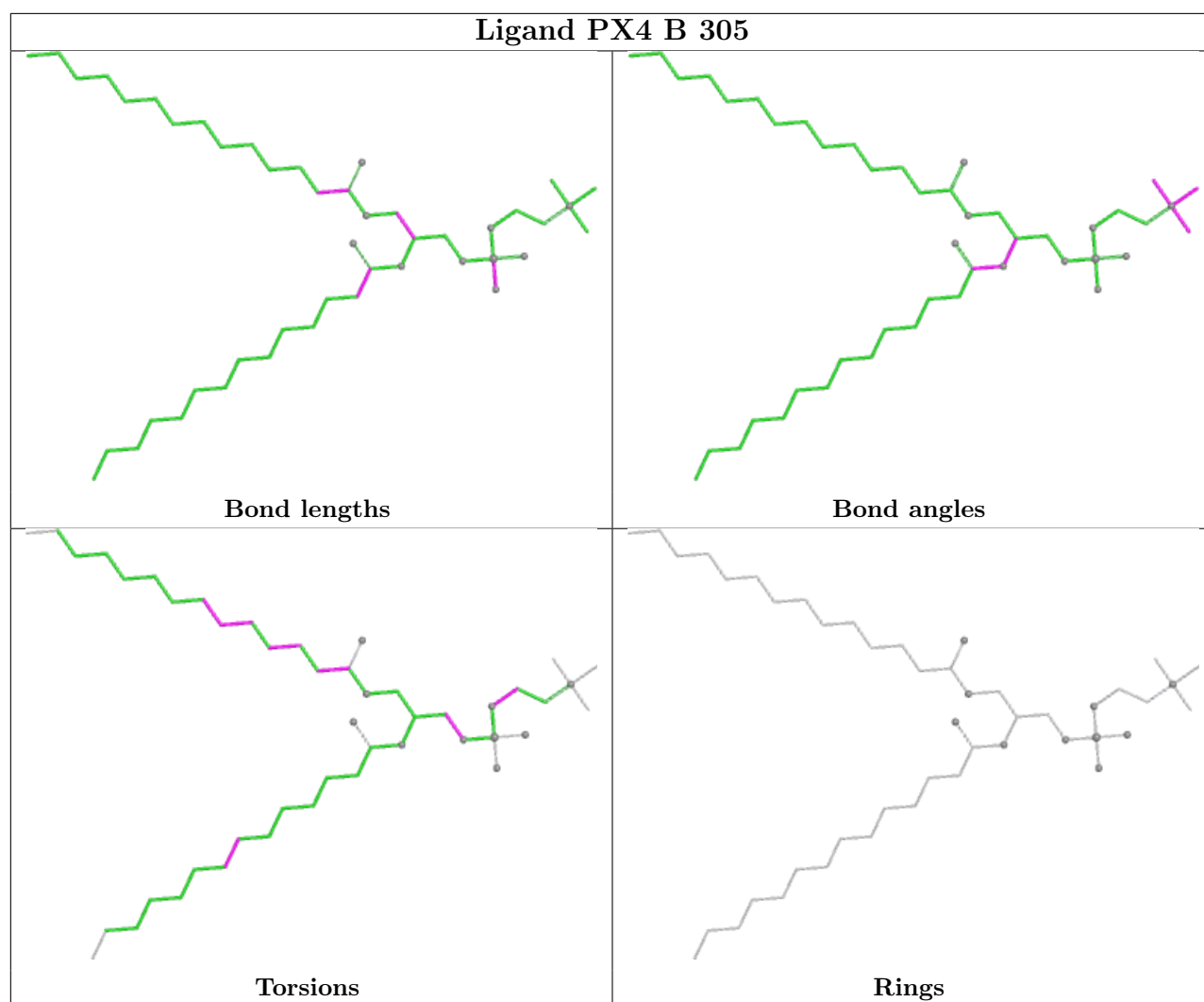


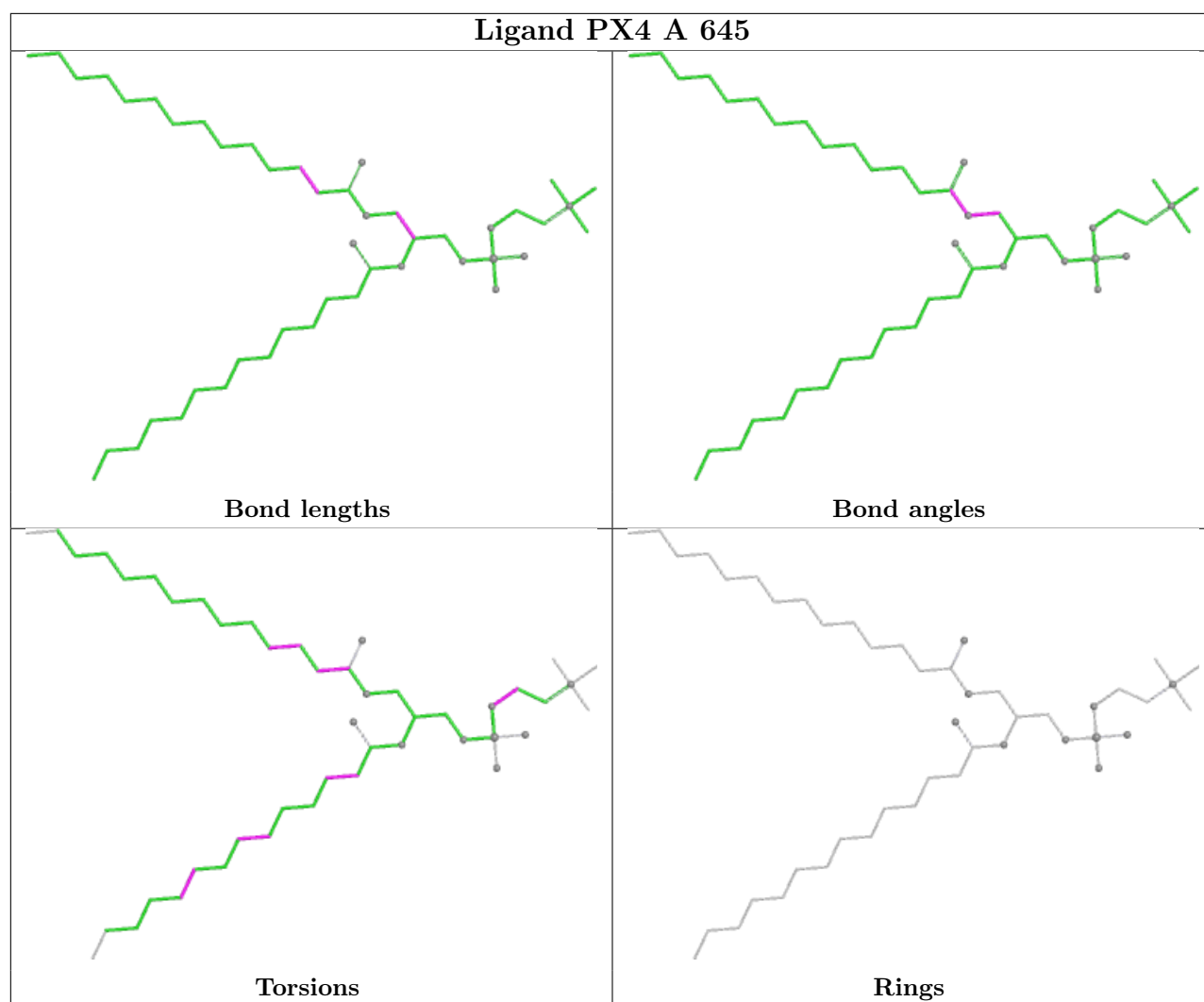


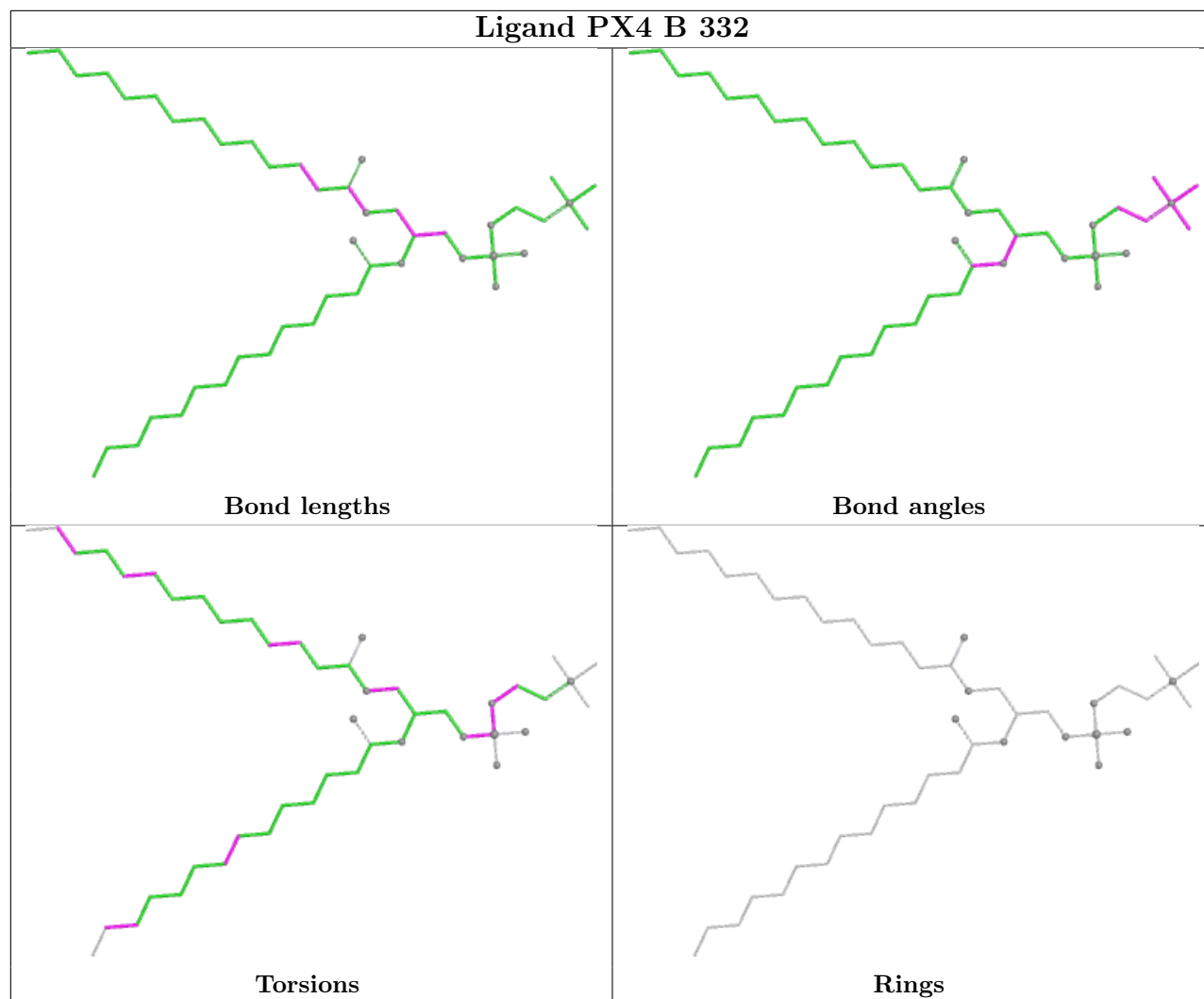


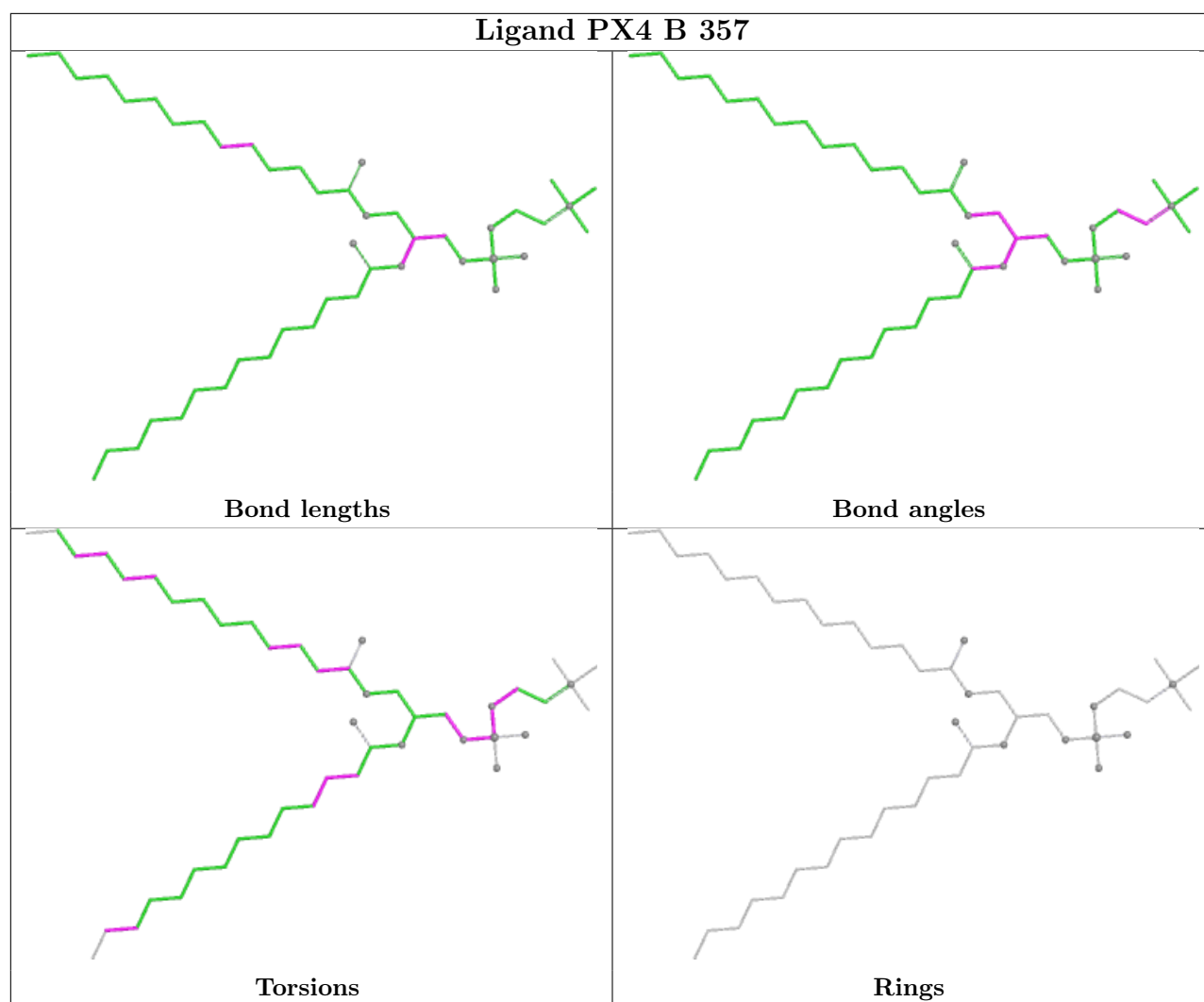


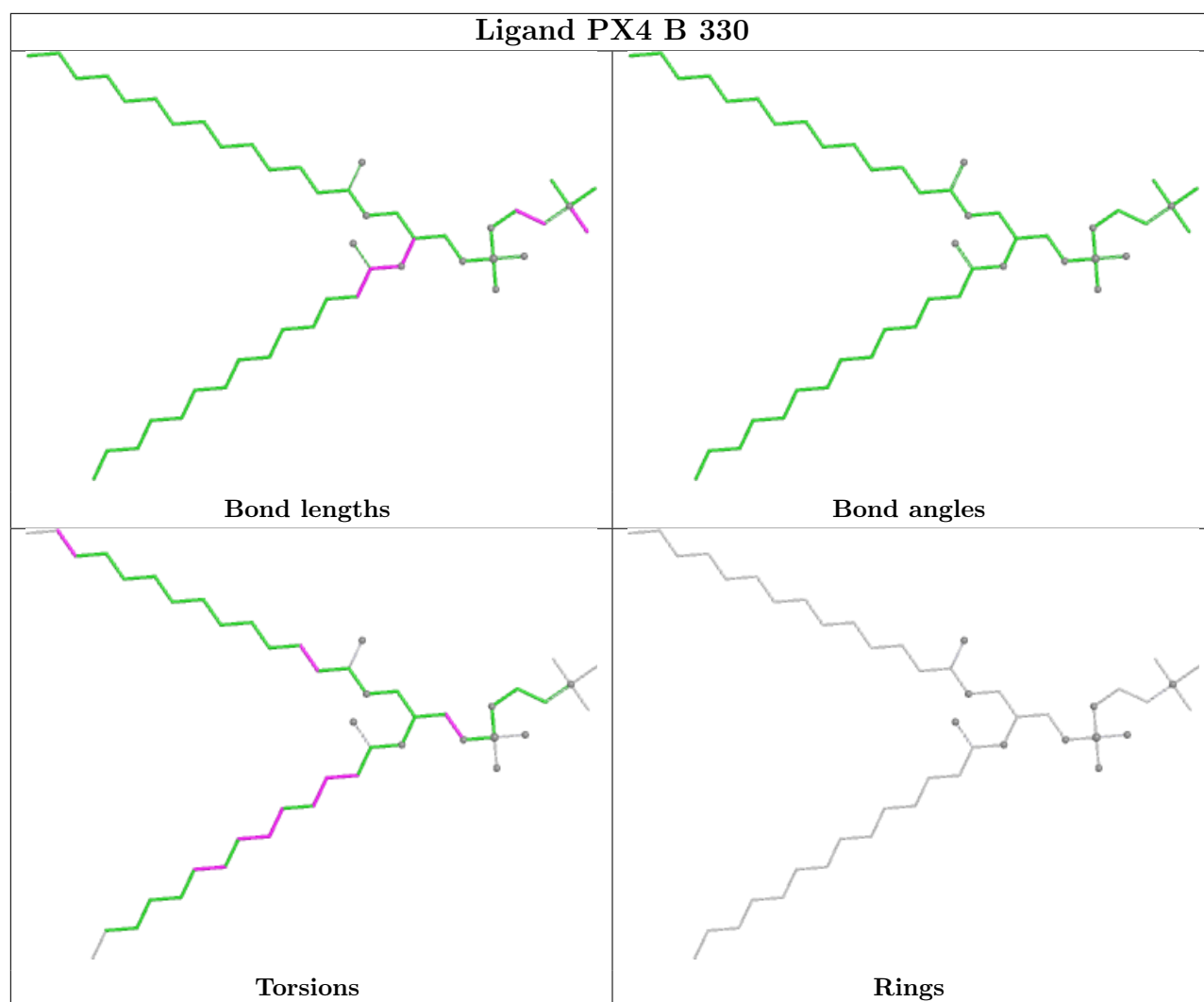


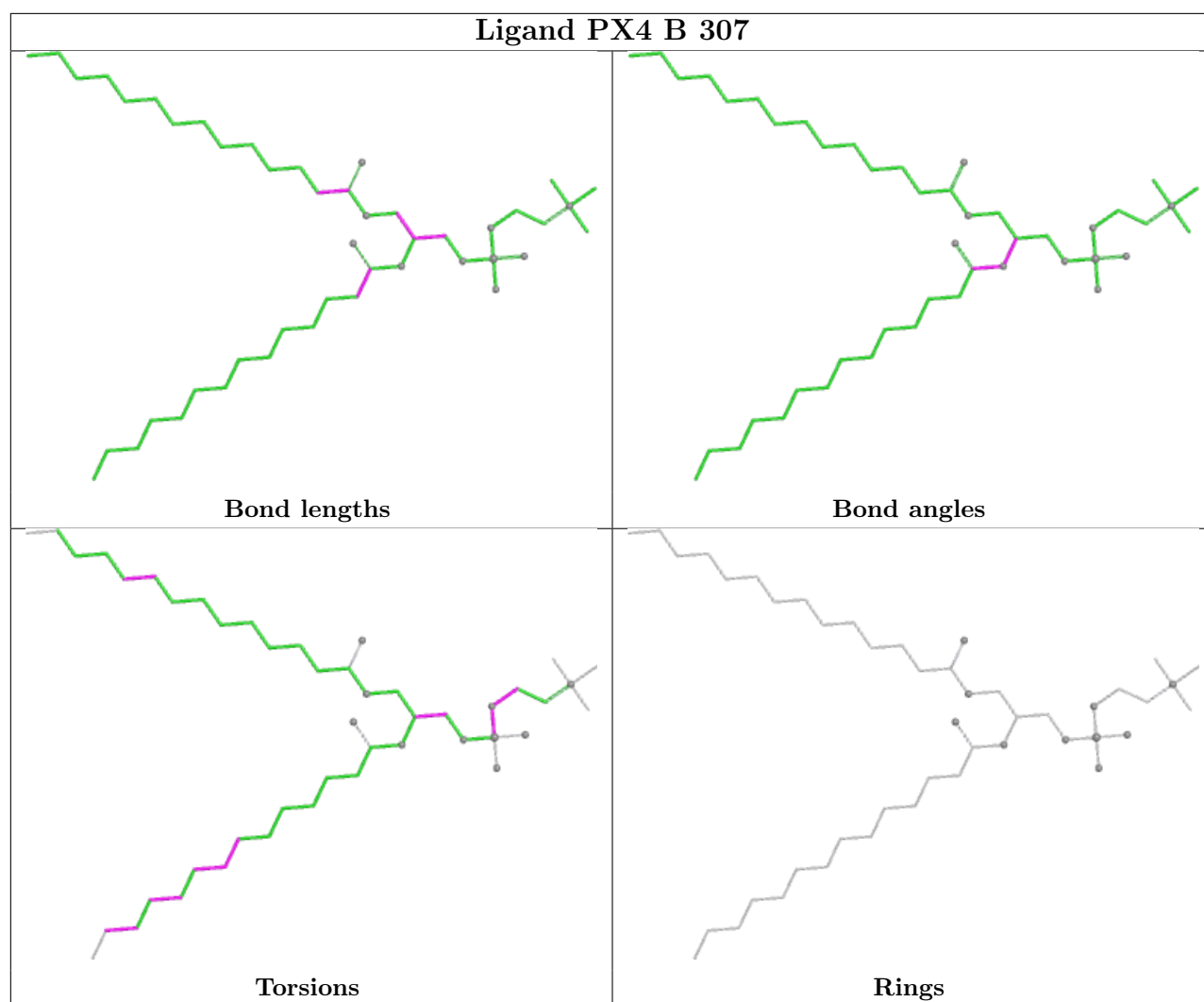


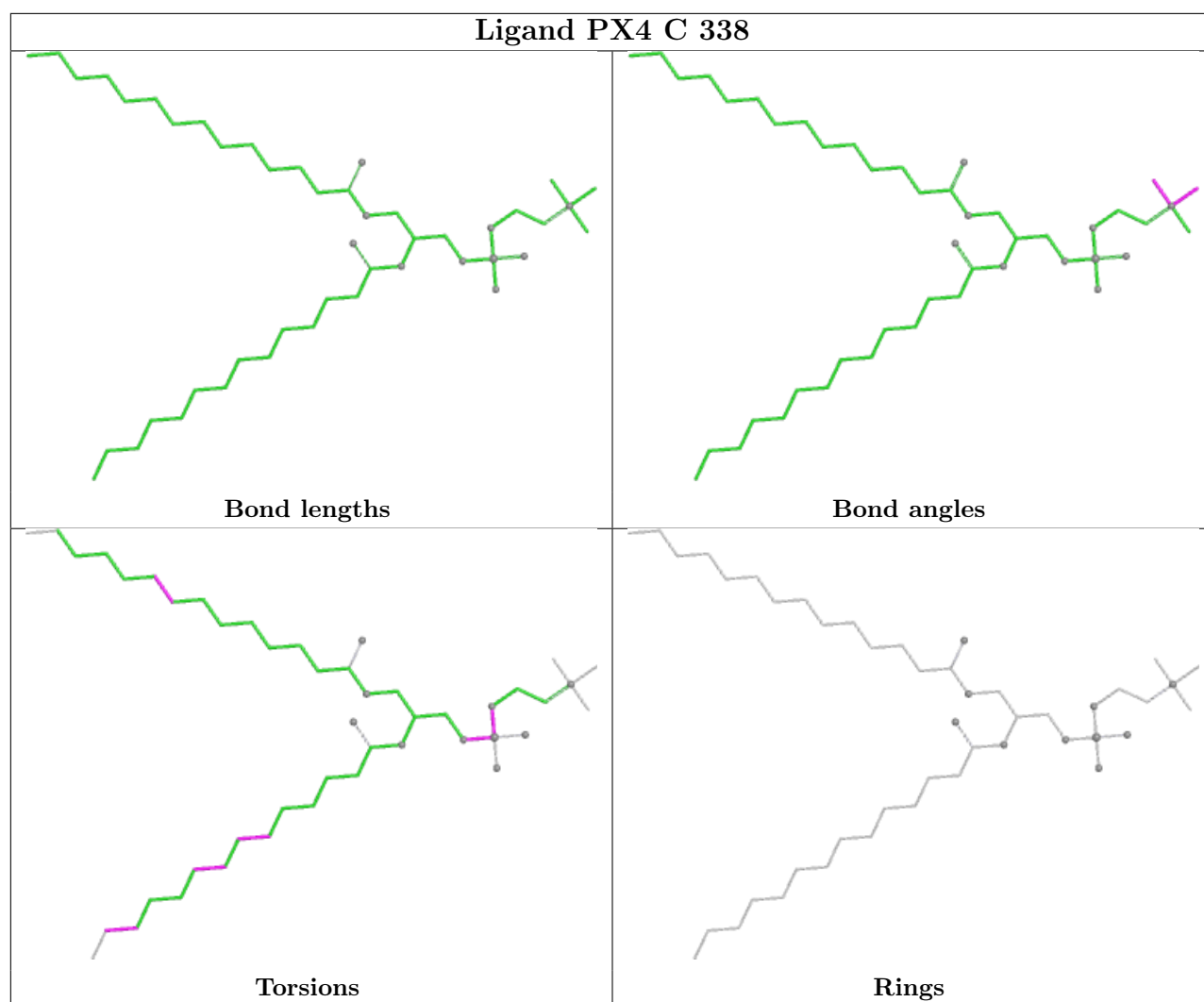


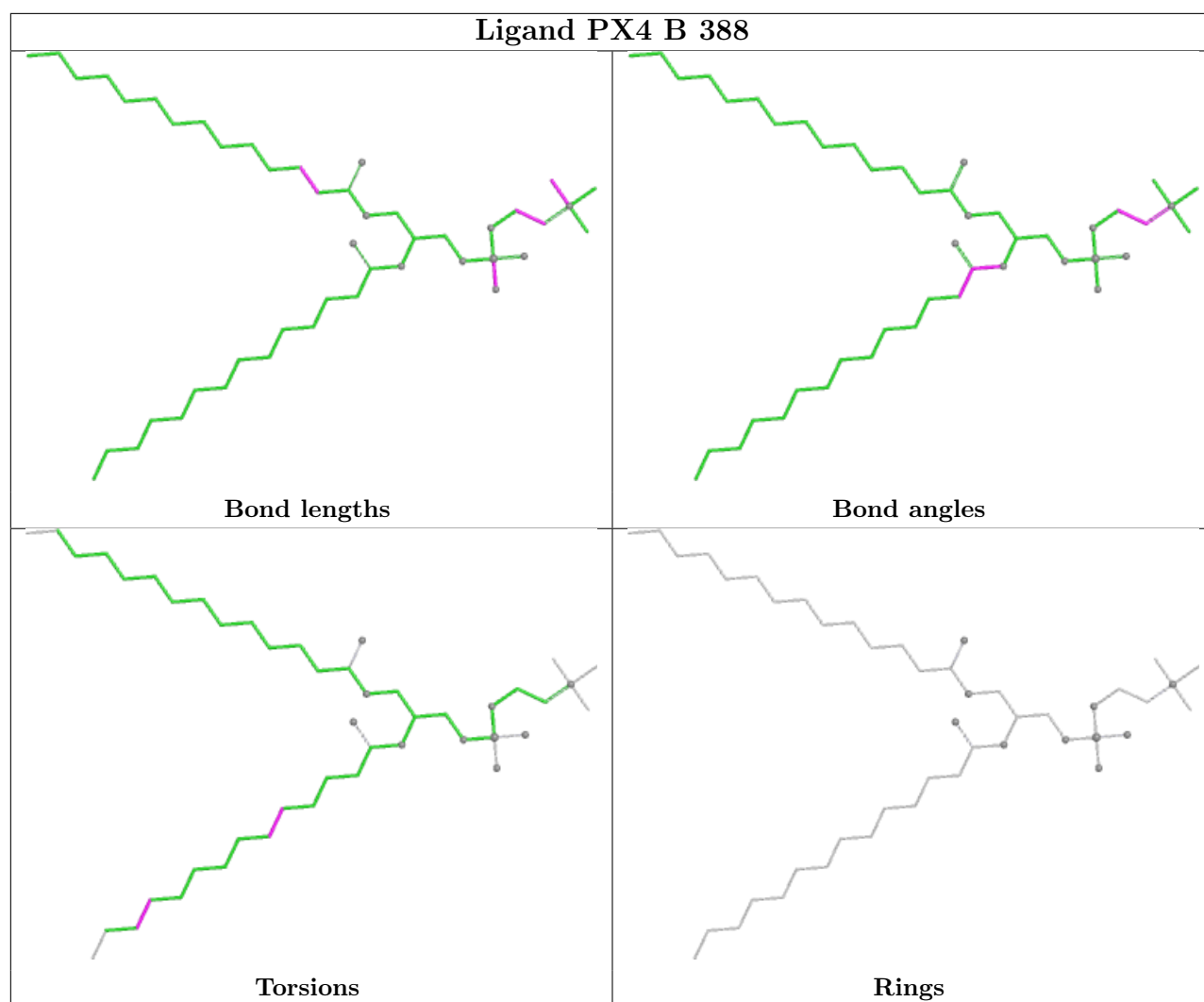


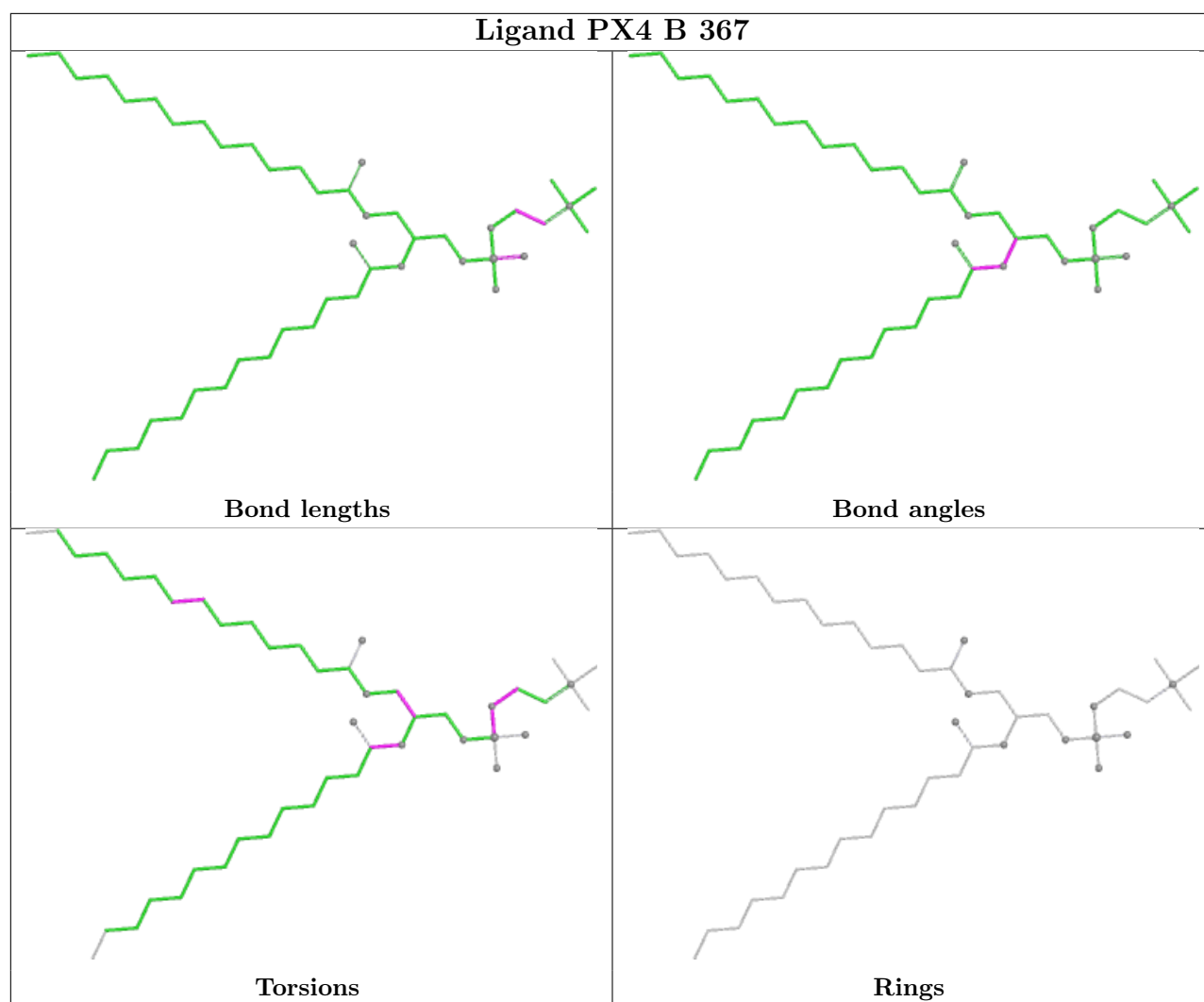


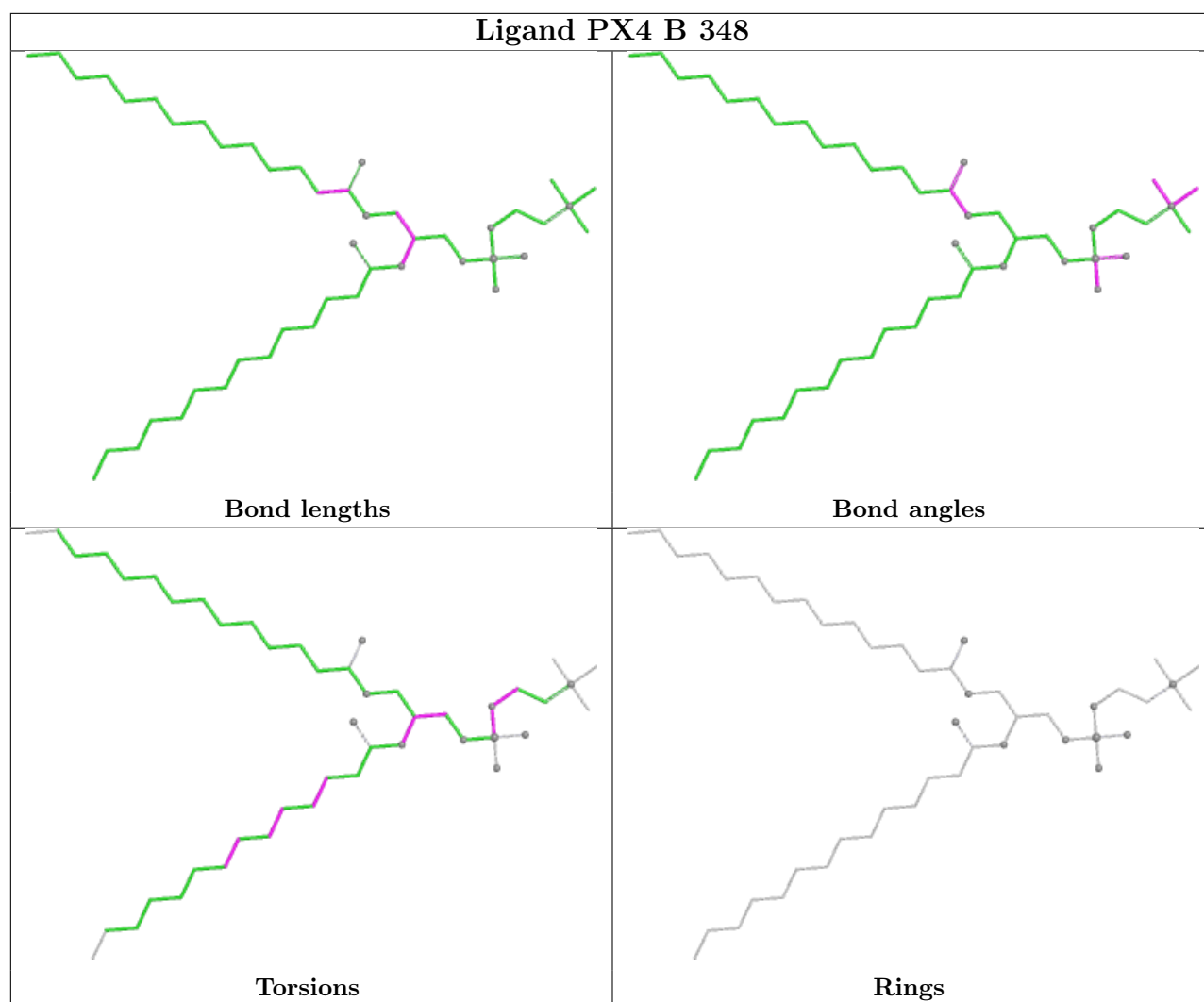


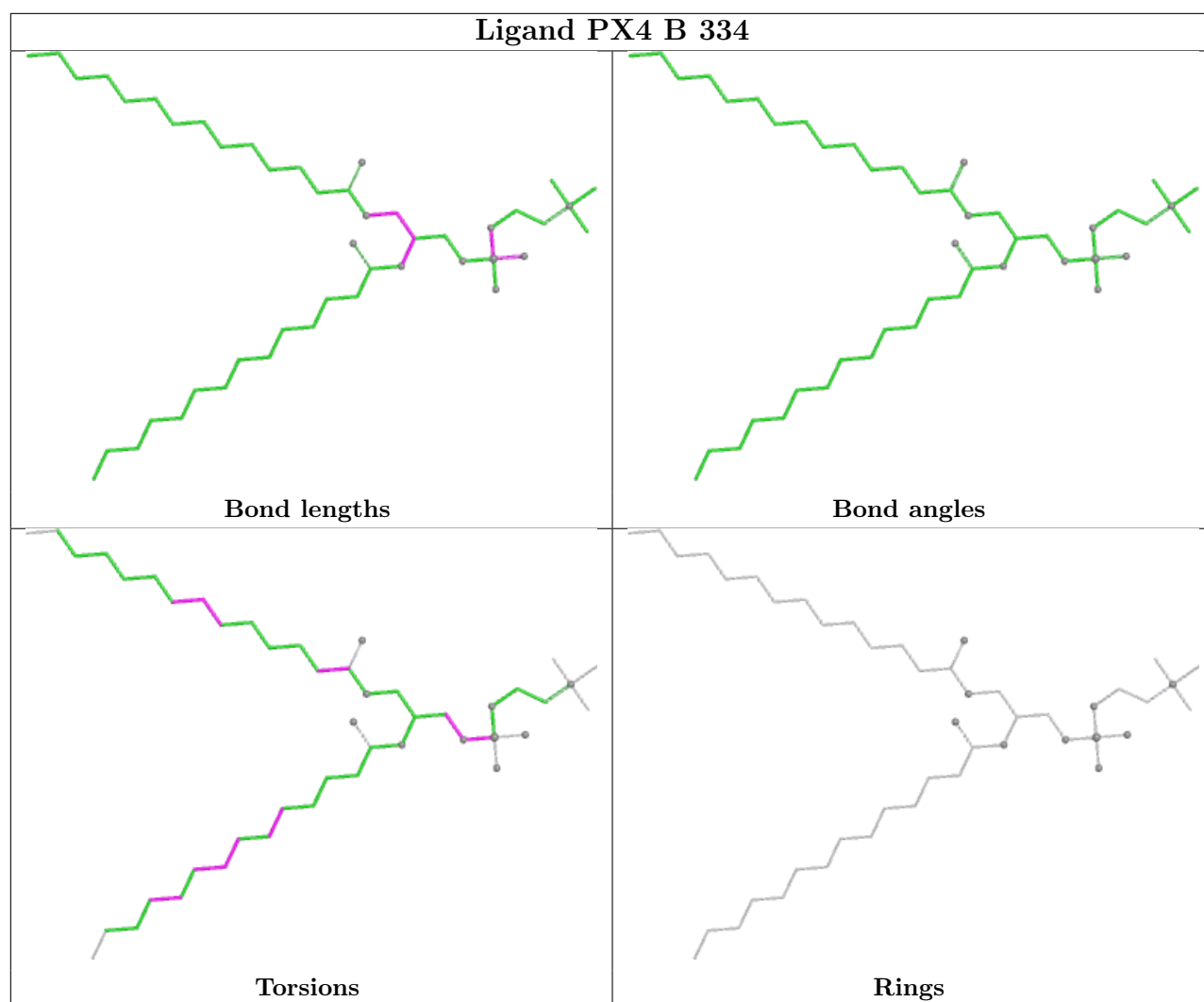


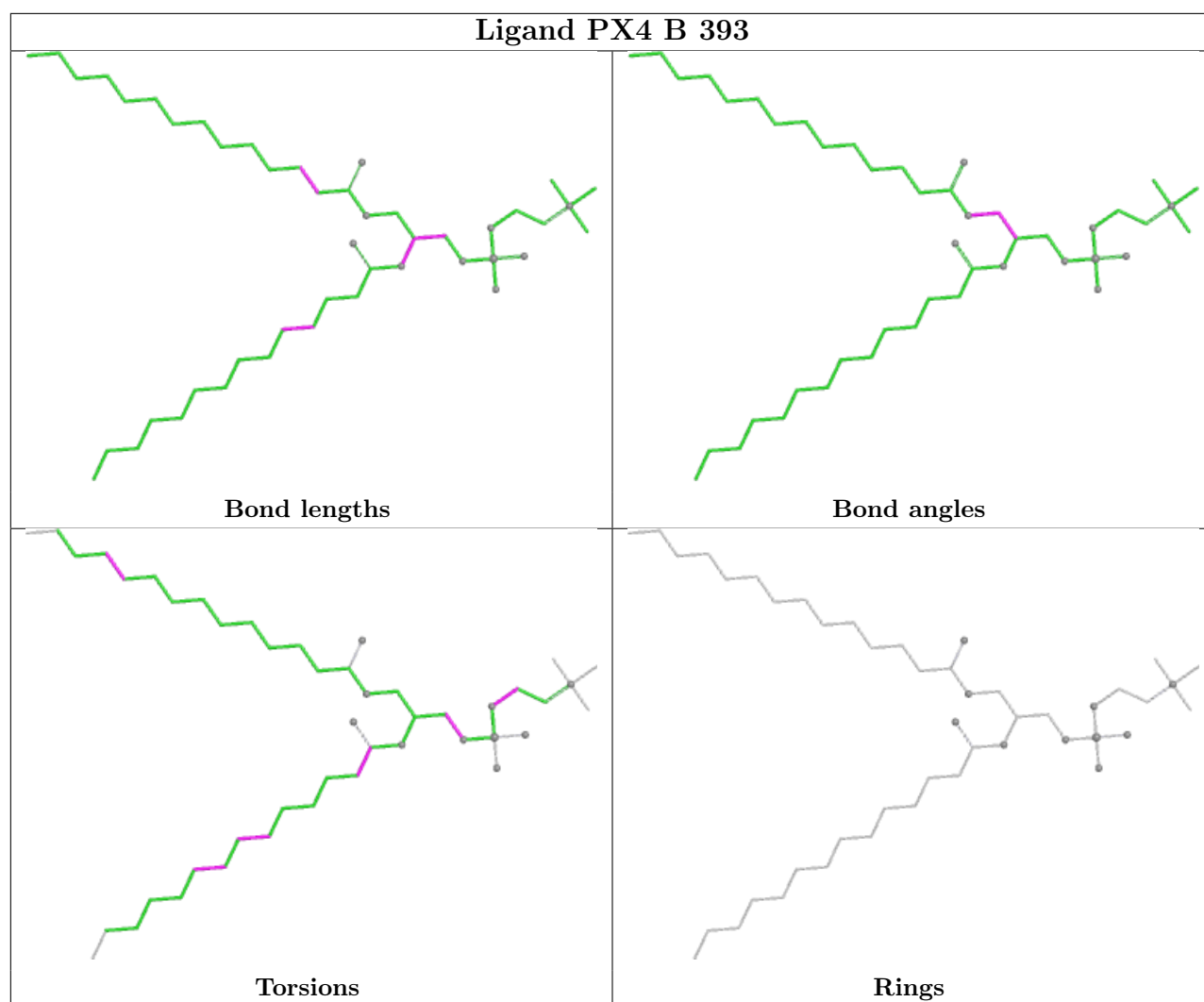


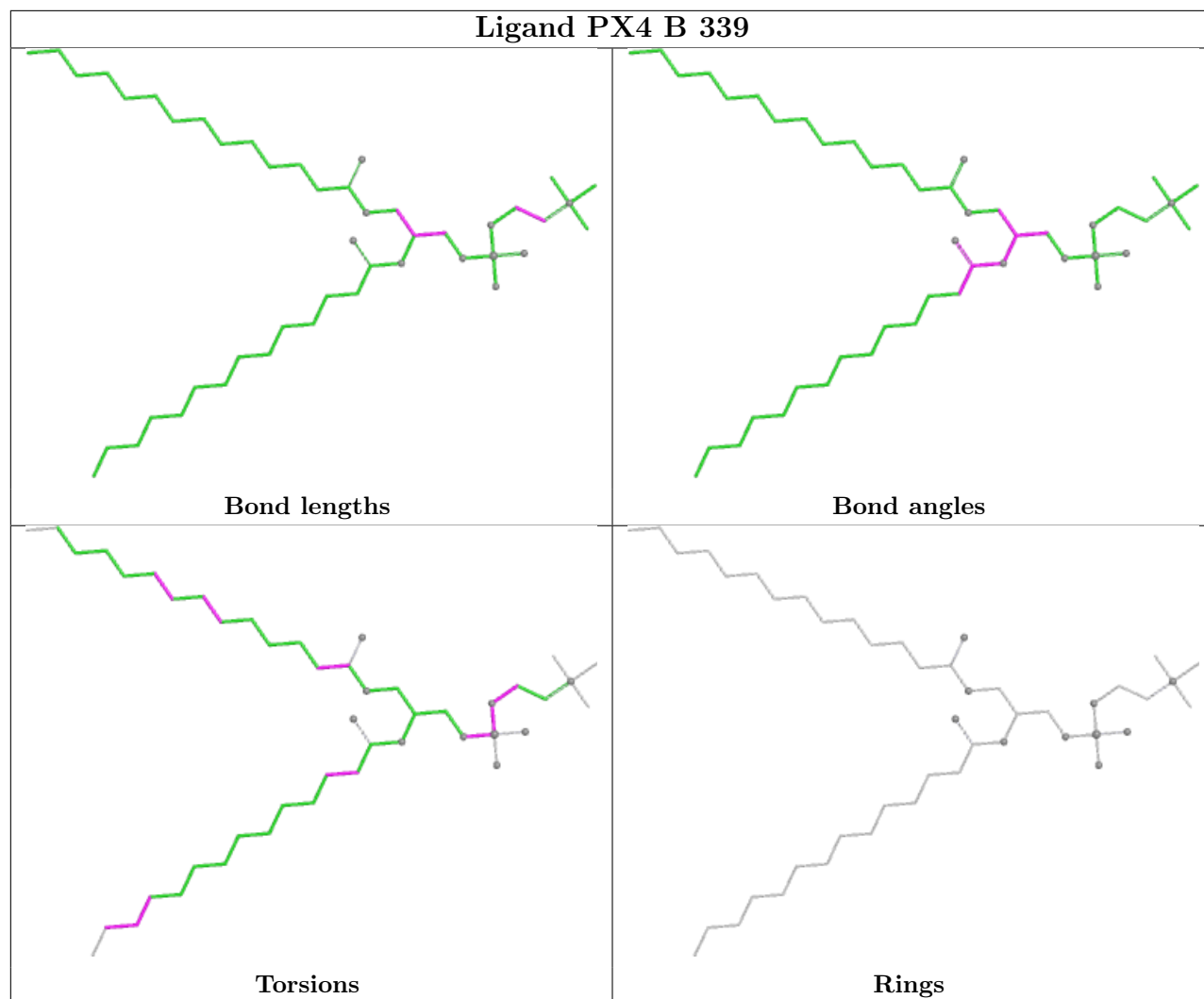


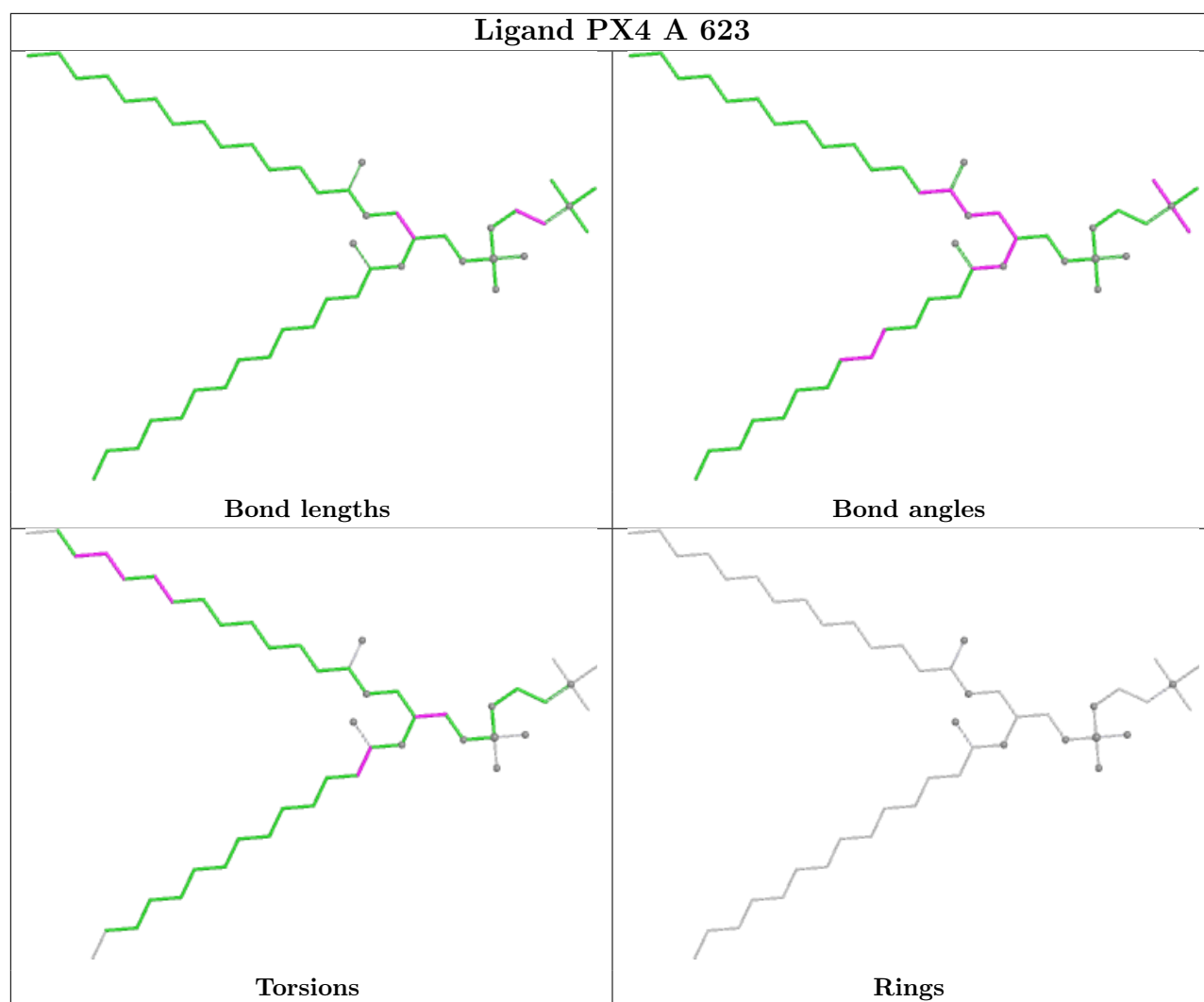


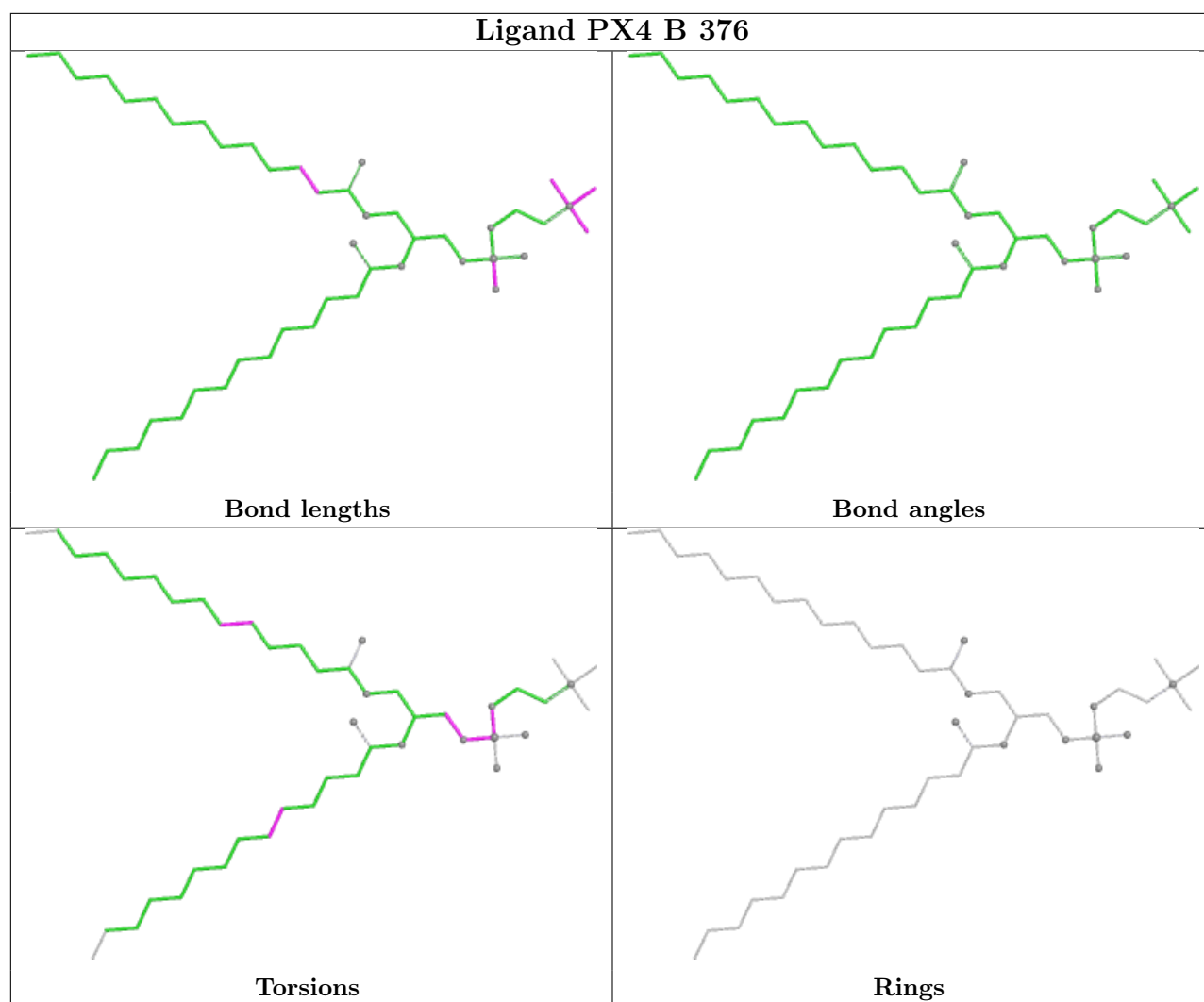


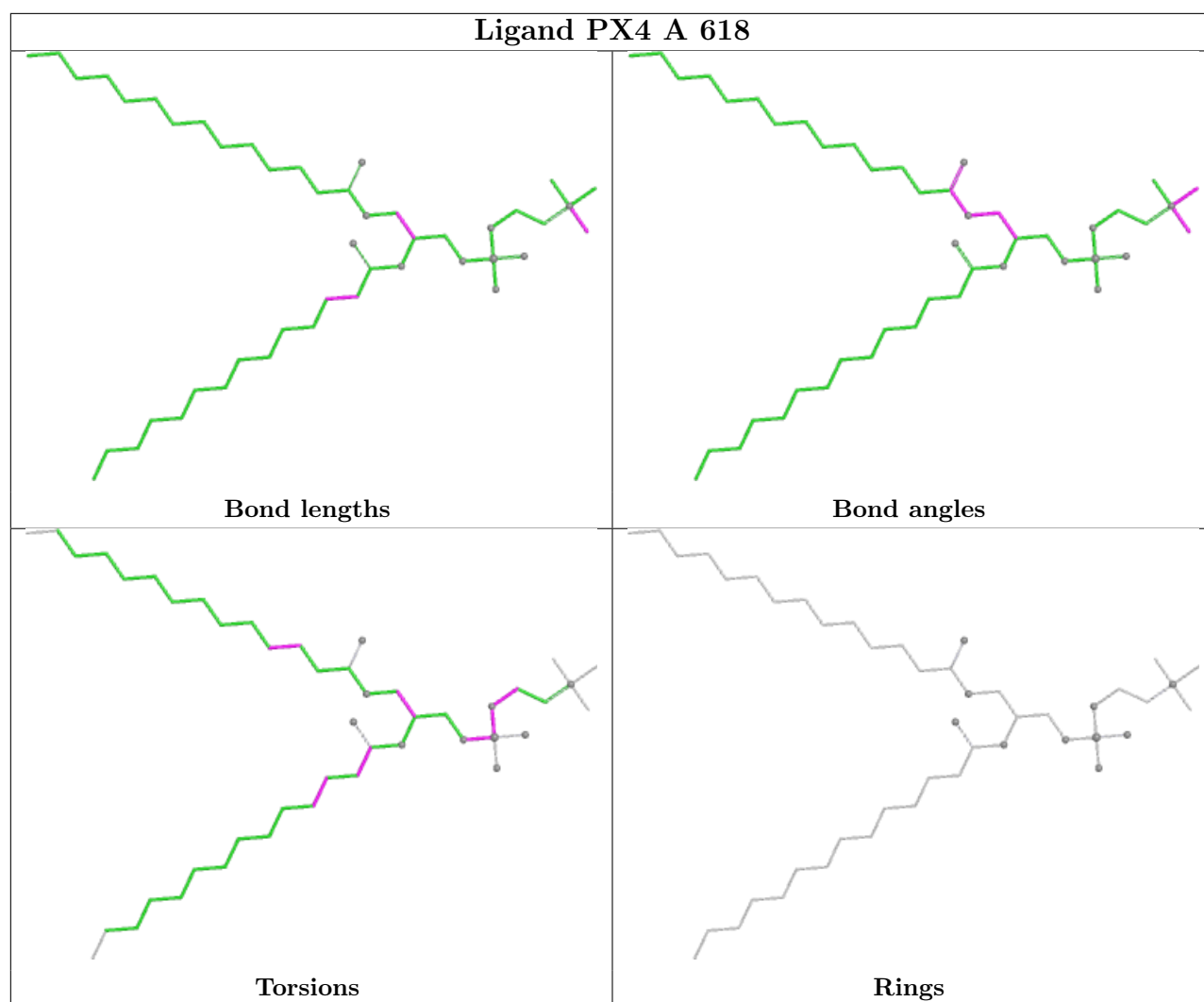


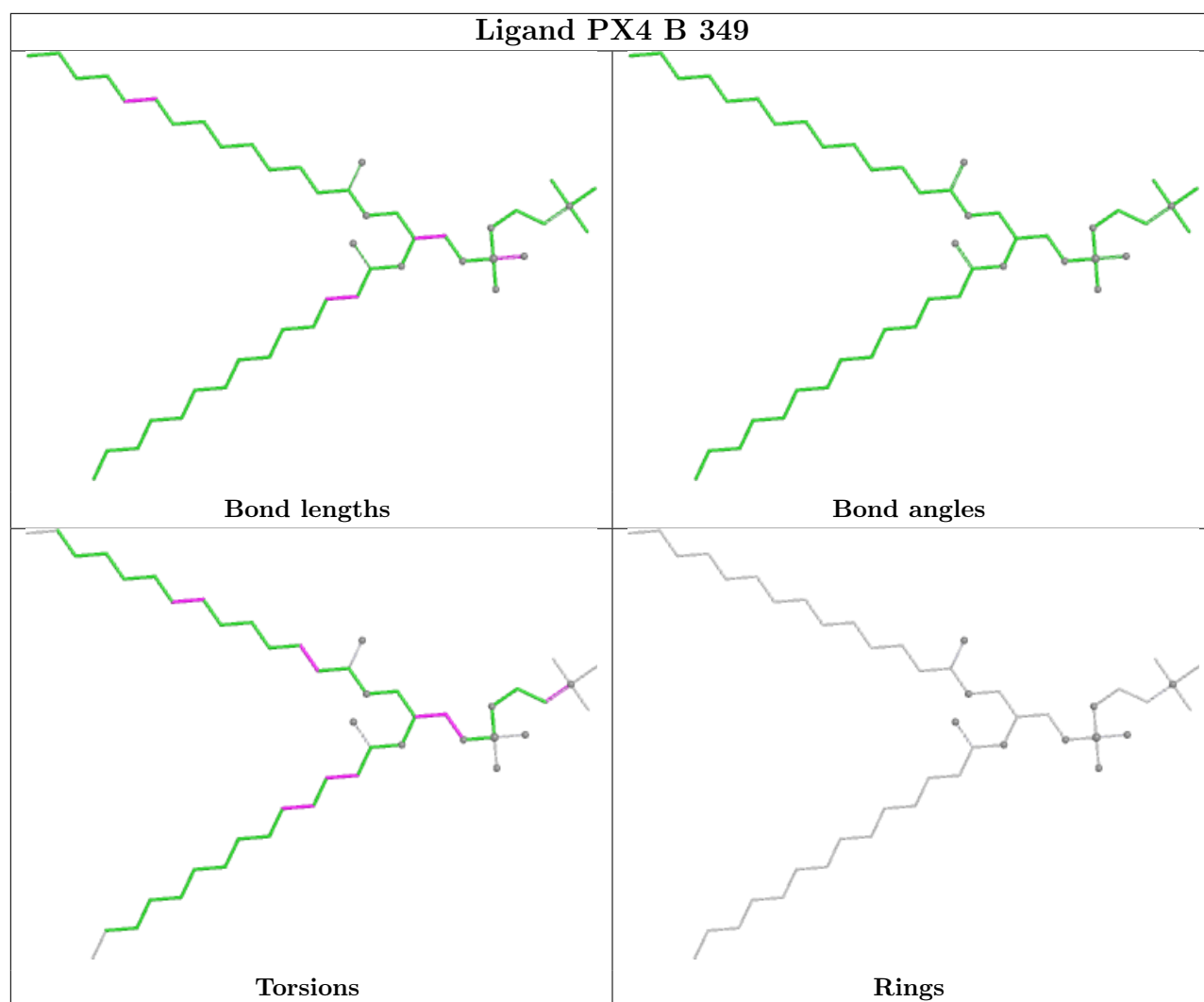


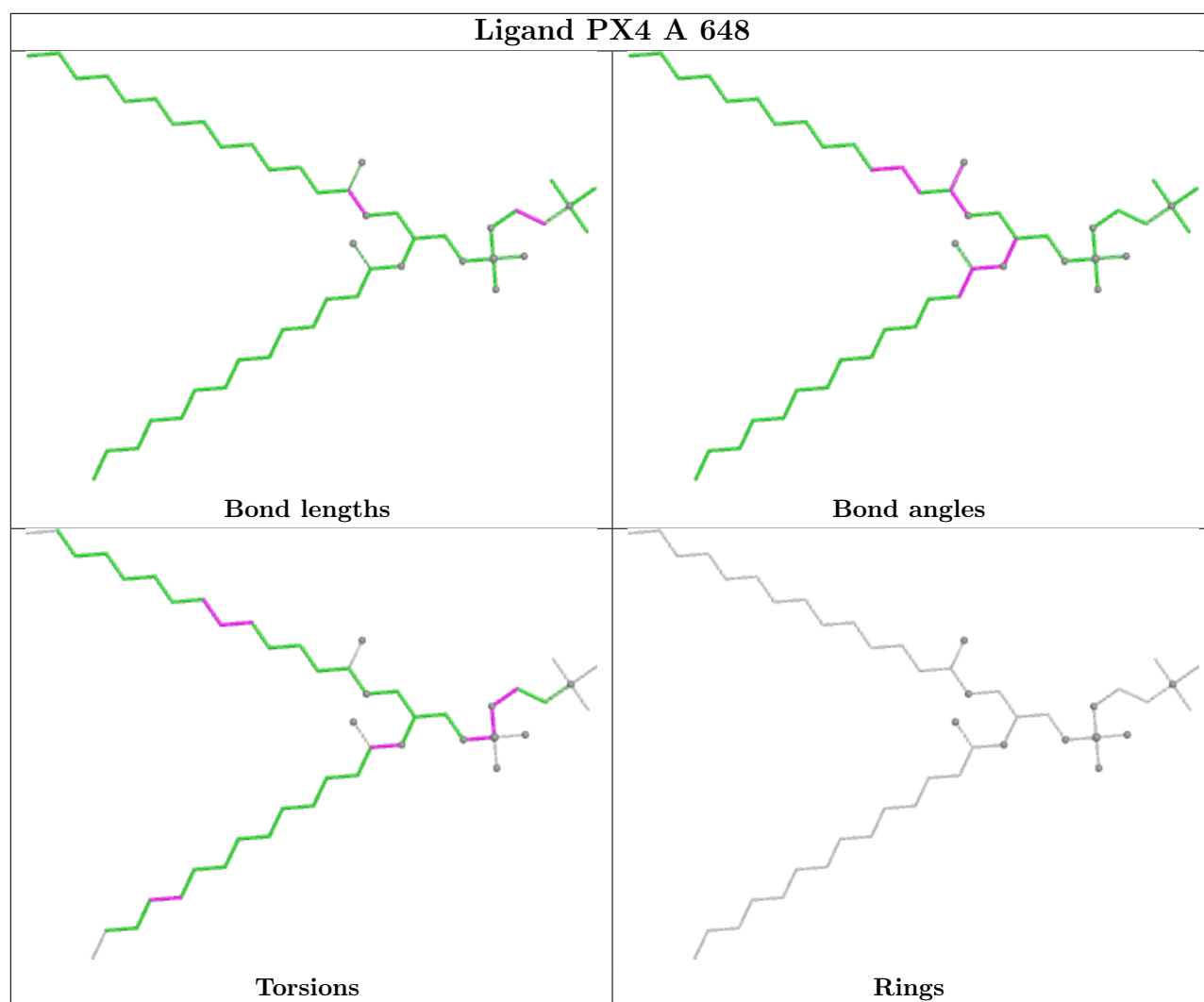


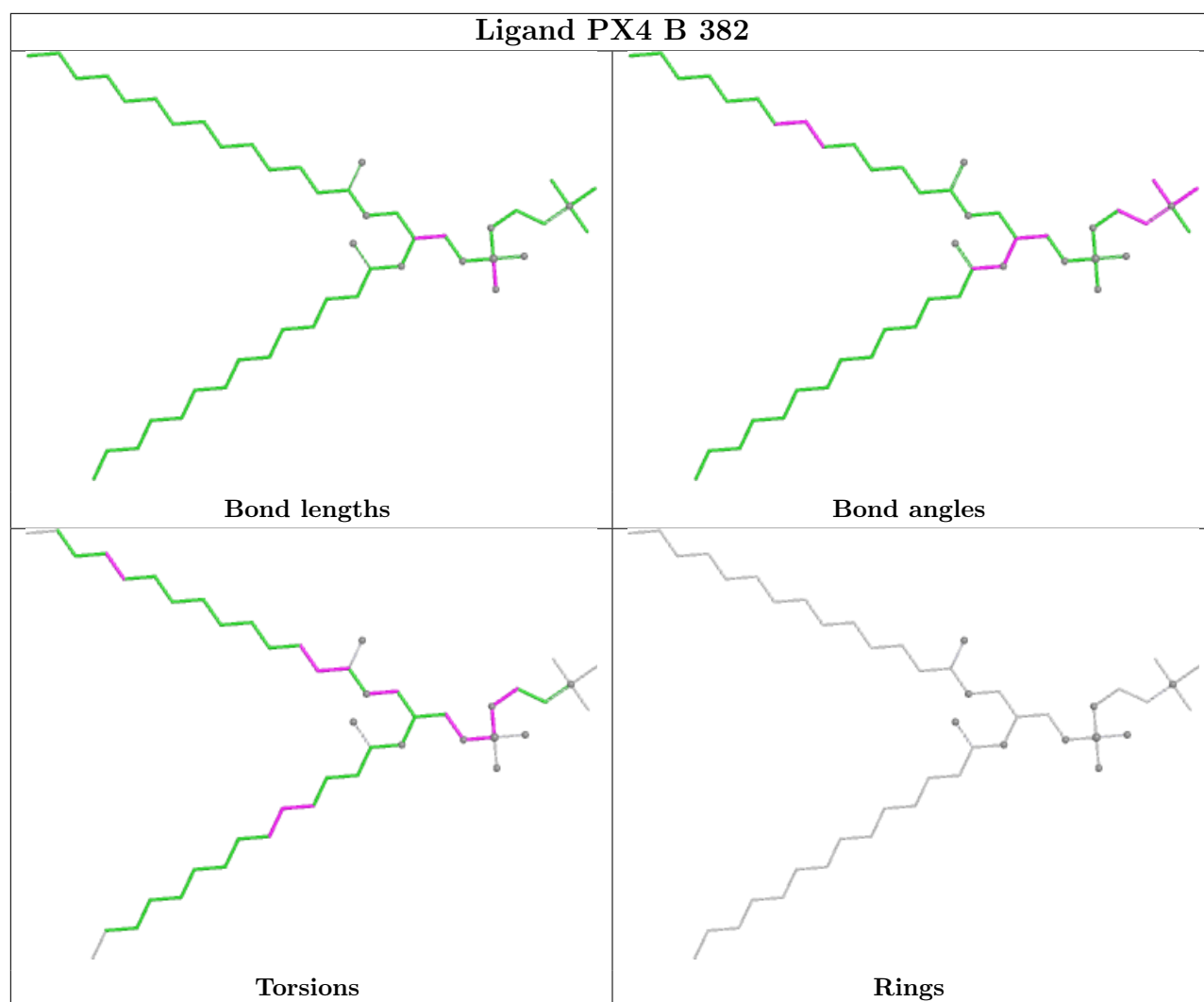


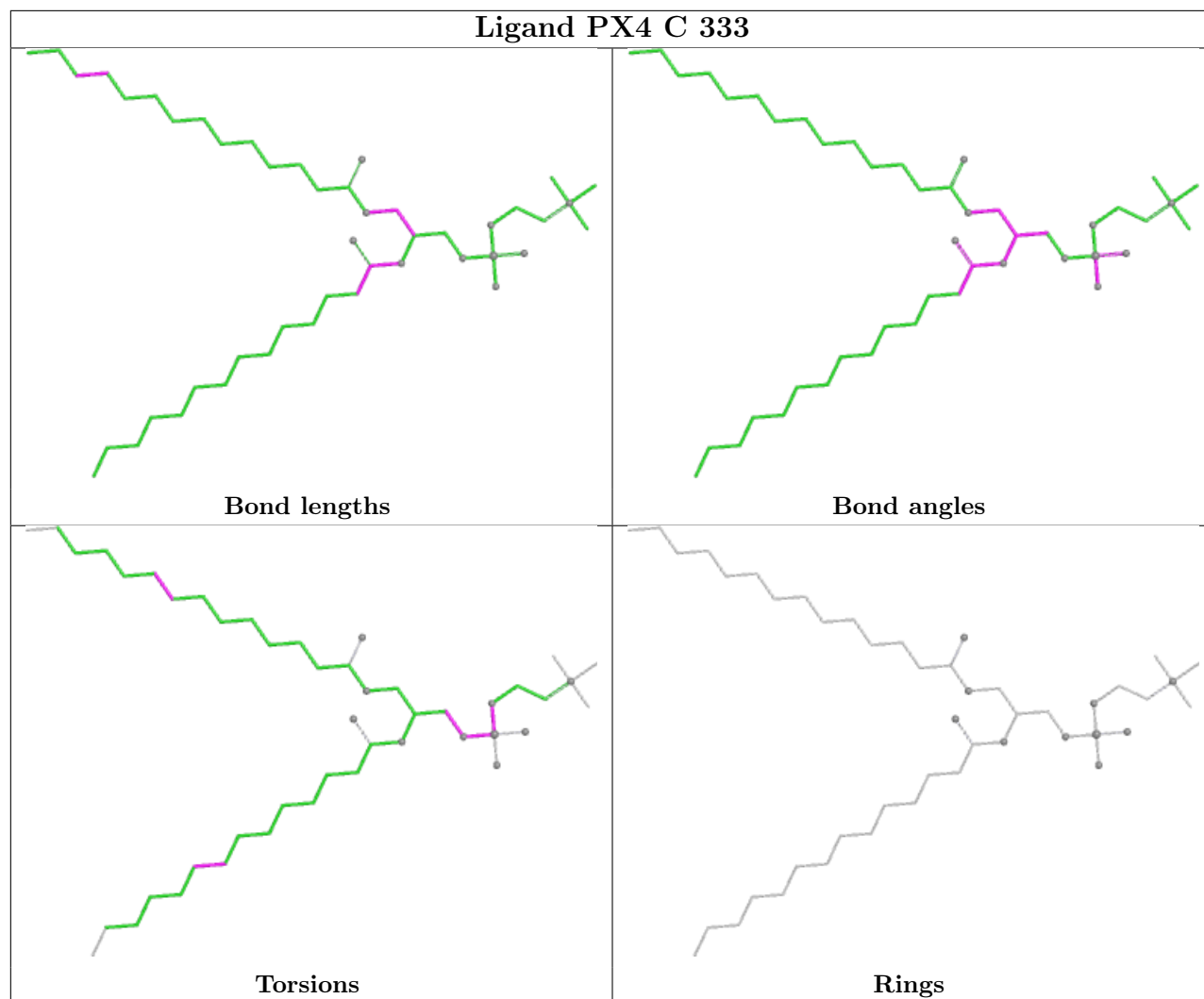


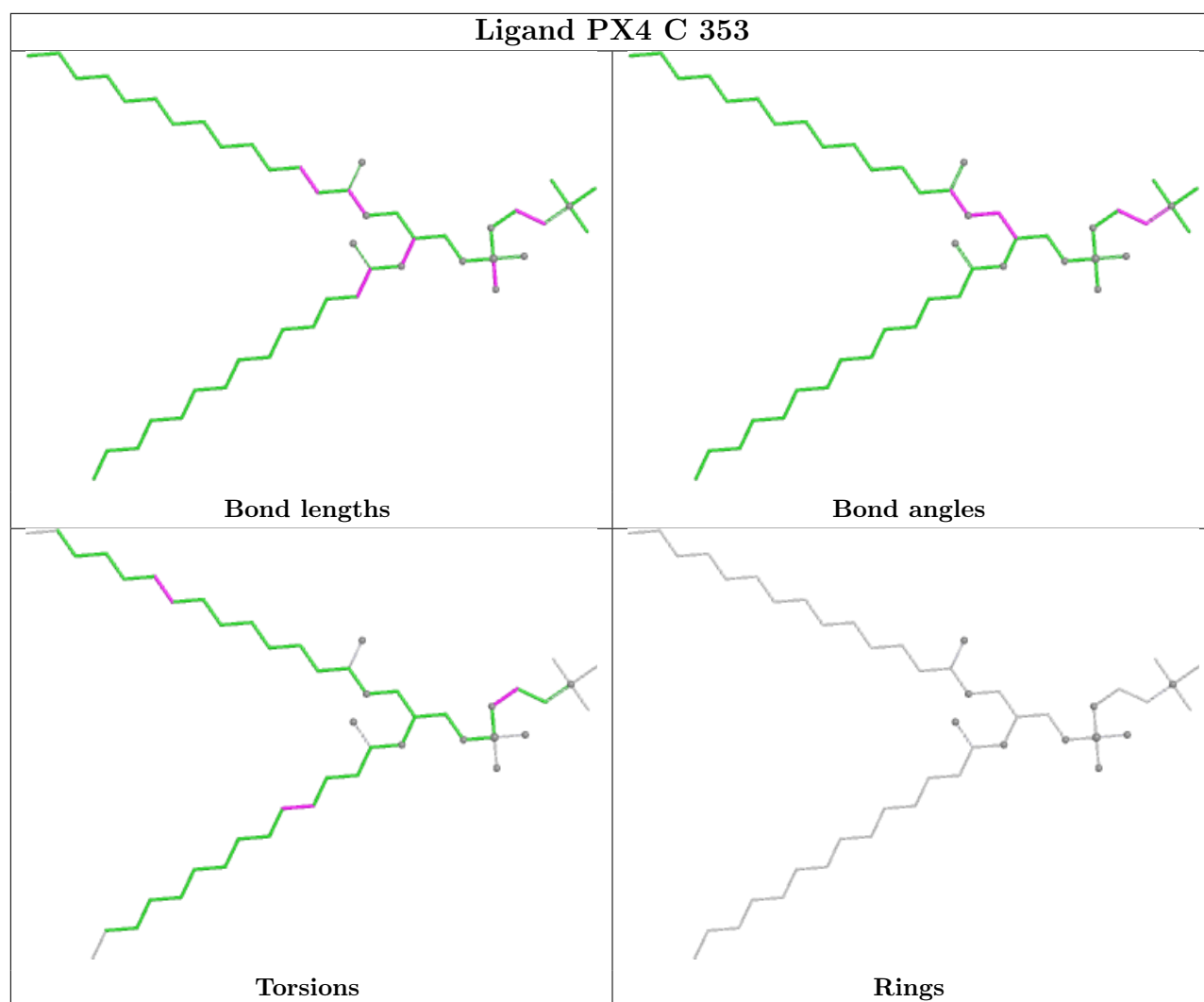


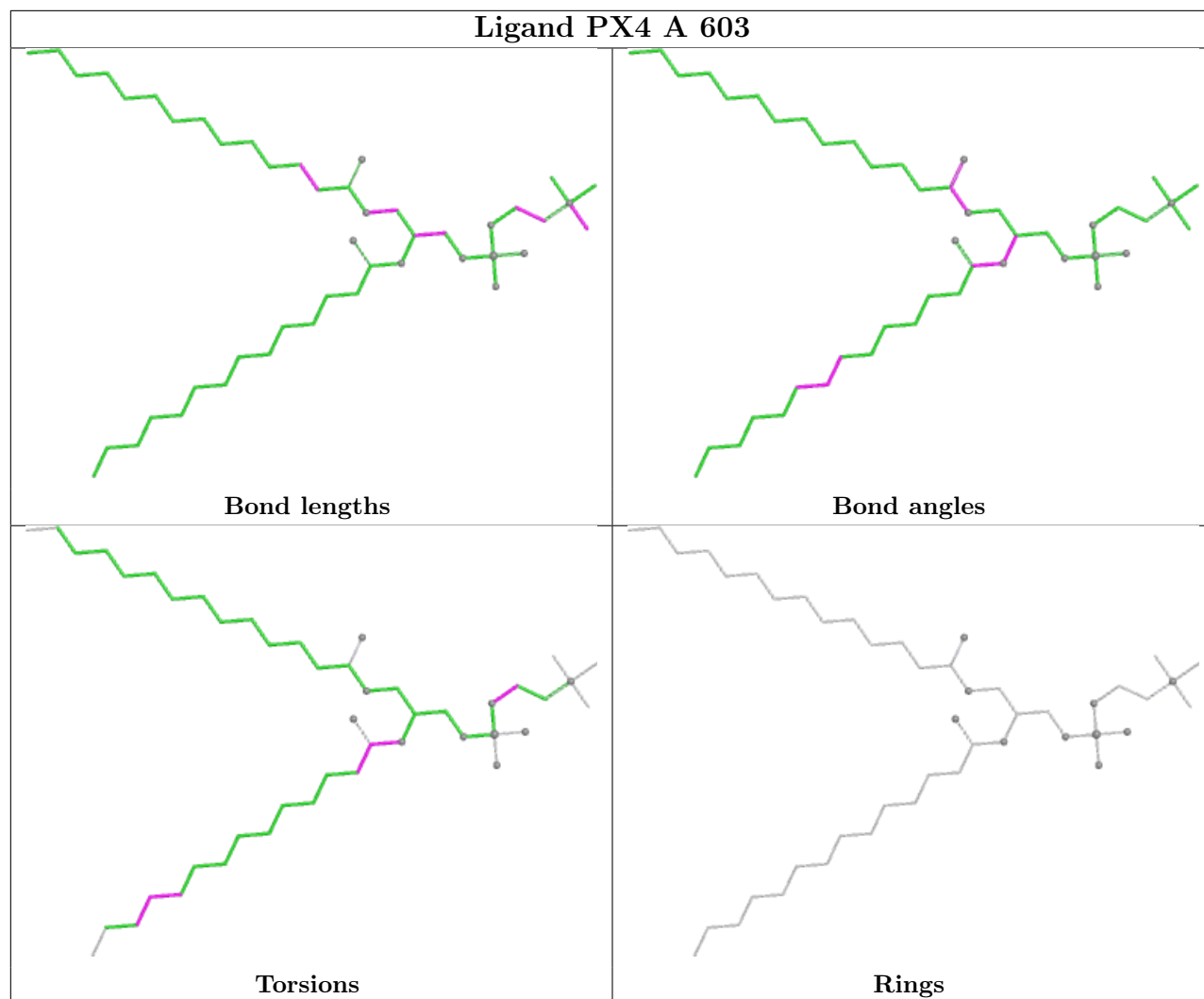


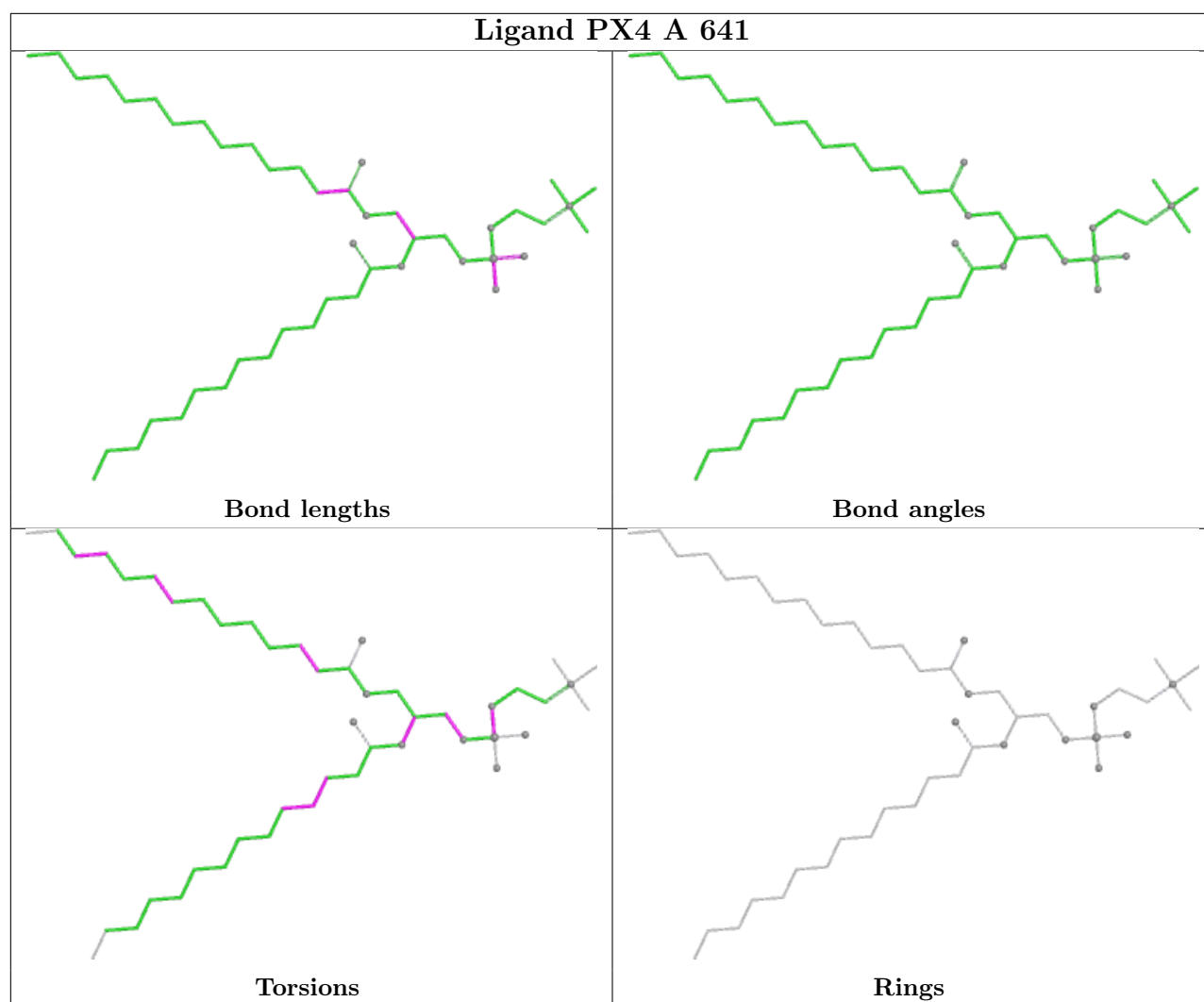


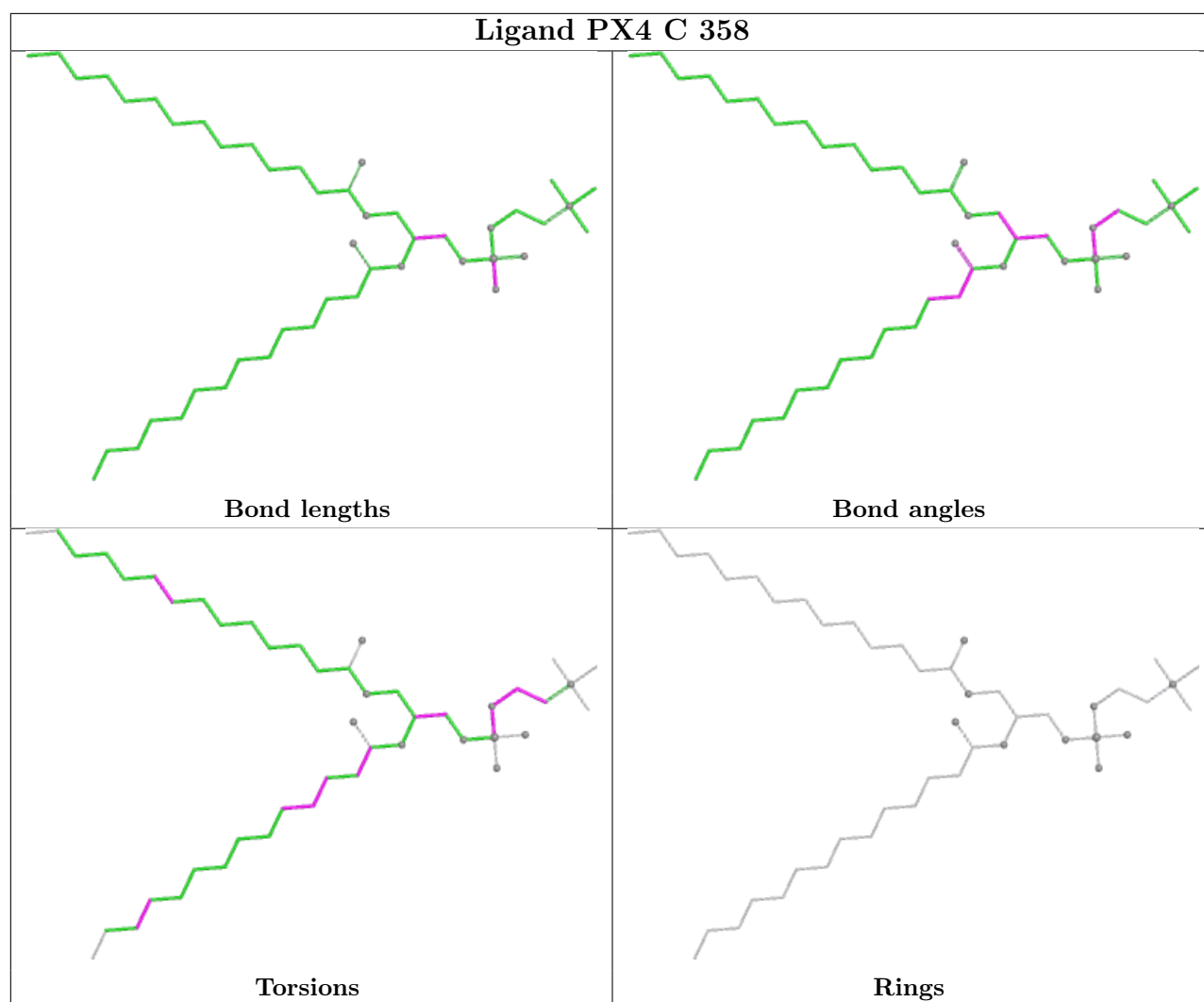


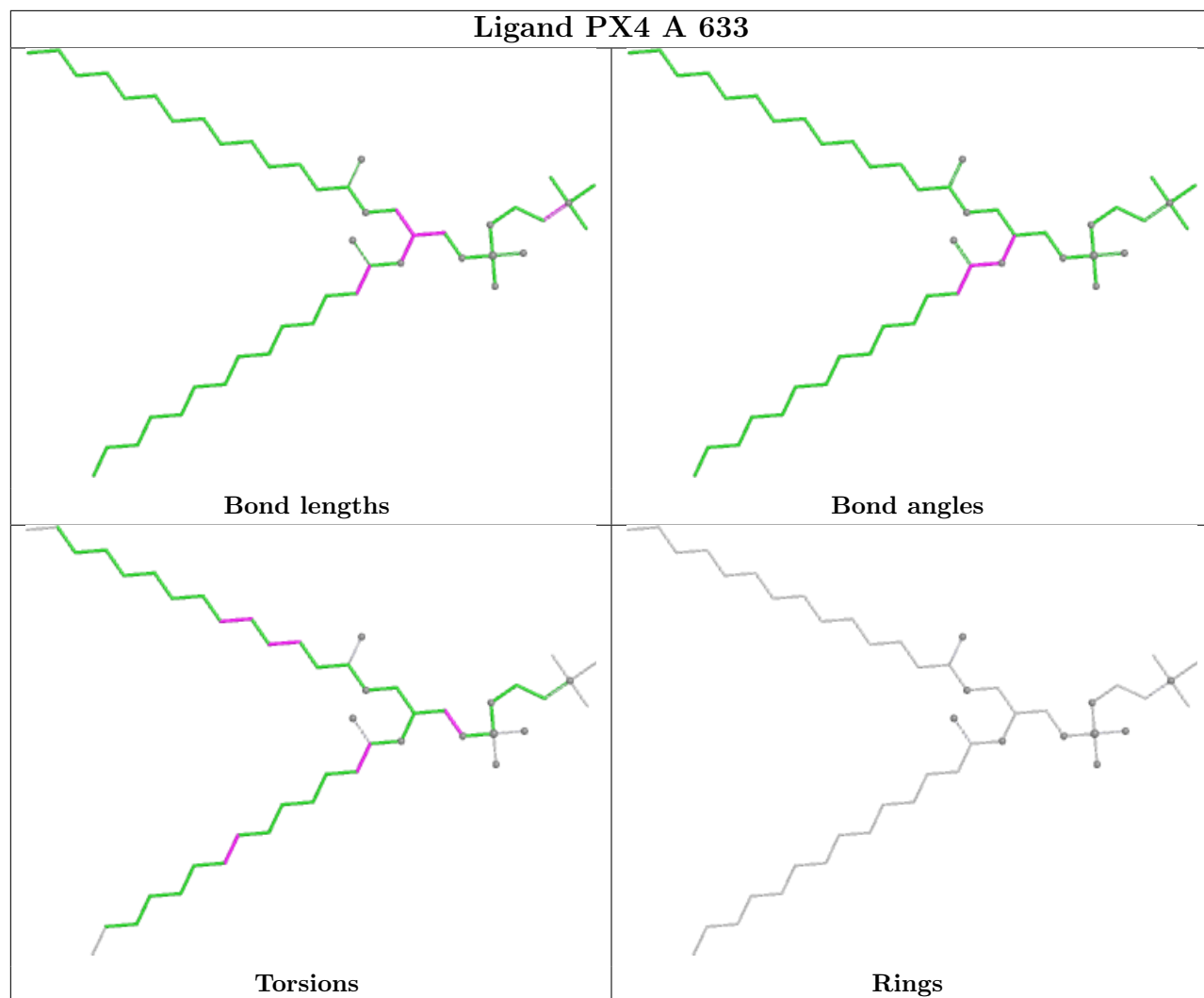


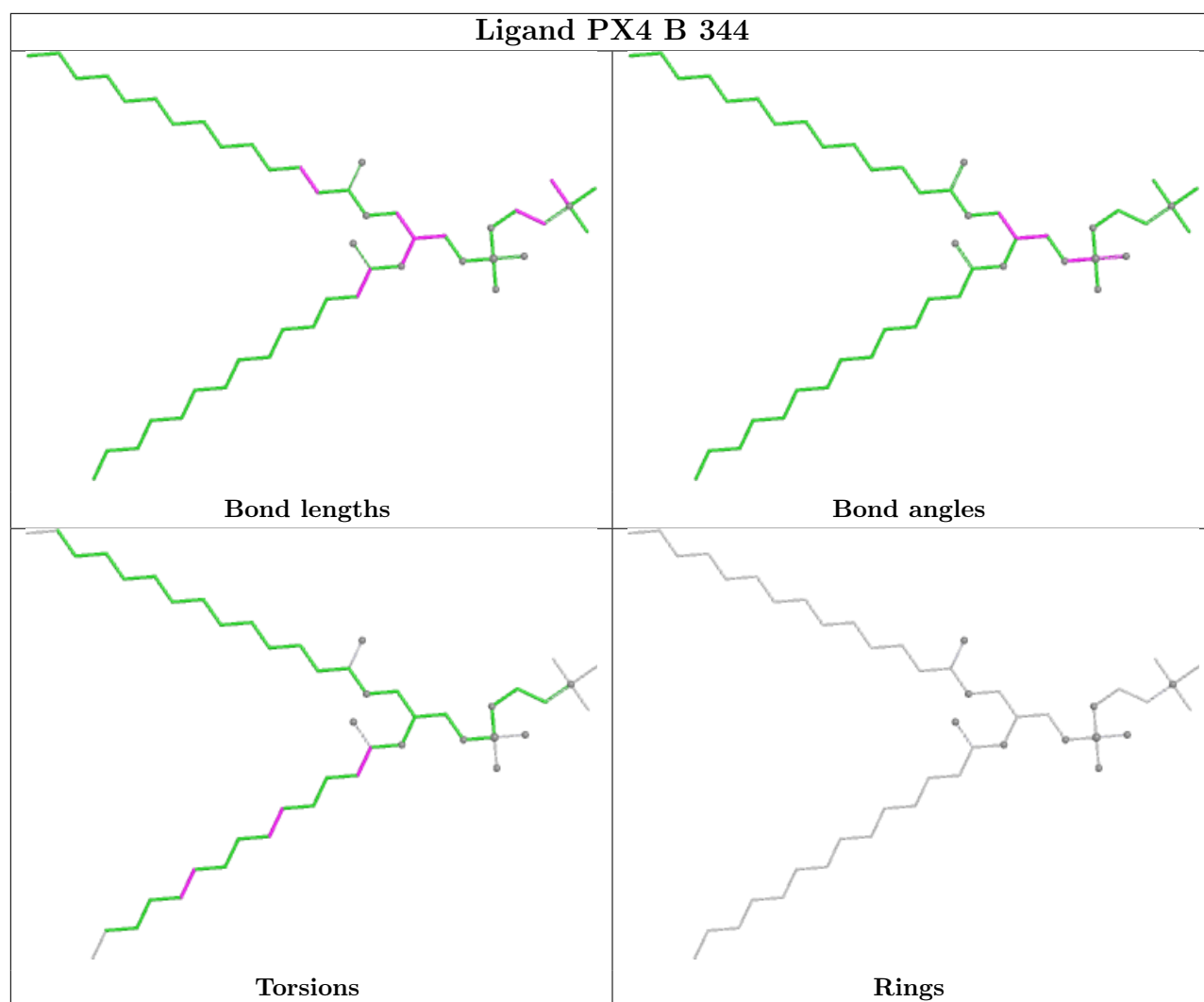


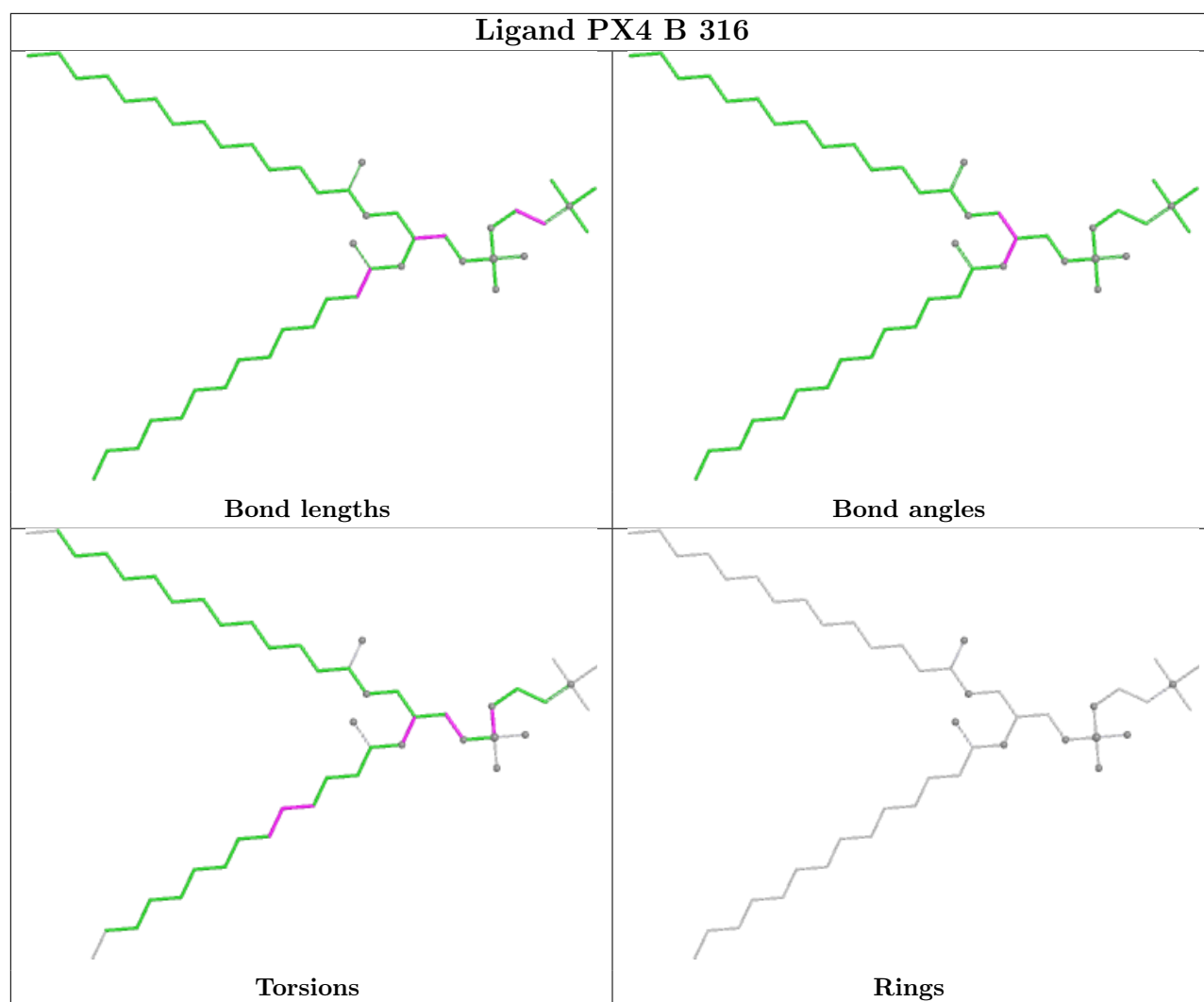


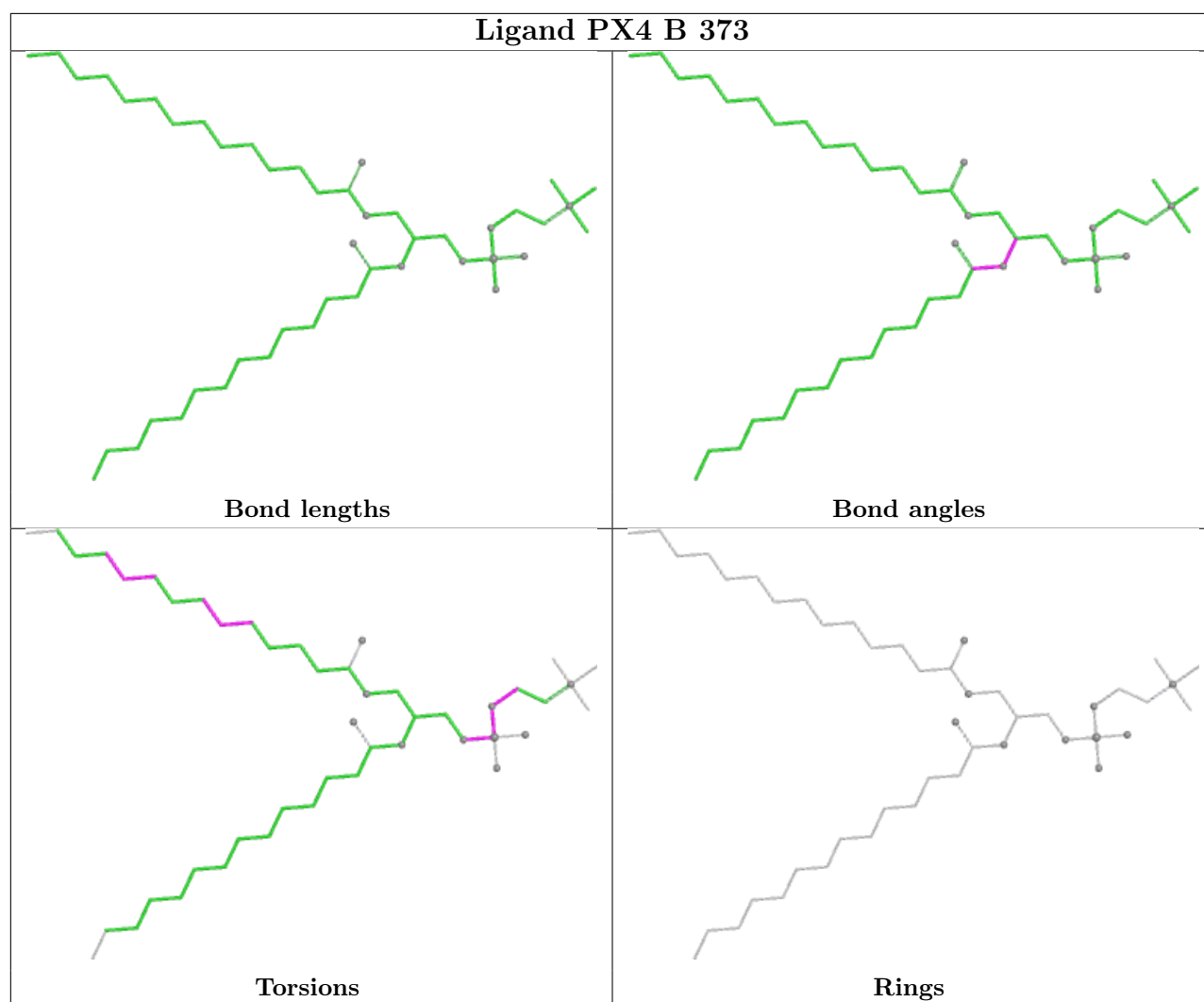


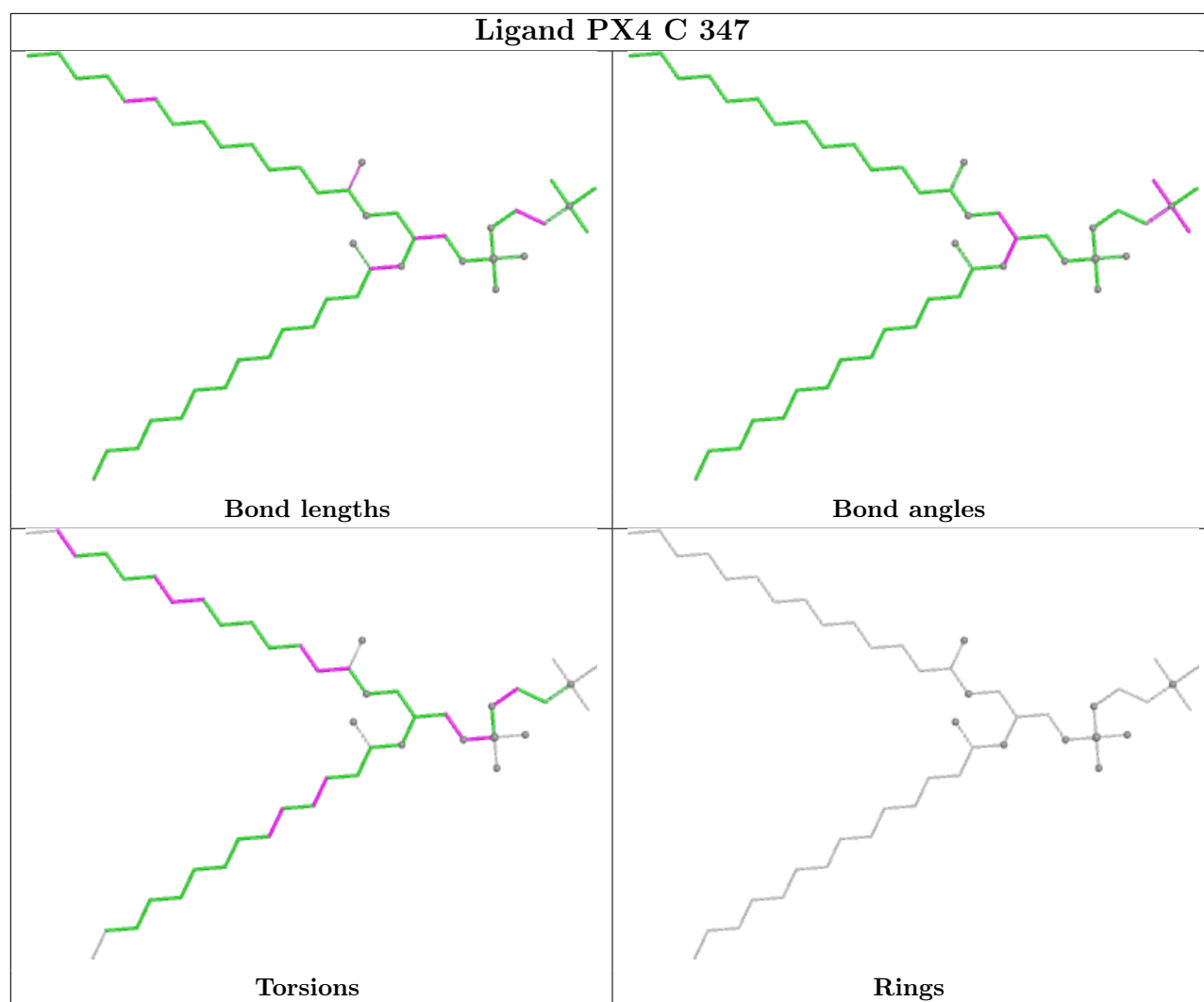


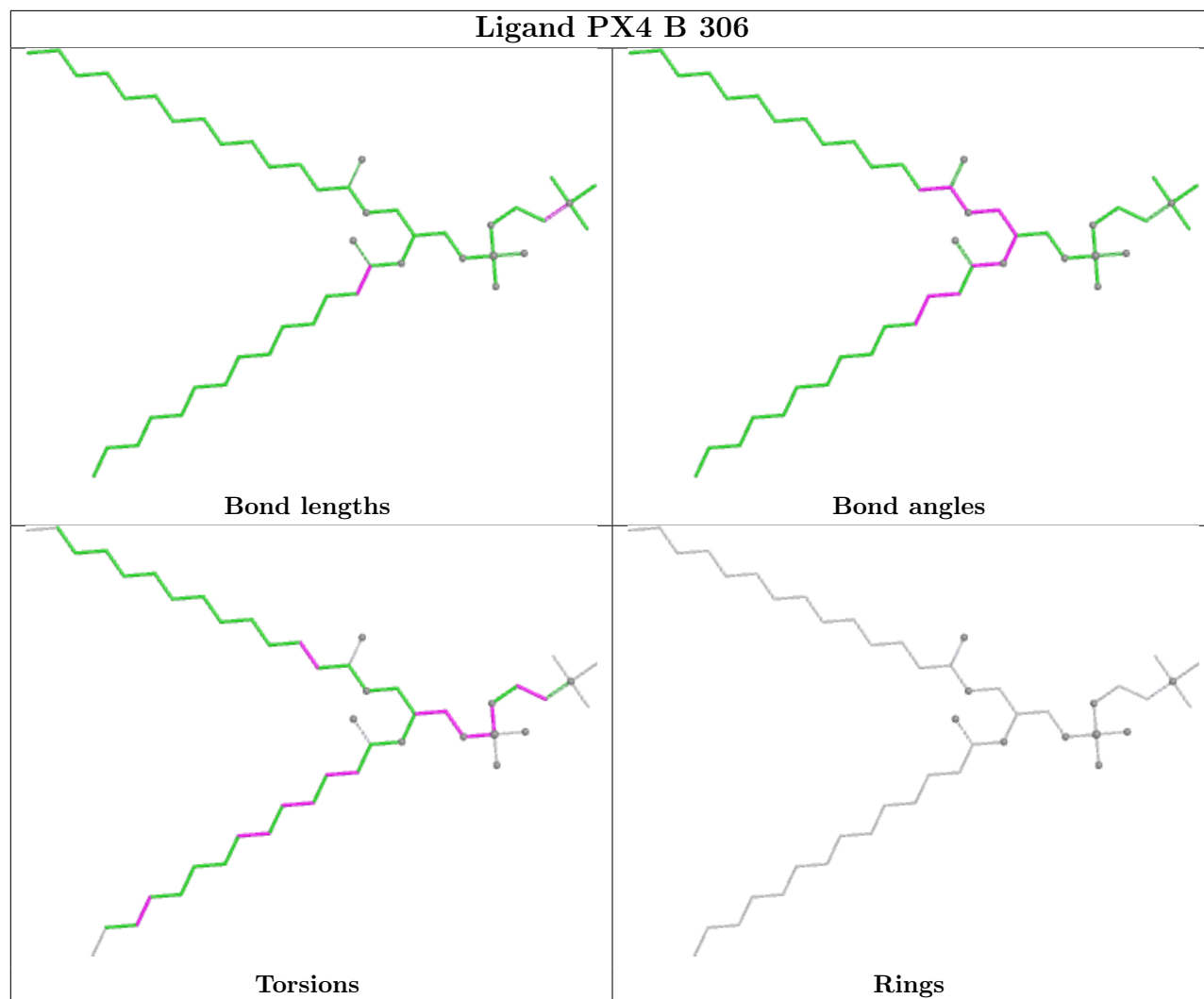


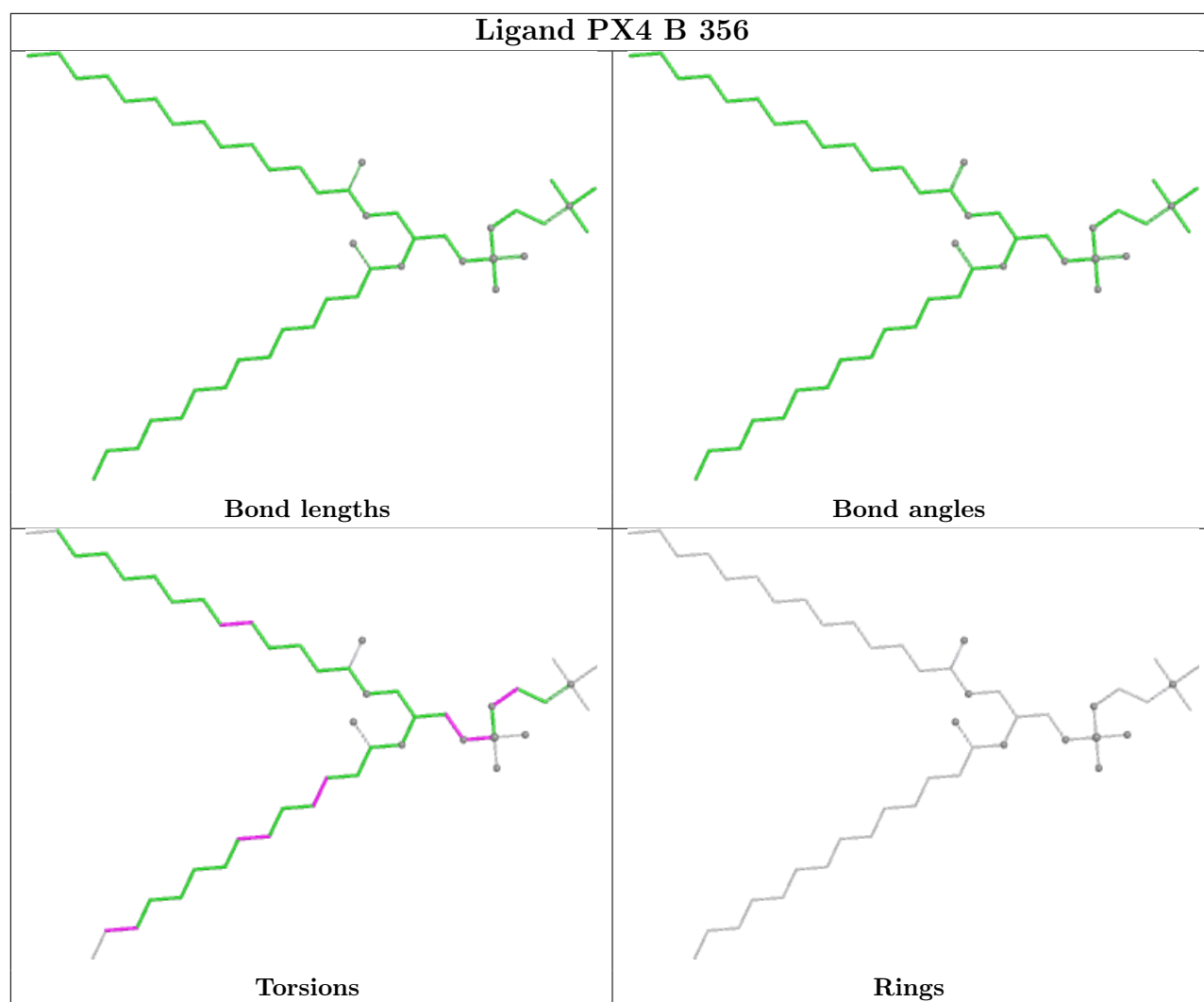


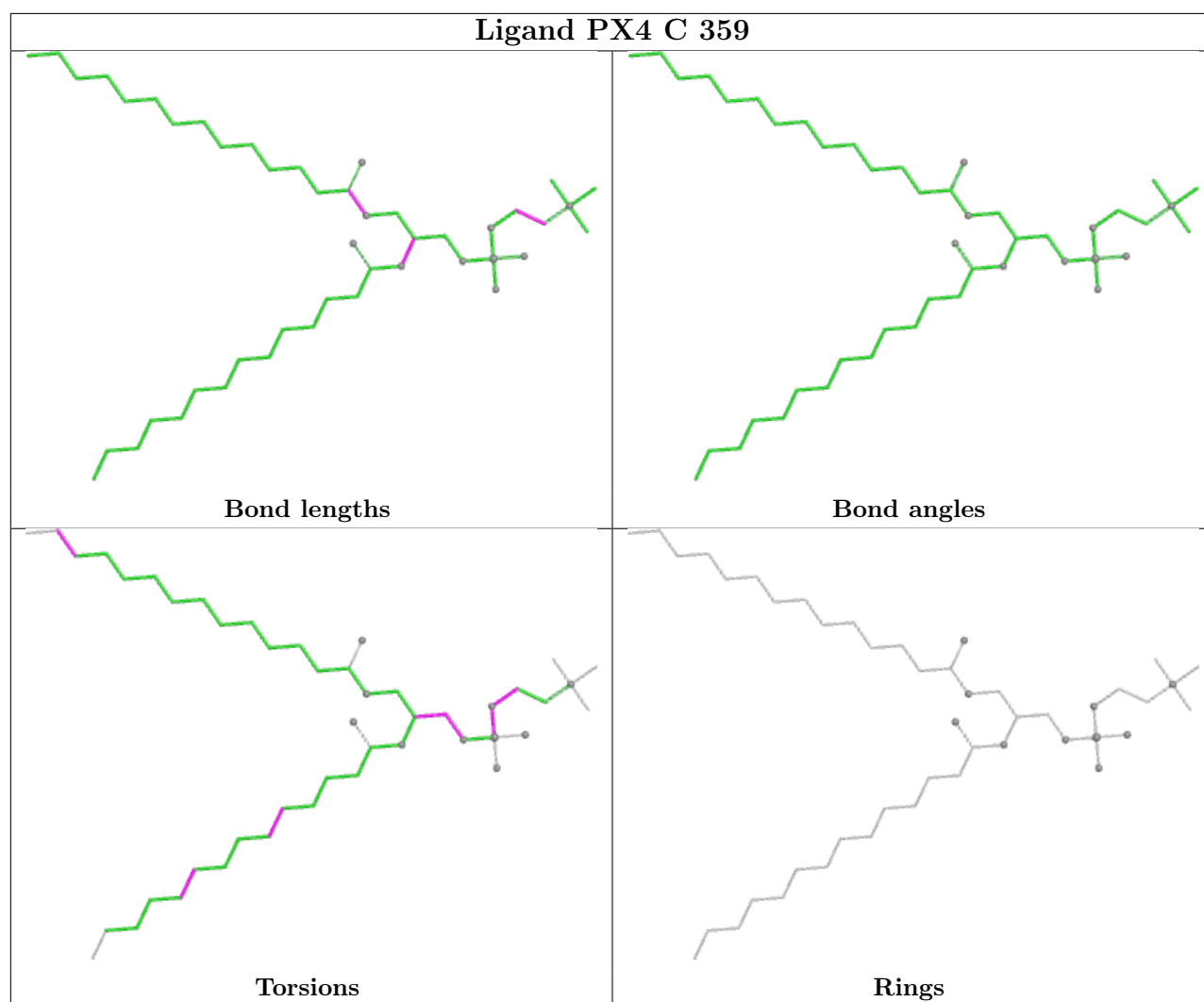


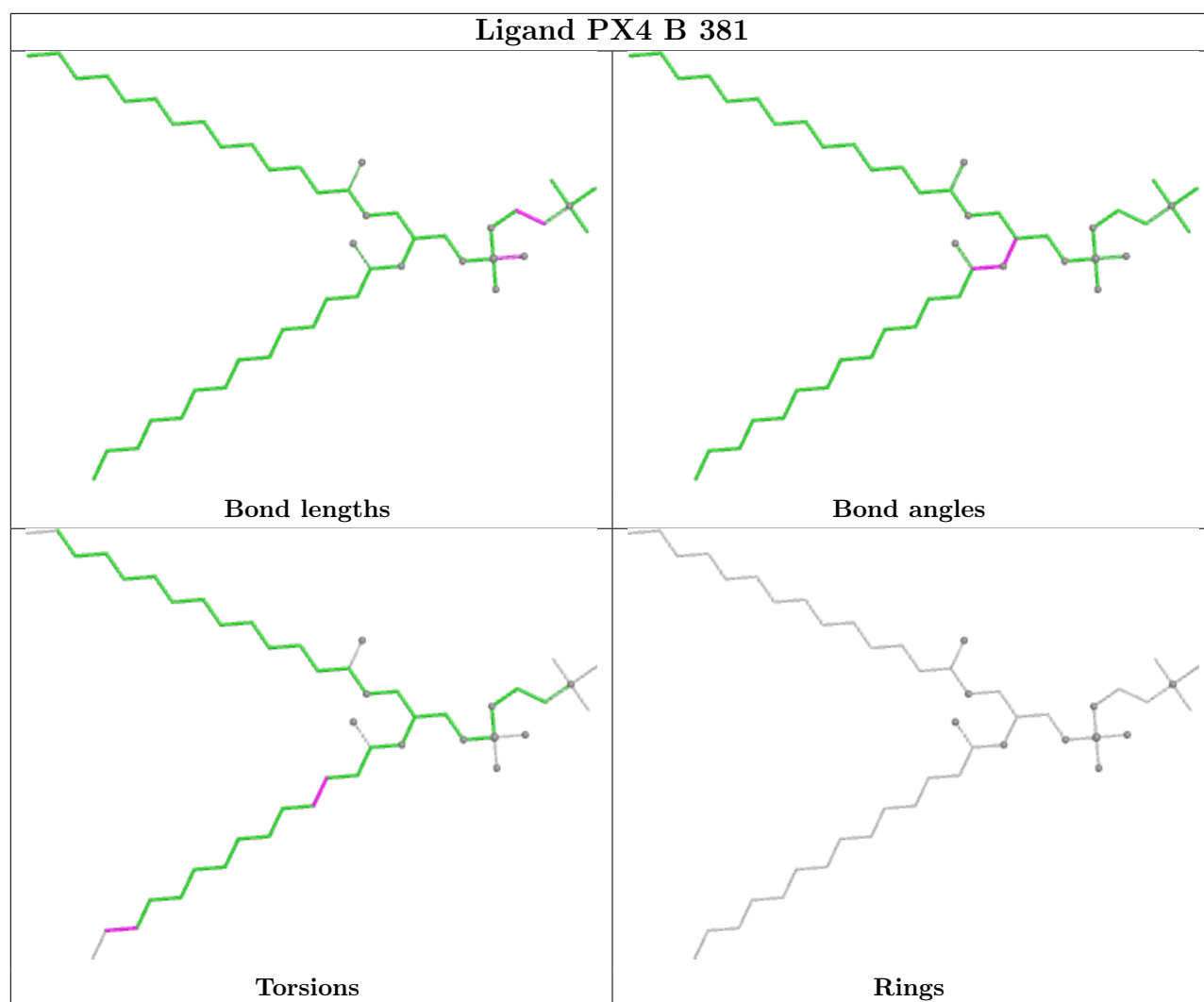


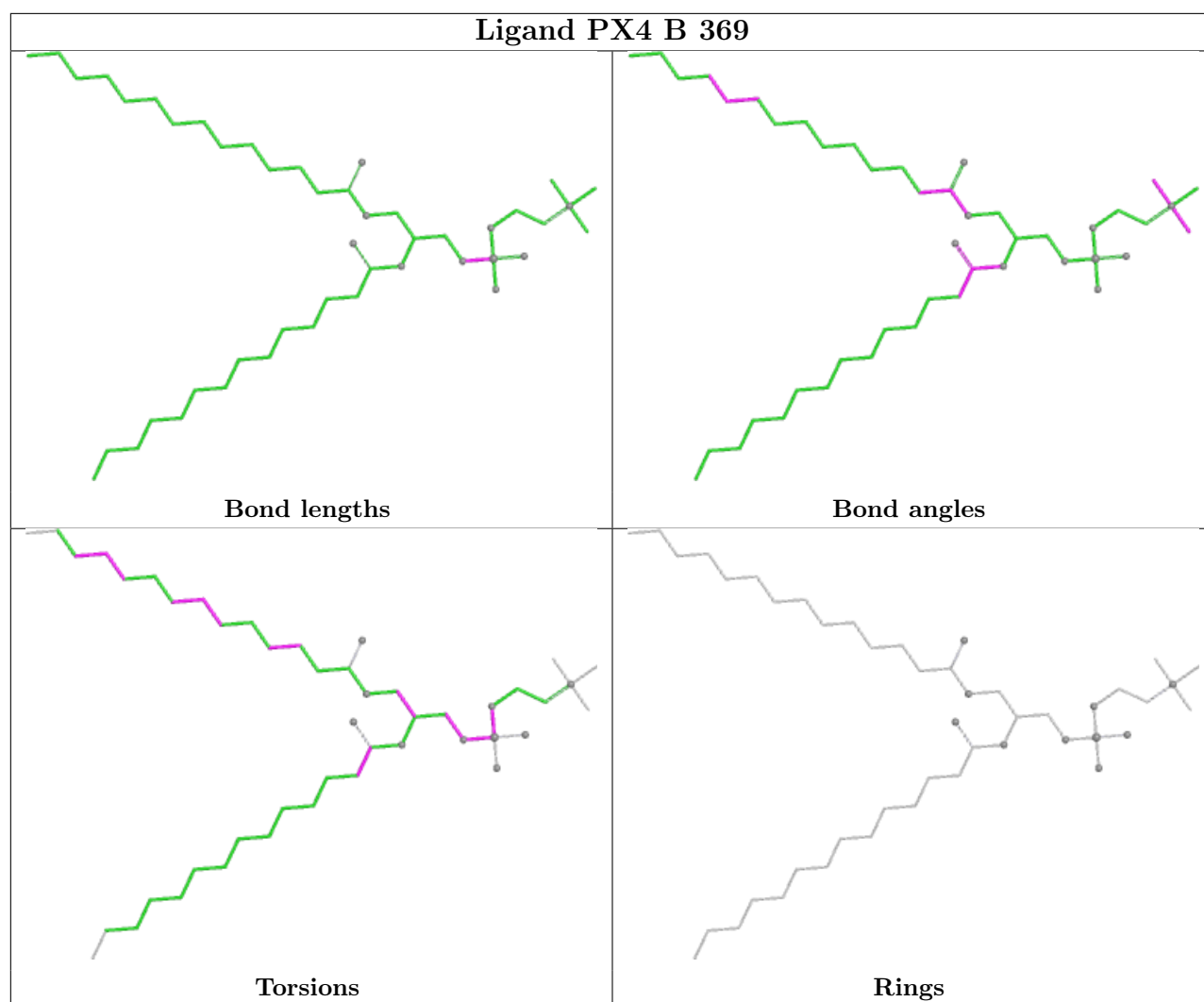


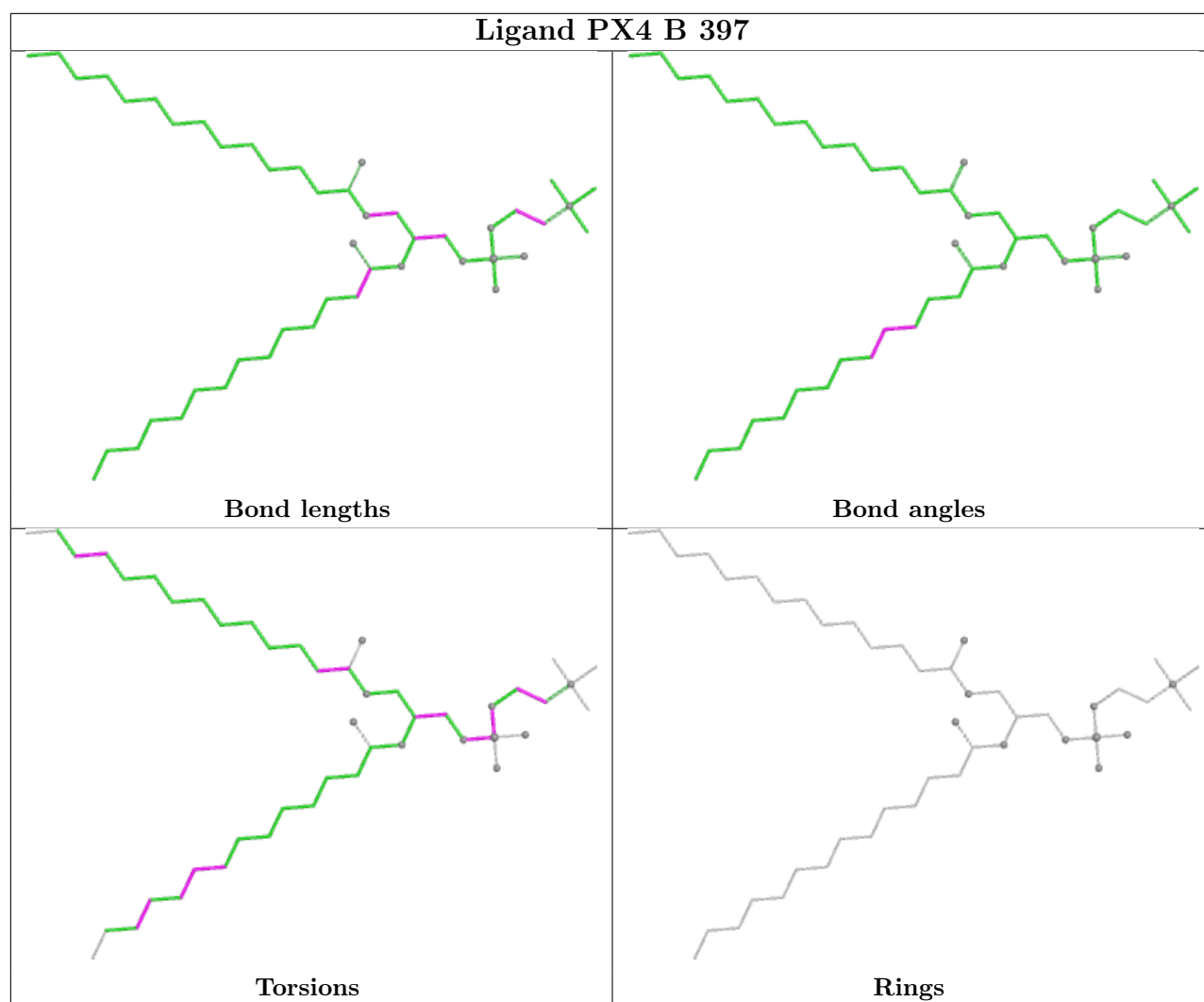












6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 4% for the well-defined parts and 4% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *Deposition_nmr_coordinates_6Aug18.txt*

7.1.1 Bookkeeping

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

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

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

| Nucleus | # values | Correction \pm precision, ppm | Suggested action |
|------------------------|----------|---------------------------------|--------------------------|
| $^{13}\text{C}_\alpha$ | 0 | — | None (insufficient data) |
| $^{13}\text{C}_\beta$ | 0 | — | None (insufficient data) |
| $^{13}\text{C}'$ | 0 | — | None (insufficient data) |
| ^{15}N | 92 | 1.12 ± 0.83 | None needed (imprecise) |

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 4%, i.e. 324 atoms were assigned a chemical shift out of a possible 8785. 0 out of 99 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | ^1H | ^{13}C | ^{15}N |
|-----------|---------------|---------------|-----------------|-----------------|
| Backbone | 184/3048 (6%) | 92/1233 (7%) | 0/1230 (0%) | 92/585 (16%) |
| Sidechain | 140/4970 (3%) | 105/3181 (3%) | 35/1554 (2%) | 0/235 (0%) |

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| | Total | ¹ H | ¹³ C | ¹⁵ N |
|----------|---------------|----------------|-----------------|-----------------|
| Aromatic | 0/767 (0%) | 0/377 (0%) | 0/364 (0%) | 0/26 (0%) |
| Overall | 324/8785 (4%) | 197/4791 (4%) | 35/3148 (1%) | 92/846 (11%) |

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

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

7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots [i](#)

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

Random coil index (RCI) for chain A:

