



Full wwPDB NMR Structure Validation Report ⓘ

Jun 23, 2024 – 04:12 AM EDT

PDB ID : 6CC9
BMRB ID : 30400
Title : NMR data-driven model of GTPase KRas-GMPPNP:Cmpd2 complex tethered to a nanodisc
Authors : Fang, Z.; Marshall, C.B.; Nishikawa, T.; Gossert, A.D.; Jansen, J.M.; Jahnke, W.; Ikura, M.
Deposited on : 2018-02-06

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

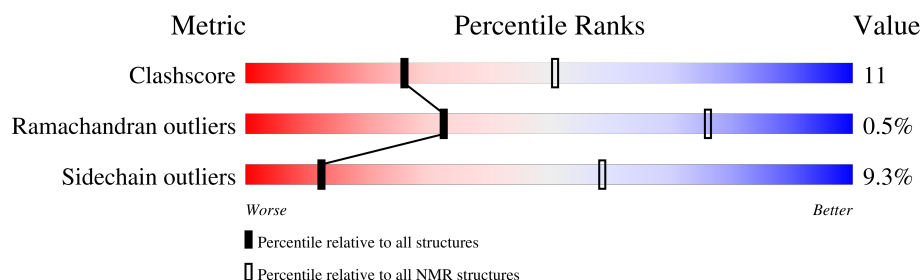
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 3%.

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 | 200 | 68% 10% 20% . |
| 1 | C | 200 | 86% 12% .. |
| 2 | B | 187 | 81% 10% 7% . |

2 Ensemble composition and analysis

This entry contains 10 models. Model 8 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:239-A:395, C:401-C:596 (353) | 0.44 | 8 |
| 2 | B:2-B:172 (171) | 0.88 | 8 |

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 2 clusters and 2 single-model clusters were found.

| Cluster number | Models |
|-----------------------|------------------|
| 1 | 2, 3, 6, 7, 8, 9 |
| 2 | 4, 10 |
| Single-model clusters | 1; 5 |

3 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9535 atoms, of which 429 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Apolipoprotein A-I.

| Mol | Chain | Residues | Atoms | | | | | | Trace |
|-----|-------|----------|-------|------|----|-----|-----|---|-------|
| 1 | A | 198 | Total | C | H | N | O | S | 0 |
| | | | 1645 | 1019 | 22 | 287 | 314 | 3 | |
| 1 | C | 198 | Total | C | H | N | O | S | 0 |
| | | | 1646 | 1019 | 22 | 287 | 315 | 3 | |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| A | 199 | GLY | - | expression tag | UNP P02647 |
| A | 200 | PRO | - | expression tag | UNP P02647 |
| C | 397 | GLY | - | expression tag | UNP P02647 |
| C | 398 | PRO | - | expression tag | UNP P02647 |

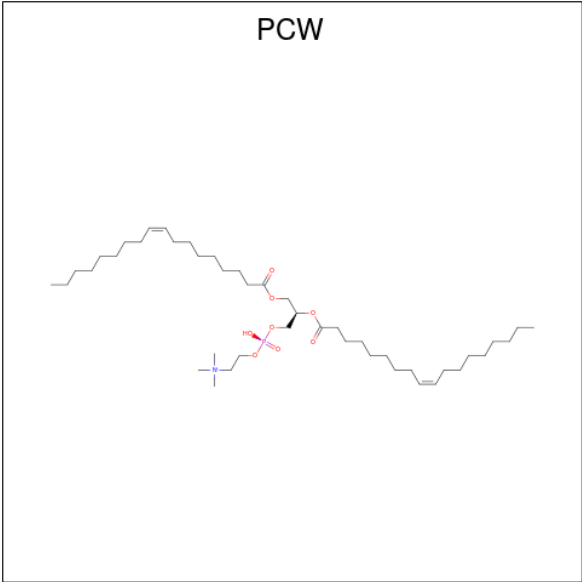
- Molecule 2 is a protein called GTPase KRas.

| Mol | Chain | Residues | Atoms | | | | | | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|-------|
| 2 | B | 185 | Total | C | H | N | O | S | 0 |
| | | | 1842 | 926 | 363 | 257 | 287 | 9 | |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|---------------------|------------|
| B | -1 | GLY | - | expression tag | UNP P01116 |
| B | 0 | SER | - | expression tag | UNP P01116 |
| B | 12 | VAL | GLY | engineered mutation | UNP P01116 |

- Molecule 3 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PCW) (formula: $C_{44}H_{85}NO_8P$).



| Mol | Chain | Residues | Atoms | | | | |
|-----|-------|----------|-------|----|---|---|---|
| 3 | A | 1 | Total | C | N | O | P |
| | | | 54 | 44 | 1 | 8 | 1 |
| 3 | A | 1 | Total | C | N | O | P |
| | | | 54 | 44 | 1 | 8 | 1 |
| 3 | A | 1 | Total | C | N | O | P |
| | | | 54 | 44 | 1 | 8 | 1 |
| 3 | A | 1 | Total | C | N | O | P |
| | | | 54 | 44 | 1 | 8 | 1 |
| 3 | A | 1 | Total | C | N | O | P |
| | | | 54 | 44 | 1 | 8 | 1 |
| 3 | A | 1 | Total | C | N | O | P |
| | | | 54 | 44 | 1 | 8 | 1 |
| 3 | A | 1 | Total | C | N | O | P |
| | | | 54 | 44 | 1 | 8 | 1 |
| 3 | A | 1 | Total | C | N | O | P |
| | | | 54 | 44 | 1 | 8 | 1 |
| 3 | B | 1 | Total | C | N | O | P |
| | | | 54 | 44 | 1 | 8 | 1 |
| 3 | B | 1 | Total | C | N | O | P |
| | | | 54 | 44 | 1 | 8 | 1 |
| 3 | B | 1 | Total | C | N | O | P |
| | | | 54 | 44 | 1 | 8 | 1 |
| 3 | B | 1 | Total | C | N | O | P |
| | | | 54 | 44 | 1 | 8 | 1 |

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| Mol | Chain | Residues | Atoms | | | | |
|-----|-------|----------|-------|----|---|---|---|
| 3 | B | 1 | Total | C | N | O | P |
| | | | 54 | 44 | 1 | 8 | 1 |
| 3 | B | 1 | Total | C | N | O | P |
| | | | 54 | 44 | 1 | 8 | 1 |
| 3 | B | 1 | Total | C | N | O | P |
| | | | 54 | 44 | 1 | 8 | 1 |
| 3 | B | 1 | Total | C | N | O | P |
| | | | 54 | 44 | 1 | 8 | 1 |
| 3 | B | 1 | Total | C | N | O | P |
| | | | 54 | 44 | 1 | 8 | 1 |
| 3 | B | 1 | Total | C | N | O | P |
| | | | 54 | 44 | 1 | 8 | 1 |
| 3 | B | 1 | Total | C | N | O | P |
| | | | 54 | 44 | 1 | 8 | 1 |
| 3 | B | 1 | Total | C | N | O | P |
| | | | 54 | 44 | 1 | 8 | 1 |
| 3 | B | 1 | Total | C | N | O | P |
| | | | 54 | 44 | 1 | 8 | 1 |
| 3 | B | 1 | Total | C | N | O | P |
| | | | 54 | 44 | 1 | 8 | 1 |
| 3 | B | 1 | Total | C | N | O | P |
| | | | 54 | 44 | 1 | 8 | 1 |
| 3 | B | 1 | Total | C | N | O | P |
| | | | 54 | 44 | 1 | 8 | 1 |
| 3 | B | 1 | Total | C | N | O | P |
| | | | 54 | 44 | 1 | 8 | 1 |
| 3 | B | 1 | Total | C | N | O | P |
| | | | 54 | 44 | 1 | 8 | 1 |
| 3 | B | 1 | Total | C | N | O | P |
| | | | 54 | 44 | 1 | 8 | 1 |
| 3 | B | 1 | Total | C | N | O | P |
| | | | 54 | 44 | 1 | 8 | 1 |
| 3 | B | 1 | Total | C | N | O | P |
| | | | 54 | 44 | 1 | 8 | 1 |
| 3 | B | 1 | Total | C | N | O | P |
| | | | 54 | 44 | 1 | 8 | 1 |

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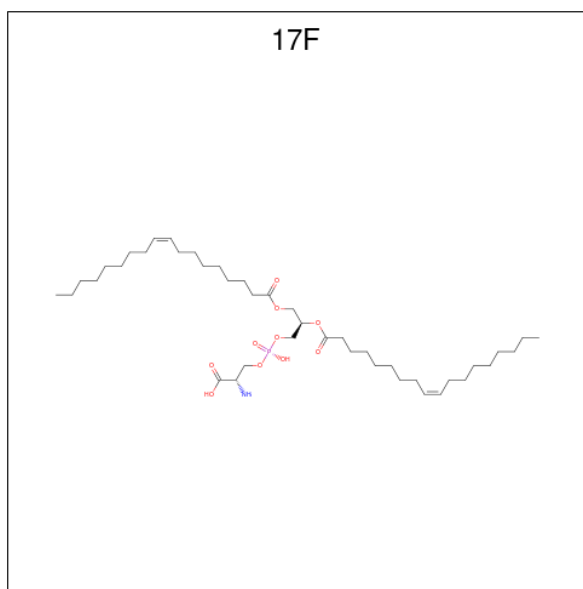
| Mol | Chain | Residues | Atoms | | | | |
|-----|-------|----------|-------|----|---|---|---|
| 3 | B | 1 | Total | C | N | O | P |
| | | | 54 | 44 | 1 | 8 | 1 |
| 3 | B | 1 | Total | C | N | O | P |
| | | | 54 | 44 | 1 | 8 | 1 |
| 3 | B | 1 | Total | C | N | O | P |
| | | | 54 | 44 | 1 | 8 | 1 |
| 3 | C | 1 | Total | C | N | O | P |
| | | | 54 | 44 | 1 | 8 | 1 |
| 3 | C | 1 | Total | C | N | O | P |
| | | | 54 | 44 | 1 | 8 | 1 |
| 3 | C | 1 | Total | C | N | O | P |
| | | | 54 | 44 | 1 | 8 | 1 |
| 3 | C | 1 | Total | C | N | O | P |
| | | | 54 | 44 | 1 | 8 | 1 |
| 3 | C | 1 | Total | C | N | O | P |
| | | | 54 | 44 | 1 | 8 | 1 |
| 3 | C | 1 | Total | C | N | O | P |
| | | | 54 | 44 | 1 | 8 | 1 |
| 3 | C | 1 | Total | C | N | O | P |
| | | | 54 | 44 | 1 | 8 | 1 |
| 3 | C | 1 | Total | C | N | O | P |
| | | | 54 | 44 | 1 | 8 | 1 |
| 3 | C | 1 | Total | C | N | O | P |
| | | | 54 | 44 | 1 | 8 | 1 |
| 3 | C | 1 | Total | C | N | O | P |
| | | | 54 | 44 | 1 | 8 | 1 |
| 3 | C | 1 | Total | C | N | O | P |
| | | | 54 | 44 | 1 | 8 | 1 |
| 3 | C | 1 | Total | C | N | O | P |
| | | | 54 | 44 | 1 | 8 | 1 |
| 3 | C | 1 | Total | C | N | O | P |
| | | | 54 | 44 | 1 | 8 | 1 |
| 3 | C | 1 | Total | C | N | O | P |
| | | | 54 | 44 | 1 | 8 | 1 |
| 3 | C | 1 | Total | C | N | O | P |
| | | | 54 | 44 | 1 | 8 | 1 |
| 3 | C | 1 | Total | C | N | O | P |
| | | | 54 | 44 | 1 | 8 | 1 |
| 3 | C | 1 | Total | C | N | O | P |
| | | | 54 | 44 | 1 | 8 | 1 |

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| Mol | Chain | Residues | Atoms | | | | |
|-----|-------|----------|-------|----|---|---|---|
| 3 | C | 1 | Total | C | N | O | P |
| | | | 54 | 44 | 1 | 8 | 1 |
| 3 | C | 1 | Total | C | N | O | P |
| | | | 54 | 44 | 1 | 8 | 1 |
| 3 | C | 1 | Total | C | N | O | P |
| | | | 54 | 44 | 1 | 8 | 1 |
| 3 | C | 1 | Total | C | N | O | P |
| | | | 54 | 44 | 1 | 8 | 1 |
| 3 | C | 1 | Total | C | N | O | P |
| | | | 54 | 44 | 1 | 8 | 1 |
| 3 | C | 1 | Total | C | N | O | P |
| | | | 54 | 44 | 1 | 8 | 1 |

- Molecule 4 is O-[(S)-({(2R)-2,3-bis[(9Z)-octadec-9-enoyloxy]propyl}oxy)(hydroxy)phosphoryl]-L-serine (three-letter code: 17F) (formula: C₄₂H₇₈NO₁₀P).



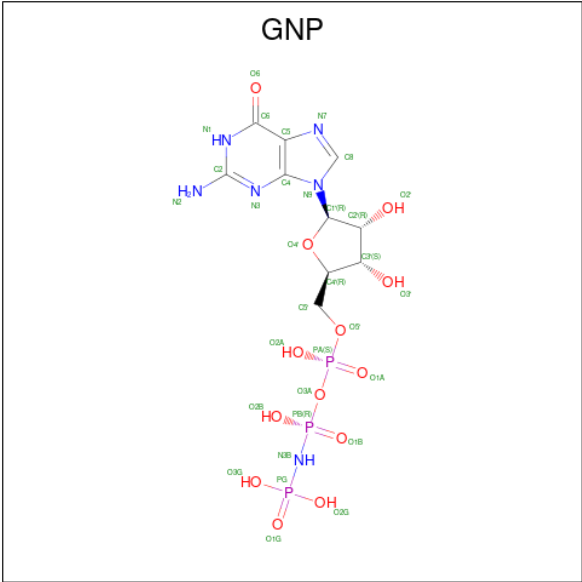
| Mol | Chain | Residues | Atoms | | | | |
|-----|-------|----------|-------|----|---|----|---|
| 4 | A | 1 | Total | C | N | O | P |
| | | | 54 | 42 | 1 | 10 | 1 |
| 4 | B | 1 | Total | C | N | O | P |
| | | | 54 | 42 | 1 | 10 | 1 |
| 4 | B | 1 | Total | C | N | O | P |
| | | | 54 | 42 | 1 | 10 | 1 |

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| Mol | Chain | Residues | Atoms | | | | |
|-----|-------|----------|-------|----|---|----|---|
| 4 | B | 1 | Total | C | N | O | P |
| | | | 54 | 42 | 1 | 10 | 1 |
| 4 | B | 1 | Total | C | N | O | P |
| | | | 54 | 42 | 1 | 10 | 1 |
| 4 | B | 1 | Total | C | N | O | P |
| | | | 54 | 42 | 1 | 10 | 1 |
| 4 | B | 1 | Total | C | N | O | P |
| | | | 54 | 42 | 1 | 10 | 1 |
| 4 | B | 1 | Total | C | N | O | P |
| | | | 54 | 42 | 1 | 10 | 1 |
| 4 | B | 1 | Total | C | N | O | P |
| | | | 54 | 42 | 1 | 10 | 1 |
| 4 | C | 1 | Total | C | N | O | P |
| | | | 54 | 42 | 1 | 10 | 1 |
| 4 | C | 1 | Total | C | N | O | P |
| | | | 54 | 42 | 1 | 10 | 1 |
| 4 | C | 1 | Total | C | N | O | P |
| | | | 54 | 42 | 1 | 10 | 1 |
| 4 | C | 1 | Total | C | N | O | P |
| | | | 54 | 42 | 1 | 10 | 1 |
| 4 | C | 1 | Total | C | N | O | P |
| | | | 54 | 42 | 1 | 10 | 1 |
| 4 | C | 1 | Total | C | N | O | P |
| | | | 54 | 42 | 1 | 10 | 1 |
| 4 | C | 1 | Total | C | N | O | P |
| | | | 54 | 42 | 1 | 10 | 1 |

- Molecule 5 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: C₁₀H₁₇N₆O₁₃P₃).

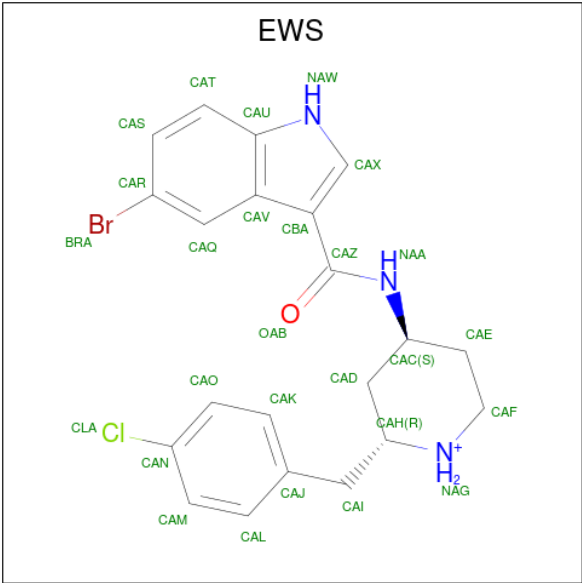


| Mol | Chain | Residues | Atoms | | | | |
|-----|-------|----------|-------|----|---|----|---|
| | | | Total | C | N | O | P |
| 5 | B | 1 | 32 | 10 | 6 | 13 | 3 |

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | |
|-----|-------|----------|-------|----|
| | | | Total | Mg |
| 6 | B | 1 | 1 | 1 |

- Molecule 7 is (2R,4S)-4-[(5-bromo-1H-indole-3-carbonyl)amino]-2-[(4-chlorophenyl)methyl]piperidin-1-ium (three-letter code: EWS) (formula: C₂₁H₂₂BrClN₃O).



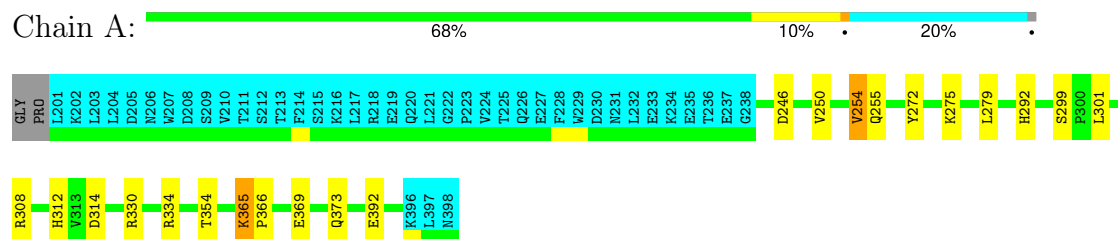
| Mol | Chain | Residues | Atoms | | | | | | |
|-----|-------|----------|-------|----|----|----|----|---|---|
| | | | Total | Br | C | Cl | H | N | O |
| 7 | B | 1 | 49 | 1 | 21 | 1 | 22 | 3 | 1 |

4 Residue-property plots [i](#)

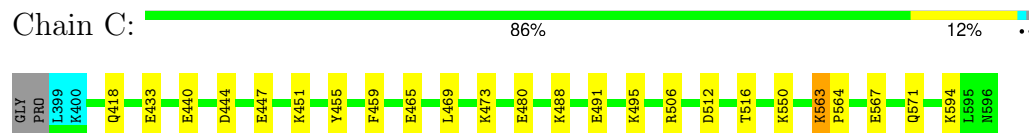
4.1 Average score per residue in the NMR ensemble

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

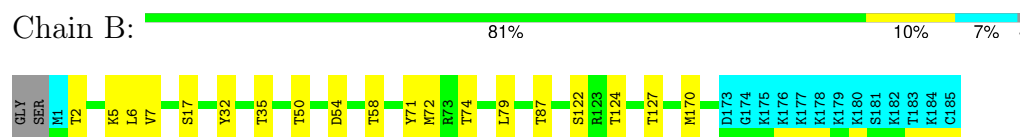
- Molecule 1: Apolipoprotein A-I



- Molecule 1: Apolipoprotein A-I



- Molecule 2: GTPase KRas



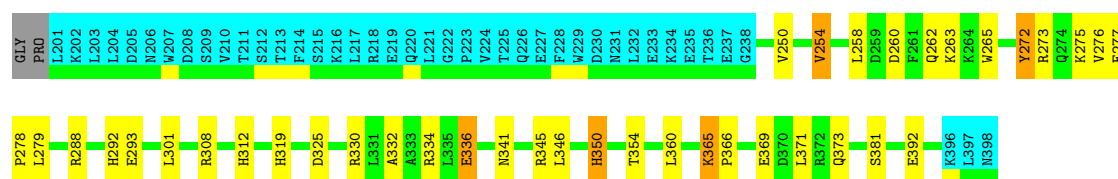
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

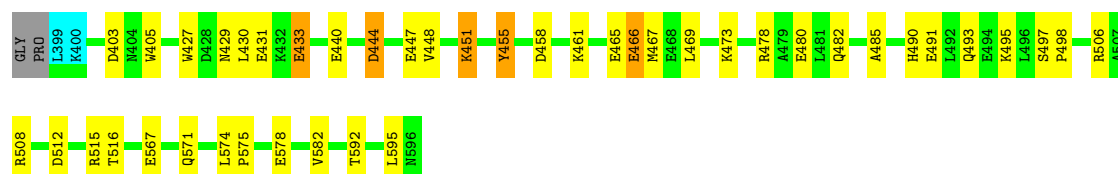
- Molecule 1: Apolipoprotein A-I





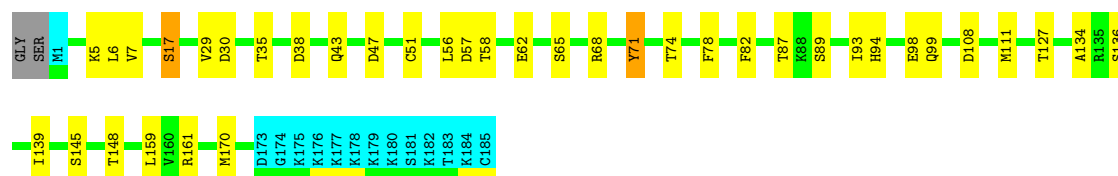
• Molecule 1: Apolipoprotein A-I

Chain C: 76% 19% ...



• Molecule 2: GTPase KRas

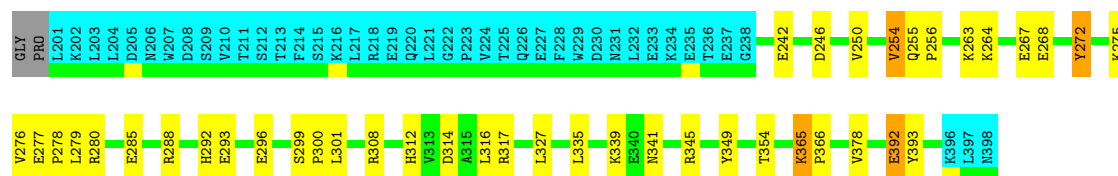
Chain B: 71% 19% 7%



4.2.2 Score per residue for model 2

• Molecule 1: Apolipoprotein A-I

Chain A: 58% 19% 20%



• Molecule 1: Apolipoprotein A-I

Chain C: 76% 18%



• Molecule 2: GTPase KRas

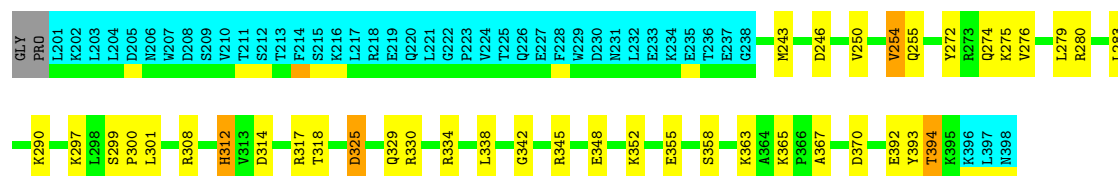
Chain B: 



4.2.3 Score per residue for model 3

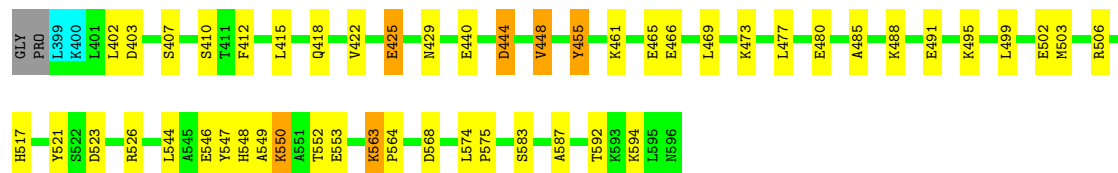
- Molecule 1: Apolipoprotein A-I

Chain A: 



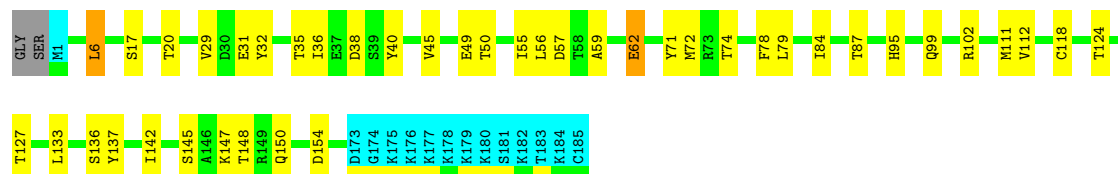
- Molecule 1: Apolipoprotein A-I

Chain C: 



- Molecule 2: GTPase KRas

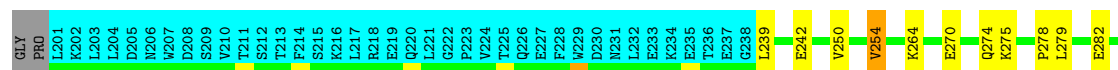
Chain B: 

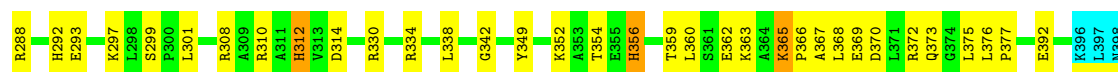


4.2.4 Score per residue for model 4

- Molecule 1: Apolipoprotein A-I

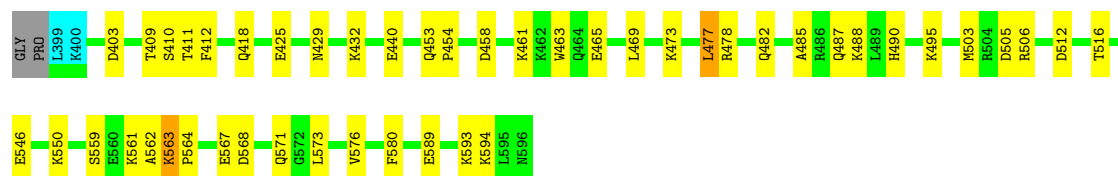
Chain A: 





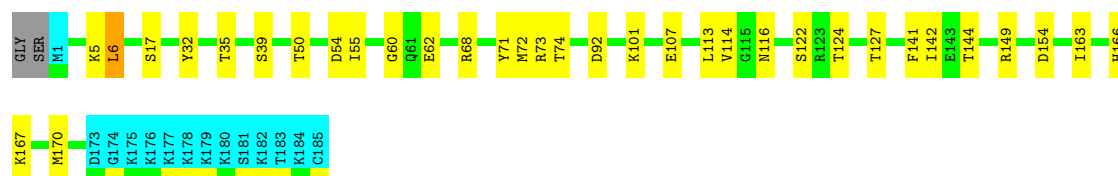
• Molecule 1: Apolipoprotein A-I

Chain C: 74% 22% ...



• Molecule 2: GTPase KRas

Chain B: 73% 18% 7%



4.2.5 Score per residue for model 5

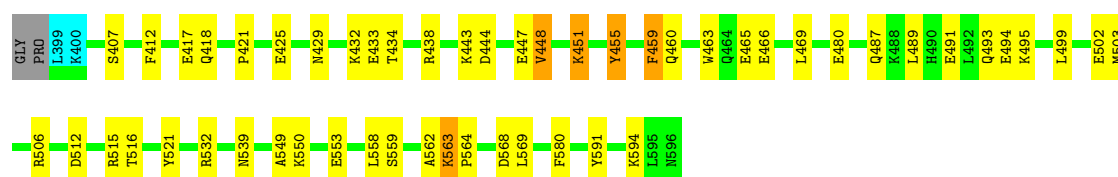
• Molecule 1: Apolipoprotein A-I

Chain A: 56% 21% 20%



• Molecule 1: Apolipoprotein A-I

Chain C: 72% 24% ...



• Molecule 2: GTPase KRas

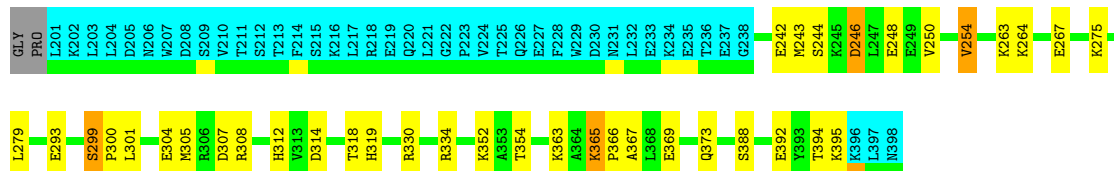
Chain B: 80% 11% 7%



4.2.6 Score per residue for model 6

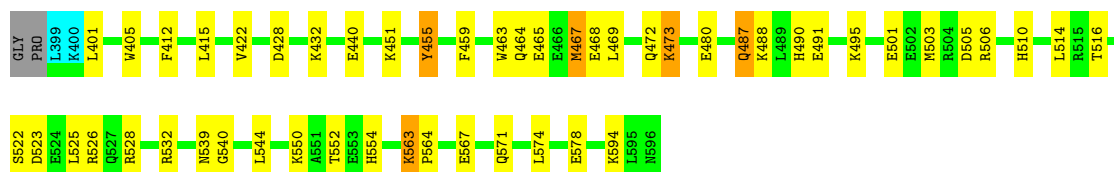
- Molecule 1: Apolipoprotein A-I

Chain A: 60% 17% 20%



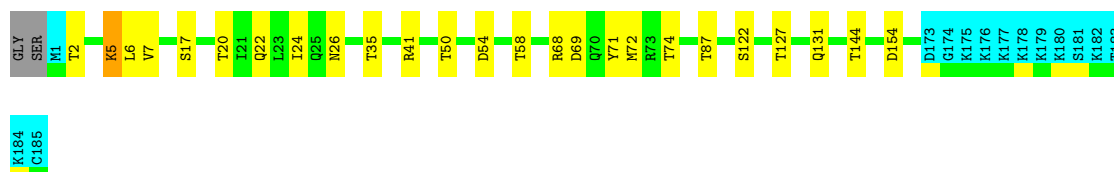
- Molecule 1: Apolipoprotein A-I

Chain C: 72% 23%



- Molecule 2: GTPase KRas

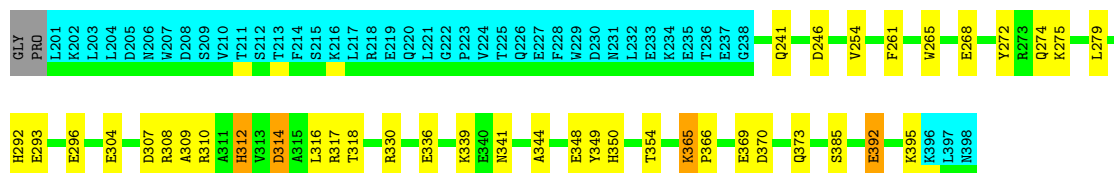
Chain B: 78% 13% 7%




4.2.7 Score per residue for model 7

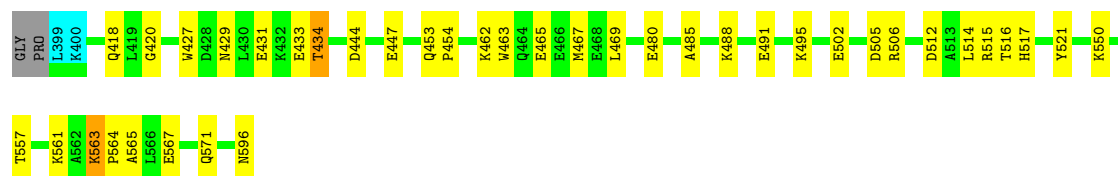
- Molecule 1: Apolipoprotein A-I

Chain A: 58% 18% 20%



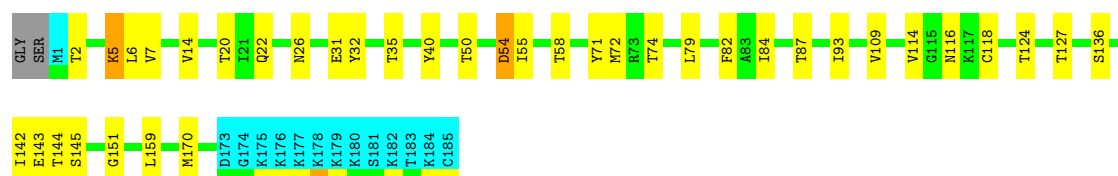
- Molecule 1: Apolipoprotein A-I

Chain C: 



- Molecule 2: GTPase KRas

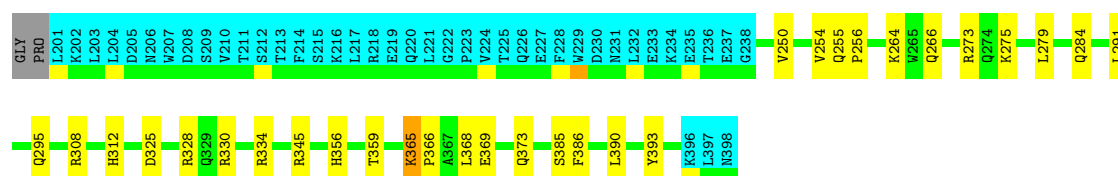
Chain B: 




4.2.8 Score per residue for model 8 (medoid)

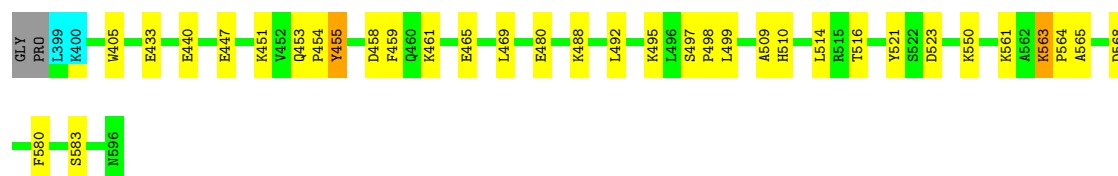
- Molecule 1: Apolipoprotein A-I

Chain A: 



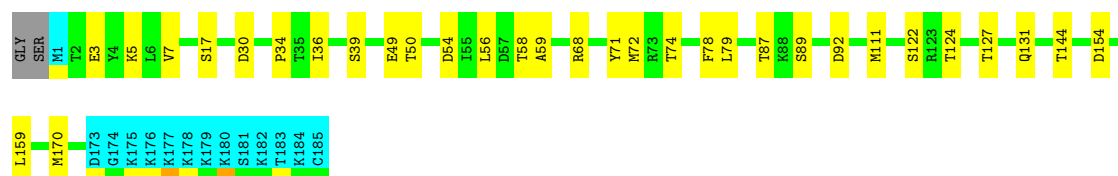
- Molecule 1: Apolipoprotein A-I

Chain C: 



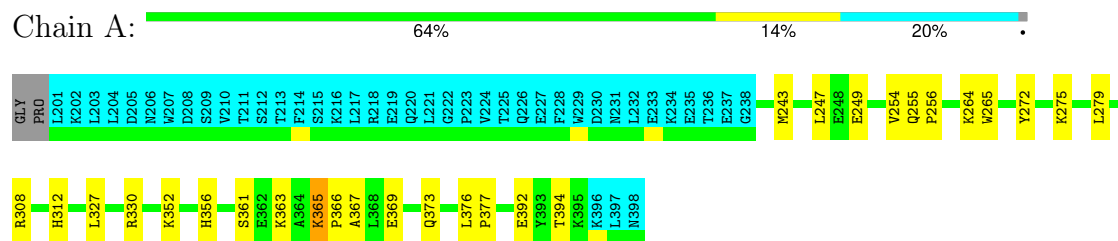
- Molecule 2: GTPase KRas

Chain B: 

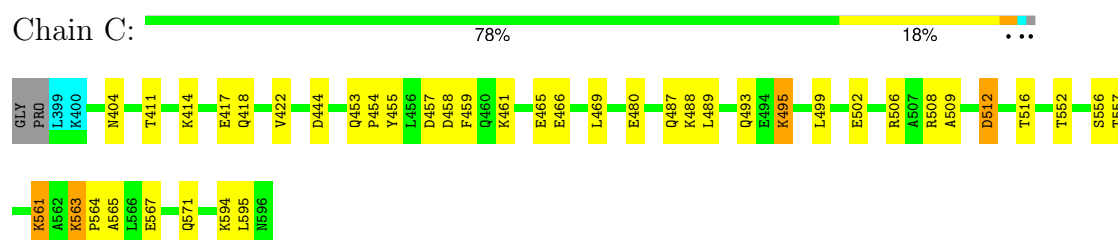


4.2.9 Score per residue for model 9

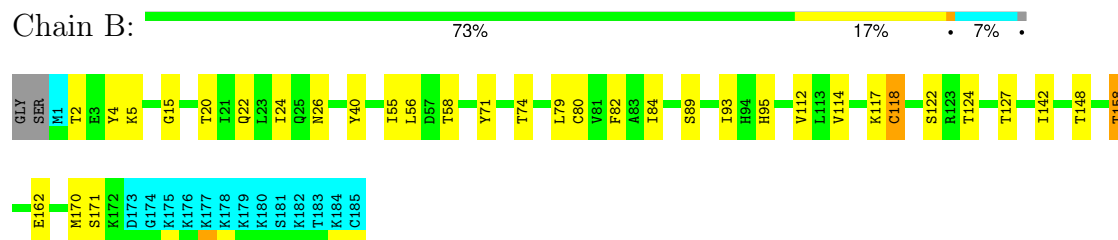
• Molecule 1: Apolipoprotein A-I



• Molecule 1: Apolipoprotein A-I

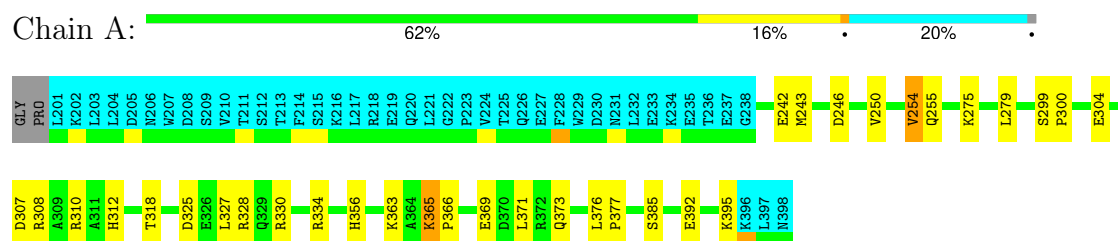


• Molecule 2: GTPase KRas

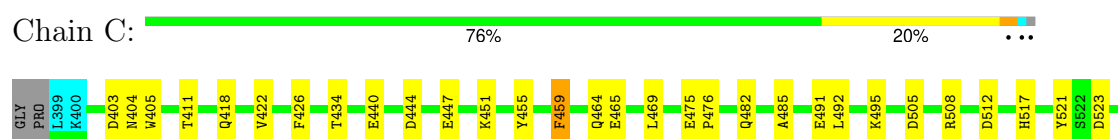


4.2.10 Score per residue for model 10

• Molecule 1: Apolipoprotein A-I

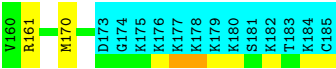
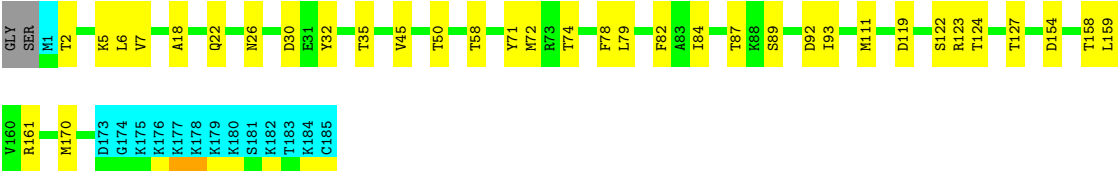


• Molecule 1: Apolipoprotein A-I





● Molecule 2: GTPase KRas



5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing*.

Of the 3000 calculated structures, 10 were deposited, based on the following criterion: *10 structures for lowest energy*.

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

| Software name | Classification | Version |
|---------------|-----------------------|---------|
| CNS | refinement | |
| HADDOCK | structure calculation | |

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 | 268 |
| Number of shifts mapped to atoms | 192 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 76 |
| Number of shifts with mapping warnings | 0 |
| Assignment completeness (well-defined parts) | 3% |

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: GNP, EWS, 17F, PCW, MG

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-----------------------|-------------|-----------------------|
| | | RMSZ | #Z>5 | RMSZ | #Z>5 |
| 1 | A | 0.26±0.00 | 0±0/1305 (0.0± 0.0%) | 0.40±0.01 | 0±0/1752 (0.0± 0.0%) |
| 1 | C | 0.26±0.00 | 0±0/1634 (0.0± 0.0%) | 0.41±0.00 | 0±0/2196 (0.0± 0.0%) |
| 2 | B | 0.27±0.00 | 0±0/1390 (0.0± 0.0%) | 0.41±0.06 | 0±0/1875 (0.0± 0.0%) |
| All | All | 0.26 | 0/43290 (0.0%) | 0.41 | 2/58230 (0.0%) |

There are no bond-length outliers.

All unique angle outliers are listed below.

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|----------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 2 | B | 5 | LYS | CD-CE-NZ | 18.53 | 154.32 | 111.70 | 6 | 2 |

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1 | A | 1284 | 18 | 1297 | 28±5 |
| 1 | C | 1607 | 22 | 1603 | 34±7 |
| 2 | B | 1368 | 322 | 1356 | 17±5 |
| 3 | A | 540 | 0 | 840 | 32±9 |
| 3 | B | 1512 | 0 | 2351 | 78±17 |
| 3 | C | 1404 | 0 | 2182 | 63±16 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 4 | A | 54 | 0 | 76 | 5±2 |
| 4 | B | 432 | 0 | 608 | 37±5 |
| 4 | C | 378 | 0 | 532 | 26±7 |
| 5 | B | 32 | 0 | 13 | 1±1 |
| 7 | B | 27 | 22 | 0 | 9±4 |
| All | All | 86390 | 3840 | 108600 | 2177 |

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 11.

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

| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 2:B:72:MET:HA | 7:B:239:EWS:BRA | 1.57 | 1.53 | 3 | 5 |
| 1:A:308:ARG:CD | 1:C:469:LEU:HD11 | 1.48 | 1.34 | 10 | 1 |
| 1:A:393:TYR:CE1 | 3:A:406:PCW:H271 | 1.45 | 1.46 | 8 | 1 |
| 1:A:393:TYR:CD1 | 3:A:406:PCW:C27 | 1.43 | 2.01 | 8 | 2 |
| 1:A:393:TYR:CD1 | 3:A:406:PCW:H271 | 1.37 | 1.51 | 8 | 1 |
| 1:A:393:TYR:HD1 | 3:A:406:PCW:C27 | 1.33 | 1.31 | 8 | 1 |
| 1:C:465:GLU:O | 1:C:469:LEU:HG | 1.28 | 1.19 | 9 | 9 |
| 2:B:72:MET:HB3 | 7:B:239:EWS:BRA | 1.26 | 1.83 | 10 | 1 |
| 1:C:465:GLU:O | 1:C:469:LEU:CG | 1.26 | 1.82 | 4 | 6 |
| 1:A:308:ARG:CG | 1:C:469:LEU:HD11 | 1.21 | 1.63 | 10 | 3 |
| 3:B:221:PCW:C5 | 3:C:601:PCW:H61 | 1.20 | 1.64 | 4 | 1 |
| 2:B:71:TYR:O | 7:B:239:EWS:BRA | 1.20 | 2.13 | 7 | 7 |
| 3:A:403:PCW:C38 | 3:B:218:PCW:H471 | 1.18 | 1.67 | 1 | 1 |
| 1:A:308:ARG:CD | 1:C:469:LEU:CD1 | 1.18 | 2.21 | 10 | 1 |
| 3:B:221:PCW:O4P | 3:C:601:PCW:C6 | 1.16 | 1.93 | 4 | 1 |
| 2:B:72:MET:CA | 7:B:239:EWS:BRA | 1.16 | 2.48 | 3 | 3 |
| 1:A:308:ARG:HG3 | 1:C:469:LEU:CD1 | 1.14 | 1.72 | 6 | 4 |
| 2:B:7:VAL:HG13 | 7:B:239:EWS:CAS | 1.14 | 1.70 | 1 | 3 |
| 3:C:601:PCW:H441 | 4:C:627:17F:H54 | 1.14 | 1.18 | 8 | 1 |
| 1:A:308:ARG:HD3 | 1:C:469:LEU:CD1 | 1.11 | 1.75 | 10 | 2 |
| 1:A:393:TYR:HD1 | 3:A:406:PCW:H272 | 1.11 | 0.99 | 8 | 1 |
| 3:C:601:PCW:H483 | 3:C:605:PCW:C48 | 1.11 | 1.75 | 10 | 1 |
| 3:C:620:PCW:C16 | 4:C:633:17F:H29 | 1.10 | 1.76 | 4 | 1 |
| 1:A:368:LEU:HD11 | 4:B:230:17F:H54 | 1.10 | 1.18 | 8 | 1 |
| 3:B:221:PCW:H161 | 3:C:601:PCW:C38 | 1.10 | 1.72 | 10 | 1 |
| 3:B:221:PCW:H161 | 3:C:601:PCW:H372 | 1.09 | 1.25 | 8 | 1 |
| 2:B:72:MET:CB | 7:B:239:EWS:BRA | 1.08 | 2.55 | 10 | 1 |
| 3:B:221:PCW:C5 | 3:C:601:PCW:C6 | 1.08 | 2.32 | 4 | 1 |
| 1:C:488:LYS:HD2 | 3:C:620:PCW:H281 | 1.07 | 1.25 | 8 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:308:ARG:CG | 1:C:469:LEU:CD1 | 1.05 | 2.34 | 10 | 2 |
| 3:B:207:PCW:H222 | 3:C:601:PCW:H452 | 1.05 | 1.27 | 8 | 1 |
| 3:B:207:PCW:C22 | 3:C:601:PCW:H452 | 1.05 | 1.79 | 8 | 1 |
| 2:B:7:VAL:HB | 7:B:239:EWS:CAT | 1.05 | 1.81 | 10 | 3 |
| 3:C:620:PCW:C14 | 4:C:633:17F:H59 | 1.05 | 1.81 | 4 | 1 |
| 1:C:567:GLU:O | 1:C:571:GLN:HG3 | 1.05 | 1.48 | 9 | 7 |
| 1:A:308:ARG:CD | 1:C:469:LEU:HD21 | 1.04 | 1.82 | 7 | 2 |
| 3:C:601:PCW:C48 | 3:C:605:PCW:H481 | 1.04 | 1.82 | 10 | 1 |
| 3:A:403:PCW:H20 | 3:C:606:PCW:H282 | 1.04 | 1.30 | 1 | 1 |
| 3:B:221:PCW:H51 | 3:C:601:PCW:H61 | 1.03 | 1.30 | 4 | 1 |
| 1:A:308:ARG:HG3 | 1:C:469:LEU:HD11 | 1.02 | 1.26 | 2 | 3 |
| 1:A:349:TYR:CE2 | 3:A:401:PCW:H262 | 1.02 | 1.89 | 7 | 1 |
| 3:B:221:PCW:H181 | 3:C:601:PCW:H411 | 1.02 | 1.23 | 10 | 1 |
| 3:A:403:PCW:H222 | 3:C:606:PCW:H282 | 1.01 | 1.28 | 1 | 1 |
| 3:A:403:PCW:H382 | 3:B:218:PCW:H471 | 1.01 | 1.18 | 1 | 1 |
| 3:C:601:PCW:C48 | 3:C:605:PCW:C48 | 1.01 | 2.37 | 10 | 1 |
| 1:A:308:ARG:HG3 | 1:C:469:LEU:HD21 | 1.00 | 1.27 | 1 | 6 |
| 1:A:308:ARG:HD2 | 1:C:469:LEU:HD21 | 1.00 | 1.33 | 10 | 2 |
| 3:B:217:PCW:H432 | 3:B:223:PCW:H451 | 0.99 | 1.32 | 5 | 1 |
| 3:B:223:PCW:H471 | 4:C:632:17F:H76 | 0.99 | 1.34 | 5 | 1 |
| 3:B:223:PCW:H281 | 1:C:521:TYR:CE2 | 0.98 | 1.93 | 5 | 1 |
| 1:C:488:LYS:NZ | 3:C:620:PCW:H261 | 0.98 | 1.72 | 4 | 1 |
| 3:B:221:PCW:H141 | 3:C:601:PCW:H351 | 0.98 | 1.31 | 4 | 1 |
| 3:B:221:PCW:H411 | 3:C:601:PCW:H39 | 0.97 | 1.35 | 10 | 1 |
| 1:A:369:GLU:O | 1:A:373:GLN:HG3 | 0.97 | 1.58 | 1 | 8 |
| 3:C:620:PCW:H162 | 4:C:633:17F:C1X | 0.96 | 1.90 | 4 | 1 |
| 1:A:308:ARG:HD3 | 1:C:469:LEU:HD11 | 0.95 | 0.97 | 10 | 2 |
| 3:B:217:PCW:H451 | 3:B:223:PCW:H462 | 0.95 | 1.32 | 5 | 1 |
| 3:B:221:PCW:C12 | 3:C:601:PCW:H362 | 0.95 | 1.77 | 10 | 1 |
| 3:C:620:PCW:H131 | 4:C:633:17F:H56 | 0.94 | 1.38 | 4 | 1 |
| 1:C:488:LYS:HD3 | 3:C:620:PCW:H283 | 0.94 | 1.34 | 9 | 1 |
| 3:A:410:PCW:H332 | 4:C:630:17F:H29 | 0.94 | 1.35 | 1 | 2 |
| 3:B:221:PCW:H52 | 3:C:601:PCW:C6 | 0.93 | 1.90 | 4 | 1 |
| 3:B:201:PCW:H361 | 3:B:220:PCW:H352 | 0.93 | 1.39 | 10 | 1 |
| 3:B:221:PCW:H161 | 3:C:601:PCW:C39 | 0.93 | 1.93 | 10 | 1 |
| 3:B:216:PCW:H62 | 3:C:601:PCW:C7 | 0.93 | 1.92 | 4 | 1 |
| 1:A:297:LYS:HE2 | 1:C:477:LEU:HG | 0.92 | 1.39 | 4 | 1 |
| 3:B:216:PCW:H62 | 3:C:601:PCW:H73 | 0.92 | 1.41 | 4 | 1 |
| 2:B:7:VAL:HA | 7:B:239:EWS:NAW | 0.92 | 1.78 | 5 | 1 |
| 3:C:620:PCW:H162 | 4:C:633:17F:H29 | 0.92 | 0.94 | 4 | 2 |
| 3:A:403:PCW:H222 | 3:C:606:PCW:C28 | 0.92 | 1.94 | 1 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 3:B:210:PCW:H322 | 3:B:214:PCW:H132 | 0.92 | 1.42 | 4 | 1 |
| 1:C:465:GLU:O | 1:C:469:LEU:CB | 0.92 | 2.16 | 4 | 2 |
| 3:C:601:PCW:H483 | 3:C:605:PCW:H481 | 0.91 | 1.32 | 10 | 1 |
| 3:B:221:PCW:H241 | 3:C:601:PCW:C19 | 0.90 | 1.94 | 10 | 2 |
| 3:B:205:PCW:H41 | 3:B:222:PCW:H71 | 0.90 | 1.41 | 10 | 1 |
| 1:C:488:LYS:NZ | 3:C:620:PCW:C26 | 0.90 | 2.34 | 4 | 1 |
| 3:B:221:PCW:O4P | 3:C:601:PCW:H63 | 0.90 | 1.65 | 4 | 1 |
| 1:A:393:TYR:CE1 | 3:A:406:PCW:C27 | 0.90 | 2.40 | 8 | 1 |
| 3:C:618:PCW:H352 | 3:C:626:PCW:H162 | 0.89 | 1.43 | 5 | 2 |
| 3:B:211:PCW:H332 | 4:B:226:17F:H19 | 0.89 | 1.44 | 10 | 1 |
| 3:B:211:PCW:H362 | 4:B:226:17F:H8 | 0.89 | 1.44 | 10 | 2 |
| 3:B:217:PCW:H472 | 3:B:223:PCW:H483 | 0.88 | 1.43 | 5 | 1 |
| 3:B:221:PCW:H211 | 3:C:601:PCW:H411 | 0.88 | 1.44 | 4 | 1 |
| 3:B:201:PCW:H31 | 3:B:203:PCW:H342 | 0.88 | 1.43 | 7 | 1 |
| 3:C:620:PCW:H141 | 4:C:633:17F:H59 | 0.88 | 1.45 | 4 | 1 |
| 1:C:488:LYS:HD2 | 3:C:620:PCW:H272 | 0.88 | 1.43 | 4 | 1 |
| 1:A:393:TYR:HE1 | 3:A:406:PCW:H271 | 0.88 | 1.22 | 8 | 1 |
| 3:B:221:PCW:C18 | 3:C:601:PCW:H411 | 0.87 | 2.00 | 10 | 1 |
| 1:A:393:TYR:CD1 | 3:A:406:PCW:H272 | 0.87 | 1.83 | 8 | 1 |
| 3:B:223:PCW:C47 | 4:C:632:17F:H76 | 0.86 | 1.99 | 5 | 1 |
| 1:C:488:LYS:HZ1 | 3:C:620:PCW:H261 | 0.86 | 1.22 | 4 | 1 |
| 2:B:72:MET:CG | 7:B:239:EWS:BRA | 0.86 | 2.79 | 10 | 2 |
| 3:B:221:PCW:C16 | 3:C:601:PCW:C39 | 0.86 | 2.53 | 10 | 1 |
| 1:A:308:ARG:HD2 | 1:C:469:LEU:CD2 | 0.86 | 2.00 | 10 | 1 |
| 3:B:221:PCW:H161 | 3:C:601:PCW:H381 | 0.86 | 1.48 | 10 | 1 |
| 3:A:410:PCW:H372 | 4:C:630:17F:H36 | 0.85 | 1.46 | 2 | 2 |
| 3:C:618:PCW:H362 | 3:C:626:PCW:H152 | 0.85 | 1.48 | 9 | 2 |
| 1:A:393:TYR:CD1 | 3:A:406:PCW:H283 | 0.85 | 2.06 | 2 | 1 |
| 2:B:7:VAL:HG13 | 7:B:239:EWS:CAT | 0.84 | 2.02 | 1 | 2 |
| 3:B:221:PCW:H272 | 3:C:601:PCW:H221 | 0.84 | 1.48 | 2 | 2 |
| 3:B:221:PCW:C4 | 3:C:601:PCW:C6 | 0.84 | 2.55 | 4 | 1 |
| 3:B:223:PCW:H481 | 4:C:632:17F:H78 | 0.84 | 1.49 | 5 | 1 |
| 3:B:210:PCW:H71 | 4:B:226:17F:HN1A | 0.84 | 1.32 | 3 | 1 |
| 1:C:465:GLU:O | 1:C:469:LEU:CD1 | 0.84 | 2.24 | 4 | 2 |
| 4:A:407:17F:H9A | 3:B:205:PCW:H332 | 0.84 | 1.47 | 9 | 1 |
| 3:A:406:PCW:H121 | 4:A:407:17F:H57 | 0.83 | 1.51 | 1 | 4 |
| 3:B:221:PCW:H241 | 3:C:601:PCW:H19 | 0.83 | 1.50 | 10 | 1 |
| 4:C:630:17F:H1 | 4:C:630:17F:H4 | 0.83 | 1.48 | 1 | 3 |
| 3:B:207:PCW:C22 | 3:C:601:PCW:C45 | 0.83 | 2.56 | 8 | 1 |
| 4:B:230:17F:H1 | 4:B:230:17F:H4 | 0.83 | 1.46 | 9 | 1 |
| 1:C:488:LYS:CG | 3:C:620:PCW:H281 | 0.82 | 2.03 | 3 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 3:B:221:PCW:C11 | 3:C:601:PCW:H362 | 0.82 | 2.03 | 10 | 1 |
| 2:B:5:LYS:HD3 | 7:B:239:EWS:CAX | 0.82 | 2.05 | 8 | 3 |
| 4:C:628:17F:H65 | 4:C:632:17F:H11 | 0.82 | 1.48 | 1 | 4 |
| 3:A:406:PCW:H342 | 4:B:227:17F:H11 | 0.81 | 1.50 | 6 | 2 |
| 3:B:207:PCW:H221 | 3:C:601:PCW:C45 | 0.81 | 2.05 | 8 | 1 |
| 1:C:563:LYS:HB2 | 1:C:564:PRO:HD3 | 0.81 | 1.52 | 2 | 9 |
| 3:B:221:PCW:O4P | 3:C:601:PCW:H62 | 0.81 | 1.71 | 4 | 1 |
| 1:A:279:LEU:HD22 | 1:C:495:LYS:HG2 | 0.80 | 1.53 | 10 | 7 |
| 3:A:410:PCW:H121 | 4:C:630:17F:H30 | 0.80 | 1.54 | 9 | 7 |
| 1:C:488:LYS:HD3 | 3:C:620:PCW:C28 | 0.80 | 2.05 | 9 | 1 |
| 3:A:403:PCW:H382 | 3:B:218:PCW:C47 | 0.80 | 2.05 | 1 | 1 |
| 4:C:630:17F:H2 | 4:C:630:17F:H4A | 0.80 | 1.52 | 9 | 5 |
| 3:B:214:PCW:H281 | 4:C:627:17F:H78 | 0.80 | 1.52 | 6 | 1 |
| 3:B:223:PCW:H481 | 4:C:632:17F:C42 | 0.80 | 2.06 | 5 | 1 |
| 1:A:365:LYS:HB2 | 1:A:366:PRO:HD3 | 0.79 | 1.55 | 4 | 8 |
| 4:B:226:17F:H47 | 4:C:628:17F:H55 | 0.79 | 1.54 | 5 | 1 |
| 3:B:206:PCW:H332 | 3:B:211:PCW:H342 | 0.79 | 1.52 | 6 | 1 |
| 3:C:618:PCW:H372 | 3:C:626:PCW:H152 | 0.79 | 1.55 | 3 | 2 |
| 3:B:221:PCW:C16 | 3:C:601:PCW:C40 | 0.79 | 2.61 | 10 | 1 |
| 3:B:221:PCW:H73 | 4:B:229:17F:H1 | 0.79 | 1.55 | 4 | 1 |
| 3:A:402:PCW:H41 | 4:A:407:17F:H1 | 0.79 | 1.55 | 10 | 1 |
| 3:C:607:PCW:H182 | 3:C:615:PCW:H351 | 0.78 | 1.56 | 7 | 2 |
| 1:C:488:LYS:HZ1 | 3:C:620:PCW:C26 | 0.78 | 1.90 | 4 | 1 |
| 3:C:607:PCW:H462 | 4:C:633:17F:H43 | 0.78 | 1.56 | 4 | 3 |
| 1:A:308:ARG:HD3 | 1:C:469:LEU:HD21 | 0.78 | 1.54 | 7 | 1 |
| 3:B:208:PCW:H73 | 3:B:218:PCW:H42 | 0.78 | 1.56 | 5 | 1 |
| 2:B:7:VAL:CB | 7:B:239:EWS:CAT | 0.78 | 2.60 | 10 | 1 |
| 1:C:488:LYS:HD2 | 3:C:620:PCW:C28 | 0.78 | 2.08 | 8 | 1 |
| 3:B:211:PCW:H121 | 4:B:226:17F:H18A | 0.78 | 1.55 | 7 | 3 |
| 1:C:466:GLU:OE1 | 1:C:469:LEU:HD12 | 0.77 | 1.78 | 1 | 1 |
| 3:B:211:PCW:H152 | 4:B:226:17F:H4 | 0.77 | 1.53 | 5 | 1 |
| 3:B:211:PCW:H382 | 4:B:226:17F:H8 | 0.77 | 1.54 | 7 | 4 |
| 2:B:5:LYS:HD3 | 7:B:239:EWS:CBA | 0.77 | 2.10 | 8 | 3 |
| 3:A:408:PCW:H351 | 3:A:410:PCW:H341 | 0.77 | 1.55 | 2 | 1 |
| 3:C:607:PCW:H381 | 3:C:615:PCW:H412 | 0.77 | 1.56 | 5 | 1 |
| 3:B:204:PCW:H122 | 3:B:212:PCW:H371 | 0.77 | 1.56 | 5 | 1 |
| 3:B:201:PCW:H371 | 4:B:228:17F:H37 | 0.77 | 1.56 | 10 | 1 |
| 1:A:349:TYR:CE2 | 3:A:401:PCW:C26 | 0.76 | 2.67 | 7 | 1 |
| 3:B:221:PCW:H162 | 3:C:601:PCW:C40 | 0.76 | 2.10 | 10 | 1 |
| 3:C:606:PCW:H361 | 3:C:612:PCW:H151 | 0.76 | 1.56 | 1 | 2 |
| 4:B:226:17F:H11 | 4:B:232:17F:H59 | 0.76 | 1.56 | 1 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 3:B:206:PCW:H121 | 3:B:220:PCW:H82 | 0.76 | 1.55 | 7 | 1 |
| 1:C:567:GLU:O | 1:C:571:GLN:CG | 0.76 | 2.34 | 9 | 3 |
| 3:C:611:PCW:H352 | 3:C:623:PCW:H382 | 0.75 | 1.58 | 4 | 1 |
| 3:B:221:PCW:H421 | 4:B:229:17F:H66 | 0.75 | 1.56 | 1 | 1 |
| 3:C:618:PCW:H381 | 3:C:626:PCW:H171 | 0.75 | 1.56 | 5 | 3 |
| 3:C:618:PCW:H361 | 3:C:626:PCW:H212 | 0.75 | 1.58 | 6 | 3 |
| 3:B:202:PCW:H341 | 3:B:202:PCW:H122 | 0.75 | 1.58 | 4 | 2 |
| 3:B:217:PCW:H73 | 4:B:226:17F:HN1A | 0.75 | 1.41 | 4 | 2 |
| 3:B:201:PCW:H351 | 3:B:220:PCW:H341 | 0.75 | 1.58 | 5 | 1 |
| 3:B:218:PCW:H231 | 3:C:626:PCW:H282 | 0.75 | 1.56 | 5 | 1 |
| 3:A:403:PCW:C39 | 3:B:218:PCW:H471 | 0.75 | 2.11 | 1 | 1 |
| 3:C:621:PCW:H431 | 4:C:632:17F:H58 | 0.75 | 1.57 | 2 | 3 |
| 3:B:210:PCW:H71 | 4:B:226:17F:N1 | 0.75 | 1.97 | 3 | 1 |
| 3:B:209:PCW:H252 | 3:C:601:PCW:H471 | 0.75 | 1.59 | 4 | 1 |
| 3:B:220:PCW:H341 | 4:B:228:17F:H30 | 0.74 | 1.56 | 3 | 1 |
| 3:B:203:PCW:H421 | 4:B:228:17F:H11 | 0.74 | 1.59 | 4 | 1 |
| 3:C:624:PCW:H372 | 3:C:625:PCW:H152 | 0.74 | 1.56 | 4 | 1 |
| 3:C:606:PCW:H141 | 3:C:612:PCW:H121 | 0.74 | 1.58 | 3 | 1 |
| 1:A:308:ARG:CD | 1:C:469:LEU:CG | 0.74 | 2.66 | 10 | 1 |
| 3:B:213:PCW:H141 | 4:B:228:17F:H18 | 0.74 | 1.58 | 6 | 1 |
| 1:A:393:TYR:HD1 | 3:A:406:PCW:H283 | 0.74 | 1.43 | 2 | 1 |
| 3:C:601:PCW:C44 | 4:C:627:17F:H54 | 0.74 | 2.09 | 8 | 1 |
| 3:B:221:PCW:H261 | 3:C:601:PCW:H20 | 0.74 | 1.60 | 9 | 1 |
| 3:A:403:PCW:C20 | 3:C:606:PCW:H282 | 0.73 | 2.11 | 1 | 1 |
| 3:B:206:PCW:H20 | 3:B:220:PCW:H181 | 0.73 | 1.59 | 1 | 1 |
| 3:C:618:PCW:H352 | 3:C:626:PCW:H152 | 0.73 | 1.58 | 4 | 2 |
| 3:B:221:PCW:H52 | 3:C:601:PCW:H62 | 0.73 | 1.58 | 4 | 1 |
| 3:B:223:PCW:H281 | 1:C:521:TYR:HE2 | 0.73 | 1.40 | 5 | 1 |
| 3:B:221:PCW:H281 | 3:C:601:PCW:H242 | 0.73 | 1.59 | 6 | 1 |
| 4:B:227:17F:H64 | 3:C:619:PCW:H481 | 0.73 | 1.61 | 1 | 1 |
| 1:A:393:TYR:HD1 | 3:A:406:PCW:C28 | 0.73 | 1.96 | 2 | 1 |
| 2:B:79:LEU:HG | 2:B:159:LEU:HD22 | 0.73 | 1.61 | 7 | 4 |
| 2:B:5:LYS:CE | 7:B:239:EWS:OAB | 0.73 | 2.36 | 8 | 3 |
| 3:B:222:PCW:H52 | 4:B:227:17F:HN1A | 0.73 | 1.44 | 7 | 1 |
| 3:B:221:PCW:H361 | 4:B:229:17F:H34 | 0.73 | 1.61 | 8 | 1 |
| 1:A:356:HIS:CD2 | 3:A:401:PCW:C27 | 0.73 | 2.72 | 9 | 1 |
| 3:B:217:PCW:C45 | 3:B:223:PCW:H462 | 0.73 | 2.13 | 5 | 1 |
| 3:B:223:PCW:C48 | 4:C:632:17F:C42 | 0.73 | 2.67 | 5 | 1 |
| 2:B:5:LYS:HB3 | 7:B:239:EWS:CAX | 0.73 | 2.14 | 4 | 3 |
| 3:C:624:PCW:H372 | 3:C:625:PCW:H162 | 0.73 | 1.59 | 10 | 1 |
| 3:B:204:PCW:H271 | 3:B:218:PCW:H181 | 0.72 | 1.61 | 6 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 4:A:407:17F:H35 | 4:B:227:17F:H34 | 0.72 | 1.60 | 2 | 1 |
| 3:A:403:PCW:C22 | 3:C:606:PCW:H262 | 0.72 | 2.13 | 1 | 1 |
| 3:B:213:PCW:H131 | 3:B:213:PCW:H332 | 0.72 | 1.61 | 5 | 1 |
| 3:B:211:PCW:O1P | 3:B:215:PCW:H82 | 0.72 | 1.84 | 4 | 1 |
| 3:A:406:PCW:H121 | 4:A:407:17F:H33 | 0.72 | 1.62 | 10 | 2 |
| 3:B:221:PCW:C28 | 3:C:601:PCW:H242 | 0.72 | 2.15 | 6 | 1 |
| 3:B:223:PCW:H281 | 1:C:521:TYR:CD2 | 0.72 | 2.19 | 5 | 1 |
| 3:B:217:PCW:H40 | 3:B:223:PCW:H451 | 0.71 | 1.59 | 5 | 1 |
| 2:B:5:LYS:NZ | 7:B:239:EWS:OAB | 0.71 | 2.21 | 7 | 3 |
| 3:A:403:PCW:H20 | 3:C:606:PCW:C28 | 0.71 | 2.13 | 1 | 1 |
| 3:B:223:PCW:C28 | 1:C:521:TYR:CE2 | 0.71 | 2.71 | 5 | 1 |
| 3:A:409:PCW:H181 | 3:C:613:PCW:H341 | 0.71 | 1.61 | 2 | 1 |
| 2:B:56:LEU:HD22 | 7:B:239:EWS:CAQ | 0.71 | 2.14 | 8 | 2 |
| 3:B:207:PCW:H81 | 4:B:228:17F:HN1 | 0.71 | 1.45 | 8 | 1 |
| 3:B:221:PCW:C16 | 3:C:601:PCW:H372 | 0.71 | 2.10 | 8 | 1 |
| 1:A:307:ASP:HA | 1:A:310:ARG:HD2 | 0.71 | 1.63 | 10 | 2 |
| 4:C:630:17F:H1 | 4:C:630:17F:C4 | 0.71 | 2.15 | 1 | 3 |
| 3:B:211:PCW:H331 | 4:B:226:17F:H19 | 0.71 | 1.62 | 2 | 1 |
| 1:C:465:GLU:O | 1:C:469:LEU:HB2 | 0.71 | 1.86 | 4 | 1 |
| 1:C:488:LYS:HD3 | 3:C:620:PCW:H281 | 0.71 | 1.61 | 7 | 1 |
| 2:B:5:LYS:HE2 | 7:B:239:EWS:OAB | 0.71 | 1.85 | 9 | 2 |
| 3:B:207:PCW:H481 | 3:C:604:PCW:H261 | 0.71 | 1.62 | 9 | 1 |
| 3:B:215:PCW:H52 | 3:B:217:PCW:H321 | 0.71 | 1.62 | 6 | 2 |
| 1:A:260:ASP:HA | 1:A:263:LYS:HE2 | 0.71 | 1.60 | 1 | 1 |
| 3:A:408:PCW:H172 | 3:A:408:PCW:H382 | 0.70 | 1.62 | 1 | 1 |
| 3:C:620:PCW:C14 | 4:C:633:17F:C32 | 0.70 | 2.66 | 4 | 1 |
| 3:B:223:PCW:C28 | 1:C:521:TYR:HE2 | 0.70 | 1.98 | 5 | 1 |
| 3:B:217:PCW:H39 | 4:B:226:17F:H62 | 0.70 | 1.63 | 1 | 1 |
| 1:A:316:LEU:HG | 1:C:462:LYS:HE3 | 0.70 | 1.63 | 7 | 2 |
| 3:B:204:PCW:H322 | 3:B:212:PCW:H332 | 0.70 | 1.62 | 5 | 1 |
| 2:B:5:LYS:CD | 7:B:239:EWS:CAX | 0.70 | 2.69 | 8 | 3 |
| 1:C:485:ALA:CB | 3:C:620:PCW:H272 | 0.70 | 2.17 | 1 | 1 |
| 3:C:606:PCW:H351 | 3:C:612:PCW:H382 | 0.70 | 1.62 | 2 | 8 |
| 1:A:356:HIS:CD2 | 3:A:401:PCW:H272 | 0.70 | 2.20 | 9 | 1 |
| 3:B:233:PCW:H351 | 3:B:233:PCW:H122 | 0.70 | 1.62 | 9 | 4 |
| 3:B:211:PCW:H321 | 4:B:226:17F:H5 | 0.70 | 1.64 | 4 | 2 |
| 1:A:275:LYS:O | 1:A:279:LEU:HG | 0.70 | 1.87 | 1 | 9 |
| 3:A:403:PCW:H351 | 3:B:212:PCW:H462 | 0.70 | 1.63 | 1 | 1 |
| 1:C:473:LYS:HG2 | 4:C:629:17F:H76 | 0.70 | 1.64 | 6 | 1 |
| 2:B:7:VAL:HG22 | 7:B:239:EWS:CAS | 0.70 | 2.16 | 2 | 1 |
| 3:A:408:PCW:H31 | 3:C:610:PCW:H352 | 0.69 | 1.63 | 1 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:341:ASN:HD21 | 1:C:433:GLU:HA | 0.69 | 1.48 | 5 | 4 |
| 3:B:219:PCW:H441 | 3:B:225:PCW:H441 | 0.69 | 1.64 | 1 | 1 |
| 3:B:216:PCW:H42 | 4:B:229:17F:H1 | 0.69 | 1.64 | 2 | 1 |
| 3:C:609:PCW:H371 | 3:C:624:PCW:H361 | 0.69 | 1.64 | 10 | 1 |
| 4:B:227:17F:H10 | 4:B:227:17F:H58 | 0.69 | 1.64 | 6 | 2 |
| 1:A:393:TYR:CD1 | 3:A:406:PCW:C28 | 0.69 | 2.76 | 2 | 3 |
| 3:C:624:PCW:H39 | 3:C:625:PCW:H421 | 0.69 | 1.62 | 2 | 1 |
| 3:C:613:PCW:H281 | 3:C:623:PCW:H242 | 0.69 | 1.63 | 3 | 1 |
| 3:A:403:PCW:C22 | 3:C:606:PCW:H282 | 0.69 | 2.14 | 1 | 1 |
| 3:C:615:PCW:H211 | 4:C:629:17F:H41 | 0.69 | 1.64 | 5 | 1 |
| 3:B:211:PCW:H332 | 4:B:226:17F:C19 | 0.69 | 2.18 | 10 | 1 |
| 1:C:453:GLN:HB2 | 1:C:454:PRO:HD3 | 0.69 | 1.61 | 7 | 5 |
| 3:A:409:PCW:H242 | 3:A:410:PCW:H231 | 0.69 | 1.62 | 10 | 1 |
| 1:A:308:ARG:HD2 | 1:C:469:LEU:CG | 0.69 | 2.17 | 10 | 1 |
| 3:B:210:PCW:H142 | 3:B:214:PCW:H151 | 0.68 | 1.64 | 5 | 4 |
| 3:B:221:PCW:C12 | 3:C:601:PCW:C36 | 0.68 | 2.55 | 10 | 1 |
| 4:B:226:17F:H42 | 4:B:232:17F:H66 | 0.68 | 1.64 | 10 | 1 |
| 4:C:632:17F:H8A | 4:C:632:17F:H32 | 0.68 | 1.63 | 9 | 2 |
| 1:C:485:ALA:HB1 | 3:C:620:PCW:H272 | 0.68 | 1.64 | 1 | 2 |
| 3:A:406:PCW:H341 | 4:B:227:17F:H9 | 0.68 | 1.65 | 10 | 1 |
| 3:A:403:PCW:H52 | 4:B:231:17F:N1 | 0.68 | 2.03 | 7 | 1 |
| 2:B:56:LEU:HD23 | 7:B:239:EWS:BRA | 0.68 | 2.43 | 8 | 2 |
| 3:B:204:PCW:H421 | 3:B:222:PCW:H182 | 0.68 | 1.65 | 10 | 1 |
| 2:B:56:LEU:CD2 | 7:B:239:EWS:BRA | 0.68 | 2.97 | 8 | 2 |
| 3:B:211:PCW:H322 | 4:B:226:17F:H19 | 0.68 | 1.64 | 1 | 1 |
| 2:B:72:MET:C | 7:B:239:EWS:BRA | 0.68 | 2.87 | 4 | 1 |
| 3:B:212:PCW:H152 | 4:B:231:17F:H6A | 0.68 | 1.66 | 4 | 1 |
| 3:B:217:PCW:H151 | 4:B:226:17F:H34 | 0.68 | 1.66 | 7 | 1 |
| 1:A:308:ARG:CD | 1:C:469:LEU:CD2 | 0.68 | 2.69 | 7 | 2 |
| 3:A:406:PCW:H152 | 4:A:407:17F:H33 | 0.68 | 1.66 | 3 | 1 |
| 3:C:607:PCW:H411 | 3:C:615:PCW:H432 | 0.68 | 1.66 | 3 | 2 |
| 3:B:210:PCW:H211 | 3:C:607:PCW:H461 | 0.68 | 1.66 | 4 | 1 |
| 3:A:406:PCW:H341 | 4:A:407:17F:H32 | 0.68 | 1.65 | 6 | 1 |
| 2:B:158:THR:HA | 2:B:161:ARG:HD2 | 0.68 | 1.66 | 10 | 1 |
| 3:C:618:PCW:H122 | 3:C:626:PCW:H182 | 0.67 | 1.64 | 4 | 1 |
| 3:C:607:PCW:H242 | 3:C:615:PCW:H431 | 0.67 | 1.66 | 10 | 4 |
| 3:B:207:PCW:H83 | 4:B:228:17F:N1 | 0.67 | 2.03 | 3 | 1 |
| 1:C:418:GLN:O | 1:C:422:VAL:HB | 0.67 | 1.88 | 9 | 3 |
| 1:C:488:LYS:CD | 3:C:620:PCW:H272 | 0.67 | 2.18 | 4 | 1 |
| 3:A:403:PCW:C22 | 3:C:606:PCW:C26 | 0.67 | 2.73 | 1 | 1 |
| 3:A:405:PCW:H431 | 3:C:609:PCW:H231 | 0.67 | 1.66 | 3 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 3:B:217:PCW:H40 | 3:B:223:PCW:C45 | 0.67 | 2.19 | 5 | 1 |
| 3:A:410:PCW:H322 | 4:C:630:17F:H37 | 0.67 | 1.66 | 8 | 2 |
| 3:A:401:PCW:H321 | 3:B:203:PCW:H152 | 0.67 | 1.66 | 8 | 1 |
| 3:C:606:PCW:H372 | 3:C:612:PCW:H182 | 0.67 | 1.67 | 10 | 3 |
| 4:B:232:17F:H49 | 3:C:624:PCW:H261 | 0.67 | 1.65 | 5 | 1 |
| 3:C:623:PCW:H371 | 3:C:623:PCW:H122 | 0.67 | 1.64 | 6 | 1 |
| 2:B:38:ASP:HB3 | 2:B:57:ASP:HB3 | 0.67 | 1.65 | 1 | 2 |
| 3:C:601:PCW:H422 | 4:C:627:17F:H54 | 0.67 | 1.65 | 3 | 1 |
| 4:B:236:17F:H57 | 3:C:622:PCW:H141 | 0.67 | 1.66 | 6 | 1 |
| 2:B:7:VAL:CG1 | 7:B:239:EWS:CAS | 0.67 | 2.73 | 10 | 2 |
| 1:A:352:LYS:HG2 | 1:C:422:VAL:HG13 | 0.67 | 1.66 | 9 | 1 |
| 3:A:408:PCW:H371 | 3:A:410:PCW:H362 | 0.67 | 1.65 | 2 | 2 |
| 1:A:308:ARG:CB | 1:C:469:LEU:HD11 | 0.67 | 2.20 | 10 | 3 |
| 3:C:618:PCW:H381 | 3:C:626:PCW:H161 | 0.67 | 1.66 | 8 | 2 |
| 3:C:617:PCW:H372 | 3:C:618:PCW:H121 | 0.67 | 1.67 | 3 | 1 |
| 3:B:217:PCW:H451 | 3:B:223:PCW:C46 | 0.67 | 2.18 | 5 | 1 |
| 3:B:202:PCW:H351 | 3:B:214:PCW:H321 | 0.66 | 1.65 | 6 | 1 |
| 3:B:201:PCW:H221 | 4:B:227:17F:H65 | 0.66 | 1.68 | 1 | 1 |
| 3:A:401:PCW:H61 | 3:B:213:PCW:H11 | 0.66 | 1.67 | 8 | 1 |
| 3:B:213:PCW:H251 | 3:B:213:PCW:H462 | 0.66 | 1.67 | 8 | 1 |
| 1:A:349:TYR:OH | 3:A:401:PCW:C22 | 0.66 | 2.44 | 4 | 1 |
| 3:A:410:PCW:H331 | 4:C:630:17F:H29 | 0.66 | 1.65 | 4 | 1 |
| 3:C:618:PCW:H351 | 3:C:626:PCW:H182 | 0.66 | 1.67 | 10 | 2 |
| 3:B:215:PCW:H81 | 3:B:219:PCW:H73 | 0.66 | 1.65 | 4 | 1 |
| 3:A:410:PCW:H382 | 4:C:630:17F:H36 | 0.66 | 1.67 | 9 | 4 |
| 1:A:308:ARG:HD3 | 1:C:469:LEU:CD2 | 0.66 | 2.21 | 7 | 1 |
| 3:A:406:PCW:H351 | 4:A:407:17F:H56 | 0.66 | 1.68 | 1 | 1 |
| 3:B:201:PCW:H271 | 3:C:611:PCW:H472 | 0.66 | 1.68 | 2 | 1 |
| 3:C:601:PCW:C48 | 3:C:605:PCW:H483 | 0.66 | 2.19 | 10 | 1 |
| 3:A:403:PCW:H222 | 3:C:606:PCW:H262 | 0.66 | 1.67 | 1 | 1 |
| 3:C:624:PCW:H351 | 3:C:625:PCW:H152 | 0.66 | 1.67 | 1 | 4 |
| 3:B:216:PCW:H73 | 4:B:229:17F:H4A | 0.66 | 1.68 | 8 | 1 |
| 3:C:607:PCW:H482 | 4:C:633:17F:H39 | 0.66 | 1.64 | 8 | 1 |
| 3:B:214:PCW:H181 | 4:B:229:17F:H35 | 0.66 | 1.68 | 2 | 1 |
| 1:A:349:TYR:OH | 3:A:401:PCW:H221 | 0.66 | 1.89 | 4 | 1 |
| 2:B:5:LYS:HG3 | 7:B:239:EWS:OAB | 0.66 | 1.90 | 1 | 1 |
| 3:C:606:PCW:H381 | 3:C:612:PCW:H152 | 0.66 | 1.66 | 2 | 1 |
| 3:B:221:PCW:H82 | 4:B:229:17F:O1 | 0.66 | 1.91 | 8 | 1 |
| 3:B:207:PCW:H131 | 3:B:216:PCW:H411 | 0.66 | 1.67 | 4 | 1 |
| 1:C:485:ALA:CB | 3:C:620:PCW:H271 | 0.66 | 2.21 | 7 | 1 |
| 4:B:228:17F:H68 | 3:C:624:PCW:H481 | 0.66 | 1.66 | 8 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 3:C:617:PCW:H372 | 3:C:618:PCW:H142 | 0.65 | 1.68 | 4 | 2 |
| 3:C:620:PCW:H142 | 4:C:633:17F:H59 | 0.65 | 1.68 | 4 | 1 |
| 3:A:408:PCW:H321 | 3:C:610:PCW:H39 | 0.65 | 1.68 | 10 | 1 |
| 3:B:207:PCW:H131 | 3:B:216:PCW:H382 | 0.65 | 1.69 | 6 | 2 |
| 3:B:208:PCW:H151 | 3:B:222:PCW:H351 | 0.65 | 1.67 | 4 | 1 |
| 3:B:209:PCW:H252 | 3:C:601:PCW:C47 | 0.65 | 2.21 | 4 | 1 |
| 3:B:201:PCW:H11 | 4:B:230:17F:HN1 | 0.65 | 1.50 | 5 | 2 |
| 2:B:56:LEU:HD22 | 7:B:239:EWS:CAR | 0.65 | 2.20 | 8 | 1 |
| 2:B:82:PHE:HB3 | 2:B:93:ILE:HD11 | 0.65 | 1.67 | 7 | 5 |
| 1:C:547:TYR:HA | 1:C:550:LYS:HB2 | 0.65 | 1.69 | 3 | 1 |
| 2:B:7:VAL:HA | 7:B:239:EWS:CAT | 0.65 | 2.22 | 1 | 1 |
| 3:B:203:PCW:H12 | 3:B:213:PCW:H332 | 0.65 | 1.68 | 4 | 1 |
| 1:A:349:TYR:CZ | 3:A:401:PCW:H221 | 0.65 | 2.27 | 4 | 1 |
| 3:B:211:PCW:H172 | 4:B:226:17F:H6 | 0.65 | 1.68 | 7 | 1 |
| 3:B:201:PCW:H12 | 4:B:230:17F:O1 | 0.65 | 1.92 | 5 | 2 |
| 3:B:221:PCW:H441 | 3:C:605:PCW:H471 | 0.65 | 1.68 | 3 | 1 |
| 3:B:223:PCW:C48 | 4:C:632:17F:H76 | 0.65 | 2.22 | 5 | 1 |
| 1:A:308:ARG:CG | 1:C:469:LEU:HD21 | 0.64 | 2.15 | 3 | 2 |
| 3:A:406:PCW:H122 | 4:A:407:17F:H20 | 0.64 | 1.66 | 3 | 1 |
| 3:B:207:PCW:H483 | 3:C:601:PCW:H211 | 0.64 | 1.69 | 4 | 1 |
| 3:C:607:PCW:H472 | 4:C:633:17F:H42 | 0.64 | 1.69 | 10 | 1 |
| 3:B:207:PCW:H222 | 3:C:601:PCW:H361 | 0.64 | 1.69 | 1 | 1 |
| 3:B:201:PCW:H212 | 4:B:230:17F:H20A | 0.64 | 1.69 | 8 | 1 |
| 3:A:410:PCW:H361 | 4:C:630:17F:H12A | 0.64 | 1.67 | 3 | 2 |
| 1:C:488:LYS:HG2 | 3:C:620:PCW:H281 | 0.64 | 1.68 | 3 | 1 |
| 3:B:213:PCW:H381 | 3:B:213:PCW:H182 | 0.64 | 1.69 | 6 | 1 |
| 3:C:603:PCW:H332 | 3:C:607:PCW:H132 | 0.64 | 1.68 | 8 | 1 |
| 3:A:405:PCW:H181 | 4:B:228:17F:H58 | 0.64 | 1.67 | 4 | 1 |
| 1:C:497:SER:HB2 | 1:C:498:PRO:HD3 | 0.64 | 1.69 | 8 | 2 |
| 1:A:308:ARG:HG3 | 1:C:469:LEU:CD2 | 0.64 | 2.16 | 3 | 6 |
| 3:A:403:PCW:H222 | 3:C:606:PCW:C26 | 0.64 | 2.22 | 1 | 1 |
| 3:A:409:PCW:H351 | 3:B:235:PCW:H412 | 0.64 | 1.69 | 9 | 1 |
| 3:C:607:PCW:H182 | 3:C:615:PCW:H352 | 0.64 | 1.69 | 9 | 1 |
| 3:B:221:PCW:C16 | 3:C:601:PCW:C38 | 0.64 | 2.64 | 10 | 1 |
| 3:A:409:PCW:H82 | 4:C:630:17F:HN1A | 0.64 | 1.53 | 2 | 1 |
| 3:B:209:PCW:H372 | 4:B:228:17F:H34 | 0.64 | 1.70 | 3 | 1 |
| 3:B:221:PCW:C4 | 3:C:601:PCW:H61 | 0.64 | 2.21 | 4 | 1 |
| 3:B:216:PCW:H20 | 3:C:604:PCW:H482 | 0.64 | 1.67 | 2 | 1 |
| 3:B:210:PCW:H352 | 3:B:214:PCW:H141 | 0.64 | 1.67 | 10 | 1 |
| 1:C:465:GLU:O | 1:C:469:LEU:HD12 | 0.63 | 1.92 | 4 | 2 |
| 1:A:349:TYR:CZ | 3:A:401:PCW:H282 | 0.63 | 2.28 | 7 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:C:595:LEU:HD11 | 4:C:630:17F:H55 | 0.63 | 1.69 | 1 | 2 |
| 3:A:406:PCW:H331 | 4:A:407:17F:H56 | 0.63 | 1.70 | 3 | 1 |
| 3:C:618:PCW:H371 | 3:C:626:PCW:H412 | 0.63 | 1.69 | 7 | 1 |
| 3:A:403:PCW:C37 | 3:B:218:PCW:H471 | 0.63 | 2.23 | 1 | 1 |
| 3:A:402:PCW:H332 | 3:B:205:PCW:H32 | 0.63 | 1.69 | 7 | 2 |
| 3:A:410:PCW:H351 | 4:C:630:17F:H12A | 0.63 | 1.71 | 6 | 2 |
| 3:C:620:PCW:H131 | 4:C:633:17F:C31 | 0.63 | 2.19 | 4 | 1 |
| 3:B:207:PCW:H221 | 3:C:601:PCW:H451 | 0.63 | 1.70 | 8 | 1 |
| 3:B:235:PCW:H32 | 3:C:602:PCW:H11 | 0.63 | 1.70 | 9 | 1 |
| 3:C:618:PCW:H352 | 3:C:626:PCW:H172 | 0.63 | 1.68 | 2 | 1 |
| 3:B:208:PCW:H20 | 3:B:222:PCW:H461 | 0.63 | 1.68 | 3 | 1 |
| 3:C:611:PCW:H151 | 3:C:623:PCW:H452 | 0.63 | 1.69 | 3 | 2 |
| 3:B:223:PCW:C27 | 1:C:521:TYR:HE2 | 0.63 | 2.06 | 5 | 1 |
| 3:A:406:PCW:H483 | 4:B:227:17F:H41 | 0.63 | 1.71 | 1 | 1 |
| 1:A:299:SER:HB2 | 1:A:300:PRO:HD3 | 0.63 | 1.69 | 5 | 4 |
| 3:B:221:PCW:H262 | 1:C:459:PHE:CZ | 0.63 | 2.28 | 5 | 1 |
| 3:B:223:PCW:C47 | 4:C:632:17F:C42 | 0.63 | 2.76 | 5 | 1 |
| 3:A:405:PCW:H352 | 3:B:216:PCW:H421 | 0.63 | 1.71 | 4 | 1 |
| 3:C:620:PCW:C16 | 4:C:633:17F:C1X | 0.63 | 2.67 | 4 | 1 |
| 3:A:409:PCW:H181 | 3:C:613:PCW:H122 | 0.63 | 1.71 | 6 | 2 |
| 3:A:410:PCW:H322 | 4:C:630:17F:H29 | 0.63 | 1.71 | 10 | 1 |
| 3:B:234:PCW:H151 | 3:C:622:PCW:H162 | 0.62 | 1.70 | 10 | 1 |
| 3:B:211:PCW:H381 | 4:B:226:17F:H20A | 0.62 | 1.71 | 1 | 1 |
| 3:B:212:PCW:H331 | 4:B:231:17F:H11 | 0.62 | 1.71 | 9 | 1 |
| 3:B:207:PCW:H441 | 3:B:216:PCW:H272 | 0.62 | 1.71 | 7 | 1 |
| 3:B:223:PCW:H19 | 3:B:225:PCW:H251 | 0.62 | 1.70 | 7 | 1 |
| 4:B:236:17F:H10 | 4:C:628:17F:H38 | 0.62 | 1.69 | 5 | 3 |
| 2:B:5:LYS:CG | 7:B:239:EWS:OAB | 0.62 | 2.48 | 1 | 1 |
| 3:A:406:PCW:H241 | 3:A:408:PCW:H272 | 0.62 | 1.72 | 4 | 1 |
| 3:A:406:PCW:H51 | 4:B:227:17F:O2 | 0.62 | 1.94 | 5 | 1 |
| 3:C:618:PCW:H362 | 3:C:626:PCW:H412 | 0.62 | 1.71 | 6 | 1 |
| 3:B:235:PCW:H342 | 3:C:623:PCW:H121 | 0.62 | 1.72 | 7 | 1 |
| 4:A:407:17F:H50 | 3:C:623:PCW:H252 | 0.62 | 1.71 | 5 | 1 |
| 3:C:609:PCW:H352 | 3:C:624:PCW:H361 | 0.62 | 1.70 | 5 | 1 |
| 3:B:204:PCW:H131 | 4:B:231:17F:H19 | 0.62 | 1.70 | 8 | 1 |
| 3:B:221:PCW:H141 | 3:C:601:PCW:C36 | 0.62 | 2.25 | 8 | 1 |
| 3:B:210:PCW:H181 | 3:B:214:PCW:H181 | 0.62 | 1.69 | 4 | 1 |
| 3:B:204:PCW:H32 | 3:B:208:PCW:H12 | 0.62 | 1.70 | 5 | 1 |
| 4:B:228:17F:H36 | 4:B:232:17F:H37 | 0.62 | 1.72 | 8 | 1 |
| 3:B:206:PCW:H40 | 4:B:226:17F:H73 | 0.62 | 1.71 | 1 | 1 |
| 3:C:604:PCW:H51 | 4:C:627:17F:N1 | 0.62 | 2.10 | 5 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 3:B:209:PCW:H151 | 3:B:216:PCW:H151 | 0.61 | 1.72 | 4 | 1 |
| 4:B:236:17F:H32 | 3:C:622:PCW:H172 | 0.61 | 1.72 | 2 | 5 |
| 3:B:203:PCW:H31 | 3:B:213:PCW:H351 | 0.61 | 1.72 | 10 | 1 |
| 2:B:7:VAL:HA | 7:B:239:EWS:CAU | 0.61 | 2.25 | 1 | 2 |
| 1:C:574:LEU:HB2 | 1:C:575:PRO:HD3 | 0.61 | 1.72 | 3 | 1 |
| 1:A:301:LEU:HD22 | 1:C:473:LYS:HE2 | 0.61 | 1.72 | 6 | 1 |
| 2:B:7:VAL:HB | 7:B:239:EWS:CAS | 0.61 | 2.25 | 8 | 2 |
| 3:B:202:PCW:H352 | 3:B:215:PCW:H152 | 0.61 | 1.73 | 10 | 1 |
| 3:C:605:PCW:H161 | 4:C:629:17F:H18 | 0.61 | 1.70 | 6 | 1 |
| 3:A:406:PCW:H352 | 4:A:407:17F:H56 | 0.61 | 1.73 | 8 | 2 |
| 3:C:620:PCW:H142 | 4:C:633:17F:C32 | 0.61 | 2.25 | 4 | 1 |
| 3:A:409:PCW:H472 | 3:C:613:PCW:H182 | 0.61 | 1.72 | 6 | 1 |
| 1:A:301:LEU:HD13 | 1:C:473:LYS:HG2 | 0.61 | 1.72 | 4 | 2 |
| 3:B:224:PCW:H12 | 3:B:224:PCW:H52 | 0.61 | 1.71 | 5 | 1 |
| 2:B:72:MET:HG2 | 7:B:239:EWS:BRA | 0.61 | 2.51 | 10 | 2 |
| 3:A:410:PCW:C33 | 4:C:630:17F:H29 | 0.61 | 2.20 | 1 | 2 |
| 2:B:56:LEU:HD22 | 7:B:239:EWS:CAD | 0.61 | 2.25 | 1 | 1 |
| 3:B:203:PCW:H12 | 3:B:213:PCW:H322 | 0.61 | 1.73 | 1 | 1 |
| 1:A:356:HIS:HD2 | 3:A:401:PCW:H272 | 0.61 | 1.53 | 9 | 1 |
| 4:B:227:17F:H10A | 4:B:227:17F:H58 | 0.61 | 1.71 | 7 | 1 |
| 3:A:404:PCW:C7 | 7:B:239:EWS:OAB | 0.61 | 2.49 | 10 | 1 |
| 3:C:601:PCW:H482 | 3:C:605:PCW:H481 | 0.61 | 1.67 | 10 | 1 |
| 3:C:607:PCW:H332 | 3:C:615:PCW:H361 | 0.60 | 1.73 | 2 | 1 |
| 3:B:206:PCW:H321 | 3:B:211:PCW:H342 | 0.60 | 1.71 | 1 | 1 |
| 3:A:405:PCW:H381 | 3:B:207:PCW:H372 | 0.60 | 1.73 | 7 | 1 |
| 3:B:224:PCW:H61 | 4:B:229:17F:O4 | 0.60 | 1.96 | 1 | 1 |
| 3:C:603:PCW:H431 | 3:C:607:PCW:H11 | 0.60 | 1.73 | 1 | 1 |
| 3:A:405:PCW:H332 | 3:B:216:PCW:H40 | 0.60 | 1.73 | 3 | 2 |
| 1:A:352:LYS:HZ2 | 1:C:425:GLU:HB3 | 0.60 | 1.54 | 4 | 1 |
| 3:C:607:PCW:H462 | 4:C:633:17F:H42 | 0.60 | 1.72 | 5 | 1 |
| 3:B:233:PCW:H381 | 3:B:233:PCW:H141 | 0.60 | 1.72 | 10 | 2 |
| 1:A:393:TYR:CD1 | 3:A:406:PCW:H281 | 0.60 | 2.31 | 3 | 1 |
| 3:B:221:PCW:C16 | 3:C:601:PCW:C41 | 0.60 | 2.79 | 10 | 1 |
| 3:B:217:PCW:H61 | 4:B:226:17F:N1 | 0.60 | 2.12 | 2 | 1 |
| 3:A:404:PCW:H182 | 3:B:225:PCW:H381 | 0.60 | 1.71 | 4 | 1 |
| 3:B:221:PCW:C41 | 3:C:601:PCW:H39 | 0.60 | 2.22 | 10 | 1 |
| 3:C:604:PCW:H352 | 3:C:605:PCW:H352 | 0.60 | 1.74 | 10 | 1 |
| 3:C:605:PCW:H162 | 4:C:629:17F:H18 | 0.60 | 1.70 | 10 | 1 |
| 3:B:204:PCW:H142 | 3:B:212:PCW:H381 | 0.60 | 1.72 | 1 | 1 |
| 3:C:609:PCW:H412 | 3:C:624:PCW:H211 | 0.60 | 1.73 | 4 | 3 |
| 3:C:601:PCW:C40 | 4:C:627:17F:H54 | 0.60 | 2.26 | 4 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 3:B:203:PCW:H72 | 4:B:230:17F:H6A | 0.60 | 1.72 | 6 | 1 |
| 3:B:210:PCW:H51 | 4:B:229:17F:H6A | 0.60 | 1.74 | 9 | 1 |
| 3:A:409:PCW:H63 | 4:C:630:17F:HN1A | 0.60 | 1.57 | 2 | 1 |
| 3:C:606:PCW:H362 | 3:C:612:PCW:H351 | 0.60 | 1.72 | 10 | 5 |
| 3:B:223:PCW:H471 | 4:C:631:17F:H67 | 0.60 | 1.72 | 2 | 1 |
| 2:B:40:TYR:HE1 | 2:B:57:ASP:HB2 | 0.60 | 1.57 | 3 | 1 |
| 1:C:488:LYS:HZ2 | 3:C:620:PCW:C26 | 0.60 | 2.10 | 4 | 1 |
| 3:B:211:PCW:H331 | 4:B:226:17F:H5 | 0.60 | 1.73 | 6 | 3 |
| 3:A:410:PCW:H382 | 4:C:630:17F:H12A | 0.60 | 1.73 | 1 | 1 |
| 1:C:561:LYS:HA | 1:C:565:ALA:HB3 | 0.60 | 1.73 | 9 | 1 |
| 3:B:221:PCW:H132 | 3:C:601:PCW:H351 | 0.60 | 1.66 | 10 | 1 |
| 3:A:403:PCW:C39 | 3:B:218:PCW:C47 | 0.59 | 2.80 | 1 | 1 |
| 3:C:615:PCW:H181 | 4:C:627:17F:H76 | 0.59 | 1.73 | 1 | 1 |
| 3:B:210:PCW:H252 | 3:C:607:PCW:H471 | 0.59 | 1.73 | 10 | 1 |
| 3:C:618:PCW:H331 | 3:C:626:PCW:H19 | 0.59 | 1.74 | 4 | 1 |
| 3:B:203:PCW:H161 | 4:B:230:17F:H34 | 0.59 | 1.74 | 4 | 1 |
| 3:C:607:PCW:H221 | 3:C:615:PCW:H411 | 0.59 | 1.73 | 5 | 3 |
| 4:C:630:17F:H2 | 4:C:630:17F:C4 | 0.59 | 2.27 | 9 | 2 |
| 3:B:203:PCW:H482 | 4:B:228:17F:H57 | 0.59 | 1.74 | 6 | 1 |
| 1:A:264:LYS:HE3 | 1:C:509:ALA:HB1 | 0.59 | 1.74 | 9 | 2 |
| 1:C:503:MET:HA | 1:C:506:ARG:HD2 | 0.59 | 1.74 | 6 | 5 |
| 3:B:218:PCW:H31 | 3:B:219:PCW:H121 | 0.59 | 1.73 | 4 | 1 |
| 4:B:227:17F:H69 | 3:C:613:PCW:H232 | 0.59 | 1.73 | 7 | 1 |
| 1:A:250:VAL:O | 1:A:254:VAL:HB | 0.59 | 1.97 | 4 | 8 |
| 1:A:369:GLU:O | 1:A:373:GLN:CG | 0.59 | 2.43 | 1 | 2 |
| 3:C:615:PCW:H171 | 4:C:627:17F:H77 | 0.59 | 1.74 | 2 | 1 |
| 1:C:488:LYS:HD3 | 3:C:620:PCW:H272 | 0.59 | 1.73 | 6 | 1 |
| 3:C:613:PCW:H151 | 3:C:613:PCW:H382 | 0.59 | 1.73 | 9 | 1 |
| 3:B:234:PCW:H461 | 3:B:234:PCW:H252 | 0.59 | 1.73 | 7 | 1 |
| 3:A:406:PCW:H321 | 4:A:407:17F:H32 | 0.59 | 1.75 | 1 | 1 |
| 2:B:78:PHE:HB2 | 2:B:111:MET:HG2 | 0.59 | 1.73 | 10 | 3 |
| 1:C:488:LYS:HD3 | 3:C:620:PCW:C27 | 0.59 | 2.28 | 6 | 1 |
| 3:C:621:PCW:H412 | 4:C:632:17F:H34 | 0.59 | 1.75 | 10 | 1 |
| 4:B:226:17F:H65 | 3:C:622:PCW:H482 | 0.59 | 1.75 | 3 | 1 |
| 4:B:226:17F:H72 | 4:B:236:17F:H54 | 0.59 | 1.75 | 4 | 1 |
| 3:C:617:PCW:H331 | 3:C:618:PCW:H141 | 0.59 | 1.75 | 10 | 1 |
| 1:A:288:ARG:O | 1:A:292:HIS:HB2 | 0.58 | 1.98 | 5 | 3 |
| 3:C:606:PCW:H141 | 3:C:612:PCW:H152 | 0.58 | 1.74 | 1 | 1 |
| 3:A:405:PCW:H212 | 3:C:609:PCW:H241 | 0.58 | 1.73 | 6 | 2 |
| 3:C:605:PCW:H212 | 4:C:629:17F:H47 | 0.58 | 1.75 | 7 | 1 |
| 3:B:201:PCW:H262 | 4:B:230:17F:H65 | 0.58 | 1.75 | 9 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 3:B:206:PCW:H171 | 4:B:232:17F:H62 | 0.58 | 1.75 | 10 | 1 |
| 1:A:330:ARG:O | 1:A:334:ARG:HG2 | 0.58 | 1.98 | 4 | 5 |
| 3:A:401:PCW:H462 | 3:C:623:PCW:H481 | 0.58 | 1.73 | 2 | 1 |
| 2:B:114:VAL:HG12 | 2:B:142:ILE:HB | 0.58 | 1.75 | 4 | 3 |
| 3:A:406:PCW:H121 | 4:A:407:17F:H20 | 0.58 | 1.75 | 5 | 1 |
| 3:B:206:PCW:H51 | 3:B:211:PCW:H332 | 0.58 | 1.75 | 1 | 1 |
| 3:C:615:PCW:H422 | 4:C:632:17F:H47 | 0.58 | 1.76 | 5 | 2 |
| 3:A:401:PCW:H482 | 3:C:614:PCW:H222 | 0.58 | 1.75 | 3 | 1 |
| 3:C:604:PCW:H82 | 4:C:627:17F:HN1A | 0.58 | 1.57 | 2 | 1 |
| 3:A:405:PCW:H421 | 4:B:228:17F:H70 | 0.58 | 1.73 | 10 | 1 |
| 3:B:220:PCW:H11 | 3:B:222:PCW:H322 | 0.58 | 1.74 | 10 | 1 |
| 3:B:221:PCW:O11 | 3:C:601:PCW:H362 | 0.58 | 1.97 | 10 | 1 |
| 3:A:401:PCW:H331 | 3:A:405:PCW:H211 | 0.58 | 1.73 | 2 | 1 |
| 3:B:202:PCW:H351 | 3:B:214:PCW:H331 | 0.58 | 1.75 | 4 | 1 |
| 1:C:488:LYS:CE | 3:C:620:PCW:H261 | 0.58 | 2.28 | 4 | 1 |
| 2:B:36:ILE:HA | 2:B:59:ALA:HB2 | 0.58 | 1.76 | 8 | 2 |
| 3:B:204:PCW:H382 | 3:B:205:PCW:H142 | 0.58 | 1.76 | 3 | 1 |
| 3:B:221:PCW:H262 | 1:C:459:PHE:HZ | 0.58 | 1.56 | 5 | 1 |
| 1:A:242:GLU:HB3 | 1:C:532:ARG:HH21 | 0.58 | 1.58 | 5 | 2 |
| 3:B:221:PCW:H272 | 3:C:601:PCW:C22 | 0.58 | 2.29 | 6 | 2 |
| 2:B:40:TYR:HB2 | 2:B:55:ILE:HB | 0.58 | 1.75 | 7 | 2 |
| 3:B:208:PCW:H361 | 3:B:222:PCW:H121 | 0.58 | 1.74 | 10 | 1 |
| 3:A:401:PCW:H361 | 3:B:213:PCW:H212 | 0.58 | 1.75 | 1 | 1 |
| 3:A:410:PCW:H332 | 4:C:630:17F:C1X | 0.58 | 2.25 | 5 | 2 |
| 3:B:206:PCW:H141 | 3:B:222:PCW:H362 | 0.58 | 1.76 | 6 | 1 |
| 3:B:203:PCW:H41 | 4:B:230:17F:H2 | 0.58 | 1.75 | 8 | 1 |
| 2:B:7:VAL:CG1 | 7:B:239:EWS:CAT | 0.58 | 2.81 | 10 | 2 |
| 3:C:606:PCW:H341 | 3:C:612:PCW:H121 | 0.58 | 1.74 | 6 | 2 |
| 3:A:405:PCW:H152 | 4:B:228:17F:H59 | 0.58 | 1.74 | 1 | 2 |
| 3:A:403:PCW:H381 | 3:B:218:PCW:H452 | 0.58 | 1.74 | 2 | 1 |
| 3:A:404:PCW:H152 | 3:B:225:PCW:H251 | 0.58 | 1.76 | 10 | 1 |
| 3:B:207:PCW:H483 | 3:C:601:PCW:C21 | 0.57 | 2.29 | 4 | 1 |
| 3:C:615:PCW:H171 | 4:C:633:17F:H10 | 0.57 | 1.76 | 9 | 1 |
| 3:B:221:PCW:H51 | 4:B:229:17F:HN1 | 0.57 | 1.58 | 4 | 1 |
| 3:C:615:PCW:H221 | 4:C:629:17F:H38 | 0.57 | 1.75 | 9 | 2 |
| 3:A:406:PCW:C34 | 4:B:227:17F:H11 | 0.57 | 2.28 | 8 | 1 |
| 3:B:233:PCW:H382 | 3:B:233:PCW:H422 | 0.57 | 1.76 | 10 | 1 |
| 3:B:207:PCW:H212 | 3:C:601:PCW:H412 | 0.57 | 1.76 | 2 | 1 |
| 1:C:523:ASP:HA | 1:C:526:ARG:HD2 | 0.57 | 1.74 | 2 | 3 |
| 3:C:609:PCW:H82 | 3:C:625:PCW:H2 | 0.57 | 1.76 | 5 | 1 |
| 3:A:403:PCW:H52 | 4:B:231:17F:HN1 | 0.57 | 1.58 | 7 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 3:B:201:PCW:H152 | 3:B:201:PCW:H211 | 0.57 | 1.76 | 1 | 1 |
| 3:B:212:PCW:H322 | 4:B:231:17F:H11 | 0.57 | 1.75 | 1 | 1 |
| 3:B:210:PCW:H81 | 4:B:226:17F:O1 | 0.57 | 1.99 | 4 | 1 |
| 4:B:226:17F:H73 | 4:B:236:17F:H50 | 0.57 | 1.74 | 6 | 1 |
| 4:C:628:17F:H64 | 4:C:632:17F:H11 | 0.57 | 1.75 | 6 | 1 |
| 3:B:222:PCW:H52 | 4:B:227:17F:N1 | 0.57 | 2.12 | 7 | 1 |
| 4:B:236:17F:H56 | 3:C:622:PCW:H141 | 0.57 | 1.77 | 7 | 2 |
| 3:C:620:PCW:C13 | 4:C:633:17F:H56 | 0.57 | 2.24 | 4 | 1 |
| 3:C:623:PCW:H40 | 3:C:624:PCW:H211 | 0.57 | 1.76 | 8 | 1 |
| 3:A:405:PCW:H39 | 3:B:216:PCW:H451 | 0.57 | 1.76 | 3 | 1 |
| 1:A:368:LEU:CD1 | 4:B:230:17F:H54 | 0.57 | 2.12 | 8 | 1 |
| 3:B:201:PCW:H32 | 4:B:230:17F:H1A | 0.57 | 1.75 | 5 | 1 |
| 3:B:201:PCW:H361 | 4:B:227:17F:H31 | 0.57 | 1.77 | 5 | 1 |
| 3:B:220:PCW:H42 | 4:B:232:17F:H19A | 0.57 | 1.75 | 6 | 1 |
| 3:C:604:PCW:H31 | 3:C:625:PCW:H332 | 0.57 | 1.76 | 8 | 1 |
| 3:B:220:PCW:H12 | 3:B:222:PCW:H322 | 0.57 | 1.77 | 1 | 1 |
| 3:A:405:PCW:H162 | 3:C:609:PCW:H252 | 0.57 | 1.75 | 3 | 2 |
| 1:C:491:GLU:HG2 | 1:C:495:LYS:HE3 | 0.57 | 1.75 | 3 | 1 |
| 3:C:607:PCW:H262 | 3:C:615:PCW:H452 | 0.57 | 1.75 | 4 | 1 |
| 3:B:210:PCW:H382 | 3:B:214:PCW:H152 | 0.57 | 1.76 | 5 | 1 |
| 3:A:410:PCW:C31 | 4:C:630:17F:H11 | 0.57 | 2.29 | 7 | 1 |
| 2:B:170:MET:SD | 3:B:211:PCW:H42 | 0.57 | 2.40 | 7 | 1 |
| 1:A:334:ARG:HD2 | 1:C:440:GLU:OE1 | 0.57 | 1.99 | 3 | 6 |
| 1:C:491:GLU:HB3 | 1:C:495:LYS:HE2 | 0.57 | 1.76 | 7 | 5 |
| 3:B:213:PCW:H221 | 3:B:213:PCW:H441 | 0.57 | 1.77 | 5 | 1 |
| 4:B:229:17F:H54 | 3:C:607:PCW:H241 | 0.57 | 1.76 | 6 | 1 |
| 1:A:368:LEU:HD11 | 4:B:230:17F:C30 | 0.57 | 2.12 | 8 | 1 |
| 4:B:229:17F:H75 | 4:C:629:17F:H54 | 0.57 | 1.75 | 2 | 1 |
| 4:C:627:17F:H10A | 4:C:629:17F:H31 | 0.57 | 1.76 | 3 | 1 |
| 3:B:213:PCW:H31 | 3:B:213:PCW:O1P | 0.57 | 2.00 | 4 | 1 |
| 3:B:204:PCW:H12 | 3:B:212:PCW:O2P | 0.57 | 2.00 | 7 | 1 |
| 3:B:234:PCW:H39 | 3:C:602:PCW:H283 | 0.57 | 1.77 | 7 | 1 |
| 3:B:207:PCW:H352 | 3:B:216:PCW:H421 | 0.57 | 1.77 | 10 | 1 |
| 1:A:352:LYS:NZ | 1:C:425:GLU:HB2 | 0.56 | 2.15 | 3 | 1 |
| 3:B:202:PCW:H182 | 3:B:215:PCW:H242 | 0.56 | 1.77 | 6 | 1 |
| 1:A:308:ARG:HD3 | 1:C:469:LEU:CG | 0.56 | 2.30 | 7 | 1 |
| 3:B:208:PCW:H62 | 3:B:219:PCW:H41 | 0.56 | 1.76 | 9 | 1 |
| 3:B:209:PCW:H472 | 4:B:228:17F:H68 | 0.56 | 1.75 | 10 | 1 |
| 3:B:206:PCW:H461 | 4:B:226:17F:H78 | 0.56 | 1.74 | 4 | 1 |
| 1:C:512:ASP:HA | 1:C:515:ARG:HD2 | 0.56 | 1.77 | 5 | 2 |
| 3:A:405:PCW:H182 | 3:C:609:PCW:H252 | 0.56 | 1.77 | 8 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 3:A:408:PCW:H73 | 3:A:410:PCW:O1P | 0.56 | 2.00 | 1 | 1 |
| 3:B:214:PCW:H262 | 4:C:633:17F:H48 | 0.56 | 1.77 | 1 | 1 |
| 3:C:619:PCW:H381 | 3:C:619:PCW:H151 | 0.56 | 1.76 | 1 | 2 |
| 1:A:393:TYR:CE1 | 3:A:406:PCW:H283 | 0.56 | 2.34 | 2 | 1 |
| 3:A:409:PCW:H461 | 3:C:613:PCW:H172 | 0.56 | 1.76 | 2 | 1 |
| 3:B:221:PCW:H342 | 4:B:229:17F:H19 | 0.56 | 1.77 | 2 | 1 |
| 3:B:201:PCW:H11 | 4:B:230:17F:N1 | 0.56 | 2.15 | 5 | 1 |
| 3:B:217:PCW:H432 | 3:B:223:PCW:C45 | 0.56 | 2.20 | 5 | 1 |
| 3:B:209:PCW:H442 | 4:B:232:17F:H43 | 0.56 | 1.75 | 9 | 1 |
| 3:C:601:PCW:H483 | 3:C:605:PCW:C47 | 0.56 | 2.29 | 10 | 1 |
| 1:C:451:LYS:O | 1:C:455:TYR:HB2 | 0.56 | 1.99 | 8 | 6 |
| 3:A:404:PCW:H352 | 3:B:225:PCW:H132 | 0.56 | 1.77 | 2 | 1 |
| 3:B:207:PCW:C7 | 4:B:228:17F:HN1 | 0.56 | 2.13 | 4 | 1 |
| 3:C:603:PCW:H40 | 4:C:628:17F:H6 | 0.56 | 1.77 | 2 | 1 |
| 3:B:203:PCW:H151 | 3:B:213:PCW:H372 | 0.56 | 1.76 | 3 | 1 |
| 3:B:201:PCW:C37 | 4:B:228:17F:H37 | 0.56 | 2.29 | 10 | 1 |
| 2:B:94:HIS:O | 2:B:98:GLU:HG2 | 0.56 | 2.00 | 1 | 1 |
| 4:B:228:17F:H62 | 3:C:624:PCW:H481 | 0.56 | 1.76 | 2 | 1 |
| 4:C:630:17F:H4A | 4:C:630:17F:O4 | 0.56 | 2.00 | 2 | 1 |
| 3:C:621:PCW:H211 | 4:C:631:17F:H31 | 0.56 | 1.78 | 3 | 1 |
| 1:C:488:LYS:NZ | 3:C:620:PCW:C25 | 0.56 | 2.68 | 4 | 1 |
| 3:B:216:PCW:H71 | 4:B:229:17F:H19 | 0.56 | 1.78 | 9 | 1 |
| 3:C:623:PCW:H122 | 3:C:623:PCW:H381 | 0.56 | 1.76 | 9 | 1 |
| 1:A:277:GLU:HB2 | 1:A:278:PRO:HD3 | 0.56 | 1.77 | 2 | 1 |
| 3:B:209:PCW:H471 | 3:C:609:PCW:H482 | 0.56 | 1.77 | 5 | 1 |
| 3:C:614:PCW:H222 | 3:C:614:PCW:H472 | 0.56 | 1.78 | 6 | 1 |
| 3:A:409:PCW:H51 | 4:C:630:17F:HN1A | 0.56 | 1.59 | 10 | 1 |
| 3:B:208:PCW:H451 | 3:B:234:PCW:H241 | 0.56 | 1.76 | 10 | 1 |
| 3:B:216:PCW:O1P | 3:B:221:PCW:H73 | 0.56 | 2.01 | 2 | 1 |
| 4:B:236:17F:H30 | 3:C:622:PCW:H271 | 0.56 | 1.77 | 2 | 1 |
| 3:B:201:PCW:H73 | 4:B:227:17F:O5 | 0.56 | 2.01 | 3 | 1 |
| 2:B:5:LYS:HD2 | 7:B:239:EWS:CAX | 0.56 | 2.30 | 7 | 1 |
| 3:C:615:PCW:H40 | 4:C:632:17F:H55 | 0.56 | 1.77 | 8 | 1 |
| 3:B:221:PCW:H411 | 3:C:601:PCW:C39 | 0.56 | 2.23 | 10 | 1 |
| 3:B:212:PCW:H81 | 4:B:231:17F:O2 | 0.56 | 2.01 | 1 | 1 |
| 3:B:203:PCW:H40 | 4:B:228:17F:H11 | 0.56 | 1.75 | 2 | 1 |
| 3:B:204:PCW:H52 | 3:B:205:PCW:H81 | 0.56 | 1.78 | 3 | 1 |
| 3:C:611:PCW:H161 | 3:C:619:PCW:H19 | 0.56 | 1.77 | 4 | 1 |
| 3:B:204:PCW:H142 | 3:B:212:PCW:H39 | 0.56 | 1.76 | 5 | 1 |
| 3:C:605:PCW:H19 | 4:C:627:17F:H59 | 0.56 | 1.78 | 7 | 1 |
| 3:C:621:PCW:H442 | 4:C:632:17F:H37 | 0.56 | 1.78 | 7 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 3:A:404:PCW:H222 | 4:C:631:17F:H50 | 0.56 | 1.78 | 1 | 1 |
| 4:B:227:17F:H44 | 3:C:613:PCW:H241 | 0.56 | 1.78 | 1 | 1 |
| 2:B:72:MET:HG3 | 7:B:239:EWS:BRA | 0.56 | 2.56 | 3 | 1 |
| 3:B:209:PCW:H442 | 4:B:228:17F:H61 | 0.56 | 1.78 | 4 | 1 |
| 3:C:618:PCW:H382 | 3:C:626:PCW:H171 | 0.56 | 1.79 | 10 | 2 |
| 3:B:210:PCW:H321 | 4:B:229:17F:H10A | 0.56 | 1.76 | 10 | 1 |
| 3:C:609:PCW:H372 | 3:C:624:PCW:H181 | 0.56 | 1.77 | 10 | 1 |
| 3:C:620:PCW:H322 | 4:C:633:17F:H77 | 0.55 | 1.77 | 1 | 1 |
| 1:C:508:ARG:O | 1:C:512:ASP:HB2 | 0.55 | 2.01 | 9 | 3 |
| 3:B:210:PCW:H211 | 3:B:214:PCW:H40 | 0.55 | 1.77 | 3 | 1 |
| 3:B:201:PCW:H212 | 4:B:230:17F:H58 | 0.55 | 1.78 | 6 | 1 |
| 3:B:209:PCW:H131 | 3:B:216:PCW:H152 | 0.55 | 1.78 | 10 | 1 |
| 3:B:203:PCW:H151 | 3:B:213:PCW:H39 | 0.55 | 1.78 | 1 | 1 |
| 2:B:79:LEU:HD23 | 2:B:112:VAL:HB | 0.55 | 1.78 | 9 | 2 |
| 3:B:216:PCW:H52 | 4:B:229:17F:HN1 | 0.55 | 1.60 | 3 | 1 |
| 4:B:230:17F:H1 | 4:B:230:17F:C4 | 0.55 | 2.24 | 9 | 1 |
| 2:B:56:LEU:CD2 | 7:B:239:EWS:CAR | 0.55 | 2.84 | 8 | 1 |
| 3:B:208:PCW:H381 | 3:B:222:PCW:H141 | 0.55 | 1.78 | 10 | 1 |
| 3:B:221:PCW:C27 | 3:C:601:PCW:H221 | 0.55 | 2.26 | 2 | 2 |
| 1:C:444:ASP:O | 1:C:448:VAL:HB | 0.55 | 2.02 | 3 | 2 |
| 3:B:201:PCW:H422 | 3:B:220:PCW:H441 | 0.55 | 1.76 | 8 | 1 |
| 4:B:230:17F:H74 | 3:C:611:PCW:H222 | 0.55 | 1.79 | 2 | 1 |
| 3:B:218:PCW:H73 | 4:B:231:17F:HN1A | 0.55 | 1.59 | 6 | 1 |
| 3:C:601:PCW:H482 | 3:C:605:PCW:C48 | 0.55 | 2.25 | 10 | 1 |
| 1:A:345:ARG:HA | 1:C:429:ASN:HD21 | 0.55 | 1.61 | 3 | 2 |
| 3:B:212:PCW:H362 | 4:B:231:17F:H10A | 0.55 | 1.78 | 5 | 2 |
| 3:B:210:PCW:H61 | 4:B:229:17F:H2 | 0.55 | 1.77 | 2 | 1 |
| 1:A:393:TYR:CE1 | 3:A:411:PCW:H272 | 0.55 | 2.35 | 3 | 1 |
| 3:B:204:PCW:H412 | 3:B:205:PCW:H151 | 0.55 | 1.79 | 6 | 1 |
| 4:B:228:17F:H53 | 3:C:624:PCW:H271 | 0.55 | 1.78 | 9 | 1 |
| 1:C:478:ARG:O | 1:C:482:GLN:HB2 | 0.55 | 2.02 | 4 | 2 |
| 3:A:405:PCW:H283 | 3:C:609:PCW:H261 | 0.55 | 1.79 | 4 | 1 |
| 3:C:606:PCW:H351 | 3:C:612:PCW:H381 | 0.55 | 1.78 | 7 | 1 |
| 3:C:604:PCW:H51 | 4:C:627:17F:HN1A | 0.55 | 1.61 | 1 | 2 |
| 3:B:218:PCW:H41 | 4:B:231:17F:O1 | 0.55 | 2.01 | 3 | 1 |
| 1:A:352:LYS:NZ | 1:C:425:GLU:HB3 | 0.55 | 2.17 | 4 | 1 |
| 3:A:406:PCW:H331 | 4:A:407:17F:H32 | 0.55 | 1.79 | 5 | 2 |
| 3:C:605:PCW:H82 | 3:C:607:PCW:H142 | 0.55 | 1.78 | 1 | 2 |
| 3:A:404:PCW:H282 | 3:C:618:PCW:H412 | 0.55 | 1.78 | 3 | 1 |
| 3:C:603:PCW:H39 | 4:C:628:17F:H6 | 0.55 | 1.78 | 4 | 1 |
| 3:B:206:PCW:H31 | 3:B:206:PCW:H51 | 0.55 | 1.78 | 6 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 3:B:213:PCW:H121 | 4:B:228:17F:H6 | 0.55 | 1.79 | 6 | 1 |
| 3:C:611:PCW:H412 | 3:C:611:PCW:H19 | 0.55 | 1.78 | 6 | 1 |
| 3:B:221:PCW:H141 | 3:C:601:PCW:H332 | 0.55 | 1.79 | 2 | 1 |
| 3:A:405:PCW:H132 | 3:A:405:PCW:H331 | 0.54 | 1.78 | 1 | 1 |
| 2:B:6:LEU:HD22 | 2:B:159:LEU:HD23 | 0.54 | 1.79 | 1 | 2 |
| 3:B:214:PCW:H441 | 3:B:217:PCW:H251 | 0.54 | 1.78 | 4 | 1 |
| 3:C:605:PCW:H172 | 4:C:629:17F:H18 | 0.54 | 1.78 | 5 | 1 |
| 3:B:203:PCW:O31 | 4:B:230:17F:H6 | 0.54 | 2.02 | 6 | 2 |
| 3:C:609:PCW:H382 | 3:C:624:PCW:H422 | 0.54 | 1.78 | 10 | 1 |
| 3:B:204:PCW:O2P | 3:B:222:PCW:H71 | 0.54 | 2.01 | 1 | 1 |
| 3:C:618:PCW:H431 | 3:C:618:PCW:H162 | 0.54 | 1.78 | 2 | 1 |
| 3:B:217:PCW:H281 | 4:C:632:17F:H70 | 0.54 | 1.79 | 7 | 2 |
| 3:B:217:PCW:H272 | 4:C:632:17F:H38 | 0.54 | 1.79 | 4 | 1 |
| 3:B:216:PCW:H411 | 3:B:224:PCW:H222 | 0.54 | 1.80 | 5 | 1 |
| 2:B:62:GLU:HG2 | 2:B:68:ARG:HD3 | 0.54 | 1.77 | 1 | 1 |
| 3:B:201:PCW:H122 | 4:B:227:17F:H18A | 0.54 | 1.78 | 3 | 1 |
| 1:C:502:GLU:HG2 | 1:C:506:ARG:HE | 0.54 | 1.63 | 3 | 2 |
| 1:C:458:ASP:HA | 1:C:461:LYS:HE3 | 0.54 | 1.78 | 4 | 1 |
| 1:C:488:LYS:HZ1 | 3:C:620:PCW:C25 | 0.54 | 2.15 | 4 | 1 |
| 3:B:204:PCW:H352 | 3:B:222:PCW:H161 | 0.54 | 1.79 | 5 | 1 |
| 4:B:231:17F:H33 | 4:B:231:17F:H8 | 0.54 | 1.80 | 5 | 2 |
| 1:A:349:TYR:HE2 | 3:A:401:PCW:C26 | 0.54 | 2.10 | 7 | 1 |
| 3:C:607:PCW:H261 | 3:C:615:PCW:H432 | 0.54 | 1.78 | 8 | 1 |
| 3:A:408:PCW:H171 | 3:A:411:PCW:H152 | 0.54 | 1.80 | 1 | 1 |
| 3:C:614:PCW:H171 | 3:C:614:PCW:H381 | 0.54 | 1.80 | 9 | 2 |
| 3:C:621:PCW:H411 | 4:C:632:17F:H34 | 0.54 | 1.80 | 4 | 2 |
| 3:B:201:PCW:H32 | 4:B:227:17F:N1 | 0.54 | 2.17 | 8 | 1 |
| 1:A:332:ALA:O | 1:A:336:GLU:HB2 | 0.54 | 2.03 | 1 | 1 |
| 3:C:613:PCW:H132 | 3:C:619:PCW:H382 | 0.54 | 1.78 | 2 | 2 |
| 3:B:211:PCW:H121 | 4:B:226:17F:H18 | 0.54 | 1.80 | 6 | 1 |
| 3:B:223:PCW:H481 | 4:C:631:17F:H61 | 0.54 | 1.78 | 9 | 1 |
| 4:C:632:17F:H61 | 4:C:633:17F:H71 | 0.54 | 1.77 | 9 | 1 |
| 3:A:408:PCW:H2 | 3:A:410:PCW:H332 | 0.54 | 1.78 | 10 | 1 |
| 3:B:210:PCW:H162 | 3:B:214:PCW:H361 | 0.54 | 1.78 | 10 | 1 |
| 3:B:210:PCW:H422 | 4:B:229:17F:H72 | 0.54 | 1.80 | 1 | 1 |
| 3:B:224:PCW:H83 | 4:B:226:17F:H4A | 0.54 | 1.79 | 2 | 1 |
| 3:B:211:PCW:H332 | 4:B:226:17F:O10 | 0.54 | 2.02 | 5 | 1 |
| 3:A:406:PCW:H362 | 4:A:407:17F:H56 | 0.54 | 1.79 | 6 | 1 |
| 3:B:214:PCW:H241 | 4:C:633:17F:H52 | 0.54 | 1.79 | 1 | 1 |
| 3:C:610:PCW:H20 | 3:C:616:PCW:H483 | 0.54 | 1.78 | 1 | 1 |
| 1:C:492:LEU:HD11 | 3:C:620:PCW:H482 | 0.54 | 1.79 | 10 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:393:TYR:HB3 | 3:A:406:PCW:H281 | 0.54 | 1.79 | 3 | 1 |
| 1:A:341:ASN:ND2 | 1:C:433:GLU:HA | 0.54 | 2.17 | 5 | 1 |
| 3:C:605:PCW:H2 | 3:C:605:PCW:O2P | 0.54 | 2.02 | 5 | 1 |
| 1:A:325:ASP:HA | 1:A:328:ARG:HD2 | 0.54 | 1.79 | 8 | 2 |
| 3:B:203:PCW:H281 | 3:C:611:PCW:H242 | 0.54 | 1.80 | 8 | 1 |
| 3:A:403:PCW:C38 | 3:B:218:PCW:C47 | 0.54 | 2.63 | 1 | 1 |
| 1:A:308:ARG:CB | 1:C:469:LEU:CD1 | 0.54 | 2.84 | 10 | 1 |
| 3:B:203:PCW:H362 | 3:B:213:PCW:H381 | 0.54 | 1.79 | 3 | 3 |
| 4:C:627:17F:H71 | 4:C:629:17F:H53 | 0.54 | 1.80 | 4 | 1 |
| 4:C:627:17F:H66 | 4:C:629:17F:H55 | 0.54 | 1.80 | 8 | 1 |
| 2:B:8:VAL:HG22 | 2:B:79:LEU:HD12 | 0.53 | 1.81 | 2 | 1 |
| 1:C:465:GLU:HB3 | 1:C:469:LEU:HD11 | 0.53 | 1.80 | 4 | 2 |
| 3:C:606:PCW:H172 | 3:C:616:PCW:H411 | 0.53 | 1.80 | 4 | 1 |
| 3:B:214:PCW:H282 | 3:C:615:PCW:H432 | 0.53 | 1.80 | 6 | 1 |
| 1:C:544:LEU:O | 1:C:548:HIS:HB2 | 0.53 | 2.03 | 3 | 1 |
| 3:C:607:PCW:H372 | 3:C:615:PCW:H412 | 0.53 | 1.79 | 3 | 2 |
| 1:A:244:SER:O | 1:A:248:GLU:HB2 | 0.53 | 2.03 | 6 | 1 |
| 3:B:219:PCW:H472 | 3:B:223:PCW:H431 | 0.53 | 1.80 | 7 | 1 |
| 3:B:201:PCW:H361 | 3:B:220:PCW:C35 | 0.53 | 2.25 | 10 | 1 |
| 3:B:220:PCW:H352 | 3:B:220:PCW:H152 | 0.53 | 1.79 | 9 | 2 |
| 3:B:209:PCW:H131 | 3:B:216:PCW:H142 | 0.53 | 1.78 | 3 | 1 |
| 1:C:546:GLU:O | 1:C:550:LYS:HD2 | 0.53 | 2.03 | 10 | 2 |
| 1:C:514:LEU:HA | 1:C:517:HIS:HB2 | 0.53 | 1.80 | 7 | 1 |
| 3:B:221:PCW:H141 | 3:C:601:PCW:C37 | 0.53 | 2.32 | 8 | 1 |
| 3:B:201:PCW:H351 | 3:B:220:PCW:H342 | 0.53 | 1.81 | 2 | 1 |
| 1:C:528:ARG:HB3 | 1:C:532:ARG:NH2 | 0.53 | 2.16 | 10 | 2 |
| 3:C:611:PCW:H332 | 3:C:623:PCW:H411 | 0.53 | 1.79 | 6 | 1 |
| 3:B:213:PCW:H72 | 4:B:230:17F:O1 | 0.53 | 2.04 | 8 | 2 |
| 3:C:607:PCW:H372 | 3:C:615:PCW:H411 | 0.53 | 1.79 | 9 | 1 |
| 3:C:603:PCW:H411 | 4:C:628:17F:H9A | 0.53 | 1.80 | 1 | 1 |
| 1:C:473:LYS:O | 1:C:477:LEU:HB2 | 0.53 | 2.03 | 4 | 2 |
| 3:B:215:PCW:H83 | 3:B:217:PCW:P | 0.53 | 2.44 | 4 | 1 |
| 3:C:611:PCW:H422 | 3:C:624:PCW:H271 | 0.53 | 1.79 | 3 | 1 |
| 3:B:223:PCW:H281 | 1:C:521:TYR:OH | 0.53 | 2.03 | 10 | 1 |
| 4:B:226:17F:H71 | 3:C:622:PCW:H483 | 0.53 | 1.80 | 4 | 1 |
| 3:B:213:PCW:H82 | 3:B:213:PCW:H322 | 0.53 | 1.80 | 7 | 1 |
| 3:B:201:PCW:H32 | 4:B:227:17F:HN1A | 0.53 | 1.64 | 8 | 1 |
| 3:A:404:PCW:H12 | 3:B:218:PCW:H352 | 0.53 | 1.80 | 2 | 1 |
| 1:C:495:LYS:O | 1:C:499:LEU:HB2 | 0.53 | 2.04 | 2 | 5 |
| 3:A:409:PCW:H412 | 3:C:619:PCW:H412 | 0.53 | 1.79 | 4 | 1 |
| 3:B:211:PCW:H121 | 4:B:226:17F:C18 | 0.53 | 2.34 | 6 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:308:ARG:HG3 | 1:C:469:LEU:HD13 | 0.53 | 1.76 | 10 | 1 |
| 3:B:210:PCW:H362 | 3:B:214:PCW:H161 | 0.53 | 1.79 | 5 | 1 |
| 1:C:469:LEU:O | 1:C:473:LYS:HB2 | 0.53 | 2.03 | 6 | 1 |
| 3:B:215:PCW:H83 | 3:B:217:PCW:H11 | 0.53 | 1.80 | 7 | 1 |
| 3:B:207:PCW:H71 | 4:B:228:17F:H1 | 0.53 | 1.81 | 10 | 1 |
| 3:C:608:PCW:H31 | 4:C:631:17F:H4A | 0.52 | 1.81 | 1 | 3 |
| 3:A:405:PCW:H142 | 3:C:609:PCW:H271 | 0.52 | 1.82 | 6 | 1 |
| 3:B:201:PCW:H381 | 4:B:227:17F:H56 | 0.52 | 1.79 | 6 | 1 |
| 4:B:236:17F:H40 | 4:B:236:17F:H72 | 0.52 | 1.80 | 7 | 1 |
| 3:B:216:PCW:H462 | 3:C:604:PCW:H481 | 0.52 | 1.79 | 2 | 1 |
| 3:C:611:PCW:H283 | 3:C:614:PCW:H441 | 0.52 | 1.81 | 3 | 1 |
| 3:B:206:PCW:H231 | 3:B:220:PCW:H422 | 0.52 | 1.81 | 4 | 1 |
| 3:B:235:PCW:H341 | 3:C:623:PCW:H331 | 0.52 | 1.82 | 4 | 1 |
| 4:B:236:17F:H70 | 3:C:603:PCW:H282 | 0.52 | 1.81 | 6 | 1 |
| 4:B:232:17F:H70 | 3:B:233:PCW:H281 | 0.52 | 1.81 | 7 | 1 |
| 2:B:170:MET:SD | 3:B:208:PCW:H61 | 0.52 | 2.45 | 10 | 1 |
| 3:B:206:PCW:H19 | 4:B:226:17F:H37 | 0.52 | 1.82 | 4 | 1 |
| 3:B:222:PCW:H40 | 3:B:234:PCW:H252 | 0.52 | 1.81 | 4 | 1 |
| 3:B:221:PCW:H461 | 3:C:605:PCW:H242 | 0.52 | 1.80 | 5 | 1 |
| 1:A:388:SER:HB3 | 1:C:594:LYS:HE2 | 0.52 | 1.81 | 6 | 1 |
| 3:B:201:PCW:H351 | 3:B:220:PCW:C34 | 0.52 | 2.33 | 5 | 1 |
| 3:B:221:PCW:H51 | 4:B:229:17F:H1 | 0.52 | 1.81 | 7 | 1 |
| 3:B:210:PCW:H151 | 3:B:217:PCW:H141 | 0.52 | 1.80 | 8 | 1 |
| 3:A:406:PCW:H361 | 4:B:227:17F:H11 | 0.52 | 1.81 | 9 | 2 |
| 3:C:603:PCW:O1P | 3:C:605:PCW:H72 | 0.52 | 2.03 | 5 | 1 |
| 4:C:628:17F:H5 | 4:C:632:17F:H1A | 0.52 | 1.82 | 10 | 2 |
| 3:B:233:PCW:H141 | 3:B:233:PCW:H371 | 0.52 | 1.80 | 1 | 1 |
| 1:A:310:ARG:O | 1:A:314:ASP:HB2 | 0.52 | 2.05 | 7 | 2 |
| 3:C:618:PCW:O3 | 3:C:626:PCW:H161 | 0.52 | 2.04 | 5 | 1 |
| 3:A:406:PCW:H452 | 3:A:409:PCW:H282 | 0.52 | 1.81 | 6 | 1 |
| 3:C:614:PCW:H412 | 3:C:614:PCW:H172 | 0.52 | 1.81 | 8 | 1 |
| 3:B:207:PCW:H211 | 3:B:209:PCW:H272 | 0.52 | 1.81 | 5 | 1 |
| 3:A:405:PCW:H162 | 3:C:609:PCW:H271 | 0.52 | 1.79 | 6 | 1 |
| 3:B:221:PCW:C15 | 3:C:601:PCW:H351 | 0.52 | 2.35 | 8 | 1 |
| 3:B:221:PCW:H161 | 3:C:601:PCW:C40 | 0.52 | 2.28 | 10 | 1 |
| 4:B:232:17F:H54 | 3:C:624:PCW:H241 | 0.52 | 1.81 | 3 | 1 |
| 3:C:609:PCW:H382 | 3:C:624:PCW:H381 | 0.52 | 1.81 | 3 | 1 |
| 3:A:405:PCW:H331 | 3:B:209:PCW:H351 | 0.52 | 1.81 | 6 | 1 |
| 3:A:410:PCW:C12 | 4:C:630:17F:H30 | 0.52 | 2.35 | 8 | 3 |
| 3:A:409:PCW:H211 | 3:C:613:PCW:H161 | 0.52 | 1.81 | 7 | 1 |
| 3:C:603:PCW:H431 | 3:C:607:PCW:H321 | 0.52 | 1.81 | 7 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 3:A:406:PCW:H452 | 3:C:613:PCW:H221 | 0.52 | 1.82 | 8 | 1 |
| 2:B:30:ASP:HA | 5:B:237:GNP:H3' | 0.52 | 1.81 | 10 | 2 |
| 3:B:211:PCW:H151 | 4:B:229:17F:H12 | 0.52 | 1.80 | 10 | 1 |
| 4:B:227:17F:H44 | 3:C:613:PCW:C24 | 0.52 | 2.35 | 1 | 1 |
| 3:C:607:PCW:H261 | 3:C:615:PCW:H431 | 0.52 | 1.82 | 2 | 1 |
| 3:C:621:PCW:H481 | 3:C:622:PCW:H481 | 0.52 | 1.82 | 8 | 2 |
| 1:C:488:LYS:HZ2 | 3:C:620:PCW:C27 | 0.52 | 2.18 | 4 | 1 |
| 3:B:219:PCW:O31 | 3:B:225:PCW:H41 | 0.52 | 2.05 | 5 | 1 |
| 2:B:7:VAL:HG11 | 7:B:239:EWS:CAS | 0.52 | 2.35 | 10 | 1 |
| 3:C:606:PCW:H431 | 3:C:612:PCW:H162 | 0.52 | 1.82 | 1 | 1 |
| 3:B:206:PCW:H32 | 3:B:208:PCW:O1P | 0.52 | 2.05 | 10 | 2 |
| 3:A:401:PCW:H472 | 3:C:611:PCW:H242 | 0.52 | 1.81 | 5 | 1 |
| 3:B:201:PCW:H212 | 4:B:230:17F:H59 | 0.52 | 1.82 | 9 | 1 |
| 1:C:595:LEU:CD1 | 4:C:630:17F:H55 | 0.51 | 2.35 | 1 | 2 |
| 3:B:216:PCW:H42 | 4:B:229:17F:C1 | 0.51 | 2.34 | 2 | 1 |
| 3:B:207:PCW:H162 | 3:B:209:PCW:H181 | 0.51 | 1.81 | 6 | 1 |
| 3:B:201:PCW:C1 | 4:B:230:17F:HN1 | 0.51 | 2.17 | 7 | 1 |
| 2:B:16:LYS:HB2 | 5:B:237:GNP:O2B | 0.51 | 2.05 | 2 | 1 |
| 3:A:403:PCW:H71 | 4:B:231:17F:N1 | 0.51 | 2.19 | 6 | 1 |
| 3:B:212:PCW:H171 | 4:B:231:17F:H34 | 0.51 | 1.82 | 9 | 1 |
| 3:A:406:PCW:H342 | 4:B:227:17F:C9 | 0.51 | 2.35 | 1 | 1 |
| 3:A:410:PCW:H121 | 4:C:630:17F:C1X | 0.51 | 2.35 | 1 | 1 |
| 3:B:201:PCW:H40 | 3:C:623:PCW:H242 | 0.51 | 1.81 | 1 | 1 |
| 3:B:206:PCW:H442 | 4:B:226:17F:H70 | 0.51 | 1.80 | 2 | 1 |
| 3:B:224:PCW:H142 | 4:B:232:17F:H9 | 0.51 | 1.81 | 6 | 1 |
| 3:C:605:PCW:H221 | 4:C:629:17F:H52 | 0.51 | 1.83 | 6 | 1 |
| 1:A:349:TYR:CD2 | 3:A:401:PCW:H262 | 0.51 | 2.35 | 7 | 1 |
| 3:C:603:PCW:H61 | 3:C:625:PCW:H251 | 0.51 | 1.82 | 8 | 1 |
| 3:B:221:PCW:H41 | 4:B:229:17F:O1 | 0.51 | 2.06 | 1 | 2 |
| 3:B:222:PCW:H483 | 3:C:622:PCW:H181 | 0.51 | 1.82 | 1 | 1 |
| 1:C:417:GLU:O | 1:C:421:PRO:HD2 | 0.51 | 2.05 | 2 | 2 |
| 3:A:401:PCW:O1P | 3:A:405:PCW:H11 | 0.51 | 2.06 | 3 | 1 |
| 3:B:211:PCW:H131 | 3:B:217:PCW:H82 | 0.51 | 1.83 | 8 | 2 |
| 3:A:406:PCW:H472 | 4:B:227:17F:H41 | 0.51 | 1.83 | 5 | 1 |
| 3:A:404:PCW:H462 | 3:B:225:PCW:H232 | 0.51 | 1.81 | 9 | 1 |
| 3:A:406:PCW:H132 | 4:A:407:17F:H20A | 0.51 | 1.83 | 1 | 2 |
| 3:B:206:PCW:H332 | 3:B:211:PCW:H321 | 0.51 | 1.82 | 1 | 1 |
| 3:C:620:PCW:H322 | 4:C:633:17F:C42 | 0.51 | 2.36 | 1 | 1 |
| 3:B:204:PCW:H422 | 3:B:205:PCW:H172 | 0.51 | 1.81 | 2 | 1 |
| 3:B:224:PCW:H281 | 3:B:233:PCW:H283 | 0.51 | 1.81 | 6 | 1 |
| 3:A:404:PCW:H172 | 3:B:225:PCW:H381 | 0.51 | 1.83 | 7 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 4:B:232:17F:H4 | 4:B:232:17F:HN1 | 0.51 | 1.65 | 9 | 1 |
| 1:C:489:LEU:O | 1:C:493:GLN:HB2 | 0.51 | 2.06 | 9 | 1 |
| 3:C:618:PCW:H431 | 3:C:626:PCW:H19 | 0.51 | 1.81 | 10 | 1 |
| 3:A:403:PCW:H362 | 3:B:218:PCW:H451 | 0.51 | 1.82 | 1 | 1 |
| 3:A:410:PCW:O2P | 3:A:411:PCW:H52 | 0.51 | 2.06 | 1 | 3 |
| 3:B:202:PCW:H442 | 3:B:215:PCW:H283 | 0.51 | 1.82 | 1 | 1 |
| 4:C:628:17F:H9 | 4:C:628:17F:H18A | 0.51 | 1.82 | 9 | 1 |
| 2:B:71:TYR:CD2 | 7:B:239:EWS:CAO | 0.51 | 2.94 | 10 | 1 |
| 3:B:211:PCW:H122 | 4:B:226:17F:C19 | 0.51 | 2.36 | 10 | 1 |
| 3:B:211:PCW:H82 | 3:B:219:PCW:C32 | 0.51 | 2.35 | 4 | 1 |
| 3:C:621:PCW:H461 | 4:C:632:17F:H35 | 0.51 | 1.83 | 5 | 1 |
| 3:A:408:PCW:H422 | 3:B:205:PCW:H452 | 0.51 | 1.82 | 6 | 1 |
| 3:B:212:PCW:H121 | 4:B:231:17F:H6A | 0.51 | 1.83 | 10 | 1 |
| 1:C:447:GLU:O | 1:C:451:LYS:HB2 | 0.51 | 2.06 | 5 | 2 |
| 3:C:615:PCW:C18 | 4:C:633:17F:H12 | 0.51 | 2.36 | 2 | 1 |
| 3:A:405:PCW:H361 | 3:A:405:PCW:H141 | 0.51 | 1.83 | 3 | 1 |
| 3:C:618:PCW:H342 | 3:C:626:PCW:H371 | 0.51 | 1.82 | 4 | 1 |
| 3:B:201:PCW:H42 | 4:B:230:17F:H2 | 0.51 | 1.83 | 7 | 1 |
| 3:B:220:PCW:H251 | 4:B:232:17F:H76 | 0.51 | 1.82 | 9 | 1 |
| 3:A:410:PCW:H352 | 4:C:630:17F:H29 | 0.51 | 1.82 | 2 | 1 |
| 2:B:43:GLN:OE1 | 3:B:202:PCW:H62 | 0.51 | 2.06 | 2 | 1 |
| 3:B:219:PCW:H471 | 3:B:223:PCW:H432 | 0.51 | 1.83 | 4 | 1 |
| 4:B:236:17F:H34 | 4:B:236:17F:H10A | 0.51 | 1.82 | 5 | 1 |
| 4:B:228:17F:H8 | 4:B:232:17F:H9A | 0.51 | 1.82 | 9 | 2 |
| 3:A:404:PCW:H231 | 3:B:225:PCW:H422 | 0.51 | 1.82 | 10 | 1 |
| 1:C:492:LEU:CD1 | 3:C:620:PCW:H482 | 0.51 | 2.36 | 10 | 1 |
| 3:B:220:PCW:H83 | 3:B:222:PCW:H321 | 0.51 | 1.82 | 7 | 1 |
| 3:A:409:PCW:H471 | 3:C:613:PCW:H182 | 0.50 | 1.83 | 1 | 1 |
| 3:B:202:PCW:H212 | 3:B:215:PCW:H232 | 0.50 | 1.83 | 4 | 1 |
| 3:B:213:PCW:H141 | 4:B:228:17F:H9 | 0.50 | 1.82 | 9 | 1 |
| 3:C:603:PCW:H242 | 4:C:632:17F:H53 | 0.50 | 1.82 | 9 | 1 |
| 3:C:601:PCW:C39 | 4:C:627:17F:H54 | 0.50 | 2.36 | 4 | 1 |
| 1:A:239:LEU:O | 1:A:243:MET:HB2 | 0.50 | 2.06 | 5 | 1 |
| 3:A:404:PCW:H32 | 3:B:218:PCW:H372 | 0.50 | 1.83 | 5 | 1 |
| 3:A:405:PCW:H232 | 3:C:609:PCW:H261 | 0.50 | 1.81 | 8 | 1 |
| 1:A:275:LYS:O | 1:A:279:LEU:HB2 | 0.50 | 2.07 | 9 | 1 |
| 4:B:236:17F:H57 | 3:C:622:PCW:H161 | 0.50 | 1.83 | 9 | 1 |
| 3:B:220:PCW:H212 | 3:B:235:PCW:H262 | 0.50 | 1.82 | 4 | 1 |
| 3:A:409:PCW:H372 | 3:B:235:PCW:H371 | 0.50 | 1.84 | 5 | 1 |
| 1:C:421:PRO:O | 1:C:425:GLU:HG2 | 0.50 | 2.06 | 5 | 1 |
| 3:B:203:PCW:H132 | 3:B:213:PCW:H351 | 0.50 | 1.84 | 9 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 3:A:403:PCW:H342 | 3:B:212:PCW:H272 | 0.50 | 1.83 | 1 | 1 |
| 3:B:203:PCW:H431 | 4:B:228:17F:H12A | 0.50 | 1.83 | 3 | 1 |
| 3:B:212:PCW:H261 | 3:B:212:PCW:H462 | 0.50 | 1.83 | 6 | 1 |
| 3:B:233:PCW:H242 | 3:C:609:PCW:H441 | 0.50 | 1.83 | 6 | 1 |
| 3:B:214:PCW:H283 | 4:C:633:17F:H52 | 0.50 | 1.82 | 7 | 1 |
| 4:C:632:17F:H61 | 4:C:633:17F:H69 | 0.50 | 1.83 | 8 | 1 |
| 1:C:414:LYS:HA | 1:C:417:GLU:HG3 | 0.50 | 1.82 | 9 | 1 |
| 3:C:603:PCW:H332 | 3:C:607:PCW:H121 | 0.50 | 1.81 | 9 | 1 |
| 2:B:72:MET:SD | 7:B:239:EWS:BRA | 0.50 | 3.24 | 10 | 1 |
| 3:A:406:PCW:H342 | 4:B:227:17F:H9 | 0.50 | 1.84 | 1 | 1 |
| 1:C:491:GLU:O | 1:C:495:LYS:HG3 | 0.50 | 2.06 | 5 | 5 |
| 1:A:279:LEU:HB3 | 1:C:495:LYS:HE3 | 0.50 | 1.83 | 2 | 1 |
| 3:B:207:PCW:H441 | 3:B:209:PCW:H241 | 0.50 | 1.82 | 4 | 1 |
| 3:A:403:PCW:H412 | 3:B:218:PCW:H462 | 0.50 | 1.84 | 5 | 1 |
| 3:B:204:PCW:H32 | 3:B:208:PCW:C1 | 0.50 | 2.36 | 5 | 1 |
| 3:A:404:PCW:H81 | 3:B:225:PCW:O2P | 0.50 | 2.06 | 7 | 1 |
| 3:B:209:PCW:H31 | 3:B:224:PCW:H132 | 0.50 | 1.83 | 7 | 2 |
| 1:C:492:LEU:HD13 | 3:C:620:PCW:H441 | 0.50 | 1.84 | 8 | 1 |
| 3:B:202:PCW:H181 | 3:B:215:PCW:H242 | 0.50 | 1.83 | 9 | 1 |
| 3:C:607:PCW:H283 | 4:C:632:17F:H52 | 0.50 | 1.84 | 1 | 1 |
| 3:C:621:PCW:H483 | 4:C:632:17F:H35 | 0.50 | 1.84 | 1 | 1 |
| 3:B:209:PCW:H83 | 4:B:228:17F:N1 | 0.50 | 2.21 | 2 | 1 |
| 3:B:210:PCW:H152 | 3:B:214:PCW:H352 | 0.50 | 1.84 | 6 | 1 |
| 1:C:525:LEU:HD23 | 1:C:528:ARG:HD2 | 0.50 | 1.83 | 6 | 1 |
| 3:B:208:PCW:H441 | 3:B:234:PCW:H262 | 0.50 | 1.84 | 7 | 1 |
| 1:A:276:VAL:O | 1:A:280:ARG:HB2 | 0.50 | 2.07 | 2 | 2 |
| 4:A:407:17F:H10A | 3:B:205:PCW:H361 | 0.50 | 1.83 | 2 | 1 |
| 3:C:606:PCW:H431 | 3:C:612:PCW:H172 | 0.50 | 1.82 | 3 | 1 |
| 3:B:222:PCW:H332 | 3:B:222:PCW:H131 | 0.50 | 1.82 | 5 | 1 |
| 3:C:615:PCW:H182 | 4:C:629:17F:H42 | 0.50 | 1.83 | 5 | 1 |
| 3:C:601:PCW:H483 | 3:C:601:PCW:H212 | 0.50 | 1.83 | 7 | 1 |
| 3:C:605:PCW:H162 | 4:C:627:17F:H34 | 0.50 | 1.82 | 8 | 1 |
| 3:A:410:PCW:O3 | 4:C:630:17F:H30 | 0.50 | 2.05 | 7 | 2 |
| 3:C:615:PCW:H221 | 4:C:629:17F:H42 | 0.50 | 1.83 | 1 | 1 |
| 2:B:84:ILE:HD11 | 2:B:118:CYS:HA | 0.50 | 1.84 | 3 | 3 |
| 3:B:222:PCW:H131 | 3:B:222:PCW:H351 | 0.50 | 1.83 | 5 | 1 |
| 3:B:209:PCW:O11 | 3:B:216:PCW:H131 | 0.50 | 2.07 | 6 | 1 |
| 3:A:403:PCW:H342 | 3:B:212:PCW:C27 | 0.50 | 2.37 | 1 | 1 |
| 4:C:630:17F:C4 | 4:C:630:17F:H1 | 0.50 | 2.37 | 2 | 1 |
| 3:B:204:PCW:H52 | 3:B:205:PCW:H61 | 0.50 | 1.82 | 3 | 1 |
| 3:B:211:PCW:H352 | 4:B:226:17F:O10 | 0.50 | 2.06 | 3 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 3:B:214:PCW:H281 | 4:C:627:17F:H75 | 0.50 | 1.84 | 3 | 1 |
| 3:B:203:PCW:H481 | 4:B:228:17F:H20 | 0.50 | 1.84 | 6 | 2 |
| 3:B:205:PCW:H221 | 3:B:205:PCW:H461 | 0.50 | 1.84 | 6 | 1 |
| 1:A:312:HIS:HE1 | 1:C:465:GLU:HB2 | 0.49 | 1.66 | 9 | 4 |
| 1:A:279:LEU:HD22 | 1:C:495:LYS:HE2 | 0.49 | 1.83 | 3 | 1 |
| 3:A:409:PCW:C6 | 4:C:630:17F:HN1A | 0.49 | 2.20 | 3 | 1 |
| 3:C:606:PCW:H361 | 3:C:612:PCW:H152 | 0.49 | 1.84 | 7 | 3 |
| 3:B:219:PCW:H351 | 3:B:225:PCW:H351 | 0.49 | 1.84 | 7 | 1 |
| 3:B:234:PCW:H141 | 3:C:602:PCW:H461 | 0.49 | 1.82 | 7 | 1 |
| 1:C:485:ALA:HB1 | 3:C:620:PCW:H271 | 0.49 | 1.82 | 7 | 1 |
| 3:A:408:PCW:H322 | 3:C:610:PCW:H371 | 0.49 | 1.84 | 8 | 1 |
| 3:A:409:PCW:H262 | 3:C:613:PCW:H181 | 0.49 | 1.83 | 8 | 1 |
| 3:C:607:PCW:H352 | 3:C:615:PCW:H381 | 0.49 | 1.83 | 8 | 1 |
| 1:A:363:LYS:HD3 | 1:C:411:THR:HG23 | 0.49 | 1.84 | 9 | 2 |
| 3:B:209:PCW:H19 | 3:B:216:PCW:H211 | 0.49 | 1.82 | 1 | 1 |
| 4:B:227:17F:H10 | 4:B:227:17F:H33 | 0.49 | 1.84 | 8 | 2 |
| 3:B:201:PCW:H82 | 3:B:222:PCW:O2P | 0.49 | 2.07 | 4 | 1 |
| 3:B:225:PCW:H282 | 3:C:626:PCW:H481 | 0.49 | 1.82 | 1 | 1 |
| 3:C:607:PCW:H471 | 4:C:633:17F:H39 | 0.49 | 1.84 | 9 | 2 |
| 1:A:365:LYS:O | 1:A:369:GLU:HB2 | 0.49 | 2.06 | 8 | 1 |
| 3:B:221:PCW:C13 | 3:C:601:PCW:C35 | 0.49 | 2.67 | 10 | 1 |
| 3:A:410:PCW:H352 | 4:C:630:17F:C1X | 0.49 | 2.37 | 2 | 1 |
| 3:B:201:PCW:H42 | 4:B:232:17F:N1 | 0.49 | 2.22 | 2 | 1 |
| 1:A:338:LEU:O | 1:A:342:GLY:HA3 | 0.49 | 2.08 | 3 | 2 |
| 3:A:406:PCW:H121 | 4:A:407:17F:H20A | 0.49 | 1.84 | 4 | 1 |
| 4:A:407:17F:H37 | 3:B:222:PCW:C3 | 0.49 | 2.36 | 5 | 1 |
| 4:B:236:17F:H47 | 4:B:236:17F:H76 | 0.49 | 1.85 | 5 | 1 |
| 1:A:308:ARG:HD2 | 1:C:465:GLU:OE1 | 0.49 | 2.08 | 6 | 1 |
| 3:B:212:PCW:H151 | 4:B:231:17F:H10 | 0.49 | 1.83 | 6 | 1 |
| 3:B:211:PCW:H231 | 4:B:229:17F:H44 | 0.49 | 1.83 | 8 | 1 |
| 3:A:402:PCW:H122 | 4:B:231:17F:H76 | 0.49 | 1.82 | 9 | 1 |
| 1:A:301:LEU:HB3 | 1:C:473:LYS:HE2 | 0.49 | 1.84 | 1 | 1 |
| 1:A:314:ASP:HA | 1:A:317:ARG:HD2 | 0.49 | 1.82 | 2 | 3 |
| 3:A:409:PCW:H82 | 4:C:630:17F:N1 | 0.49 | 2.23 | 2 | 1 |
| 3:C:607:PCW:H482 | 4:C:633:17F:H42 | 0.49 | 1.83 | 2 | 1 |
| 3:B:221:PCW:P | 3:C:601:PCW:H63 | 0.49 | 2.48 | 4 | 1 |
| 3:C:606:PCW:H381 | 3:C:612:PCW:H162 | 0.49 | 1.85 | 6 | 2 |
| 2:B:7:VAL:HG13 | 7:B:239:EWS:CAU | 0.49 | 2.38 | 5 | 1 |
| 3:B:204:PCW:H121 | 3:B:208:PCW:H352 | 0.49 | 1.82 | 5 | 1 |
| 3:A:402:PCW:C32 | 3:B:205:PCW:H32 | 0.49 | 2.37 | 6 | 1 |
| 2:B:5:LYS:HG2 | 2:B:54:ASP:HB3 | 0.49 | 1.83 | 6 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 3:B:214:PCW:H261 | 3:C:615:PCW:H472 | 0.49 | 1.83 | 7 | 1 |
| 2:B:15:GLY:HA2 | 5:B:237:GNP:O2B | 0.49 | 2.07 | 9 | 1 |
| 3:A:405:PCW:H461 | 3:C:609:PCW:H20 | 0.49 | 1.83 | 10 | 1 |
| 3:B:223:PCW:C28 | 1:C:521:TYR:OH | 0.49 | 2.61 | 10 | 1 |
| 3:A:406:PCW:H322 | 4:B:227:17F:H6A | 0.49 | 1.83 | 1 | 1 |
| 4:B:236:17F:H11A | 3:C:622:PCW:H272 | 0.49 | 1.85 | 3 | 1 |
| 1:C:574:LEU:O | 1:C:578:GLU:HG3 | 0.49 | 2.07 | 6 | 1 |
| 3:C:607:PCW:H272 | 3:C:615:PCW:H451 | 0.49 | 1.85 | 10 | 1 |
| 2:B:6:LEU:O | 7:B:239:EWS:NAW | 0.49 | 2.46 | 1 | 1 |
| 3:B:210:PCW:H142 | 3:B:214:PCW:H162 | 0.49 | 1.84 | 1 | 1 |
| 2:B:116:ASN:HA | 2:B:144:THR:O | 0.49 | 2.08 | 7 | 2 |
| 3:B:211:PCW:H151 | 4:B:226:17F:H20 | 0.49 | 1.83 | 4 | 1 |
| 1:C:489:LEU:O | 1:C:493:GLN:HG3 | 0.49 | 2.08 | 5 | 1 |
| 2:B:5:LYS:CG | 7:B:239:EWS:CAX | 0.49 | 2.91 | 8 | 1 |
| 4:B:226:17F:H39 | 4:C:628:17F:H55 | 0.49 | 1.83 | 8 | 1 |
| 3:B:202:PCW:H231 | 3:B:215:PCW:H242 | 0.49 | 1.85 | 2 | 1 |
| 3:B:207:PCW:H242 | 3:B:216:PCW:H182 | 0.49 | 1.84 | 2 | 1 |
| 1:C:488:LYS:HG2 | 3:C:620:PCW:C28 | 0.49 | 2.36 | 3 | 1 |
| 1:C:466:GLU:OE1 | 1:C:469:LEU:CD1 | 0.49 | 2.58 | 1 | 1 |
| 3:C:601:PCW:H461 | 3:C:601:PCW:H171 | 0.49 | 1.84 | 2 | 1 |
| 3:B:215:PCW:H461 | 4:C:632:17F:H75 | 0.49 | 1.85 | 3 | 1 |
| 3:C:615:PCW:C19 | 4:C:633:17F:H12 | 0.49 | 2.38 | 4 | 2 |
| 3:A:402:PCW:H11 | 3:B:212:PCW:H31 | 0.49 | 1.84 | 6 | 1 |
| 3:B:221:PCW:H212 | 4:C:627:17F:H54 | 0.49 | 1.84 | 10 | 1 |
| 4:C:627:17F:H68 | 4:C:629:17F:H53 | 0.49 | 1.84 | 10 | 1 |
| 3:B:202:PCW:H71 | 3:B:217:PCW:H31 | 0.49 | 1.85 | 1 | 1 |
| 3:B:221:PCW:H242 | 3:C:601:PCW:H172 | 0.49 | 1.85 | 2 | 1 |
| 1:C:517:HIS:O | 1:C:521:TYR:HB2 | 0.49 | 2.07 | 7 | 3 |
| 3:B:210:PCW:H121 | 3:B:214:PCW:H341 | 0.49 | 1.85 | 10 | 1 |
| 3:B:214:PCW:H232 | 4:B:229:17F:H50 | 0.49 | 1.83 | 10 | 1 |
| 3:B:207:PCW:H83 | 4:B:228:17F:HN1A | 0.48 | 1.64 | 3 | 1 |
| 3:A:406:PCW:C16 | 4:A:407:17F:H33 | 0.48 | 2.38 | 6 | 1 |
| 3:C:612:PCW:H242 | 3:C:612:PCW:H422 | 0.48 | 1.84 | 6 | 1 |
| 1:A:336:GLU:HA | 1:A:339:LYS:HE3 | 0.48 | 1.85 | 7 | 1 |
| 2:B:143:GLU:O | 2:B:151:GLY:HA3 | 0.48 | 2.08 | 7 | 1 |
| 3:C:615:PCW:H212 | 4:C:629:17F:H42 | 0.48 | 1.84 | 8 | 1 |
| 4:A:407:17F:H50 | 3:C:613:PCW:H283 | 0.48 | 1.84 | 10 | 1 |
| 4:B:236:17F:H77 | 3:C:603:PCW:H272 | 0.48 | 1.85 | 1 | 1 |
| 1:A:268:GLU:O | 1:A:272:TYR:HB2 | 0.48 | 2.08 | 2 | 3 |
| 4:B:231:17F:H12A | 4:B:231:17F:H61 | 0.48 | 1.85 | 3 | 1 |
| 3:C:605:PCW:H261 | 4:C:629:17F:H66 | 0.48 | 1.85 | 4 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 4:B:228:17F:O8 | 4:B:232:17F:H6A | 0.48 | 2.08 | 6 | 1 |
| 3:B:204:PCW:H141 | 3:B:208:PCW:H371 | 0.48 | 1.85 | 7 | 1 |
| 3:C:604:PCW:H31 | 3:C:625:PCW:H341 | 0.48 | 1.86 | 7 | 1 |
| 3:B:214:PCW:H231 | 4:B:229:17F:H39 | 0.48 | 1.84 | 1 | 1 |
| 3:C:610:PCW:H62 | 3:C:617:PCW:H61 | 0.48 | 1.85 | 1 | 1 |
| 2:B:147:LYS:HG3 | 5:B:237:GNP:HN1 | 0.48 | 1.69 | 3 | 1 |
| 3:A:405:PCW:H2 | 4:B:228:17F:H19 | 0.48 | 1.84 | 6 | 1 |
| 4:A:407:17F:H44 | 3:B:220:PCW:H421 | 0.48 | 1.85 | 6 | 1 |
| 3:C:626:PCW:H41 | 3:C:626:PCW:O31 | 0.48 | 2.08 | 6 | 1 |
| 1:C:479:ALA:O | 1:C:483:GLU:HG2 | 0.48 | 2.08 | 2 | 1 |
| 3:A:409:PCW:H142 | 3:A:410:PCW:H172 | 0.48 | 1.84 | 3 | 1 |
| 1:A:359:THR:HA | 1:A:362:GLU:OE1 | 0.48 | 2.09 | 4 | 1 |
| 3:C:615:PCW:H231 | 4:C:629:17F:H45 | 0.48 | 1.85 | 5 | 1 |
| 3:A:408:PCW:H11 | 3:C:610:PCW:H321 | 0.48 | 1.85 | 7 | 1 |
| 1:A:291:LEU:O | 1:A:295:GLN:HG3 | 0.48 | 2.08 | 8 | 1 |
| 3:B:215:PCW:H121 | 3:B:217:PCW:H122 | 0.48 | 1.84 | 9 | 1 |
| 3:C:615:PCW:H20 | 4:C:633:17F:H40 | 0.48 | 1.85 | 10 | 1 |
| 3:B:224:PCW:H71 | 4:B:229:17F:O5 | 0.48 | 2.08 | 2 | 1 |
| 1:C:563:LYS:HB2 | 1:C:564:PRO:CD | 0.48 | 2.39 | 10 | 5 |
| 4:C:627:17F:H10A | 4:C:629:17F:H19 | 0.48 | 1.86 | 2 | 1 |
| 3:B:204:PCW:H142 | 3:B:208:PCW:H362 | 0.48 | 1.84 | 4 | 1 |
| 3:C:607:PCW:O11 | 3:C:615:PCW:H51 | 0.48 | 2.08 | 7 | 1 |
| 3:A:405:PCW:H142 | 3:C:609:PCW:H272 | 0.48 | 1.85 | 10 | 1 |
| 2:B:17:SER:HB2 | 2:B:29:VAL:HG21 | 0.48 | 1.84 | 1 | 1 |
| 1:A:255:GLN:HB2 | 1:A:256:PRO:CD | 0.48 | 2.39 | 2 | 4 |
| 3:B:204:PCW:O2P | 3:B:204:PCW:H73 | 0.48 | 2.08 | 2 | 1 |
| 1:A:297:LYS:O | 1:A:301:LEU:HB2 | 0.48 | 2.08 | 3 | 2 |
| 3:B:208:PCW:H272 | 3:B:219:PCW:H272 | 0.48 | 1.85 | 4 | 1 |
| 3:A:406:PCW:H331 | 4:B:227:17F:C8 | 0.48 | 2.39 | 6 | 1 |
| 3:B:208:PCW:H39 | 3:B:234:PCW:H272 | 0.48 | 1.84 | 8 | 1 |
| 3:C:604:PCW:H152 | 3:C:625:PCW:H462 | 0.48 | 1.84 | 9 | 1 |
| 3:A:401:PCW:H41 | 3:B:213:PCW:O11 | 0.48 | 2.09 | 1 | 1 |
| 3:B:210:PCW:H71 | 4:B:229:17F:O4 | 0.48 | 2.08 | 2 | 1 |
| 3:B:203:PCW:H422 | 4:B:228:17F:H40 | 0.48 | 1.86 | 3 | 1 |
| 3:B:214:PCW:H221 | 3:C:615:PCW:H483 | 0.48 | 1.85 | 4 | 1 |
| 2:B:22:GLN:O | 2:B:26:ASN:HA | 0.48 | 2.08 | 9 | 4 |
| 4:B:236:17F:H73 | 4:C:628:17F:H72 | 0.48 | 1.86 | 4 | 1 |
| 3:B:212:PCW:H152 | 4:B:231:17F:H59 | 0.48 | 1.84 | 5 | 1 |
| 3:A:402:PCW:H152 | 3:A:402:PCW:H351 | 0.48 | 1.84 | 9 | 1 |
| 3:B:203:PCW:O2 | 3:B:213:PCW:H322 | 0.48 | 2.08 | 9 | 1 |
| 3:A:405:PCW:H151 | 4:B:228:17F:H33 | 0.48 | 1.86 | 10 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 2:B:71:TYR:CD1 | 7:B:239:EWS:BRA | 0.48 | 3.22 | 1 | 1 |
| 3:A:401:PCW:H261 | 3:C:614:PCW:H281 | 0.48 | 1.86 | 4 | 1 |
| 3:A:406:PCW:H382 | 4:B:227:17F:H8A | 0.48 | 1.84 | 4 | 1 |
| 3:B:214:PCW:H81 | 4:B:229:17F:O1 | 0.48 | 2.09 | 4 | 1 |
| 3:A:405:PCW:H152 | 3:C:609:PCW:H262 | 0.48 | 1.84 | 5 | 1 |
| 1:C:559:SER:HB2 | 1:C:563:LYS:HE2 | 0.48 | 1.85 | 5 | 1 |
| 3:B:206:PCW:H162 | 3:B:208:PCW:H161 | 0.48 | 1.86 | 9 | 1 |
| 3:B:210:PCW:H122 | 3:B:214:PCW:H162 | 0.48 | 1.86 | 9 | 1 |
| 3:B:215:PCW:H40 | 4:C:632:17F:H76 | 0.48 | 1.84 | 9 | 1 |
| 3:B:235:PCW:H251 | 3:C:622:PCW:H251 | 0.48 | 1.86 | 9 | 1 |
| 3:C:614:PCW:H412 | 3:C:619:PCW:H20 | 0.48 | 1.86 | 9 | 1 |
| 1:A:352:LYS:HZ2 | 1:C:425:GLU:CB | 0.48 | 2.22 | 4 | 1 |
| 2:B:5:LYS:HB3 | 7:B:239:EWS:NAW | 0.48 | 2.23 | 6 | 2 |
| 3:B:207:PCW:H63 | 4:B:228:17F:HN1 | 0.48 | 1.68 | 6 | 1 |
| 3:A:403:PCW:H51 | 4:B:231:17F:H4 | 0.48 | 1.86 | 7 | 1 |
| 3:B:221:PCW:H82 | 4:B:229:17F:C3 | 0.48 | 2.39 | 7 | 1 |
| 3:B:213:PCW:H83 | 4:B:230:17F:O1 | 0.48 | 2.08 | 8 | 1 |
| 1:A:308:ARG:CG | 1:C:469:LEU:CD2 | 0.48 | 2.91 | 10 | 1 |
| 3:B:217:PCW:H483 | 3:B:219:PCW:H481 | 0.48 | 1.85 | 10 | 1 |
| 3:C:621:PCW:H162 | 4:C:632:17F:H6 | 0.47 | 1.85 | 1 | 1 |
| 3:B:220:PCW:H121 | 3:B:220:PCW:H372 | 0.47 | 1.85 | 2 | 2 |
| 3:C:615:PCW:H212 | 4:C:629:17F:H41 | 0.47 | 1.85 | 2 | 1 |
| 3:C:603:PCW:H332 | 3:C:607:PCW:H122 | 0.47 | 1.86 | 3 | 1 |
| 3:A:410:PCW:H331 | 4:C:630:17F:C1X | 0.47 | 2.39 | 4 | 1 |
| 3:B:201:PCW:H432 | 4:B:228:17F:H45 | 0.47 | 1.84 | 5 | 1 |
| 2:B:5:LYS:HD3 | 2:B:54:ASP:HB3 | 0.47 | 1.85 | 7 | 1 |
| 2:B:3:GLU:HG3 | 3:B:223:PCW:H81 | 0.47 | 1.85 | 8 | 1 |
| 3:B:205:PCW:H483 | 3:C:610:PCW:H432 | 0.47 | 1.86 | 8 | 1 |
| 1:A:273:ARG:HA | 1:A:276:VAL:HG12 | 0.47 | 1.85 | 1 | 1 |
| 1:C:430:LEU:HA | 1:C:433:GLU:HB2 | 0.47 | 1.86 | 1 | 1 |
| 3:C:608:PCW:H31 | 4:C:631:17F:C4 | 0.47 | 2.39 | 1 | 2 |
| 1:A:363:LYS:O | 1:A:367:ALA:HB3 | 0.47 | 2.10 | 4 | 4 |
| 3:C:621:PCW:H442 | 4:C:632:17F:H12 | 0.47 | 1.84 | 4 | 1 |
| 3:B:203:PCW:H52 | 3:B:203:PCW:H2 | 0.47 | 1.85 | 10 | 1 |
| 1:C:488:LYS:CB | 3:C:620:PCW:H281 | 0.47 | 2.38 | 3 | 1 |
| 3:C:605:PCW:H152 | 4:C:627:17F:H34 | 0.47 | 1.86 | 6 | 1 |
| 1:A:242:GLU:HB3 | 1:C:532:ARG:NH2 | 0.47 | 2.24 | 10 | 1 |
| 3:C:607:PCW:H132 | 3:C:615:PCW:H342 | 0.47 | 1.86 | 10 | 1 |
| 3:A:402:PCW:O1P | 3:B:212:PCW:H51 | 0.47 | 2.09 | 6 | 1 |
| 3:B:220:PCW:H142 | 4:B:232:17F:H60 | 0.47 | 1.86 | 8 | 1 |
| 3:A:404:PCW:H72 | 7:B:239:EWS:OAB | 0.47 | 2.08 | 10 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 3:A:406:PCW:H51 | 4:B:230:17F:N1 | 0.47 | 2.24 | 1 | 1 |
| 3:B:210:PCW:H282 | 3:B:214:PCW:H40 | 0.47 | 1.86 | 2 | 1 |
| 3:B:211:PCW:H62 | 3:B:211:PCW:H12 | 0.47 | 1.85 | 2 | 1 |
| 3:C:615:PCW:H182 | 4:C:633:17F:H12 | 0.47 | 1.87 | 2 | 1 |
| 3:B:209:PCW:H382 | 3:B:224:PCW:H221 | 0.47 | 1.86 | 3 | 1 |
| 3:B:204:PCW:H342 | 3:B:212:PCW:H12 | 0.47 | 1.87 | 4 | 1 |
| 1:C:429:ASN:HA | 1:C:432:LYS:HD2 | 0.47 | 1.85 | 4 | 2 |
| 4:B:236:17F:H43 | 4:B:236:17F:H75 | 0.47 | 1.85 | 5 | 1 |
| 3:B:216:PCW:O1P | 3:C:601:PCW:H71 | 0.47 | 2.09 | 7 | 1 |
| 3:C:623:PCW:H39 | 3:C:623:PCW:H141 | 0.47 | 1.86 | 8 | 1 |
| 3:B:202:PCW:H332 | 3:B:215:PCW:H141 | 0.47 | 1.86 | 1 | 1 |
| 3:B:216:PCW:H32 | 4:B:229:17F:H2 | 0.47 | 1.87 | 1 | 1 |
| 4:B:236:17F:H73 | 4:C:628:17F:H68 | 0.47 | 1.86 | 1 | 2 |
| 4:B:230:17F:H78 | 3:C:619:PCW:H451 | 0.47 | 1.85 | 2 | 1 |
| 2:B:5:LYS:HD3 | 7:B:239:EWS:OAB | 0.47 | 2.08 | 6 | 1 |
| 3:B:221:PCW:H121 | 3:C:601:PCW:H351 | 0.47 | 1.85 | 6 | 1 |
| 3:B:221:PCW:H452 | 3:C:605:PCW:H471 | 0.47 | 1.87 | 6 | 1 |
| 3:B:201:PCW:H361 | 4:B:227:17F:H20 | 0.47 | 1.86 | 7 | 1 |
| 3:A:402:PCW:H482 | 3:C:610:PCW:H261 | 0.47 | 1.87 | 8 | 1 |
| 3:A:406:PCW:H121 | 4:A:407:17F:C31 | 0.47 | 2.34 | 8 | 1 |
| 3:C:607:PCW:H332 | 3:C:615:PCW:H341 | 0.47 | 1.86 | 8 | 1 |
| 3:B:210:PCW:O2P | 3:B:214:PCW:H41 | 0.47 | 2.09 | 10 | 1 |
| 3:C:604:PCW:H12 | 3:C:625:PCW:H332 | 0.47 | 1.86 | 1 | 1 |
| 3:C:607:PCW:H352 | 3:C:615:PCW:H382 | 0.47 | 1.85 | 1 | 1 |
| 3:A:408:PCW:H151 | 3:A:411:PCW:H152 | 0.47 | 1.84 | 2 | 1 |
| 3:B:208:PCW:H82 | 3:B:219:PCW:O1P | 0.47 | 2.10 | 2 | 1 |
| 3:C:621:PCW:H132 | 4:C:632:17F:H4A | 0.47 | 1.87 | 2 | 2 |
| 3:B:211:PCW:C12 | 4:B:226:17F:H18A | 0.47 | 2.39 | 3 | 1 |
| 3:C:607:PCW:H152 | 3:C:615:PCW:H321 | 0.47 | 1.85 | 7 | 2 |
| 3:B:209:PCW:H451 | 3:B:224:PCW:H242 | 0.47 | 1.86 | 4 | 1 |
| 3:B:205:PCW:H152 | 3:B:205:PCW:H351 | 0.47 | 1.85 | 6 | 1 |
| 3:B:216:PCW:H231 | 3:C:604:PCW:H462 | 0.47 | 1.86 | 6 | 1 |
| 4:B:232:17F:H4A | 4:B:232:17F:O10 | 0.47 | 2.09 | 6 | 1 |
| 3:C:626:PCW:H422 | 4:C:631:17F:H48 | 0.47 | 1.86 | 6 | 1 |
| 3:B:209:PCW:H131 | 3:B:216:PCW:H122 | 0.47 | 1.87 | 7 | 1 |
| 3:C:603:PCW:H252 | 4:C:628:17F:H39 | 0.47 | 1.85 | 8 | 1 |
| 3:A:408:PCW:H11 | 3:C:610:PCW:H352 | 0.47 | 1.87 | 9 | 1 |
| 3:B:224:PCW:H82 | 4:B:226:17F:O1 | 0.47 | 2.09 | 9 | 1 |
| 3:C:615:PCW:H151 | 4:C:633:17F:H8 | 0.47 | 1.85 | 9 | 1 |
| 3:A:409:PCW:H222 | 3:A:410:PCW:H212 | 0.47 | 1.86 | 10 | 1 |
| 3:B:203:PCW:H251 | 4:B:230:17F:H64 | 0.47 | 1.87 | 10 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 3:B:205:PCW:H461 | 3:C:610:PCW:H272 | 0.47 | 1.87 | 10 | 1 |
| 3:C:607:PCW:H152 | 3:C:615:PCW:H352 | 0.47 | 1.87 | 1 | 1 |
| 3:B:203:PCW:H482 | 3:B:213:PCW:H19 | 0.47 | 1.86 | 3 | 1 |
| 3:B:220:PCW:H131 | 4:B:232:17F:H31 | 0.47 | 1.87 | 3 | 1 |
| 4:B:236:17F:H68 | 3:C:603:PCW:H271 | 0.47 | 1.86 | 3 | 1 |
| 1:C:549:ALA:O | 1:C:553:GLU:HG3 | 0.47 | 2.09 | 3 | 2 |
| 3:B:208:PCW:H41 | 3:B:219:PCW:H32 | 0.47 | 1.86 | 4 | 1 |
| 3:B:233:PCW:H62 | 3:B:233:PCW:H331 | 0.47 | 1.87 | 6 | 2 |
| 3:A:411:PCW:H452 | 3:C:616:PCW:H251 | 0.47 | 1.87 | 1 | 1 |
| 3:C:613:PCW:H31 | 3:C:613:PCW:O31 | 0.47 | 2.08 | 1 | 8 |
| 1:C:586:SER:O | 1:C:590:GLU:HG3 | 0.47 | 2.10 | 10 | 2 |
| 3:B:204:PCW:H231 | 3:B:218:PCW:H212 | 0.47 | 1.87 | 3 | 1 |
| 1:A:375:LEU:HD11 | 4:B:230:17F:H54 | 0.47 | 1.87 | 4 | 1 |
| 3:B:203:PCW:H322 | 3:B:213:PCW:H352 | 0.47 | 1.86 | 9 | 1 |
| 3:B:201:PCW:O2P | 3:B:213:PCW:H72 | 0.47 | 2.10 | 2 | 1 |
| 3:A:405:PCW:H161 | 4:B:228:17F:H34 | 0.47 | 1.87 | 4 | 1 |
| 3:B:204:PCW:H162 | 3:B:208:PCW:H382 | 0.47 | 1.86 | 4 | 1 |
| 3:A:410:PCW:H462 | 3:A:411:PCW:H241 | 0.47 | 1.86 | 6 | 1 |
| 4:B:227:17F:H58 | 4:B:227:17F:C10 | 0.47 | 2.39 | 9 | 2 |
| 3:A:406:PCW:H341 | 4:B:227:17F:H9A | 0.47 | 1.87 | 7 | 1 |
| 3:B:211:PCW:O11 | 3:B:217:PCW:H12 | 0.47 | 2.10 | 7 | 1 |
| 3:B:234:PCW:H62 | 3:C:617:PCW:O1P | 0.47 | 2.10 | 7 | 1 |
| 3:A:402:PCW:H372 | 4:B:231:17F:H74 | 0.47 | 1.87 | 8 | 1 |
| 3:B:207:PCW:H232 | 3:B:216:PCW:H162 | 0.47 | 1.86 | 9 | 1 |
| 3:B:209:PCW:H161 | 3:B:224:PCW:H211 | 0.47 | 1.86 | 10 | 1 |
| 3:B:214:PCW:H212 | 4:B:229:17F:H36 | 0.46 | 1.86 | 1 | 1 |
| 3:C:621:PCW:H432 | 4:C:632:17F:H69 | 0.46 | 1.87 | 2 | 1 |
| 3:B:206:PCW:O2P | 3:B:211:PCW:H82 | 0.46 | 2.10 | 3 | 1 |
| 1:A:376:LEU:HB2 | 1:A:377:PRO:CD | 0.46 | 2.40 | 9 | 3 |
| 3:B:223:PCW:H471 | 4:C:632:17F:C42 | 0.46 | 2.25 | 5 | 1 |
| 3:C:603:PCW:H421 | 3:C:607:PCW:H11 | 0.46 | 1.86 | 5 | 1 |
| 1:A:309:ALA:HA | 1:A:312:HIS:HB2 | 0.46 | 1.86 | 7 | 1 |
| 3:B:221:PCW:O31 | 3:B:221:PCW:H12 | 0.46 | 2.10 | 7 | 1 |
| 4:B:226:17F:H40 | 4:B:236:17F:H42 | 0.46 | 1.87 | 10 | 1 |
| 3:C:605:PCW:H221 | 4:C:627:17F:H37 | 0.46 | 1.85 | 10 | 1 |
| 1:C:440:GLU:O | 1:C:444:ASP:HB2 | 0.46 | 2.10 | 1 | 1 |
| 3:B:211:PCW:O3 | 4:B:226:17F:H4 | 0.46 | 2.11 | 3 | 1 |
| 1:A:356:HIS:HD2 | 3:A:401:PCW:C27 | 0.46 | 2.16 | 9 | 1 |
| 3:B:212:PCW:H241 | 3:B:218:PCW:H451 | 0.46 | 1.87 | 4 | 1 |
| 1:C:465:GLU:C | 1:C:469:LEU:HD12 | 0.46 | 2.30 | 4 | 1 |
| 3:A:405:PCW:O2P | 3:B:207:PCW:H72 | 0.46 | 2.10 | 7 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 3:C:607:PCW:H341 | 3:C:615:PCW:H362 | 0.46 | 1.87 | 9 | 1 |
| 3:C:612:PCW:H161 | 3:C:617:PCW:H19 | 0.46 | 1.88 | 9 | 1 |
| 3:B:213:PCW:H441 | 3:B:213:PCW:H251 | 0.46 | 1.88 | 1 | 1 |
| 3:A:401:PCW:H482 | 3:C:614:PCW:H221 | 0.46 | 1.86 | 2 | 1 |
| 3:C:626:PCW:H40 | 4:C:631:17F:H44 | 0.46 | 1.87 | 6 | 2 |
| 1:A:372:ARG:O | 1:A:376:LEU:HG | 0.46 | 2.10 | 4 | 1 |
| 3:A:401:PCW:H481 | 3:C:614:PCW:H20 | 0.46 | 1.86 | 4 | 1 |
| 3:A:406:PCW:H381 | 4:B:227:17F:H11 | 0.46 | 1.87 | 4 | 1 |
| 3:B:207:PCW:H231 | 3:C:601:PCW:H322 | 0.46 | 1.87 | 4 | 1 |
| 1:A:351:ALA:O | 1:A:355:GLU:HG2 | 0.46 | 2.10 | 5 | 1 |
| 3:B:208:PCW:H62 | 4:B:231:17F:O1 | 0.46 | 2.10 | 5 | 1 |
| 3:B:218:PCW:H41 | 3:B:219:PCW:O11 | 0.46 | 2.10 | 7 | 1 |
| 3:B:201:PCW:H32 | 4:B:230:17F:O1 | 0.46 | 2.10 | 10 | 1 |
| 4:B:226:17F:H35 | 4:B:236:17F:H50 | 0.46 | 1.86 | 10 | 1 |
| 3:C:603:PCW:H411 | 4:C:628:17F:C7 | 0.46 | 2.40 | 10 | 1 |
| 3:B:206:PCW:H482 | 3:B:218:PCW:H221 | 0.46 | 1.88 | 1 | 1 |
| 1:C:573:LEU:HA | 1:C:576:VAL:HG12 | 0.46 | 1.86 | 4 | 2 |
| 3:B:203:PCW:O2 | 3:B:213:PCW:H321 | 0.46 | 2.11 | 5 | 1 |
| 3:B:233:PCW:H481 | 3:C:603:PCW:H2 | 0.46 | 1.87 | 5 | 1 |
| 3:C:617:PCW:H411 | 3:C:618:PCW:H182 | 0.46 | 1.88 | 7 | 1 |
| 3:C:608:PCW:H73 | 4:C:631:17F:O1 | 0.46 | 2.10 | 8 | 1 |
| 3:B:202:PCW:H332 | 3:B:215:PCW:H152 | 0.46 | 1.88 | 9 | 1 |
| 4:C:628:17F:H1A | 4:C:628:17F:H4 | 0.46 | 1.86 | 1 | 1 |
| 4:C:630:17F:C4 | 4:C:630:17F:C1 | 0.46 | 2.92 | 1 | 3 |
| 2:B:45:VAL:HG22 | 2:B:50:THR:HG23 | 0.46 | 1.88 | 10 | 2 |
| 3:A:409:PCW:H483 | 3:C:619:PCW:H40 | 0.46 | 1.86 | 4 | 1 |
| 3:A:403:PCW:H442 | 3:A:404:PCW:H141 | 0.46 | 1.87 | 5 | 1 |
| 2:B:171:SER:HA | 3:B:209:PCW:H61 | 0.46 | 1.86 | 5 | 1 |
| 3:B:209:PCW:H381 | 4:B:228:17F:H20A | 0.46 | 1.87 | 7 | 1 |
| 1:C:561:LYS:O | 1:C:565:ALA:HB3 | 0.46 | 2.10 | 8 | 2 |
| 3:B:201:PCW:H371 | 4:B:228:17F:H41 | 0.46 | 1.87 | 9 | 1 |
| 1:A:392:GLU:HA | 1:A:395:LYS:HG2 | 0.46 | 1.87 | 10 | 1 |
| 3:B:212:PCW:H382 | 4:B:231:17F:H10A | 0.46 | 1.88 | 4 | 1 |
| 2:B:5:LYS:CD | 7:B:239:EWS:OAB | 0.46 | 2.63 | 6 | 1 |
| 3:B:210:PCW:H352 | 3:B:214:PCW:H142 | 0.46 | 1.86 | 7 | 1 |
| 3:C:611:PCW:H411 | 3:C:611:PCW:H19 | 0.46 | 1.86 | 8 | 1 |
| 3:B:212:PCW:H352 | 4:B:231:17F:H29 | 0.46 | 1.87 | 9 | 1 |
| 3:B:221:PCW:H422 | 4:B:229:17F:H63 | 0.46 | 1.86 | 9 | 1 |
| 3:C:606:PCW:H142 | 3:C:612:PCW:H171 | 0.46 | 1.87 | 10 | 1 |
| 3:A:409:PCW:H351 | 3:B:235:PCW:H382 | 0.46 | 1.87 | 5 | 1 |
| 3:B:214:PCW:H281 | 4:C:627:17F:H73 | 0.46 | 1.88 | 7 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 3:B:219:PCW:H452 | 3:B:219:PCW:H232 | 0.46 | 1.87 | 8 | 1 |
| 3:B:209:PCW:H131 | 3:B:224:PCW:H182 | 0.46 | 1.87 | 9 | 1 |
| 1:A:272:TYR:HD2 | 1:C:506:ARG:HH22 | 0.46 | 1.53 | 1 | 1 |
| 1:A:365:LYS:CB | 1:A:366:PRO:HD3 | 0.46 | 2.38 | 6 | 5 |
| 3:A:408:PCW:H252 | 3:A:411:PCW:H251 | 0.46 | 1.87 | 1 | 1 |
| 3:A:410:PCW:H382 | 4:C:630:17F:C12 | 0.46 | 2.40 | 1 | 1 |
| 2:B:145:SER:HB3 | 2:B:148:THR:HG22 | 0.46 | 1.88 | 1 | 1 |
| 1:C:563:LYS:CB | 1:C:564:PRO:HD3 | 0.46 | 2.36 | 2 | 3 |
| 3:A:410:PCW:H51 | 3:A:410:PCW:H11 | 0.46 | 1.87 | 5 | 1 |
| 3:B:213:PCW:H141 | 4:B:228:17F:O9 | 0.46 | 2.11 | 5 | 1 |
| 3:B:206:PCW:O2P | 3:B:211:PCW:H12 | 0.46 | 2.11 | 7 | 1 |
| 3:C:605:PCW:H451 | 4:C:627:17F:H51 | 0.46 | 1.88 | 8 | 1 |
| 3:A:408:PCW:H351 | 3:A:410:PCW:C34 | 0.46 | 2.34 | 2 | 1 |
| 1:A:352:LYS:HZ1 | 1:C:425:GLU:HB2 | 0.46 | 1.70 | 3 | 1 |
| 1:A:315:ALA:O | 1:A:319:HIS:HB2 | 0.46 | 2.11 | 5 | 1 |
| 3:A:409:PCW:H461 | 3:C:613:PCW:H171 | 0.46 | 1.88 | 5 | 1 |
| 3:B:201:PCW:H52 | 3:B:222:PCW:H42 | 0.46 | 1.86 | 6 | 1 |
| 3:C:607:PCW:H222 | 3:C:615:PCW:H411 | 0.46 | 1.87 | 6 | 1 |
| 3:C:609:PCW:H412 | 3:C:624:PCW:H222 | 0.46 | 1.88 | 8 | 1 |
| 3:B:205:PCW:H52 | 3:B:212:PCW:O2P | 0.46 | 2.11 | 9 | 1 |
| 3:B:219:PCW:H411 | 3:B:223:PCW:H372 | 0.46 | 1.86 | 9 | 1 |
| 3:B:225:PCW:H19 | 3:B:225:PCW:H381 | 0.46 | 1.87 | 9 | 1 |
| 3:C:621:PCW:H252 | 3:C:622:PCW:H431 | 0.46 | 1.87 | 9 | 1 |
| 3:B:210:PCW:H132 | 3:B:217:PCW:H151 | 0.45 | 1.87 | 1 | 1 |
| 4:B:236:17F:H33 | 3:C:622:PCW:H19 | 0.45 | 1.87 | 10 | 2 |
| 1:C:455:TYR:OH | 3:C:601:PCW:H231 | 0.45 | 2.10 | 9 | 2 |
| 3:C:622:PCW:H282 | 4:C:628:17F:H52 | 0.45 | 1.87 | 3 | 2 |
| 3:B:222:PCW:H481 | 3:C:622:PCW:H181 | 0.45 | 1.86 | 4 | 1 |
| 3:C:603:PCW:H412 | 3:C:607:PCW:H31 | 0.45 | 1.88 | 6 | 1 |
| 1:A:355:GLU:OE1 | 1:A:355:GLU:HA | 0.45 | 2.11 | 3 | 1 |
| 3:C:615:PCW:H19 | 4:C:633:17F:H12 | 0.45 | 1.88 | 4 | 1 |
| 3:B:204:PCW:H2 | 3:B:208:PCW:H322 | 0.45 | 1.87 | 5 | 1 |
| 3:B:208:PCW:H451 | 4:B:231:17F:H48 | 0.45 | 1.88 | 5 | 1 |
| 1:C:466:GLU:HA | 1:C:469:LEU:HD12 | 0.45 | 1.87 | 5 | 1 |
| 3:C:618:PCW:O3 | 3:C:626:PCW:H162 | 0.45 | 2.11 | 6 | 1 |
| 3:B:220:PCW:H442 | 3:B:222:PCW:H221 | 0.45 | 1.88 | 8 | 1 |
| 3:B:221:PCW:H172 | 3:C:601:PCW:H381 | 0.45 | 1.88 | 8 | 1 |
| 3:A:404:PCW:H20 | 3:B:225:PCW:H252 | 0.45 | 1.88 | 9 | 1 |
| 3:A:406:PCW:H472 | 3:A:409:PCW:H262 | 0.45 | 1.86 | 9 | 1 |
| 1:A:346:LEU:O | 1:A:350:HIS:HB2 | 0.45 | 2.11 | 1 | 1 |
| 3:C:603:PCW:H231 | 4:C:632:17F:H54 | 0.45 | 1.87 | 1 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 3:C:604:PCW:H131 | 3:C:625:PCW:H372 | 0.45 | 1.88 | 3 | 1 |
| 3:B:217:PCW:H232 | 4:B:226:17F:H64 | 0.45 | 1.88 | 5 | 1 |
| 3:B:210:PCW:H181 | 3:B:214:PCW:H19 | 0.45 | 1.88 | 6 | 1 |
| 3:A:411:PCW:H431 | 3:C:616:PCW:H261 | 0.45 | 1.88 | 9 | 1 |
| 3:C:611:PCW:H31 | 3:C:619:PCW:O3 | 0.45 | 2.11 | 9 | 1 |
| 3:B:201:PCW:H371 | 4:B:228:17F:C21 | 0.45 | 2.37 | 10 | 1 |
| 3:B:207:PCW:C21 | 3:C:601:PCW:H412 | 0.45 | 2.40 | 2 | 1 |
| 3:B:221:PCW:H131 | 3:B:221:PCW:H341 | 0.45 | 1.88 | 3 | 1 |
| 3:C:607:PCW:H181 | 3:C:615:PCW:H352 | 0.45 | 1.89 | 4 | 1 |
| 1:A:352:LYS:HG2 | 1:C:422:VAL:HG22 | 0.45 | 1.88 | 6 | 1 |
| 3:B:204:PCW:P | 3:B:212:PCW:O2P | 0.45 | 2.74 | 6 | 1 |
| 3:B:212:PCW:H121 | 4:B:231:17F:H9A | 0.45 | 1.88 | 7 | 1 |
| 3:B:216:PCW:H71 | 4:B:229:17F:H19A | 0.45 | 1.88 | 8 | 1 |
| 3:C:603:PCW:H441 | 3:C:607:PCW:H11 | 0.45 | 1.88 | 8 | 1 |
| 3:A:402:PCW:O2P | 3:B:205:PCW:H32 | 0.45 | 2.11 | 9 | 1 |
| 3:B:203:PCW:H122 | 4:B:230:17F:O8 | 0.45 | 2.11 | 10 | 1 |
| 3:B:210:PCW:H232 | 3:B:214:PCW:H461 | 0.45 | 1.87 | 10 | 1 |
| 4:B:230:17F:H9 | 4:B:230:17F:H19 | 0.45 | 1.88 | 10 | 1 |
| 3:A:403:PCW:C39 | 3:B:218:PCW:C48 | 0.45 | 2.95 | 1 | 1 |
| 3:A:403:PCW:H221 | 3:C:606:PCW:C26 | 0.45 | 2.40 | 1 | 1 |
| 3:B:203:PCW:H41 | 4:B:230:17F:O2 | 0.45 | 2.11 | 3 | 1 |
| 3:C:607:PCW:H232 | 3:C:615:PCW:H411 | 0.45 | 1.88 | 3 | 1 |
| 2:B:163:ILE:HG22 | 2:B:167:LYS:HE2 | 0.45 | 1.87 | 4 | 1 |
| 4:B:227:17F:H33 | 4:B:227:17F:O8 | 0.45 | 2.12 | 5 | 1 |
| 3:B:213:PCW:N | 4:B:232:17F:N1 | 0.45 | 2.65 | 7 | 1 |
| 3:A:409:PCW:H62 | 4:C:630:17F:H1A | 0.45 | 1.87 | 9 | 1 |
| 3:B:202:PCW:H162 | 3:B:215:PCW:H182 | 0.45 | 1.88 | 9 | 1 |
| 3:B:234:PCW:H172 | 3:B:234:PCW:H421 | 0.45 | 1.87 | 9 | 1 |
| 3:B:210:PCW:H51 | 4:B:226:17F:H2 | 0.45 | 1.88 | 10 | 1 |
| 3:C:615:PCW:H212 | 4:C:629:17F:H45 | 0.45 | 1.88 | 10 | 1 |
| 1:C:464:GLN:O | 1:C:468:GLU:HG3 | 0.45 | 2.12 | 6 | 1 |
| 3:A:410:PCW:H472 | 3:A:411:PCW:H283 | 0.45 | 1.87 | 7 | 1 |
| 3:A:409:PCW:H261 | 3:C:613:PCW:H181 | 0.45 | 1.88 | 10 | 1 |
| 3:B:221:PCW:H61 | 4:B:229:17F:O2 | 0.45 | 2.11 | 10 | 1 |
| 3:B:221:PCW:C17 | 3:C:601:PCW:H411 | 0.45 | 2.41 | 10 | 1 |
| 3:C:603:PCW:C40 | 4:C:628:17F:H6 | 0.45 | 2.42 | 2 | 1 |
| 1:C:455:TYR:CE1 | 3:C:601:PCW:H252 | 0.45 | 2.47 | 3 | 1 |
| 1:A:363:LYS:HG2 | 1:C:411:THR:HG22 | 0.45 | 1.87 | 4 | 1 |
| 3:B:211:PCW:H372 | 4:B:226:17F:H19A | 0.45 | 1.89 | 5 | 1 |
| 3:B:233:PCW:H51 | 4:B:236:17F:O2 | 0.45 | 2.12 | 6 | 1 |
| 3:B:223:PCW:H461 | 3:C:622:PCW:H452 | 0.45 | 1.87 | 7 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 3:B:234:PCW:H442 | 3:B:234:PCW:H212 | 0.45 | 1.89 | 7 | 1 |
| 3:B:221:PCW:H141 | 3:C:601:PCW:H372 | 0.45 | 1.88 | 8 | 1 |
| 3:B:212:PCW:H172 | 4:B:231:17F:H34 | 0.45 | 1.89 | 5 | 1 |
| 4:B:226:17F:H20A | 4:B:229:17F:H10 | 0.45 | 1.88 | 6 | 1 |
| 1:C:487:GLN:O | 1:C:491:GLU:HG3 | 0.45 | 2.12 | 6 | 1 |
| 3:B:209:PCW:H342 | 4:B:228:17F:O8 | 0.45 | 2.12 | 1 | 1 |
| 1:C:461:LYS:O | 1:C:465:GLU:HG3 | 0.45 | 2.11 | 1 | 2 |
| 3:A:408:PCW:H251 | 3:A:411:PCW:H232 | 0.45 | 1.87 | 2 | 1 |
| 3:B:214:PCW:H271 | 3:C:615:PCW:H432 | 0.45 | 1.89 | 2 | 1 |
| 3:C:611:PCW:H182 | 3:C:619:PCW:H181 | 0.45 | 1.89 | 2 | 3 |
| 3:A:405:PCW:H242 | 3:C:609:PCW:H261 | 0.45 | 1.88 | 3 | 1 |
| 3:B:220:PCW:H451 | 3:B:235:PCW:H232 | 0.45 | 1.88 | 5 | 1 |
| 4:B:236:17F:H72 | 3:C:603:PCW:H262 | 0.45 | 1.89 | 5 | 1 |
| 3:A:406:PCW:H331 | 4:B:227:17F:H8A | 0.45 | 1.88 | 6 | 1 |
| 3:B:235:PCW:H11 | 3:C:602:PCW:H11 | 0.45 | 1.88 | 6 | 1 |
| 3:B:208:PCW:H261 | 3:B:219:PCW:H283 | 0.45 | 1.88 | 7 | 1 |
| 3:B:217:PCW:H342 | 3:B:217:PCW:H152 | 0.45 | 1.87 | 7 | 1 |
| 1:A:327:LEU:HD23 | 1:A:330:ARG:HD3 | 0.45 | 1.88 | 9 | 1 |
| 4:B:236:17F:H44 | 4:C:628:17F:H78 | 0.45 | 1.88 | 10 | 1 |
| 3:B:234:PCW:H251 | 3:C:617:PCW:H481 | 0.45 | 1.89 | 1 | 1 |
| 3:B:213:PCW:H121 | 4:B:228:17F:O9 | 0.45 | 2.12 | 9 | 2 |
| 1:C:431:GLU:HA | 1:C:434:THR:OG1 | 0.45 | 2.12 | 7 | 1 |
| 3:B:201:PCW:H362 | 3:B:220:PCW:H382 | 0.45 | 1.89 | 8 | 1 |
| 3:B:204:PCW:H422 | 3:B:205:PCW:H351 | 0.45 | 1.88 | 8 | 1 |
| 4:C:628:17F:H6A | 4:C:632:17F:HN1 | 0.45 | 1.72 | 8 | 1 |
| 3:A:405:PCW:H40 | 3:C:609:PCW:H20 | 0.44 | 1.89 | 2 | 1 |
| 3:C:615:PCW:H421 | 4:C:632:17F:H52 | 0.44 | 1.89 | 3 | 1 |
| 3:A:410:PCW:H352 | 4:C:630:17F:H37 | 0.44 | 1.89 | 7 | 1 |
| 3:B:203:PCW:H483 | 4:B:228:17F:H57 | 0.44 | 1.87 | 7 | 1 |
| 3:B:203:PCW:H411 | 3:B:213:PCW:H162 | 0.44 | 1.89 | 7 | 1 |
| 3:C:611:PCW:H382 | 3:C:611:PCW:H171 | 0.44 | 1.89 | 7 | 1 |
| 4:C:628:17F:H65 | 4:C:632:17F:H29 | 0.44 | 1.89 | 7 | 1 |
| 4:B:227:17F:H65 | 3:C:623:PCW:H281 | 0.44 | 1.90 | 9 | 1 |
| 3:C:607:PCW:H322 | 3:C:615:PCW:H341 | 0.44 | 1.88 | 10 | 1 |
| 3:C:613:PCW:H171 | 3:C:613:PCW:H431 | 0.44 | 1.88 | 10 | 1 |
| 3:B:206:PCW:H451 | 3:B:208:PCW:H282 | 0.44 | 1.90 | 1 | 1 |
| 2:B:5:LYS:HA | 2:B:54:ASP:O | 0.44 | 2.12 | 2 | 1 |
| 3:B:204:PCW:H42 | 3:B:218:PCW:O4P | 0.44 | 2.12 | 1 | 1 |
| 3:B:208:PCW:O1P | 3:B:211:PCW:H83 | 0.44 | 2.13 | 1 | 1 |
| 3:A:406:PCW:H231 | 4:A:407:17F:H75 | 0.44 | 1.88 | 2 | 1 |
| 3:C:611:PCW:H141 | 3:C:619:PCW:H172 | 0.44 | 1.88 | 2 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 3:B:212:PCW:H332 | 4:B:231:17F:H8A | 0.44 | 1.88 | 4 | 1 |
| 4:B:227:17F:H58 | 4:B:227:17F:H9A | 0.44 | 1.88 | 5 | 1 |
| 3:B:223:PCW:H462 | 3:C:622:PCW:H452 | 0.44 | 1.88 | 9 | 1 |
| 4:B:230:17F:H2 | 4:B:230:17F:O2 | 0.44 | 2.12 | 9 | 1 |
| 3:C:622:PCW:H73 | 3:C:622:PCW:H331 | 0.44 | 1.88 | 9 | 1 |
| 4:A:407:17F:H54 | 3:B:204:PCW:H481 | 0.44 | 1.89 | 1 | 1 |
| 3:B:201:PCW:H382 | 3:B:220:PCW:H361 | 0.44 | 1.89 | 2 | 1 |
| 2:B:113:LEU:O | 2:B:141:PHE:HA | 0.44 | 2.12 | 4 | 1 |
| 3:A:403:PCW:H432 | 3:B:218:PCW:H472 | 0.44 | 1.89 | 10 | 1 |
| 4:B:236:17F:H10 | 4:C:628:17F:H41 | 0.44 | 1.90 | 10 | 1 |
| 1:C:530:ALA:O | 1:C:534:GLU:HG2 | 0.44 | 2.12 | 2 | 1 |
| 3:B:220:PCW:H251 | 4:B:232:17F:H75 | 0.44 | 1.90 | 3 | 1 |
| 3:A:404:PCW:H261 | 4:C:631:17F:H49 | 0.44 | 1.88 | 4 | 1 |
| 3:B:219:PCW:O2P | 3:B:225:PCW:H62 | 0.44 | 2.13 | 4 | 1 |
| 4:B:229:17F:H4 | 4:B:229:17F:H2 | 0.44 | 1.89 | 4 | 1 |
| 3:C:607:PCW:H121 | 3:C:615:PCW:O31 | 0.44 | 2.12 | 4 | 1 |
| 1:A:307:ASP:HA | 1:A:310:ARG:CD | 0.44 | 2.41 | 5 | 1 |
| 1:A:242:GLU:OE1 | 1:C:528:ARG:HA | 0.44 | 2.12 | 6 | 1 |
| 3:A:401:PCW:H40 | 3:B:203:PCW:H271 | 0.44 | 1.88 | 6 | 1 |
| 3:B:211:PCW:H242 | 3:B:216:PCW:H161 | 0.44 | 1.90 | 6 | 1 |
| 3:B:224:PCW:H52 | 4:B:226:17F:P1 | 0.44 | 2.52 | 8 | 1 |
| 3:B:204:PCW:H372 | 3:B:222:PCW:H141 | 0.44 | 1.89 | 9 | 1 |
| 3:B:210:PCW:H52 | 4:B:229:17F:HN1 | 0.44 | 1.72 | 9 | 1 |
| 1:C:455:TYR:O | 1:C:459:PHE:HB2 | 0.44 | 2.12 | 10 | 1 |
| 3:C:611:PCW:H172 | 3:C:623:PCW:H451 | 0.44 | 1.89 | 2 | 1 |
| 3:B:221:PCW:H182 | 3:C:601:PCW:H412 | 0.44 | 1.90 | 3 | 1 |
| 3:C:618:PCW:H122 | 3:C:626:PCW:H181 | 0.44 | 1.89 | 3 | 2 |
| 3:B:210:PCW:C14 | 3:B:214:PCW:H151 | 0.44 | 2.40 | 5 | 1 |
| 3:B:221:PCW:H411 | 3:C:601:PCW:H372 | 0.44 | 1.89 | 7 | 1 |
| 3:C:605:PCW:H221 | 4:C:629:17F:H51 | 0.44 | 1.89 | 8 | 1 |
| 4:A:407:17F:H20A | 4:A:407:17F:H8 | 0.44 | 1.88 | 10 | 1 |
| 1:A:277:GLU:HB3 | 1:A:278:PRO:CD | 0.44 | 2.43 | 1 | 1 |
| 4:A:407:17F:H30 | 4:B:227:17F:H19 | 0.44 | 1.89 | 2 | 1 |
| 3:B:208:PCW:H332 | 3:B:222:PCW:H362 | 0.44 | 1.90 | 4 | 1 |
| 3:A:404:PCW:H40 | 3:B:225:PCW:H261 | 0.44 | 1.89 | 5 | 1 |
| 1:A:243:MET:HA | 1:A:246:ASP:HB2 | 0.44 | 1.90 | 6 | 1 |
| 1:A:299:SER:HB2 | 1:A:300:PRO:CD | 0.44 | 2.42 | 10 | 2 |
| 3:B:210:PCW:H73 | 4:B:226:17F:H2 | 0.44 | 1.89 | 6 | 1 |
| 1:C:428:ASP:O | 1:C:432:LYS:HG3 | 0.44 | 2.12 | 6 | 1 |
| 3:A:405:PCW:O2P | 3:B:207:PCW:H83 | 0.44 | 2.13 | 7 | 1 |
| 3:A:409:PCW:H211 | 3:C:613:PCW:H142 | 0.44 | 1.87 | 8 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 3:B:216:PCW:H32 | 4:B:229:17F:HN1 | 0.44 | 1.71 | 8 | 1 |
| 3:A:410:PCW:C32 | 4:C:630:17F:H29 | 0.44 | 2.43 | 10 | 1 |
| 3:C:607:PCW:H142 | 3:C:615:PCW:H321 | 0.44 | 1.90 | 10 | 1 |
| 3:B:218:PCW:H152 | 3:B:219:PCW:H121 | 0.44 | 1.90 | 1 | 1 |
| 3:B:219:PCW:H482 | 4:C:631:17F:H63 | 0.44 | 1.89 | 1 | 1 |
| 3:B:204:PCW:H322 | 3:B:222:PCW:H121 | 0.44 | 1.89 | 2 | 1 |
| 1:C:458:ASP:O | 1:C:462:LYS:HG3 | 0.44 | 2.13 | 2 | 1 |
| 3:B:205:PCW:H19 | 3:B:205:PCW:H412 | 0.44 | 1.89 | 3 | 1 |
| 4:A:407:17F:H41 | 4:B:227:17F:H31 | 0.44 | 1.87 | 7 | 1 |
| 3:B:207:PCW:H162 | 3:B:209:PCW:H211 | 0.44 | 1.90 | 7 | 1 |
| 1:A:345:ARG:HD3 | 1:C:433:GLU:OE2 | 0.44 | 2.13 | 8 | 1 |
| 3:B:201:PCW:H181 | 4:B:230:17F:H18 | 0.44 | 1.89 | 8 | 1 |
| 3:B:207:PCW:H422 | 3:B:209:PCW:H231 | 0.44 | 1.90 | 10 | 1 |
| 3:B:233:PCW:H82 | 4:B:236:17F:O1 | 0.44 | 2.13 | 10 | 1 |
| 3:C:618:PCW:C35 | 3:C:626:PCW:H212 | 0.44 | 2.43 | 10 | 1 |
| 1:C:485:ALA:HA | 1:C:488:LYS:HG2 | 0.44 | 1.90 | 4 | 1 |
| 2:B:62:GLU:OE1 | 2:B:68:ARG:HD3 | 0.44 | 2.13 | 5 | 1 |
| 3:C:609:PCW:H132 | 3:C:625:PCW:H40 | 0.44 | 1.89 | 5 | 1 |
| 3:A:409:PCW:H211 | 3:C:613:PCW:H171 | 0.44 | 1.89 | 6 | 1 |
| 3:A:401:PCW:O1P | 3:A:405:PCW:H12 | 0.44 | 2.12 | 7 | 1 |
| 3:A:410:PCW:H322 | 4:C:630:17F:C21 | 0.44 | 2.41 | 8 | 1 |
| 3:B:216:PCW:H11 | 4:B:229:17F:N1 | 0.44 | 2.28 | 8 | 1 |
| 3:C:621:PCW:H422 | 4:C:632:17F:H34 | 0.44 | 1.88 | 9 | 1 |
| 3:B:221:PCW:C17 | 3:C:601:PCW:C41 | 0.44 | 2.96 | 10 | 1 |
| 3:C:618:PCW:H412 | 3:C:626:PCW:C17 | 0.44 | 2.43 | 10 | 1 |
| 3:B:220:PCW:H331 | 3:B:220:PCW:H132 | 0.43 | 1.90 | 1 | 1 |
| 1:C:512:ASP:O | 1:C:515:ARG:HB2 | 0.43 | 2.13 | 1 | 1 |
| 3:A:406:PCW:H462 | 4:A:407:17F:H74 | 0.43 | 1.90 | 5 | 1 |
| 3:B:221:PCW:H362 | 4:B:229:17F:H58 | 0.43 | 1.90 | 5 | 1 |
| 3:C:626:PCW:H271 | 4:C:631:17F:H41 | 0.43 | 1.89 | 5 | 1 |
| 1:A:392:GLU:HA | 1:A:395:LYS:HD2 | 0.43 | 1.89 | 7 | 1 |
| 1:C:567:GLU:HG2 | 1:C:571:GLN:NE2 | 0.43 | 2.27 | 9 | 1 |
| 3:B:212:PCW:H351 | 4:B:231:17F:H8A | 0.43 | 1.88 | 1 | 1 |
| 1:A:278:PRO:O | 1:A:282:GLU:HG3 | 0.43 | 2.12 | 5 | 2 |
| 3:C:615:PCW:H222 | 4:C:633:17F:H41 | 0.43 | 1.90 | 8 | 2 |
| 3:A:405:PCW:H152 | 4:B:228:17F:H34 | 0.43 | 1.88 | 6 | 1 |
| 1:C:491:GLU:HB3 | 1:C:495:LYS:CE | 0.43 | 2.44 | 7 | 2 |
| 3:C:605:PCW:H171 | 4:C:627:17F:H34 | 0.43 | 1.90 | 9 | 1 |
| 3:B:221:PCW:H241 | 3:C:601:PCW:C20 | 0.43 | 2.40 | 10 | 1 |
| 3:C:608:PCW:H82 | 4:C:631:17F:O1 | 0.43 | 2.12 | 10 | 1 |
| 3:C:609:PCW:O1P | 3:C:614:PCW:H32 | 0.43 | 2.13 | 10 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 3:A:403:PCW:H222 | 3:C:606:PCW:C27 | 0.43 | 2.41 | 1 | 1 |
| 1:C:485:ALA:HA | 3:C:620:PCW:H271 | 0.43 | 1.90 | 3 | 1 |
| 3:C:603:PCW:H251 | 3:C:607:PCW:H281 | 0.43 | 1.88 | 3 | 1 |
| 3:C:606:PCW:H171 | 3:C:616:PCW:H39 | 0.43 | 1.88 | 3 | 1 |
| 3:C:621:PCW:H441 | 4:C:632:17F:H37 | 0.43 | 1.89 | 3 | 1 |
| 3:B:210:PCW:H122 | 3:B:214:PCW:H121 | 0.43 | 1.88 | 4 | 1 |
| 4:B:226:17F:H51 | 4:C:628:17F:H54 | 0.43 | 1.90 | 4 | 1 |
| 3:C:620:PCW:C13 | 4:C:633:17F:H59 | 0.43 | 2.39 | 4 | 1 |
| 2:B:32:TYR:HD1 | 5:B:237:GNP:HNB3 | 0.43 | 1.56 | 5 | 1 |
| 3:B:212:PCW:H252 | 3:B:218:PCW:H412 | 0.43 | 1.91 | 5 | 1 |
| 3:B:203:PCW:H40 | 4:B:228:17F:H12A | 0.43 | 1.90 | 7 | 1 |
| 1:C:458:ASP:HA | 1:C:461:LYS:HD2 | 0.43 | 1.90 | 9 | 1 |
| 3:C:607:PCW:H151 | 3:C:615:PCW:C35 | 0.43 | 2.43 | 10 | 1 |
| 3:B:207:PCW:H42 | 3:B:216:PCW:H351 | 0.43 | 1.90 | 2 | 1 |
| 2:B:40:TYR:CE1 | 2:B:57:ASP:HB2 | 0.43 | 2.44 | 3 | 1 |
| 1:A:376:LEU:HB2 | 1:A:377:PRO:HD3 | 0.43 | 1.91 | 9 | 2 |
| 1:A:291:LEU:HD23 | 1:A:294:LEU:HD12 | 0.43 | 1.88 | 5 | 1 |
| 3:B:219:PCW:O2P | 3:B:225:PCW:H82 | 0.43 | 2.13 | 6 | 1 |
| 3:B:233:PCW:H83 | 3:C:602:PCW:H32 | 0.43 | 1.90 | 6 | 1 |
| 1:A:330:ARG:HD3 | 1:C:444:ASP:OD2 | 0.43 | 2.14 | 7 | 1 |
| 3:B:203:PCW:H19 | 4:B:230:17F:H10 | 0.43 | 1.89 | 7 | 1 |
| 3:B:208:PCW:H352 | 3:B:222:PCW:H352 | 0.43 | 1.89 | 10 | 1 |
| 3:C:618:PCW:H122 | 3:C:626:PCW:H171 | 0.43 | 1.91 | 2 | 1 |
| 3:B:203:PCW:H441 | 3:B:213:PCW:H262 | 0.43 | 1.90 | 3 | 1 |
| 3:B:221:PCW:H222 | 3:C:601:PCW:H483 | 0.43 | 1.90 | 3 | 1 |
| 3:B:235:PCW:O4P | 3:B:235:PCW:H2 | 0.43 | 2.13 | 4 | 1 |
| 3:B:215:PCW:H73 | 3:B:217:PCW:O1P | 0.43 | 2.13 | 5 | 1 |
| 3:B:216:PCW:H241 | 3:C:605:PCW:H461 | 0.43 | 1.90 | 8 | 1 |
| 1:A:356:HIS:HA | 1:C:418:GLN:OE1 | 0.43 | 2.13 | 10 | 1 |
| 3:A:408:PCW:O31 | 3:A:410:PCW:H332 | 0.43 | 2.13 | 10 | 1 |
| 2:B:84:ILE:HD12 | 2:B:123:ARG:HG3 | 0.43 | 1.90 | 10 | 1 |
| 3:B:204:PCW:O3P | 3:B:222:PCW:H61 | 0.43 | 2.13 | 1 | 1 |
| 1:A:263:LYS:O | 1:A:267:GLU:HG3 | 0.43 | 2.14 | 6 | 2 |
| 2:B:14:VAL:HG23 | 2:B:16:LYS:HG2 | 0.43 | 1.91 | 2 | 1 |
| 3:B:201:PCW:H132 | 4:B:230:17F:H18 | 0.43 | 1.91 | 3 | 1 |
| 3:B:214:PCW:H42 | 3:B:217:PCW:H61 | 0.43 | 1.90 | 4 | 1 |
| 3:B:212:PCW:H332 | 4:B:231:17F:H11 | 0.43 | 1.89 | 6 | 1 |
| 3:B:223:PCW:H451 | 3:C:622:PCW:H431 | 0.43 | 1.90 | 6 | 1 |
| 3:B:221:PCW:H141 | 3:C:601:PCW:H362 | 0.43 | 1.91 | 8 | 1 |
| 3:C:618:PCW:O1P | 3:C:626:PCW:H2 | 0.43 | 2.12 | 9 | 1 |
| 3:B:209:PCW:O31 | 3:B:216:PCW:H31 | 0.43 | 2.13 | 10 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 4:B:228:17F:H47 | 3:C:611:PCW:H462 | 0.43 | 1.89 | 1 | 1 |
| 3:C:605:PCW:H171 | 4:C:629:17F:H18 | 0.43 | 1.91 | 1 | 1 |
| 3:B:204:PCW:H231 | 3:B:212:PCW:H461 | 0.43 | 1.91 | 2 | 1 |
| 1:A:365:LYS:HB2 | 1:A:366:PRO:CD | 0.43 | 2.43 | 9 | 2 |
| 3:A:410:PCW:H381 | 4:C:630:17F:H36 | 0.43 | 1.90 | 4 | 2 |
| 3:B:222:PCW:H71 | 3:B:222:PCW:O31 | 0.43 | 2.13 | 6 | 1 |
| 3:B:206:PCW:H431 | 3:B:217:PCW:H382 | 0.43 | 1.89 | 8 | 1 |
| 2:B:68:ARG:O | 2:B:72:MET:HB2 | 0.43 | 2.13 | 4 | 3 |
| 3:A:406:PCW:H321 | 4:B:227:17F:O7 | 0.43 | 2.14 | 5 | 1 |
| 1:C:510:HIS:O | 1:C:514:LEU:HG | 0.43 | 2.14 | 8 | 2 |
| 3:B:222:PCW:H272 | 3:B:235:PCW:H221 | 0.43 | 1.89 | 4 | 1 |
| 3:B:210:PCW:C7 | 4:B:226:17F:HN1A | 0.43 | 2.26 | 5 | 1 |
| 3:B:235:PCW:H32 | 3:C:602:PCW:H31 | 0.43 | 1.91 | 5 | 1 |
| 3:A:402:PCW:H471 | 4:B:231:17F:H46 | 0.43 | 1.90 | 8 | 1 |
| 3:C:611:PCW:H221 | 3:C:619:PCW:H242 | 0.43 | 1.91 | 8 | 1 |
| 3:A:406:PCW:H282 | 3:A:411:PCW:H481 | 0.43 | 1.90 | 10 | 1 |
| 3:B:217:PCW:H131 | 4:B:226:17F:H63 | 0.43 | 1.90 | 10 | 1 |
| 1:A:258:LEU:O | 1:A:262:GLN:HB2 | 0.43 | 2.14 | 1 | 1 |
| 3:B:215:PCW:H72 | 3:B:219:PCW:H63 | 0.43 | 1.91 | 1 | 1 |
| 1:A:335:LEU:O | 1:A:339:LYS:HG3 | 0.43 | 2.13 | 2 | 1 |
| 3:B:211:PCW:H382 | 4:B:226:17F:H10 | 0.43 | 1.91 | 4 | 1 |
| 4:B:236:17F:H8A | 4:C:628:17F:H41 | 0.43 | 1.91 | 4 | 1 |
| 3:B:204:PCW:H181 | 3:B:218:PCW:H132 | 0.43 | 1.90 | 5 | 1 |
| 3:B:206:PCW:H351 | 3:B:211:PCW:H331 | 0.43 | 1.90 | 5 | 1 |
| 3:B:214:PCW:H40 | 3:B:215:PCW:H39 | 0.43 | 1.91 | 5 | 1 |
| 1:A:304:GLU:O | 1:A:308:ARG:HG2 | 0.43 | 2.14 | 6 | 1 |
| 1:A:344:ALA:O | 1:A:348:GLU:HG2 | 0.43 | 2.14 | 7 | 1 |
| 3:B:201:PCW:H42 | 4:B:230:17F:C2 | 0.43 | 2.44 | 7 | 1 |
| 4:C:633:17F:H58 | 4:C:633:17F:H30 | 0.43 | 1.90 | 7 | 1 |
| 1:A:386:PHE:O | 1:A:390:LEU:HG | 0.43 | 2.14 | 8 | 1 |
| 4:B:228:17F:H39 | 4:B:232:17F:H38 | 0.43 | 1.91 | 8 | 1 |
| 3:B:205:PCW:C4 | 3:B:222:PCW:H71 | 0.43 | 2.30 | 10 | 1 |
| 1:A:270:GLU:O | 1:A:274:GLN:HB2 | 0.42 | 2.14 | 5 | 1 |
| 4:B:231:17F:H50 | 3:C:610:PCW:H483 | 0.42 | 1.91 | 5 | 1 |
| 2:B:20:THR:O | 2:B:24:ILE:HG12 | 0.42 | 2.14 | 6 | 2 |
| 3:B:208:PCW:H19 | 3:B:222:PCW:H442 | 0.42 | 1.90 | 6 | 1 |
| 1:A:279:LEU:HB3 | 1:C:495:LYS:HD3 | 0.42 | 1.90 | 7 | 1 |
| 3:B:224:PCW:H52 | 4:B:226:17F:O1 | 0.42 | 2.14 | 8 | 1 |
| 3:C:607:PCW:H151 | 3:C:615:PCW:H351 | 0.42 | 1.90 | 10 | 1 |
| 3:A:401:PCW:H441 | 3:C:614:PCW:H272 | 0.42 | 1.90 | 1 | 1 |
| 3:C:604:PCW:H371 | 3:C:605:PCW:H331 | 0.42 | 1.91 | 1 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 3:B:209:PCW:H332 | 3:B:224:PCW:H19 | 0.42 | 1.90 | 3 | 1 |
| 3:B:235:PCW:C34 | 3:C:623:PCW:H331 | 0.42 | 2.44 | 4 | 1 |
| 3:C:625:PCW:O11 | 3:C:625:PCW:H52 | 0.42 | 2.15 | 7 | 1 |
| 3:B:207:PCW:H71 | 4:B:228:17F:C1 | 0.42 | 2.44 | 10 | 1 |
| 3:C:605:PCW:H242 | 4:C:629:17F:H52 | 0.42 | 1.92 | 10 | 1 |
| 3:B:211:PCW:H131 | 3:B:217:PCW:H2 | 0.42 | 1.90 | 1 | 1 |
| 3:C:604:PCW:H52 | 3:C:604:PCW:C1 | 0.42 | 2.44 | 2 | 1 |
| 3:A:404:PCW:H11 | 3:B:218:PCW:H372 | 0.42 | 1.89 | 3 | 1 |
| 2:B:6:LEU:O | 2:B:55:ILE:HA | 0.42 | 2.14 | 3 | 2 |
| 2:B:59:ALA:HB3 | 2:B:62:GLU:HG2 | 0.42 | 1.91 | 3 | 1 |
| 3:B:209:PCW:H342 | 4:B:228:17F:H18A | 0.42 | 1.90 | 3 | 1 |
| 3:C:607:PCW:C15 | 3:C:615:PCW:H321 | 0.42 | 2.45 | 3 | 2 |
| 3:A:402:PCW:H321 | 3:B:205:PCW:H32 | 0.42 | 1.91 | 6 | 1 |
| 3:A:406:PCW:C31 | 4:A:407:17F:H31 | 0.42 | 2.44 | 8 | 1 |
| 3:C:610:PCW:H272 | 3:C:610:PCW:H482 | 0.42 | 1.92 | 8 | 1 |
| 4:B:236:17F:H75 | 3:C:603:PCW:H271 | 0.42 | 1.92 | 9 | 1 |
| 3:B:204:PCW:H412 | 3:B:205:PCW:H382 | 0.42 | 1.91 | 10 | 1 |
| 3:B:209:PCW:H151 | 3:B:216:PCW:H142 | 0.42 | 1.90 | 2 | 1 |
| 2:B:145:SER:HB2 | 2:B:150:GLN:HB2 | 0.42 | 1.92 | 3 | 1 |
| 3:B:224:PCW:H11 | 4:B:232:17F:H6 | 0.42 | 1.91 | 4 | 1 |
| 1:A:304:GLU:O | 1:A:308:ARG:HG3 | 0.42 | 2.14 | 7 | 1 |
| 3:C:609:PCW:H382 | 3:C:624:PCW:H431 | 0.42 | 1.89 | 7 | 1 |
| 4:B:232:17F:H49 | 3:C:609:PCW:H451 | 0.42 | 1.91 | 9 | 1 |
| 3:A:410:PCW:H442 | 3:A:410:PCW:H272 | 0.42 | 1.92 | 10 | 1 |
| 3:B:210:PCW:H71 | 4:B:226:17F:O1 | 0.42 | 2.14 | 1 | 1 |
| 3:B:219:PCW:H461 | 3:B:223:PCW:H482 | 0.42 | 1.89 | 1 | 1 |
| 3:B:233:PCW:H41 | 4:B:236:17F:O2 | 0.42 | 2.15 | 8 | 2 |
| 4:C:628:17F:H4A | 4:C:632:17F:HN1 | 0.42 | 1.75 | 3 | 1 |
| 3:A:406:PCW:H321 | 4:A:407:17F:H8 | 0.42 | 1.91 | 4 | 1 |
| 2:B:62:GLU:HB3 | 2:B:68:ARG:NH1 | 0.42 | 2.30 | 4 | 1 |
| 3:B:233:PCW:H172 | 3:C:624:PCW:C15 | 0.42 | 2.44 | 4 | 1 |
| 2:B:170:MET:HB3 | 3:B:211:PCW:H52 | 0.42 | 1.92 | 9 | 1 |
| 3:B:217:PCW:H222 | 4:B:226:17F:H65 | 0.42 | 1.91 | 9 | 1 |
| 3:C:618:PCW:H372 | 3:C:626:PCW:H412 | 0.42 | 1.91 | 9 | 1 |
| 3:A:405:PCW:H432 | 3:C:609:PCW:H231 | 0.42 | 1.92 | 10 | 1 |
| 3:A:406:PCW:H211 | 4:A:407:17F:H70 | 0.42 | 1.90 | 2 | 1 |
| 3:C:610:PCW:H482 | 3:C:610:PCW:H252 | 0.42 | 1.89 | 2 | 1 |
| 1:A:356:HIS:O | 1:A:360:LEU:HB2 | 0.42 | 2.14 | 4 | 1 |
| 3:B:215:PCW:H11 | 3:B:223:PCW:O1P | 0.42 | 2.15 | 4 | 1 |
| 3:B:212:PCW:H412 | 4:B:231:17F:H57 | 0.42 | 1.90 | 5 | 1 |
| 3:C:615:PCW:H222 | 4:C:633:17F:H35 | 0.42 | 1.91 | 6 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 3:B:207:PCW:H71 | 4:B:228:17F:HN1 | 0.42 | 1.74 | 7 | 1 |
| 4:A:407:17F:H37 | 4:B:227:17F:H19 | 0.42 | 1.91 | 10 | 1 |
| 3:B:211:PCW:H11 | 3:B:217:PCW:O1P | 0.42 | 2.14 | 10 | 1 |
| 4:A:407:17F:H30 | 4:B:227:17F:O10 | 0.42 | 2.15 | 1 | 1 |
| 2:B:78:PHE:O | 2:B:111:MET:HA | 0.42 | 2.15 | 3 | 1 |
| 2:B:133:LEU:HG | 2:B:137:TYR:HE2 | 0.42 | 1.73 | 3 | 1 |
| 3:B:214:PCW:H241 | 3:C:615:PCW:H471 | 0.42 | 1.92 | 3 | 1 |
| 3:B:221:PCW:C7 | 4:B:229:17F:H1 | 0.42 | 2.36 | 4 | 1 |
| 3:B:201:PCW:H40 | 3:C:623:PCW:H272 | 0.42 | 1.90 | 5 | 1 |
| 3:A:409:PCW:H2 | 3:A:409:PCW:O1P | 0.42 | 2.14 | 7 | 2 |
| 3:B:219:PCW:H231 | 3:B:219:PCW:H461 | 0.42 | 1.92 | 7 | 1 |
| 3:A:406:PCW:H331 | 4:A:407:17F:H31 | 0.42 | 1.91 | 8 | 1 |
| 1:C:458:ASP:HA | 1:C:461:LYS:NZ | 0.42 | 2.30 | 8 | 1 |
| 3:C:625:PCW:O11 | 3:C:625:PCW:H83 | 0.42 | 2.15 | 8 | 1 |
| 3:C:608:PCW:C1 | 4:C:631:17F:H4A | 0.42 | 2.44 | 2 | 1 |
| 1:A:325:ASP:O | 1:A:329:GLN:HG3 | 0.42 | 2.15 | 3 | 1 |
| 3:B:210:PCW:H73 | 4:B:226:17F:P1 | 0.42 | 2.55 | 10 | 1 |
| 3:C:615:PCW:H242 | 4:C:629:17F:H45 | 0.42 | 1.92 | 1 | 1 |
| 1:C:589:GLU:O | 1:C:593:LYS:HG3 | 0.42 | 2.14 | 4 | 1 |
| 3:C:605:PCW:H481 | 4:C:627:17F:H53 | 0.42 | 1.91 | 4 | 1 |
| 3:B:210:PCW:H41 | 4:B:226:17F:O5 | 0.42 | 2.15 | 5 | 1 |
| 3:B:214:PCW:H381 | 3:B:217:PCW:H162 | 0.42 | 1.90 | 6 | 1 |
| 3:A:401:PCW:H362 | 3:B:213:PCW:H432 | 0.42 | 1.92 | 8 | 1 |
| 3:B:207:PCW:H232 | 3:C:601:PCW:H421 | 0.42 | 1.90 | 8 | 1 |
| 3:C:607:PCW:H283 | 3:C:615:PCW:H422 | 0.42 | 1.92 | 3 | 1 |
| 4:B:226:17F:H45 | 4:B:232:17F:H62 | 0.42 | 1.91 | 4 | 1 |
| 3:C:605:PCW:H212 | 4:C:627:17F:H37 | 0.42 | 1.92 | 6 | 1 |
| 3:B:210:PCW:H82 | 4:B:229:17F:H6A | 0.42 | 1.91 | 7 | 1 |
| 3:A:410:PCW:H132 | 4:C:630:17F:H11A | 0.42 | 1.92 | 8 | 1 |
| 3:B:216:PCW:H221 | 3:C:604:PCW:H462 | 0.42 | 1.91 | 8 | 1 |
| 1:C:427:TRP:O | 1:C:431:GLU:HG2 | 0.41 | 2.15 | 1 | 1 |
| 3:B:218:PCW:H71 | 4:B:231:17F:H2 | 0.41 | 1.90 | 2 | 1 |
| 3:B:209:PCW:H73 | 3:B:216:PCW:H12 | 0.41 | 1.92 | 3 | 1 |
| 3:B:221:PCW:H371 | 4:B:229:17F:H31 | 0.41 | 1.91 | 3 | 1 |
| 3:B:211:PCW:H82 | 3:B:219:PCW:H321 | 0.41 | 1.91 | 4 | 1 |
| 3:A:408:PCW:H39 | 3:A:410:PCW:H432 | 0.41 | 1.92 | 5 | 1 |
| 3:C:602:PCW:H63 | 3:C:602:PCW:O11 | 0.41 | 2.15 | 6 | 1 |
| 1:C:574:LEU:HB2 | 1:C:575:PRO:CD | 0.41 | 2.45 | 1 | 1 |
| 3:B:211:PCW:H121 | 4:B:226:17F:O9 | 0.41 | 2.14 | 3 | 1 |
| 3:A:409:PCW:H63 | 4:C:630:17F:N1 | 0.41 | 2.30 | 4 | 1 |
| 1:C:488:LYS:NZ | 3:C:620:PCW:C27 | 0.41 | 2.83 | 4 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 3:B:209:PCW:H61 | 3:B:216:PCW:O2P | 0.41 | 2.14 | 6 | 1 |
| 3:B:205:PCW:H62 | 3:B:212:PCW:O2P | 0.41 | 2.14 | 7 | 1 |
| 3:B:210:PCW:H20 | 4:C:633:17F:H51 | 0.41 | 1.91 | 9 | 1 |
| 3:C:603:PCW:H371 | 3:C:607:PCW:C3 | 0.41 | 2.46 | 9 | 1 |
| 3:C:612:PCW:H241 | 3:C:612:PCW:H452 | 0.41 | 1.91 | 9 | 1 |
| 3:B:215:PCW:H83 | 3:B:217:PCW:O2P | 0.41 | 2.14 | 1 | 1 |
| 1:A:243:MET:HA | 1:A:246:ASP:HB3 | 0.41 | 1.92 | 3 | 1 |
| 3:B:212:PCW:H461 | 3:B:218:PCW:H442 | 0.41 | 1.91 | 4 | 1 |
| 3:B:203:PCW:O31 | 3:B:203:PCW:H41 | 0.41 | 2.16 | 6 | 1 |
| 3:A:411:PCW:H172 | 3:A:411:PCW:H211 | 0.41 | 1.92 | 10 | 1 |
| 4:B:236:17F:H6A | 3:C:603:PCW:H142 | 0.41 | 1.92 | 10 | 1 |
| 3:B:203:PCW:H132 | 3:B:213:PCW:H372 | 0.41 | 1.91 | 1 | 1 |
| 1:A:345:ARG:O | 1:A:349:TYR:HB2 | 0.41 | 2.15 | 2 | 1 |
| 3:B:204:PCW:O1P | 3:B:222:PCW:H81 | 0.41 | 2.14 | 3 | 1 |
| 4:A:407:17F:H37 | 3:B:222:PCW:H32 | 0.41 | 1.91 | 5 | 1 |
| 3:B:220:PCW:O2P | 3:B:222:PCW:H322 | 0.41 | 2.15 | 5 | 1 |
| 3:A:405:PCW:H331 | 3:B:209:PCW:H361 | 0.41 | 1.91 | 7 | 1 |
| 3:B:207:PCW:H71 | 4:B:228:17F:O3 | 0.41 | 2.15 | 7 | 1 |
| 4:A:407:17F:H54 | 3:C:613:PCW:H281 | 0.41 | 1.92 | 9 | 1 |
| 3:B:212:PCW:H432 | 4:B:231:17F:H60 | 0.41 | 1.93 | 1 | 1 |
| 3:B:216:PCW:H52 | 3:B:216:PCW:O31 | 0.41 | 2.14 | 1 | 1 |
| 1:C:458:ASP:HA | 1:C:461:LYS:HE2 | 0.41 | 1.91 | 1 | 1 |
| 1:A:264:LYS:O | 1:A:268:GLU:HG3 | 0.41 | 2.15 | 2 | 1 |
| 1:C:576:VAL:O | 1:C:580:PHE:HB2 | 0.41 | 2.15 | 2 | 1 |
| 3:A:401:PCW:H381 | 3:B:213:PCW:H483 | 0.41 | 1.92 | 3 | 1 |
| 3:B:210:PCW:H332 | 3:B:214:PCW:H142 | 0.41 | 1.91 | 3 | 1 |
| 3:B:208:PCW:H432 | 3:B:234:PCW:H221 | 0.41 | 1.92 | 5 | 1 |
| 3:B:209:PCW:H151 | 3:B:216:PCW:H171 | 0.41 | 1.92 | 5 | 1 |
| 1:C:502:GLU:O | 1:C:506:ARG:HG3 | 0.41 | 2.15 | 9 | 3 |
| 3:C:615:PCW:H442 | 4:C:632:17F:H47 | 0.41 | 1.93 | 5 | 1 |
| 4:B:232:17F:H44 | 3:C:609:PCW:H482 | 0.41 | 1.93 | 6 | 1 |
| 3:C:604:PCW:H131 | 3:C:625:PCW:H381 | 0.41 | 1.93 | 6 | 1 |
| 3:A:409:PCW:H121 | 3:C:613:PCW:H2 | 0.41 | 1.92 | 9 | 1 |
| 1:A:330:ARG:HH12 | 1:C:448:VAL:HG23 | 0.41 | 1.76 | 1 | 1 |
| 1:A:285:GLU:HA | 1:A:288:ARG:HD2 | 0.41 | 1.92 | 2 | 1 |
| 2:B:71:TYR:HD1 | 7:B:239:EWS:BRA | 0.41 | 2.53 | 2 | 1 |
| 3:B:201:PCW:H212 | 4:B:230:17F:H33 | 0.41 | 1.92 | 2 | 1 |
| 3:B:218:PCW:H172 | 3:B:225:PCW:H372 | 0.41 | 1.91 | 2 | 1 |
| 3:C:611:PCW:O31 | 3:C:623:PCW:H361 | 0.41 | 2.15 | 2 | 1 |
| 1:A:239:LEU:HA | 1:A:242:GLU:HB2 | 0.41 | 1.91 | 4 | 1 |
| 1:A:290:LYS:HE3 | 1:C:487:GLN:OE1 | 0.41 | 2.16 | 5 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 3:B:220:PCW:H71 | 4:B:232:17F:O1 | 0.41 | 2.16 | 8 | 1 |
| 3:A:410:PCW:C38 | 4:C:630:17F:H36 | 0.41 | 2.44 | 9 | 1 |
| 3:A:404:PCW:H352 | 3:B:225:PCW:H162 | 0.41 | 1.91 | 10 | 1 |
| 3:B:213:PCW:H161 | 3:B:213:PCW:H342 | 0.41 | 1.91 | 10 | 1 |
| 3:B:208:PCW:H341 | 3:B:222:PCW:H362 | 0.41 | 1.90 | 1 | 1 |
| 3:B:235:PCW:H481 | 3:C:610:PCW:H452 | 0.41 | 1.91 | 1 | 1 |
| 3:C:626:PCW:O31 | 3:C:626:PCW:H42 | 0.41 | 2.15 | 1 | 1 |
| 3:B:208:PCW:H242 | 3:B:218:PCW:H281 | 0.41 | 1.93 | 3 | 1 |
| 2:B:101:LYS:HE3 | 2:B:107:GLU:HA | 0.41 | 1.93 | 4 | 1 |
| 3:B:201:PCW:H172 | 4:B:227:17F:O8 | 0.41 | 2.15 | 4 | 1 |
| 3:B:233:PCW:H451 | 3:B:233:PCW:H321 | 0.41 | 1.93 | 5 | 1 |
| 4:B:226:17F:H70 | 4:B:236:17F:H55 | 0.41 | 1.92 | 6 | 1 |
| 3:B:221:PCW:H132 | 3:C:601:PCW:H12 | 0.41 | 1.92 | 7 | 1 |
| 3:B:205:PCW:O2P | 3:B:212:PCW:H73 | 0.41 | 2.16 | 10 | 1 |
| 1:A:341:ASN:O | 1:A:345:ARG:HG3 | 0.41 | 2.16 | 2 | 1 |
| 3:A:411:PCW:H162 | 4:C:630:17F:H38 | 0.41 | 1.92 | 2 | 1 |
| 3:B:206:PCW:H32 | 3:B:220:PCW:H63 | 0.41 | 1.91 | 4 | 1 |
| 3:A:405:PCW:H322 | 3:B:207:PCW:H322 | 0.41 | 1.92 | 5 | 1 |
| 3:B:201:PCW:H132 | 4:B:227:17F:O8 | 0.41 | 2.16 | 6 | 1 |
| 1:C:540:GLY:O | 1:C:544:LEU:HG | 0.41 | 2.16 | 6 | 1 |
| 3:A:406:PCW:H131 | 4:A:407:17F:H20A | 0.41 | 1.92 | 7 | 1 |
| 3:B:224:PCW:H151 | 4:B:232:17F:H9 | 0.41 | 1.92 | 7 | 1 |
| 3:B:203:PCW:H321 | 3:B:213:PCW:H81 | 0.41 | 1.92 | 9 | 1 |
| 1:A:330:ARG:NH2 | 1:C:447:GLU:HB3 | 0.41 | 2.31 | 10 | 1 |
| 3:B:221:PCW:H452 | 4:C:627:17F:H50 | 0.41 | 1.93 | 1 | 1 |
| 1:C:490:HIS:HA | 1:C:493:GLN:OE1 | 0.41 | 2.15 | 1 | 1 |
| 1:C:578:GLU:O | 1:C:582:VAL:HG23 | 0.41 | 2.16 | 1 | 1 |
| 1:A:375:LEU:HD11 | 4:B:230:17F:C30 | 0.41 | 2.46 | 4 | 1 |
| 3:B:204:PCW:H151 | 3:B:212:PCW:H39 | 0.41 | 1.92 | 4 | 1 |
| 4:B:226:17F:C40 | 4:B:236:17F:H54 | 0.41 | 2.45 | 4 | 1 |
| 1:C:465:GLU:C | 1:C:469:LEU:CD1 | 0.41 | 2.85 | 4 | 1 |
| 1:A:277:GLU:HB2 | 1:A:278:PRO:CD | 0.41 | 2.45 | 5 | 1 |
| 4:A:407:17F:C2X | 3:B:201:PCW:H381 | 0.41 | 2.45 | 5 | 1 |
| 3:A:406:PCW:H341 | 4:A:407:17F:C1Y | 0.41 | 2.43 | 6 | 1 |
| 3:B:219:PCW:H381 | 3:B:223:PCW:H372 | 0.41 | 1.92 | 6 | 1 |
| 3:B:220:PCW:H2 | 3:B:220:PCW:H41 | 0.41 | 1.91 | 6 | 1 |
| 3:C:611:PCW:H152 | 3:C:623:PCW:H431 | 0.41 | 1.92 | 6 | 1 |
| 3:C:621:PCW:H482 | 4:C:632:17F:H35 | 0.41 | 1.92 | 6 | 1 |
| 3:A:404:PCW:O1P | 3:B:218:PCW:H71 | 0.41 | 2.15 | 7 | 1 |
| 3:B:205:PCW:H371 | 3:B:205:PCW:H19 | 0.41 | 1.93 | 7 | 1 |
| 3:C:607:PCW:H282 | 3:C:615:PCW:H451 | 0.41 | 1.93 | 7 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 3:B:206:PCW:H40 | 3:B:217:PCW:H351 | 0.41 | 1.92 | 10 | 1 |
| 4:A:407:17F:H51 | 3:C:623:PCW:H251 | 0.41 | 1.93 | 2 | 1 |
| 3:B:207:PCW:H82 | 3:B:209:PCW:O2P | 0.41 | 2.16 | 3 | 1 |
| 3:B:204:PCW:N | 3:B:204:PCW:O2P | 0.41 | 2.54 | 4 | 1 |
| 3:C:617:PCW:H181 | 3:C:617:PCW:H152 | 0.41 | 1.65 | 4 | 1 |
| 3:B:201:PCW:H372 | 4:B:227:17F:H32 | 0.41 | 1.93 | 8 | 1 |
| 3:B:206:PCW:H431 | 3:B:217:PCW:H411 | 0.41 | 1.91 | 8 | 1 |
| 3:B:216:PCW:H32 | 4:B:229:17F:N1 | 0.41 | 2.31 | 8 | 1 |
| 1:A:264:LYS:CE | 1:C:509:ALA:HB1 | 0.41 | 2.44 | 9 | 1 |
| 3:B:224:PCW:H421 | 4:B:226:17F:H49 | 0.41 | 1.93 | 9 | 1 |
| 3:C:607:PCW:H251 | 3:C:615:PCW:H441 | 0.41 | 1.93 | 9 | 1 |
| 3:B:209:PCW:O1P | 3:B:216:PCW:H12 | 0.40 | 2.16 | 1 | 1 |
| 3:B:207:PCW:H172 | 3:B:209:PCW:H241 | 0.40 | 1.92 | 2 | 1 |
| 3:C:615:PCW:H222 | 4:C:633:17F:H40 | 0.40 | 1.92 | 3 | 1 |
| 3:B:207:PCW:H11 | 4:B:228:17F:O1 | 0.40 | 2.16 | 4 | 1 |
| 3:B:207:PCW:H19 | 3:C:601:PCW:H122 | 0.40 | 1.92 | 4 | 1 |
| 3:B:209:PCW:H39 | 4:B:228:17F:H18A | 0.40 | 1.92 | 4 | 1 |
| 3:B:220:PCW:C4 | 4:B:232:17F:H19A | 0.40 | 2.46 | 6 | 1 |
| 3:B:213:PCW:C6 | 4:B:232:17F:HN1A | 0.40 | 2.28 | 7 | 1 |
| 3:B:218:PCW:H283 | 3:B:234:PCW:H462 | 0.40 | 1.93 | 9 | 1 |
| 3:B:210:PCW:O1P | 3:B:217:PCW:H41 | 0.40 | 2.16 | 10 | 1 |
| 3:A:409:PCW:H232 | 3:C:613:PCW:H172 | 0.40 | 1.93 | 3 | 1 |
| 1:C:488:LYS:HB3 | 3:C:620:PCW:H281 | 0.40 | 1.93 | 3 | 1 |
| 3:C:603:PCW:H481 | 4:C:633:17F:H60 | 0.40 | 1.93 | 3 | 1 |
| 1:A:349:TYR:OH | 3:A:401:PCW:H222 | 0.40 | 2.15 | 4 | 1 |
| 1:C:559:SER:HA | 1:C:562:ALA:HB3 | 0.40 | 1.94 | 4 | 2 |
| 3:A:401:PCW:H483 | 3:C:623:PCW:H482 | 0.40 | 1.93 | 5 | 1 |
| 3:B:201:PCW:C1 | 4:B:230:17F:H1A | 0.40 | 2.45 | 5 | 1 |
| 3:A:401:PCW:H51 | 3:B:203:PCW:H12 | 0.40 | 1.92 | 6 | 1 |
| 3:B:210:PCW:H83 | 4:B:229:17F:H2 | 0.40 | 1.93 | 7 | 1 |
| 3:B:217:PCW:H152 | 3:B:217:PCW:C34 | 0.40 | 2.46 | 7 | 1 |
| 1:A:243:MET:O | 1:A:247:LEU:HB2 | 0.40 | 2.16 | 9 | 1 |
| 4:A:407:17F:H52 | 3:B:201:PCW:H411 | 0.40 | 1.93 | 9 | 1 |
| 3:A:408:PCW:C32 | 3:C:610:PCW:H39 | 0.40 | 2.43 | 10 | 1 |
| 3:B:206:PCW:H162 | 4:B:226:17F:H37 | 0.40 | 1.91 | 10 | 1 |
| 1:C:475:GLU:HB2 | 1:C:476:PRO:CD | 0.40 | 2.46 | 10 | 1 |
| 3:B:202:PCW:C7 | 3:B:217:PCW:H31 | 0.40 | 2.46 | 1 | 1 |
| 3:A:404:PCW:H72 | 3:B:225:PCW:O2P | 0.40 | 2.15 | 2 | 1 |
| 3:B:210:PCW:H171 | 3:B:214:PCW:H352 | 0.40 | 1.92 | 2 | 1 |
| 3:B:221:PCW:H51 | 4:B:229:17F:N1 | 0.40 | 2.30 | 4 | 1 |
| 3:A:403:PCW:H462 | 3:A:404:PCW:H372 | 0.40 | 1.92 | 5 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 3:B:233:PCW:H381 | 3:B:233:PCW:C42 | 0.40 | 2.47 | 5 | 1 |
| 4:B:236:17F:H72 | 3:C:603:PCW:H282 | 0.40 | 1.92 | 5 | 1 |
| 1:C:412:PHE:O | 1:C:415:LEU:HB2 | 0.40 | 2.16 | 6 | 1 |
| 3:A:404:PCW:H322 | 3:A:404:PCW:H41 | 0.40 | 1.92 | 7 | 1 |
| 3:B:201:PCW:H41 | 4:B:230:17F:O1 | 0.40 | 2.16 | 7 | 1 |
| 3:C:613:PCW:H72 | 3:C:619:PCW:H12 | 0.40 | 1.93 | 7 | 1 |
| 3:B:220:PCW:O1P | 3:B:220:PCW:H2 | 0.40 | 2.17 | 8 | 1 |
| 3:A:409:PCW:H62 | 4:C:630:17F:N1 | 0.40 | 2.32 | 9 | 1 |
| 3:A:410:PCW:H462 | 3:A:411:PCW:H231 | 0.40 | 1.93 | 9 | 1 |
| 2:B:158:THR:O | 2:B:162:GLU:HG2 | 0.40 | 2.16 | 9 | 1 |
| 4:B:236:17F:C31 | 3:C:622:PCW:H141 | 0.40 | 2.47 | 9 | 1 |
| 3:B:211:PCW:C36 | 4:B:226:17F:H8 | 0.40 | 2.32 | 10 | 1 |
| 1:A:260:ASP:HA | 1:A:263:LYS:CE | 0.40 | 2.38 | 1 | 1 |
| 1:C:508:ARG:O | 1:C:512:ASP:HB3 | 0.40 | 2.16 | 1 | 1 |
| 3:A:406:PCW:H351 | 4:A:407:17F:H32 | 0.40 | 1.92 | 5 | 1 |
| 3:B:211:PCW:H251 | 3:B:211:PCW:H461 | 0.40 | 1.93 | 6 | 1 |
| 3:C:611:PCW:H19 | 3:C:611:PCW:H381 | 0.40 | 1.93 | 6 | 1 |
| 3:B:233:PCW:H381 | 3:B:233:PCW:H422 | 0.40 | 1.92 | 9 | 1 |
| 3:A:411:PCW:H41 | 3:A:411:PCW:O11 | 0.40 | 2.16 | 1 | 1 |
| 2:B:134:ALA:HB1 | 2:B:139:ILE:O | 0.40 | 2.16 | 1 | 1 |
| 1:A:352:LYS:O | 1:A:356:HIS:HB2 | 0.40 | 2.17 | 4 | 1 |
| 3:B:206:PCW:H431 | 3:B:206:PCW:H372 | 0.40 | 1.94 | 4 | 1 |
| 4:B:226:17F:H74 | 3:C:621:PCW:H483 | 0.40 | 1.93 | 5 | 1 |
| 1:C:434:THR:HB | 1:C:438:ARG:CZ | 0.40 | 2.47 | 5 | 1 |
| 3:B:208:PCW:H361 | 3:B:234:PCW:H282 | 0.40 | 1.92 | 6 | 1 |
| 3:B:217:PCW:H421 | 3:B:223:PCW:H382 | 0.40 | 1.92 | 6 | 1 |
| 1:C:463:TRP:O | 1:C:467:MET:HB2 | 0.40 | 2.17 | 6 | 1 |
| 1:A:268:GLU:OE1 | 1:C:506:ARG:HD3 | 0.40 | 2.17 | 7 | 1 |
| 3:A:410:PCW:H381 | 4:C:630:17F:H12A | 0.40 | 1.94 | 7 | 1 |
| 4:B:228:17F:C2X | 4:B:232:17F:H37 | 0.40 | 2.43 | 8 | 1 |
| 3:C:611:PCW:H372 | 3:C:624:PCW:H283 | 0.40 | 1.93 | 8 | 1 |
| 2:B:18:ALA:HB2 | 5:B:237:GNP:O2A | 0.40 | 2.15 | 10 | 1 |
| 3:C:603:PCW:H371 | 3:C:603:PCW:H412 | 0.40 | 1.94 | 10 | 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 | 157/200 (78%) | 153±1 (98±1%) | 3±1 (2±1%) | 1±0 (1±0%) | 29 | 74 |
| 1 | C | 195/200 (98%) | 190±1 (98±1%) | 4±2 (2±1%) | 1±0 (1±0%) | 32 | 76 |
| 2 | B | 171/187 (91%) | 160±4 (94±2%) | 10±4 (6±3%) | 0±0 (0±0%) | 44 | 80 |
| All | All | 5230/5870 (89%) | 5036 (96%) | 169 (3%) | 25 (0%) | 32 | 76 |

All 8 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 | 365 | LYS | 10 |
| 1 | C | 563 | LYS | 9 |
| 2 | B | 60 | GLY | 1 |
| 2 | B | 119 | ASP | 1 |
| 2 | B | 14 | VAL | 1 |
| 1 | C | 420 | GLY | 1 |
| 2 | B | 34 | PRO | 1 |
| 2 | B | 117 | LYS | 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 | 135/175 (77%) | 123±3 (91±2%) | 12±3 (9±2%) | 14 | 60 |
| 1 | C | 172/175 (98%) | 157±3 (91±2%) | 15±3 (9±2%) | 14 | 60 |
| 2 | B | 152/166 (92%) | 136±2 (89±1%) | 16±2 (11±1%) | 10 | 55 |
| All | All | 4590/5160 (89%) | 4162 (91%) | 428 (9%) | 12 | 59 |

All 173 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | A | 254 | VAL | 9 |
| 2 | B | 74 | THR | 9 |
| 2 | B | 127 | THR | 9 |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | A | 392 | GLU | 8 |
| 2 | B | 35 | THR | 8 |
| 2 | B | 58 | THR | 8 |
| 2 | B | 87 | THR | 8 |
| 1 | C | 516 | THR | 8 |
| 1 | A | 312 | HIS | 8 |
| 2 | B | 124 | THR | 8 |
| 1 | C | 550 | LYS | 8 |
| 1 | C | 480 | GLU | 7 |
| 2 | B | 122 | SER | 7 |
| 1 | A | 354 | THR | 6 |
| 1 | C | 455 | TYR | 6 |
| 2 | B | 2 | THR | 6 |
| 1 | A | 293 | GLU | 5 |
| 2 | B | 17 | SER | 5 |
| 1 | A | 246 | ASP | 5 |
| 2 | B | 32 | TYR | 5 |
| 1 | C | 594 | LYS | 5 |
| 1 | A | 318 | THR | 5 |
| 2 | B | 6 | LEU | 5 |
| 2 | B | 154 | ASP | 5 |
| 1 | C | 459 | PHE | 5 |
| 1 | A | 265 | TRP | 4 |
| 1 | A | 272 | TYR | 4 |
| 2 | B | 89 | SER | 4 |
| 2 | B | 170 | MET | 4 |
| 1 | C | 403 | ASP | 4 |
| 1 | C | 405 | TRP | 4 |
| 1 | C | 444 | ASP | 4 |
| 1 | C | 580 | PHE | 4 |
| 1 | A | 370 | ASP | 4 |
| 1 | C | 568 | ASP | 4 |
| 2 | B | 50 | THR | 4 |
| 1 | C | 505 | ASP | 4 |
| 1 | A | 319 | HIS | 3 |
| 1 | A | 350 | HIS | 3 |
| 2 | B | 136 | SER | 3 |
| 1 | C | 447 | GLU | 3 |
| 1 | C | 451 | LYS | 3 |
| 1 | C | 466 | GLU | 3 |
| 1 | C | 467 | MET | 3 |
| 1 | A | 292 | HIS | 3 |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 2 | B | 95 | HIS | 3 |
| 2 | B | 148 | THR | 3 |
| 1 | C | 407 | SER | 3 |
| 1 | C | 512 | ASP | 3 |
| 1 | A | 274 | GLN | 3 |
| 1 | A | 394 | THR | 3 |
| 2 | B | 20 | THR | 3 |
| 1 | C | 412 | PHE | 3 |
| 1 | C | 552 | THR | 3 |
| 2 | B | 54 | ASP | 3 |
| 2 | B | 92 | ASP | 3 |
| 1 | C | 418 | GLN | 3 |
| 1 | C | 463 | TRP | 3 |
| 1 | C | 487 | GLN | 3 |
| 1 | A | 314 | ASP | 3 |
| 1 | A | 385 | SER | 3 |
| 1 | A | 325 | ASP | 2 |
| 1 | A | 371 | LEU | 2 |
| 2 | B | 99 | GLN | 2 |
| 2 | B | 108 | ASP | 2 |
| 1 | C | 592 | THR | 2 |
| 1 | A | 296 | GLU | 2 |
| 1 | A | 327 | LEU | 2 |
| 2 | B | 102 | ARG | 2 |
| 2 | B | 145 | SER | 2 |
| 1 | A | 255 | GLN | 2 |
| 2 | B | 31 | GLU | 2 |
| 2 | B | 49 | GLU | 2 |
| 1 | C | 410 | SER | 2 |
| 1 | C | 448 | VAL | 2 |
| 1 | C | 583 | SER | 2 |
| 1 | A | 264 | LYS | 2 |
| 1 | A | 299 | SER | 2 |
| 1 | A | 356 | HIS | 2 |
| 2 | B | 39 | SER | 2 |
| 1 | C | 490 | HIS | 2 |
| 1 | C | 546 | GLU | 2 |
| 1 | C | 561 | LYS | 2 |
| 2 | B | 158 | THR | 2 |
| 2 | B | 131 | GLN | 2 |
| 2 | B | 144 | THR | 2 |
| 1 | C | 434 | THR | 2 |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | C | 523 | ASP | 2 |
| 1 | C | 404 | ASN | 2 |
| 1 | A | 336 | GLU | 1 |
| 1 | A | 360 | LEU | 1 |
| 1 | A | 381 | SER | 1 |
| 2 | B | 30 | ASP | 1 |
| 2 | B | 43 | GLN | 1 |
| 2 | B | 47 | ASP | 1 |
| 2 | B | 51 | CYS | 1 |
| 2 | B | 65 | SER | 1 |
| 2 | B | 71 | TYR | 1 |
| 2 | B | 161 | ARG | 1 |
| 1 | C | 433 | GLU | 1 |
| 1 | A | 378 | VAL | 1 |
| 2 | B | 3 | GLU | 1 |
| 2 | B | 106 | SER | 1 |
| 2 | B | 114 | VAL | 1 |
| 2 | B | 132 | ASP | 1 |
| 2 | B | 153 | ASP | 1 |
| 1 | C | 548 | HIS | 1 |
| 1 | C | 559 | SER | 1 |
| 1 | C | 576 | VAL | 1 |
| 1 | C | 584 | PHE | 1 |
| 1 | A | 283 | LEU | 1 |
| 1 | A | 290 | LYS | 1 |
| 1 | A | 348 | GLU | 1 |
| 1 | A | 358 | SER | 1 |
| 2 | B | 29 | VAL | 1 |
| 2 | B | 62 | GLU | 1 |
| 2 | B | 142 | ILE | 1 |
| 1 | C | 402 | LEU | 1 |
| 1 | C | 415 | LEU | 1 |
| 1 | C | 425 | GLU | 1 |
| 1 | C | 461 | LYS | 1 |
| 1 | A | 270 | GLU | 1 |
| 1 | A | 368 | LEU | 1 |
| 2 | B | 73 | ARG | 1 |
| 2 | B | 149 | ARG | 1 |
| 2 | B | 166 | HIS | 1 |
| 1 | C | 409 | THR | 1 |
| 1 | C | 477 | LEU | 1 |
| 2 | B | 16 | LYS | 1 |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 2 | B | 96 | TYR | 1 |
| 1 | C | 443 | LYS | 1 |
| 1 | C | 460 | GLN | 1 |
| 1 | C | 494 | GLU | 1 |
| 1 | C | 558 | LEU | 1 |
| 1 | A | 305 | MET | 1 |
| 1 | A | 307 | ASP | 1 |
| 2 | B | 41 | ARG | 1 |
| 2 | B | 69 | ASP | 1 |
| 1 | C | 401 | LEU | 1 |
| 1 | C | 472 | GLN | 1 |
| 1 | C | 473 | LYS | 1 |
| 1 | C | 501 | GLU | 1 |
| 1 | C | 522 | SER | 1 |
| 1 | C | 554 | HIS | 1 |
| 1 | A | 241 | GLN | 1 |
| 1 | A | 261 | PHE | 1 |
| 2 | B | 109 | VAL | 1 |
| 1 | C | 427 | TRP | 1 |
| 1 | C | 429 | ASN | 1 |
| 1 | C | 596 | ASN | 1 |
| 1 | A | 266 | GLN | 1 |
| 1 | A | 273 | ARG | 1 |
| 1 | A | 284 | GLN | 1 |
| 1 | A | 359 | THR | 1 |
| 1 | C | 521 | TYR | 1 |
| 1 | A | 249 | GLU | 1 |
| 1 | A | 361 | SER | 1 |
| 2 | B | 4 | TYR | 1 |
| 2 | B | 80 | CYS | 1 |
| 2 | B | 118 | CYS | 1 |
| 2 | B | 171 | SER | 1 |
| 1 | C | 457 | ASP | 1 |
| 1 | C | 495 | LYS | 1 |
| 1 | C | 556 | SER | 1 |
| 1 | C | 557 | THR | 1 |
| 1 | A | 243 | MET | 1 |
| 1 | A | 304 | GLU | 1 |
| 2 | B | 119 | ASP | 1 |
| 1 | C | 426 | PHE | 1 |
| 1 | C | 464 | GLN | 1 |
| 1 | C | 482 | GLN | 1 |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | C | 560 | GLU | 1 |
| 1 | C | 566 | LEU | 1 |

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.6 Ligand geometry ⓘ

Of 83 ligands modelled in this entry, 1 is monoatomic - leaving 82 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 | PCW | B | 225 | - | 53,53,53 | 1.05±0.01 | 4±1 (7±1%) |
| 3 | PCW | A | 402 | - | 53,53,53 | 1.05±0.01 | 4±0 (7±0%) |
| 3 | PCW | B | 208 | - | 53,53,53 | 1.05±0.01 | 5±0 (9±0%) |
| 3 | PCW | B | 221 | - | 53,53,53 | 1.07±0.01 | 5±0 (9±0%) |
| 3 | PCW | B | 212 | - | 53,53,53 | 1.05±0.01 | 5±0 (9±0%) |
| 4 | 17F | C | 633 | - | 52,53,53 | 0.92±0.01 | 1±0 (1±0%) |
| 3 | PCW | C | 603 | - | 53,53,53 | 1.04±0.01 | 4±0 (6±0%) |
| 3 | PCW | A | 411 | - | 53,53,53 | 1.04±0.01 | 4±0 (7±0%) |
| 3 | PCW | A | 401 | - | 53,53,53 | 1.04±0.02 | 4±0 (7±0%) |
| 3 | PCW | C | 611 | - | 53,53,53 | 1.04±0.01 | 4±0 (7±0%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | |
|-----|------|-------|-----|------|--------------|-----------|------------|
| | | | | | Counts | RMSZ | #Z>2 |
| 3 | PCW | C | 604 | - | 53,53,53 | 1.05±0.01 | 4±0 (6±0%) |
| 4 | 17F | C | 627 | - | 52,53,53 | 0.92±0.01 | 1±0 (1±0%) |
| 4 | 17F | C | 628 | - | 52,53,53 | 0.91±0.01 | 0±0 (0±0%) |
| 3 | PCW | C | 620 | - | 53,53,53 | 1.04±0.01 | 5±0 (8±0%) |
| 3 | PCW | A | 406 | - | 53,53,53 | 1.06±0.01 | 5±0 (9±0%) |
| 3 | PCW | C | 605 | - | 53,53,53 | 1.06±0.01 | 5±0 (8±0%) |
| 3 | PCW | B | 216 | - | 53,53,53 | 1.05±0.01 | 4±0 (6±0%) |
| 4 | 17F | B | 228 | - | 52,53,53 | 0.92±0.01 | 0±0 (0±0%) |
| 4 | 17F | C | 632 | - | 52,53,53 | 0.92±0.01 | 1±0 (1±0%) |
| 3 | PCW | C | 625 | - | 53,53,53 | 1.04±0.01 | 4±1 (7±1%) |
| 3 | PCW | B | 219 | - | 53,53,53 | 1.04±0.01 | 4±0 (7±0%) |
| 3 | PCW | B | 211 | - | 53,53,53 | 1.05±0.01 | 4±0 (6±0%) |
| 3 | PCW | C | 616 | - | 53,53,53 | 1.05±0.01 | 4±0 (7±0%) |
| 4 | 17F | B | 232 | - | 52,53,53 | 0.92±0.01 | 1±0 (1±0%) |
| 4 | 17F | B | 231 | - | 52,53,53 | 0.92±0.01 | 1±0 (1±0%) |
| 4 | 17F | A | 407 | - | 52,53,53 | 0.91±0.01 | 0±0 (0±0%) |
| 3 | PCW | C | 609 | - | 53,53,53 | 1.04±0.01 | 4±0 (6±0%) |
| 3 | PCW | C | 615 | - | 53,53,53 | 1.05±0.01 | 4±0 (6±0%) |
| 3 | PCW | A | 410 | - | 53,53,53 | 1.07±0.01 | 4±0 (7±0%) |
| 3 | PCW | B | 233 | - | 53,53,53 | 1.06±0.01 | 4±0 (7±0%) |
| 3 | PCW | C | 606 | - | 53,53,53 | 1.04±0.01 | 4±0 (8±0%) |
| 3 | PCW | B | 213 | - | 53,53,53 | 1.05±0.01 | 3±0 (6±0%) |
| 3 | PCW | B | 201 | - | 53,53,53 | 1.05±0.01 | 4±0 (7±0%) |
| 4 | 17F | C | 630 | - | 52,53,53 | 0.91±0.01 | 0±0 (0±0%) |
| 3 | PCW | B | 224 | - | 53,53,53 | 1.05±0.01 | 5±0 (9±0%) |
| 4 | 17F | B | 236 | - | 52,53,53 | 0.92±0.01 | 1±0 (1±0%) |
| 3 | PCW | C | 614 | - | 53,53,53 | 1.04±0.01 | 4±0 (6±0%) |
| 3 | PCW | C | 626 | - | 53,53,53 | 1.04±0.01 | 5±0 (8±0%) |
| 3 | PCW | B | 222 | - | 53,53,53 | 1.06±0.01 | 4±0 (7±0%) |
| 3 | PCW | B | 202 | - | 53,53,53 | 1.05±0.01 | 4±0 (7±0%) |
| 3 | PCW | B | 235 | - | 53,53,53 | 1.04±0.01 | 4±0 (6±0%) |
| 4 | 17F | B | 230 | - | 52,53,53 | 0.92±0.01 | 1±0 (1±0%) |
| 3 | PCW | B | 220 | - | 53,53,53 | 1.04±0.01 | 4±0 (6±0%) |
| 3 | PCW | B | 206 | - | 53,53,53 | 1.05±0.01 | 4±0 (8±0%) |
| 3 | PCW | C | 602 | - | 53,53,53 | 1.05±0.01 | 4±0 (7±0%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | |
|-----|------|-------|-----|------|--------------|-----------|-------------|
| | | | | | Counts | RMSZ | #Z>2 |
| 3 | PCW | C | 612 | - | 53,53,53 | 1.04±0.01 | 4±0 (7±0%) |
| 5 | GNP | B | 237 | - | 29,34,34 | 1.73±0.02 | 8±0 (25±1%) |
| 3 | PCW | B | 210 | - | 53,53,53 | 1.05±0.01 | 4±0 (6±0%) |
| 3 | PCW | C | 613 | - | 53,53,53 | 1.08±0.01 | 6±0 (10±0%) |
| 4 | 17F | C | 629 | - | 52,53,53 | 0.92±0.01 | 1±0 (1±0%) |
| 3 | PCW | B | 218 | - | 53,53,53 | 1.06±0.01 | 4±0 (7±0%) |
| 3 | PCW | C | 621 | - | 53,53,53 | 1.05±0.01 | 4±0 (8±0%) |
| 3 | PCW | B | 223 | - | 53,53,53 | 1.05±0.01 | 4±0 (7±0%) |
| 3 | PCW | B | 204 | - | 53,53,53 | 1.04±0.01 | 4±0 (6±0%) |
| 3 | PCW | A | 403 | - | 53,53,53 | 1.05±0.01 | 5±0 (8±0%) |
| 4 | 17F | C | 631 | - | 52,53,53 | 0.92±0.01 | 1±0 (1±0%) |
| 3 | PCW | A | 405 | - | 53,53,53 | 1.04±0.01 | 4±0 (7±0%) |
| 3 | PCW | B | 217 | - | 53,53,53 | 1.05±0.01 | 4±0 (6±0%) |
| 3 | PCW | C | 608 | - | 53,53,53 | 1.05±0.01 | 5±0 (8±0%) |
| 4 | 17F | B | 227 | - | 52,53,53 | 0.93±0.01 | 1±0 (1±0%) |
| 3 | PCW | B | 234 | - | 53,53,53 | 1.04±0.01 | 4±0 (7±0%) |
| 3 | PCW | B | 214 | - | 53,53,53 | 1.05±0.02 | 4±0 (7±0%) |
| 3 | PCW | C | 607 | - | 53,53,53 | 1.04±0.01 | 4±0 (6±0%) |
| 4 | 17F | B | 226 | - | 52,53,53 | 0.92±0.01 | 1±0 (1±0%) |
| 3 | PCW | C | 619 | - | 53,53,53 | 1.04±0.01 | 3±0 (6±0%) |
| 3 | PCW | C | 624 | - | 53,53,53 | 1.05±0.01 | 4±0 (7±0%) |
| 3 | PCW | B | 215 | - | 53,53,53 | 1.05±0.01 | 5±0 (9±0%) |
| 3 | PCW | C | 617 | - | 53,53,53 | 1.04±0.01 | 4±0 (6±0%) |
| 3 | PCW | A | 408 | - | 53,53,53 | 1.04±0.01 | 4±0 (6±0%) |
| 3 | PCW | C | 622 | - | 53,53,53 | 1.06±0.01 | 4±0 (7±0%) |
| 3 | PCW | B | 203 | - | 53,53,53 | 1.05±0.01 | 4±0 (7±0%) |
| 3 | PCW | C | 623 | - | 53,53,53 | 1.04±0.01 | 4±0 (6±0%) |
| 3 | PCW | C | 601 | - | 53,53,53 | 1.04±0.01 | 5±0 (8±0%) |
| 3 | PCW | C | 610 | - | 53,53,53 | 1.04±0.01 | 4±0 (6±0%) |
| 3 | PCW | B | 207 | - | 53,53,53 | 1.05±0.01 | 4±0 (7±0%) |
| 3 | PCW | B | 205 | - | 53,53,53 | 1.04±0.01 | 4±1 (8±1%) |
| 3 | PCW | B | 209 | - | 53,53,53 | 1.05±0.01 | 5±0 (8±0%) |
| 3 | PCW | C | 618 | - | 53,53,53 | 1.05±0.01 | 4±0 (7±0%) |
| 7 | EWS | B | 239 | - | 29,30,30 | 3.25±0.00 | 9±0 (31±0%) |
| 3 | PCW | A | 404 | - | 53,53,53 | 1.05±0.01 | 4±0 (6±0%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | |
|-----|------|-------|-----|------|--------------|-----------|------------|
| | | | | | Counts | RMSZ | #Z>2 |
| 4 | 17F | B | 229 | - | 52,53,53 | 0.92±0.01 | 1±0 (1±0%) |
| 3 | PCW | A | 409 | - | 53,53,53 | 1.05±0.01 | 4±0 (6±0%) |

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

| Mol | Type | Chain | Res | Link | Bond angles | | |
|-----|------|-------|-----|------|-------------|-----------|-------------|
| | | | | | Counts | RMSZ | #Z>2 |
| 3 | PCW | B | 225 | - | 59,61,61 | 2.32±0.01 | 5±0 (8±0%) |
| 3 | PCW | A | 402 | - | 59,61,61 | 2.32±0.01 | 5±0 (8±0%) |
| 3 | PCW | B | 208 | - | 59,61,61 | 0.85±0.01 | 1±0 (1±0%) |
| 3 | PCW | B | 221 | - | 59,61,61 | 0.83±0.01 | 1±0 (1±0%) |
| 3 | PCW | B | 212 | - | 59,61,61 | 0.84±0.00 | 1±0 (1±0%) |
| 4 | 17F | C | 633 | - | 54,60,60 | 1.04±0.02 | 4±0 (7±0%) |
| 3 | PCW | C | 603 | - | 59,61,61 | 2.32±0.01 | 5±0 (8±0%) |
| 3 | PCW | A | 411 | - | 59,61,61 | 2.32±0.01 | 5±0 (8±0%) |
| 3 | PCW | A | 401 | - | 59,61,61 | 2.32±0.01 | 5±0 (8±0%) |
| 3 | PCW | C | 611 | - | 59,61,61 | 2.32±0.00 | 5±0 (8±0%) |
| 3 | PCW | C | 604 | - | 59,61,61 | 2.33±0.00 | 5±0 (8±0%) |
| 4 | 17F | C | 627 | - | 54,60,60 | 1.06±0.01 | 5±0 (9±0%) |
| 4 | 17F | C | 628 | - | 54,60,60 | 1.12±0.03 | 6±0 (10±0%) |
| 3 | PCW | C | 620 | - | 59,61,61 | 0.85±0.01 | 1±0 (1±0%) |
| 3 | PCW | A | 406 | - | 59,61,61 | 0.84±0.01 | 1±0 (1±0%) |
| 3 | PCW | C | 605 | - | 59,61,61 | 0.85±0.01 | 1±0 (1±0%) |
| 3 | PCW | B | 216 | - | 59,61,61 | 2.32±0.01 | 5±0 (8±0%) |
| 4 | 17F | B | 228 | - | 54,60,60 | 1.08±0.03 | 5±1 (9±1%) |
| 4 | 17F | C | 632 | - | 54,60,60 | 1.05±0.03 | 5±0 (9±0%) |
| 3 | PCW | C | 625 | - | 59,61,61 | 2.32±0.01 | 5±0 (8±0%) |
| 3 | PCW | B | 219 | - | 59,61,61 | 2.32±0.00 | 5±0 (8±0%) |
| 3 | PCW | B | 211 | - | 59,61,61 | 2.32±0.01 | 5±0 (8±0%) |
| 3 | PCW | C | 616 | - | 59,61,61 | 2.32±0.00 | 5±0 (8±0%) |
| 4 | 17F | B | 232 | - | 54,60,60 | 1.05±0.03 | 5±0 (9±0%) |

| Mol | Type | Chain | Res | Link | Bond angles | | |
|-----|------|-------|-----|------|-------------|-----------|--------------|
| | | | | | Counts | RMSZ | #Z>2 |
| 4 | 17F | B | 231 | - | 54,60,60 | 1.06±0.03 | 5±0 (9±0%) |
| 4 | 17F | A | 407 | - | 54,60,60 | 1.77±0.03 | 10±1 (17±1%) |
| 3 | PCW | C | 609 | - | 59,61,61 | 2.32±0.01 | 5±0 (8±0%) |
| 3 | PCW | C | 615 | - | 59,61,61 | 2.32±0.01 | 5±0 (8±0%) |
| 3 | PCW | A | 410 | - | 59,61,61 | 2.33±0.01 | 5±0 (8±0%) |
| 3 | PCW | B | 233 | - | 59,61,61 | 2.31±0.01 | 5±0 (8±0%) |
| 3 | PCW | C | 606 | - | 59,61,61 | 0.84±0.01 | 1±0 (1±0%) |
| 3 | PCW | B | 213 | - | 59,61,61 | 2.32±0.01 | 5±0 (8±0%) |
| 3 | PCW | B | 201 | - | 59,61,61 | 2.32±0.01 | 5±0 (8±0%) |
| 4 | 17F | C | 630 | - | 54,60,60 | 1.80±0.03 | 10±0 (17±0%) |
| 3 | PCW | B | 224 | - | 59,61,61 | 0.84±0.01 | 1±0 (1±0%) |
| 4 | 17F | B | 236 | - | 54,60,60 | 1.05±0.03 | 5±0 (9±0%) |
| 3 | PCW | C | 614 | - | 59,61,61 | 2.32±0.01 | 5±0 (8±0%) |
| 3 | PCW | C | 626 | - | 59,61,61 | 0.84±0.01 | 1±0 (1±0%) |
| 3 | PCW | B | 222 | - | 59,61,61 | 2.32±0.01 | 5±0 (8±0%) |
| 3 | PCW | B | 202 | - | 59,61,61 | 2.32±0.00 | 5±0 (8±0%) |
| 3 | PCW | B | 235 | - | 59,61,61 | 2.32±0.01 | 5±0 (8±0%) |
| 4 | 17F | B | 230 | - | 54,60,60 | 1.10±0.05 | 5±0 (9±0%) |
| 3 | PCW | B | 220 | - | 59,61,61 | 2.32±0.01 | 5±0 (8±0%) |
| 3 | PCW | B | 206 | - | 59,61,61 | 0.84±0.01 | 1±0 (1±0%) |
| 3 | PCW | C | 602 | - | 59,61,61 | 2.32±0.00 | 5±0 (8±0%) |
| 3 | PCW | C | 612 | - | 59,61,61 | 2.32±0.01 | 5±0 (8±0%) |
| 5 | GNP | B | 237 | - | 33,54,54 | 2.23±0.01 | 7±0 (20±1%) |
| 3 | PCW | B | 210 | - | 59,61,61 | 2.32±0.01 | 5±0 (8±0%) |
| 3 | PCW | C | 613 | - | 59,61,61 | 0.83±0.01 | 1±0 (1±0%) |
| 4 | 17F | C | 629 | - | 54,60,60 | 1.04±0.02 | 5±0 (9±0%) |
| 3 | PCW | B | 218 | - | 59,61,61 | 2.32±0.01 | 5±0 (8±0%) |
| 3 | PCW | C | 621 | - | 59,61,61 | 0.84±0.01 | 1±0 (1±0%) |
| 3 | PCW | B | 223 | - | 59,61,61 | 2.32±0.00 | 5±0 (8±0%) |
| 3 | PCW | B | 204 | - | 59,61,61 | 2.77±0.01 | 9±0 (15±0%) |
| 3 | PCW | A | 403 | - | 59,61,61 | 0.85±0.01 | 1±0 (1±0%) |
| 4 | 17F | C | 631 | - | 54,60,60 | 1.05±0.03 | 5±0 (9±0%) |
| 3 | PCW | A | 405 | - | 59,61,61 | 2.32±0.01 | 5±0 (8±0%) |
| 3 | PCW | B | 217 | - | 59,61,61 | 2.32±0.01 | 5±0 (8±0%) |
| 3 | PCW | C | 608 | - | 59,61,61 | 0.84±0.01 | 1±0 (1±0%) |

| Mol | Type | Chain | Res | Link | Bond angles | | |
|-----|------|-------|-----|------|-------------|-----------|-------------|
| | | | | | Counts | RMSZ | #Z>2 |
| 4 | 17F | B | 227 | - | 54,60,60 | 1.05±0.02 | 5±0 (8±0%) |
| 3 | PCW | B | 234 | - | 59,61,61 | 2.77±0.01 | 9±0 (15±0%) |
| 3 | PCW | B | 214 | - | 59,61,61 | 2.32±0.00 | 5±0 (8±0%) |
| 3 | PCW | C | 607 | - | 59,61,61 | 2.32±0.01 | 5±0 (8±0%) |
| 4 | 17F | B | 226 | - | 54,60,60 | 1.07±0.02 | 5±0 (9±0%) |
| 3 | PCW | C | 619 | - | 59,61,61 | 2.32±0.01 | 5±0 (8±0%) |
| 3 | PCW | C | 624 | - | 59,61,61 | 2.32±0.00 | 5±0 (8±0%) |
| 3 | PCW | B | 215 | - | 59,61,61 | 0.84±0.01 | 1±0 (1±0%) |
| 3 | PCW | C | 617 | - | 59,61,61 | 2.32±0.01 | 5±0 (8±0%) |
| 3 | PCW | A | 408 | - | 59,61,61 | 2.32±0.01 | 5±0 (8±0%) |
| 3 | PCW | C | 622 | - | 59,61,61 | 2.32±0.01 | 5±0 (8±0%) |
| 3 | PCW | B | 203 | - | 59,61,61 | 2.32±0.01 | 5±0 (8±0%) |
| 3 | PCW | C | 623 | - | 59,61,61 | 2.32±0.01 | 5±0 (8±0%) |
| 3 | PCW | C | 601 | - | 59,61,61 | 0.84±0.01 | 1±0 (1±0%) |
| 3 | PCW | C | 610 | - | 59,61,61 | 2.32±0.01 | 5±0 (8±0%) |
| 3 | PCW | B | 207 | - | 59,61,61 | 2.32±0.01 | 5±0 (8±0%) |
| 3 | PCW | B | 205 | - | 59,61,61 | 0.85±0.01 | 1±0 (1±0%) |
| 3 | PCW | B | 209 | - | 59,61,61 | 0.85±0.01 | 1±0 (1±0%) |
| 3 | PCW | C | 618 | - | 59,61,61 | 2.33±0.01 | 5±0 (8±0%) |
| 7 | EWS | B | 239 | - | 35,42,42 | 0.97±0.00 | 1±0 (2±0%) |
| 3 | PCW | A | 404 | - | 59,61,61 | 2.32±0.00 | 5±0 (8±0%) |
| 4 | 17F | B | 229 | - | 54,60,60 | 1.07±0.04 | 5±0 (9±0%) |
| 3 | PCW | A | 409 | - | 59,61,61 | 2.32±0.01 | 5±0 (8±0%) |

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 | PCW | C | 604 | - | - | 0±0,57,57,57 | - |
| 3 | PCW | C | 605 | - | - | 0±0,57,57,57 | - |
| 3 | PCW | B | 201 | - | - | 0±0,57,57,57 | - |
| 4 | 17F | C | 630 | - | - | 0±0,59,59,59 | - |
| 3 | PCW | C | 613 | - | - | 0±0,57,57,57 | - |
| 4 | 17F | C | 631 | - | - | 0±0,59,59,59 | - |
| 3 | PCW | B | 206 | - | - | 0±0,57,57,57 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|--------------|-----------|
| 3 | PCW | B | 233 | - | - | 0±0,57,57,57 | - |
| 3 | PCW | B | 217 | - | - | 0±0,57,57,57 | - |
| 3 | PCW | C | 622 | - | - | 0±0,57,57,57 | - |
| 3 | PCW | B | 208 | - | - | 0±0,57,57,57 | - |
| 3 | PCW | B | 221 | - | - | 0±0,57,57,57 | - |
| 3 | PCW | B | 222 | - | - | 0±0,57,57,57 | - |
| 3 | PCW | B | 213 | - | - | 0±0,57,57,57 | - |
| 3 | PCW | B | 220 | - | - | 0±0,57,57,57 | - |
| 3 | PCW | B | 225 | - | - | 0±0,57,57,57 | - |
| 3 | PCW | C | 603 | - | - | 0±0,57,57,57 | - |
| 3 | PCW | C | 609 | - | - | 0±0,57,57,57 | - |
| 3 | PCW | B | 234 | - | - | 0±0,57,57,57 | - |
| 3 | PCW | A | 408 | - | - | 0±0,57,57,57 | - |
| 3 | PCW | B | 205 | - | - | 0±0,57,57,57 | - |
| 3 | PCW | A | 411 | - | - | 0±0,57,57,57 | - |
| 3 | PCW | C | 612 | - | - | 0±0,57,57,57 | - |
| 3 | PCW | C | 601 | - | - | 0±0,57,57,57 | - |
| 3 | PCW | B | 209 | - | - | 0±0,57,57,57 | - |
| 4 | 17F | C | 627 | - | - | 0±0,59,59,59 | - |
| 3 | PCW | B | 214 | - | - | 0±0,57,57,57 | - |
| 3 | PCW | A | 402 | - | - | 0±0,57,57,57 | - |
| 3 | PCW | B | 211 | - | - | 0±0,57,57,57 | - |
| 4 | 17F | A | 407 | - | - | 0±0,59,59,59 | - |
| 3 | PCW | C | 608 | - | - | 0±0,57,57,57 | - |
| 3 | PCW | A | 401 | - | - | 0±0,57,57,57 | - |
| 3 | PCW | C | 625 | - | - | 0±0,57,57,57 | - |
| 3 | PCW | A | 406 | - | - | 0±0,57,57,57 | - |
| 4 | 17F | B | 231 | - | - | 0±0,59,59,59 | - |
| 3 | PCW | C | 624 | - | - | 0±0,57,57,57 | - |
| 3 | PCW | B | 204 | - | - | 0±0,57,57,57 | - |
| 5 | GNP | B | 237 | - | - | 0±0,14,38,38 | 0±0,3,3,3 |
| 4 | 17F | C | 629 | - | - | 0±0,59,59,59 | - |
| 3 | PCW | B | 223 | - | - | 0±0,57,57,57 | - |
| 3 | PCW | C | 615 | - | - | 0±0,57,57,57 | - |
| 3 | PCW | C | 602 | - | - | 0±0,57,57,57 | - |
| 3 | PCW | B | 216 | - | - | 0±0,57,57,57 | - |
| 4 | 17F | B | 228 | - | - | 0±0,59,59,59 | - |
| 3 | PCW | C | 611 | - | - | 0±0,57,57,57 | - |
| 3 | PCW | B | 210 | - | - | 0±0,57,57,57 | - |
| 3 | PCW | B | 218 | - | - | 0±0,57,57,57 | - |
| 4 | 17F | B | 230 | - | - | 0±0,59,59,59 | - |
| 4 | 17F | B | 229 | - | - | 0±0,59,59,59 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|--------------|-----------|
| 3 | PCW | B | 215 | - | - | 0±0,57,57,57 | - |
| 3 | PCW | A | 405 | - | - | 0±0,57,57,57 | - |
| 3 | PCW | C | 626 | - | - | 0±0,57,57,57 | - |
| 3 | PCW | B | 235 | - | - | 0±0,57,57,57 | - |
| 3 | PCW | B | 207 | - | - | 0±0,57,57,57 | - |
| 3 | PCW | C | 607 | - | - | 0±0,57,57,57 | - |
| 3 | PCW | B | 224 | - | - | 0±0,57,57,57 | - |
| 4 | 17F | B | 236 | - | - | 0±0,59,59,59 | - |
| 3 | PCW | C | 610 | - | - | 0±0,57,57,57 | - |
| 3 | PCW | B | 203 | - | - | 0±0,57,57,57 | - |
| 3 | PCW | A | 403 | - | - | 0±0,57,57,57 | - |
| 4 | 17F | C | 633 | - | - | 0±0,59,59,59 | - |
| 4 | 17F | B | 227 | - | - | 0±0,59,59,59 | - |
| 4 | 17F | B | 232 | - | - | 0±0,59,59,59 | - |
| 3 | PCW | A | 410 | - | - | 0±0,57,57,57 | - |
| 3 | PCW | B | 202 | - | - | 0±0,57,57,57 | - |
| 3 | PCW | A | 404 | - | - | 0±0,57,57,57 | - |
| 3 | PCW | C | 606 | - | - | 0±0,57,57,57 | - |
| 3 | PCW | C | 614 | - | - | 0±0,57,57,57 | - |
| 3 | PCW | C | 621 | - | - | 0±0,57,57,57 | - |
| 3 | PCW | C | 617 | - | - | 0±0,57,57,57 | - |
| 4 | 17F | C | 628 | - | - | 0±0,59,59,59 | - |
| 3 | PCW | C | 619 | - | - | 0±0,57,57,57 | - |
| 7 | EWS | B | 239 | - | - | 0±0,10,22,22 | 1±0,4,4,4 |
| 3 | PCW | B | 219 | - | - | 0±0,57,57,57 | - |
| 3 | PCW | C | 616 | - | - | 0±0,57,57,57 | - |
| 4 | 17F | C | 632 | - | - | 0±0,59,59,59 | - |
| 3 | PCW | B | 212 | - | - | 0±0,57,57,57 | - |
| 3 | PCW | A | 409 | - | - | 0±0,57,57,57 | - |
| 3 | PCW | C | 623 | - | - | 0±0,57,57,57 | - |
| 4 | 17F | B | 226 | - | - | 0±0,59,59,59 | - |
| 3 | PCW | C | 620 | - | - | 0±0,57,57,57 | - |
| 3 | PCW | C | 618 | - | - | 0±0,57,57,57 | - |

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 |
| 7 | B | 239 | EWS | CBA-CAZ | 10.76 | 1.34 | 1.50 | 9 | 10 |
| 7 | B | 239 | EWS | CBA-CAV | 9.84 | 1.34 | 1.42 | 8 | 10 |
| 7 | B | 239 | EWS | CAI-CAJ | 5.02 | 1.39 | 1.51 | 8 | 10 |
| 5 | B | 237 | GNP | PG-O1G | 4.61 | 1.53 | 1.46 | 4 | 10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 7 | B | 239 | EWS | CAT-CAU | 3.86 | 1.35 | 1.41 | 10 | 10 |
| 5 | B | 237 | GNP | PG-O3G | 3.36 | 1.47 | 1.56 | 4 | 10 |
| 5 | B | 237 | GNP | PB-O2B | 3.29 | 1.48 | 1.56 | 1 | 10 |
| 5 | B | 237 | GNP | C6-N1 | 2.99 | 1.38 | 1.33 | 4 | 10 |
| 3 | A | 411 | PCW | C5-N | 2.94 | 1.42 | 1.51 | 1 | 10 |
| 3 | C | 615 | PCW | C5-N | 2.93 | 1.42 | 1.51 | 3 | 10 |
| 3 | B | 218 | PCW | C5-N | 2.89 | 1.42 | 1.51 | 5 | 10 |
| 3 | C | 604 | PCW | C5-N | 2.87 | 1.42 | 1.51 | 1 | 10 |
| 3 | C | 618 | PCW | C5-N | 2.87 | 1.42 | 1.51 | 4 | 10 |
| 3 | B | 222 | PCW | C5-N | 2.86 | 1.42 | 1.51 | 7 | 10 |
| 3 | A | 410 | PCW | C5-N | 2.86 | 1.42 | 1.51 | 8 | 10 |
| 3 | A | 405 | PCW | C5-N | 2.85 | 1.42 | 1.51 | 10 | 10 |
| 3 | C | 616 | PCW | C5-N | 2.85 | 1.42 | 1.51 | 6 | 10 |
| 3 | A | 404 | PCW | C5-N | 2.85 | 1.42 | 1.51 | 3 | 10 |
| 3 | B | 216 | PCW | C5-N | 2.84 | 1.42 | 1.51 | 2 | 10 |
| 3 | C | 609 | PCW | C5-N | 2.83 | 1.42 | 1.51 | 1 | 10 |
| 3 | A | 402 | PCW | C5-N | 2.83 | 1.42 | 1.51 | 4 | 10 |
| 3 | A | 409 | PCW | C5-N | 2.83 | 1.42 | 1.51 | 1 | 10 |
| 3 | C | 624 | PCW | C5-N | 2.81 | 1.42 | 1.51 | 2 | 10 |
| 7 | B | 239 | EWS | CAQ-CAV | 2.81 | 1.36 | 1.42 | 5 | 10 |
| 3 | B | 212 | PCW | C1-C2 | 2.81 | 1.59 | 1.50 | 7 | 10 |
| 3 | B | 201 | PCW | C5-N | 2.80 | 1.42 | 1.51 | 6 | 10 |
| 3 | B | 225 | PCW | C5-N | 2.80 | 1.42 | 1.51 | 3 | 10 |
| 3 | B | 220 | PCW | C5-N | 2.79 | 1.43 | 1.51 | 6 | 10 |
| 3 | B | 203 | PCW | C5-N | 2.79 | 1.43 | 1.51 | 9 | 10 |
| 3 | B | 233 | PCW | C5-N | 2.78 | 1.43 | 1.51 | 6 | 10 |
| 5 | B | 237 | GNP | PB-O3A | 2.78 | 1.55 | 1.59 | 5 | 10 |
| 3 | B | 202 | PCW | C5-N | 2.78 | 1.43 | 1.51 | 4 | 10 |
| 3 | B | 214 | PCW | C5-N | 2.78 | 1.43 | 1.51 | 7 | 10 |
| 3 | B | 219 | PCW | C5-N | 2.78 | 1.43 | 1.51 | 1 | 10 |
| 3 | C | 623 | PCW | C5-N | 2.78 | 1.43 | 1.51 | 7 | 10 |
| 3 | C | 619 | PCW | C5-N | 2.78 | 1.43 | 1.51 | 9 | 10 |
| 3 | B | 223 | PCW | C5-N | 2.77 | 1.43 | 1.51 | 6 | 10 |
| 3 | C | 603 | PCW | C5-N | 2.77 | 1.43 | 1.51 | 5 | 10 |
| 3 | B | 213 | PCW | C5-N | 2.76 | 1.43 | 1.51 | 1 | 10 |
| 3 | B | 217 | PCW | C5-N | 2.76 | 1.43 | 1.51 | 8 | 10 |
| 3 | B | 211 | PCW | C5-N | 2.76 | 1.43 | 1.51 | 6 | 10 |
| 3 | B | 235 | PCW | C5-N | 2.76 | 1.43 | 1.51 | 7 | 10 |
| 3 | C | 602 | PCW | C5-N | 2.76 | 1.43 | 1.51 | 5 | 10 |
| 3 | C | 625 | PCW | C5-N | 2.76 | 1.43 | 1.51 | 1 | 10 |
| 3 | C | 617 | PCW | C5-N | 2.76 | 1.43 | 1.51 | 2 | 10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 204 | PCW | C5-N | 2.76 | 1.43 | 1.51 | 6 | 10 |
| 3 | C | 622 | PCW | C5-N | 2.76 | 1.43 | 1.51 | 6 | 10 |
| 3 | B | 207 | PCW | C5-N | 2.74 | 1.43 | 1.51 | 1 | 10 |
| 3 | B | 208 | PCW | C1-C2 | 2.74 | 1.59 | 1.50 | 2 | 10 |
| 5 | B | 237 | GNP | PG-O2G | 2.73 | 1.49 | 1.56 | 3 | 10 |
| 7 | B | 239 | EWS | CAQ-CAR | 2.73 | 1.41 | 1.36 | 5 | 10 |
| 3 | C | 622 | PCW | C1-C2 | 2.72 | 1.59 | 1.50 | 9 | 10 |
| 3 | B | 210 | PCW | C5-N | 2.72 | 1.43 | 1.51 | 7 | 10 |
| 3 | C | 610 | PCW | C5-N | 2.72 | 1.43 | 1.51 | 2 | 10 |
| 3 | C | 612 | PCW | C5-N | 2.71 | 1.43 | 1.51 | 9 | 10 |
| 3 | A | 401 | PCW | C5-N | 2.71 | 1.43 | 1.51 | 10 | 10 |
| 3 | C | 613 | PCW | C1-C2 | 2.71 | 1.59 | 1.50 | 5 | 10 |
| 3 | A | 406 | PCW | C1-C2 | 2.70 | 1.59 | 1.50 | 1 | 10 |
| 3 | C | 602 | PCW | C1-C2 | 2.70 | 1.59 | 1.50 | 9 | 10 |
| 3 | B | 221 | PCW | C1-C2 | 2.70 | 1.59 | 1.50 | 6 | 10 |
| 3 | C | 607 | PCW | C5-N | 2.70 | 1.43 | 1.51 | 3 | 10 |
| 3 | A | 409 | PCW | C1-C2 | 2.70 | 1.59 | 1.50 | 10 | 10 |
| 3 | B | 233 | PCW | C1-C2 | 2.69 | 1.59 | 1.50 | 5 | 10 |
| 3 | B | 209 | PCW | C1-C2 | 2.68 | 1.59 | 1.50 | 9 | 10 |
| 3 | B | 213 | PCW | C1-C2 | 2.67 | 1.59 | 1.50 | 9 | 10 |
| 3 | B | 218 | PCW | C1-C2 | 2.66 | 1.59 | 1.50 | 4 | 10 |
| 3 | A | 405 | PCW | C1-C2 | 2.66 | 1.59 | 1.50 | 10 | 10 |
| 3 | C | 625 | PCW | C1-C2 | 2.65 | 1.59 | 1.50 | 6 | 10 |
| 3 | B | 202 | PCW | C1-C2 | 2.64 | 1.59 | 1.50 | 4 | 10 |
| 3 | C | 607 | PCW | C1-C2 | 2.64 | 1.59 | 1.50 | 10 | 10 |
| 3 | B | 214 | PCW | C1-C2 | 2.64 | 1.59 | 1.50 | 3 | 10 |
| 3 | B | 203 | PCW | C1-C2 | 2.64 | 1.59 | 1.50 | 8 | 10 |
| 3 | B | 224 | PCW | C1-C2 | 2.64 | 1.59 | 1.50 | 8 | 10 |
| 3 | C | 611 | PCW | C5-N | 2.64 | 1.43 | 1.51 | 9 | 10 |
| 3 | B | 211 | PCW | C1-C2 | 2.63 | 1.59 | 1.50 | 8 | 10 |
| 3 | C | 610 | PCW | C1-C2 | 2.63 | 1.59 | 1.50 | 10 | 10 |
| 3 | C | 614 | PCW | C5-N | 2.63 | 1.43 | 1.51 | 5 | 10 |
| 3 | A | 408 | PCW | C5-N | 2.62 | 1.43 | 1.51 | 3 | 10 |
| 3 | C | 626 | PCW | C1-C2 | 2.62 | 1.59 | 1.50 | 10 | 10 |
| 3 | A | 410 | PCW | C1-C2 | 2.62 | 1.59 | 1.50 | 8 | 10 |
| 3 | B | 207 | PCW | C1-C2 | 2.61 | 1.59 | 1.50 | 5 | 10 |
| 3 | C | 615 | PCW | C1-C2 | 2.61 | 1.59 | 1.50 | 5 | 10 |
| 3 | A | 411 | PCW | C1-C2 | 2.61 | 1.59 | 1.50 | 2 | 10 |
| 3 | B | 234 | PCW | C5-N | 2.60 | 1.43 | 1.51 | 1 | 10 |
| 5 | B | 237 | GNP | C8-N7 | 2.60 | 1.29 | 1.34 | 3 | 10 |
| 3 | A | 408 | PCW | C1-C2 | 2.60 | 1.58 | 1.50 | 5 | 10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | C | 609 | PCW | C1-C2 | 2.60 | 1.58 | 1.50 | 3 | 10 |
| 3 | A | 402 | PCW | C1-C2 | 2.60 | 1.58 | 1.50 | 7 | 10 |
| 3 | B | 210 | PCW | C1-C2 | 2.60 | 1.58 | 1.50 | 10 | 10 |
| 3 | B | 217 | PCW | C1-C2 | 2.60 | 1.58 | 1.50 | 10 | 10 |
| 3 | B | 204 | PCW | C1-C2 | 2.59 | 1.58 | 1.50 | 4 | 10 |
| 3 | C | 621 | PCW | C5-N | 2.59 | 1.43 | 1.51 | 10 | 10 |
| 3 | B | 223 | PCW | C1-C2 | 2.58 | 1.58 | 1.50 | 7 | 10 |
| 3 | C | 603 | PCW | C1-C2 | 2.58 | 1.58 | 1.50 | 2 | 10 |
| 3 | C | 606 | PCW | C1-C2 | 2.58 | 1.58 | 1.50 | 9 | 10 |
| 3 | B | 216 | PCW | C1-C2 | 2.58 | 1.58 | 1.50 | 3 | 10 |
| 3 | C | 604 | PCW | C1-C2 | 2.58 | 1.58 | 1.50 | 1 | 10 |
| 3 | B | 205 | PCW | C5-N | 2.57 | 1.43 | 1.51 | 6 | 10 |
| 3 | C | 624 | PCW | C1-C2 | 2.57 | 1.58 | 1.50 | 3 | 10 |
| 3 | A | 401 | PCW | C1-C2 | 2.57 | 1.58 | 1.50 | 5 | 10 |
| 3 | C | 601 | PCW | C1-C2 | 2.57 | 1.58 | 1.50 | 1 | 10 |
| 3 | C | 614 | PCW | C1-C2 | 2.57 | 1.58 | 1.50 | 7 | 10 |
| 3 | B | 225 | PCW | C1-C2 | 2.57 | 1.58 | 1.50 | 6 | 10 |
| 3 | C | 621 | PCW | C1-C2 | 2.57 | 1.58 | 1.50 | 5 | 10 |
| 3 | C | 618 | PCW | C1-C2 | 2.56 | 1.58 | 1.50 | 3 | 10 |
| 3 | C | 611 | PCW | C1-C2 | 2.56 | 1.58 | 1.50 | 6 | 10 |
| 3 | B | 222 | PCW | C1-C2 | 2.55 | 1.58 | 1.50 | 5 | 10 |
| 3 | B | 206 | PCW | C1-C2 | 2.55 | 1.58 | 1.50 | 4 | 10 |
| 3 | C | 617 | PCW | C1-C2 | 2.54 | 1.58 | 1.50 | 7 | 10 |
| 3 | A | 403 | PCW | C5-N | 2.54 | 1.43 | 1.51 | 9 | 10 |
| 3 | B | 220 | PCW | C1-C2 | 2.54 | 1.58 | 1.50 | 2 | 10 |
| 3 | A | 404 | PCW | C1-C2 | 2.54 | 1.58 | 1.50 | 3 | 10 |
| 3 | B | 205 | PCW | C1-C2 | 2.54 | 1.58 | 1.50 | 1 | 10 |
| 3 | B | 215 | PCW | C1-C2 | 2.54 | 1.58 | 1.50 | 8 | 10 |
| 3 | A | 410 | PCW | C33-C32 | 2.53 | 1.61 | 1.52 | 3 | 10 |
| 3 | B | 219 | PCW | C1-C2 | 2.53 | 1.58 | 1.50 | 7 | 10 |
| 3 | C | 620 | PCW | C5-N | 2.53 | 1.43 | 1.51 | 1 | 10 |
| 3 | B | 235 | PCW | C1-C2 | 2.53 | 1.58 | 1.50 | 6 | 10 |
| 3 | C | 626 | PCW | C5-N | 2.53 | 1.43 | 1.51 | 2 | 10 |
| 3 | C | 616 | PCW | C1-C2 | 2.53 | 1.58 | 1.50 | 1 | 10 |
| 3 | C | 605 | PCW | C5-N | 2.52 | 1.43 | 1.51 | 7 | 10 |
| 3 | C | 620 | PCW | C1-C2 | 2.52 | 1.58 | 1.50 | 7 | 10 |
| 3 | A | 403 | PCW | C1-C2 | 2.52 | 1.58 | 1.50 | 8 | 10 |
| 3 | B | 234 | PCW | C1-C2 | 2.52 | 1.58 | 1.50 | 4 | 10 |
| 3 | A | 406 | PCW | C5-N | 2.52 | 1.43 | 1.51 | 5 | 10 |
| 3 | B | 208 | PCW | C5-N | 2.52 | 1.43 | 1.51 | 9 | 10 |
| 3 | C | 608 | PCW | C1-C2 | 2.52 | 1.58 | 1.50 | 3 | 10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | C | 605 | PCW | C1-C2 | 2.51 | 1.58 | 1.50 | 6 | 10 |
| 3 | A | 404 | PCW | C33-C32 | 2.51 | 1.61 | 1.52 | 9 | 10 |
| 3 | B | 221 | PCW | C5-N | 2.50 | 1.43 | 1.51 | 3 | 10 |
| 3 | B | 224 | PCW | C5-N | 2.50 | 1.43 | 1.51 | 4 | 10 |
| 3 | C | 612 | PCW | C1-C2 | 2.50 | 1.58 | 1.50 | 6 | 10 |
| 3 | C | 619 | PCW | C33-C32 | 2.50 | 1.61 | 1.52 | 5 | 10 |
| 3 | C | 615 | PCW | C33-C32 | 2.50 | 1.61 | 1.52 | 4 | 10 |
| 3 | B | 216 | PCW | C33-C32 | 2.49 | 1.61 | 1.52 | 2 | 10 |
| 3 | B | 209 | PCW | C5-N | 2.49 | 1.43 | 1.51 | 3 | 10 |
| 3 | C | 608 | PCW | C5-N | 2.49 | 1.43 | 1.51 | 9 | 10 |
| 3 | C | 622 | PCW | C33-C32 | 2.49 | 1.61 | 1.52 | 10 | 10 |
| 3 | B | 207 | PCW | C33-C32 | 2.49 | 1.61 | 1.52 | 9 | 10 |
| 3 | B | 210 | PCW | C33-C32 | 2.48 | 1.61 | 1.52 | 6 | 10 |
| 3 | C | 619 | PCW | C1-C2 | 2.48 | 1.58 | 1.50 | 6 | 10 |
| 3 | B | 212 | PCW | C5-N | 2.47 | 1.43 | 1.51 | 6 | 10 |
| 3 | B | 218 | PCW | C33-C32 | 2.48 | 1.61 | 1.52 | 4 | 10 |
| 3 | A | 403 | PCW | C33-C32 | 2.47 | 1.61 | 1.52 | 5 | 10 |
| 3 | C | 601 | PCW | C5-N | 2.47 | 1.43 | 1.51 | 2 | 10 |
| 3 | C | 623 | PCW | C1-C2 | 2.47 | 1.58 | 1.50 | 1 | 10 |
| 3 | C | 606 | PCW | C5-N | 2.47 | 1.43 | 1.51 | 10 | 10 |
| 3 | B | 201 | PCW | C1-C2 | 2.47 | 1.58 | 1.50 | 1 | 10 |
| 3 | C | 605 | PCW | C33-C32 | 2.47 | 1.61 | 1.52 | 7 | 10 |
| 3 | B | 202 | PCW | C33-C32 | 2.46 | 1.61 | 1.52 | 6 | 10 |
| 3 | C | 613 | PCW | C5-N | 2.46 | 1.44 | 1.51 | 10 | 10 |
| 3 | C | 626 | PCW | C33-C32 | 2.45 | 1.61 | 1.52 | 6 | 10 |
| 3 | A | 406 | PCW | C33-C32 | 2.45 | 1.61 | 1.52 | 7 | 10 |
| 3 | A | 401 | PCW | C33-C32 | 2.44 | 1.61 | 1.52 | 3 | 10 |
| 3 | B | 206 | PCW | C5-N | 2.44 | 1.44 | 1.51 | 5 | 10 |
| 3 | C | 606 | PCW | C33-C32 | 2.44 | 1.61 | 1.52 | 6 | 10 |
| 3 | B | 204 | PCW | C33-C32 | 2.43 | 1.61 | 1.52 | 10 | 10 |
| 3 | B | 219 | PCW | C33-C32 | 2.43 | 1.61 | 1.52 | 1 | 10 |
| 3 | B | 225 | PCW | C33-C32 | 2.43 | 1.61 | 1.52 | 4 | 10 |
| 3 | B | 221 | PCW | C33-C32 | 2.43 | 1.61 | 1.52 | 1 | 10 |
| 3 | B | 201 | PCW | C33-C32 | 2.43 | 1.61 | 1.52 | 4 | 10 |
| 3 | C | 603 | PCW | C33-C32 | 2.43 | 1.61 | 1.52 | 7 | 10 |
| 3 | C | 623 | PCW | C33-C32 | 2.43 | 1.61 | 1.52 | 7 | 10 |
| 3 | C | 624 | PCW | C33-C32 | 2.43 | 1.61 | 1.52 | 8 | 10 |
| 3 | A | 408 | PCW | C33-C32 | 2.43 | 1.61 | 1.52 | 2 | 10 |
| 3 | B | 205 | PCW | C33-C32 | 2.43 | 1.61 | 1.52 | 10 | 10 |
| 3 | C | 611 | PCW | C33-C32 | 2.43 | 1.61 | 1.52 | 5 | 10 |
| 3 | A | 402 | PCW | C33-C32 | 2.42 | 1.61 | 1.52 | 7 | 10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | A | 409 | PCW | C33-C32 | 2.42 | 1.61 | 1.52 | 3 | 10 |
| 3 | C | 625 | PCW | C33-C32 | 2.42 | 1.61 | 1.52 | 6 | 10 |
| 3 | C | 612 | PCW | C33-C32 | 2.42 | 1.61 | 1.52 | 8 | 10 |
| 3 | B | 234 | PCW | C33-C32 | 2.42 | 1.61 | 1.52 | 5 | 10 |
| 3 | C | 604 | PCW | C33-C32 | 2.42 | 1.61 | 1.52 | 8 | 10 |
| 3 | C | 607 | PCW | C33-C32 | 2.42 | 1.61 | 1.52 | 4 | 10 |
| 3 | B | 233 | PCW | C33-C32 | 2.42 | 1.61 | 1.52 | 3 | 10 |
| 3 | C | 601 | PCW | C33-C32 | 2.41 | 1.61 | 1.52 | 9 | 10 |
| 3 | C | 617 | PCW | C33-C32 | 2.41 | 1.61 | 1.52 | 9 | 10 |
| 3 | B | 217 | PCW | C33-C32 | 2.41 | 1.61 | 1.52 | 9 | 10 |
| 3 | C | 614 | PCW | C33-C32 | 2.41 | 1.61 | 1.52 | 8 | 10 |
| 3 | C | 618 | PCW | C33-C32 | 2.41 | 1.61 | 1.52 | 1 | 10 |
| 3 | C | 621 | PCW | C33-C32 | 2.41 | 1.61 | 1.52 | 5 | 10 |
| 3 | B | 208 | PCW | C33-C32 | 2.41 | 1.61 | 1.52 | 5 | 10 |
| 3 | B | 214 | PCW | C33-C32 | 2.41 | 1.61 | 1.52 | 4 | 10 |
| 3 | C | 609 | PCW | C33-C32 | 2.41 | 1.61 | 1.52 | 1 | 10 |
| 3 | B | 209 | PCW | C33-C32 | 2.40 | 1.61 | 1.52 | 9 | 10 |
| 3 | B | 222 | PCW | C33-C32 | 2.40 | 1.61 | 1.52 | 2 | 10 |
| 3 | B | 206 | PCW | C33-C32 | 2.40 | 1.61 | 1.52 | 9 | 10 |
| 3 | C | 602 | PCW | C33-C32 | 2.40 | 1.61 | 1.52 | 8 | 10 |
| 3 | B | 211 | PCW | C33-C32 | 2.39 | 1.60 | 1.52 | 6 | 10 |
| 3 | C | 613 | PCW | C33-C32 | 2.39 | 1.60 | 1.52 | 10 | 10 |
| 3 | C | 610 | PCW | C33-C32 | 2.39 | 1.60 | 1.52 | 7 | 10 |
| 3 | C | 616 | PCW | C33-C32 | 2.39 | 1.60 | 1.52 | 6 | 10 |
| 3 | B | 215 | PCW | C5-N | 2.38 | 1.44 | 1.51 | 5 | 10 |
| 3 | B | 215 | PCW | C33-C32 | 2.38 | 1.60 | 1.52 | 2 | 10 |
| 3 | C | 608 | PCW | C33-C32 | 2.38 | 1.60 | 1.52 | 7 | 10 |
| 7 | B | 239 | EWS | CAV-CAU | 2.38 | 1.36 | 1.42 | 2 | 10 |
| 3 | B | 213 | PCW | C33-C32 | 2.38 | 1.60 | 1.52 | 6 | 10 |
| 3 | B | 203 | PCW | C33-C32 | 2.37 | 1.60 | 1.52 | 2 | 10 |
| 3 | B | 220 | PCW | C33-C32 | 2.37 | 1.60 | 1.52 | 2 | 10 |
| 3 | B | 206 | PCW | C7-N | 2.37 | 1.43 | 1.50 | 7 | 10 |
| 3 | C | 613 | PCW | O2-C2 | 2.37 | 1.52 | 1.46 | 3 | 5 |
| 3 | A | 405 | PCW | C33-C32 | 2.36 | 1.60 | 1.52 | 10 | 10 |
| 3 | B | 224 | PCW | C33-C32 | 2.36 | 1.60 | 1.52 | 8 | 10 |
| 3 | A | 411 | PCW | C33-C32 | 2.35 | 1.60 | 1.52 | 2 | 10 |
| 3 | B | 223 | PCW | C33-C32 | 2.34 | 1.60 | 1.52 | 3 | 10 |
| 3 | C | 620 | PCW | C33-C32 | 2.34 | 1.60 | 1.52 | 5 | 10 |
| 3 | B | 212 | PCW | C33-C32 | 2.34 | 1.60 | 1.52 | 10 | 10 |
| 3 | C | 621 | PCW | C7-N | 2.32 | 1.43 | 1.50 | 9 | 10 |
| 3 | B | 235 | PCW | C33-C32 | 2.32 | 1.60 | 1.52 | 4 | 10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | C | 613 | PCW | C7-N | 2.31 | 1.43 | 1.50 | 3 | 10 |
| 3 | B | 203 | PCW | C3-C2 | 2.29 | 1.58 | 1.50 | 8 | 8 |
| 3 | B | 209 | PCW | C7-N | 2.29 | 1.43 | 1.50 | 5 | 10 |
| 3 | C | 620 | PCW | C7-N | 2.29 | 1.43 | 1.50 | 6 | 10 |
| 3 | A | 403 | PCW | C7-N | 2.29 | 1.43 | 1.50 | 9 | 9 |
| 3 | A | 406 | PCW | C7-N | 2.28 | 1.43 | 1.50 | 5 | 10 |
| 7 | B | 239 | EWS | CAO-CAN | 2.28 | 1.42 | 1.38 | 1 | 10 |
| 3 | B | 224 | PCW | C7-N | 2.27 | 1.43 | 1.50 | 7 | 10 |
| 3 | C | 608 | PCW | C7-N | 2.27 | 1.43 | 1.50 | 6 | 10 |
| 3 | B | 208 | PCW | C7-N | 2.27 | 1.43 | 1.50 | 7 | 10 |
| 3 | A | 401 | PCW | C3-C2 | 2.26 | 1.57 | 1.50 | 2 | 9 |
| 3 | A | 406 | PCW | C3-C2 | 2.26 | 1.57 | 1.50 | 7 | 9 |
| 3 | B | 212 | PCW | C7-N | 2.26 | 1.43 | 1.50 | 9 | 10 |
| 3 | B | 216 | PCW | C3-C2 | 2.26 | 1.57 | 1.50 | 8 | 7 |
| 3 | A | 410 | PCW | C3-C2 | 2.25 | 1.57 | 1.50 | 6 | 10 |
| 3 | C | 623 | PCW | C3-C2 | 2.25 | 1.57 | 1.50 | 10 | 7 |
| 3 | A | 402 | PCW | C3-C2 | 2.24 | 1.57 | 1.50 | 1 | 8 |
| 3 | B | 218 | PCW | C3-C2 | 2.24 | 1.57 | 1.50 | 2 | 8 |
| 3 | B | 212 | PCW | C3-C2 | 2.24 | 1.57 | 1.50 | 7 | 8 |
| 3 | B | 215 | PCW | C7-N | 2.24 | 1.43 | 1.50 | 1 | 10 |
| 3 | B | 221 | PCW | C3-C2 | 2.24 | 1.57 | 1.50 | 8 | 10 |
| 3 | C | 605 | PCW | C7-N | 2.24 | 1.43 | 1.50 | 1 | 10 |
| 3 | B | 221 | PCW | C7-N | 2.23 | 1.43 | 1.50 | 9 | 9 |
| 3 | C | 625 | PCW | C3-C2 | 2.23 | 1.57 | 1.50 | 5 | 8 |
| 3 | C | 608 | PCW | C3-C2 | 2.23 | 1.57 | 1.50 | 10 | 6 |
| 3 | C | 612 | PCW | C3-C2 | 2.23 | 1.57 | 1.50 | 8 | 10 |
| 3 | C | 606 | PCW | C7-N | 2.23 | 1.43 | 1.50 | 6 | 10 |
| 3 | C | 626 | PCW | C7-N | 2.23 | 1.43 | 1.50 | 8 | 10 |
| 3 | C | 602 | PCW | C3-C2 | 2.22 | 1.57 | 1.50 | 2 | 8 |
| 3 | B | 219 | PCW | C3-C2 | 2.22 | 1.57 | 1.50 | 10 | 8 |
| 3 | B | 205 | PCW | C7-N | 2.21 | 1.43 | 1.50 | 2 | 9 |
| 3 | C | 601 | PCW | C7-N | 2.21 | 1.43 | 1.50 | 6 | 9 |
| 3 | C | 616 | PCW | C3-C2 | 2.21 | 1.57 | 1.50 | 3 | 9 |
| 3 | C | 626 | PCW | C3-C2 | 2.20 | 1.57 | 1.50 | 1 | 6 |
| 3 | B | 207 | PCW | C3-C2 | 2.19 | 1.57 | 1.50 | 5 | 9 |
| 3 | C | 601 | PCW | C3-C2 | 2.19 | 1.57 | 1.50 | 8 | 8 |
| 3 | C | 614 | PCW | C3-C2 | 2.19 | 1.57 | 1.50 | 7 | 5 |
| 3 | B | 222 | PCW | C3-C2 | 2.19 | 1.57 | 1.50 | 6 | 10 |
| 3 | B | 233 | PCW | C3-C2 | 2.18 | 1.57 | 1.50 | 7 | 8 |
| 3 | B | 204 | PCW | C3-C2 | 2.18 | 1.57 | 1.50 | 4 | 6 |
| 3 | B | 234 | PCW | C3-C2 | 2.17 | 1.57 | 1.50 | 9 | 8 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | C | 611 | PCW | C3-C2 | 2.17 | 1.57 | 1.50 | 6 | 8 |
| 3 | B | 214 | PCW | C3-C2 | 2.17 | 1.57 | 1.50 | 4 | 8 |
| 3 | B | 225 | PCW | C3-C2 | 2.17 | 1.57 | 1.50 | 4 | 8 |
| 3 | A | 403 | PCW | C3-C2 | 2.17 | 1.57 | 1.50 | 6 | 7 |
| 3 | B | 223 | PCW | C3-C2 | 2.17 | 1.57 | 1.50 | 6 | 10 |
| 3 | B | 211 | PCW | C3-C2 | 2.17 | 1.57 | 1.50 | 5 | 7 |
| 3 | C | 605 | PCW | C3-C2 | 2.16 | 1.57 | 1.50 | 10 | 7 |
| 4 | B | 227 | 17F | C1X-C2X | 2.16 | 1.61 | 1.52 | 6 | 10 |
| 3 | C | 610 | PCW | C3-C2 | 2.16 | 1.57 | 1.50 | 5 | 5 |
| 3 | A | 411 | PCW | C3-C2 | 2.16 | 1.57 | 1.50 | 2 | 9 |
| 3 | A | 405 | PCW | C3-C2 | 2.15 | 1.57 | 1.50 | 5 | 9 |
| 4 | C | 630 | 17F | C1X-C2X | 2.15 | 1.61 | 1.52 | 9 | 2 |
| 3 | A | 404 | PCW | C3-C2 | 2.15 | 1.57 | 1.50 | 5 | 6 |
| 3 | B | 208 | PCW | C3-C2 | 2.15 | 1.57 | 1.50 | 3 | 9 |
| 3 | B | 201 | PCW | C3-C2 | 2.15 | 1.57 | 1.50 | 6 | 8 |
| 3 | B | 202 | PCW | C3-C2 | 2.15 | 1.57 | 1.50 | 4 | 8 |
| 3 | C | 603 | PCW | C3-C2 | 2.15 | 1.57 | 1.50 | 1 | 7 |
| 3 | C | 613 | PCW | C3-C2 | 2.15 | 1.57 | 1.50 | 5 | 10 |
| 3 | C | 622 | PCW | C3-C2 | 2.15 | 1.57 | 1.50 | 4 | 8 |
| 3 | C | 624 | PCW | C3-C2 | 2.15 | 1.57 | 1.50 | 6 | 8 |
| 4 | C | 632 | 17F | C1X-C2X | 2.15 | 1.61 | 1.52 | 3 | 8 |
| 3 | B | 215 | PCW | C3-C2 | 2.15 | 1.57 | 1.50 | 4 | 9 |
| 3 | B | 224 | PCW | C3-C2 | 2.14 | 1.57 | 1.50 | 8 | 9 |
| 3 | B | 209 | PCW | C3-C2 | 2.14 | 1.57 | 1.50 | 2 | 7 |
| 3 | B | 235 | PCW | C3-C2 | 2.14 | 1.57 | 1.50 | 7 | 7 |
| 3 | C | 619 | PCW | P-O4P | 2.14 | 1.51 | 1.59 | 2 | 1 |
| 3 | C | 604 | PCW | C3-C2 | 2.14 | 1.57 | 1.50 | 9 | 7 |
| 4 | B | 229 | 17F | C1X-C2X | 2.14 | 1.61 | 1.52 | 9 | 7 |
| 3 | B | 205 | PCW | C3-C2 | 2.13 | 1.57 | 1.50 | 6 | 6 |
| 3 | C | 609 | PCW | C3-C2 | 2.13 | 1.57 | 1.50 | 7 | 6 |
| 3 | C | 617 | PCW | C3-C2 | 2.13 | 1.57 | 1.50 | 2 | 5 |
| 3 | C | 607 | PCW | C3-C2 | 2.13 | 1.57 | 1.50 | 3 | 6 |
| 3 | C | 620 | PCW | C3-C2 | 2.13 | 1.57 | 1.50 | 10 | 7 |
| 3 | B | 210 | PCW | C3-C2 | 2.13 | 1.57 | 1.50 | 9 | 5 |
| 4 | B | 236 | 17F | C1X-C2X | 2.13 | 1.61 | 1.52 | 3 | 10 |
| 3 | B | 213 | PCW | C3-C2 | 2.13 | 1.57 | 1.50 | 7 | 4 |
| 3 | C | 606 | PCW | C3-C2 | 2.12 | 1.57 | 1.50 | 9 | 5 |
| 3 | C | 618 | PCW | C3-C2 | 2.12 | 1.57 | 1.50 | 7 | 8 |
| 3 | A | 408 | PCW | C3-C2 | 2.11 | 1.57 | 1.50 | 2 | 7 |
| 4 | B | 226 | 17F | C1X-C2X | 2.12 | 1.61 | 1.52 | 4 | 8 |
| 3 | B | 220 | PCW | C3-C2 | 2.10 | 1.57 | 1.50 | 7 | 7 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | C | 619 | PCW | C3-C2 | 2.10 | 1.57 | 1.50 | 5 | 3 |
| 4 | C | 633 | 17F | C1X-C2X | 2.10 | 1.61 | 1.52 | 7 | 9 |
| 4 | B | 230 | 17F | C1X-C2X | 2.10 | 1.61 | 1.52 | 1 | 7 |
| 3 | A | 409 | PCW | C3-C2 | 2.10 | 1.57 | 1.50 | 9 | 6 |
| 4 | A | 407 | 17F | C1X-C2X | 2.10 | 1.61 | 1.52 | 10 | 5 |
| 4 | B | 231 | 17F | C1X-C2X | 2.09 | 1.61 | 1.52 | 9 | 7 |
| 4 | C | 629 | 17F | C1X-C2X | 2.09 | 1.61 | 1.52 | 4 | 7 |
| 3 | C | 615 | PCW | C3-C2 | 2.09 | 1.57 | 1.50 | 7 | 6 |
| 4 | B | 232 | 17F | C1X-C2X | 2.09 | 1.61 | 1.52 | 2 | 8 |
| 3 | B | 217 | PCW | C3-C2 | 2.09 | 1.57 | 1.50 | 2 | 6 |
| 5 | B | 237 | GNP | O4'-C1' | 2.09 | 1.43 | 1.40 | 8 | 5 |
| 4 | C | 627 | 17F | C1X-C2X | 2.08 | 1.61 | 1.52 | 3 | 6 |
| 3 | B | 206 | PCW | C3-C2 | 2.07 | 1.57 | 1.50 | 9 | 5 |
| 3 | C | 621 | PCW | C3-C2 | 2.07 | 1.57 | 1.50 | 6 | 4 |
| 4 | C | 631 | 17F | C1X-C2X | 2.06 | 1.61 | 1.52 | 3 | 7 |
| 7 | B | 239 | EWS | CAT-CAS | 2.06 | 1.41 | 1.36 | 7 | 10 |
| 4 | B | 228 | 17F | C1X-C2X | 2.05 | 1.60 | 1.52 | 7 | 5 |
| 3 | C | 615 | PCW | P-O4P | 2.04 | 1.51 | 1.59 | 3 | 1 |
| 3 | B | 225 | PCW | P-O4P | 2.04 | 1.51 | 1.59 | 5 | 1 |
| 3 | C | 625 | PCW | P-O4P | 2.02 | 1.51 | 1.59 | 1 | 1 |
| 3 | B | 207 | PCW | P-O4P | 2.02 | 1.51 | 1.59 | 9 | 1 |
| 4 | C | 628 | 17F | C1X-C2X | 2.01 | 1.60 | 1.52 | 1 | 1 |
| 4 | C | 627 | 17F | C4-C5 | 2.01 | 1.57 | 1.50 | 2 | 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 | B | 210 | PCW | C8-N-C7 | 12.13 | 77.11 | 108.98 | 10 | 10 |
| 3 | A | 409 | PCW | C8-N-C7 | 12.06 | 77.30 | 108.98 | 6 | 10 |
| 3 | C | 604 | PCW | C8-N-C7 | 12.02 | 77.40 | 108.98 | 7 | 10 |
| 3 | C | 612 | PCW | C8-N-C7 | 12.02 | 77.41 | 108.98 | 7 | 10 |
| 3 | A | 408 | PCW | C8-N-C7 | 12.01 | 77.42 | 108.98 | 1 | 10 |
| 3 | C | 618 | PCW | C8-N-C7 | 12.01 | 77.44 | 108.98 | 4 | 10 |
| 3 | B | 225 | PCW | C8-N-C7 | 11.99 | 77.47 | 108.98 | 5 | 10 |
| 3 | A | 411 | PCW | C8-N-C7 | 11.99 | 77.49 | 108.98 | 9 | 10 |
| 3 | A | 404 | PCW | C8-N-C7 | 11.97 | 77.53 | 108.98 | 6 | 10 |
| 3 | B | 235 | PCW | C8-N-C7 | 11.97 | 77.54 | 108.98 | 6 | 10 |
| 3 | C | 610 | PCW | C8-N-C7 | 11.96 | 77.56 | 108.98 | 10 | 10 |
| 3 | C | 607 | PCW | C8-N-C7 | 11.96 | 77.57 | 108.98 | 9 | 10 |
| 3 | A | 410 | PCW | C8-N-C7 | 11.95 | 77.57 | 108.98 | 10 | 10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|---------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 211 | PCW | C8-N-C7 | 11.95 | 77.58 | 108.98 | 5 | 10 |
| 3 | C | 603 | PCW | C8-N-C7 | 11.95 | 77.59 | 108.98 | 3 | 10 |
| 3 | C | 617 | PCW | C8-N-C7 | 11.95 | 77.59 | 108.98 | 3 | 10 |
| 3 | B | 222 | PCW | C8-N-C7 | 11.95 | 77.60 | 108.98 | 5 | 10 |
| 3 | A | 401 | PCW | C8-N-C7 | 11.94 | 77.60 | 108.98 | 1 | 10 |
| 3 | C | 625 | PCW | C8-N-C7 | 11.94 | 77.60 | 108.98 | 9 | 10 |
| 3 | B | 216 | PCW | C8-N-C7 | 11.94 | 77.61 | 108.98 | 6 | 10 |
| 3 | B | 223 | PCW | C8-N-C7 | 11.94 | 77.61 | 108.98 | 6 | 10 |
| 3 | B | 201 | PCW | C8-N-C7 | 11.94 | 77.62 | 108.98 | 6 | 10 |
| 3 | B | 234 | PCW | C8-N-C7 | 11.93 | 77.64 | 108.98 | 3 | 10 |
| 3 | C | 624 | PCW | C8-N-C7 | 11.93 | 77.64 | 108.98 | 7 | 10 |
| 3 | C | 614 | PCW | C8-N-C7 | 11.93 | 77.64 | 108.98 | 4 | 10 |
| 3 | B | 214 | PCW | C8-N-C7 | 11.93 | 77.65 | 108.98 | 10 | 10 |
| 3 | A | 405 | PCW | C8-N-C7 | 11.93 | 77.65 | 108.98 | 6 | 10 |
| 3 | C | 611 | PCW | C8-N-C7 | 11.92 | 77.66 | 108.98 | 10 | 10 |
| 3 | A | 402 | PCW | C8-N-C7 | 11.92 | 77.68 | 108.98 | 10 | 10 |
| 3 | B | 217 | PCW | C8-N-C7 | 11.91 | 77.69 | 108.98 | 6 | 10 |
| 3 | B | 207 | PCW | C8-N-C7 | 11.91 | 77.69 | 108.98 | 4 | 10 |
| 3 | C | 623 | PCW | C8-N-C7 | 11.91 | 77.69 | 108.98 | 1 | 10 |
| 3 | B | 220 | PCW | C8-N-C7 | 11.91 | 77.70 | 108.98 | 5 | 10 |
| 3 | B | 204 | PCW | C8-N-C7 | 11.90 | 77.70 | 108.98 | 9 | 10 |
| 3 | C | 615 | PCW | C8-N-C7 | 11.90 | 77.71 | 108.98 | 1 | 10 |
| 3 | B | 233 | PCW | C8-N-C7 | 11.90 | 77.72 | 108.98 | 7 | 10 |
| 3 | B | 219 | PCW | C8-N-C7 | 11.90 | 77.73 | 108.98 | 10 | 10 |
| 3 | C | 602 | PCW | C8-N-C7 | 11.89 | 77.74 | 108.98 | 8 | 10 |
| 3 | B | 202 | PCW | C8-N-C7 | 11.89 | 77.74 | 108.98 | 10 | 10 |
| 3 | C | 616 | PCW | C8-N-C7 | 11.89 | 77.74 | 108.98 | 2 | 10 |
| 3 | C | 619 | PCW | C8-N-C7 | 11.89 | 77.75 | 108.98 | 5 | 10 |
| 3 | B | 203 | PCW | C8-N-C7 | 11.88 | 77.76 | 108.98 | 1 | 10 |
| 3 | B | 213 | PCW | C8-N-C7 | 11.87 | 77.79 | 108.98 | 6 | 10 |
| 3 | C | 609 | PCW | C8-N-C7 | 11.85 | 77.86 | 108.98 | 5 | 10 |
| 3 | C | 622 | PCW | C8-N-C7 | 11.84 | 77.88 | 108.98 | 4 | 10 |
| 3 | B | 218 | PCW | C8-N-C7 | 11.83 | 77.91 | 108.98 | 10 | 10 |
| 3 | A | 409 | PCW | C8-N-C6 | 10.17 | 82.27 | 108.98 | 7 | 10 |
| 3 | B | 219 | PCW | C8-N-C6 | 10.14 | 82.34 | 108.98 | 2 | 10 |
| 3 | C | 617 | PCW | C8-N-C6 | 10.13 | 82.35 | 108.98 | 2 | 10 |
| 3 | C | 624 | PCW | C8-N-C6 | 10.13 | 82.37 | 108.98 | 2 | 10 |
| 3 | A | 411 | PCW | C8-N-C6 | 10.12 | 82.40 | 108.98 | 3 | 10 |
| 3 | B | 233 | PCW | C8-N-C6 | 10.11 | 82.41 | 108.98 | 3 | 10 |
| 3 | B | 214 | PCW | C8-N-C6 | 10.11 | 82.43 | 108.98 | 1 | 10 |
| 3 | B | 220 | PCW | C8-N-C6 | 10.11 | 82.43 | 108.98 | 6 | 10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-----------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 225 | PCW | C8-N-C6 | 10.11 | 82.43 | 108.98 | 10 | 10 |
| 3 | C | 609 | PCW | C8-N-C6 | 10.11 | 82.43 | 108.98 | 2 | 10 |
| 3 | B | 203 | PCW | C8-N-C6 | 10.10 | 82.44 | 108.98 | 2 | 10 |
| 3 | B | 213 | PCW | C8-N-C6 | 10.10 | 82.45 | 108.98 | 8 | 10 |
| 3 | A | 410 | PCW | C8-N-C6 | 10.10 | 82.45 | 108.98 | 6 | 10 |
| 3 | B | 218 | PCW | C8-N-C6 | 10.10 | 82.46 | 108.98 | 2 | 10 |
| 3 | B | 204 | PCW | C8-N-C6 | 10.09 | 82.46 | 108.98 | 5 | 10 |
| 3 | C | 614 | PCW | C8-N-C6 | 10.09 | 82.46 | 108.98 | 2 | 10 |
| 3 | B | 223 | PCW | C8-N-C6 | 10.09 | 82.47 | 108.98 | 5 | 10 |
| 3 | B | 202 | PCW | C8-N-C6 | 10.08 | 82.49 | 108.98 | 6 | 10 |
| 3 | B | 222 | PCW | C8-N-C6 | 10.08 | 82.49 | 108.98 | 10 | 10 |
| 3 | C | 623 | PCW | C8-N-C6 | 10.08 | 82.49 | 108.98 | 9 | 10 |
| 3 | B | 207 | PCW | C8-N-C6 | 10.08 | 82.50 | 108.98 | 10 | 10 |
| 3 | C | 619 | PCW | C8-N-C6 | 10.08 | 82.50 | 108.98 | 3 | 10 |
| 3 | B | 217 | PCW | C8-N-C6 | 10.08 | 82.50 | 108.98 | 7 | 10 |
| 3 | C | 622 | PCW | C8-N-C6 | 10.08 | 82.51 | 108.98 | 6 | 10 |
| 3 | C | 625 | PCW | C8-N-C6 | 10.06 | 82.55 | 108.98 | 5 | 10 |
| 3 | A | 401 | PCW | C8-N-C6 | 10.06 | 82.56 | 108.98 | 8 | 10 |
| 3 | A | 405 | PCW | C8-N-C6 | 10.06 | 82.56 | 108.98 | 9 | 10 |
| 3 | C | 612 | PCW | C8-N-C6 | 10.05 | 82.56 | 108.98 | 5 | 10 |
| 3 | A | 402 | PCW | C8-N-C6 | 10.05 | 82.58 | 108.98 | 5 | 10 |
| 3 | C | 615 | PCW | C8-N-C6 | 10.05 | 82.58 | 108.98 | 2 | 10 |
| 3 | C | 607 | PCW | C8-N-C6 | 10.05 | 82.59 | 108.98 | 3 | 10 |
| 3 | A | 408 | PCW | C8-N-C6 | 10.04 | 82.59 | 108.98 | 9 | 10 |
| 3 | B | 210 | PCW | C8-N-C6 | 10.04 | 82.60 | 108.98 | 4 | 10 |
| 3 | B | 216 | PCW | C8-N-C6 | 10.04 | 82.61 | 108.98 | 9 | 10 |
| 3 | B | 234 | PCW | C8-N-C6 | 10.03 | 82.62 | 108.98 | 5 | 10 |
| 3 | C | 603 | PCW | C8-N-C6 | 10.03 | 82.64 | 108.98 | 8 | 10 |
| 3 | A | 404 | PCW | C8-N-C6 | 10.02 | 82.64 | 108.98 | 2 | 10 |
| 3 | C | 616 | PCW | C8-N-C6 | 10.02 | 82.64 | 108.98 | 8 | 10 |
| 3 | C | 611 | PCW | C8-N-C6 | 10.02 | 82.65 | 108.98 | 3 | 10 |
| 3 | C | 618 | PCW | C8-N-C6 | 10.02 | 82.65 | 108.98 | 9 | 10 |
| 3 | B | 201 | PCW | C8-N-C6 | 10.01 | 82.68 | 108.98 | 3 | 10 |
| 3 | C | 602 | PCW | C8-N-C6 | 10.01 | 82.68 | 108.98 | 9 | 10 |
| 3 | B | 235 | PCW | C8-N-C6 | 9.99 | 82.73 | 108.98 | 2 | 10 |
| 3 | C | 604 | PCW | C8-N-C6 | 9.98 | 82.76 | 108.98 | 3 | 10 |
| 3 | B | 211 | PCW | C8-N-C6 | 9.98 | 82.76 | 108.98 | 7 | 10 |
| 3 | C | 610 | PCW | C8-N-C6 | 9.95 | 82.85 | 108.98 | 7 | 10 |
| 5 | B | 237 | GNP | C5-C6-N1 | 7.95 | 112.80 | 123.42 | 8 | 10 |
| 3 | B | 234 | PCW | O4P-P-O2P | 7.60 | 78.83 | 108.94 | 6 | 10 |
| 3 | B | 204 | PCW | O4P-P-O2P | 7.58 | 78.88 | 108.94 | 3 | 10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-----------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 5 | B | 237 | GNP | C2-N1-C6 | 6.57 | 125.09 | 115.96 | 8 | 10 |
| 4 | A | 407 | 17F | O2-P1-O6 | 6.39 | 78.61 | 107.57 | 5 | 10 |
| 4 | C | 630 | 17F | O2-P1-O6 | 6.37 | 78.71 | 107.57 | 7 | 10 |
| 4 | C | 630 | 17F | O2-P1-O3 | 6.19 | 79.52 | 107.57 | 6 | 10 |
| 4 | A | 407 | 17F | O2-P1-O3 | 6.19 | 79.53 | 107.57 | 4 | 10 |
| 3 | B | 204 | PCW | O1P-P-O2P | 5.95 | 84.75 | 112.44 | 9 | 10 |
| 3 | B | 234 | PCW | O1P-P-O2P | 5.90 | 85.02 | 112.44 | 5 | 10 |
| 3 | B | 204 | PCW | O3P-P-O2P | 5.89 | 85.58 | 108.94 | 6 | 10 |
| 3 | B | 234 | PCW | O3P-P-O2P | 5.86 | 85.71 | 108.94 | 6 | 10 |
| 3 | B | 207 | PCW | C8-N-C5 | 5.54 | 87.89 | 109.91 | 6 | 10 |
| 3 | C | 616 | PCW | C8-N-C5 | 5.50 | 88.06 | 109.91 | 5 | 10 |
| 3 | A | 411 | PCW | C8-N-C5 | 5.49 | 88.09 | 109.91 | 7 | 10 |
| 3 | C | 622 | PCW | C8-N-C5 | 5.48 | 88.13 | 109.91 | 5 | 10 |
| 3 | C | 603 | PCW | C8-N-C5 | 5.47 | 88.17 | 109.91 | 7 | 10 |
| 3 | B | 217 | PCW | C8-N-C5 | 5.46 | 88.21 | 109.91 | 1 | 10 |
| 3 | C | 610 | PCW | C8-N-C5 | 5.45 | 88.24 | 109.91 | 9 | 10 |
| 3 | B | 222 | PCW | C8-N-C5 | 5.45 | 88.25 | 109.91 | 4 | 10 |
| 3 | C | 623 | PCW | C8-N-C5 | 5.45 | 88.25 | 109.91 | 8 | 10 |
| 3 | A | 408 | PCW | C8-N-C5 | 5.44 | 88.28 | 109.91 | 10 | 10 |
| 3 | B | 201 | PCW | C8-N-C5 | 5.44 | 88.27 | 109.91 | 10 | 10 |
| 3 | C | 615 | PCW | C8-N-C5 | 5.44 | 88.29 | 109.91 | 5 | 10 |
| 3 | C | 617 | PCW | C8-N-C5 | 5.44 | 88.30 | 109.91 | 9 | 10 |
| 3 | A | 405 | PCW | C8-N-C5 | 5.43 | 88.33 | 109.91 | 10 | 10 |
| 3 | C | 619 | PCW | C8-N-C5 | 5.43 | 88.33 | 109.91 | 8 | 10 |
| 3 | B | 223 | PCW | C8-N-C5 | 5.43 | 88.34 | 109.91 | 3 | 10 |
| 3 | B | 213 | PCW | C8-N-C5 | 5.42 | 88.36 | 109.91 | 10 | 10 |
| 3 | C | 625 | PCW | C8-N-C5 | 5.42 | 88.37 | 109.91 | 2 | 10 |
| 3 | B | 210 | PCW | C8-N-C5 | 5.42 | 88.38 | 109.91 | 1 | 10 |
| 3 | A | 402 | PCW | C8-N-C5 | 5.41 | 88.39 | 109.91 | 8 | 10 |
| 3 | C | 609 | PCW | C8-N-C5 | 5.41 | 88.39 | 109.91 | 6 | 10 |
| 3 | B | 218 | PCW | C8-N-C5 | 5.41 | 88.40 | 109.91 | 9 | 10 |
| 3 | C | 607 | PCW | C8-N-C5 | 5.41 | 88.40 | 109.91 | 6 | 10 |
| 3 | A | 404 | PCW | C8-N-C5 | 5.41 | 88.41 | 109.91 | 9 | 10 |
| 3 | C | 612 | PCW | C8-N-C5 | 5.41 | 88.41 | 109.91 | 4 | 10 |
| 3 | B | 216 | PCW | C8-N-C5 | 5.40 | 88.43 | 109.91 | 3 | 10 |
| 3 | B | 219 | PCW | C8-N-C5 | 5.40 | 88.44 | 109.91 | 4 | 10 |
| 3 | B | 225 | PCW | C8-N-C5 | 5.39 | 88.47 | 109.91 | 2 | 10 |
| 3 | A | 401 | PCW | C8-N-C5 | 5.39 | 88.48 | 109.91 | 2 | 10 |
| 3 | B | 234 | PCW | C8-N-C5 | 5.39 | 88.48 | 109.91 | 4 | 10 |
| 3 | C | 618 | PCW | C8-N-C5 | 5.39 | 88.50 | 109.91 | 8 | 10 |
| 3 | B | 202 | PCW | C8-N-C5 | 5.38 | 88.51 | 109.91 | 5 | 10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 214 | PCW | C8-N-C5 | 5.39 | 88.50 | 109.91 | 2 | 10 |
| 3 | B | 220 | PCW | C8-N-C5 | 5.38 | 88.52 | 109.91 | 2 | 10 |
| 3 | B | 235 | PCW | C8-N-C5 | 5.38 | 88.52 | 109.91 | 1 | 10 |
| 3 | C | 602 | PCW | C8-N-C5 | 5.38 | 88.52 | 109.91 | 10 | 10 |
| 3 | A | 410 | PCW | C8-N-C5 | 5.38 | 88.53 | 109.91 | 10 | 10 |
| 3 | B | 204 | PCW | C8-N-C5 | 5.38 | 88.53 | 109.91 | 7 | 10 |
| 3 | C | 624 | PCW | C8-N-C5 | 5.38 | 88.53 | 109.91 | 4 | 10 |
| 3 | C | 611 | PCW | C8-N-C5 | 5.38 | 88.54 | 109.91 | 8 | 10 |
| 3 | C | 604 | PCW | C8-N-C5 | 5.37 | 88.55 | 109.91 | 6 | 10 |
| 3 | C | 614 | PCW | C8-N-C5 | 5.37 | 88.57 | 109.91 | 5 | 10 |
| 3 | B | 233 | PCW | C8-N-C5 | 5.36 | 88.59 | 109.91 | 1 | 10 |
| 3 | B | 211 | PCW | C8-N-C5 | 5.35 | 88.63 | 109.91 | 2 | 10 |
| 3 | B | 203 | PCW | C8-N-C5 | 5.35 | 88.66 | 109.91 | 8 | 10 |
| 3 | A | 409 | PCW | C8-N-C5 | 5.32 | 88.75 | 109.91 | 9 | 10 |
| 4 | C | 630 | 17F | O3-C1-C2 | 5.00 | 112.42 | 108.06 | 5 | 10 |
| 4 | B | 230 | 17F | O3-C1-C2 | 4.89 | 112.32 | 108.06 | 8 | 10 |
| 4 | A | 407 | 17F | O2-P1-O1 | 4.84 | 89.91 | 112.44 | 1 | 10 |
| 4 | C | 630 | 17F | O2-P1-O1 | 4.81 | 90.06 | 112.44 | 10 | 10 |
| 4 | B | 229 | 17F | O3-C1-C2 | 4.26 | 111.77 | 108.06 | 9 | 10 |
| 4 | B | 231 | 17F | O3-C1-C2 | 4.23 | 111.75 | 108.06 | 1 | 10 |
| 4 | B | 228 | 17F | O3-C1-C2 | 4.13 | 111.66 | 108.06 | 4 | 10 |
| 4 | C | 631 | 17F | O3-C1-C2 | 4.11 | 111.64 | 108.06 | 2 | 10 |
| 4 | B | 226 | 17F | O3-C1-C2 | 4.09 | 111.62 | 108.06 | 7 | 10 |
| 4 | B | 236 | 17F | O3-C1-C2 | 3.87 | 111.43 | 108.06 | 4 | 10 |
| 4 | B | 227 | 17F | O3-C1-C2 | 3.85 | 111.41 | 108.06 | 10 | 10 |
| 4 | B | 232 | 17F | O3-C1-C2 | 3.80 | 111.37 | 108.06 | 5 | 10 |
| 4 | C | 628 | 17F | O3-C1-C2 | 3.75 | 111.33 | 108.06 | 7 | 10 |
| 5 | B | 237 | GNP | O1B-PB-N3B | 3.69 | 106.33 | 111.77 | 5 | 10 |
| 4 | C | 632 | 17F | O3-C1-C2 | 3.66 | 111.25 | 108.06 | 2 | 10 |
| 4 | C | 627 | 17F | O3-C1-C2 | 3.62 | 111.22 | 108.06 | 10 | 10 |
| 3 | B | 204 | PCW | O1P-P-O4P | 3.59 | 123.82 | 107.57 | 9 | 10 |
| 4 | A | 407 | 17F | O3-C1-C2 | 3.57 | 111.17 | 108.06 | 1 | 10 |
| 4 | C | 633 | 17F | O3-C1-C2 | 3.49 | 111.10 | 108.06 | 3 | 10 |
| 3 | B | 214 | PCW | C6-N-C5 | 3.45 | 123.63 | 109.91 | 1 | 10 |
| 4 | C | 628 | 17F | O7-C7-O8 | 3.45 | 132.26 | 123.63 | 7 | 10 |
| 3 | B | 234 | PCW | O1P-P-O4P | 3.44 | 123.18 | 107.57 | 5 | 10 |
| 4 | C | 632 | 17F | O5-C3-O4 | 3.44 | 116.27 | 124.08 | 4 | 10 |
| 4 | B | 229 | 17F | O5-C3-O4 | 3.44 | 116.28 | 124.08 | 5 | 10 |
| 4 | C | 629 | 17F | O3-C1-C2 | 3.43 | 111.05 | 108.06 | 10 | 10 |
| 3 | B | 233 | PCW | C6-N-C5 | 3.42 | 123.52 | 109.91 | 6 | 10 |
| 3 | B | 219 | PCW | C6-N-C5 | 3.42 | 123.51 | 109.91 | 4 | 10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|----------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 4 | C | 631 | 17F | O5-C3-O4 | 3.41 | 116.33 | 124.08 | 5 | 10 |
| 3 | A | 402 | PCW | C6-N-C5 | 3.41 | 123.46 | 109.91 | 5 | 10 |
| 4 | B | 226 | 17F | O5-C3-O4 | 3.40 | 116.36 | 124.08 | 3 | 10 |
| 3 | A | 409 | PCW | C6-N-C5 | 3.40 | 123.42 | 109.91 | 9 | 10 |
| 4 | B | 232 | 17F | O5-C3-O4 | 3.39 | 116.38 | 124.08 | 4 | 10 |
| 4 | B | 236 | 17F | O5-C3-O4 | 3.39 | 116.39 | 124.08 | 4 | 10 |
| 3 | A | 401 | PCW | C6-N-C5 | 3.38 | 123.36 | 109.91 | 3 | 10 |
| 4 | C | 630 | 17F | O5-C3-O4 | 3.38 | 116.41 | 124.08 | 10 | 10 |
| 4 | C | 627 | 17F | O5-C3-O4 | 3.38 | 116.41 | 124.08 | 9 | 10 |
| 3 | C | 609 | PCW | C6-N-C5 | 3.37 | 123.32 | 109.91 | 7 | 10 |
| 3 | C | 624 | PCW | C6-N-C5 | 3.37 | 123.32 | 109.91 | 2 | 10 |
| 4 | B | 227 | 17F | O5-C3-O4 | 3.37 | 116.43 | 124.08 | 9 | 10 |
| 4 | C | 628 | 17F | O5-C3-O4 | 3.37 | 116.42 | 124.08 | 4 | 10 |
| 3 | A | 408 | PCW | C6-N-C5 | 3.37 | 123.31 | 109.91 | 7 | 10 |
| 3 | C | 623 | PCW | C6-N-C5 | 3.37 | 123.31 | 109.91 | 9 | 10 |
| 3 | B | 213 | PCW | C6-N-C5 | 3.37 | 123.30 | 109.91 | 9 | 10 |
| 3 | C | 611 | PCW | C6-N-C5 | 3.37 | 123.30 | 109.91 | 8 | 10 |
| 4 | C | 629 | 17F | O5-C3-O4 | 3.37 | 116.44 | 124.08 | 7 | 10 |
| 4 | B | 228 | 17F | O5-C3-O4 | 3.36 | 116.45 | 124.08 | 1 | 10 |
| 3 | C | 622 | PCW | C6-N-C5 | 3.36 | 123.28 | 109.91 | 5 | 10 |
| 4 | B | 231 | 17F | O5-C3-O4 | 3.36 | 116.46 | 124.08 | 7 | 10 |
| 3 | C | 607 | PCW | C6-N-C5 | 3.36 | 123.26 | 109.91 | 6 | 10 |
| 3 | C | 614 | PCW | C6-N-C5 | 3.36 | 123.25 | 109.91 | 5 | 10 |
| 4 | B | 230 | 17F | O5-C3-O4 | 3.36 | 116.47 | 124.08 | 5 | 10 |
| 3 | A | 410 | PCW | C6-N-C5 | 3.35 | 123.24 | 109.91 | 9 | 10 |
| 4 | C | 633 | 17F | O5-C3-O4 | 3.35 | 116.47 | 124.08 | 9 | 10 |
| 3 | C | 603 | PCW | C6-N-C5 | 3.35 | 123.22 | 109.91 | 9 | 10 |
| 3 | B | 220 | PCW | C6-N-C5 | 3.35 | 123.21 | 109.91 | 8 | 10 |
| 3 | C | 602 | PCW | C6-N-C5 | 3.35 | 123.22 | 109.91 | 9 | 10 |
| 3 | A | 411 | PCW | C6-N-C5 | 3.34 | 123.20 | 109.91 | 7 | 10 |
| 3 | B | 223 | PCW | C6-N-C5 | 3.34 | 123.20 | 109.91 | 5 | 10 |
| 3 | C | 615 | PCW | C6-N-C5 | 3.34 | 123.18 | 109.91 | 4 | 10 |
| 3 | A | 404 | PCW | C6-N-C5 | 3.33 | 123.15 | 109.91 | 4 | 10 |
| 3 | B | 207 | PCW | C6-N-C5 | 3.33 | 123.15 | 109.91 | 2 | 10 |
| 3 | C | 625 | PCW | C6-N-C5 | 3.33 | 123.14 | 109.91 | 2 | 10 |
| 3 | C | 617 | PCW | C6-N-C5 | 3.33 | 123.14 | 109.91 | 10 | 10 |
| 4 | A | 407 | 17F | O5-C3-O4 | 3.33 | 116.53 | 124.08 | 3 | 10 |
| 3 | B | 204 | PCW | C6-N-C5 | 3.32 | 123.11 | 109.91 | 5 | 10 |
| 3 | B | 218 | PCW | C6-N-C5 | 3.32 | 123.12 | 109.91 | 1 | 10 |
| 3 | B | 225 | PCW | C6-N-C5 | 3.32 | 123.11 | 109.91 | 10 | 10 |
| 3 | C | 610 | PCW | C6-N-C5 | 3.32 | 123.09 | 109.91 | 7 | 10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|----------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 203 | PCW | C6-N-C5 | 3.31 | 123.08 | 109.91 | 2 | 10 |
| 3 | C | 616 | PCW | C6-N-C5 | 3.31 | 123.08 | 109.91 | 10 | 10 |
| 3 | B | 210 | PCW | C6-N-C5 | 3.30 | 123.04 | 109.91 | 3 | 10 |
| 3 | B | 216 | PCW | C6-N-C5 | 3.30 | 123.04 | 109.91 | 7 | 10 |
| 3 | B | 202 | PCW | C6-N-C5 | 3.30 | 123.02 | 109.91 | 5 | 10 |
| 3 | B | 201 | PCW | C6-N-C5 | 3.29 | 123.00 | 109.91 | 7 | 10 |
| 3 | B | 235 | PCW | C6-N-C5 | 3.29 | 123.00 | 109.91 | 3 | 10 |
| 3 | B | 222 | PCW | C6-N-C5 | 3.29 | 122.97 | 109.91 | 9 | 10 |
| 3 | B | 217 | PCW | C6-N-C5 | 3.28 | 122.96 | 109.91 | 1 | 10 |
| 3 | C | 619 | PCW | C6-N-C5 | 3.28 | 122.96 | 109.91 | 9 | 10 |
| 3 | C | 604 | PCW | C6-N-C5 | 3.28 | 122.96 | 109.91 | 4 | 10 |
| 3 | C | 618 | PCW | C6-N-C5 | 3.27 | 122.92 | 109.91 | 3 | 10 |
| 3 | C | 612 | PCW | C6-N-C5 | 3.27 | 122.90 | 109.91 | 4 | 10 |
| 3 | A | 405 | PCW | C6-N-C5 | 3.27 | 122.90 | 109.91 | 9 | 10 |
| 3 | B | 234 | PCW | C6-N-C5 | 3.27 | 122.89 | 109.91 | 8 | 10 |
| 3 | B | 211 | PCW | C6-N-C5 | 3.25 | 122.82 | 109.91 | 8 | 10 |
| 5 | B | 237 | GNP | N3-C2-N1 | 3.21 | 123.12 | 127.21 | 5 | 10 |
| 4 | B | 230 | 17F | O7-C7-O8 | 3.16 | 131.53 | 123.63 | 7 | 10 |
| 4 | C | 633 | 17F | O7-C7-O8 | 3.09 | 131.35 | 123.63 | 1 | 10 |
| 4 | B | 232 | 17F | O7-C7-O8 | 3.08 | 131.34 | 123.63 | 7 | 10 |
| 4 | B | 229 | 17F | O7-C7-O8 | 3.08 | 131.34 | 123.63 | 1 | 10 |
| 4 | A | 407 | 17F | O7-C7-O8 | 3.07 | 131.31 | 123.63 | 3 | 10 |
| 4 | C | 629 | 17F | O7-C7-O8 | 3.06 | 131.27 | 123.63 | 5 | 10 |
| 4 | C | 631 | 17F | O7-C7-O8 | 3.05 | 131.27 | 123.63 | 3 | 10 |
| 4 | C | 627 | 17F | O7-C7-O8 | 3.01 | 131.17 | 123.63 | 4 | 10 |
| 4 | A | 407 | 17F | O3-P1-O1 | 2.99 | 120.80 | 108.94 | 5 | 10 |
| 4 | B | 236 | 17F | O7-C7-O8 | 2.99 | 131.10 | 123.63 | 10 | 10 |
| 4 | C | 632 | 17F | O7-C7-O8 | 2.95 | 131.01 | 123.63 | 1 | 10 |
| 4 | B | 228 | 17F | O7-C7-O8 | 2.94 | 130.99 | 123.63 | 1 | 10 |
| 4 | B | 231 | 17F | O7-C7-O8 | 2.89 | 130.85 | 123.63 | 4 | 10 |
| 4 | B | 226 | 17F | O7-C7-O8 | 2.88 | 130.84 | 123.63 | 10 | 10 |
| 4 | C | 630 | 17F | O7-C7-O8 | 2.87 | 130.81 | 123.63 | 8 | 10 |
| 4 | B | 227 | 17F | O7-C7-O8 | 2.84 | 130.74 | 123.63 | 1 | 10 |
| 4 | C | 630 | 17F | O3-P1-O1 | 2.82 | 120.10 | 108.94 | 8 | 10 |
| 3 | B | 215 | PCW | C8-N-C7 | 2.75 | 101.74 | 108.98 | 4 | 10 |
| 3 | B | 224 | PCW | C8-N-C7 | 2.75 | 101.75 | 108.98 | 5 | 10 |
| 3 | C | 605 | PCW | C8-N-C7 | 2.74 | 101.78 | 108.98 | 5 | 10 |
| 5 | B | 237 | GNP | N2-C2-N3 | 2.73 | 122.05 | 117.79 | 6 | 10 |
| 3 | A | 403 | PCW | C8-N-C7 | 2.73 | 101.81 | 108.98 | 4 | 10 |
| 3 | A | 406 | PCW | C8-N-C7 | 2.72 | 101.82 | 108.98 | 3 | 10 |
| 3 | C | 620 | PCW | C8-N-C7 | 2.70 | 101.89 | 108.98 | 7 | 10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | B | 212 | PCW | C8-N-C7 | 2.69 | 101.91 | 108.98 | 4 | 10 |
| 4 | C | 628 | 17F | C5-O9-C17 | 2.68 | 111.38 | 117.80 | 2 | 10 |
| 3 | B | 221 | PCW | C8-N-C7 | 2.68 | 101.94 | 108.98 | 10 | 10 |
| 3 | B | 206 | PCW | C8-N-C7 | 2.67 | 101.96 | 108.98 | 7 | 10 |
| 3 | B | 208 | PCW | C8-N-C7 | 2.67 | 101.97 | 108.98 | 3 | 10 |
| 3 | C | 613 | PCW | C8-N-C7 | 2.67 | 101.97 | 108.98 | 1 | 10 |
| 3 | B | 205 | PCW | C8-N-C7 | 2.67 | 101.97 | 108.98 | 7 | 10 |
| 3 | C | 621 | PCW | C8-N-C7 | 2.67 | 101.97 | 108.98 | 2 | 10 |
| 3 | B | 209 | PCW | C8-N-C7 | 2.66 | 101.99 | 108.98 | 1 | 10 |
| 3 | C | 626 | PCW | C8-N-C7 | 2.64 | 102.03 | 108.98 | 10 | 10 |
| 4 | C | 633 | 17F | O9-C17-O10 | 2.64 | 129.87 | 123.70 | 10 | 10 |
| 3 | C | 606 | PCW | C8-N-C7 | 2.63 | 102.08 | 108.98 | 6 | 10 |
| 3 | C | 608 | PCW | C8-N-C7 | 2.63 | 102.08 | 108.98 | 6 | 10 |
| 3 | B | 235 | PCW | C7-N-C5 | 2.61 | 120.30 | 109.91 | 6 | 10 |
| 3 | C | 601 | PCW | C8-N-C7 | 2.59 | 102.17 | 108.98 | 6 | 10 |
| 3 | C | 610 | PCW | C7-N-C5 | 2.59 | 120.20 | 109.91 | 1 | 10 |
| 4 | A | 407 | 17F | O6-P1-O1 | 2.59 | 119.20 | 108.94 | 9 | 10 |
| 4 | C | 630 | 17F | O6-P1-O1 | 2.57 | 119.12 | 108.94 | 9 | 9 |
| 4 | C | 631 | 17F | C5-O9-C17 | 2.56 | 111.66 | 117.80 | 9 | 10 |
| 3 | C | 612 | PCW | C7-N-C5 | 2.56 | 120.09 | 109.91 | 2 | 10 |
| 3 | B | 201 | PCW | C7-N-C5 | 2.54 | 119.99 | 109.91 | 9 | 10 |
| 4 | B | 232 | 17F | C5-O9-C17 | 2.53 | 111.73 | 117.80 | 8 | 9 |
| 3 | C | 619 | PCW | C7-N-C5 | 2.53 | 119.96 | 109.91 | 7 | 10 |
| 3 | B | 220 | PCW | C7-N-C5 | 2.53 | 119.95 | 109.91 | 10 | 10 |
| 3 | A | 405 | PCW | C7-N-C5 | 2.52 | 119.92 | 109.91 | 1 | 10 |
| 4 | C | 630 | 17F | C5-O9-C17 | 2.52 | 111.77 | 117.80 | 7 | 8 |
| 3 | B | 207 | PCW | C7-N-C5 | 2.52 | 119.91 | 109.91 | 6 | 10 |
| 3 | B | 225 | PCW | C7-N-C5 | 2.51 | 119.88 | 109.91 | 7 | 10 |
| 3 | B | 222 | PCW | C7-N-C5 | 2.51 | 119.87 | 109.91 | 4 | 10 |
| 3 | A | 408 | PCW | C7-N-C5 | 2.50 | 119.87 | 109.91 | 1 | 10 |
| 3 | B | 217 | PCW | C7-N-C5 | 2.50 | 119.86 | 109.91 | 4 | 10 |
| 3 | A | 401 | PCW | C7-N-C5 | 2.49 | 119.81 | 109.91 | 1 | 10 |
| 3 | C | 622 | PCW | C7-N-C5 | 2.49 | 119.81 | 109.91 | 2 | 10 |
| 4 | A | 407 | 17F | O9-C17-O10 | 2.49 | 129.53 | 123.70 | 1 | 10 |
| 3 | B | 234 | PCW | C7-N-C5 | 2.49 | 119.80 | 109.91 | 4 | 10 |
| 3 | C | 624 | PCW | C7-N-C5 | 2.48 | 119.78 | 109.91 | 5 | 10 |
| 4 | B | 231 | 17F | C5-O9-C17 | 2.48 | 111.86 | 117.80 | 4 | 9 |
| 3 | B | 210 | PCW | C7-N-C5 | 2.48 | 119.75 | 109.91 | 6 | 10 |
| 3 | B | 203 | PCW | C7-N-C5 | 2.48 | 119.75 | 109.91 | 6 | 10 |
| 4 | C | 632 | 17F | O9-C17-O10 | 2.47 | 129.48 | 123.70 | 5 | 10 |
| 3 | B | 211 | PCW | C7-N-C5 | 2.47 | 119.73 | 109.91 | 4 | 10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 3 | C | 623 | PCW | C7-N-C5 | 2.47 | 119.71 | 109.91 | 2 | 10 |
| 4 | B | 226 | 17F | C5-O9-C17 | 2.47 | 111.89 | 117.80 | 2 | 9 |
| 3 | B | 214 | PCW | C7-N-C5 | 2.46 | 119.70 | 109.91 | 9 | 10 |
| 3 | C | 602 | PCW | C7-N-C5 | 2.46 | 119.70 | 109.91 | 5 | 10 |
| 3 | A | 404 | PCW | C7-N-C5 | 2.46 | 119.69 | 109.91 | 9 | 10 |
| 3 | C | 615 | PCW | C7-N-C5 | 2.46 | 119.69 | 109.91 | 5 | 10 |
| 3 | A | 411 | PCW | C7-N-C5 | 2.46 | 119.69 | 109.91 | 10 | 10 |
| 3 | C | 616 | PCW | C7-N-C5 | 2.46 | 119.69 | 109.91 | 5 | 10 |
| 4 | B | 230 | 17F | C5-O9-C17 | 2.46 | 111.92 | 117.80 | 4 | 10 |
| 3 | B | 218 | PCW | C7-N-C5 | 2.45 | 119.66 | 109.91 | 4 | 10 |
| 3 | B | 223 | PCW | C7-N-C5 | 2.45 | 119.66 | 109.91 | 7 | 10 |
| 3 | B | 233 | PCW | C7-N-C5 | 2.45 | 119.66 | 109.91 | 1 | 10 |
| 4 | C | 627 | 17F | O9-C17-O10 | 2.45 | 129.43 | 123.70 | 8 | 10 |
| 3 | C | 607 | PCW | C7-N-C5 | 2.44 | 119.63 | 109.91 | 10 | 10 |
| 4 | B | 229 | 17F | C5-O9-C17 | 2.44 | 111.95 | 117.80 | 8 | 9 |
| 3 | C | 603 | PCW | C7-N-C5 | 2.44 | 119.61 | 109.91 | 6 | 10 |
| 3 | C | 625 | PCW | C7-N-C5 | 2.44 | 119.61 | 109.91 | 10 | 10 |
| 3 | C | 614 | PCW | C7-N-C5 | 2.44 | 119.59 | 109.91 | 6 | 10 |
| 3 | C | 617 | PCW | C7-N-C5 | 2.43 | 119.58 | 109.91 | 9 | 10 |
| 4 | B | 228 | 17F | C5-O9-C17 | 2.43 | 111.97 | 117.80 | 7 | 10 |
| 3 | A | 402 | PCW | C7-N-C5 | 2.43 | 119.56 | 109.91 | 4 | 10 |
| 3 | B | 213 | PCW | C7-N-C5 | 2.43 | 119.55 | 109.91 | 5 | 10 |
| 3 | C | 618 | PCW | C7-N-C5 | 2.43 | 119.55 | 109.91 | 4 | 10 |
| 4 | B | 227 | 17F | C5-O9-C17 | 2.43 | 111.99 | 117.80 | 3 | 8 |
| 4 | B | 226 | 17F | O9-C17-O10 | 2.42 | 129.37 | 123.70 | 6 | 10 |
| 3 | C | 604 | PCW | C7-N-C5 | 2.42 | 119.54 | 109.91 | 7 | 10 |
| 5 | B | 237 | GNP | O1G-PG-N3B | 2.42 | 108.20 | 111.77 | 8 | 9 |
| 4 | B | 228 | 17F | O9-C17-O10 | 2.42 | 129.36 | 123.70 | 4 | 10 |
| 3 | B | 202 | PCW | C7-N-C5 | 2.42 | 119.52 | 109.91 | 9 | 10 |
| 3 | A | 409 | PCW | C7-N-C5 | 2.41 | 119.49 | 109.91 | 8 | 10 |
| 4 | B | 231 | 17F | O9-C17-O10 | 2.41 | 129.33 | 123.70 | 8 | 10 |
| 3 | B | 216 | PCW | C7-N-C5 | 2.41 | 119.47 | 109.91 | 4 | 10 |
| 3 | B | 204 | PCW | C7-N-C5 | 2.40 | 119.45 | 109.91 | 2 | 10 |
| 3 | C | 609 | PCW | C7-N-C5 | 2.40 | 119.44 | 109.91 | 5 | 10 |
| 3 | C | 611 | PCW | C7-N-C5 | 2.40 | 119.43 | 109.91 | 10 | 10 |
| 3 | A | 410 | PCW | C7-N-C5 | 2.39 | 119.42 | 109.91 | 4 | 10 |
| 3 | B | 219 | PCW | C7-N-C5 | 2.39 | 119.41 | 109.91 | 8 | 10 |
| 4 | B | 227 | 17F | O9-C17-O10 | 2.39 | 129.29 | 123.70 | 10 | 10 |
| 4 | B | 236 | 17F | O9-C17-O10 | 2.39 | 129.29 | 123.70 | 3 | 10 |
| 4 | C | 629 | 17F | O9-C17-O10 | 2.39 | 129.28 | 123.70 | 9 | 10 |
| 4 | C | 630 | 17F | O9-C17-O10 | 2.38 | 129.28 | 123.70 | 6 | 10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 4 | B | 229 | 17F | O9-C17-O10 | 2.38 | 129.27 | 123.70 | 10 | 10 |
| 4 | C | 627 | 17F | C5-O9-C17 | 2.36 | 112.15 | 117.80 | 1 | 9 |
| 4 | C | 629 | 17F | C5-O9-C17 | 2.35 | 112.17 | 117.80 | 3 | 10 |
| 4 | B | 232 | 17F | O9-C17-O10 | 2.35 | 129.19 | 123.70 | 10 | 10 |
| 4 | C | 631 | 17F | O9-C17-O10 | 2.32 | 129.13 | 123.70 | 7 | 10 |
| 4 | C | 632 | 17F | C5-O9-C17 | 2.32 | 112.25 | 117.80 | 8 | 10 |
| 4 | B | 230 | 17F | O9-C17-O10 | 2.30 | 129.08 | 123.70 | 5 | 10 |
| 4 | C | 628 | 17F | O7-C7-C8 | 2.30 | 104.83 | 111.83 | 7 | 9 |
| 7 | B | 239 | EWS | CAX-CBA-CAZ | 2.27 | 122.42 | 128.56 | 8 | 10 |
| 5 | B | 237 | GNP | C2-N3-C4 | 2.27 | 113.04 | 115.48 | 3 | 8 |
| 4 | A | 407 | 17F | C5-O9-C17 | 2.26 | 112.38 | 117.80 | 7 | 4 |
| 4 | B | 236 | 17F | C5-O9-C17 | 2.25 | 112.41 | 117.80 | 9 | 10 |
| 4 | C | 628 | 17F | O9-C17-O10 | 2.24 | 128.94 | 123.70 | 1 | 10 |
| 4 | B | 228 | 17F | C6-C5-C4 | 2.15 | 106.77 | 111.78 | 10 | 1 |
| 4 | B | 228 | 17F | O7-C6-C5 | 2.14 | 114.56 | 108.40 | 6 | 2 |
| 3 | C | 616 | PCW | C7-N-C6 | 2.12 | 114.55 | 108.98 | 2 | 1 |
| 3 | C | 618 | PCW | C7-N-C6 | 2.09 | 114.47 | 108.98 | 4 | 1 |
| 3 | A | 404 | PCW | C7-N-C6 | 2.07 | 114.40 | 108.98 | 3 | 1 |
| 3 | B | 204 | PCW | C7-N-C6 | 2.06 | 114.39 | 108.98 | 10 | 1 |
| 3 | A | 405 | PCW | C7-N-C6 | 2.05 | 114.37 | 108.98 | 8 | 2 |
| 3 | B | 204 | PCW | O1P-P-O3P | 2.05 | 116.87 | 107.57 | 6 | 3 |
| 3 | A | 409 | PCW | C7-N-C6 | 2.05 | 114.36 | 108.98 | 6 | 1 |
| 3 | B | 222 | PCW | C7-N-C6 | 2.05 | 114.36 | 108.98 | 10 | 2 |
| 3 | A | 402 | PCW | C7-N-C6 | 2.04 | 114.32 | 108.98 | 10 | 1 |
| 3 | C | 617 | PCW | C7-N-C6 | 2.03 | 114.32 | 108.98 | 5 | 2 |
| 4 | A | 407 | 17F | O7-C6-C5 | 2.03 | 114.25 | 108.40 | 3 | 1 |
| 3 | A | 401 | PCW | C7-N-C6 | 2.03 | 114.30 | 108.98 | 8 | 1 |
| 3 | B | 219 | PCW | C7-N-C6 | 2.02 | 114.29 | 108.98 | 5 | 1 |
| 3 | C | 604 | PCW | C7-N-C6 | 2.02 | 114.27 | 108.98 | 1 | 1 |
| 3 | C | 612 | PCW | C7-N-C6 | 2.02 | 114.27 | 108.98 | 10 | 1 |
| 3 | B | 207 | PCW | C7-N-C6 | 2.01 | 114.27 | 108.98 | 1 | 1 |
| 3 | B | 217 | PCW | C7-N-C6 | 2.01 | 114.26 | 108.98 | 7 | 1 |
| 3 | B | 225 | PCW | C7-N-C6 | 2.00 | 114.23 | 108.98 | 5 | 1 |
| 3 | C | 609 | PCW | C7-N-C6 | 2.00 | 114.23 | 108.98 | 10 | 1 |

There are no chirality outliers.

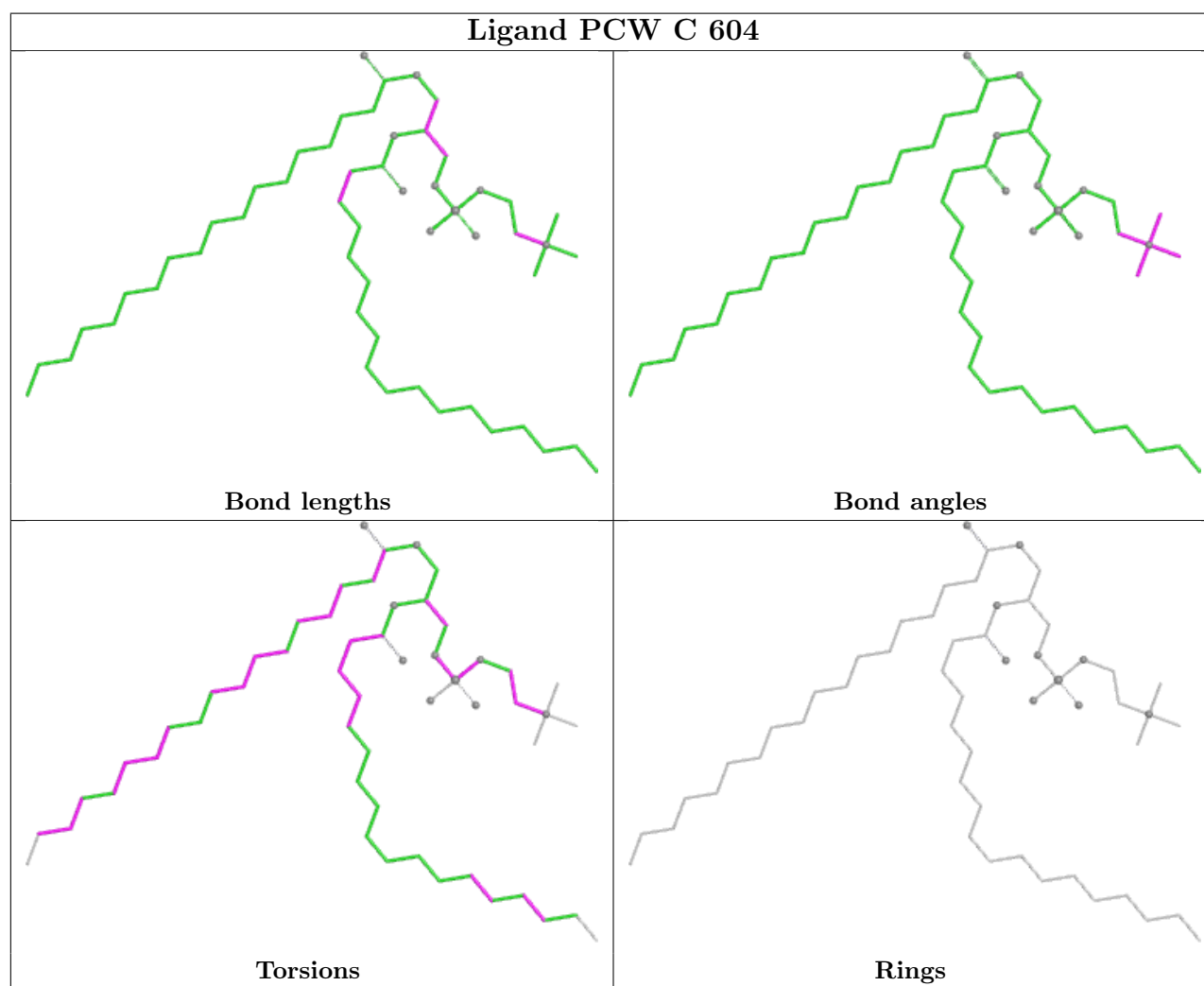
All unique torsion outliers are listed below.

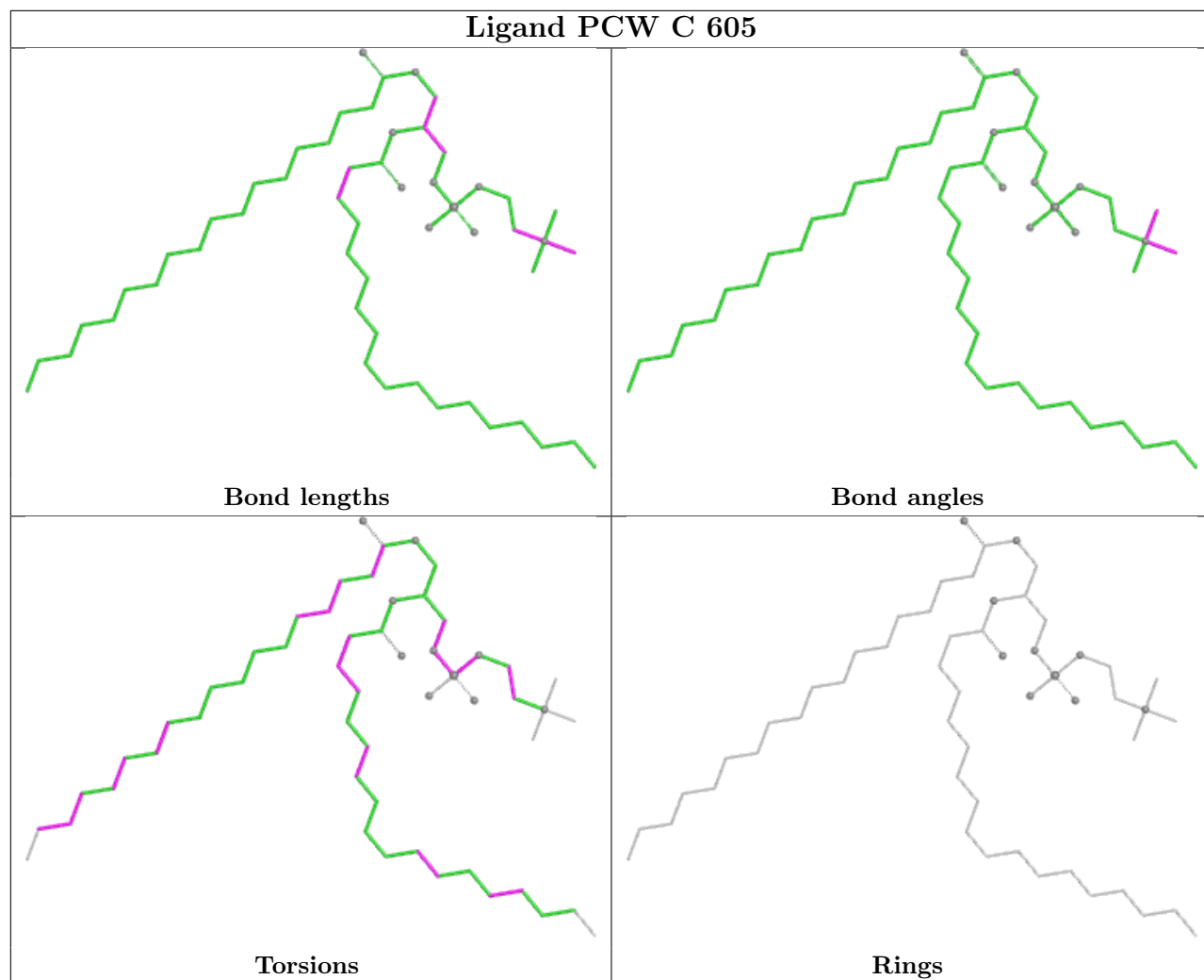
| Mol | Chain | Res | Type | Atoms | Models (Total) |
|-----|-------|-----|------|---------------|----------------|
| 5 | B | 237 | GNP | PG-N3B-PB-O1B | 1 |

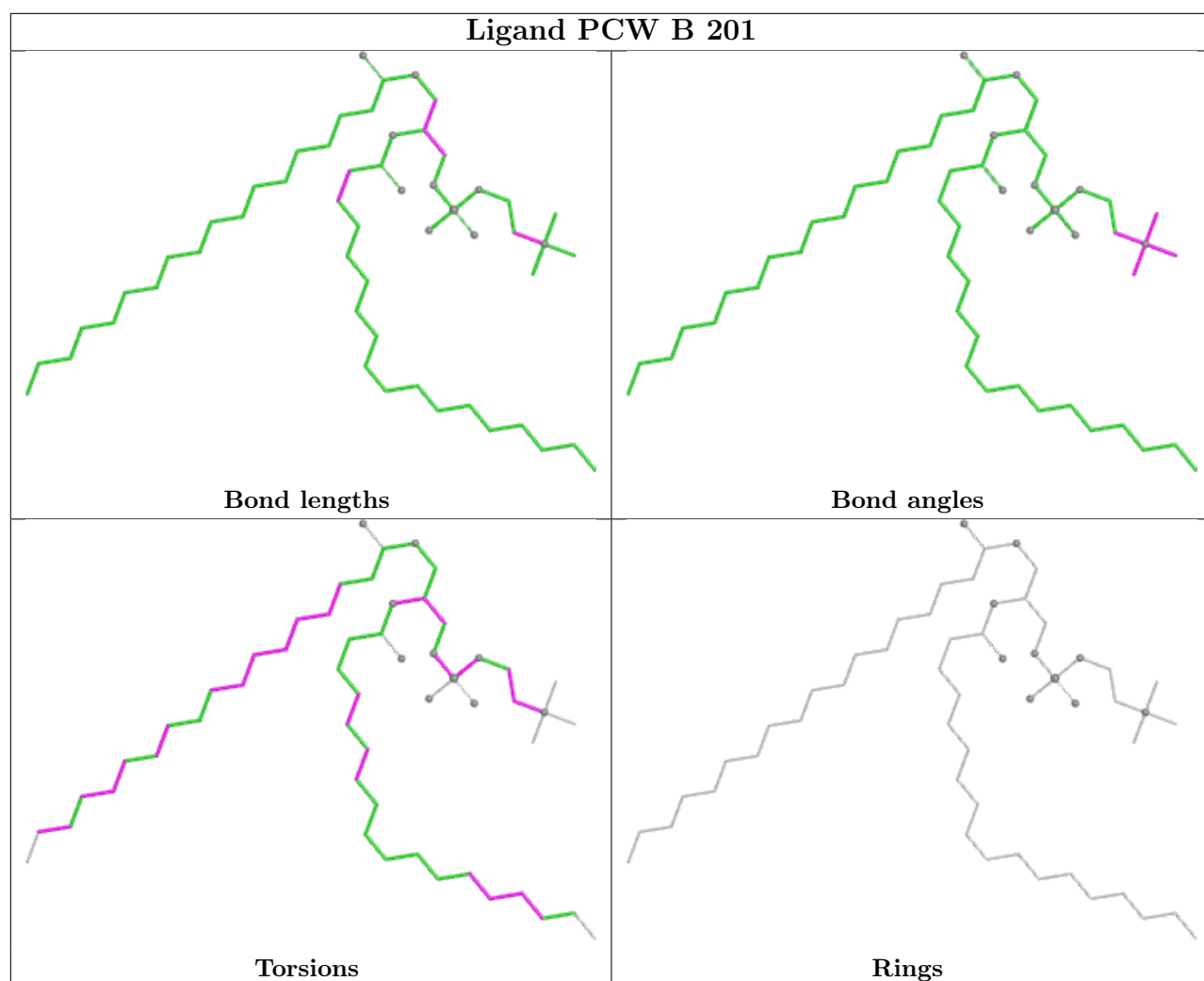
All unique ring outliers are listed below.

| Mol | Chain | Res | Type | Atoms | Models (Total) |
|-----|-------|-----|------|-------------------------|----------------|
| 7 | B | 239 | EWS | CAC-CAD-CAE-CAF-CAH-NAG | 10 |

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.



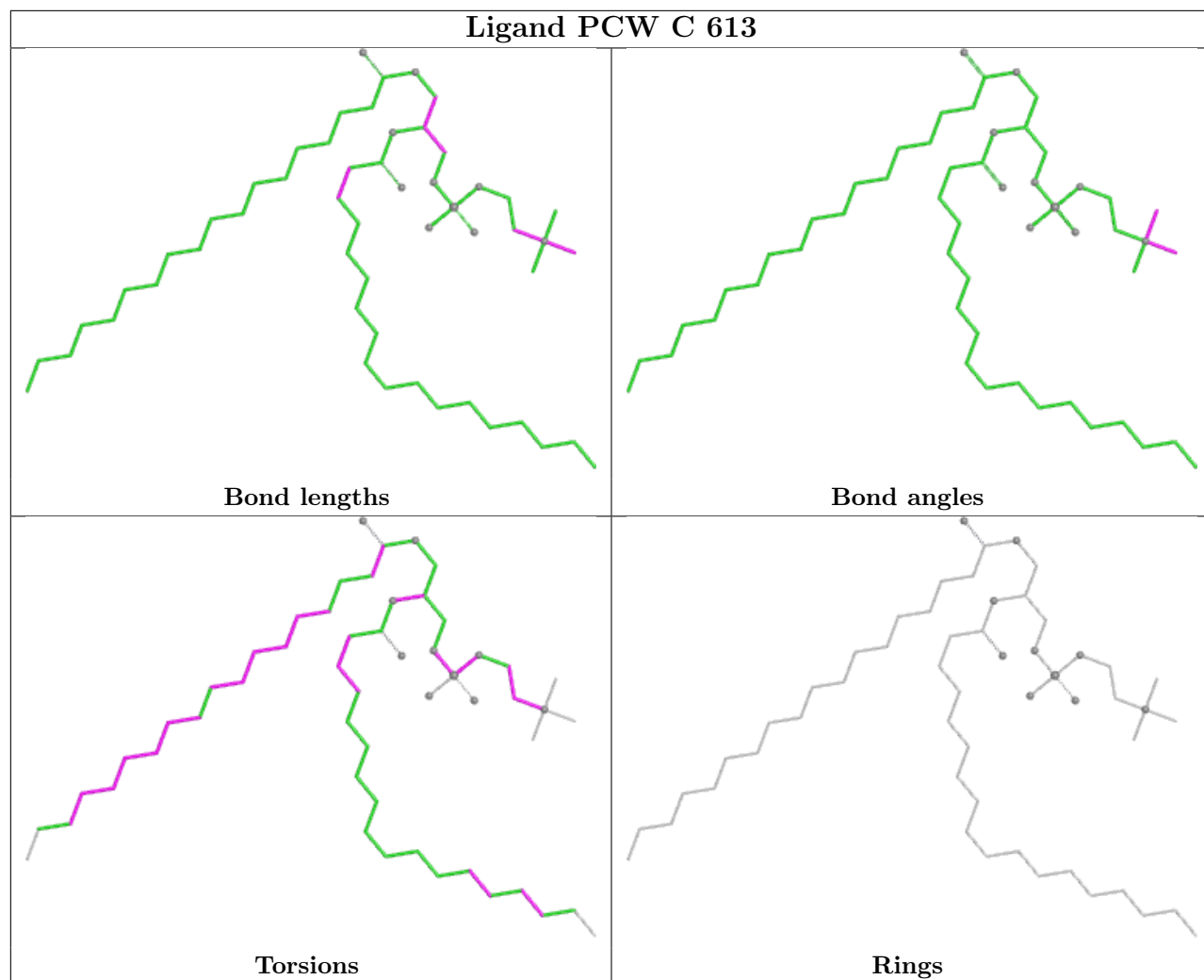


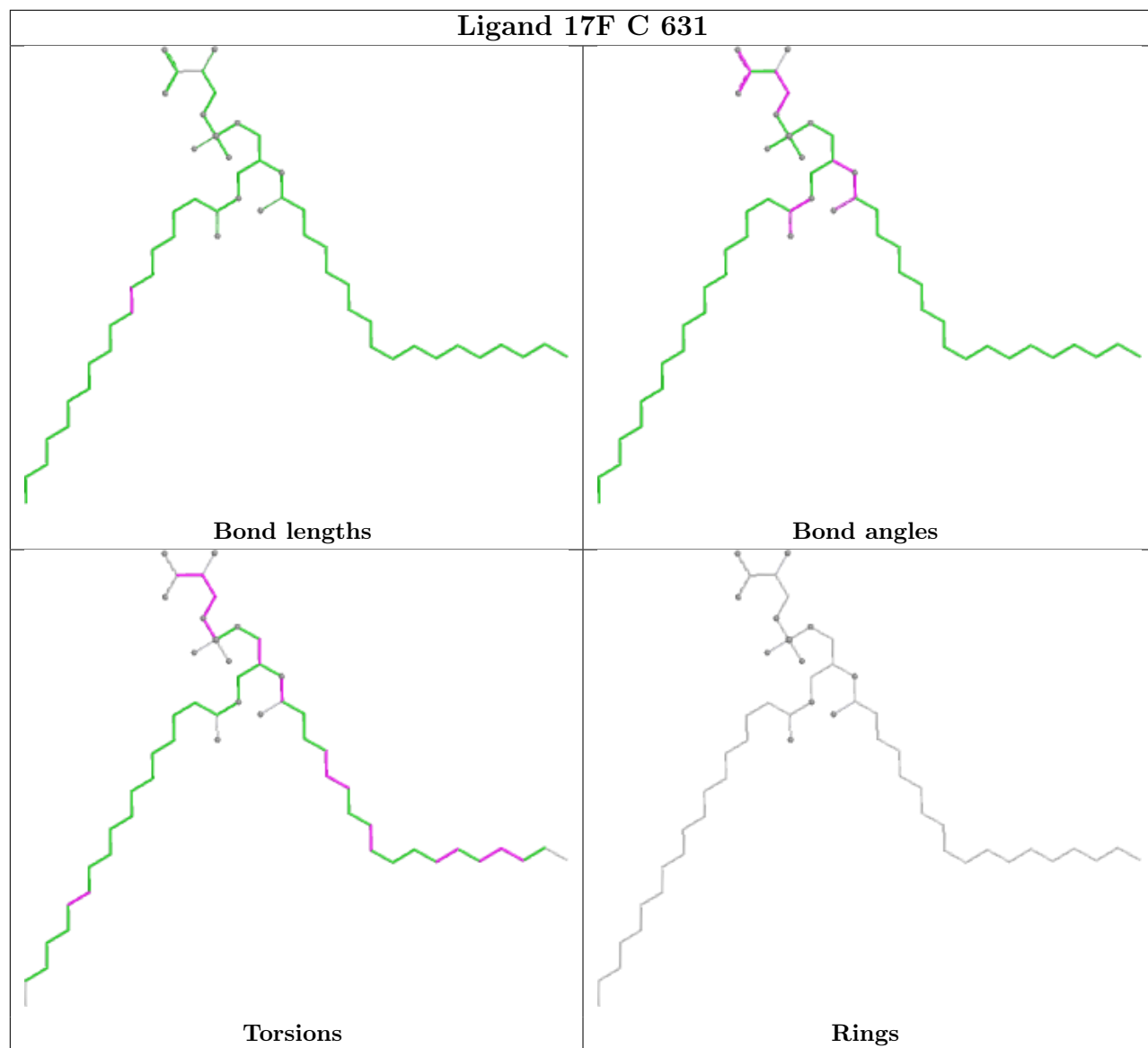


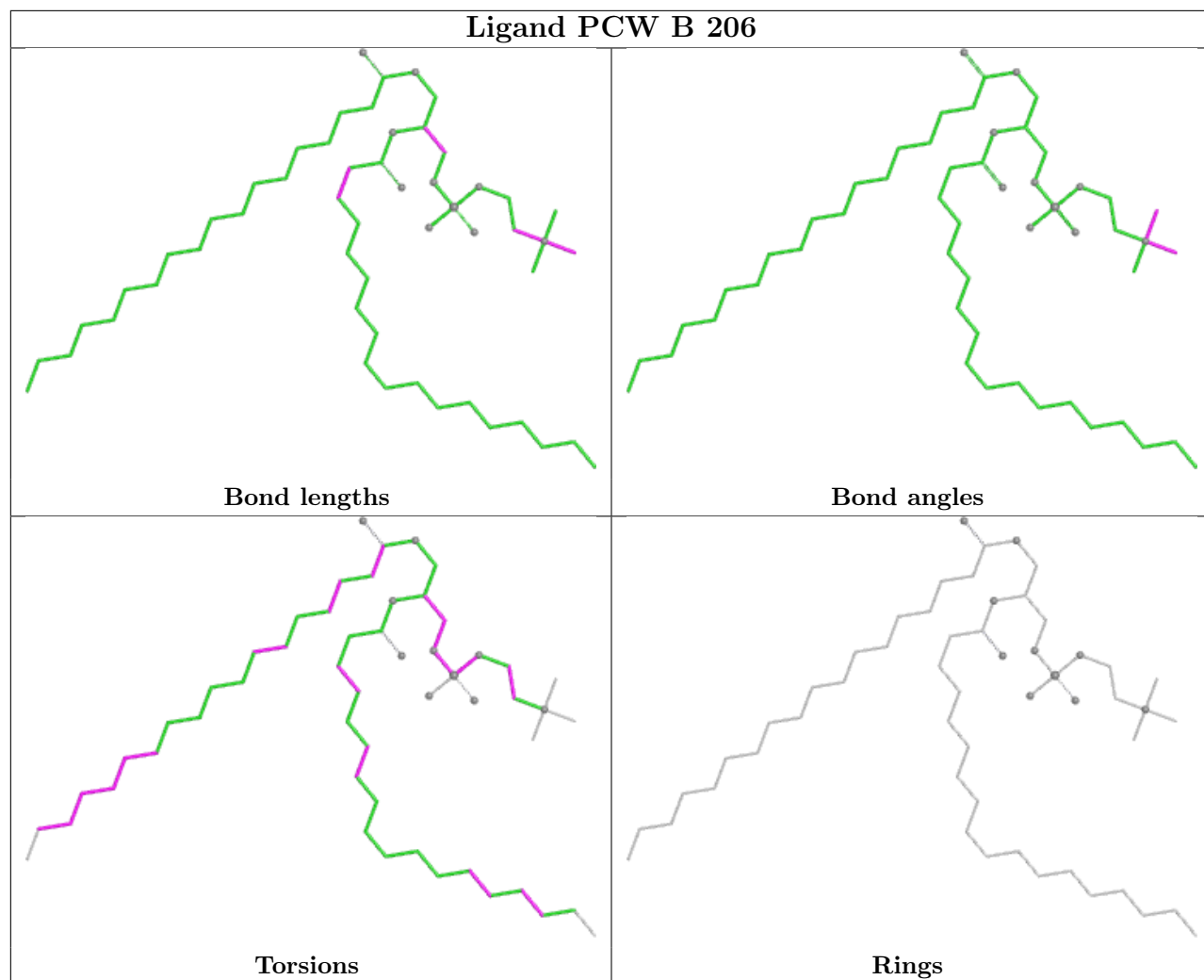
Ligand 17F C 630

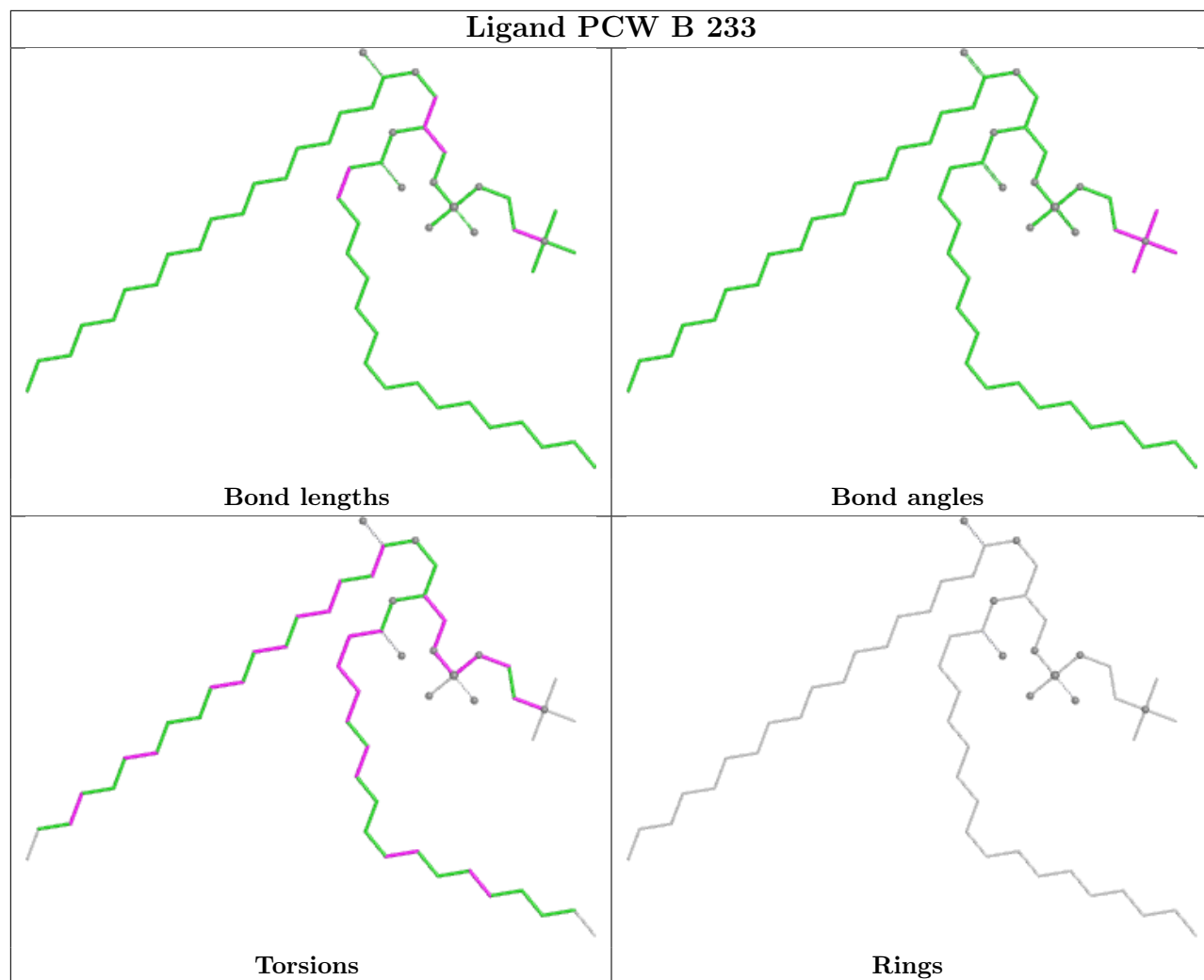
The figure displays four panels of structural data for Ligand 17F C 630, which is a complex organic molecule with a long, branched alkyl chain and a functional group at the end. The panels are arranged in a 2x2 grid:

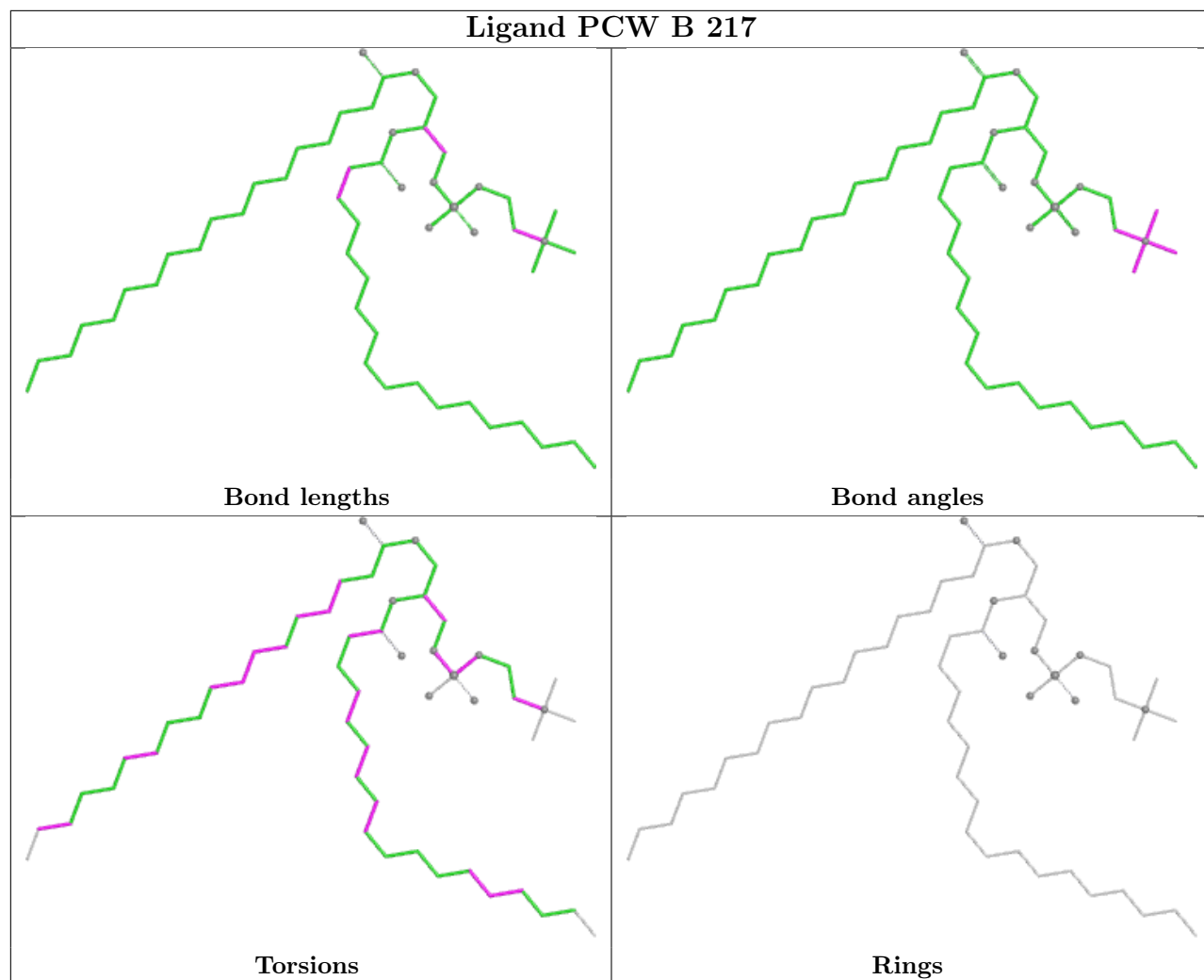
- Bond lengths:** Shows the molecule with green lines representing the bonds. The functional group at the top is highlighted in magenta.
- Bond angles:** Shows the molecule with green lines representing the bonds. The functional group at the top is highlighted in magenta.
- Torsions:** Shows the molecule with green lines representing the bonds. The functional group at the top is highlighted in magenta.
- Rings:** Shows the molecule with gray lines representing the bonds. The functional group at the top is highlighted in magenta.

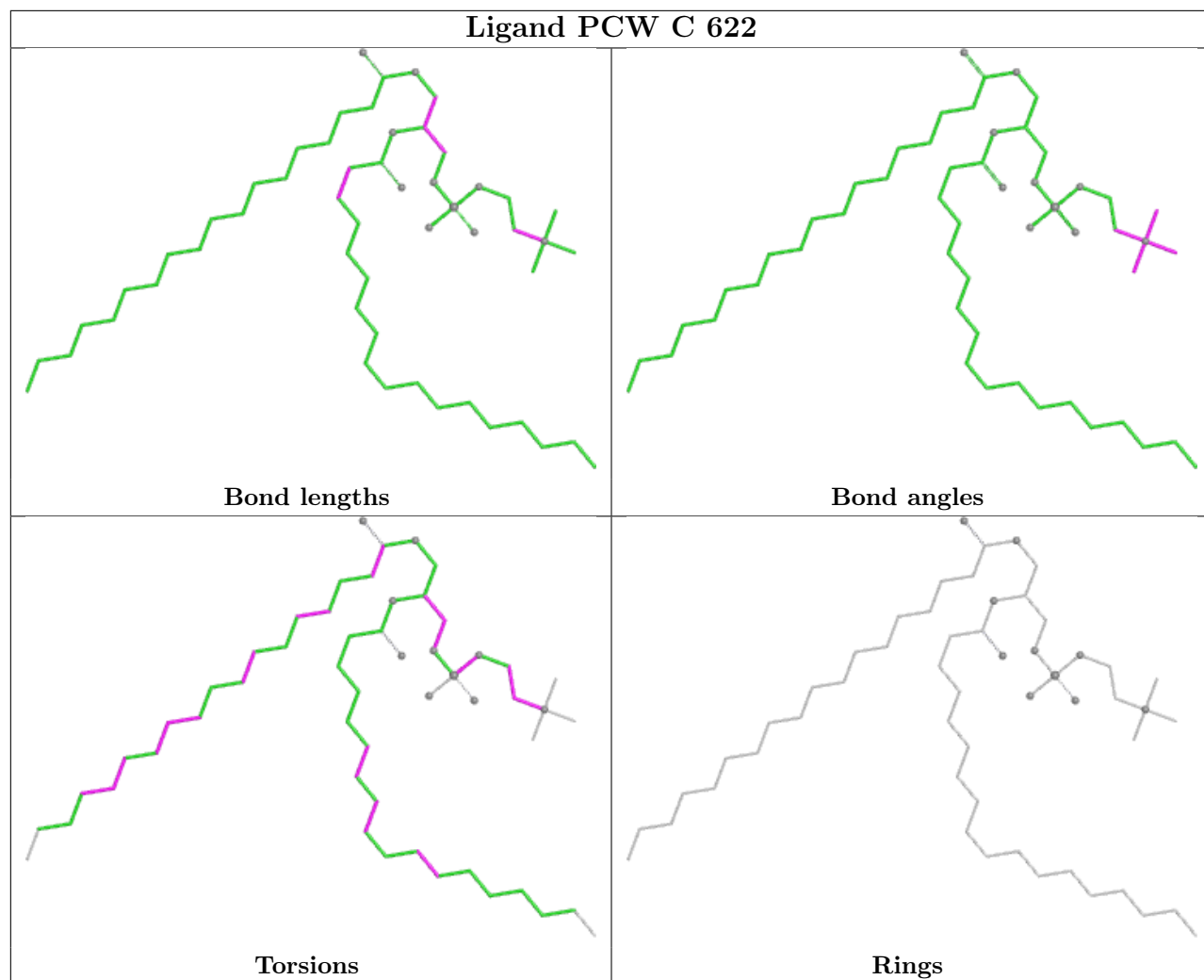


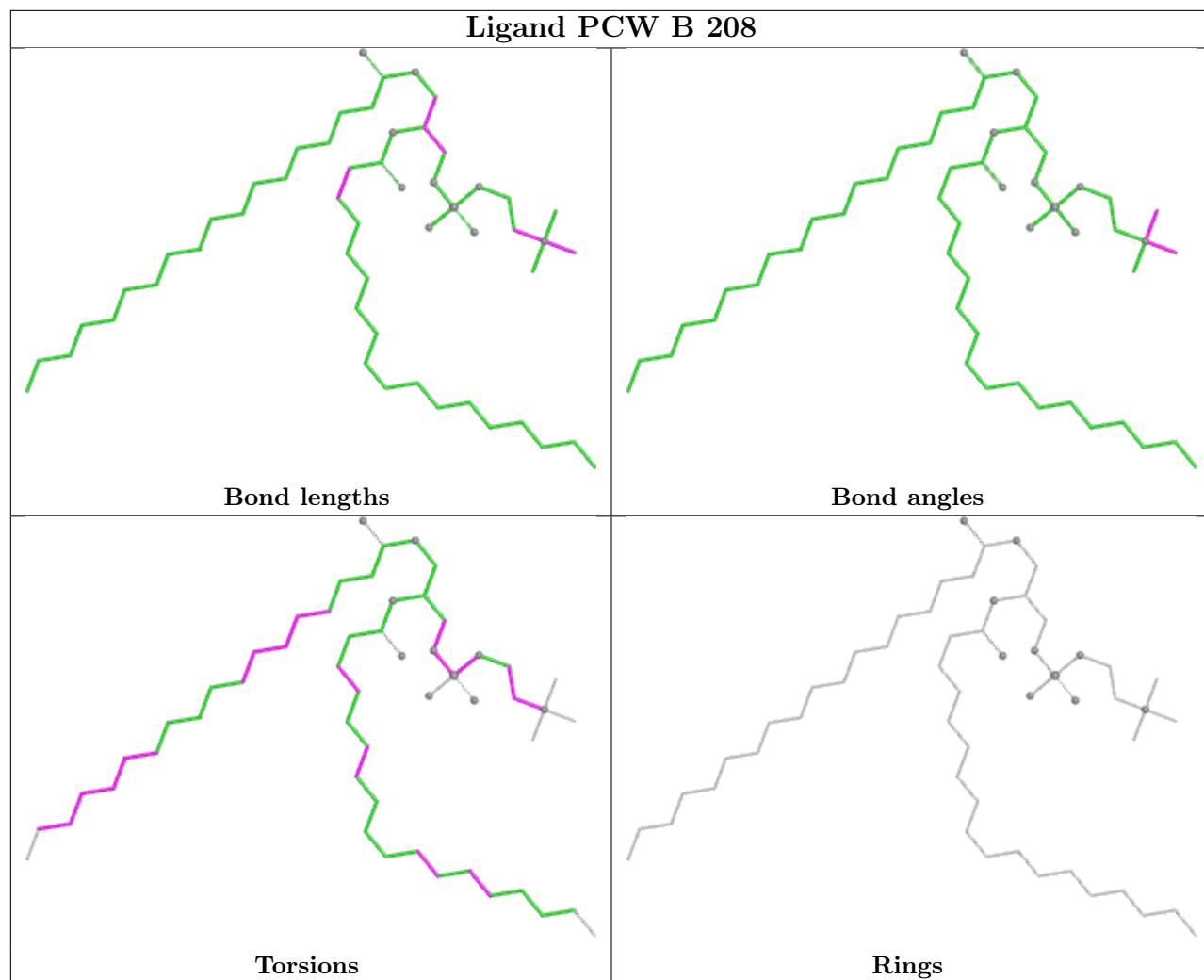


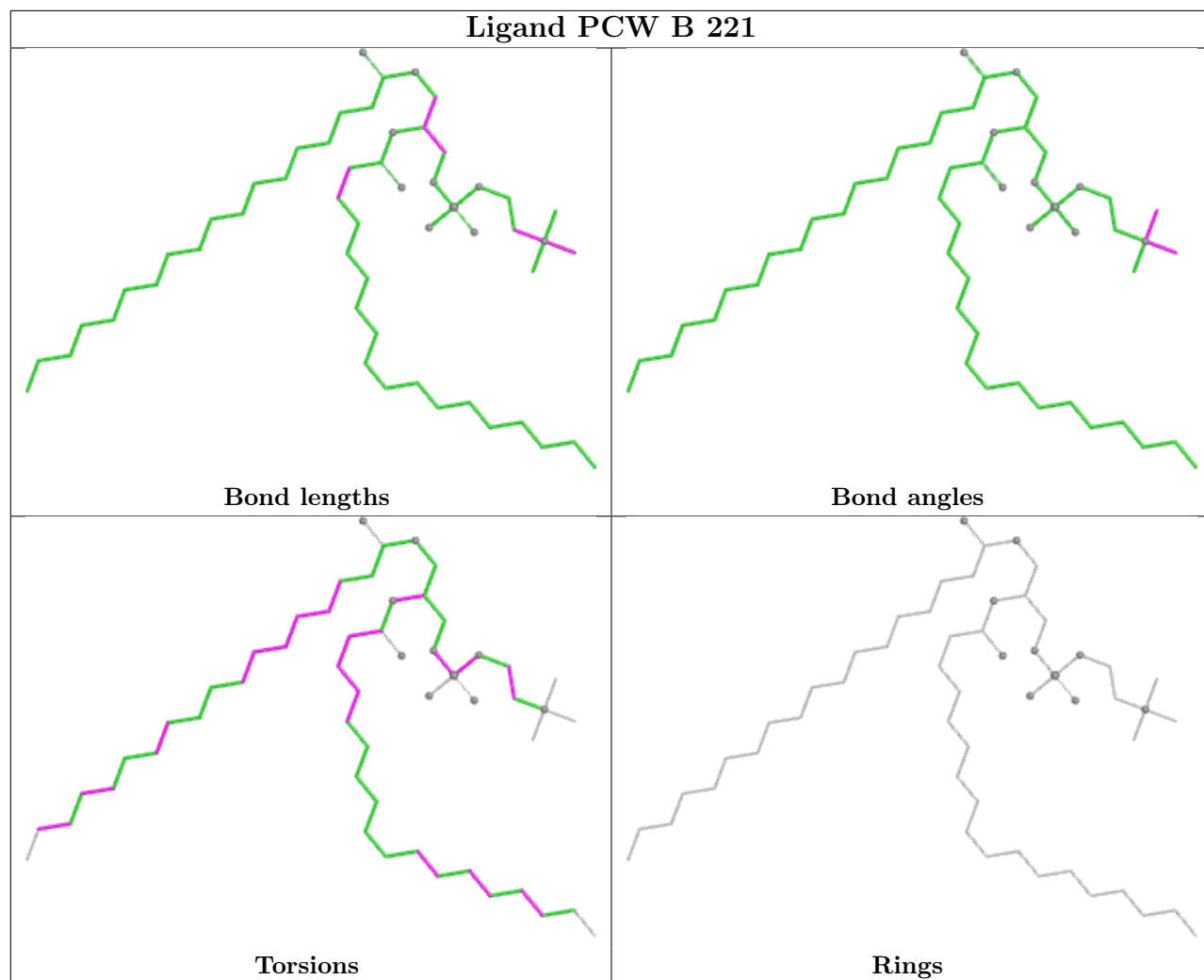


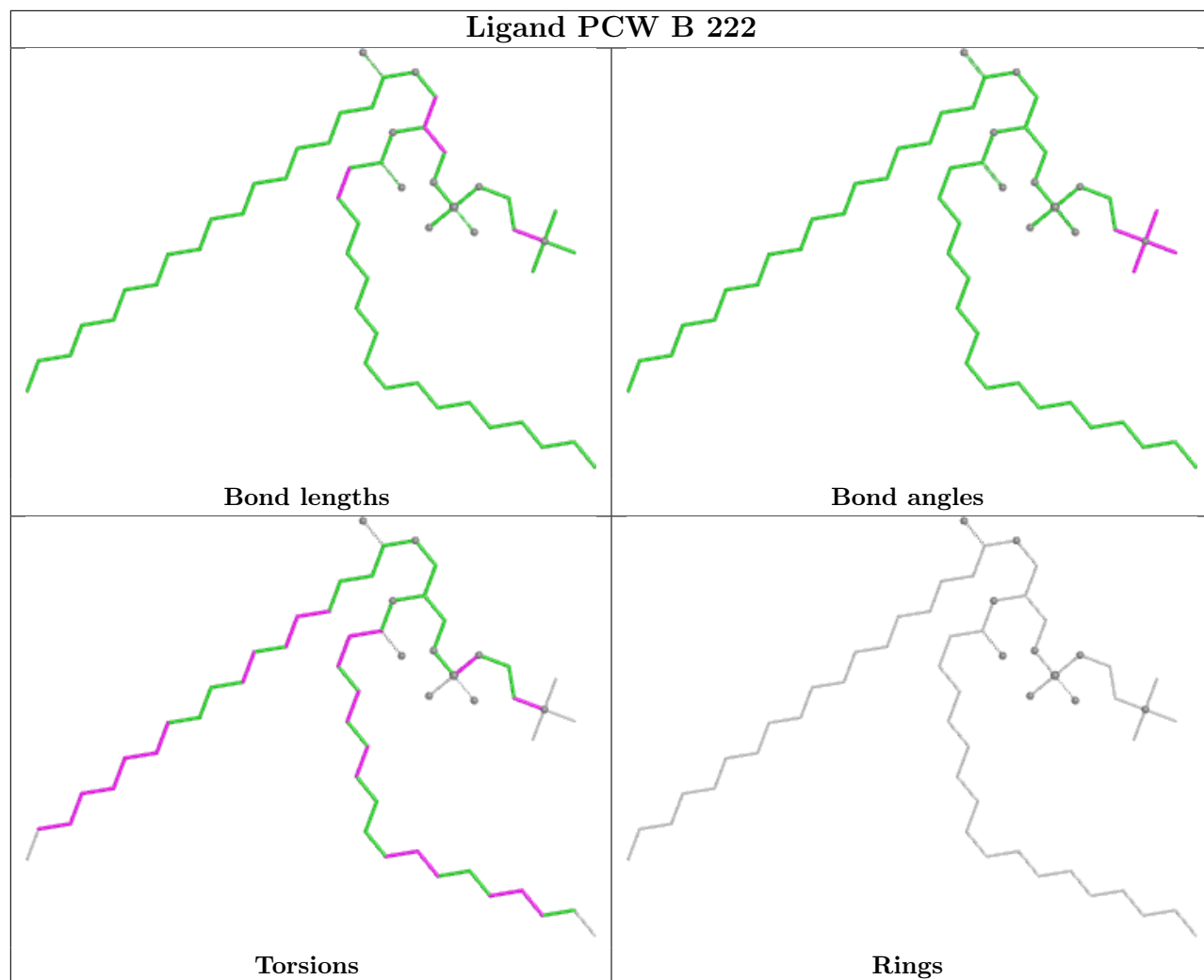


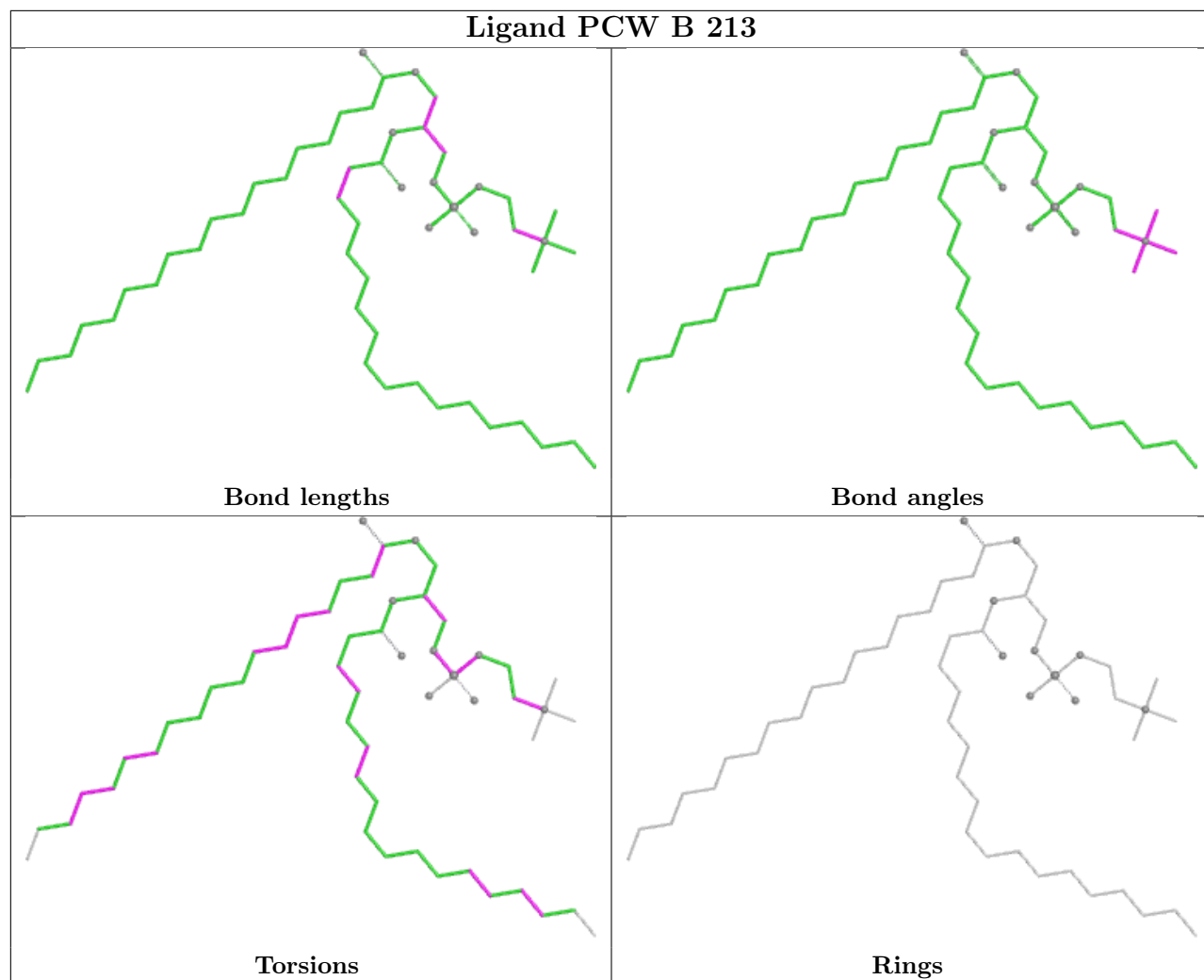


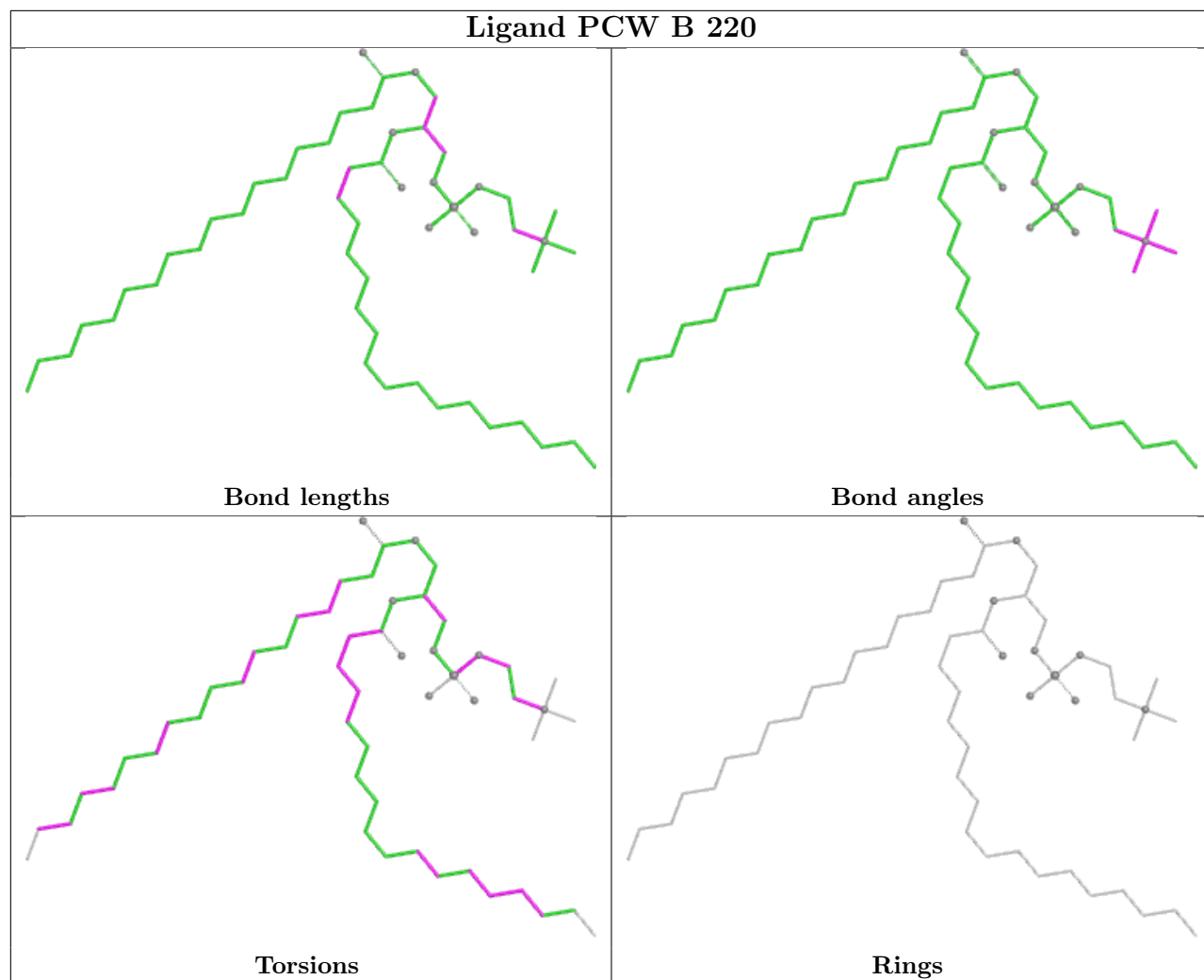


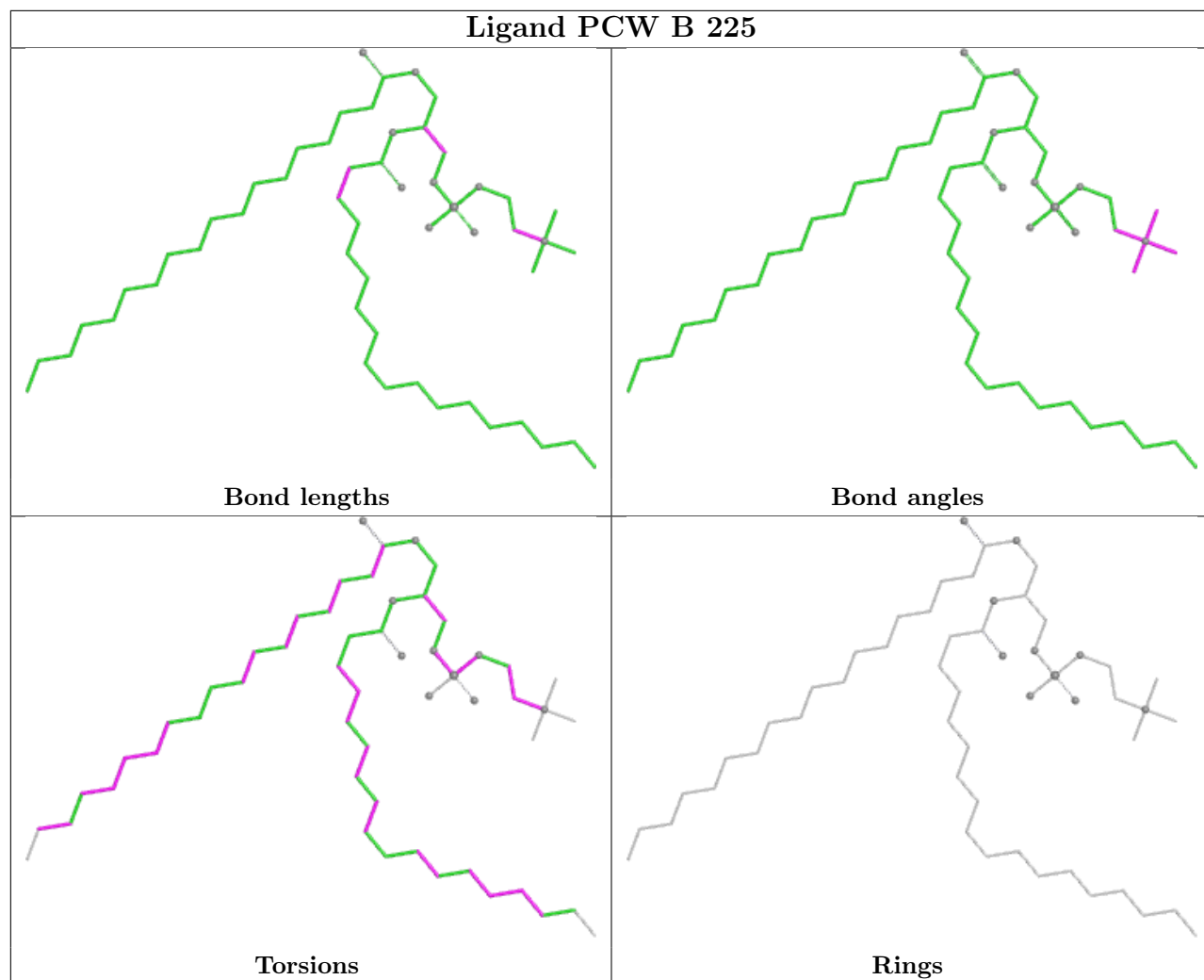


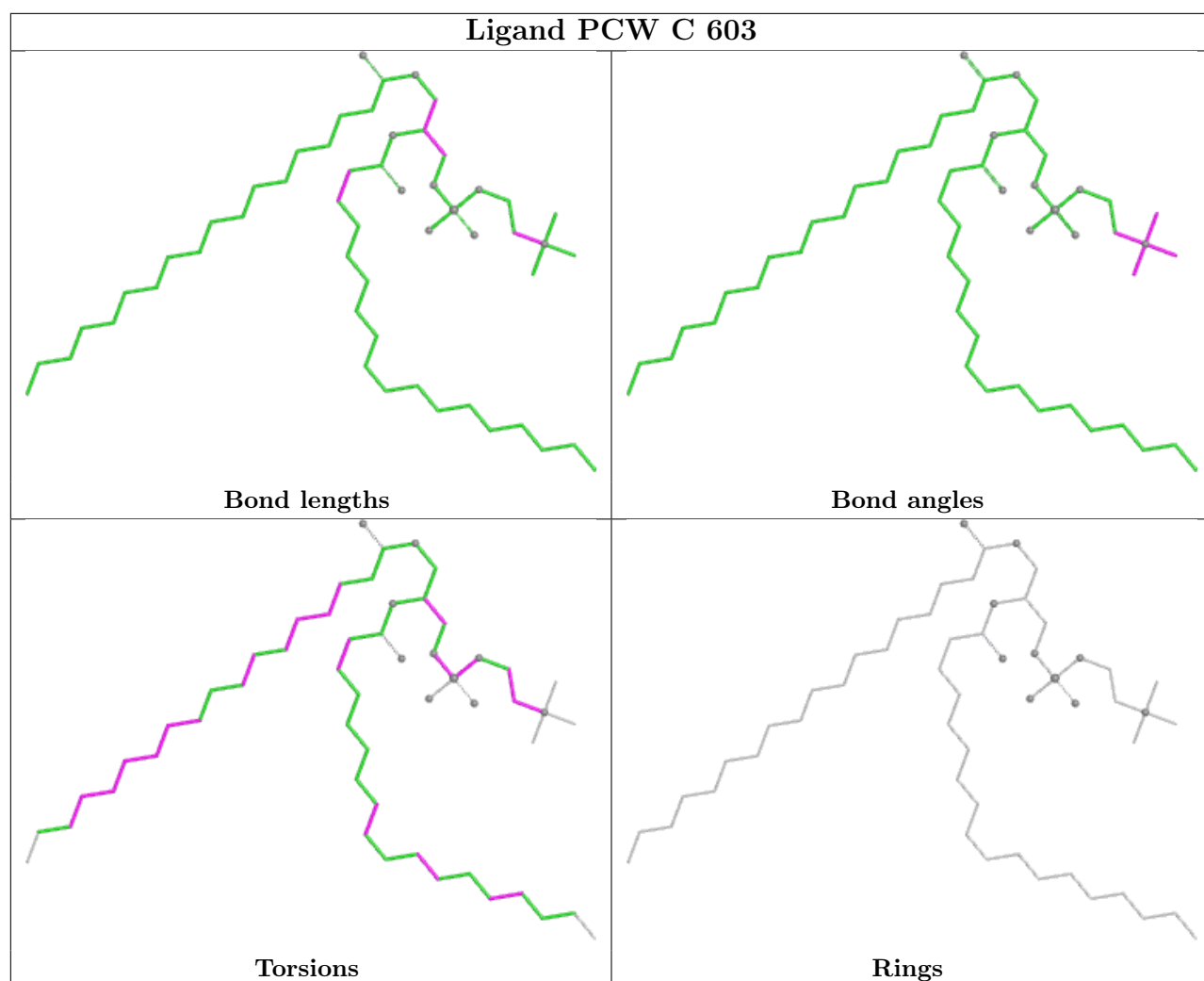


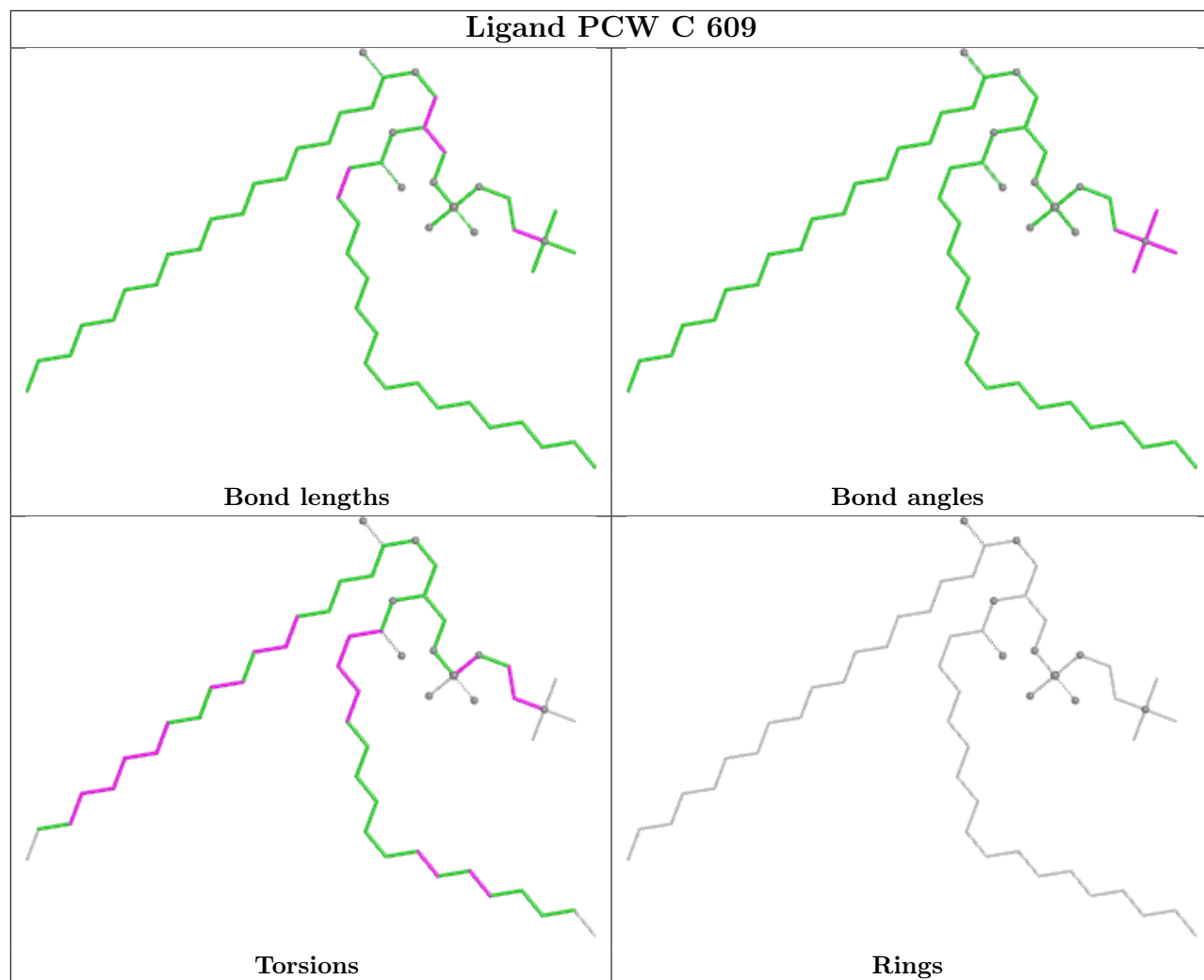


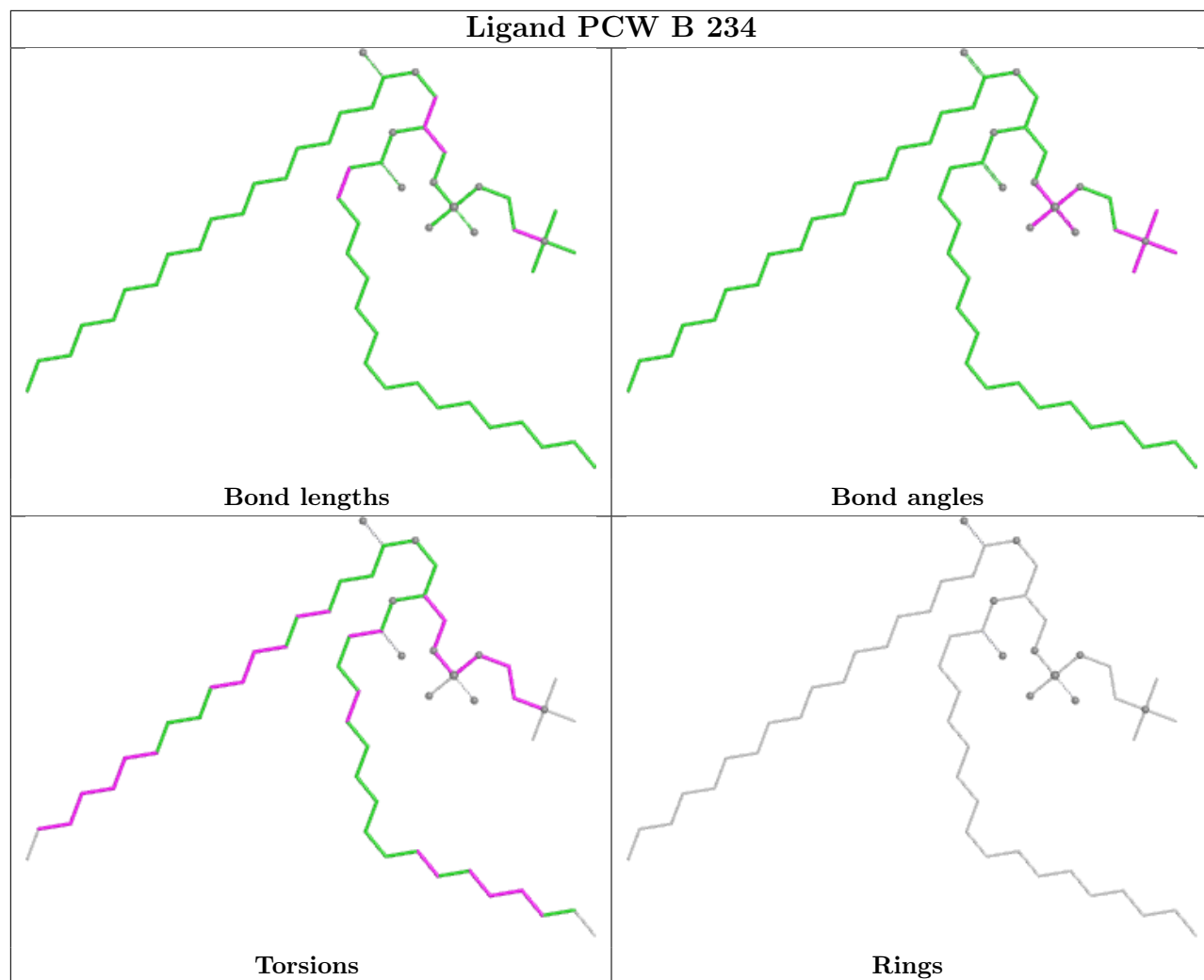


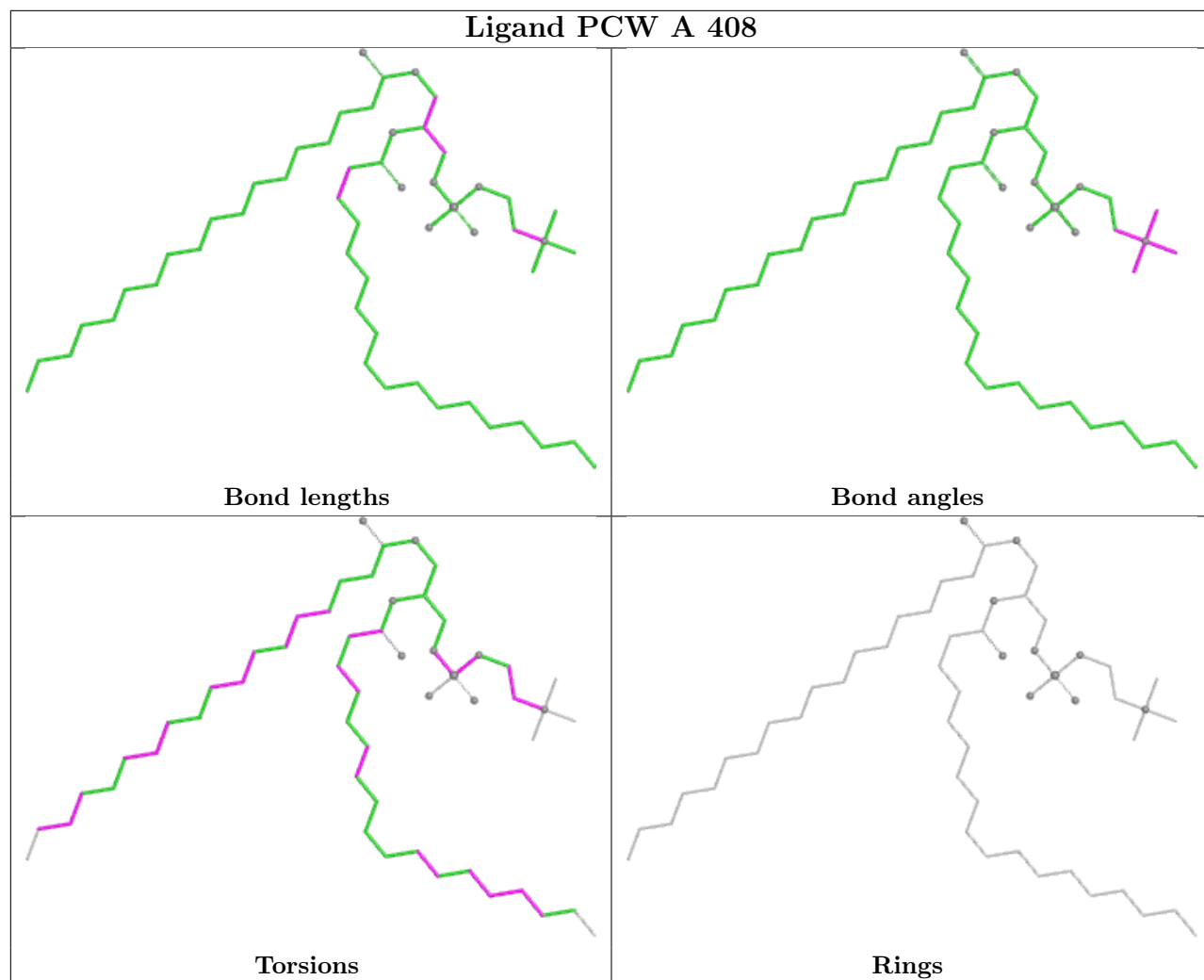


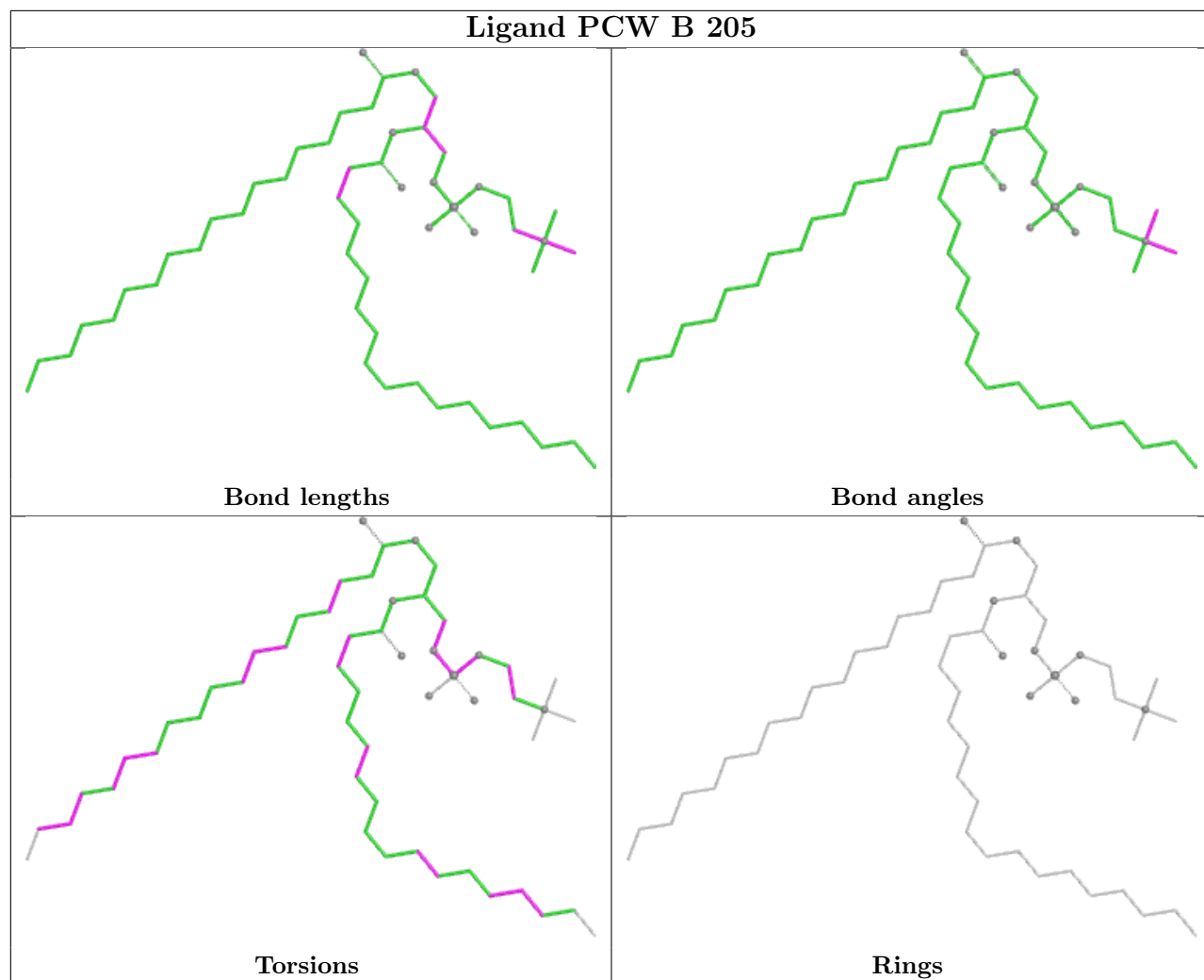


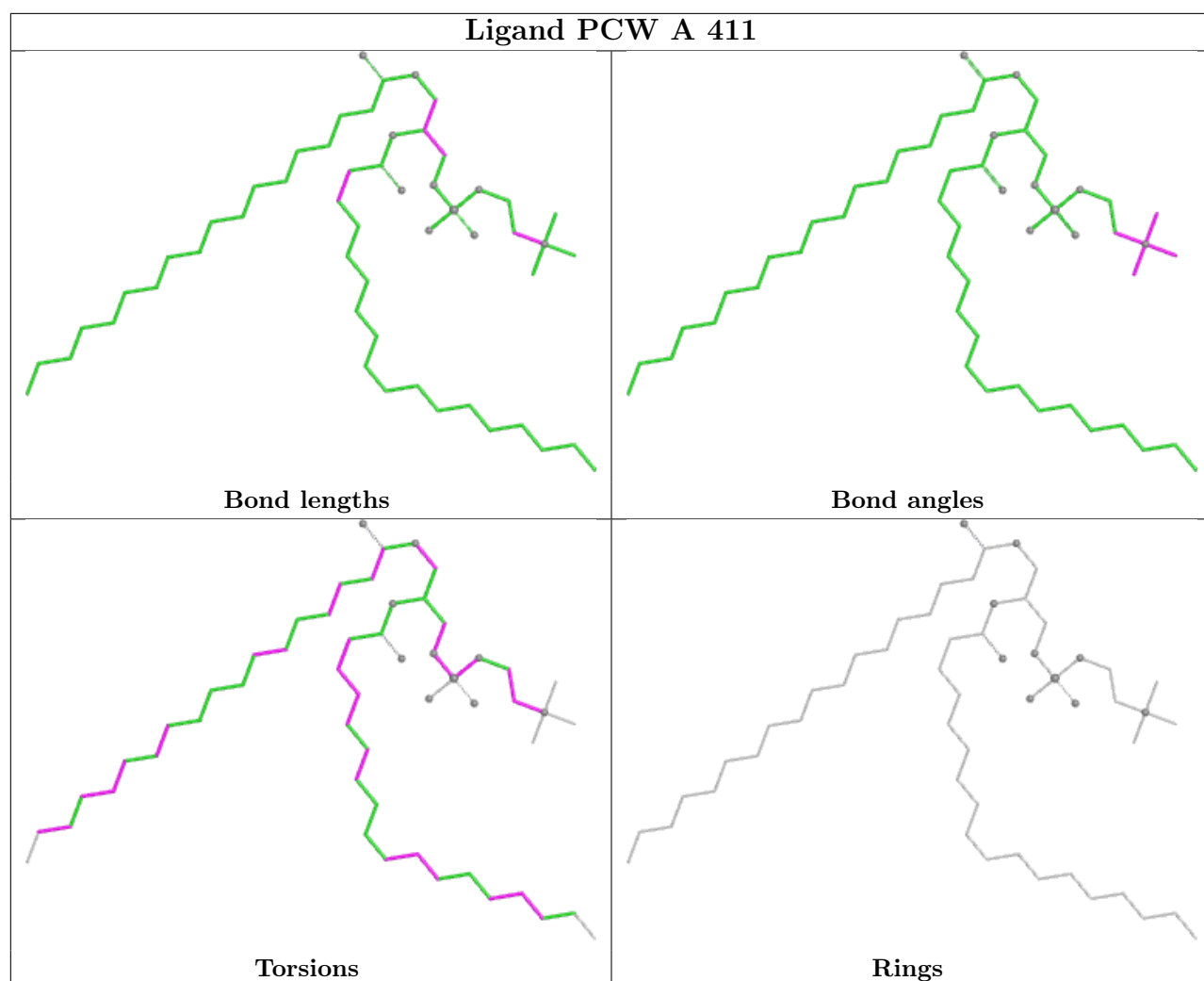


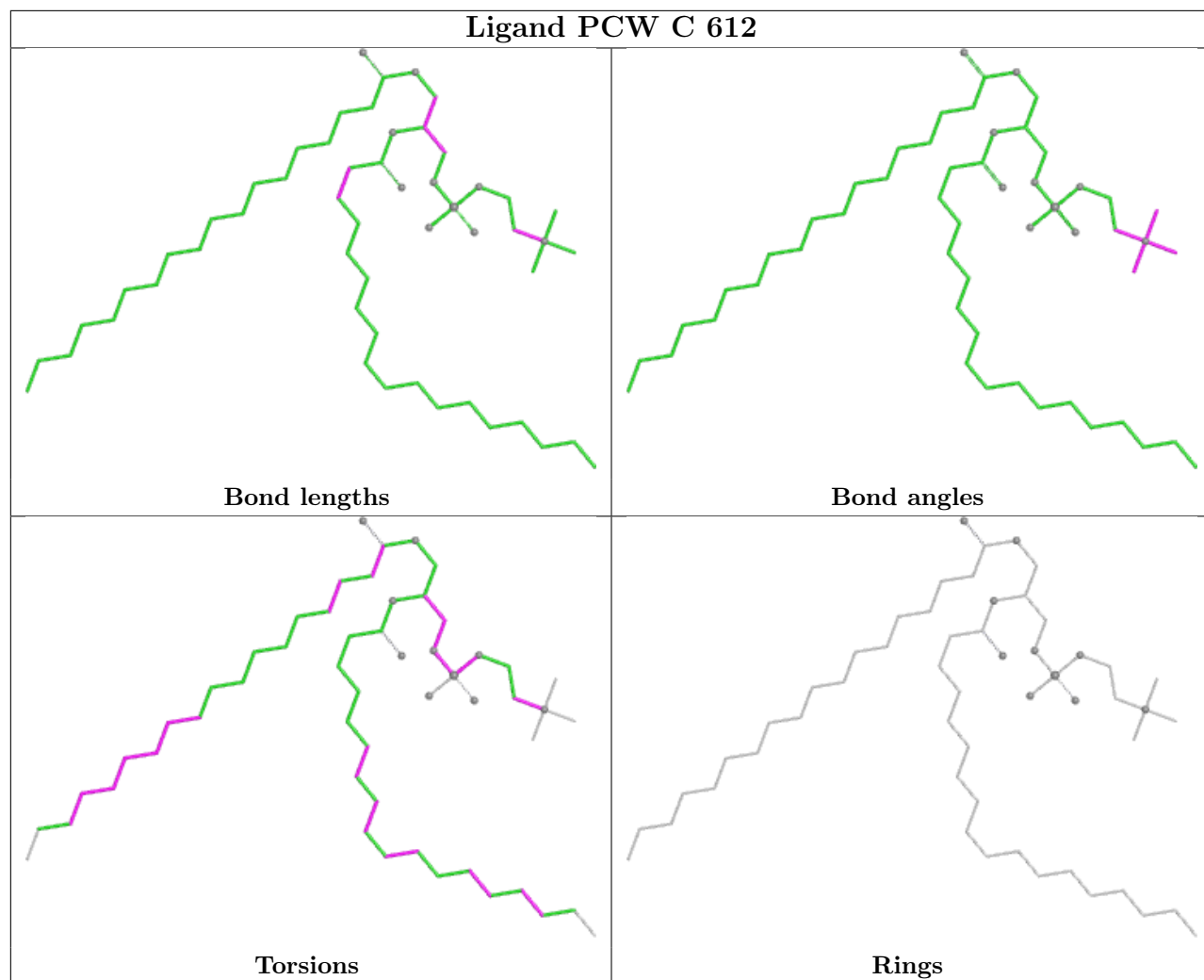


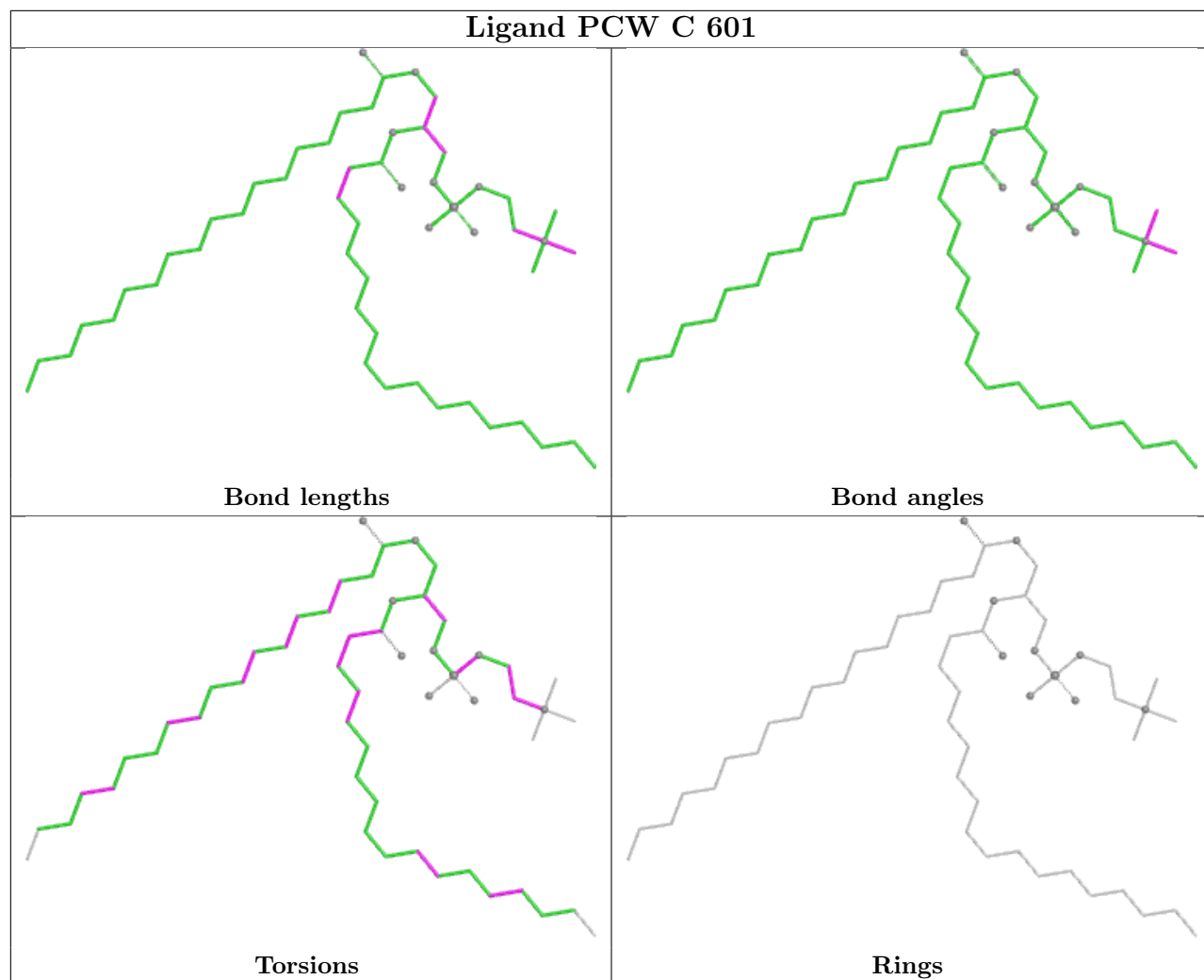


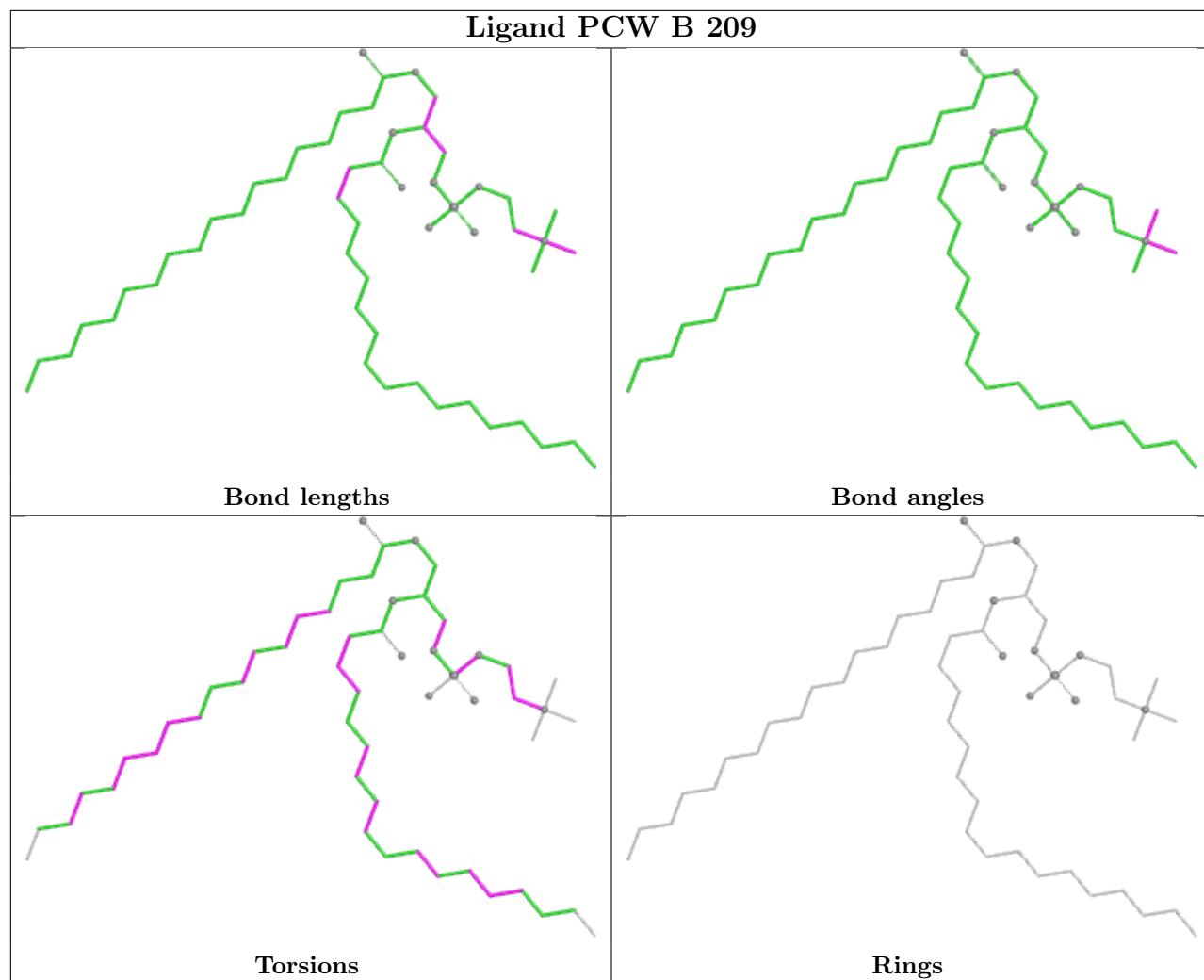


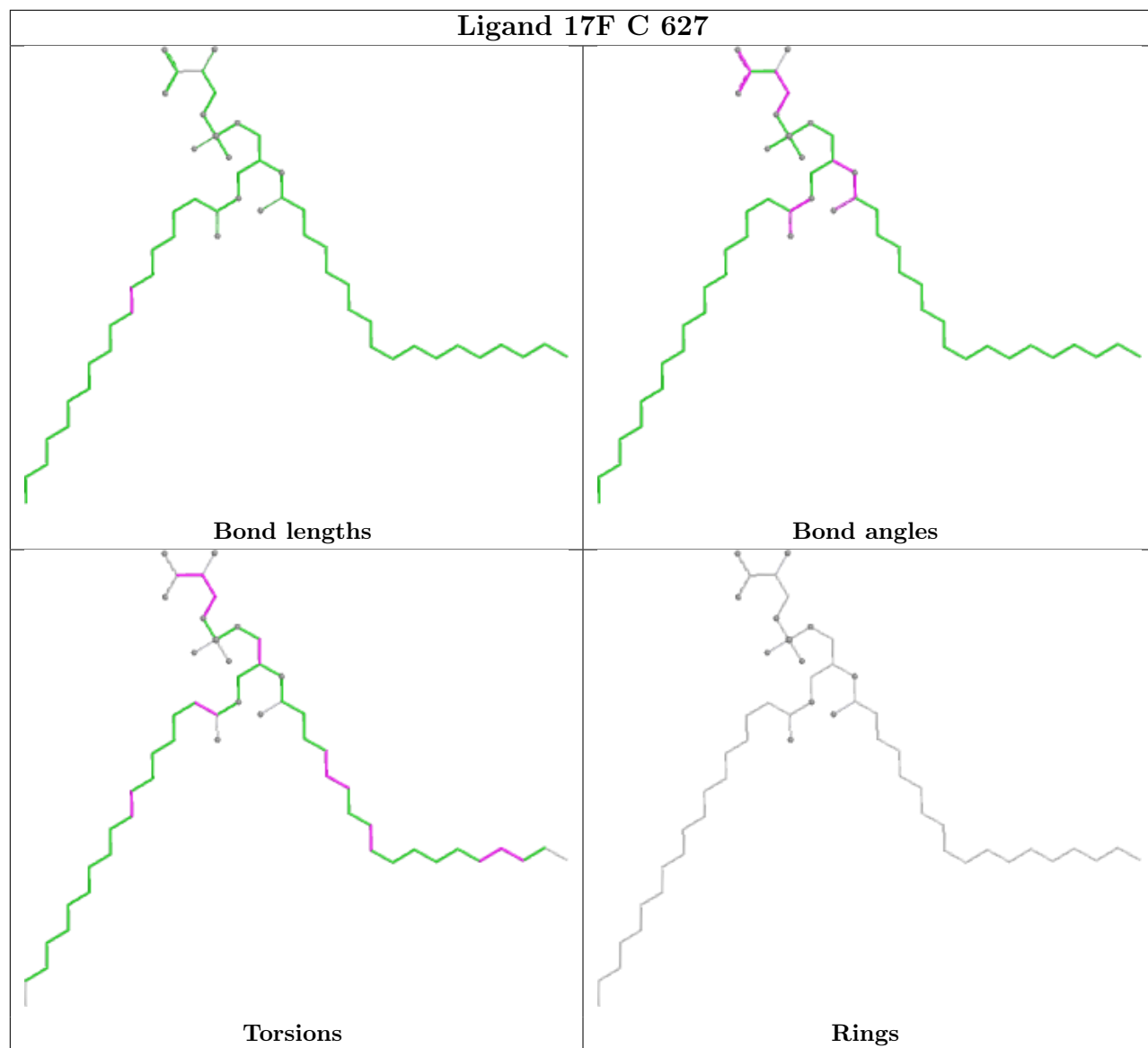


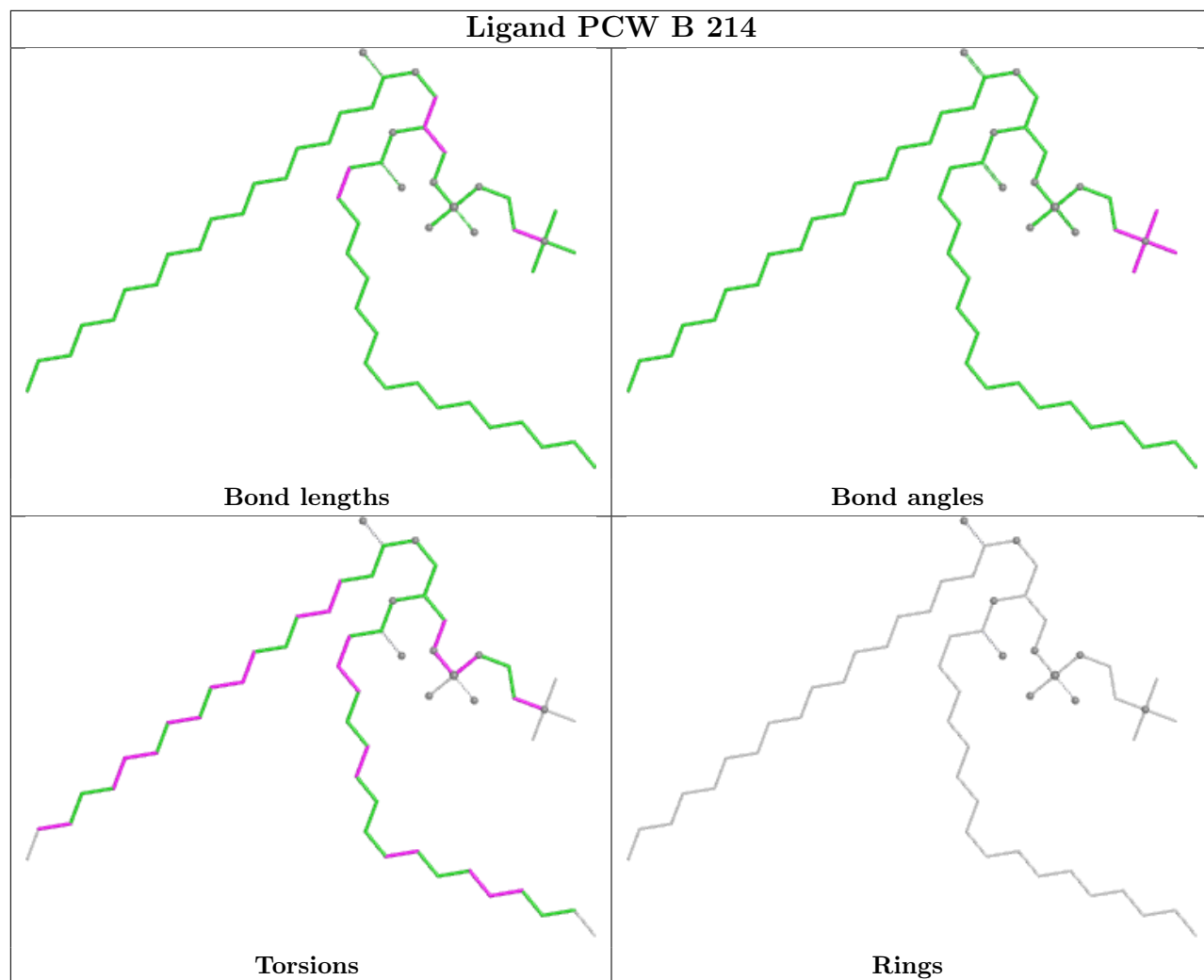


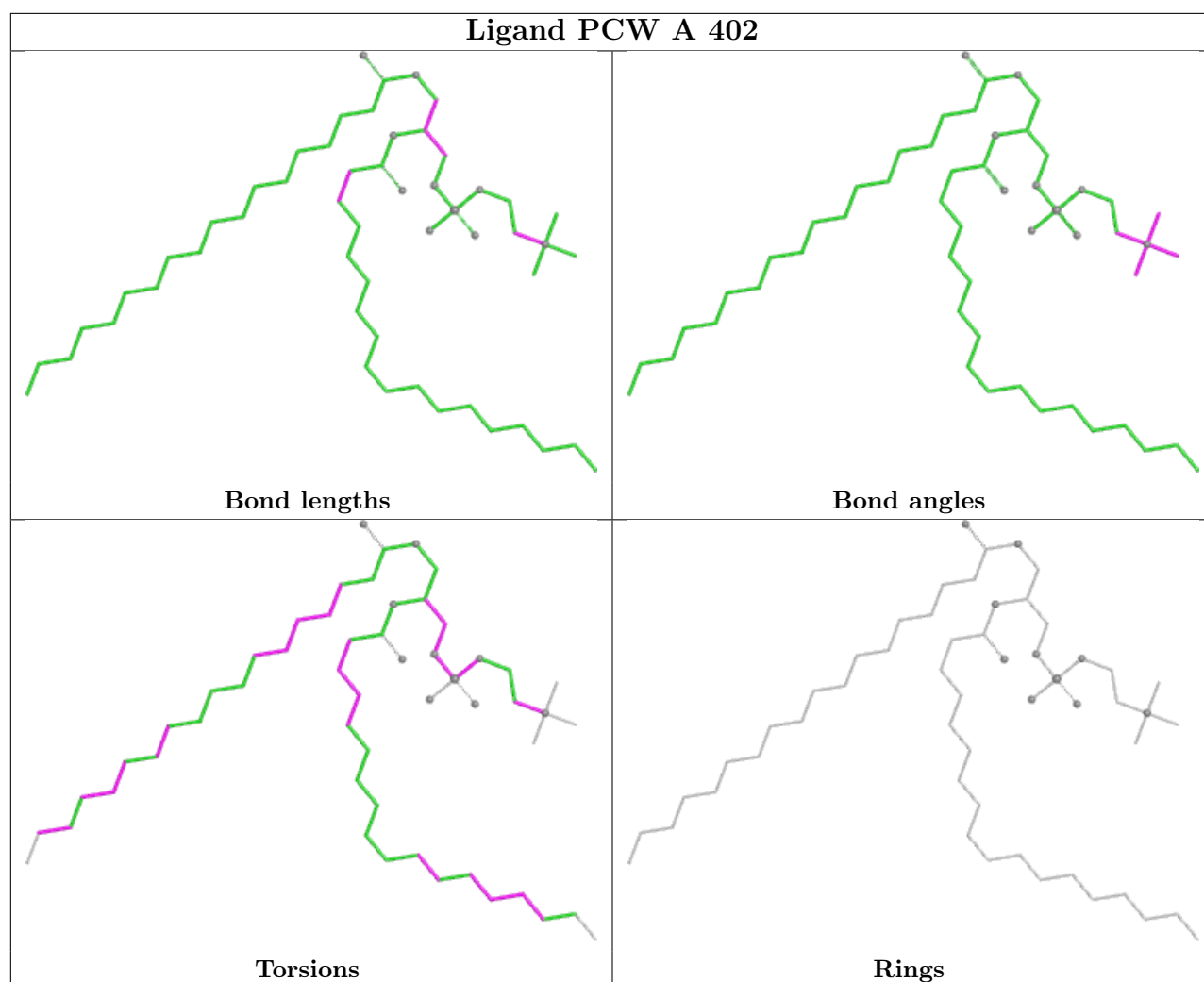


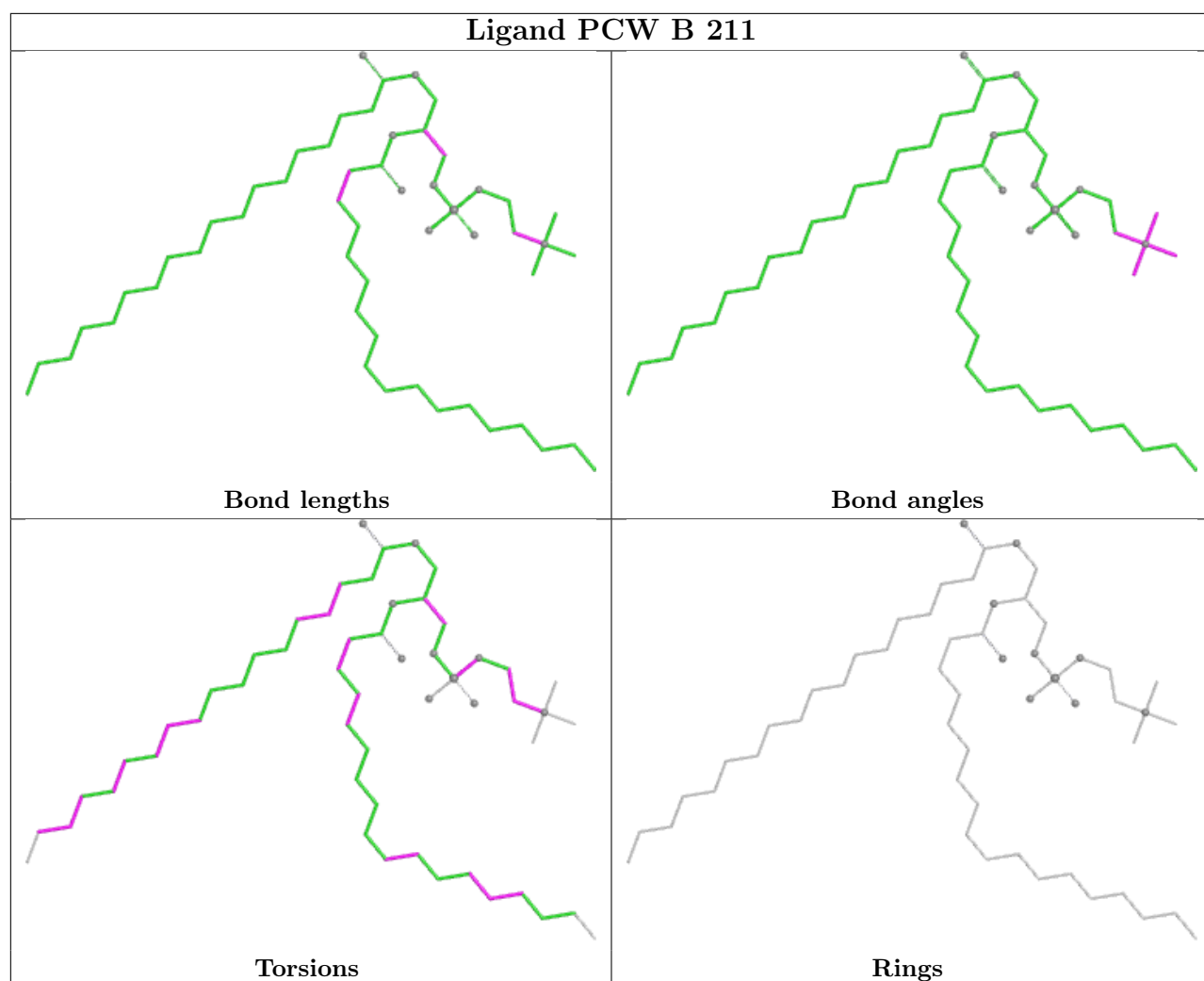


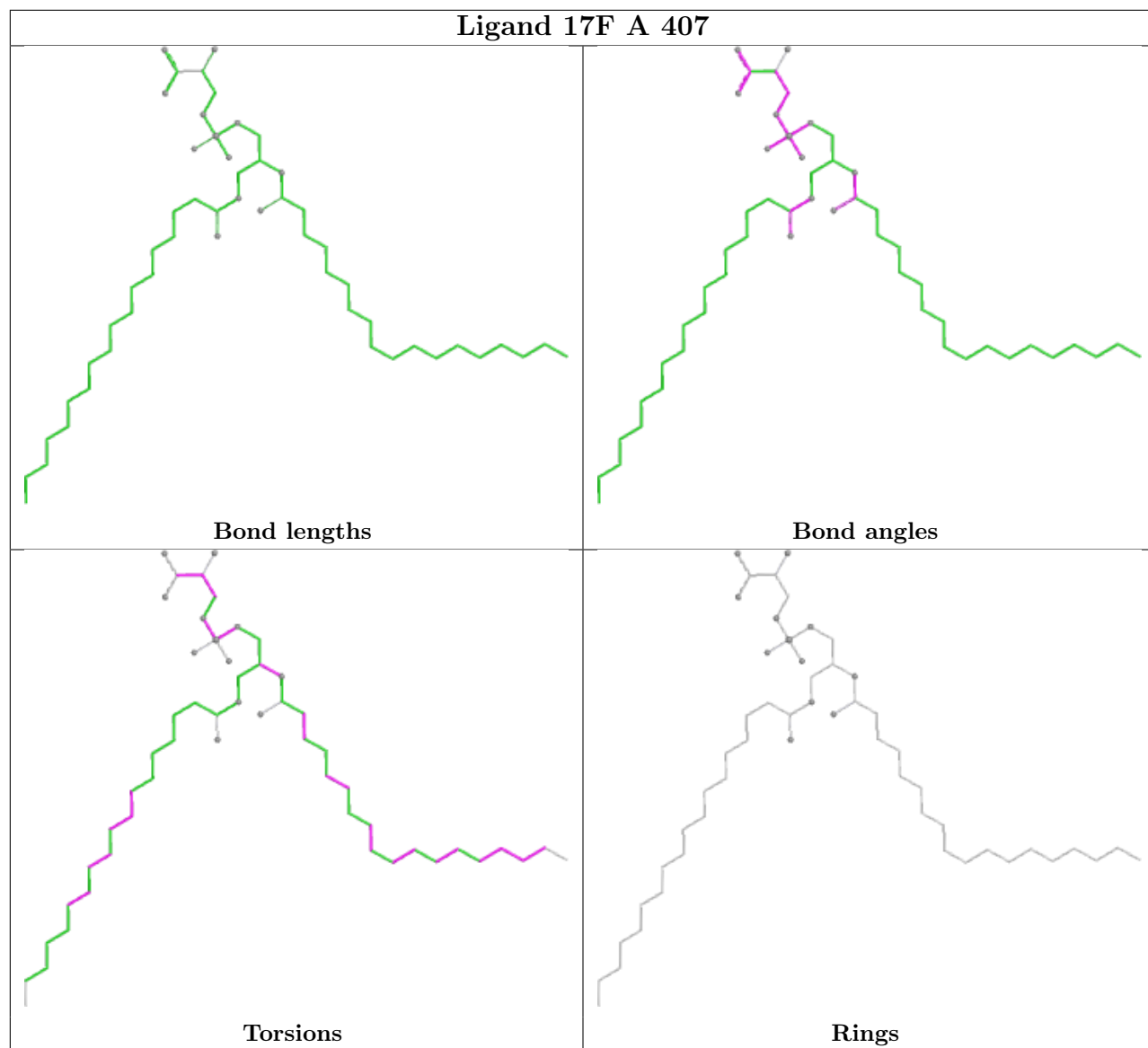


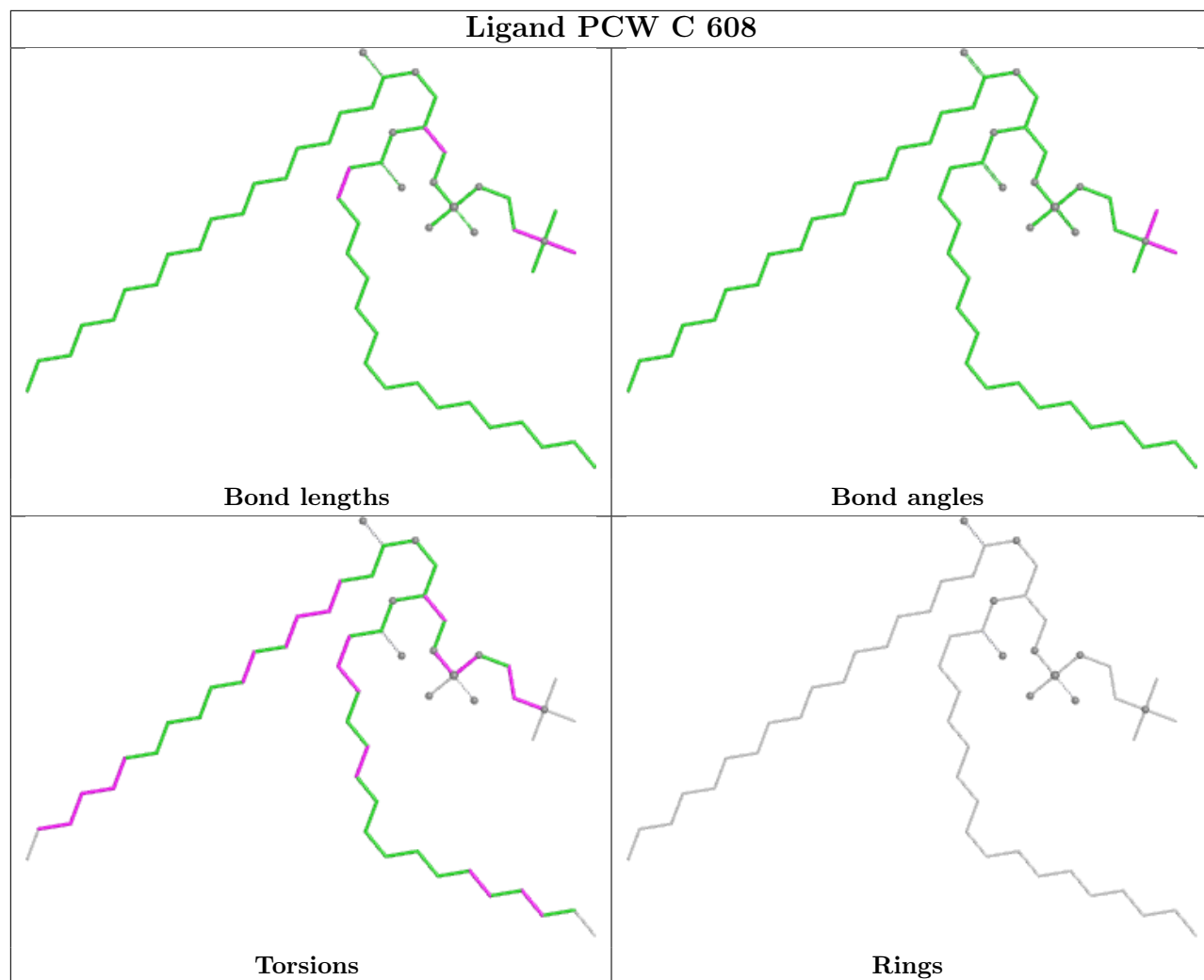


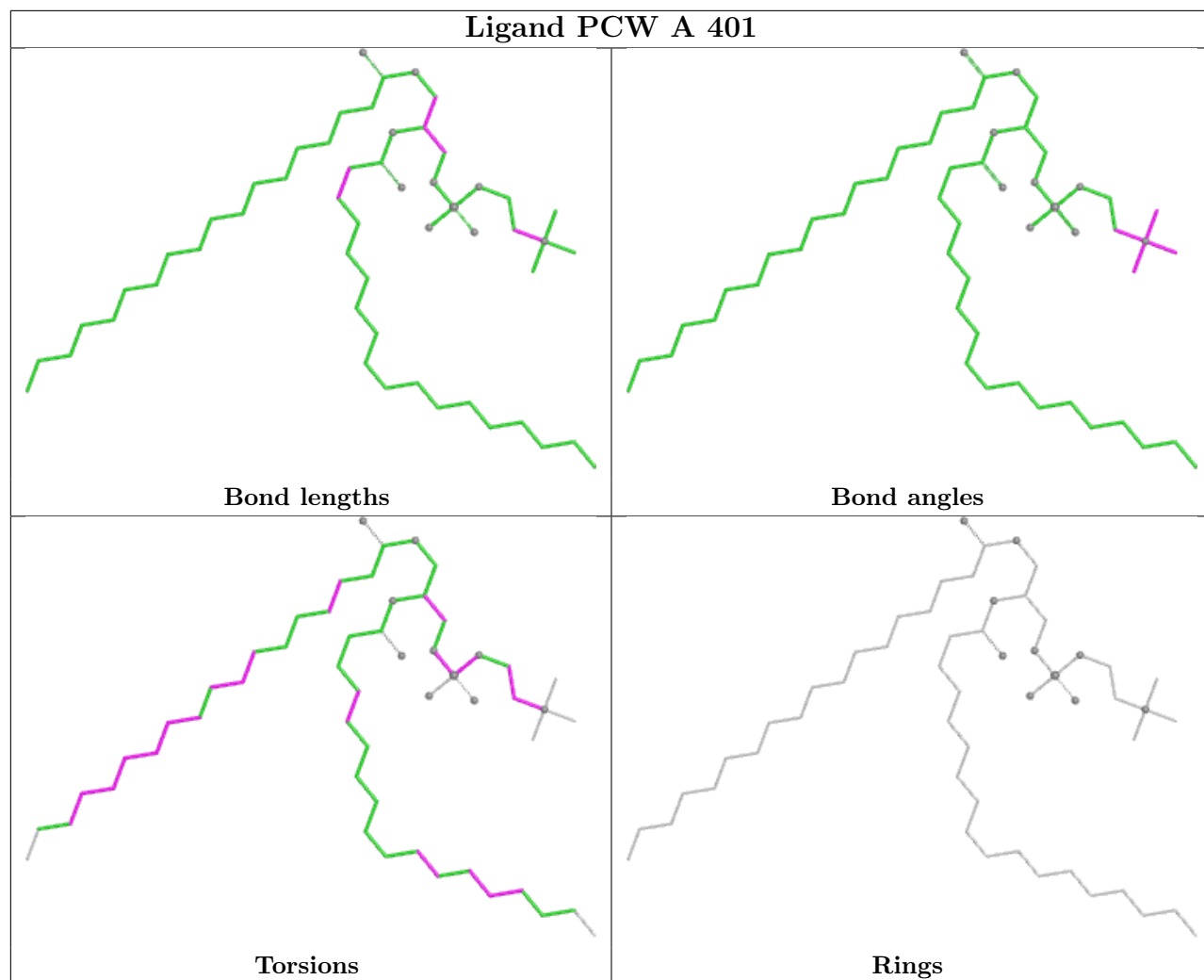


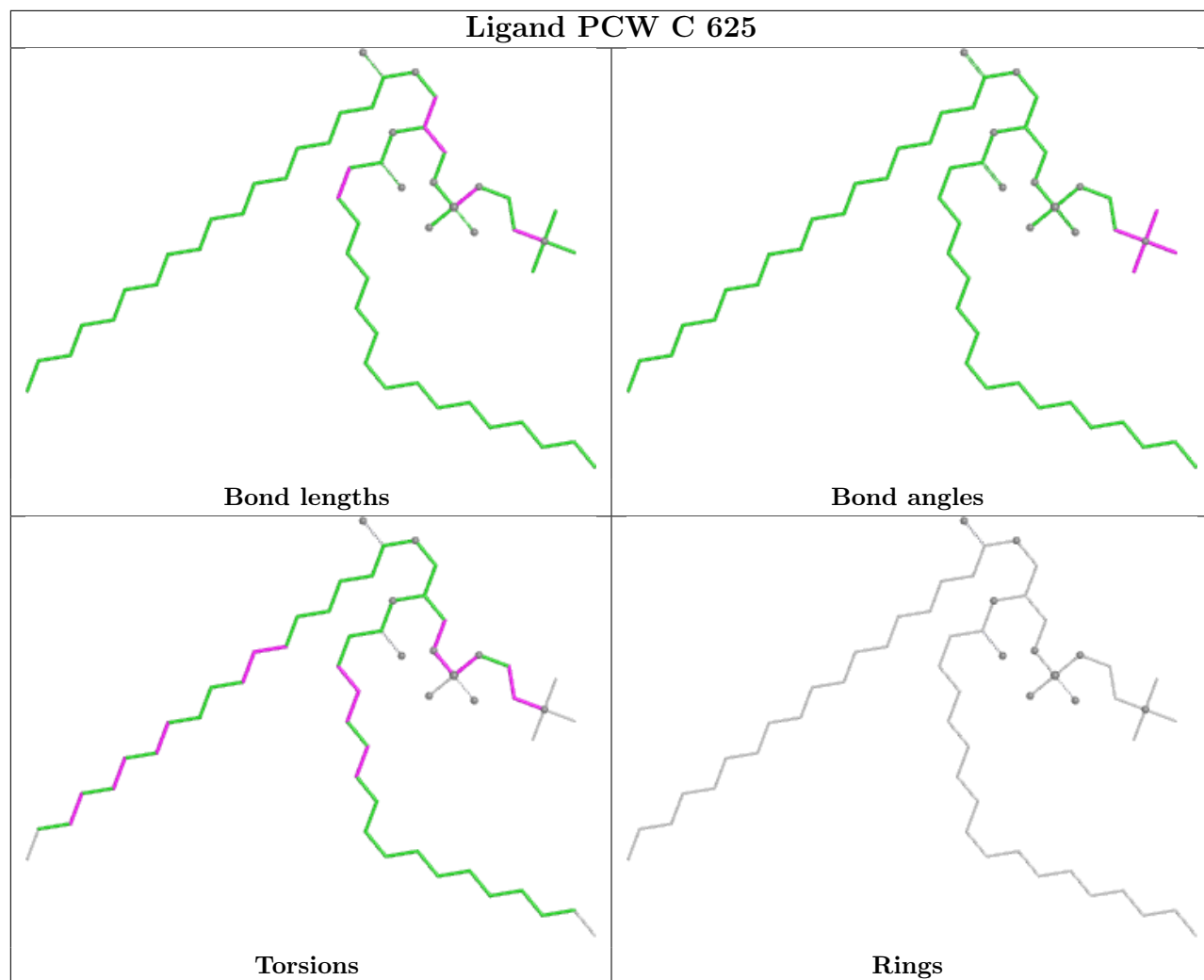


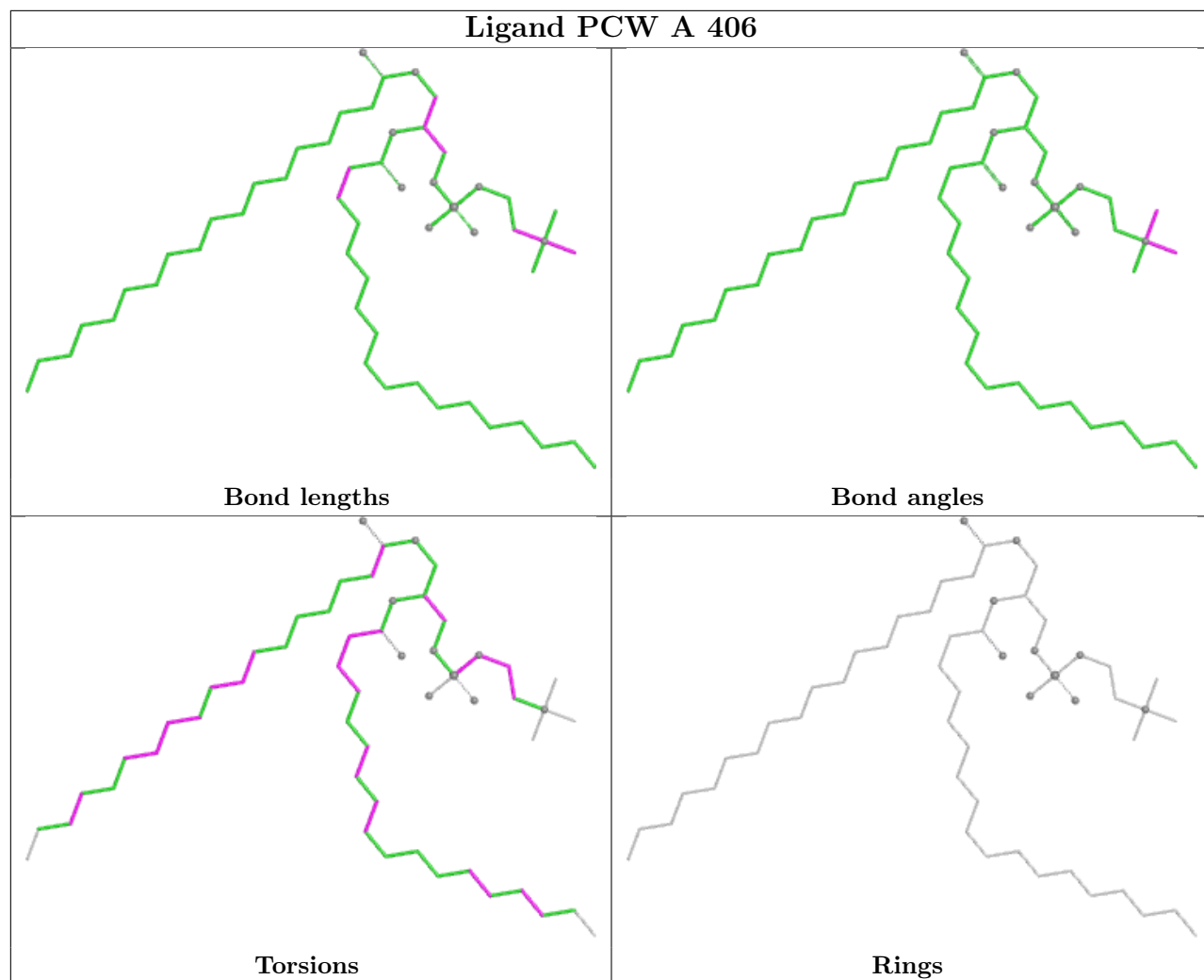


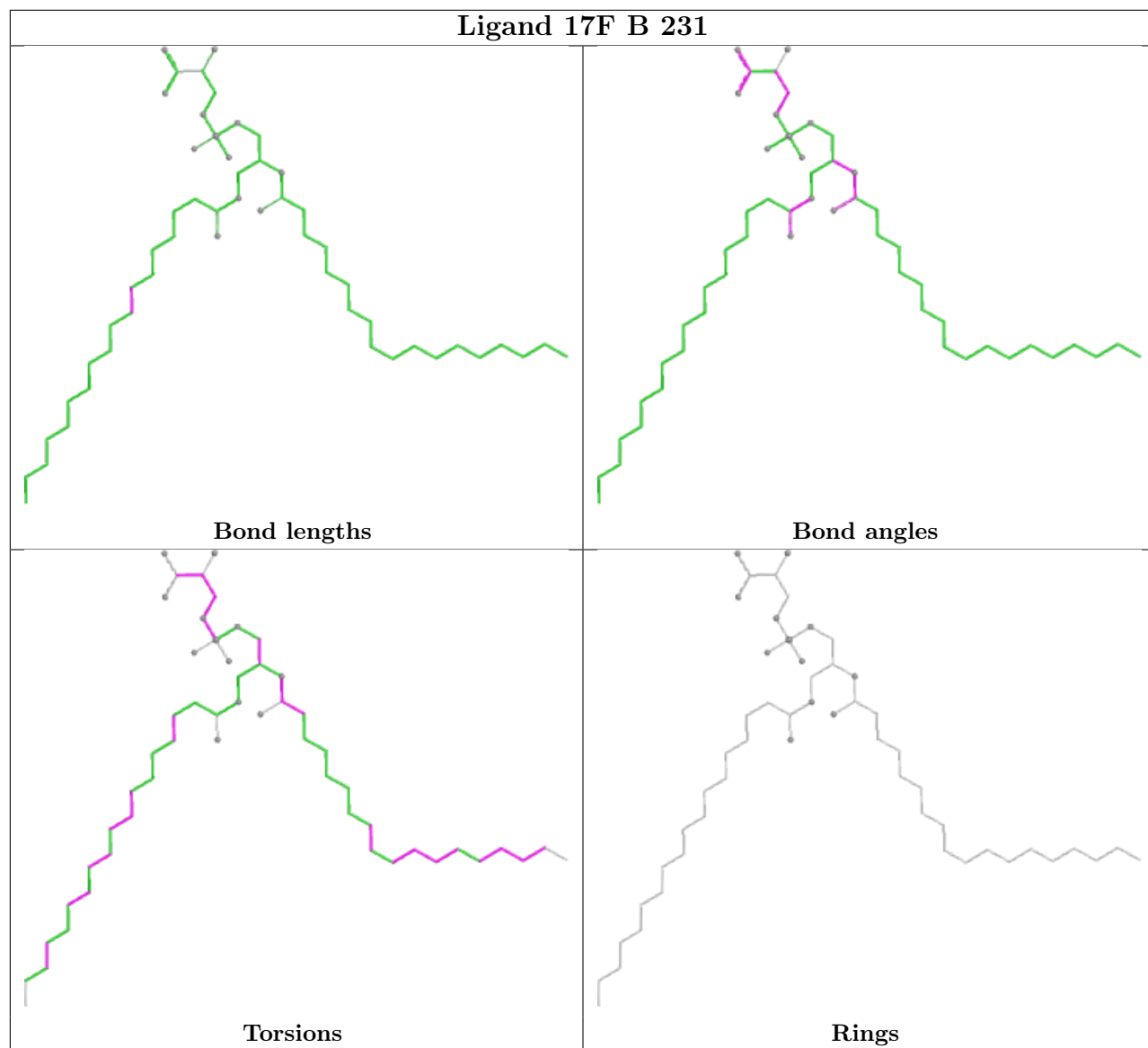


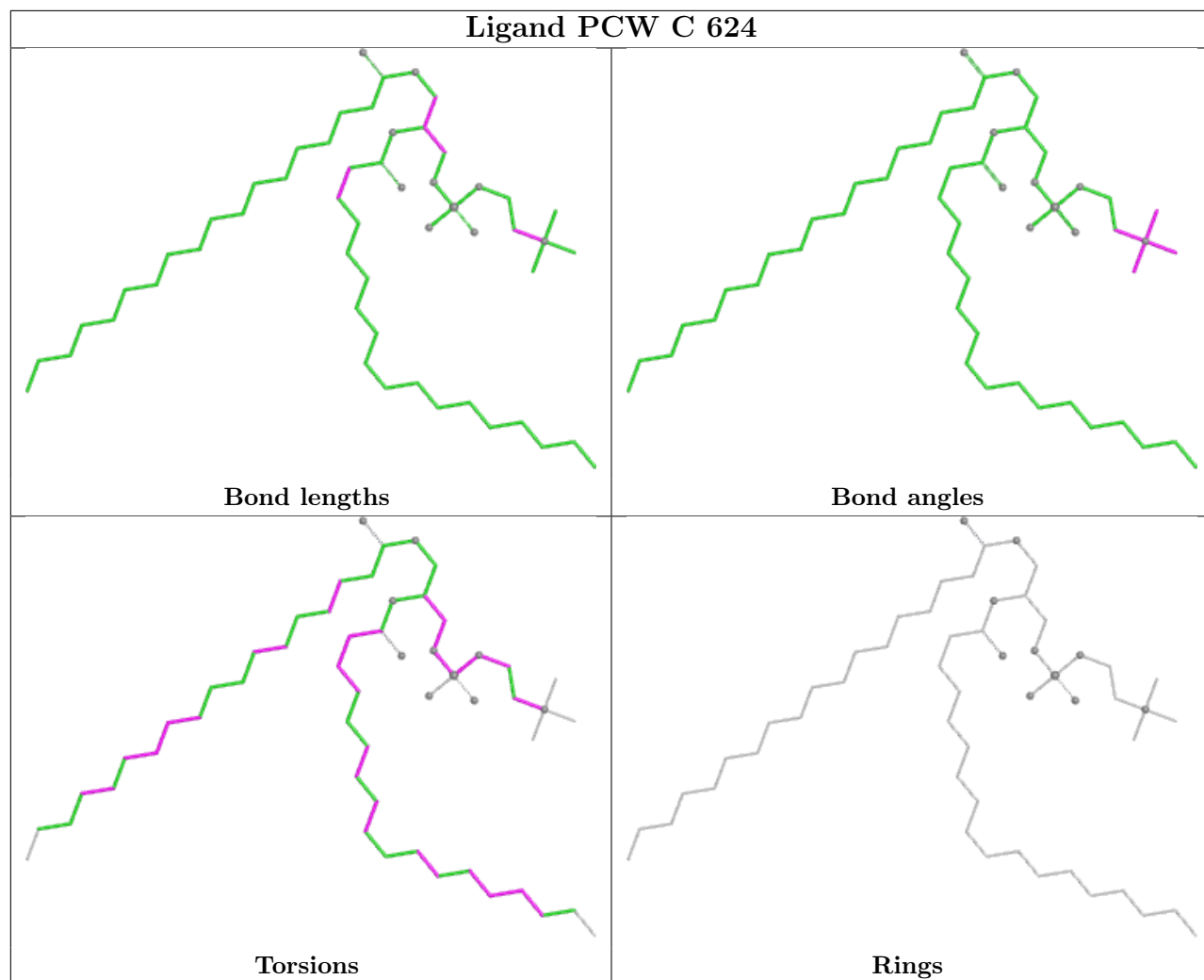


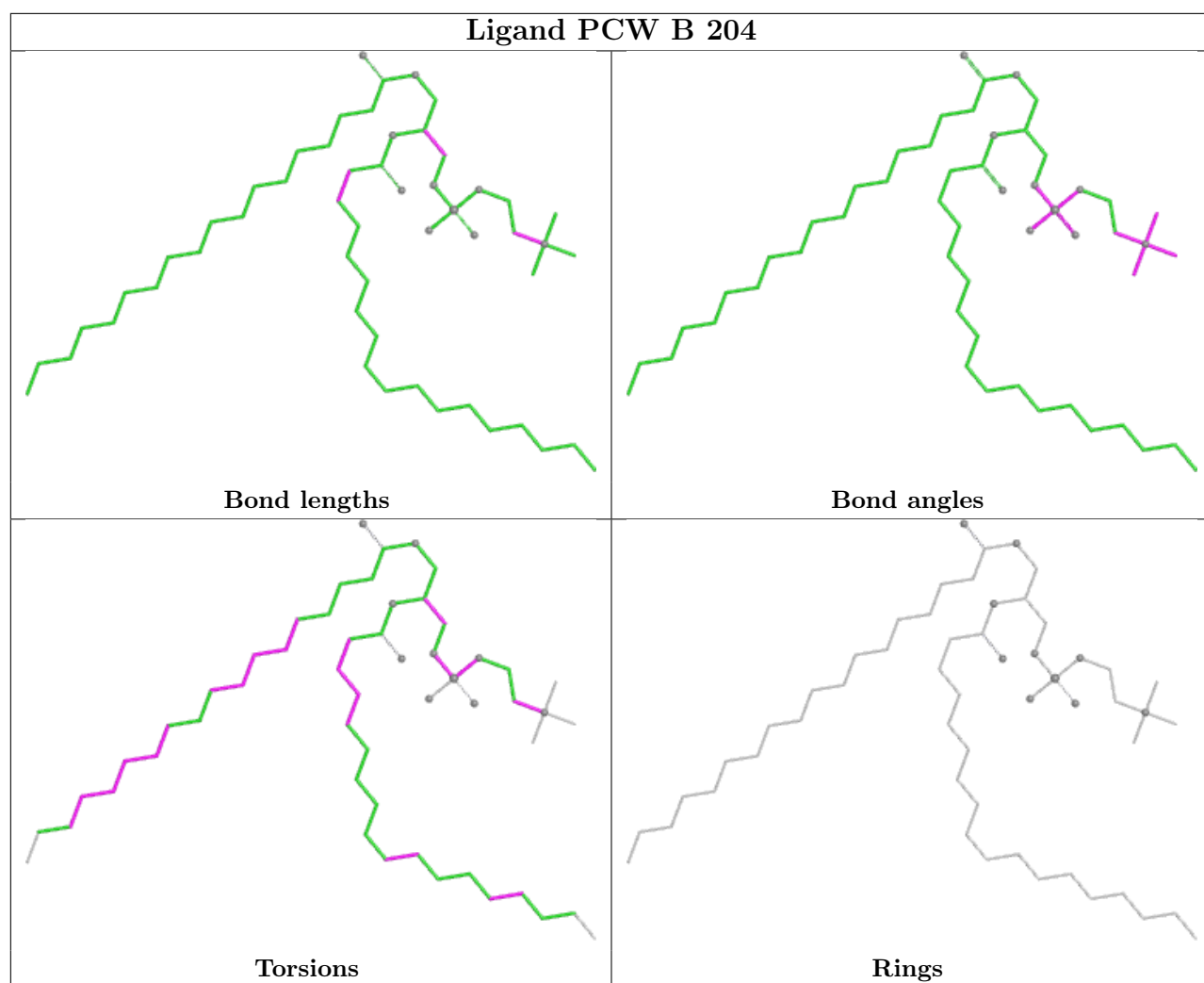


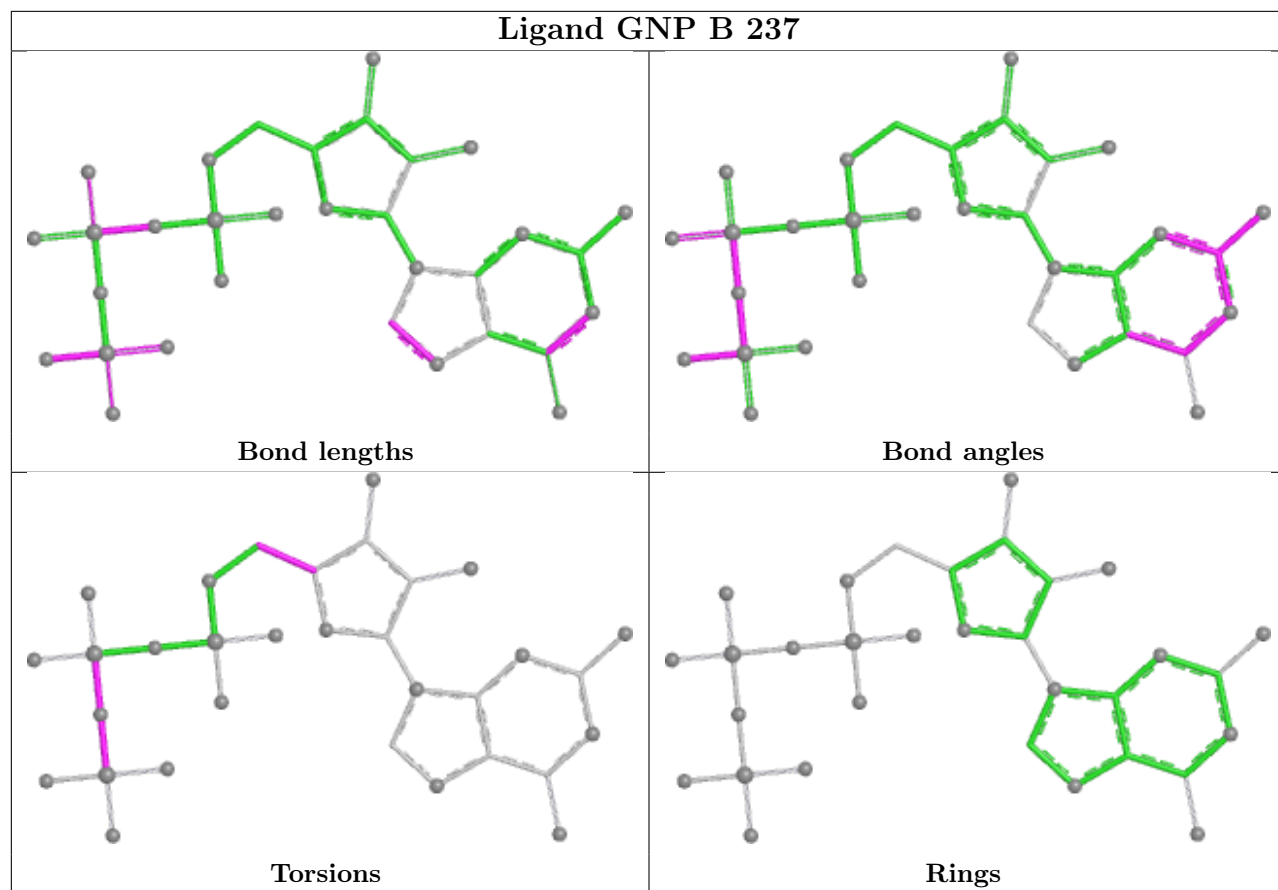


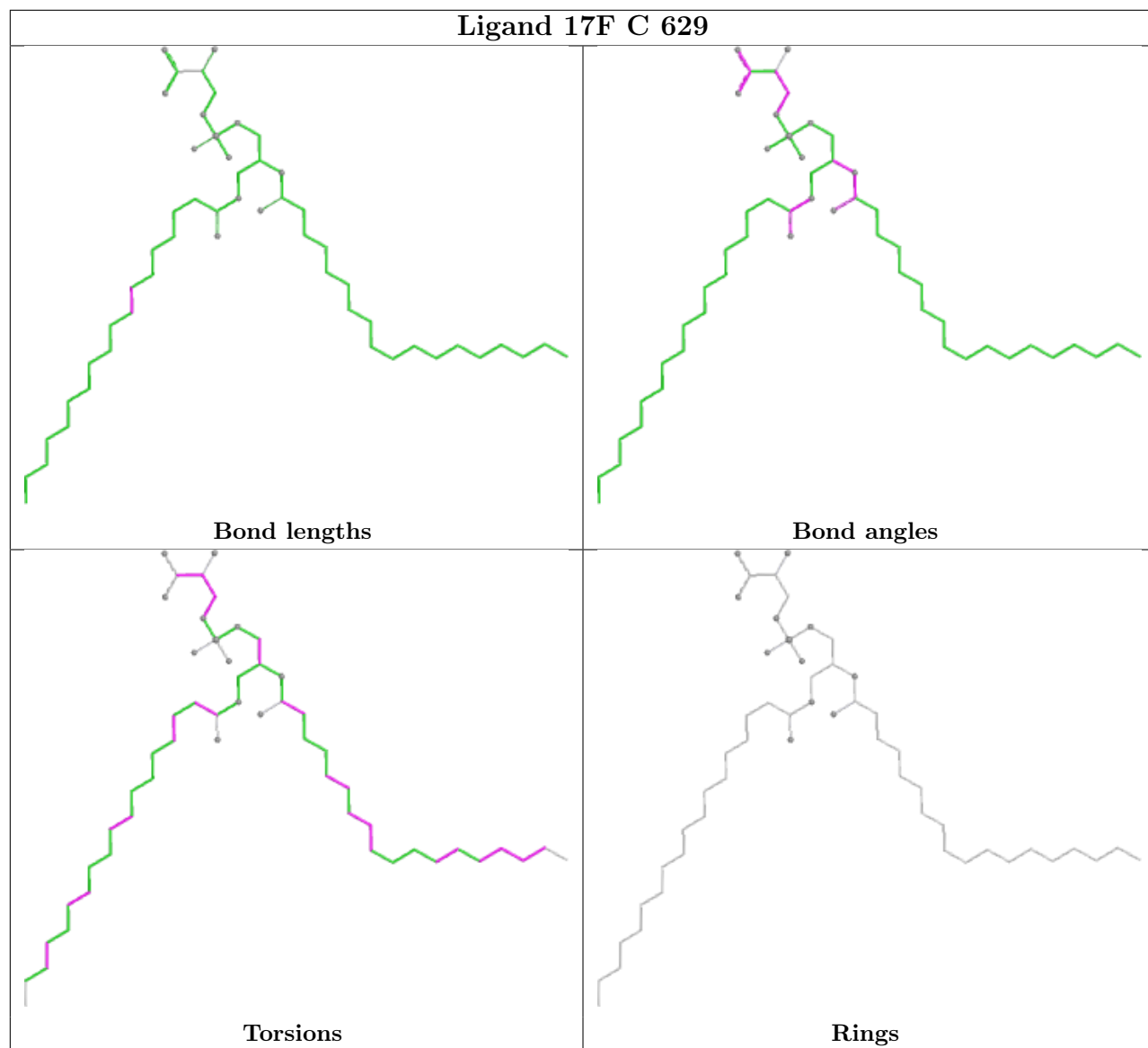


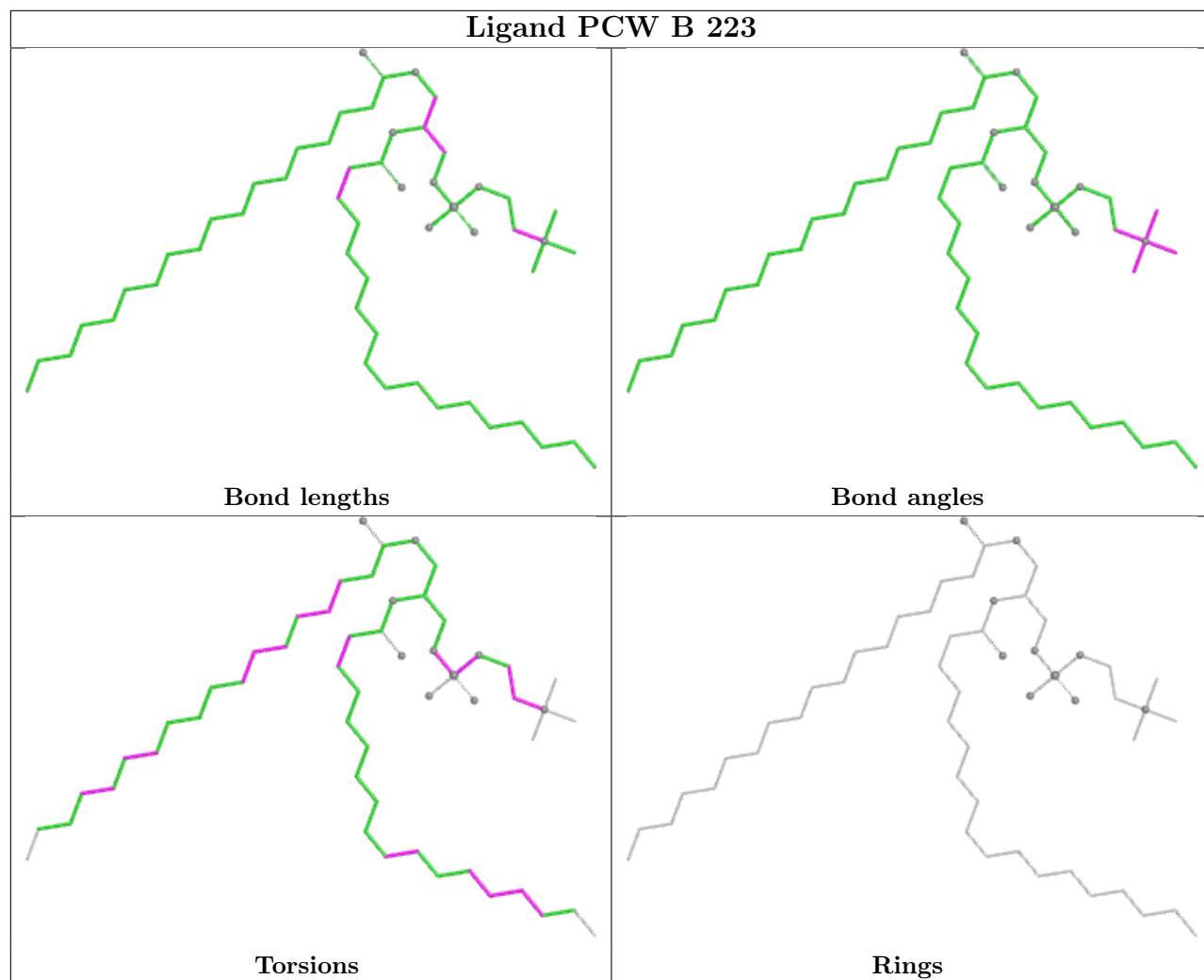


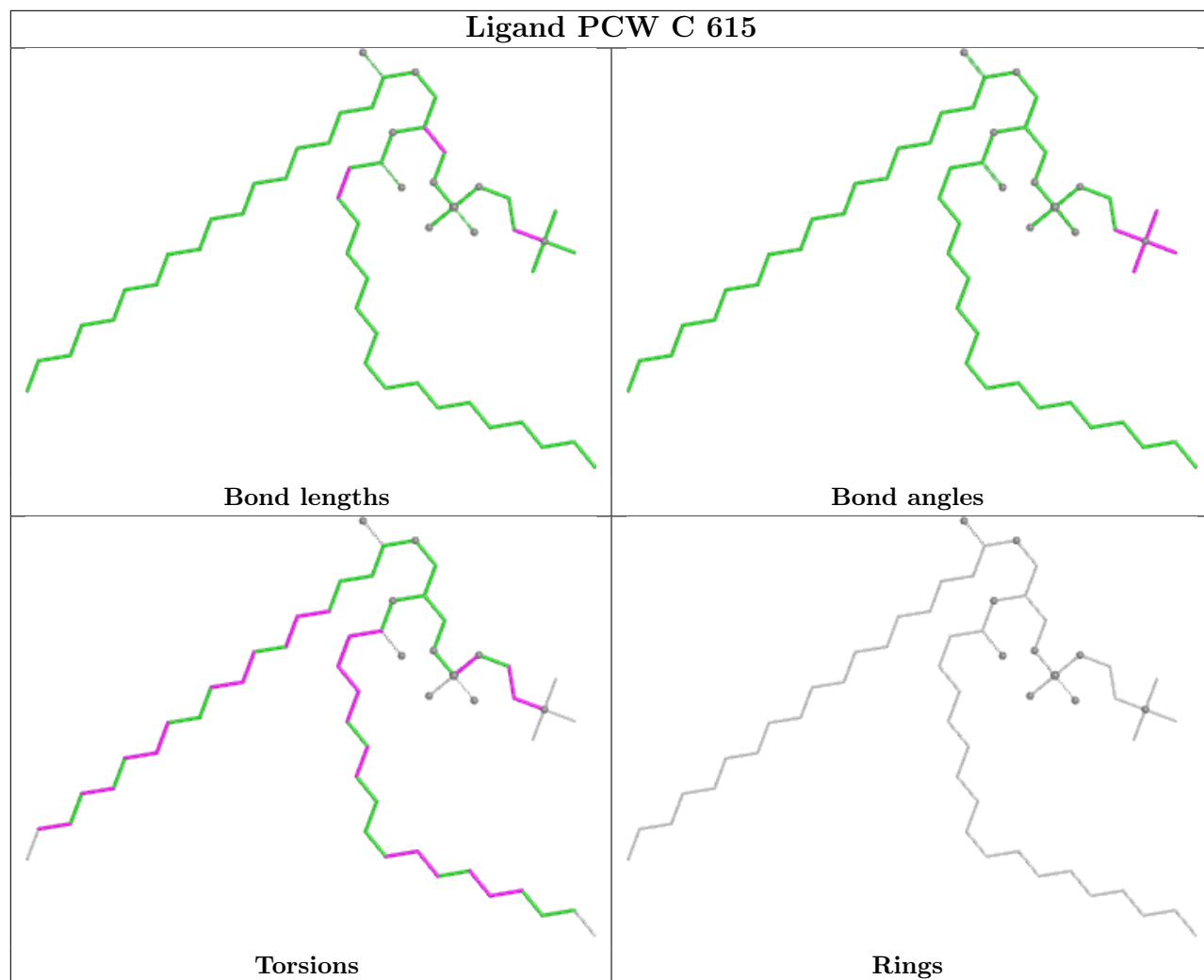


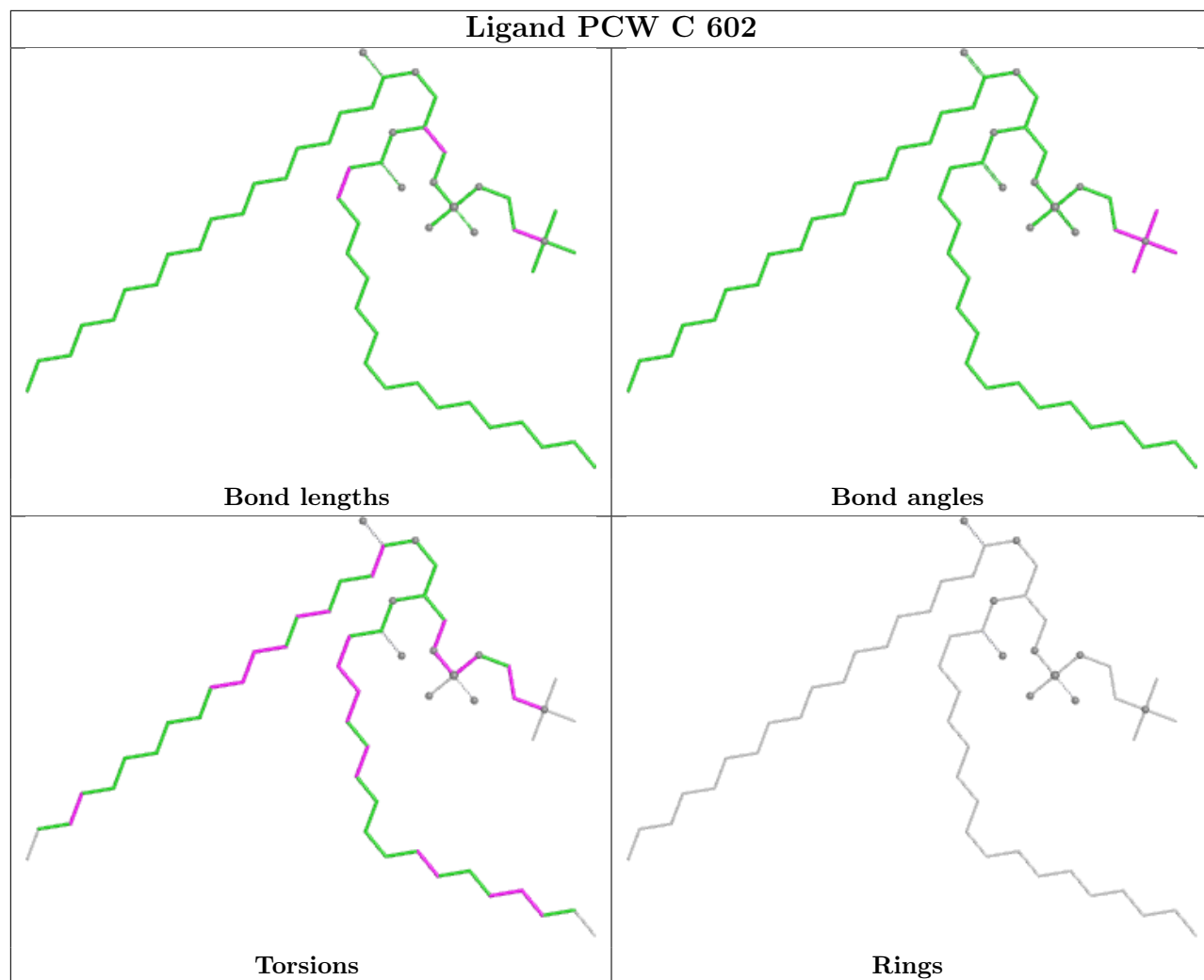


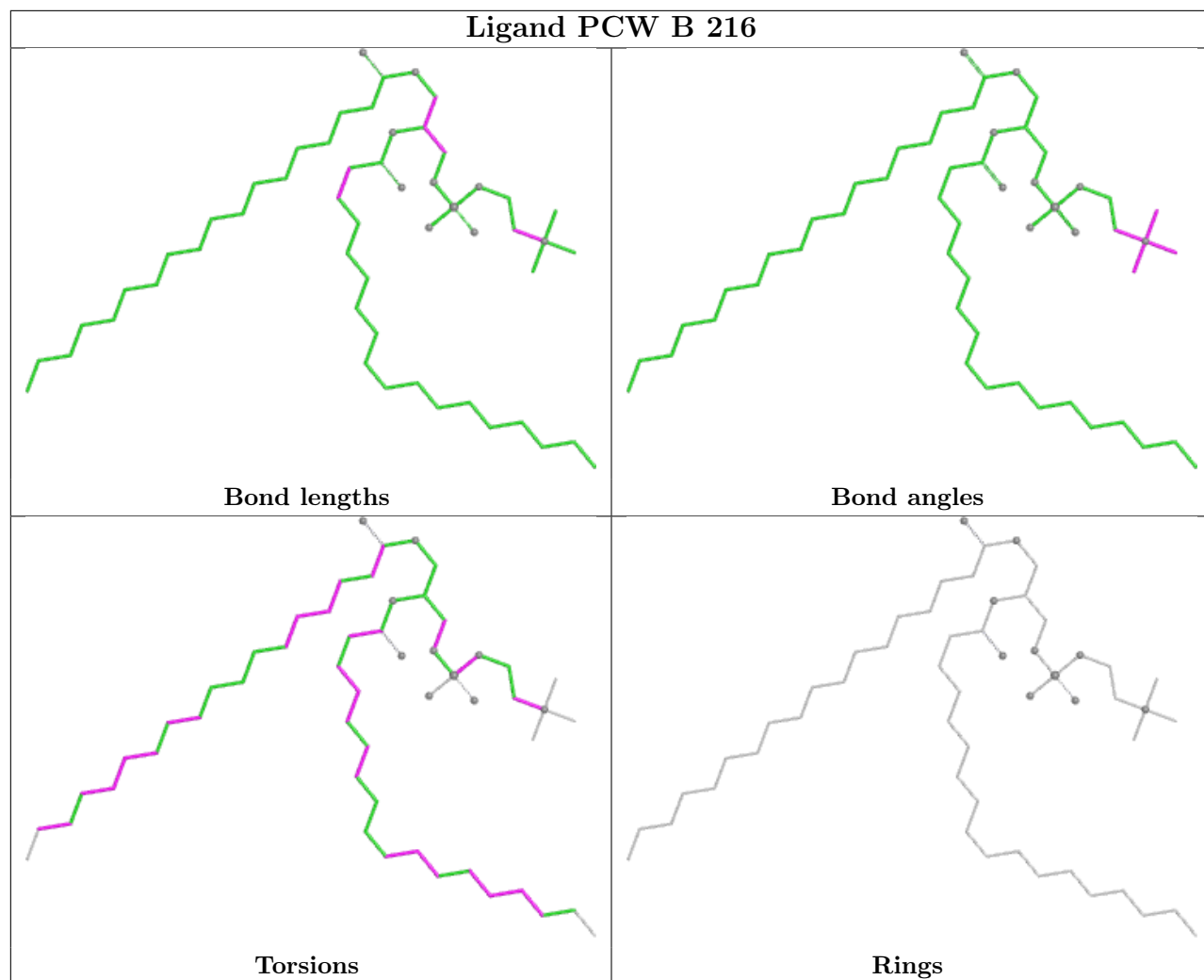


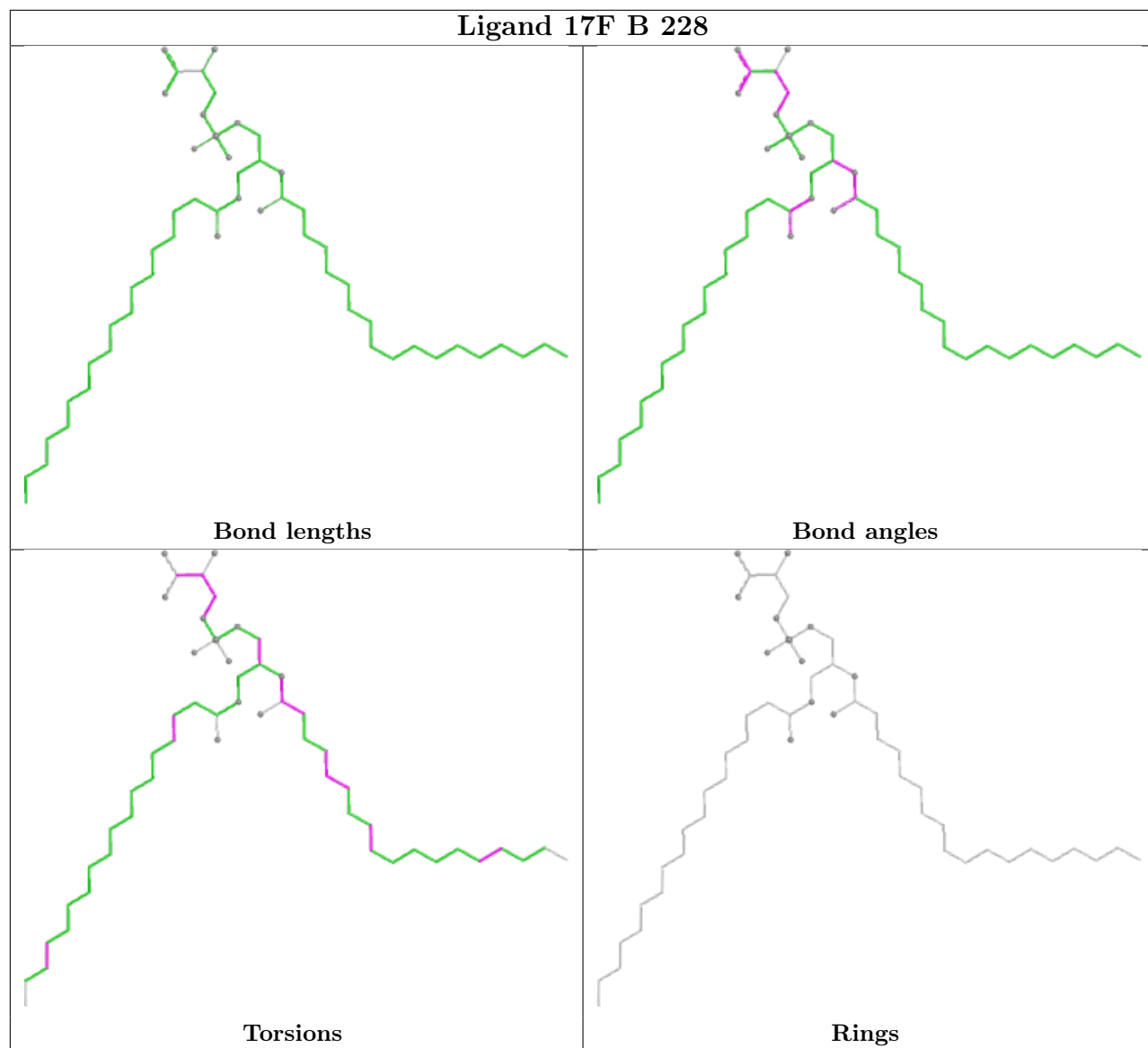


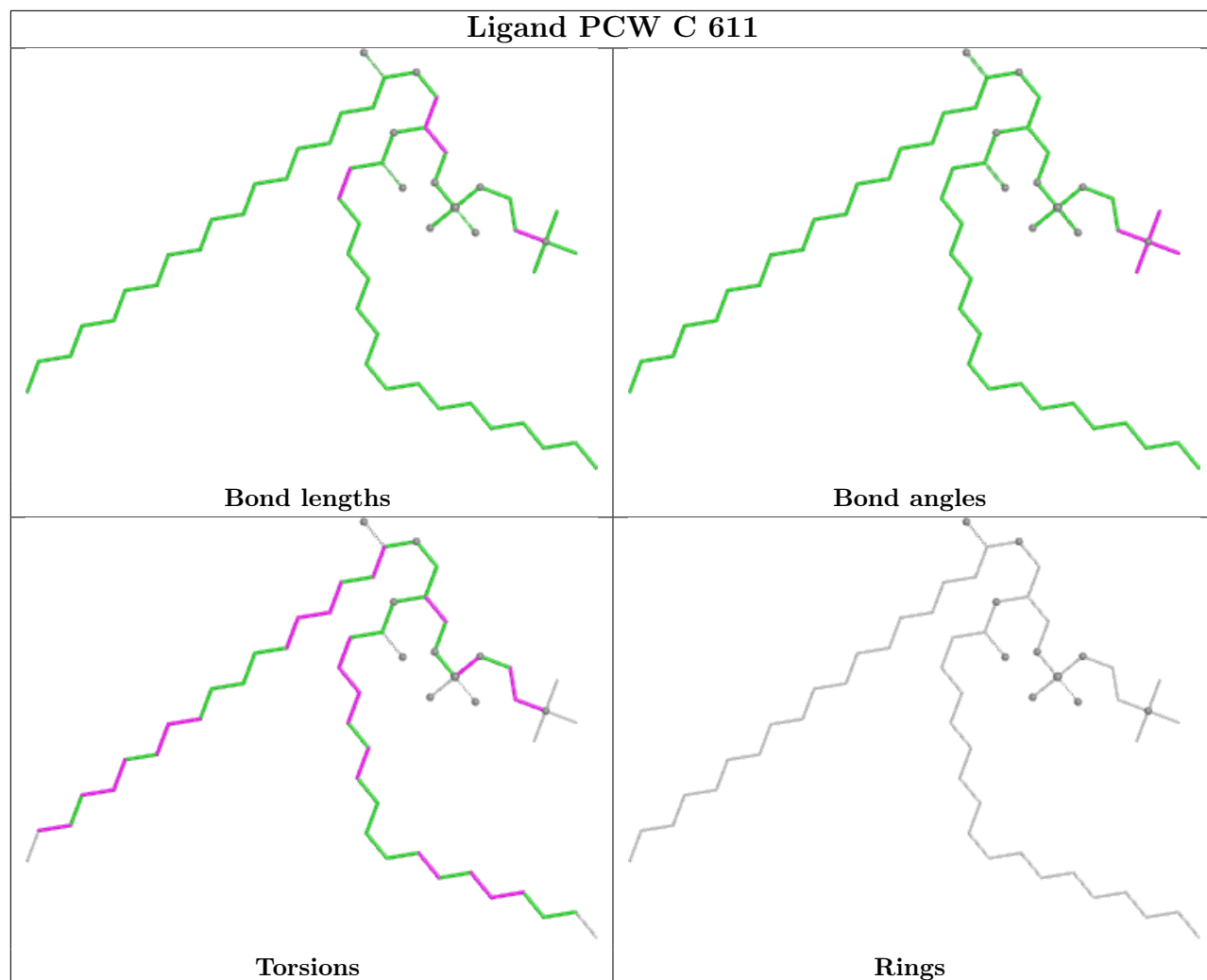


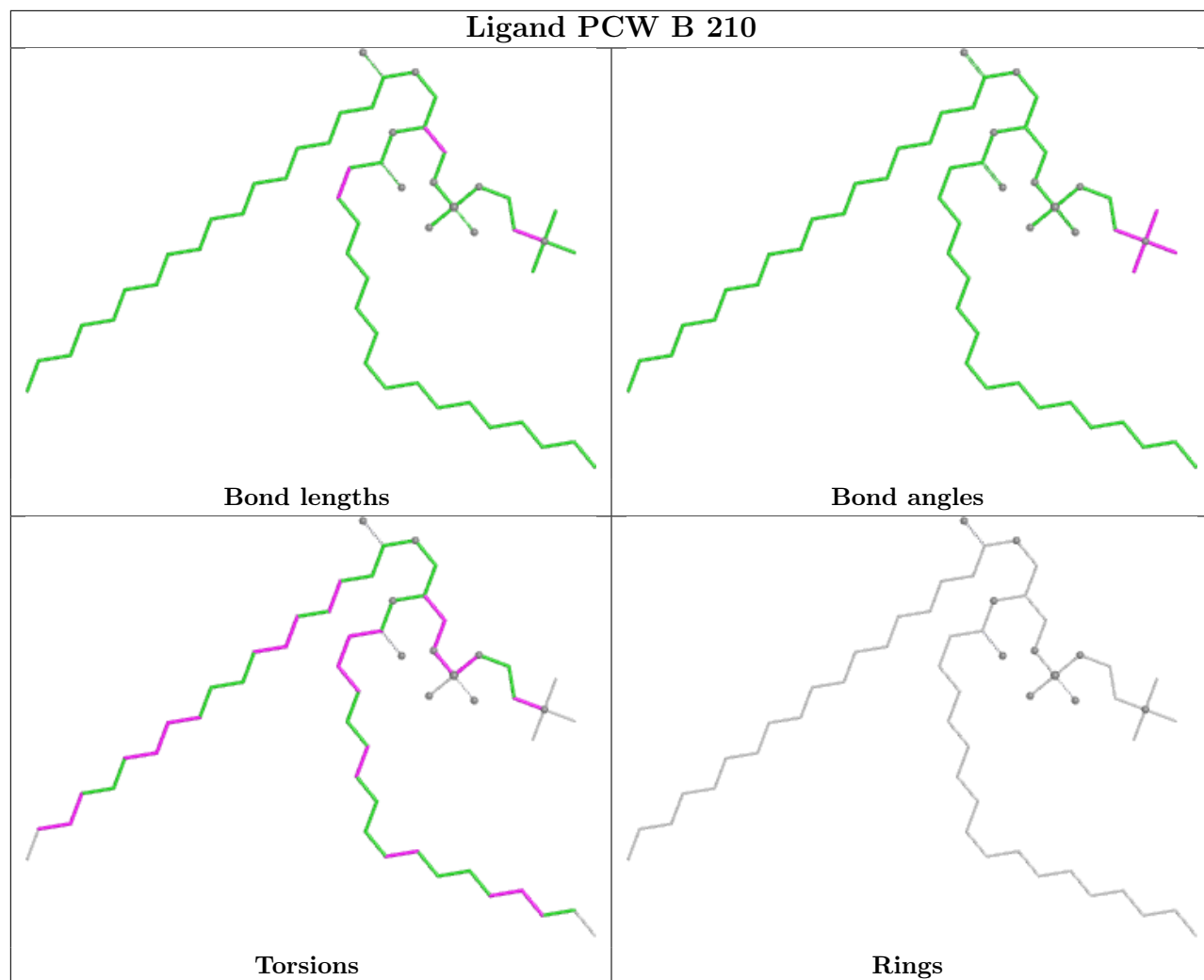


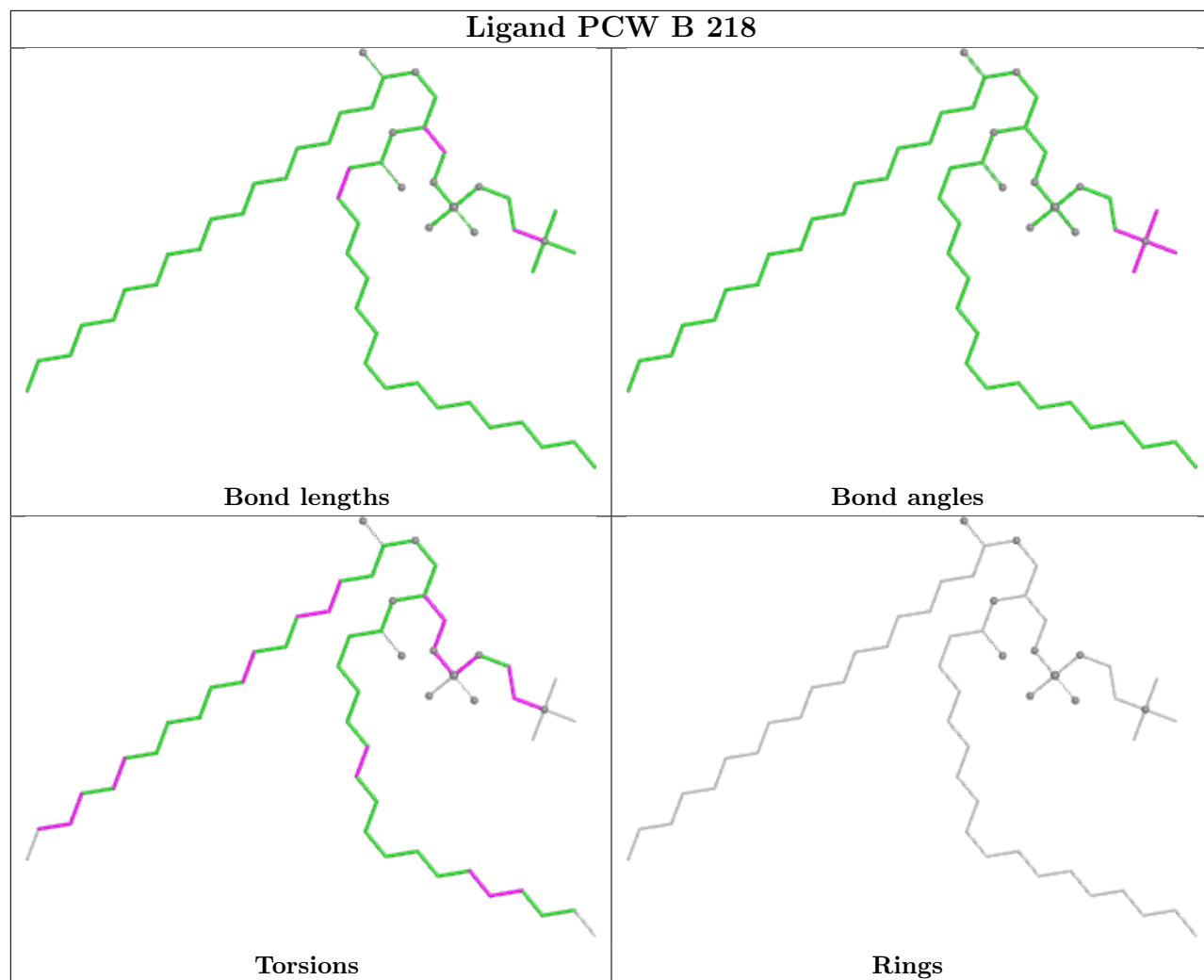


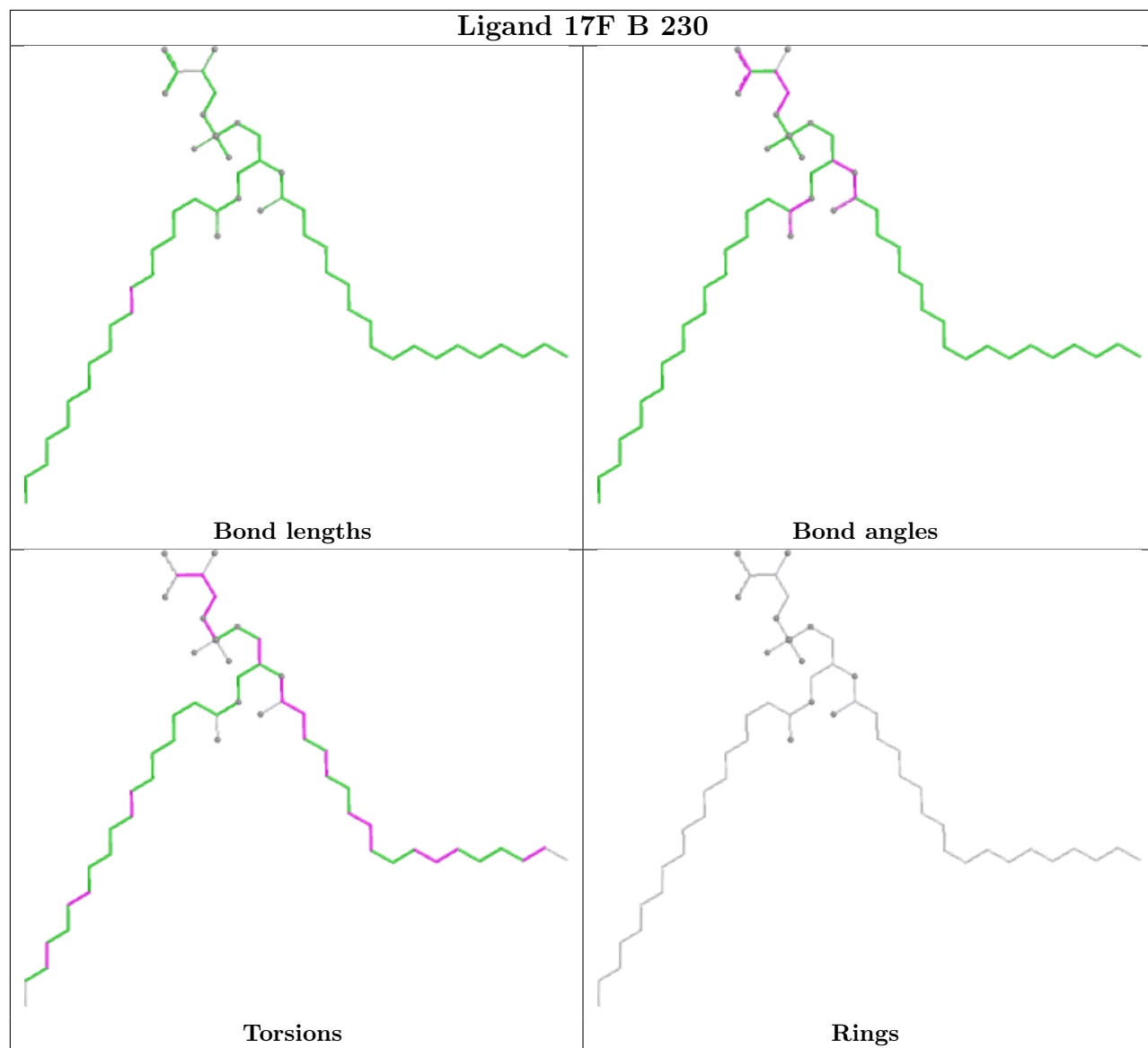


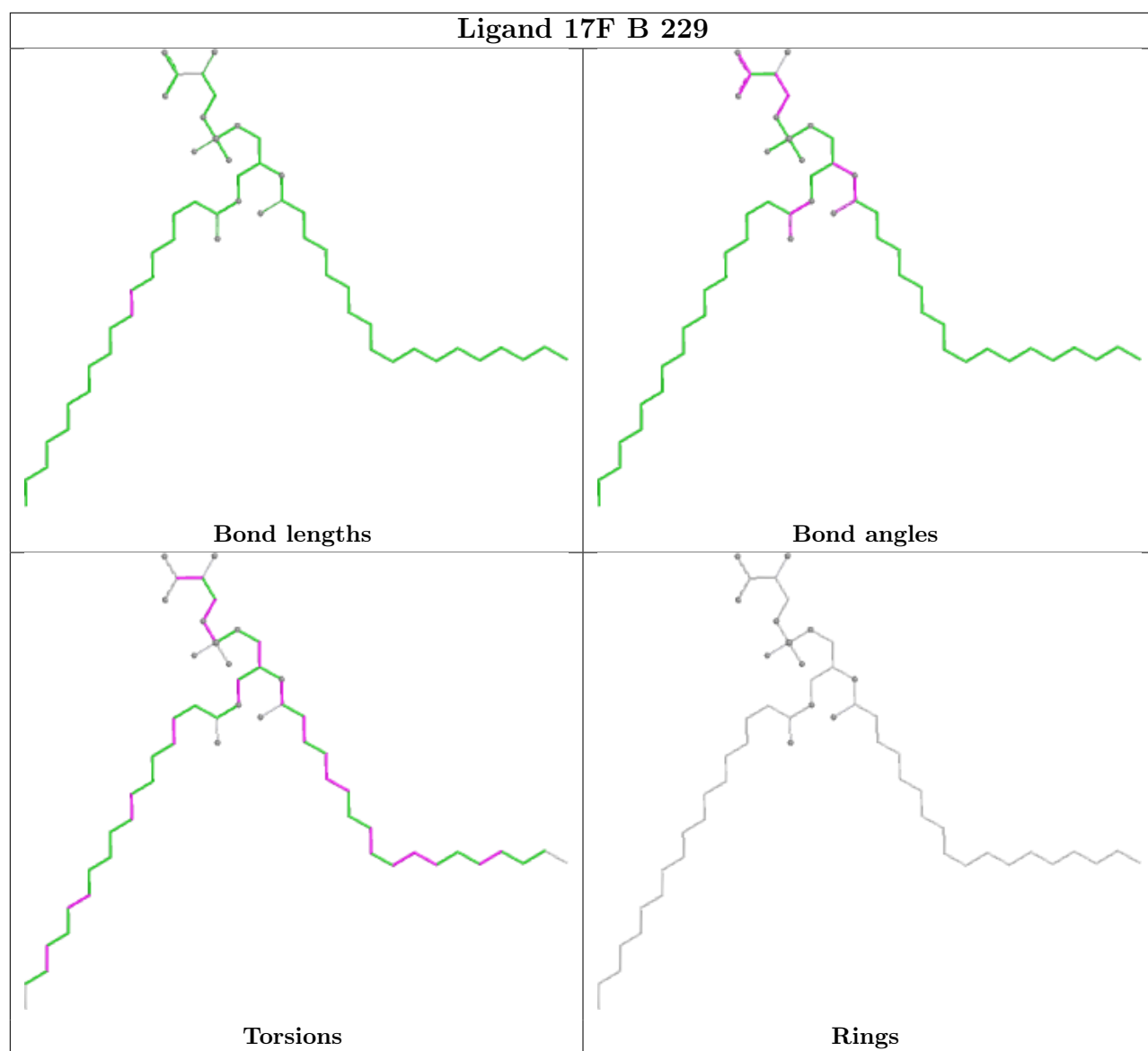


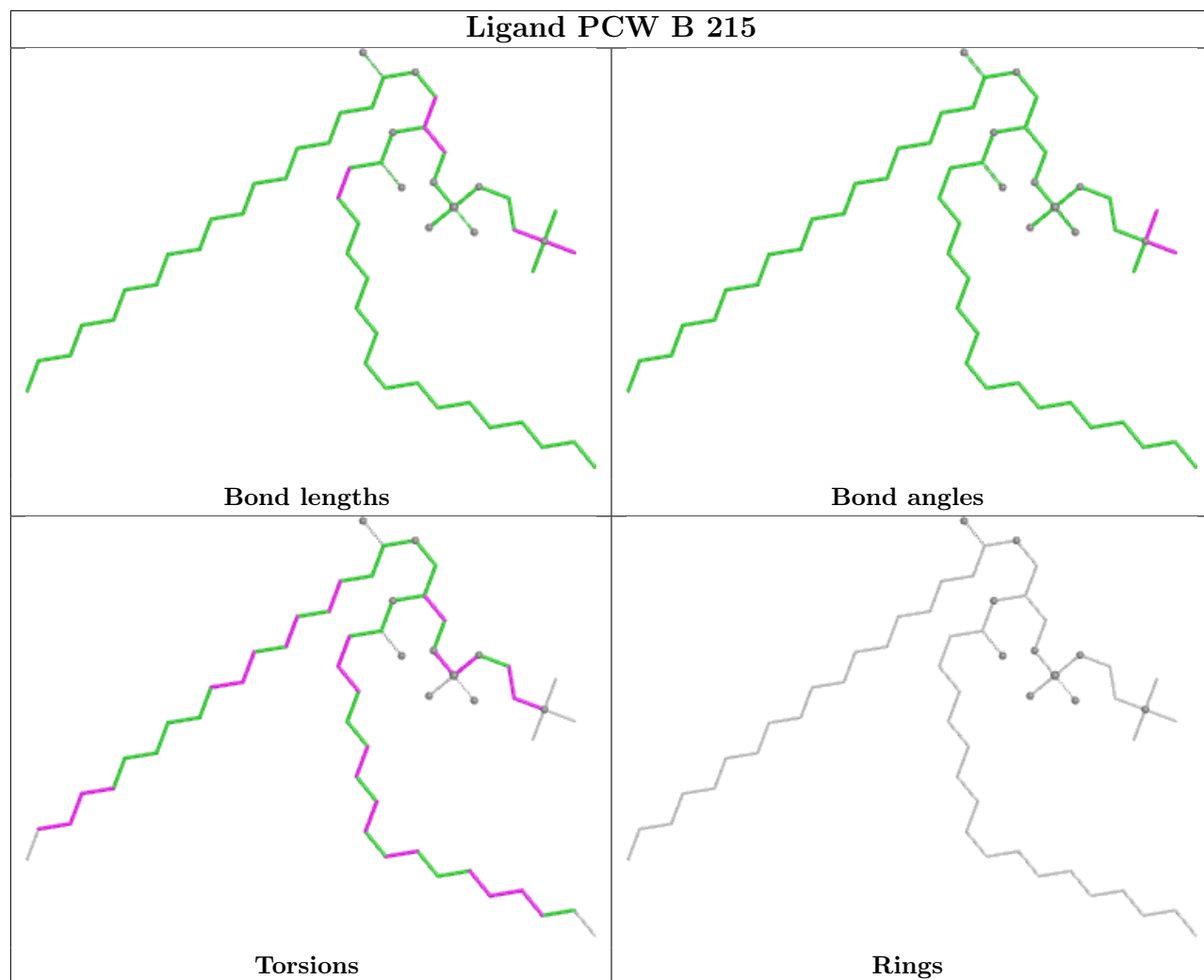


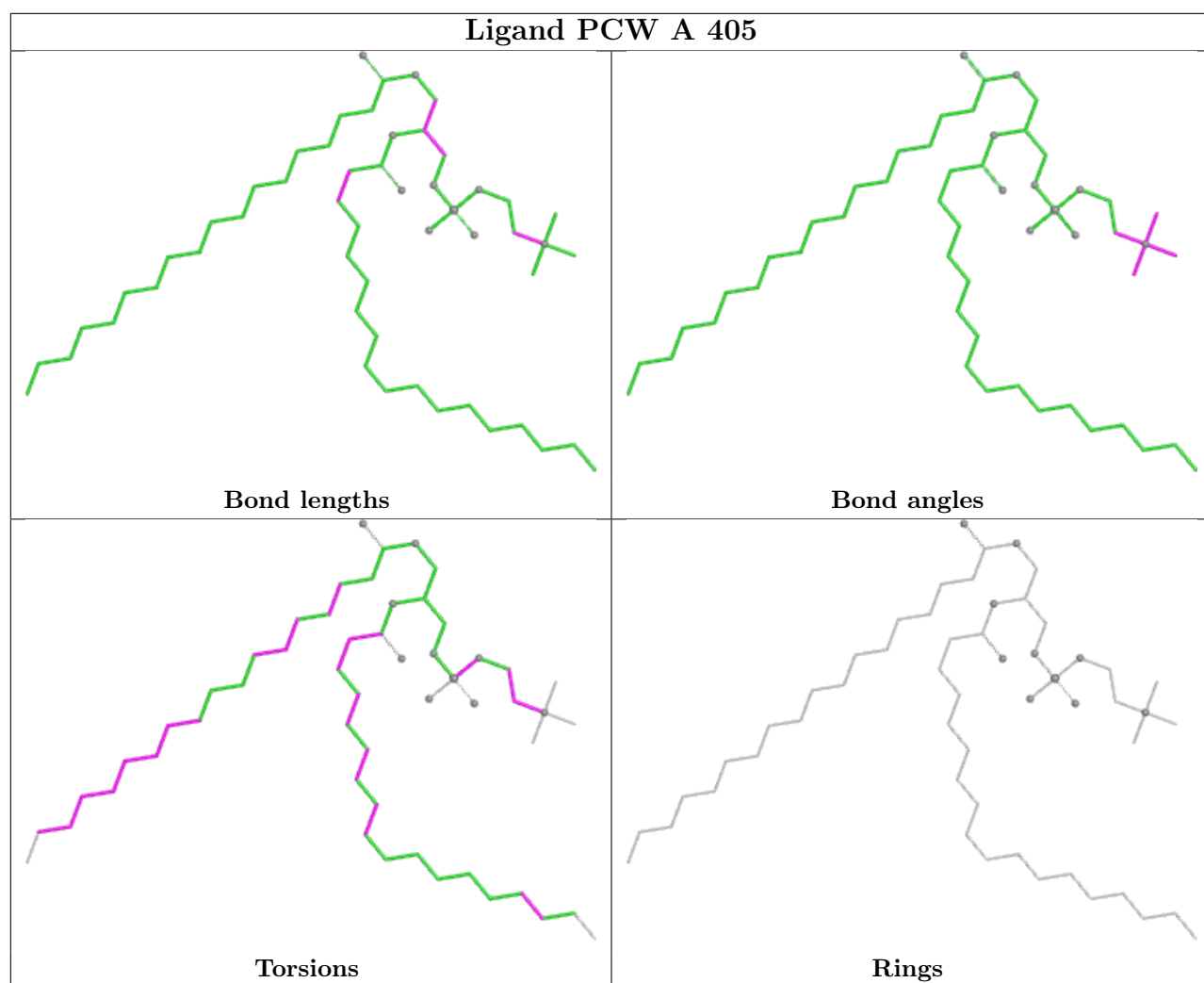


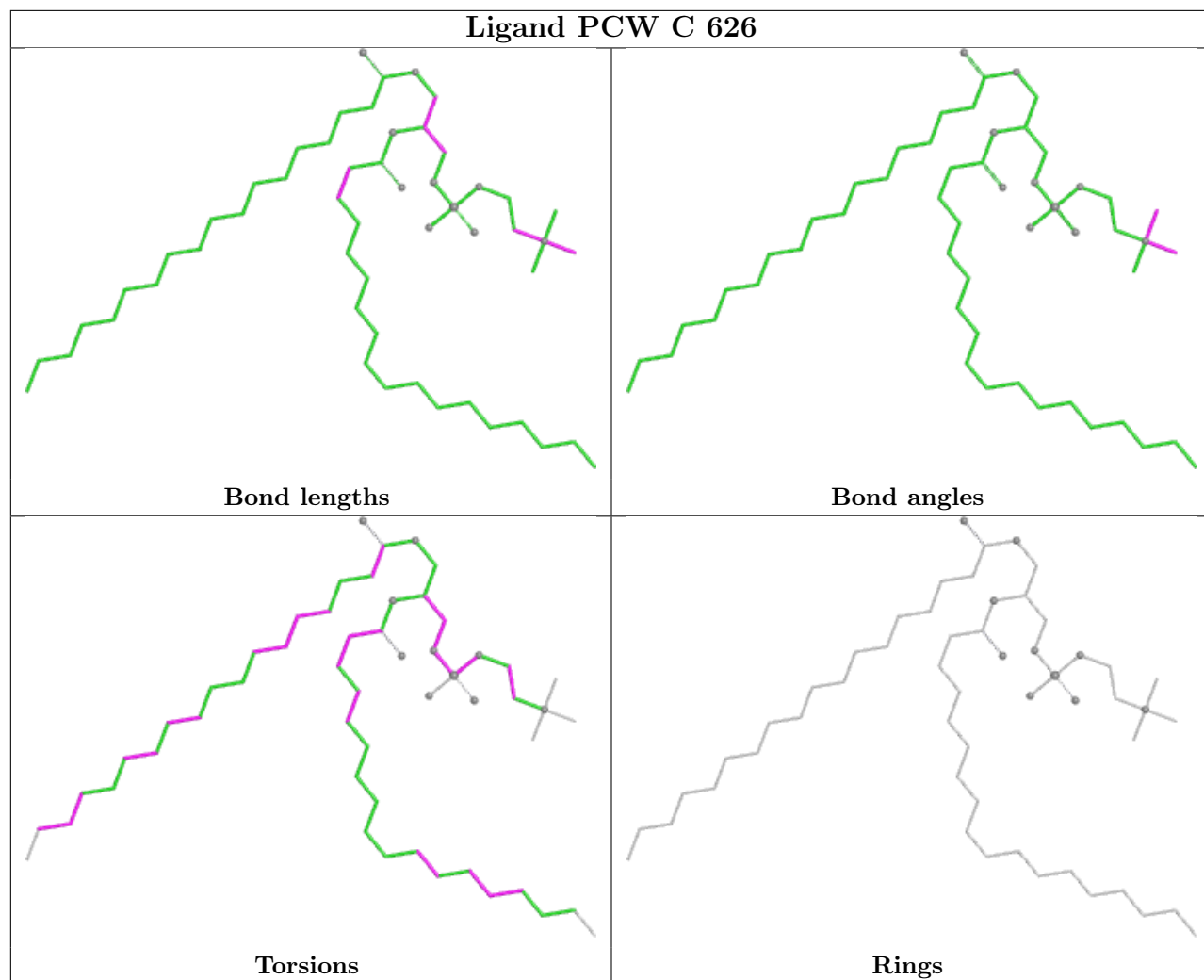


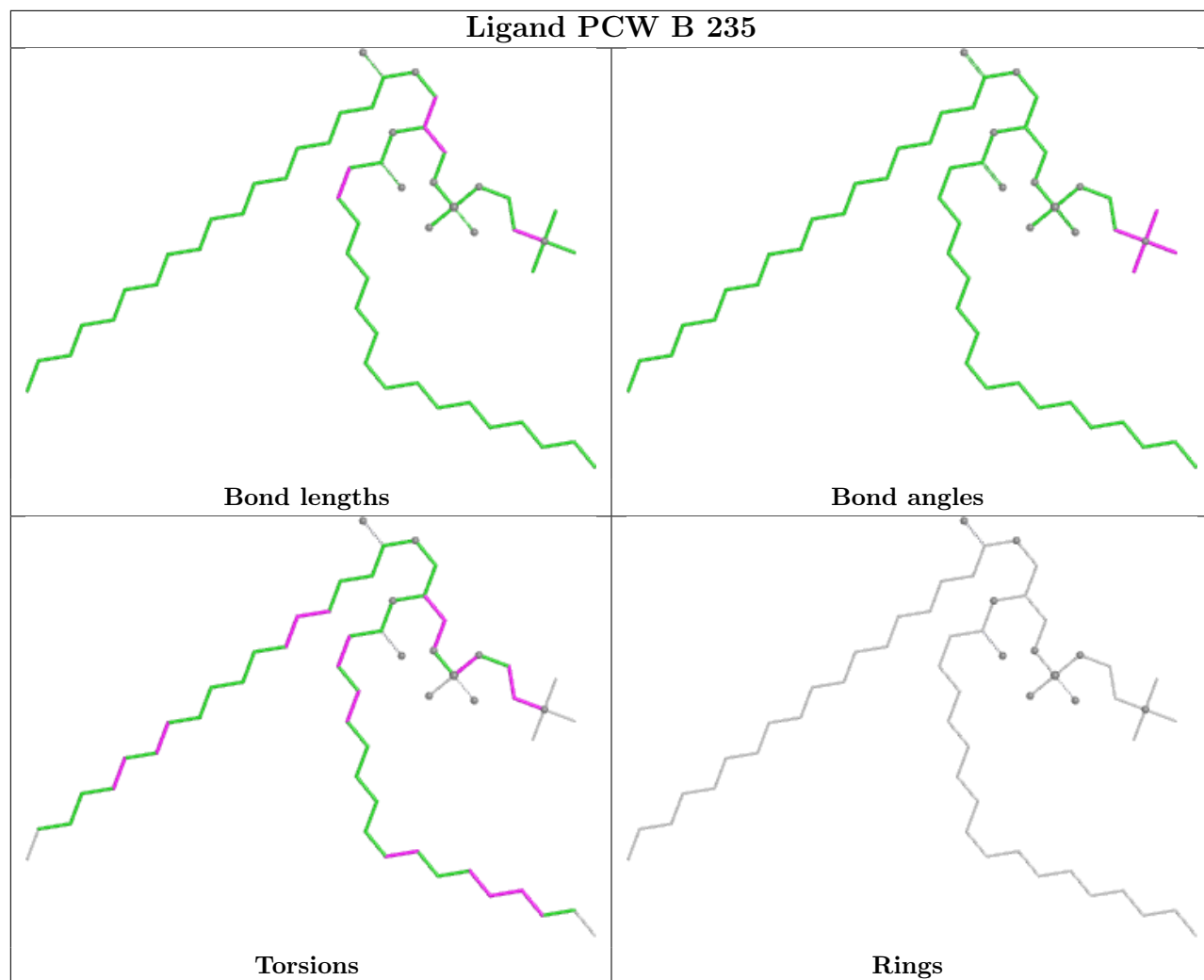


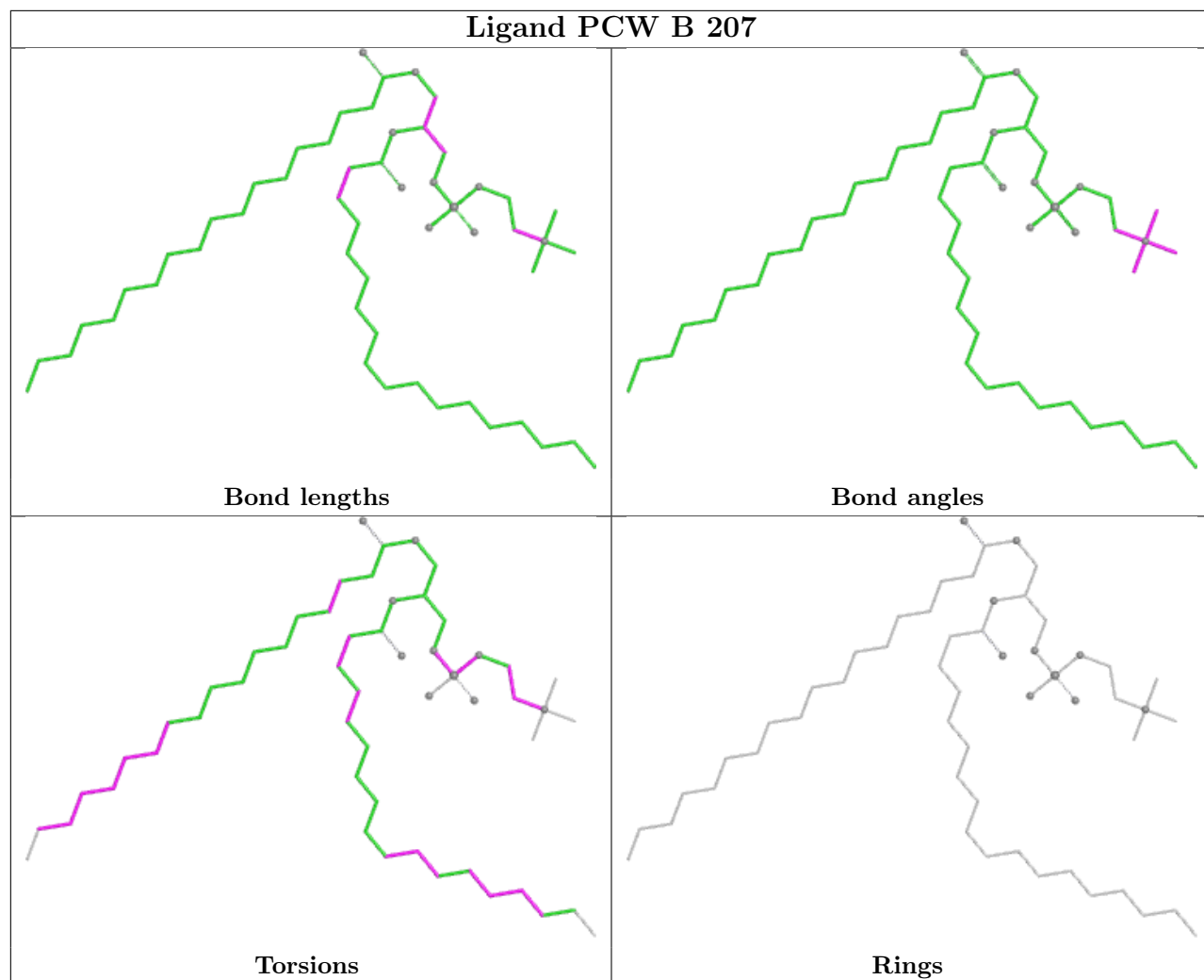


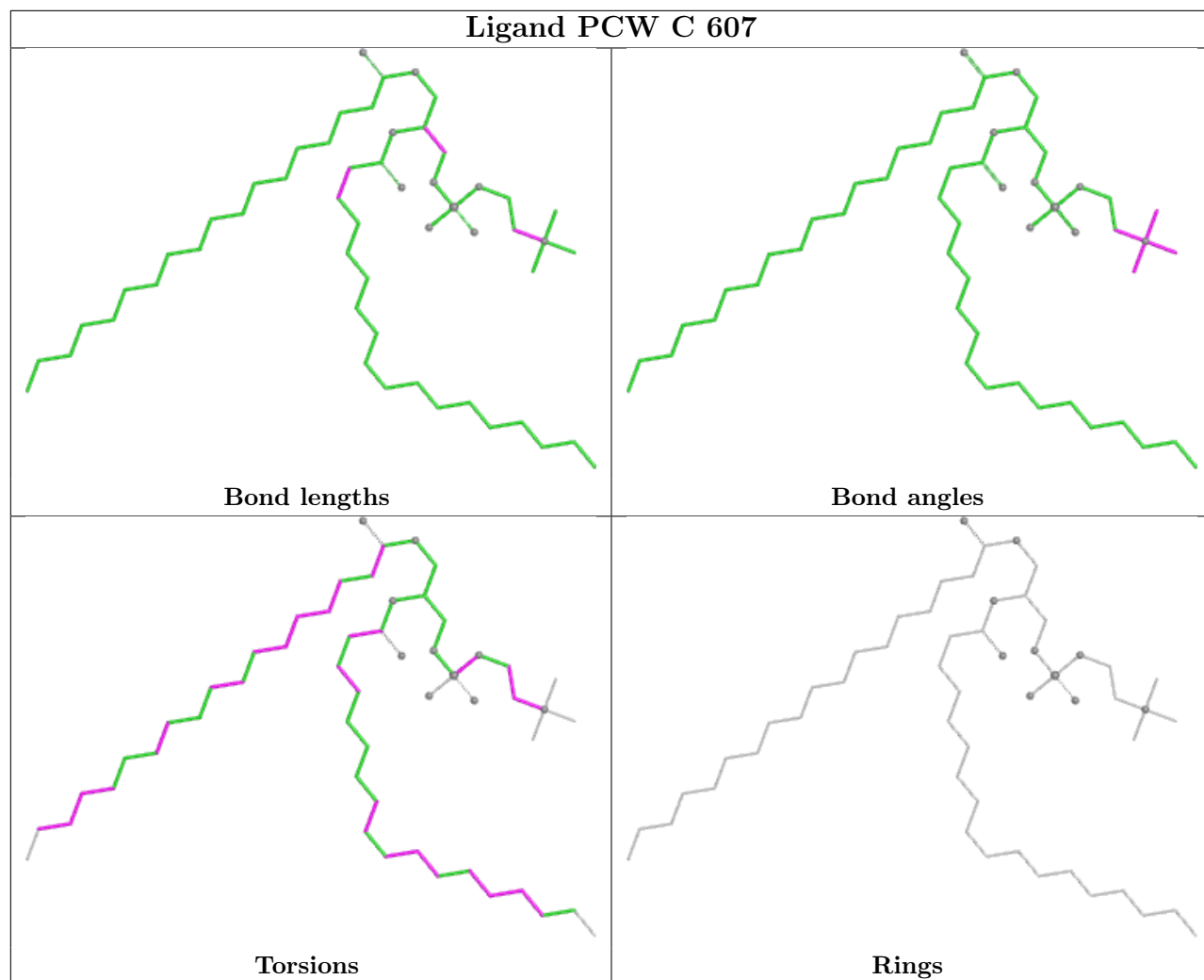


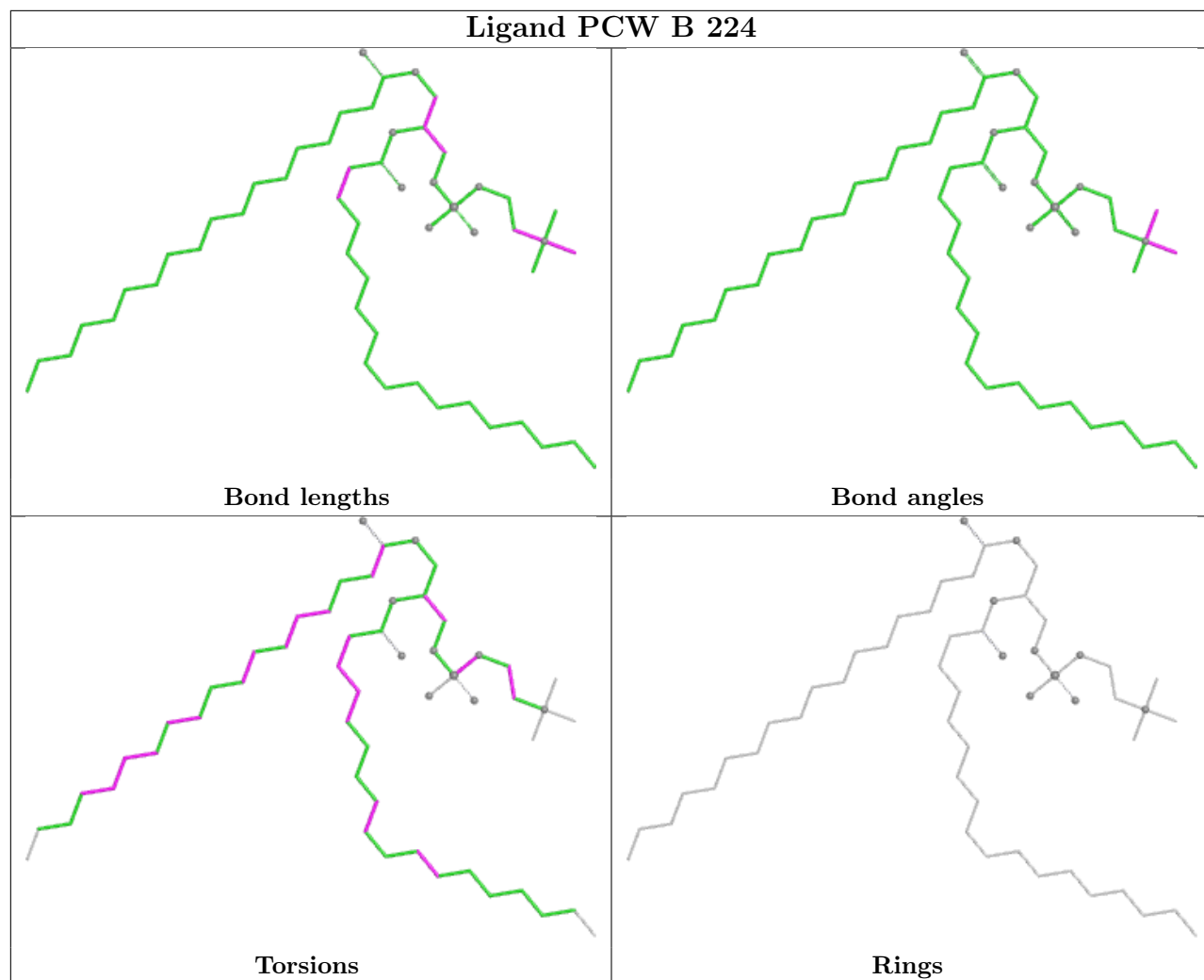


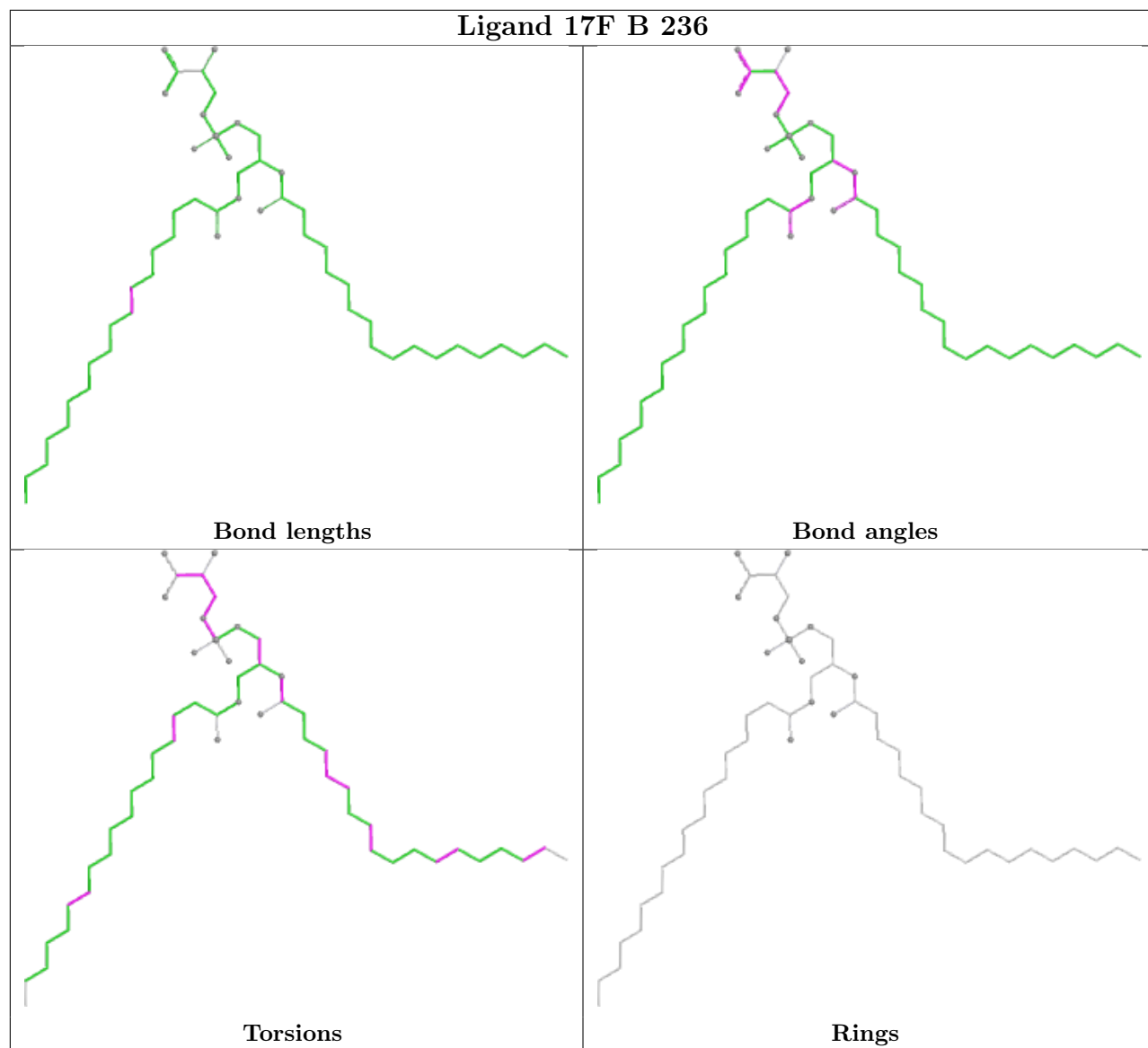


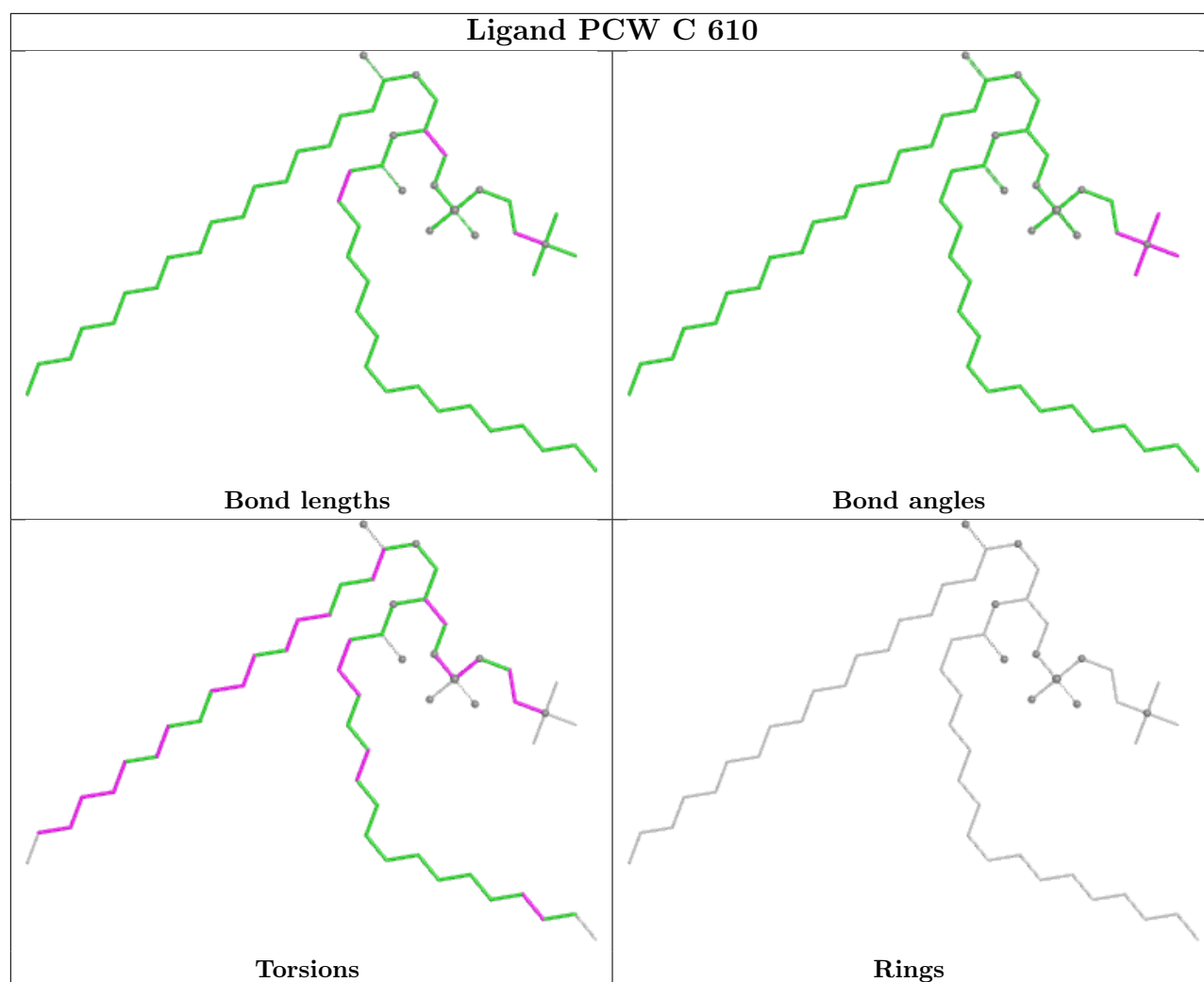


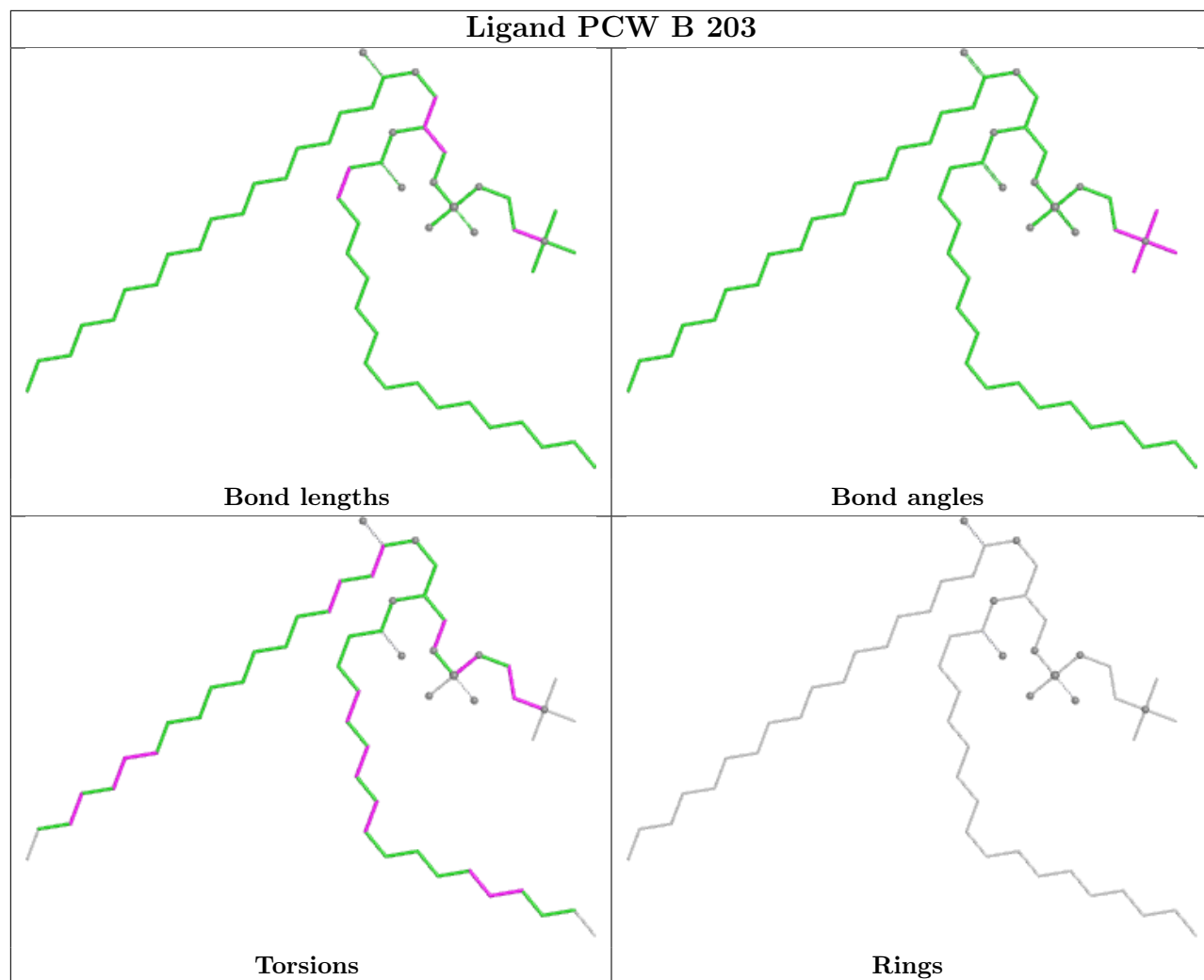


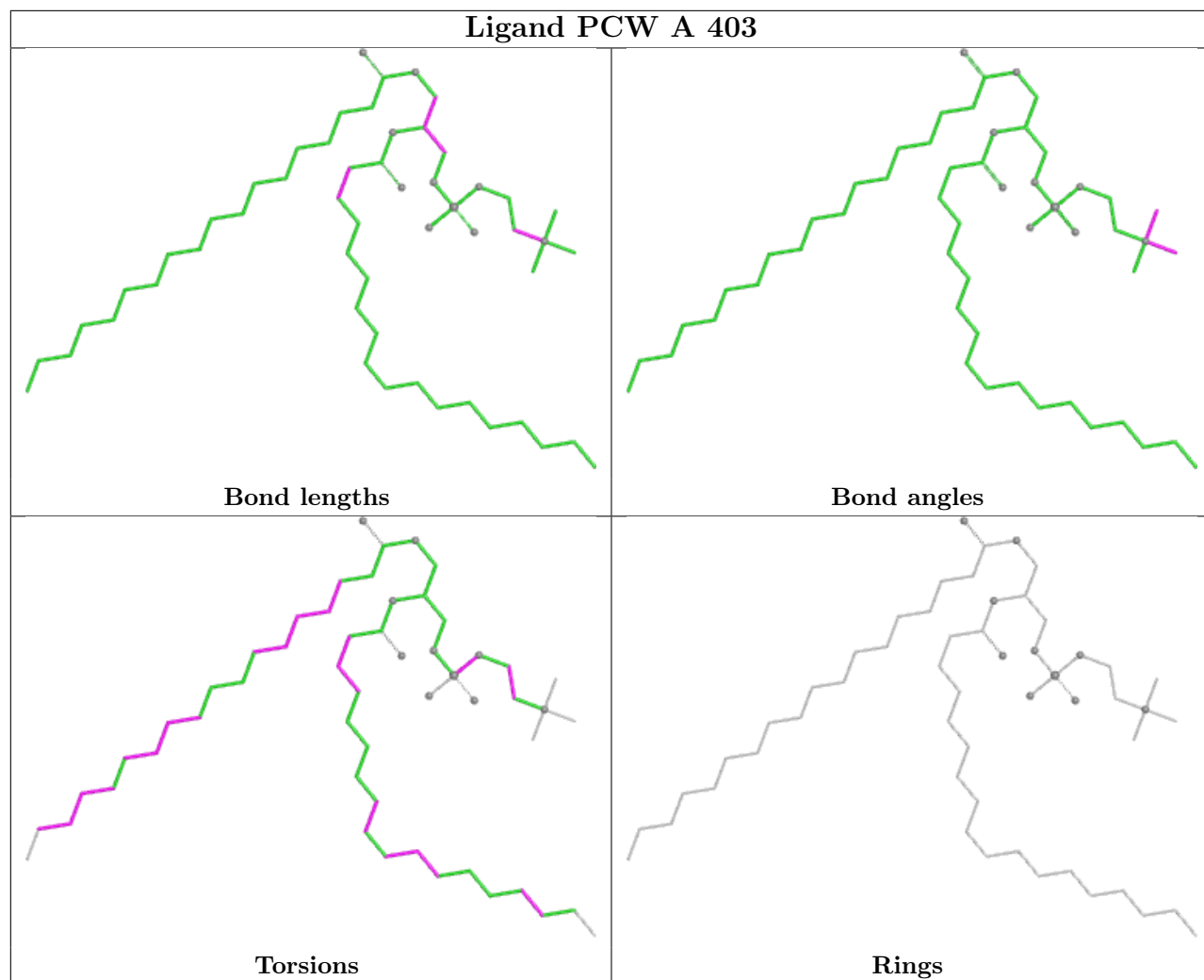


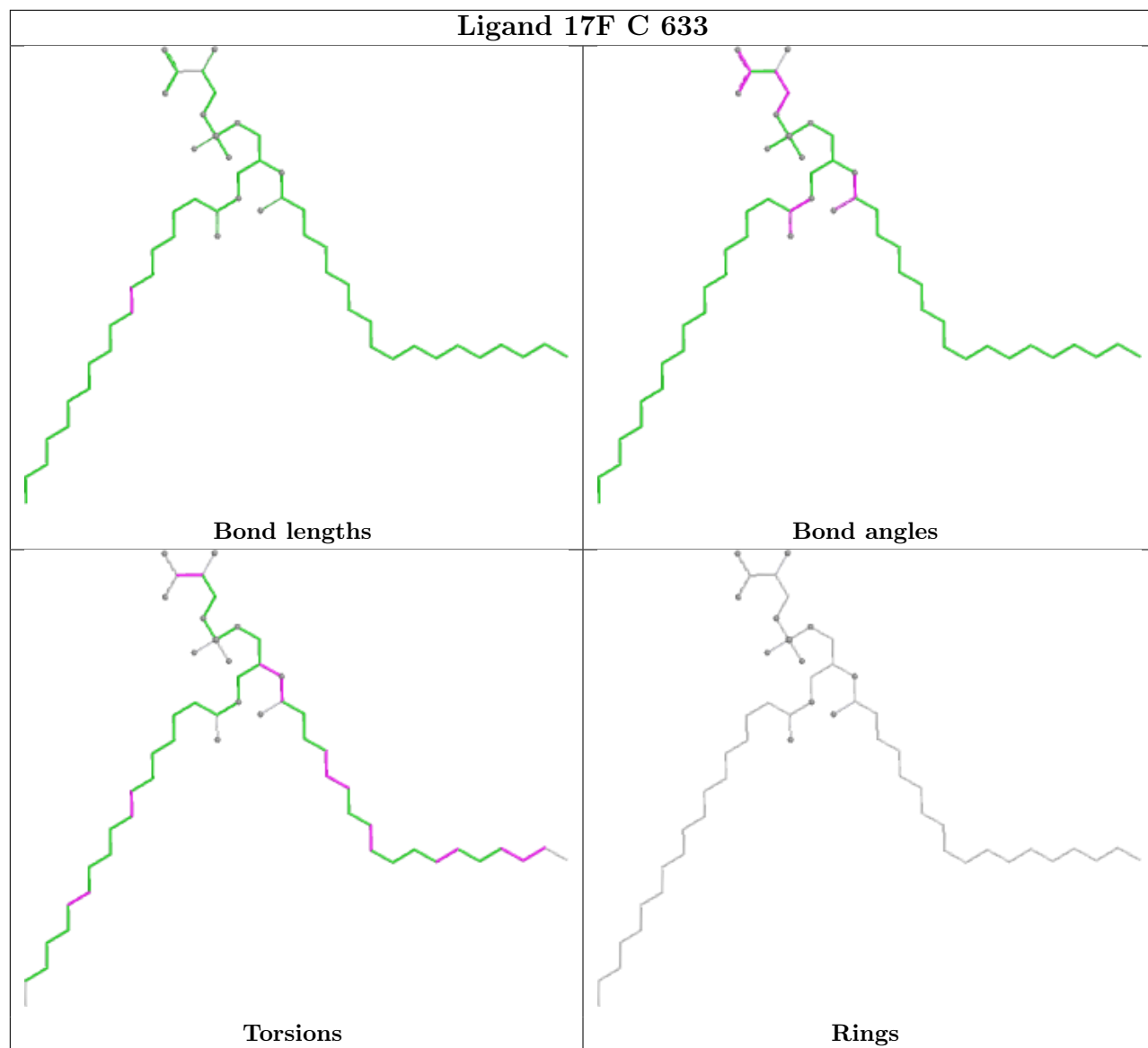


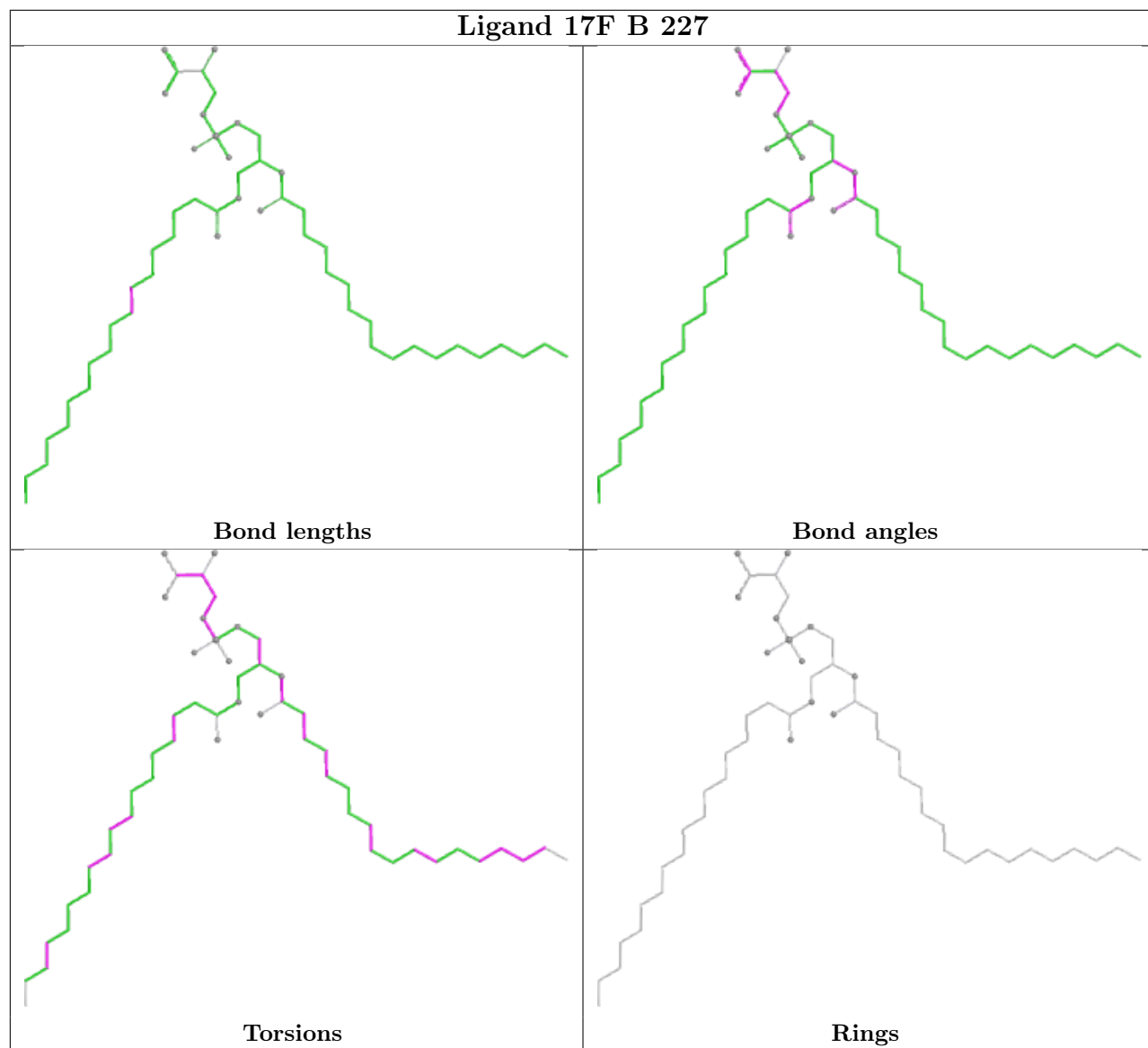


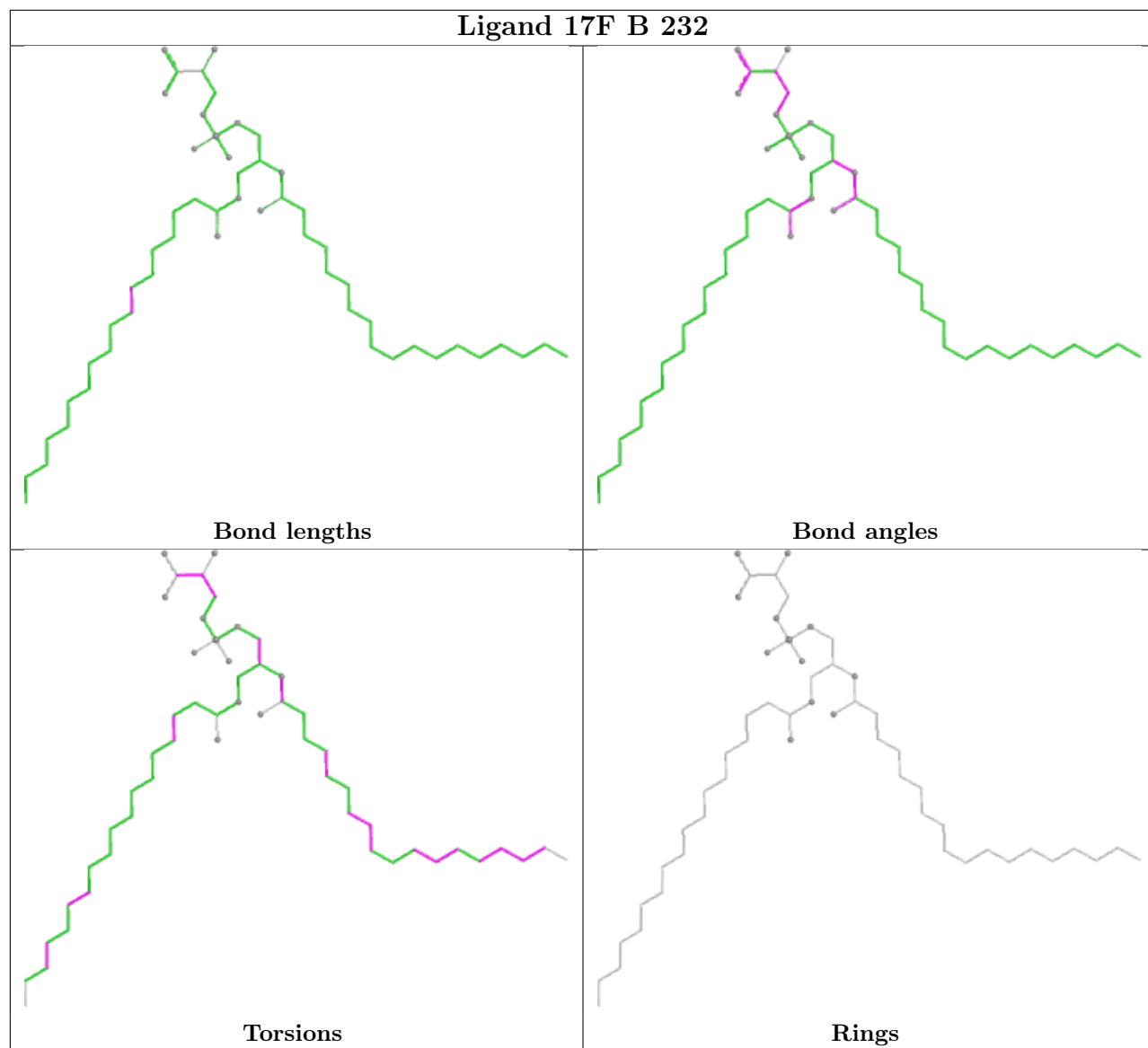


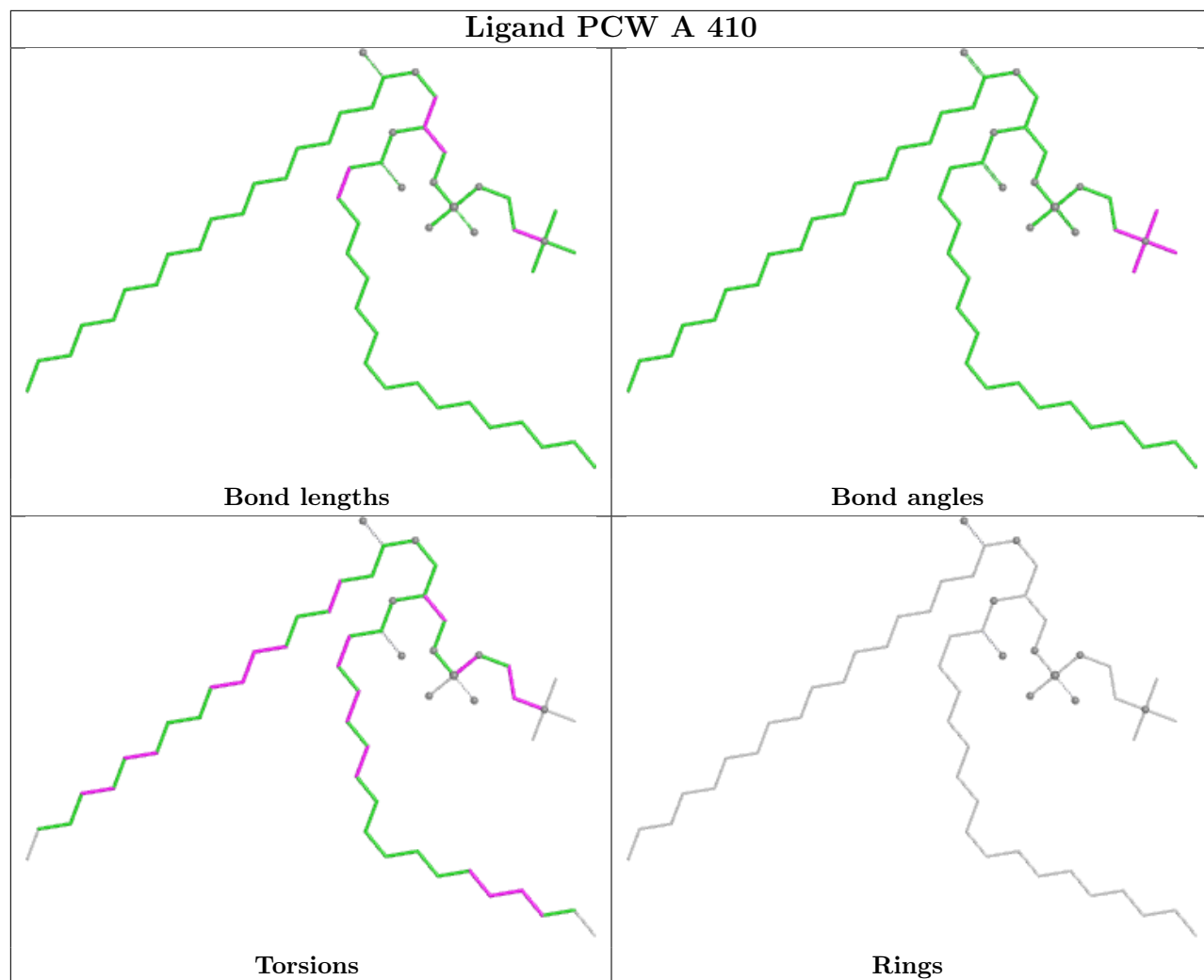


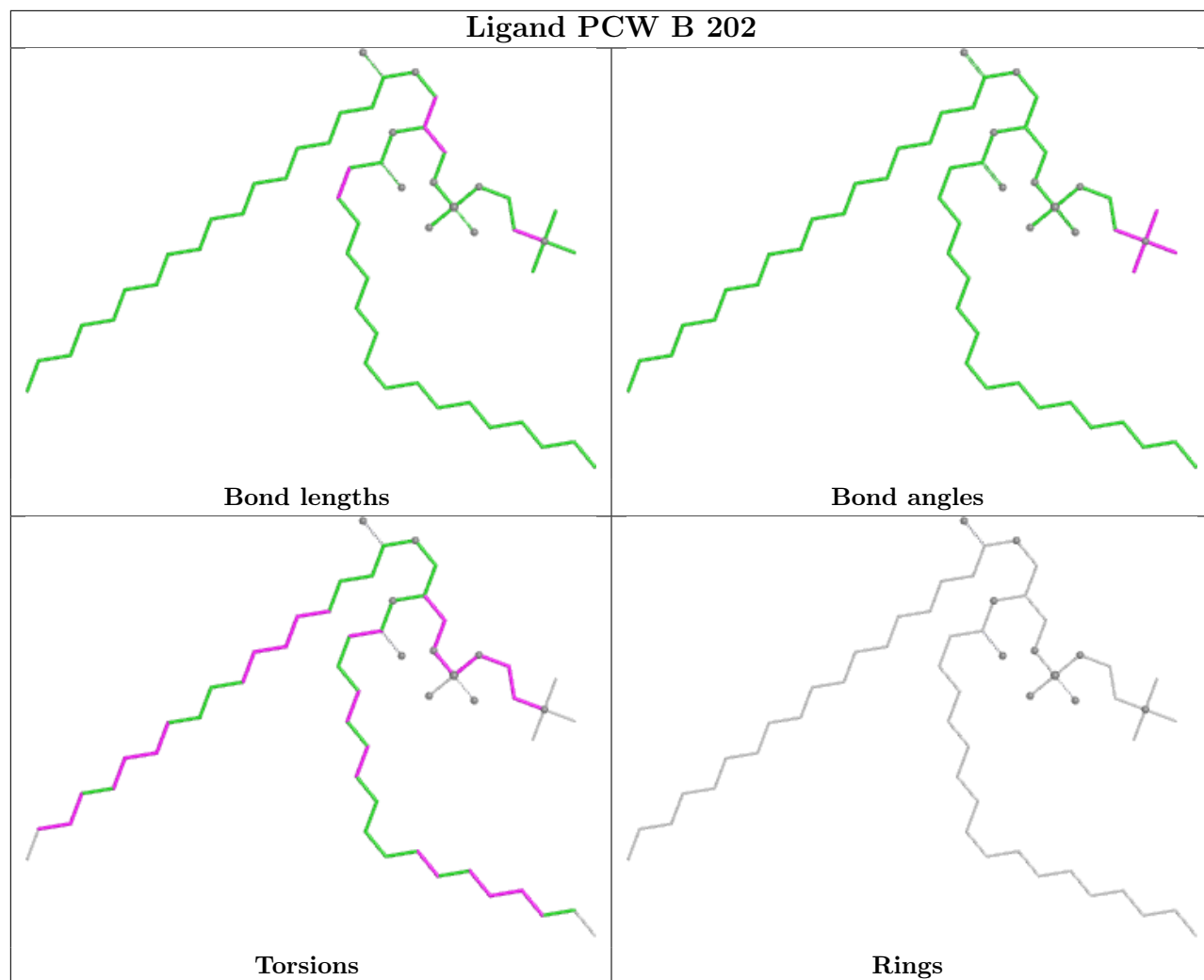


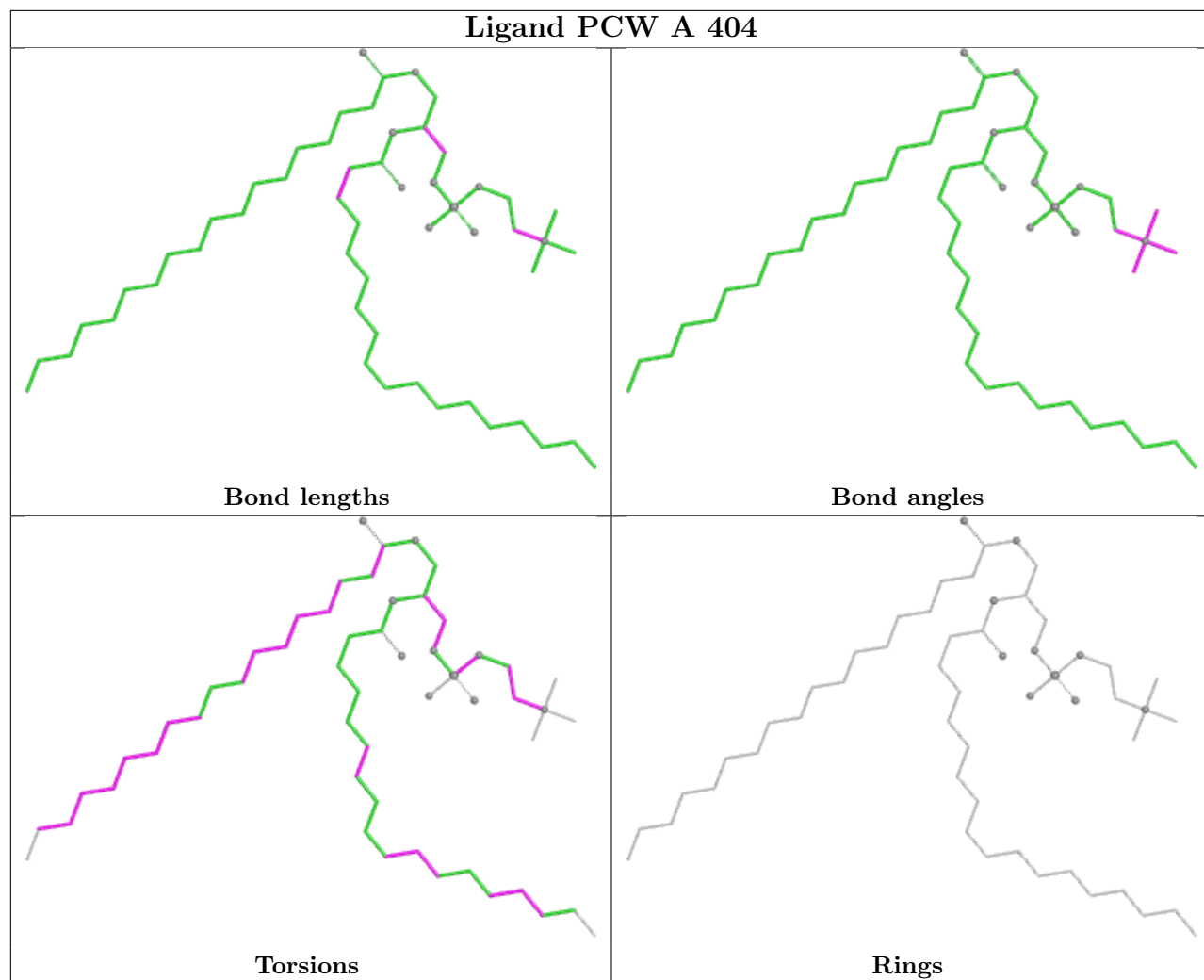


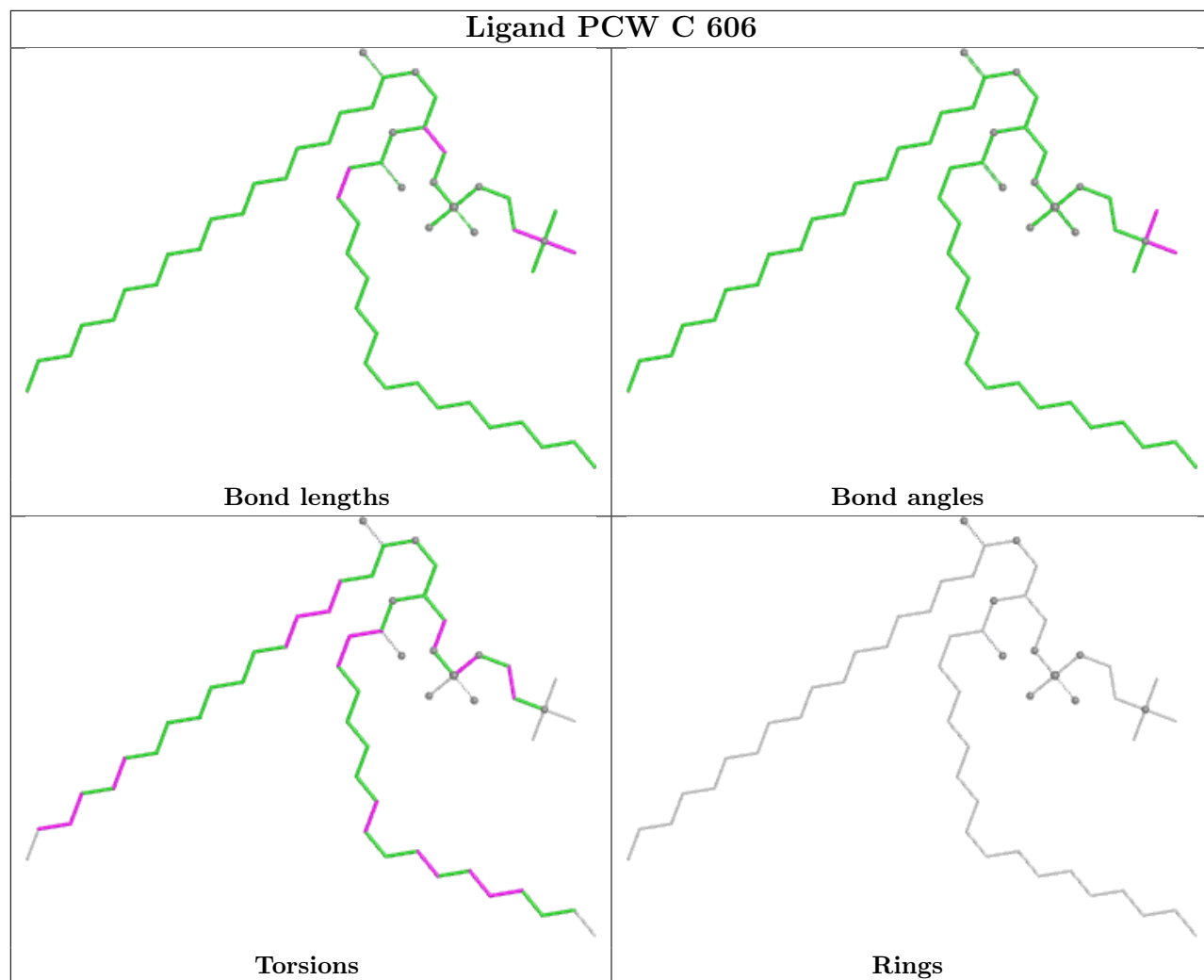


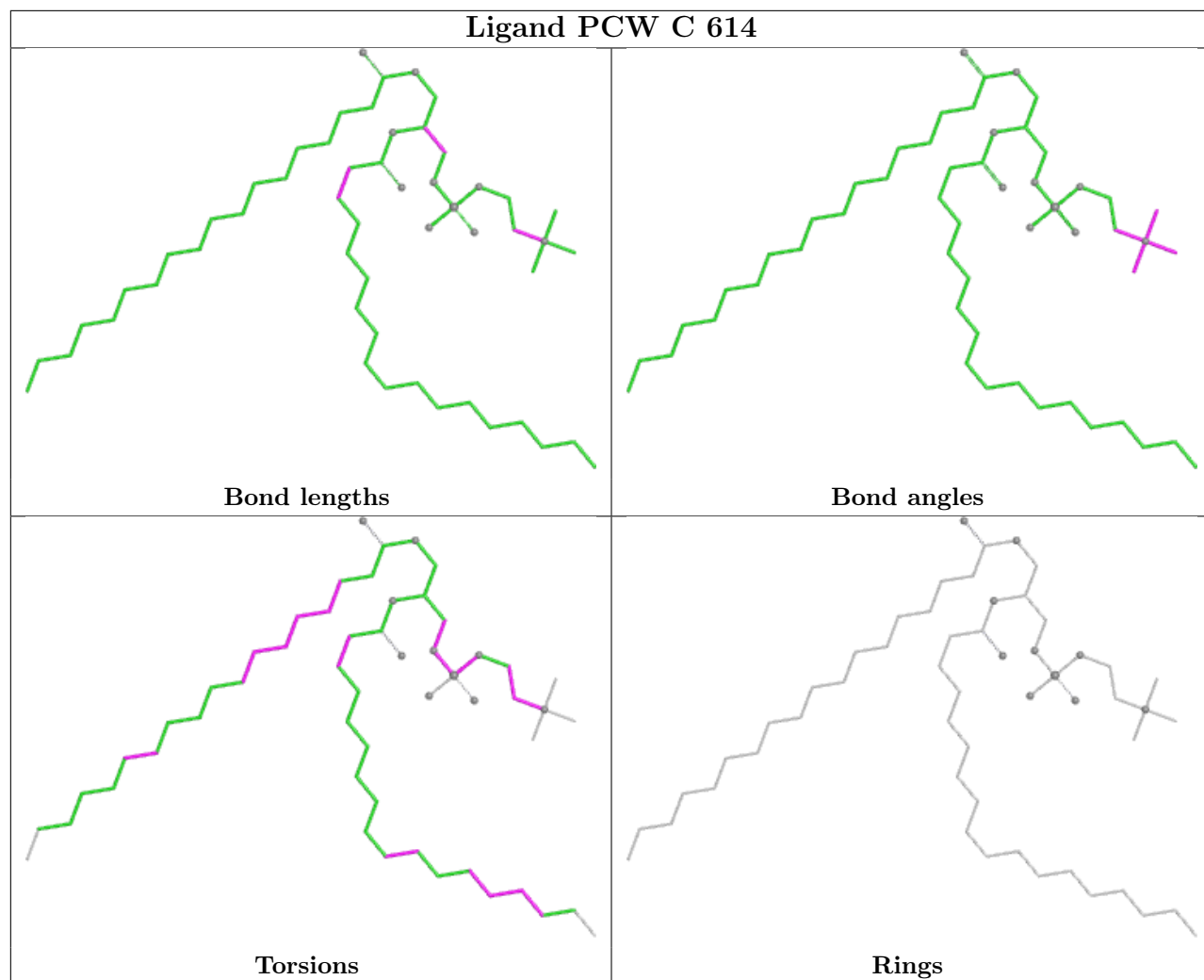


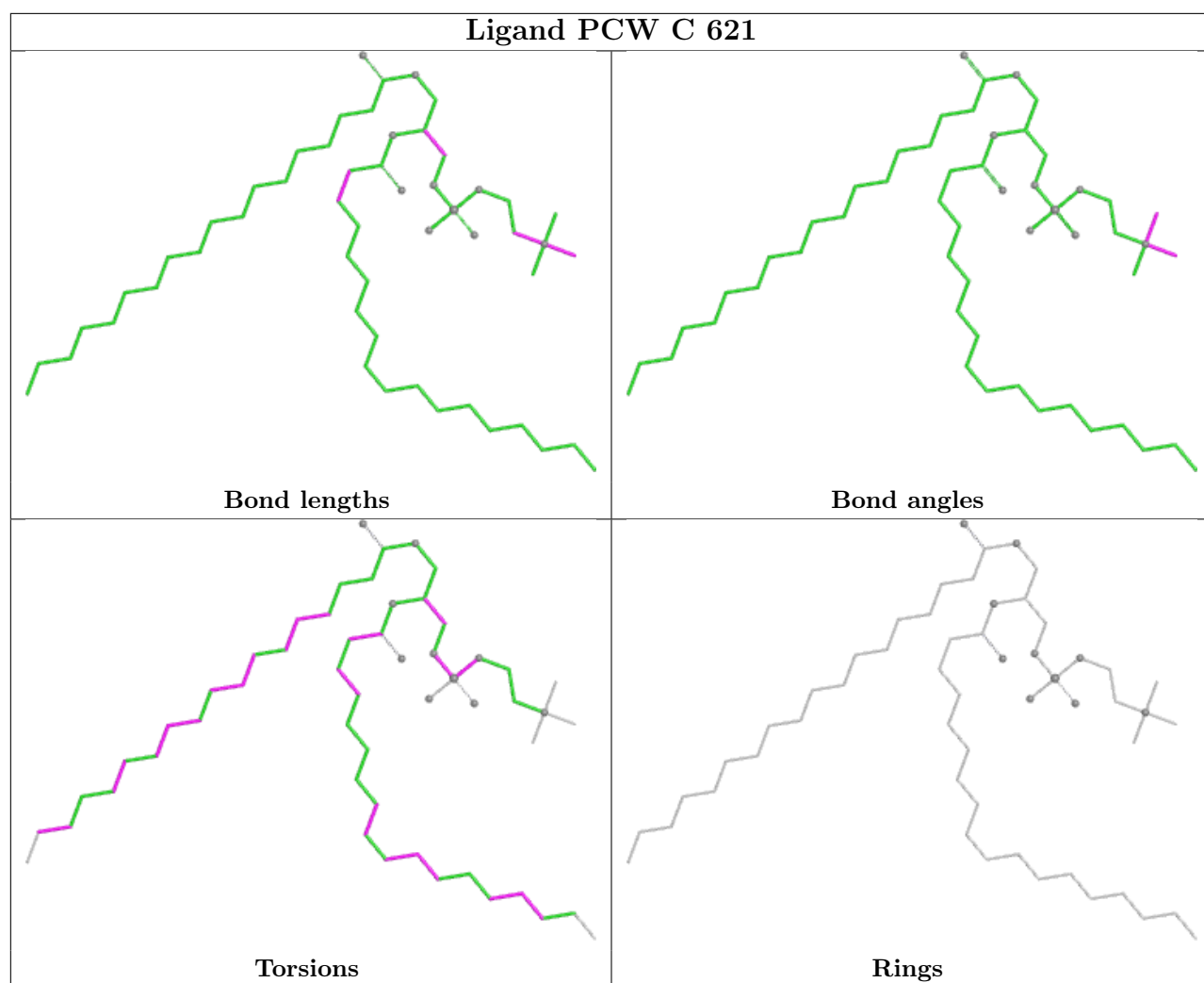


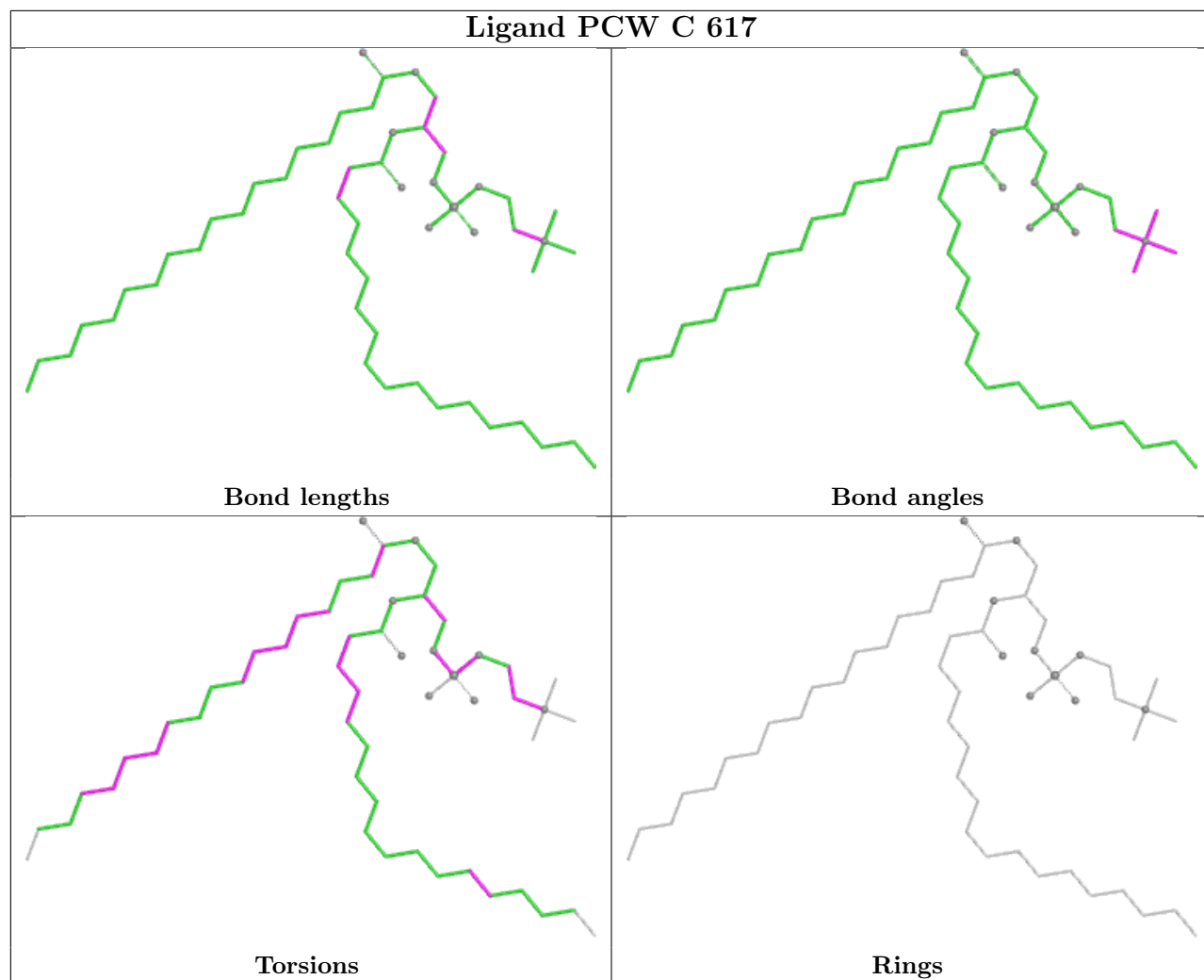


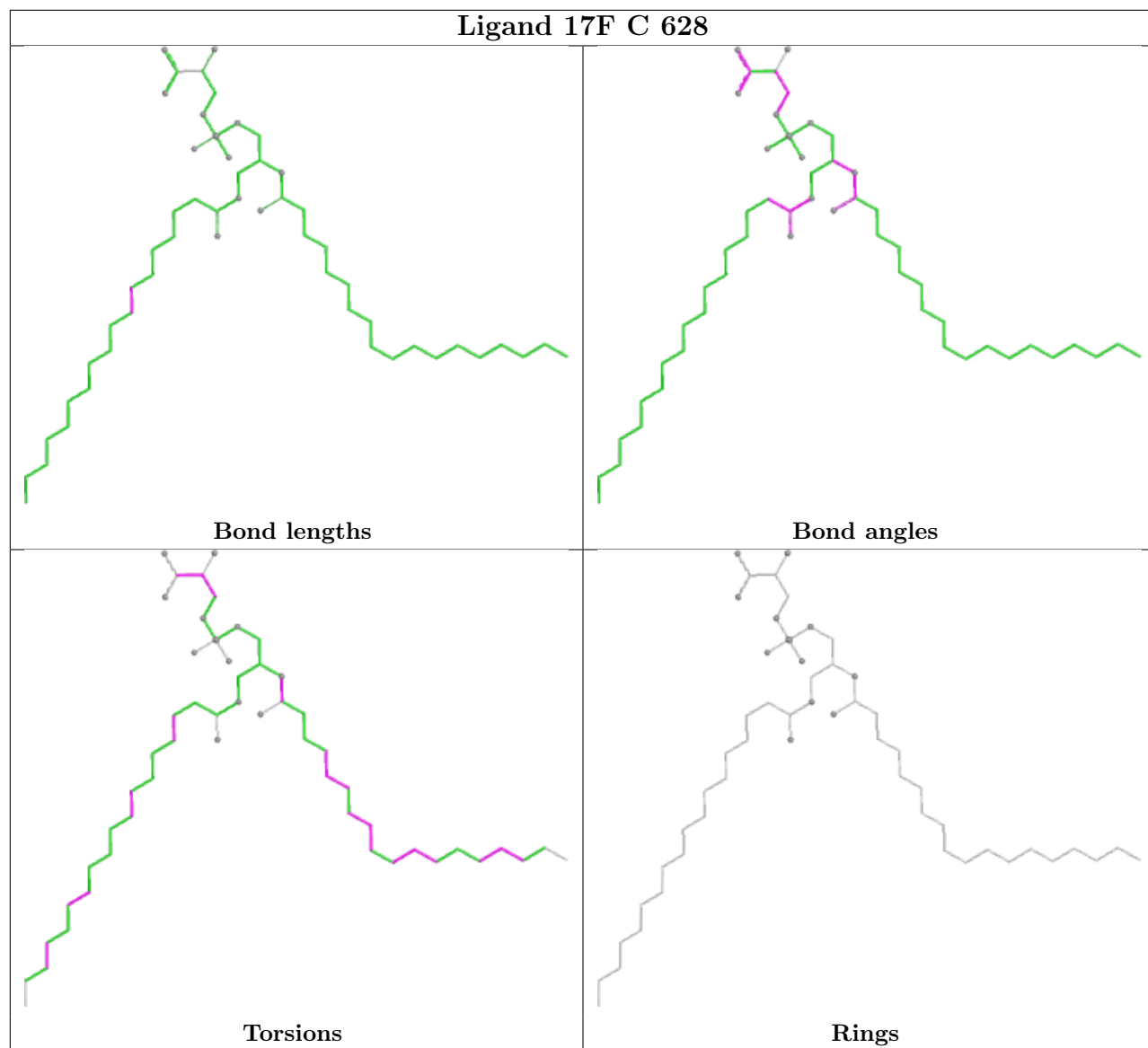


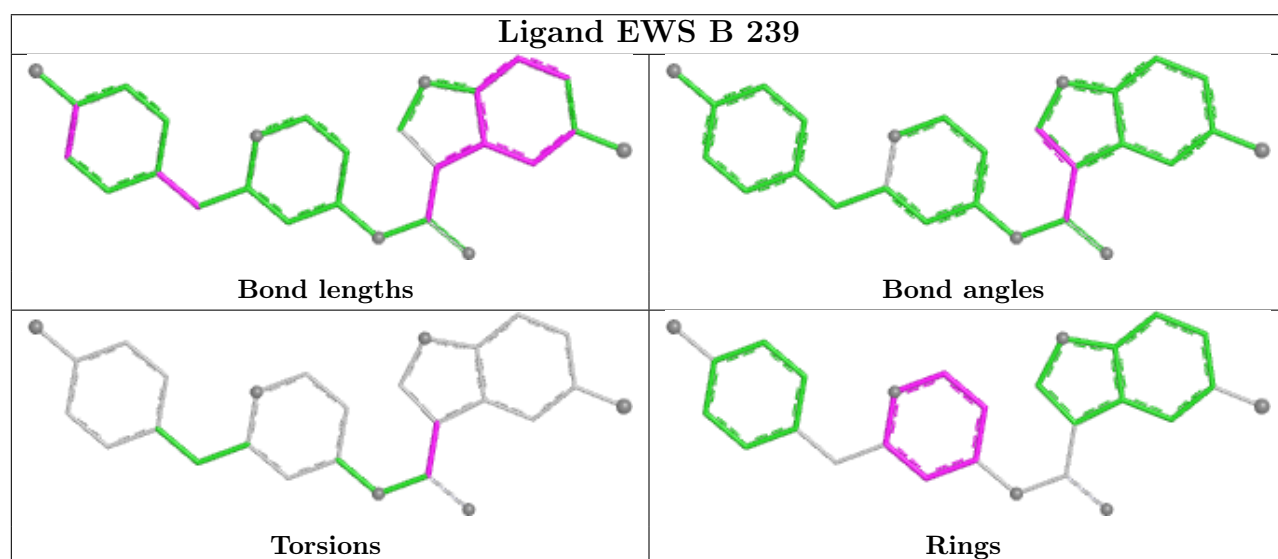
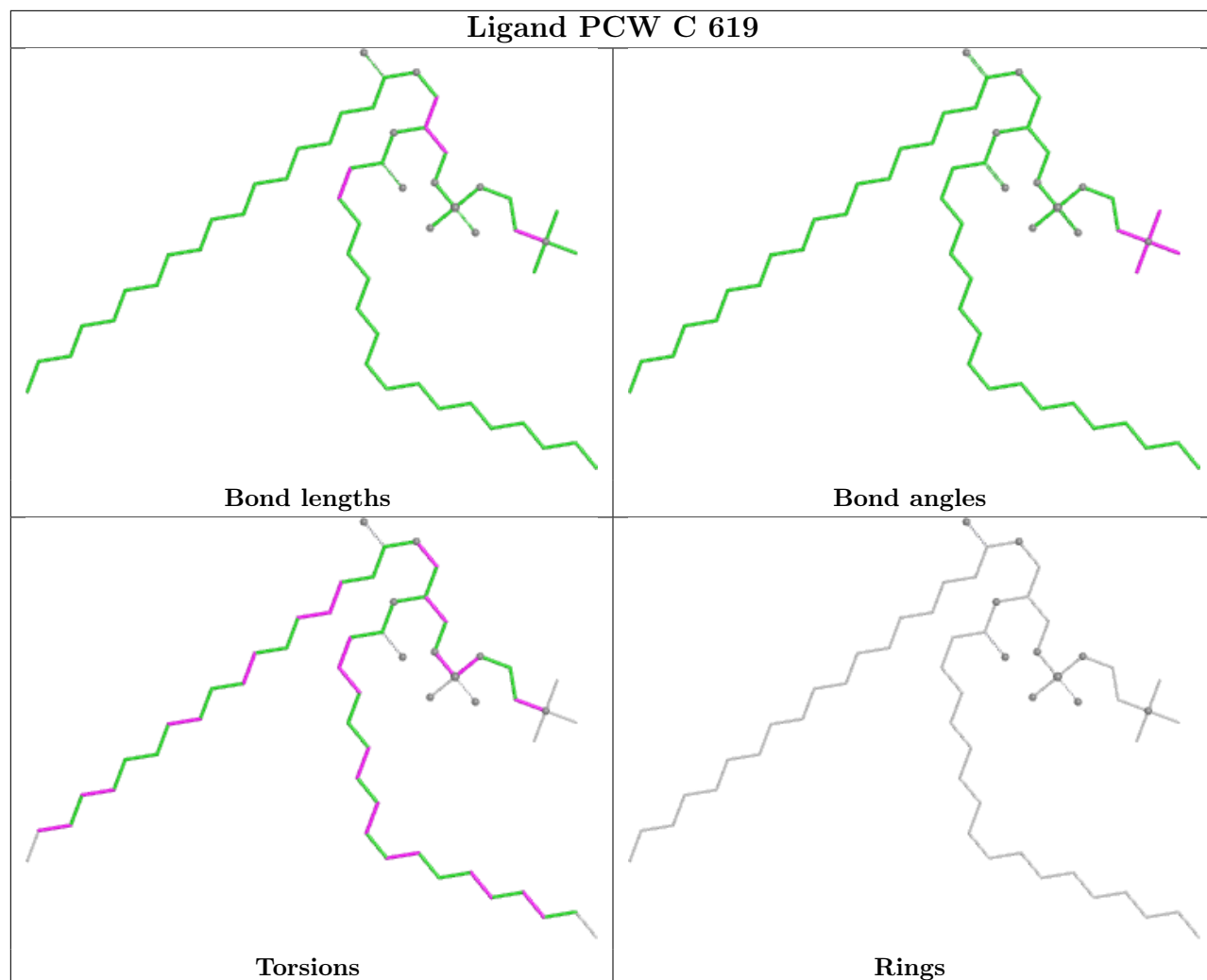


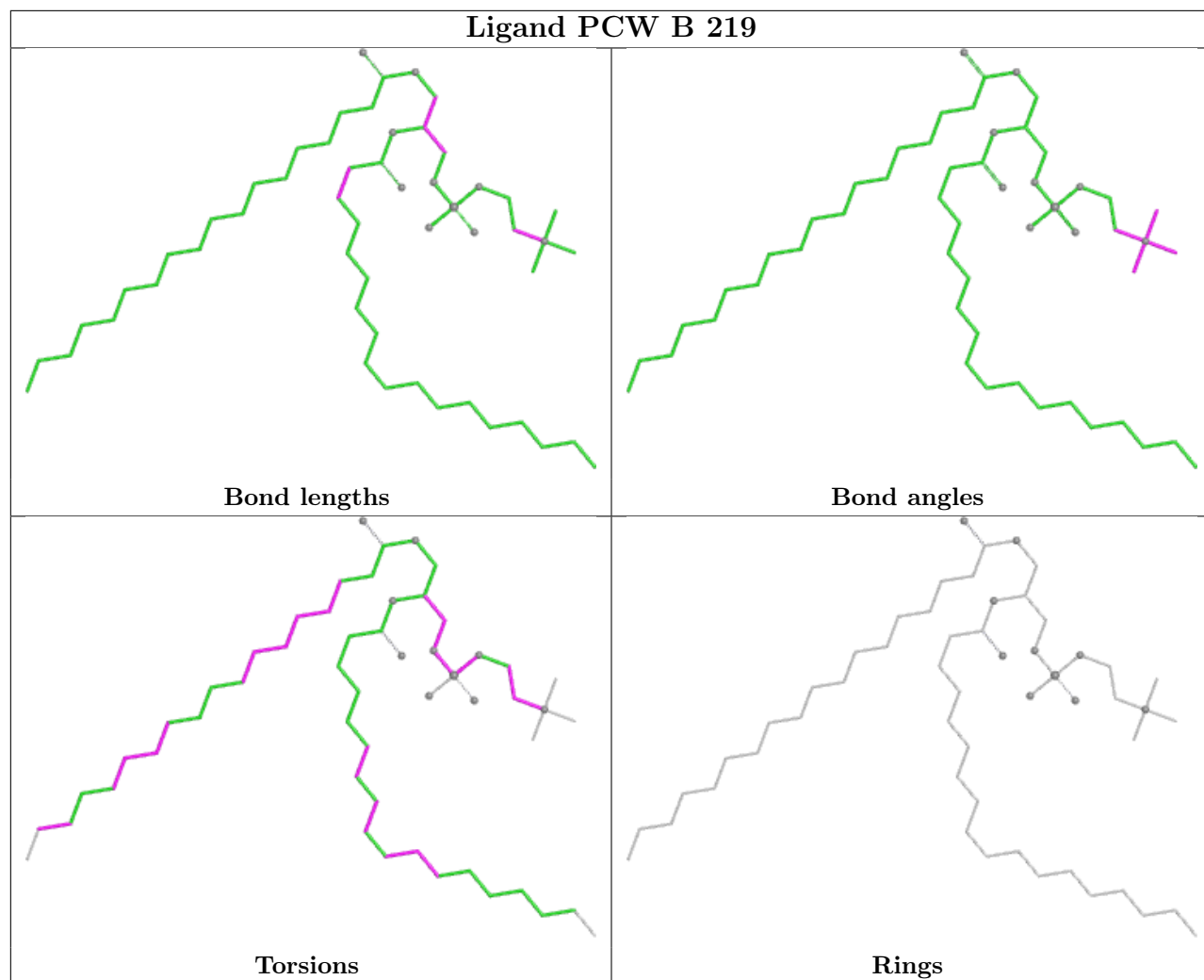


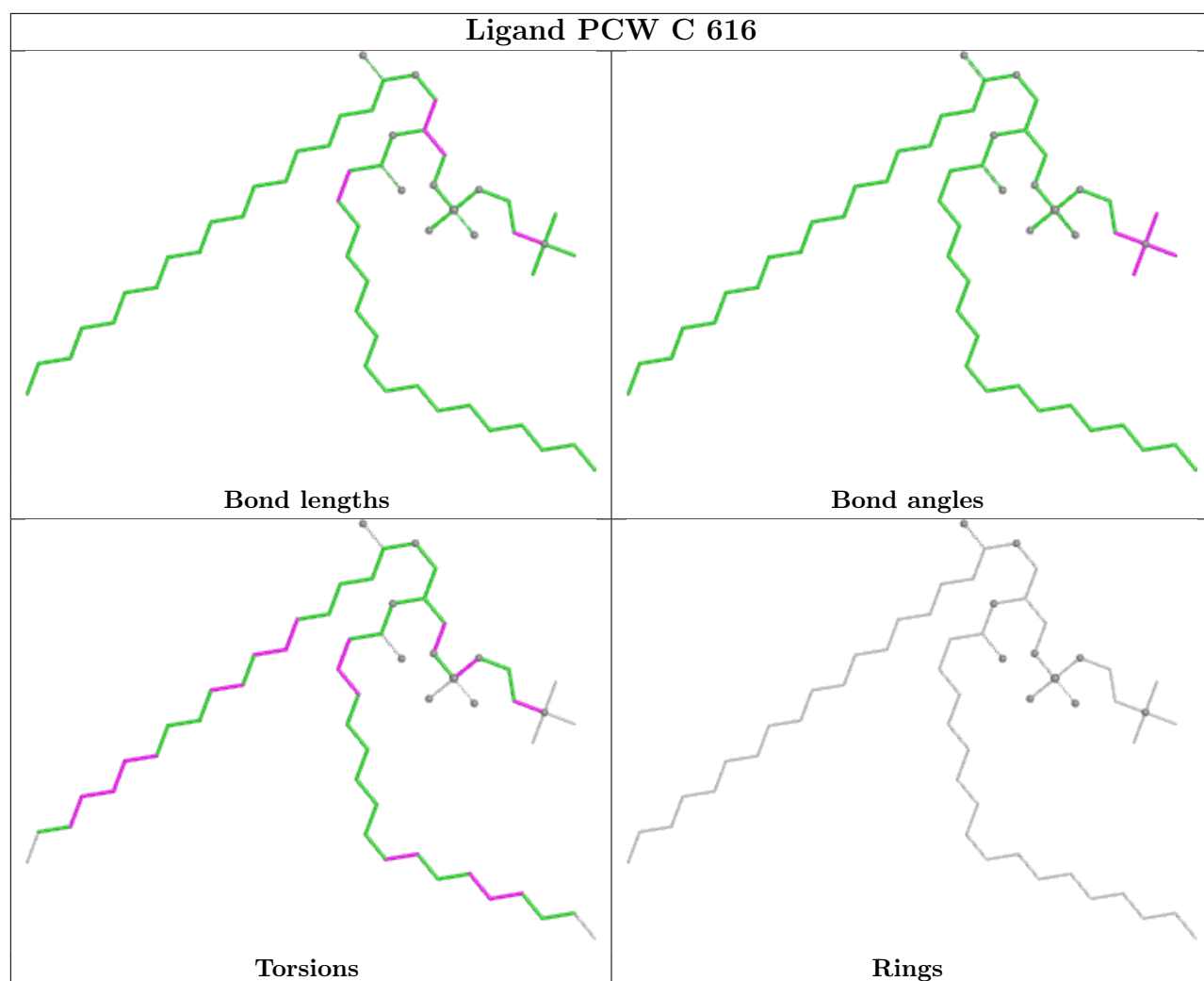


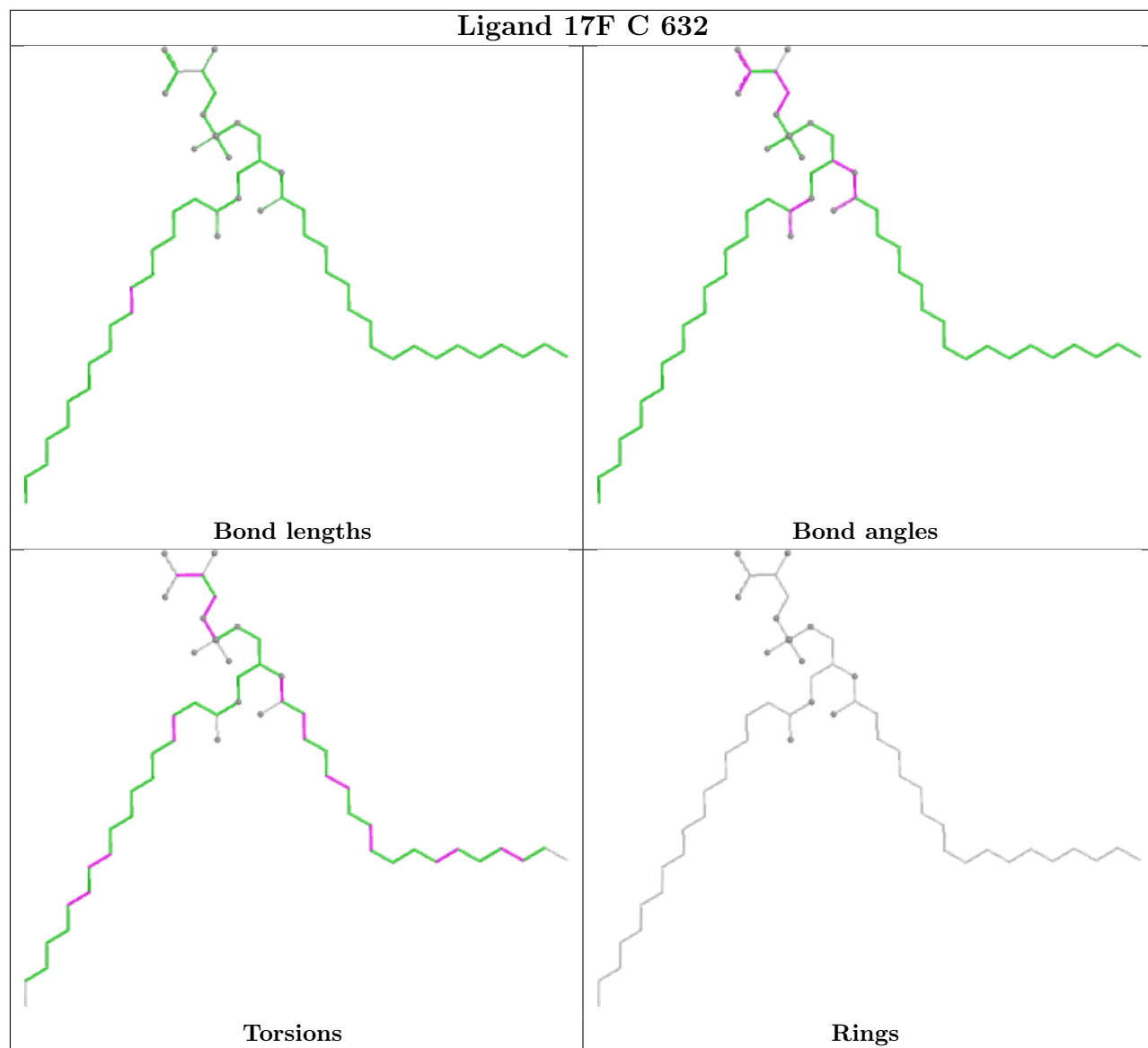


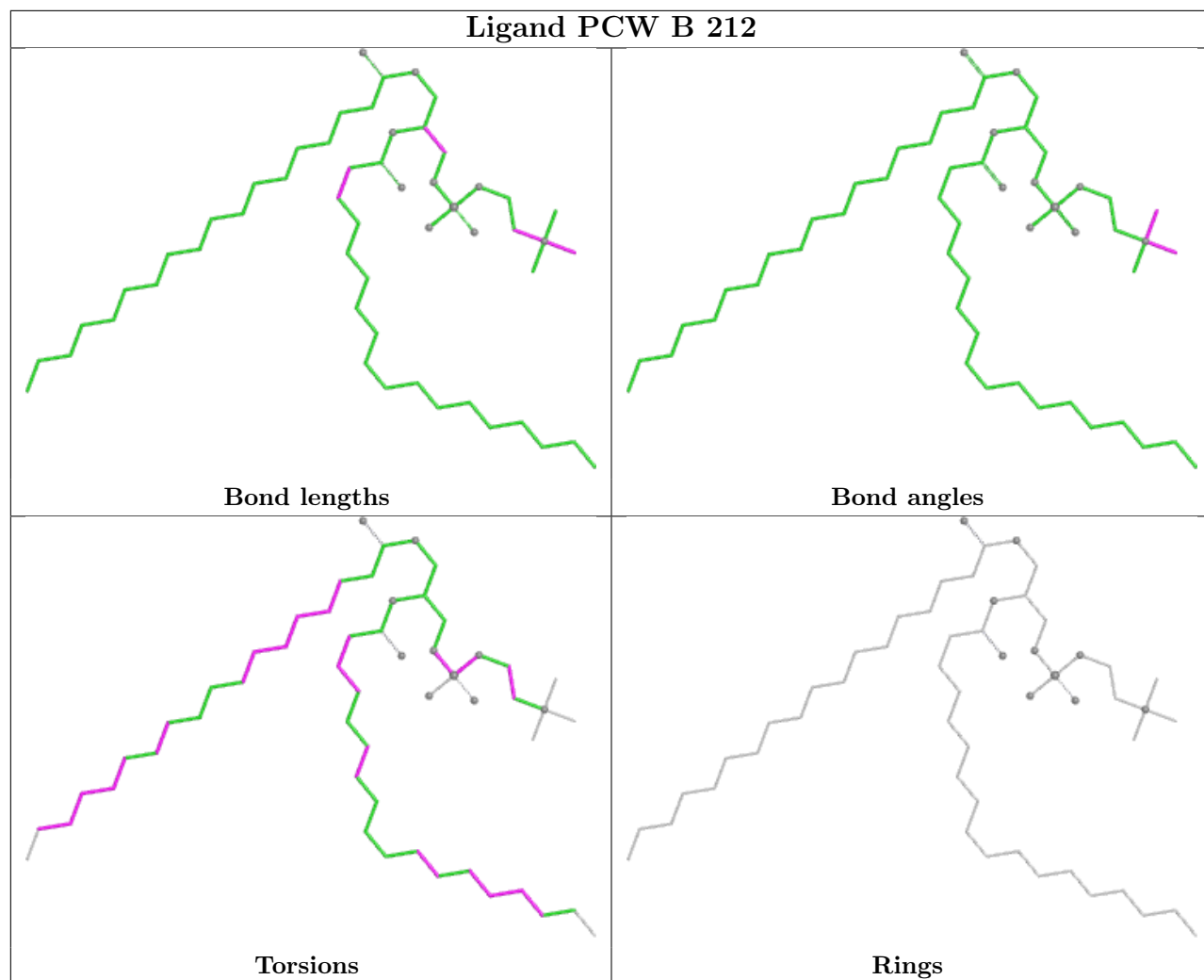


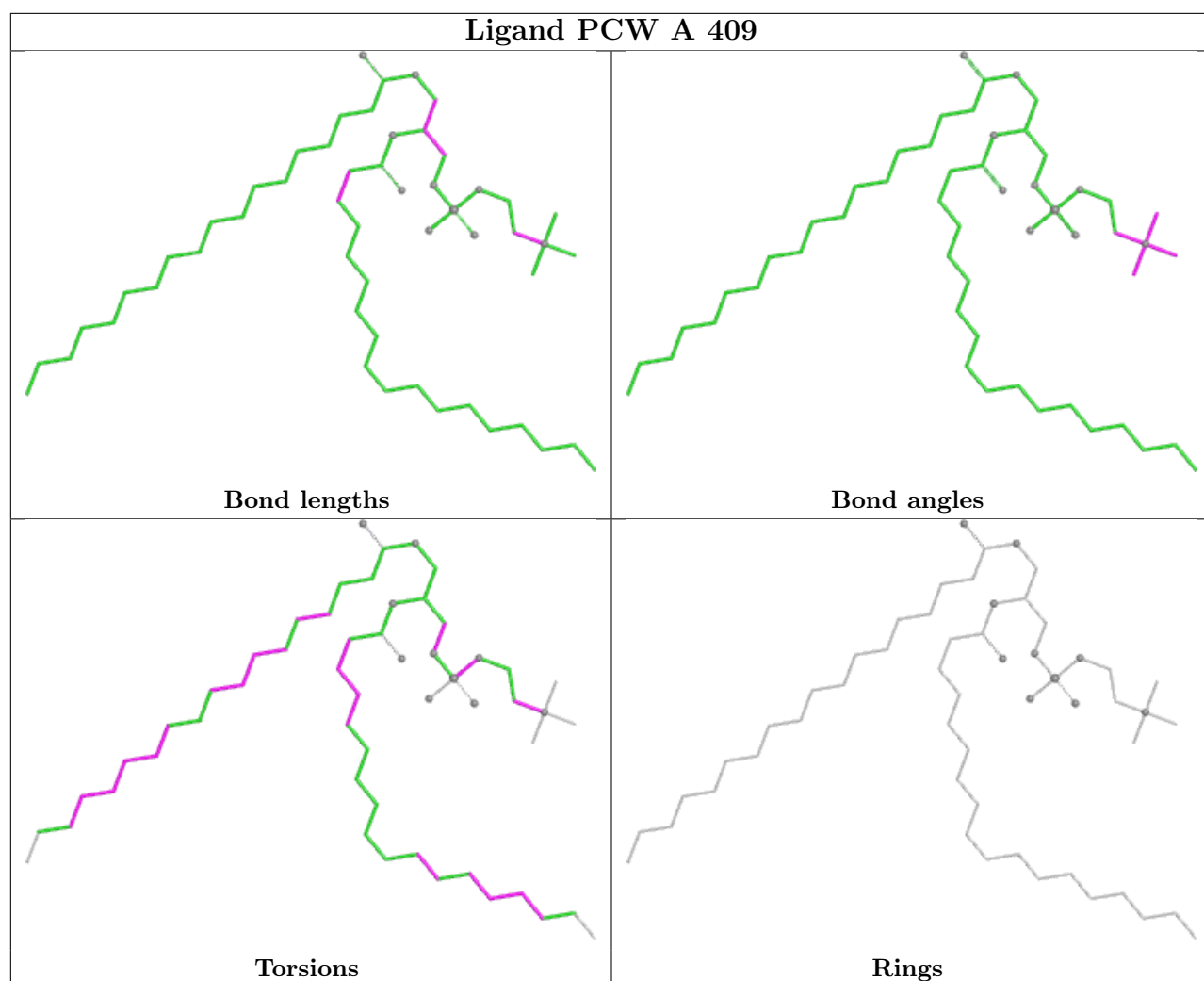


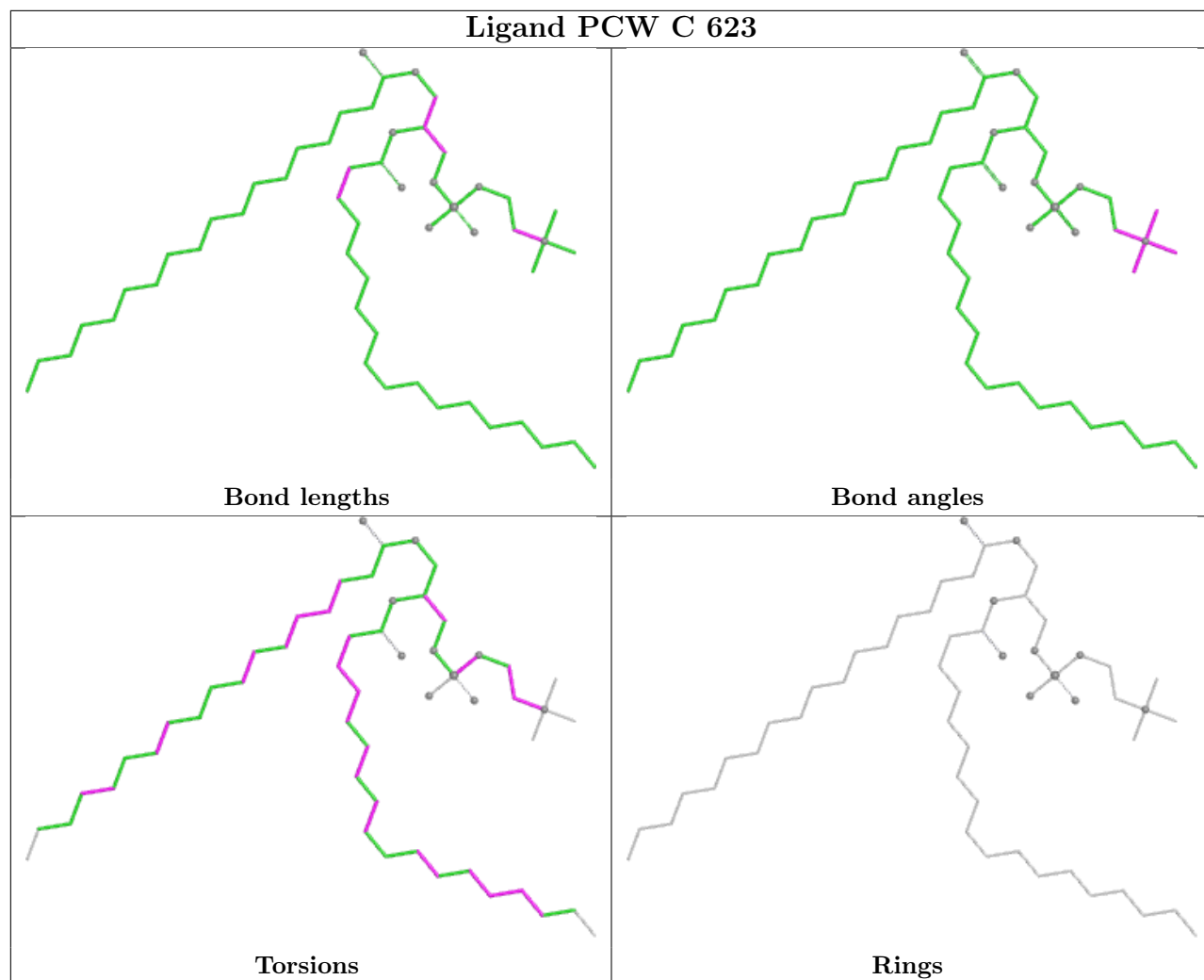


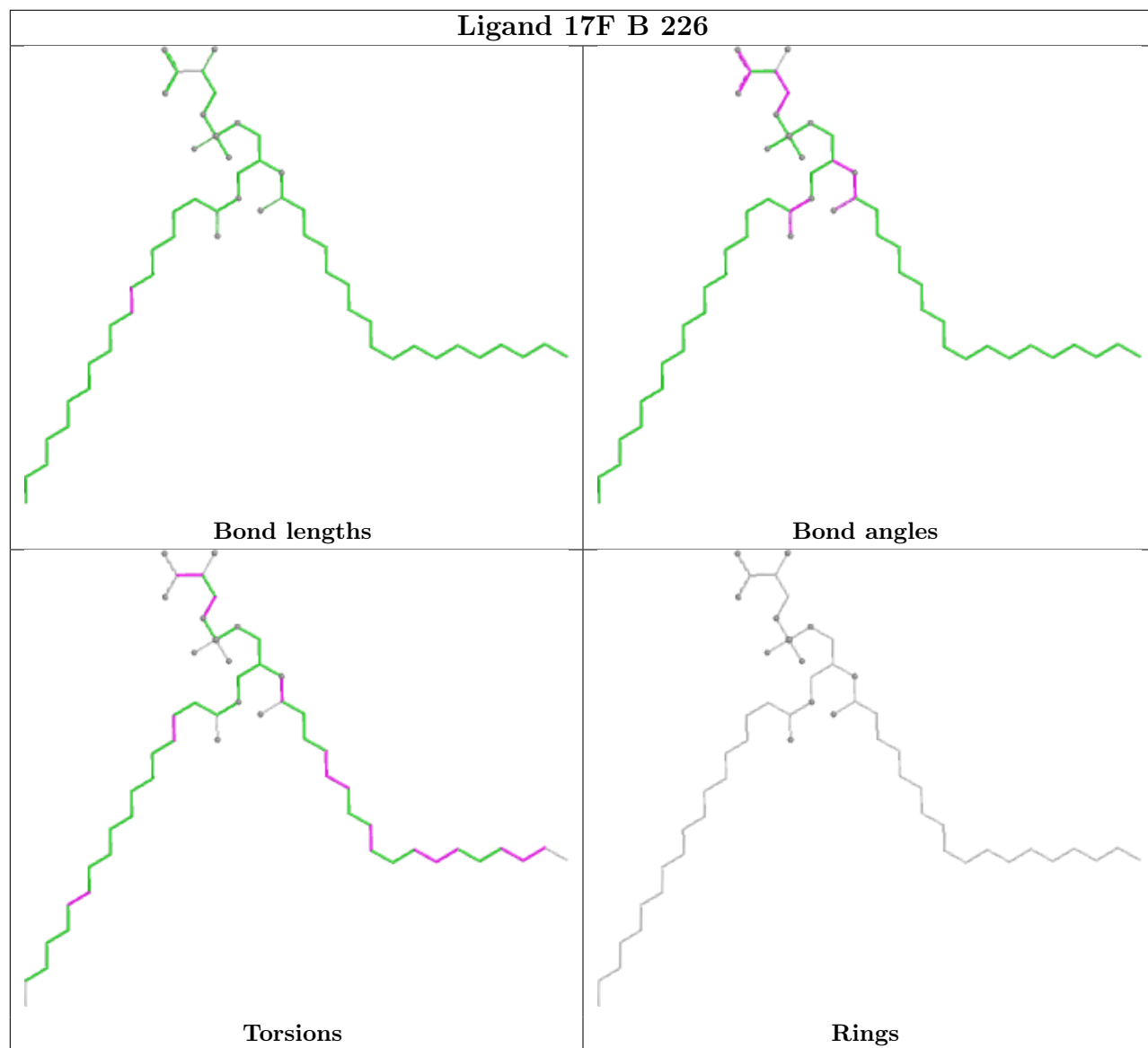


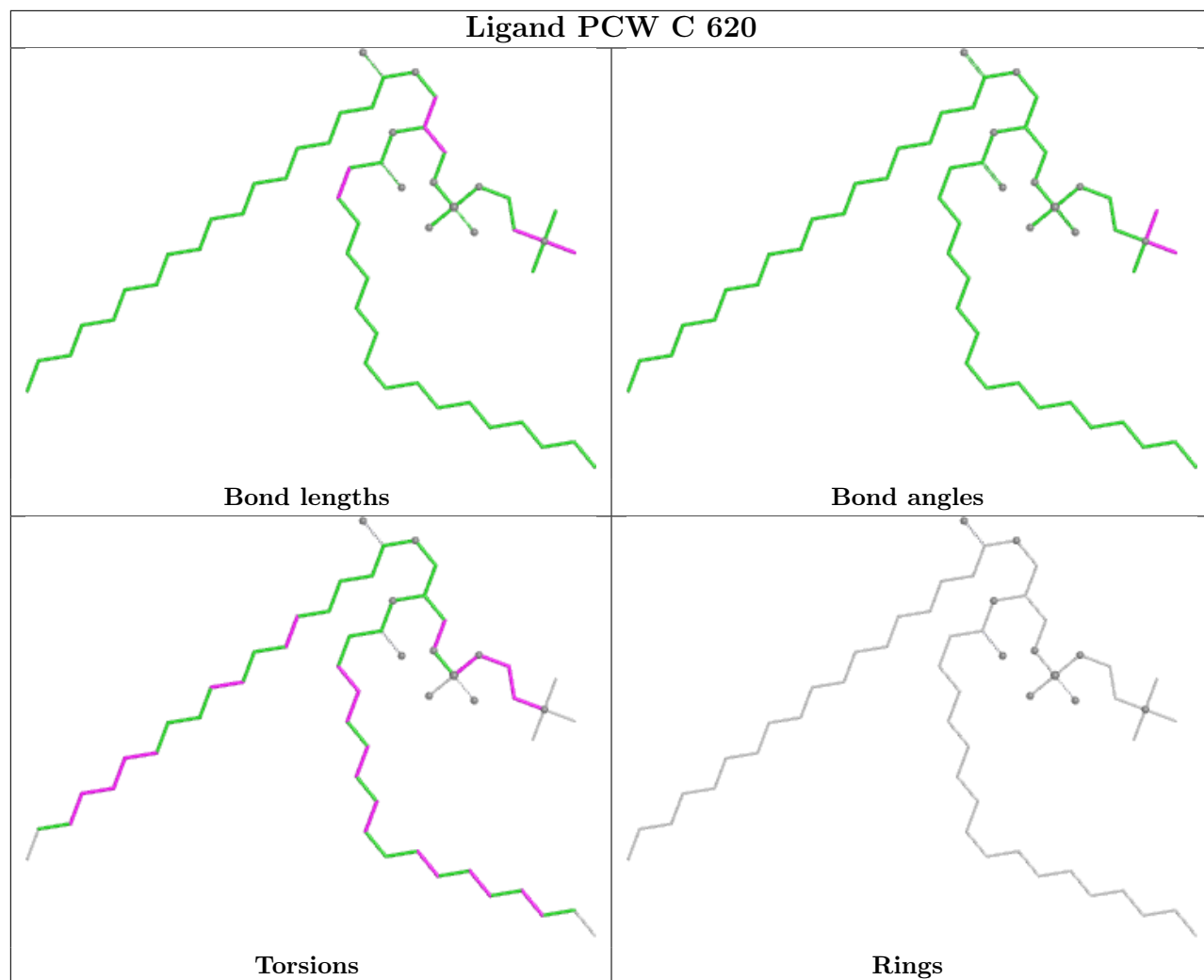


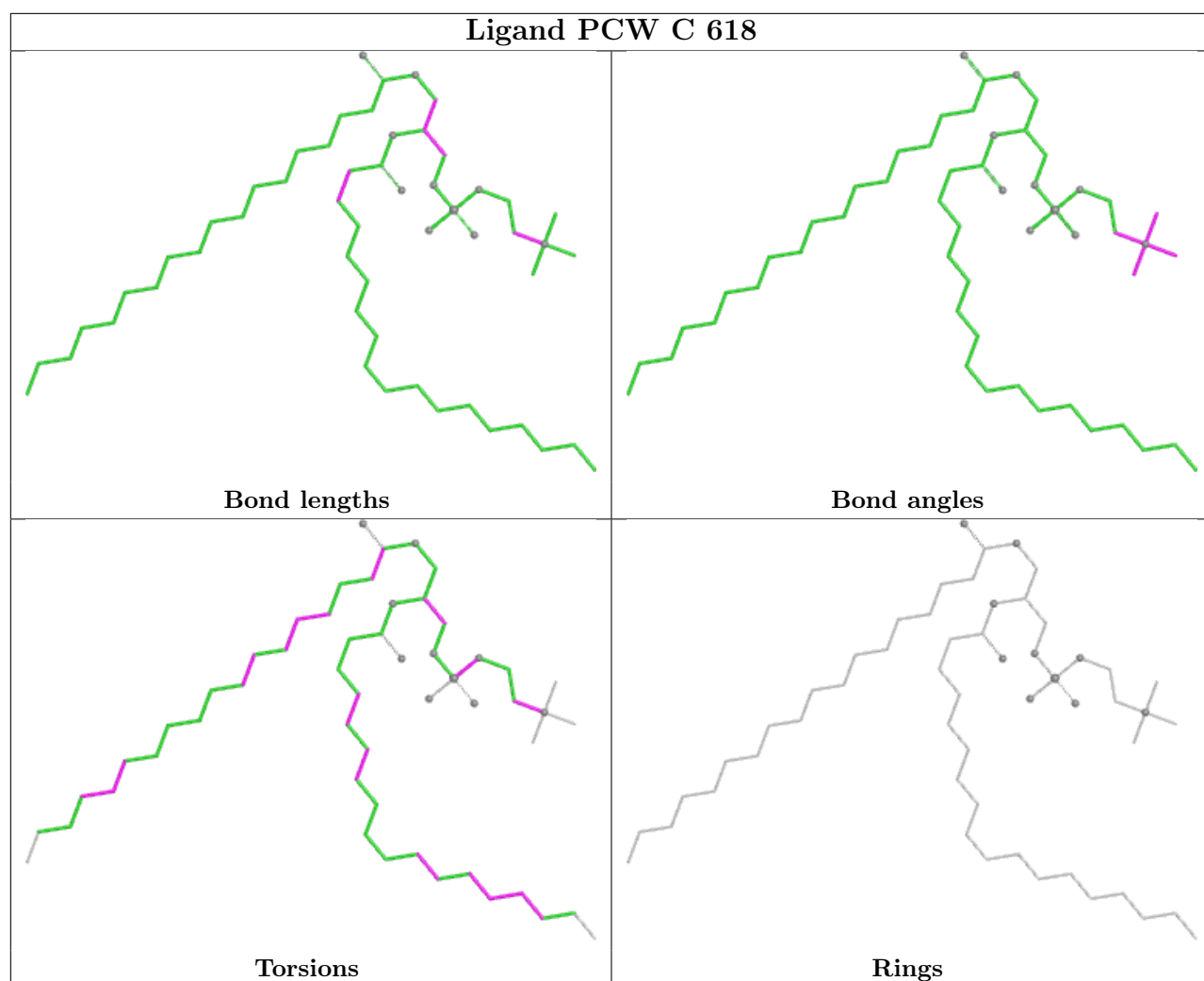












6.7 Other polymers [i](#)

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 3% for the well-defined parts and 3% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *resonance_list_nmrstar_50_51.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 | 268 |
| Number of shifts mapped to atoms | 192 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 76 |
| Number of shifts with mapping warnings | 0 |
| Number of shift outliers (ShiftChecker) | 0 |

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. All 76 occurrences are reported below.

| List ID | Chain | Res | Type | Atom | Shift Data | | |
|---------|-------|-----|------|------|------------|-------------|-----------|
| | | | | | Value | Uncertainty | Ambiguity |
| 1 | B | 1 | MET | H1 | 8.197 | . | . |
| 1 | B | 6 | LEU | HD21 | 0.865 | . | . |
| 1 | B | 6 | LEU | HD22 | 0.865 | . | . |
| 1 | B | 6 | LEU | HD23 | 0.865 | . | . |
| 1 | B | 14 | VAL | HG11 | 0.892 | . | . |
| 1 | B | 14 | VAL | HG12 | 0.892 | . | . |
| 1 | B | 14 | VAL | HG13 | 0.892 | . | . |
| 1 | B | 19 | LEU | HD11 | 0.547 | . | . |
| 1 | B | 19 | LEU | HD12 | 0.547 | . | . |
| 1 | B | 19 | LEU | HD13 | 0.547 | . | . |
| 1 | B | 21 | ILE | HD11 | 0.513 | . | . |
| 1 | B | 21 | ILE | HD12 | 0.513 | . | . |
| 1 | B | 21 | ILE | HD13 | 0.513 | . | . |
| 1 | B | 23 | LEU | HD11 | -0.325 | . | . |

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| List ID | Chain | Res | Type | Atom | Shift Data | | |
|---------|-------|-----|------|------|------------|-------------|-----------|
| | | | | | Value | Uncertainty | Ambiguity |
| 1 | B | 23 | LEU | HD12 | -0.325 | . | . |
| 1 | B | 23 | LEU | HD13 | -0.325 | . | . |
| 1 | B | 24 | ILE | HD11 | 0.389 | . | . |
| 1 | B | 24 | ILE | HD12 | 0.389 | . | . |
| 1 | B | 24 | ILE | HD13 | 0.389 | . | . |
| 1 | B | 36 | ILE | HD11 | 0.714 | . | . |
| 1 | B | 36 | ILE | HD12 | 0.714 | . | . |
| 1 | B | 36 | ILE | HD13 | 0.714 | . | . |
| 1 | B | 46 | ILE | HD11 | 0.361 | . | . |
| 1 | B | 46 | ILE | HD12 | 0.361 | . | . |
| 1 | B | 46 | ILE | HD13 | 0.361 | . | . |
| 1 | B | 55 | ILE | HD11 | 0.451 | . | . |
| 1 | B | 55 | ILE | HD12 | 0.451 | . | . |
| 1 | B | 55 | ILE | HD13 | 0.451 | . | . |
| 1 | B | 79 | LEU | HD11 | 0.023 | . | . |
| 1 | B | 79 | LEU | HD12 | 0.023 | . | . |
| 1 | B | 79 | LEU | HD13 | 0.023 | . | . |
| 1 | B | 79 | LEU | HD21 | 0.081 | . | . |
| 1 | B | 79 | LEU | HD22 | 0.081 | . | . |
| 1 | B | 79 | LEU | HD23 | 0.081 | . | . |
| 1 | B | 84 | ILE | HD11 | 0.7 | . | . |
| 1 | B | 84 | ILE | HD12 | 0.7 | . | . |
| 1 | B | 84 | ILE | HD13 | 0.7 | . | . |
| 1 | B | 93 | ILE | HD11 | 0.724 | . | . |
| 1 | B | 93 | ILE | HD12 | 0.724 | . | . |
| 1 | B | 93 | ILE | HD13 | 0.724 | . | . |
| 1 | B | 100 | ILE | HD11 | 0.234 | . | . |
| 1 | B | 100 | ILE | HD12 | 0.234 | . | . |
| 1 | B | 100 | ILE | HD13 | 0.234 | . | . |
| 1 | B | 113 | LEU | HD11 | 0.989 | . | . |
| 1 | B | 113 | LEU | HD12 | 0.989 | . | . |
| 1 | B | 113 | LEU | HD13 | 0.989 | . | . |
| 1 | B | 113 | LEU | HD21 | 1.261 | . | . |
| 1 | B | 113 | LEU | HD22 | 1.261 | . | . |
| 1 | B | 113 | LEU | HD23 | 1.261 | . | . |
| 1 | B | 120 | LEU | HD21 | 0.8 | . | . |
| 1 | B | 120 | LEU | HD22 | 0.8 | . | . |
| 1 | B | 120 | LEU | HD23 | 0.8 | . | . |
| 1 | B | 125 | VAL | HG11 | -0.21 | . | . |
| 1 | B | 125 | VAL | HG12 | -0.21 | . | . |
| 1 | B | 125 | VAL | HG13 | -0.21 | . | . |

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| List ID | Chain | Res | Type | Atom | Shift Data | | |
|---------|-------|-----|------|------|------------|-------------|-----------|
| | | | | | Value | Uncertainty | Ambiguity |
| 1 | B | 133 | LEU | HD11 | 0.344 | . | . |
| 1 | B | 133 | LEU | HD12 | 0.344 | . | . |
| 1 | B | 133 | LEU | HD13 | 0.344 | . | . |
| 1 | B | 133 | LEU | HD21 | 0.39 | . | . |
| 1 | B | 133 | LEU | HD22 | 0.39 | . | . |
| 1 | B | 133 | LEU | HD23 | 0.39 | . | . |
| 1 | B | 139 | ILE | HD11 | 0.809 | . | . |
| 1 | B | 139 | ILE | HD12 | 0.809 | . | . |
| 1 | B | 139 | ILE | HD13 | 0.809 | . | . |
| 1 | B | 142 | ILE | HD11 | 0.618 | . | . |
| 1 | B | 142 | ILE | HD12 | 0.618 | . | . |
| 1 | B | 142 | ILE | HD13 | 0.618 | . | . |
| 1 | B | 159 | LEU | HD11 | 0.613 | . | . |
| 1 | B | 159 | LEU | HD12 | 0.613 | . | . |
| 1 | B | 159 | LEU | HD13 | 0.613 | . | . |
| 1 | B | 160 | VAL | HG11 | -0.056 | . | . |
| 1 | B | 160 | VAL | HG12 | -0.056 | . | . |
| 1 | B | 160 | VAL | HG13 | -0.056 | . | . |
| 1 | B | 163 | ILE | HD11 | 0.612 | . | . |
| 1 | B | 163 | ILE | HD12 | 0.612 | . | . |
| 1 | B | 163 | ILE | HD13 | 0.612 | . | . |

7.1.2 Chemical shift referencing [i](#)

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 | 84 | -0.46 ± 0.99 | None needed (< 0.5 ppm) |

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 3%, i.e. 254 atoms were assigned a chemical shift out of a possible 7385. 0 out of 99 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | ^1H | ^{13}C | ^{15}N |
|----------|---------------|--------------|-----------------|-----------------|
| Backbone | 154/2608 (6%) | 77/1053 (7%) | 0/1048 (0%) | 77/507 (15%) |

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| | Total | ¹ H | ¹³ C | ¹⁵ N |
|-----------|---------------|----------------|-----------------|-----------------|
| Sidechain | 100/4339 (2%) | 75/2790 (3%) | 25/1354 (2%) | 0/195 (0%) |
| Aromatic | 0/438 (0%) | 0/222 (0%) | 0/208 (0%) | 0/8 (0%) |
| Overall | 254/7385 (3%) | 152/4065 (4%) | 25/2610 (1%) | 77/710 (11%) |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 3%, i.e. 267 atoms were assigned a chemical shift out of a possible 8192. 0 out of 109 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | ¹ H | ¹³ C | ¹⁵ N |
|-----------|---------------|----------------|-----------------|-----------------|
| Backbone | 167/2894 (6%) | 83/1169 (7%) | 0/1162 (0%) | 84/563 (15%) |
| Sidechain | 100/4818 (2%) | 75/3094 (2%) | 25/1508 (2%) | 0/216 (0%) |
| Aromatic | 0/480 (0%) | 0/244 (0%) | 0/228 (0%) | 0/8 (0%) |
| Overall | 267/8192 (3%) | 158/4507 (4%) | 25/2898 (1%) | 84/787 (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 B:

