



Full wwPDB EM Validation Report ⓘ

Oct 18, 2023 – 07:26 PM JST

PDB ID : 8IMN
EMDB ID : EMD-35570
Title : Rt1I-Rt1II, Rt2'I-Rt2'II, Rt3I-Rt3II cylinder in cyanobacterial phycobilisome from *Anthocerotibacter panamensis* (Cluster F)
Authors : Wang, C.H.; Yang, C.H.; Wu, H.Y.; Jiang, H.W.; Ho, M.C.; Ho, M.Y.
Deposited on : 2023-03-07
Resolution : 3.07 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>

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:

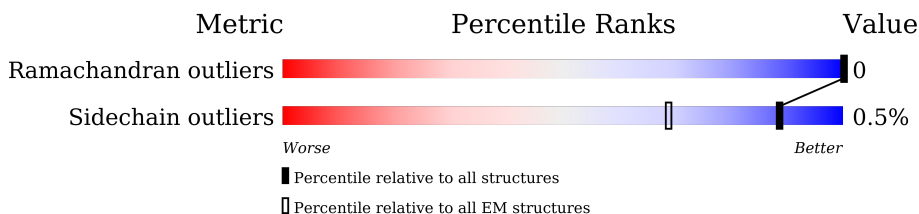
EMDB validation analysis : 0.0.1.dev70
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.07 Å.

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) | EM structures (#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Ramachandran outliers | 154571 | 4023 |
| Sidechain outliers | 154315 | 3826 |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | 5 | 1182 | |
| 2 | A | 163 | |
| 2 | B | 163 | |
| 2 | C | 163 | |
| 2 | D | 163 | |
| 2 | E | 163 | |
| 2 | F | 163 | |
| 2 | N | 163 | |
| 2 | O | 163 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 2 | P | 163 | 70% 99% |
| 2 | Q | 163 | 7% 99% |
| 2 | R | 163 | 16% 99% |
| 2 | S | 163 | 99% |
| 2 | a | 163 | 98% |
| 2 | b | 163 | 6% 100% |
| 2 | c | 163 | 25% 98% |
| 2 | d | 163 | 99% |
| 2 | e | 163 | 98% |
| 2 | f | 163 | 99% |
| 3 | G | 172 | 100% |
| 3 | H | 172 | 100% |
| 3 | I | 172 | 100% |
| 3 | J | 172 | 100% |
| 3 | K | 172 | 100% |
| 3 | L | 172 | 99% |
| 3 | T | 172 | 99% |
| 3 | U | 172 | 51% 99% |
| 3 | V | 172 | 41% 100% |
| 3 | W | 172 | 100% |
| 3 | X | 172 | 100% |
| 3 | Y | 172 | 100% |
| 3 | g | 172 | 99% |
| 3 | h | 172 | 18% 99% |
| 3 | i | 172 | 22% 100% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--------------------|
| 3 | j | 172 | <p>7% 99% 12%</p> |
| 3 | k | 172 | <p>100% 12%</p> |
| 3 | l | 172 | <p>99% 12%</p> |
| 4 | M | 78 | <p>19% 88% 12%</p> |
| 4 | Z | 78 | <p>86% 12%</p> |
| 4 | m | 78 | <p>68% 87% 12%</p> |

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 55489 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called CpcN.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 1 | 5 | 702 | 5659 | 3562 | 995 | 1093 | 9 | 0 | 0 |

- Molecule 2 is a protein called CpcA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| | | | Total | C | N | O | S | | |
| 2 | A | 162 | 1254 | 799 | 216 | 238 | 1 | 0 | 0 |
| 2 | B | 163 | 1262 | 804 | 217 | 239 | 2 | 0 | 0 |
| 2 | C | 162 | 1254 | 799 | 216 | 238 | 1 | 0 | 0 |
| 2 | D | 162 | 1254 | 799 | 216 | 238 | 1 | 0 | 0 |
| 2 | E | 162 | 1254 | 799 | 216 | 238 | 1 | 0 | 0 |
| 2 | F | 162 | 1254 | 799 | 216 | 238 | 1 | 0 | 0 |
| 2 | N | 162 | 1254 | 799 | 216 | 238 | 1 | 0 | 0 |
| 2 | O | 163 | 1262 | 804 | 217 | 239 | 2 | 0 | 0 |
| 2 | P | 162 | 1254 | 799 | 216 | 238 | 1 | 0 | 0 |
| 2 | Q | 162 | 1254 | 799 | 216 | 238 | 1 | 0 | 0 |
| 2 | R | 162 | 1254 | 799 | 216 | 238 | 1 | 0 | 0 |
| 2 | S | 162 | 1254 | 799 | 216 | 238 | 1 | 0 | 0 |
| 2 | a | 162 | 1254 | 799 | 216 | 238 | 1 | 0 | 0 |
| 2 | b | 163 | 1262 | 804 | 217 | 239 | 2 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 2 | c | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1254 | 799 | 216 | 238 | 1 | | |
| 2 | d | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1254 | 799 | 216 | 238 | 1 | | |
| 2 | e | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1254 | 799 | 216 | 238 | 1 | | |
| 2 | f | 162 | Total | C | N | O | S | 0 | 0 |
| | | | 1254 | 799 | 216 | 238 | 1 | | |

- Molecule 3 is a protein called CpcB.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 3 | G | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 807 | 226 | 252 | 8 | | |
| 3 | H | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 807 | 226 | 252 | 8 | | |
| 3 | I | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 807 | 226 | 252 | 8 | | |
| 3 | J | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 807 | 226 | 252 | 8 | | |
| 3 | K | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 807 | 226 | 252 | 8 | | |
| 3 | L | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 807 | 226 | 252 | 8 | | |
| 3 | T | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 807 | 226 | 252 | 8 | | |
| 3 | U | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 807 | 226 | 252 | 8 | | |
| 3 | V | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 807 | 226 | 252 | 8 | | |
| 3 | W | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 807 | 226 | 252 | 8 | | |
| 3 | X | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 807 | 226 | 252 | 8 | | |
| 3 | Y | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 807 | 226 | 252 | 8 | | |
| 3 | g | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 807 | 226 | 252 | 8 | | |
| 3 | h | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 807 | 226 | 252 | 8 | | |
| 3 | i | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 807 | 226 | 252 | 8 | | |

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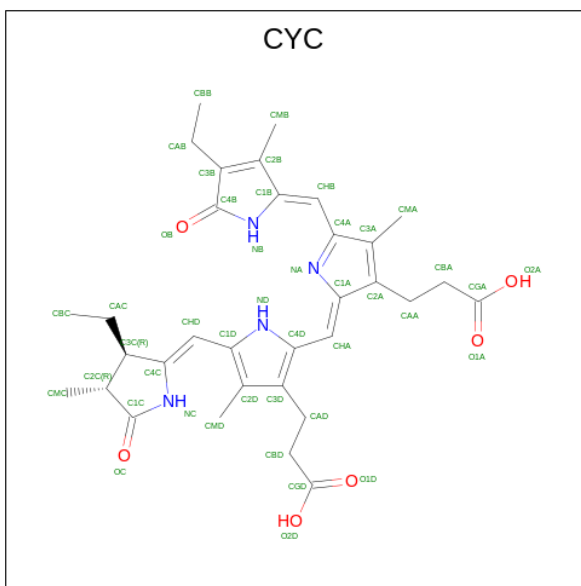
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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 3 | j | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 807 | 226 | 252 | 8 | | |
| 3 | k | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 807 | 226 | 252 | 8 | | |
| 3 | l | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1293 | 807 | 226 | 252 | 8 | | |

- Molecule 4 is a protein called CpcD.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 4 | M | 69 | Total | C | N | O | S | 0 | 0 |
| | | | 546 | 345 | 101 | 99 | 1 | | |
| 4 | Z | 69 | Total | C | N | O | S | 0 | 0 |
| | | | 546 | 345 | 101 | 99 | 1 | | |
| 4 | m | 69 | Total | C | N | O | S | 0 | 0 |
| | | | 546 | 345 | 101 | 99 | 1 | | |

- Molecule 5 is PHYCOCYANOBILIN (three-letter code: CYC) (formula: $C_{33}H_{40}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------|----|---|---|---------|
| 5 | 5 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 5 | 5 | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |
| 5 | A | 1 | Total | C | N | O | 0 |
| | | | 43 | 33 | 4 | 6 | |

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| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------------|---------|--------|--------|---------|
| | | | Total | C | N | O | |
| 5 | B | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 5 | C | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 5 | D | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 5 | E | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 5 | F | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 5 | G | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 5 | G | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 5 | H | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 5 | H | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 5 | I | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 5 | I | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 5 | J | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 5 | J | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 5 | K | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 5 | K | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 5 | L | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 5 | N | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 5 | O | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 5 | P | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 5 | Q | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 5 | R | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |

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| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------------|---------|--------|--------|---------|
| | | | Total | C | N | O | |
| 5 | S | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 5 | T | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 5 | T | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 5 | U | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 5 | U | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 5 | V | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 5 | V | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 5 | W | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 5 | W | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 5 | X | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 5 | X | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 5 | Y | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 5 | Y | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 5 | a | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 5 | b | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 5 | c | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 5 | d | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 5 | e | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 5 | f | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 5 | g | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |
| 5 | g | 1 | Total 43 | C 33 | N 4 | O 6 | 0 |

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| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------------|----|---|---|---------|
| | | | Total | C | N | O | |
| 5 | h | 1 | Total 43 | 33 | 4 | 6 | 0 |
| 5 | h | 1 | Total 43 | 33 | 4 | 6 | 0 |
| 5 | i | 1 | Total 43 | 33 | 4 | 6 | 0 |
| 5 | i | 1 | Total 43 | 33 | 4 | 6 | 0 |
| 5 | j | 1 | Total 43 | 33 | 4 | 6 | 0 |
| 5 | j | 1 | Total 43 | 33 | 4 | 6 | 0 |
| 5 | k | 1 | Total 43 | 33 | 4 | 6 | 0 |
| 5 | k | 1 | Total 43 | 33 | 4 | 6 | 0 |
| 5 | l | 1 | Total 43 | 33 | 4 | 6 | 0 |

Chain B:  99%



• Molecule 2: CpcA

Chain C:  99%



• Molecule 2: CpcA

Chain D:  99%



• Molecule 2: CpcA

Chain E:  99%



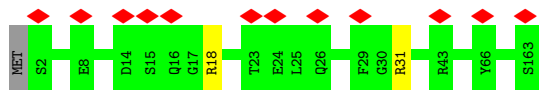
• Molecule 2: CpcA

Chain F:  99%



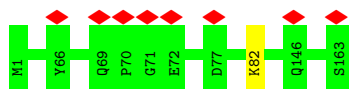
• Molecule 2: CpcA

Chain N:  98% 7%

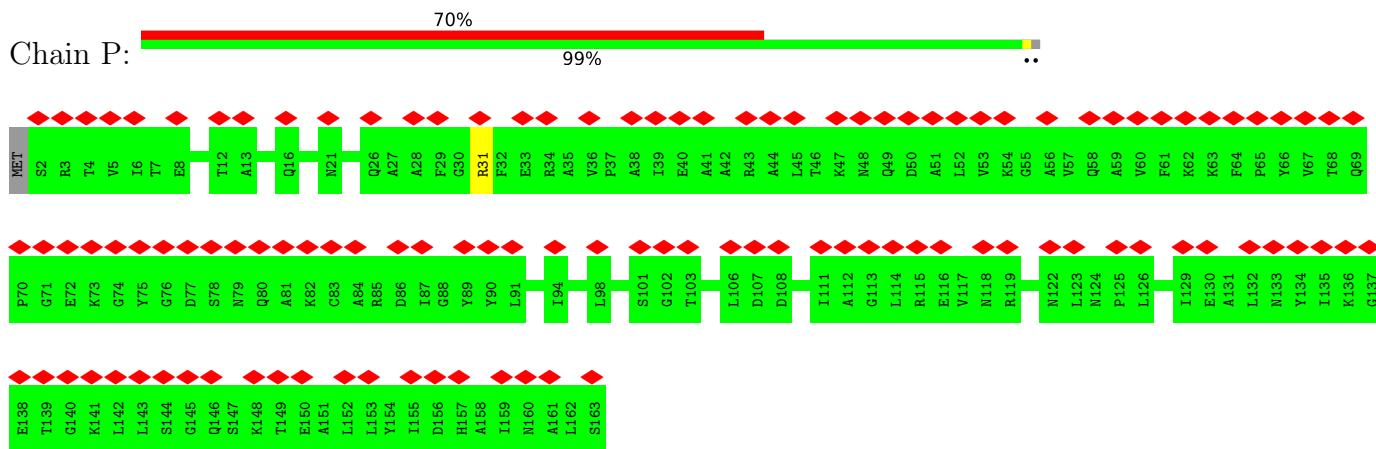


• Molecule 2: CpcA

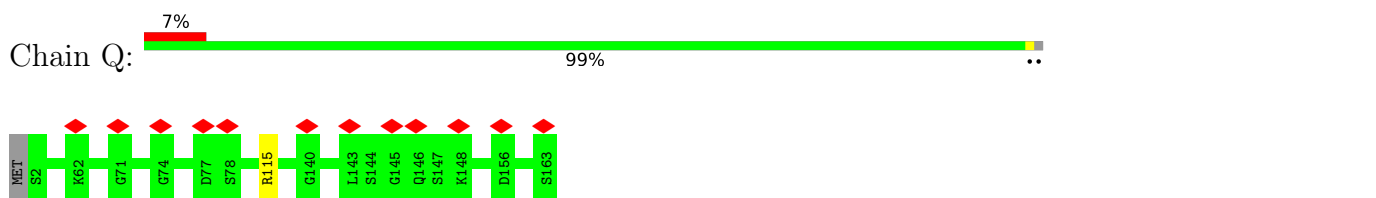
Chain O:  99% 5%



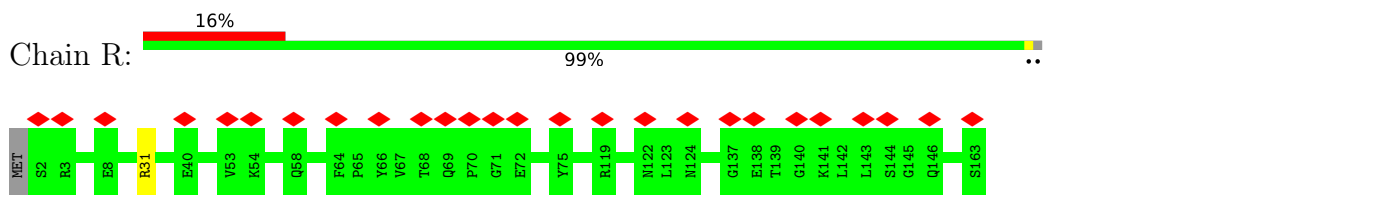
• Molecule 2: CpcA



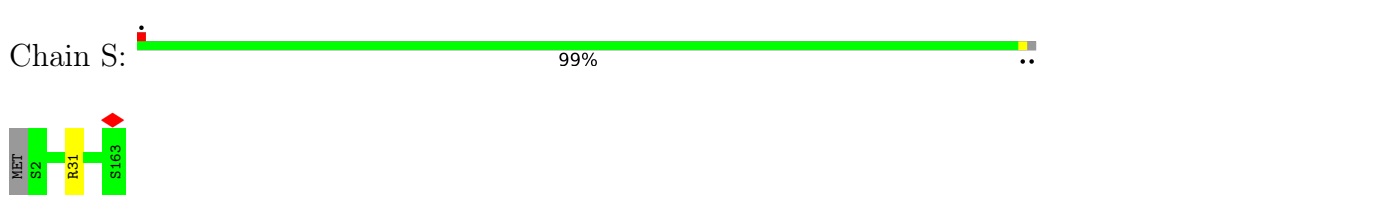
• Molecule 2: CpcA



• Molecule 2: CpcA



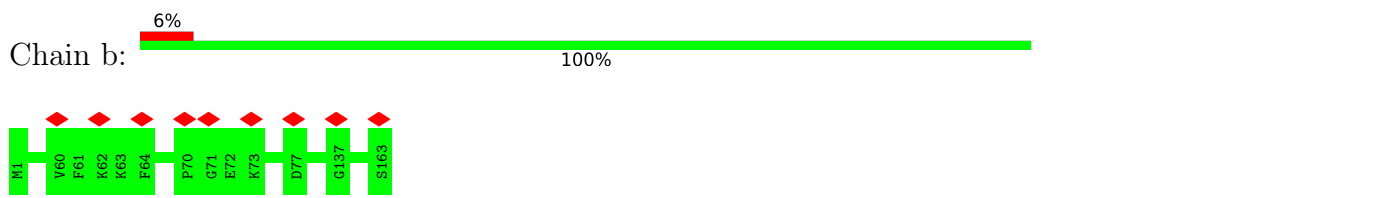
• Molecule 2: CpcA



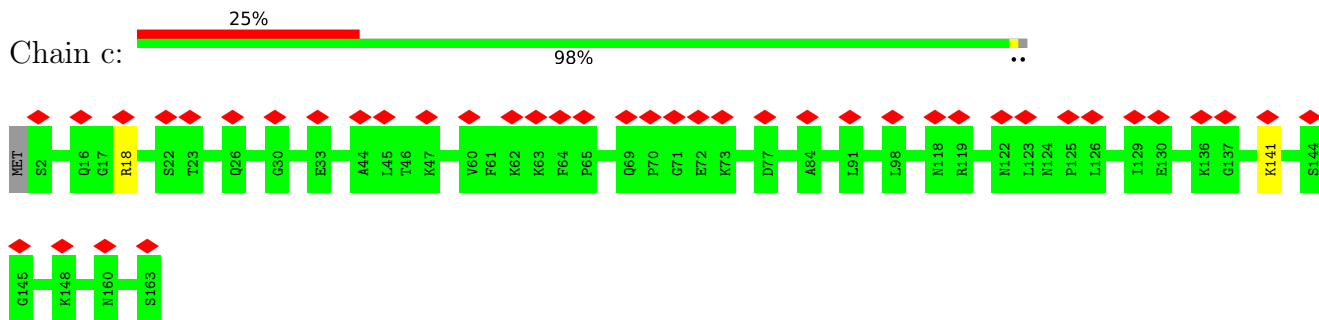
• Molecule 2: CpcA



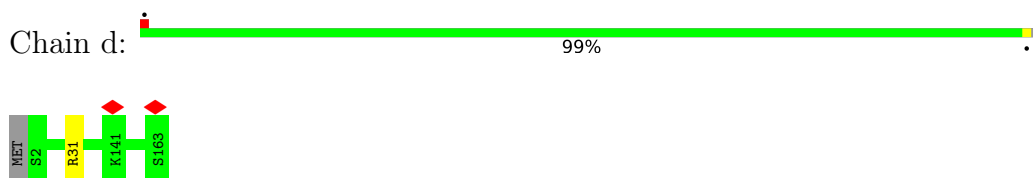
• Molecule 2: CpcA



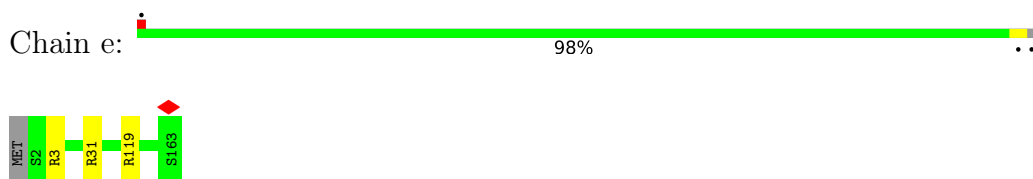
• Molecule 2: CpcA



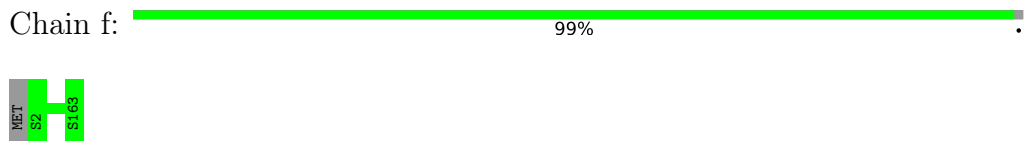
• Molecule 2: CpcA



• Molecule 2: CpcA



• Molecule 2: CpcA

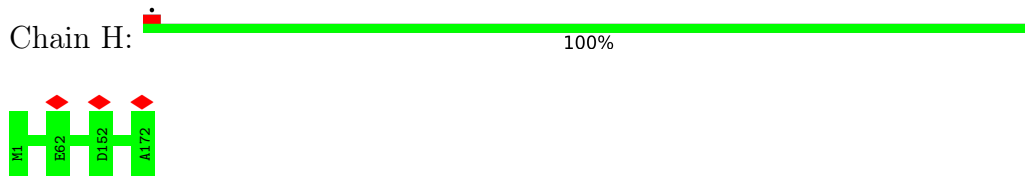


• Molecule 3: CpcB



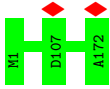
There are no outlier residues recorded for this chain.

• Molecule 3: CpcB



• Molecule 3: CpcB





• Molecule 3: CpcB



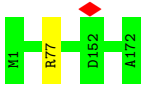
There are no outlier residues recorded for this chain.

• Molecule 3: CpcB

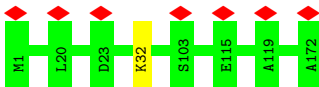


There are no outlier residues recorded for this chain.

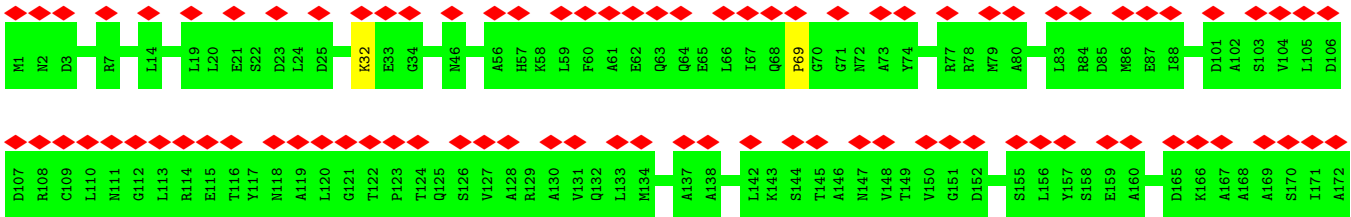
• Molecule 3: CpcB



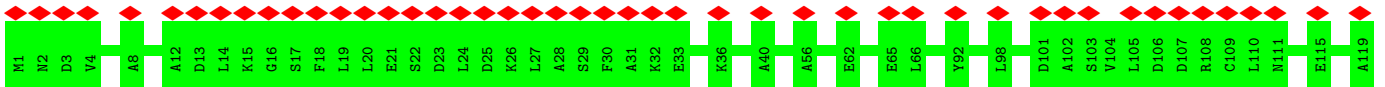
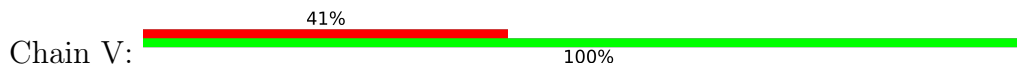
• Molecule 3: CpcB

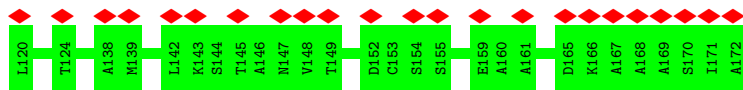


• Molecule 3: CpcB



• Molecule 3: CpcB





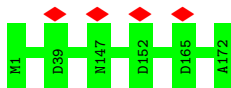
- Molecule 3: CpcB

Chain W: 100%

There are no outlier residues recorded for this chain.

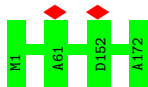
- Molecule 3: CpcB

Chain X: 100%



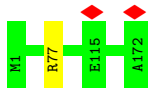
- Molecule 3: CpcB

Chain Y: 100%



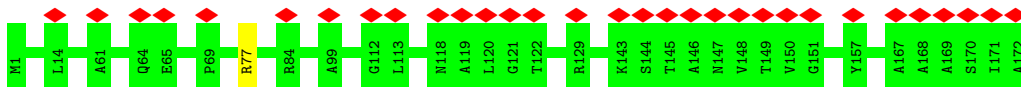
- Molecule 3: CpcB

Chain g: 99%



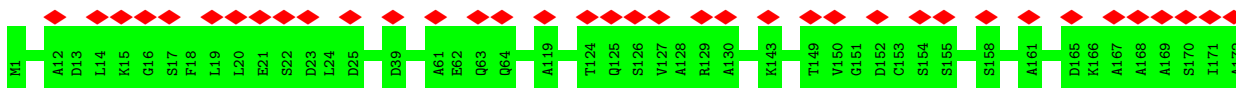
- Molecule 3: CpcB

Chain h: 18% 99%



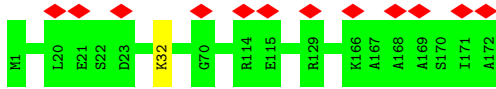
- Molecule 3: CpcB

Chain i: 22% 100%

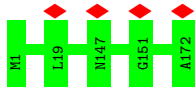


- Molecule 3: CpcB

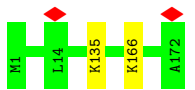
Chain j: 7% 99%



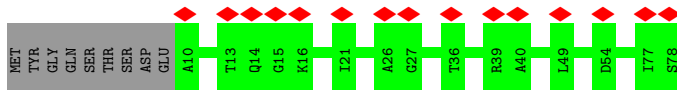
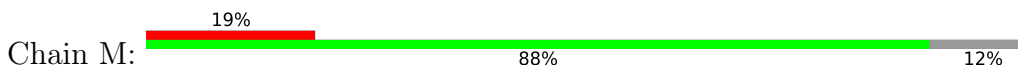
• Molecule 3: CpcB



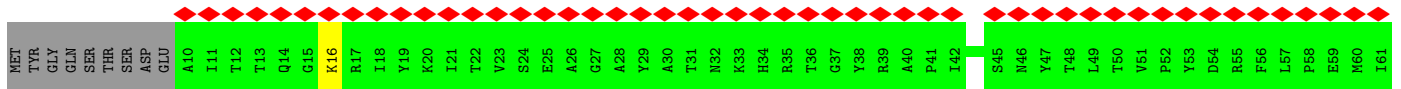
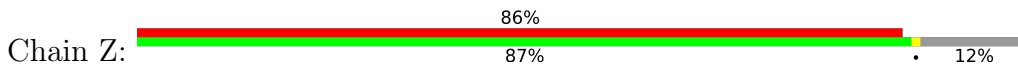
• Molecule 3: CpcB



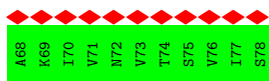
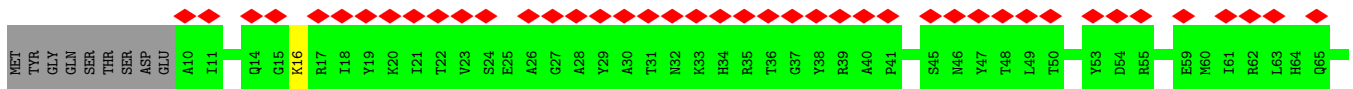
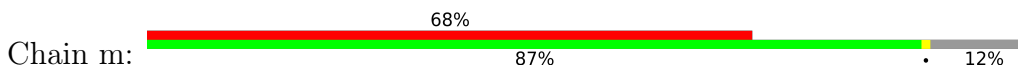
• Molecule 4: CpcD



• Molecule 4: CpcD



• Molecule 4: CpcD



4 Experimental information

| Property | Value | Source |
|--------------------------------------|-------------------------------|-----------|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 1109579 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING ONLY | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | 50 | Depositor |
| Minimum defocus (nm) | 1000 | Depositor |
| Maximum defocus (nm) | 2000 | Depositor |
| Magnification | 81000 | Depositor |
| Image detector | GATAN K3 BIOQUANTUM (6k x 4k) | Depositor |
| Maximum map value | 7.163 | Depositor |
| Minimum map value | -0.037 | Depositor |
| Average map value | 0.038 | Depositor |
| Map value standard deviation | 0.107 | Depositor |
| Recommended contour level | 0.8 | Depositor |
| Map size (\AA) | 721.48, 721.48, 721.48 | wwPDB |
| Map dimensions | 680, 680, 680 | wwPDB |
| Map angles ($^\circ$) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (\AA) | 1.061, 1.061, 1.061 | Depositor |

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CYC

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 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 | 5 | 0.32 | 0/5786 | 0.47 | 0/7836 |
| 2 | A | 0.33 | 0/1277 | 0.47 | 0/1729 |
| 2 | B | 0.37 | 0/1285 | 0.50 | 0/1739 |
| 2 | C | 0.32 | 0/1277 | 0.45 | 0/1729 |
| 2 | D | 0.38 | 0/1277 | 0.48 | 0/1729 |
| 2 | E | 0.36 | 0/1277 | 0.51 | 0/1729 |
| 2 | F | 0.40 | 0/1277 | 0.51 | 0/1729 |
| 2 | N | 0.34 | 0/1277 | 0.48 | 0/1729 |
| 2 | O | 0.32 | 0/1285 | 0.49 | 0/1739 |
| 2 | P | 0.28 | 0/1277 | 0.45 | 0/1729 |
| 2 | Q | 0.32 | 0/1277 | 0.48 | 0/1729 |
| 2 | R | 0.30 | 0/1277 | 0.50 | 0/1729 |
| 2 | S | 0.45 | 0/1277 | 0.49 | 0/1729 |
| 2 | a | 0.30 | 0/1277 | 0.49 | 0/1729 |
| 2 | b | 0.27 | 0/1285 | 0.43 | 0/1739 |
| 2 | c | 0.27 | 0/1277 | 0.44 | 0/1729 |
| 2 | d | 0.27 | 0/1277 | 0.41 | 0/1729 |
| 2 | e | 0.31 | 0/1277 | 0.50 | 0/1729 |
| 2 | f | 0.36 | 0/1277 | 0.53 | 0/1729 |
| 3 | G | 0.29 | 0/1310 | 0.48 | 0/1772 |
| 3 | H | 0.28 | 0/1310 | 0.48 | 0/1772 |
| 3 | I | 0.28 | 0/1310 | 0.42 | 0/1772 |
| 3 | J | 0.37 | 0/1310 | 0.47 | 0/1772 |
| 3 | K | 0.37 | 0/1310 | 0.44 | 0/1772 |
| 3 | L | 0.36 | 0/1310 | 0.47 | 0/1772 |
| 3 | T | 0.29 | 0/1310 | 0.49 | 0/1772 |
| 3 | U | 0.35 | 1/1310 (0.1%) | 0.62 | 3/1772 (0.2%) |
| 3 | V | 0.27 | 0/1310 | 0.47 | 0/1772 |
| 3 | W | 0.37 | 0/1310 | 0.48 | 0/1772 |
| 3 | X | 0.31 | 0/1310 | 0.46 | 0/1772 |
| 3 | Y | 0.34 | 0/1310 | 0.46 | 0/1772 |
| 3 | g | 0.27 | 0/1310 | 0.48 | 0/1772 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|----------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 3 | h | 0.25 | 0/1310 | 0.43 | 0/1772 |
| 3 | i | 0.26 | 0/1310 | 0.49 | 0/1772 |
| 3 | j | 0.29 | 0/1310 | 0.48 | 0/1772 |
| 3 | k | 0.26 | 0/1310 | 0.44 | 0/1772 |
| 3 | l | 0.31 | 0/1310 | 0.49 | 0/1772 |
| 4 | M | 0.25 | 0/556 | 0.44 | 0/753 |
| 4 | Z | 0.26 | 0/556 | 0.48 | 0/753 |
| 4 | m | 0.25 | 0/556 | 0.49 | 0/753 |
| All | All | 0.32 | 1/54044 (0.0%) | 0.48 | 3/73143 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 2 | e | 0 | 1 |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 3 | U | 69 | PRO | CG-CD | -6.43 | 1.29 | 1.50 |

All (3) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|--------|-------------|----------|
| 3 | U | 69 | PRO | CA-N-CD | -12.63 | 93.82 | 111.50 |
| 3 | U | 69 | PRO | N-CD-CG | -9.11 | 89.53 | 103.20 |
| 3 | U | 69 | PRO | CA-CB-CG | -5.34 | 93.85 | 104.00 |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 2 | e | 3 | ARG | Peptide |

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM 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 | 5 | 700/1182 (59%) | 665 (95%) | 35 (5%) | 0 | 100 | 100 |
| 2 | A | 160/163 (98%) | 155 (97%) | 5 (3%) | 0 | 100 | 100 |
| 2 | B | 161/163 (99%) | 154 (96%) | 7 (4%) | 0 | 100 | 100 |
| 2 | C | 160/163 (98%) | 155 (97%) | 5 (3%) | 0 | 100 | 100 |
| 2 | D | 160/163 (98%) | 156 (98%) | 4 (2%) | 0 | 100 | 100 |
| 2 | E | 160/163 (98%) | 153 (96%) | 7 (4%) | 0 | 100 | 100 |
| 2 | F | 160/163 (98%) | 156 (98%) | 4 (2%) | 0 | 100 | 100 |
| 2 | N | 160/163 (98%) | 156 (98%) | 4 (2%) | 0 | 100 | 100 |
| 2 | O | 161/163 (99%) | 158 (98%) | 3 (2%) | 0 | 100 | 100 |
| 2 | P | 160/163 (98%) | 156 (98%) | 4 (2%) | 0 | 100 | 100 |
| 2 | Q | 160/163 (98%) | 156 (98%) | 4 (2%) | 0 | 100 | 100 |
| 2 | R | 160/163 (98%) | 157 (98%) | 3 (2%) | 0 | 100 | 100 |
| 2 | S | 160/163 (98%) | 155 (97%) | 5 (3%) | 0 | 100 | 100 |
| 2 | a | 160/163 (98%) | 152 (95%) | 8 (5%) | 0 | 100 | 100 |
| 2 | b | 161/163 (99%) | 157 (98%) | 4 (2%) | 0 | 100 | 100 |
| 2 | c | 160/163 (98%) | 156 (98%) | 4 (2%) | 0 | 100 | 100 |
| 2 | d | 160/163 (98%) | 159 (99%) | 1 (1%) | 0 | 100 | 100 |
| 2 | e | 160/163 (98%) | 154 (96%) | 6 (4%) | 0 | 100 | 100 |
| 2 | f | 160/163 (98%) | 153 (96%) | 7 (4%) | 0 | 100 | 100 |
| 3 | G | 170/172 (99%) | 166 (98%) | 4 (2%) | 0 | 100 | 100 |
| 3 | H | 170/172 (99%) | 164 (96%) | 6 (4%) | 0 | 100 | 100 |
| 3 | I | 170/172 (99%) | 165 (97%) | 5 (3%) | 0 | 100 | 100 |
| 3 | J | 170/172 (99%) | 160 (94%) | 10 (6%) | 0 | 100 | 100 |
| 3 | K | 170/172 (99%) | 168 (99%) | 2 (1%) | 0 | 100 | 100 |
| 3 | L | 170/172 (99%) | 162 (95%) | 8 (5%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 3 | T | 170/172 (99%) | 165 (97%) | 5 (3%) | 0 | 100 | 100 |
| 3 | U | 170/172 (99%) | 167 (98%) | 3 (2%) | 0 | 100 | 100 |
| 3 | V | 170/172 (99%) | 169 (99%) | 1 (1%) | 0 | 100 | 100 |
| 3 | W | 170/172 (99%) | 161 (95%) | 9 (5%) | 0 | 100 | 100 |
| 3 | X | 170/172 (99%) | 168 (99%) | 2 (1%) | 0 | 100 | 100 |
| 3 | Y | 170/172 (99%) | 165 (97%) | 5 (3%) | 0 | 100 | 100 |
| 3 | g | 170/172 (99%) | 165 (97%) | 5 (3%) | 0 | 100 | 100 |
| 3 | h | 170/172 (99%) | 166 (98%) | 4 (2%) | 0 | 100 | 100 |
| 3 | i | 170/172 (99%) | 168 (99%) | 2 (1%) | 0 | 100 | 100 |
| 3 | j | 170/172 (99%) | 166 (98%) | 4 (2%) | 0 | 100 | 100 |
| 3 | k | 170/172 (99%) | 168 (99%) | 2 (1%) | 0 | 100 | 100 |
| 3 | l | 170/172 (99%) | 165 (97%) | 5 (3%) | 0 | 100 | 100 |
| 4 | M | 67/78 (86%) | 62 (92%) | 5 (8%) | 0 | 100 | 100 |
| 4 | Z | 67/78 (86%) | 62 (92%) | 5 (8%) | 0 | 100 | 100 |
| 4 | m | 67/78 (86%) | 65 (97%) | 2 (3%) | 0 | 100 | 100 |
| All | All | 6844/7446 (92%) | 6630 (97%) | 214 (3%) | 0 | 100 | 100 |

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM 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 | 5 | 594/1003 (59%) | 594 (100%) | 0 | 100 | 100 |
| 2 | A | 128/129 (99%) | 126 (98%) | 2 (2%) | 62 | 83 |
| 2 | B | 129/129 (100%) | 128 (99%) | 1 (1%) | 81 | 91 |
| 2 | C | 128/129 (99%) | 128 (100%) | 0 | 100 | 100 |
| 2 | D | 128/129 (99%) | 128 (100%) | 0 | 100 | 100 |
| 2 | E | 128/129 (99%) | 127 (99%) | 1 (1%) | 81 | 91 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|------------|----------|-------------|-----|
| 2 | F | 128/129 (99%) | 128 (100%) | 0 | 100 | 100 |
| 2 | N | 128/129 (99%) | 126 (98%) | 2 (2%) | 62 | 83 |
| 2 | O | 129/129 (100%) | 128 (99%) | 1 (1%) | 81 | 91 |
| 2 | P | 128/129 (99%) | 127 (99%) | 1 (1%) | 81 | 91 |
| 2 | Q | 128/129 (99%) | 127 (99%) | 1 (1%) | 81 | 91 |
| 2 | R | 128/129 (99%) | 127 (99%) | 1 (1%) | 81 | 91 |
| 2 | S | 128/129 (99%) | 127 (99%) | 1 (1%) | 81 | 91 |
| 2 | a | 128/129 (99%) | 125 (98%) | 3 (2%) | 50 | 75 |
| 2 | b | 129/129 (100%) | 129 (100%) | 0 | 100 | 100 |
| 2 | c | 128/129 (99%) | 126 (98%) | 2 (2%) | 62 | 83 |
| 2 | d | 128/129 (99%) | 127 (99%) | 1 (1%) | 81 | 91 |
| 2 | e | 128/129 (99%) | 126 (98%) | 2 (2%) | 62 | 83 |
| 2 | f | 128/129 (99%) | 128 (100%) | 0 | 100 | 100 |
| 3 | G | 133/133 (100%) | 133 (100%) | 0 | 100 | 100 |
| 3 | H | 133/133 (100%) | 133 (100%) | 0 | 100 | 100 |
| 3 | I | 133/133 (100%) | 133 (100%) | 0 | 100 | 100 |
| 3 | J | 133/133 (100%) | 133 (100%) | 0 | 100 | 100 |
| 3 | K | 133/133 (100%) | 133 (100%) | 0 | 100 | 100 |
| 3 | L | 133/133 (100%) | 132 (99%) | 1 (1%) | 81 | 91 |
| 3 | T | 133/133 (100%) | 132 (99%) | 1 (1%) | 81 | 91 |
| 3 | U | 133/133 (100%) | 132 (99%) | 1 (1%) | 81 | 91 |
| 3 | V | 133/133 (100%) | 133 (100%) | 0 | 100 | 100 |
| 3 | W | 133/133 (100%) | 133 (100%) | 0 | 100 | 100 |
| 3 | X | 133/133 (100%) | 133 (100%) | 0 | 100 | 100 |
| 3 | Y | 133/133 (100%) | 133 (100%) | 0 | 100 | 100 |
| 3 | g | 133/133 (100%) | 132 (99%) | 1 (1%) | 81 | 91 |
| 3 | h | 133/133 (100%) | 132 (99%) | 1 (1%) | 81 | 91 |
| 3 | i | 133/133 (100%) | 133 (100%) | 0 | 100 | 100 |
| 3 | j | 133/133 (100%) | 132 (99%) | 1 (1%) | 81 | 91 |
| 3 | k | 133/133 (100%) | 133 (100%) | 0 | 100 | 100 |
| 3 | l | 133/133 (100%) | 131 (98%) | 2 (2%) | 65 | 84 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 4 | M | 59/67 (88%) | 59 (100%) | 0 | 100 | 100 |
| 4 | Z | 59/67 (88%) | 58 (98%) | 1 (2%) | 60 | 82 |
| 4 | m | 59/67 (88%) | 58 (98%) | 1 (2%) | 60 | 82 |
| All | All | 5472/5920 (92%) | 5443 (100%) | 29 (0%) | 89 | 94 |

All (29) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | A | 18 | ARG |
| 2 | A | 31 | ARG |
| 2 | B | 31 | ARG |
| 2 | E | 31 | ARG |
| 3 | L | 77 | ARG |
| 2 | N | 18 | ARG |
| 2 | N | 31 | ARG |
| 2 | O | 82 | LYS |
| 2 | P | 31 | ARG |
| 2 | Q | 115 | ARG |
| 2 | R | 31 | ARG |
| 2 | S | 31 | ARG |
| 3 | T | 32 | LYS |
| 3 | U | 32 | LYS |
| 4 | Z | 16 | LYS |
| 2 | a | 18 | ARG |
| 2 | a | 31 | ARG |
| 2 | a | 82 | LYS |
| 2 | c | 18 | ARG |
| 2 | c | 141 | LYS |
| 2 | d | 31 | ARG |
| 2 | e | 31 | ARG |
| 2 | e | 119 | ARG |
| 3 | g | 77 | ARG |
| 3 | h | 77 | ARG |
| 3 | j | 32 | LYS |
| 3 | l | 135 | LYS |
| 3 | l | 166 | LYS |
| 4 | m | 16 | LYS |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 5 | 425 | HIS |
| 2 | B | 48 | ASN |
| 2 | E | 26 | GLN |
| 3 | G | 147 | ASN |
| 3 | J | 111 | ASN |
| 3 | K | 72 | ASN |
| 2 | R | 146 | GLN |
| 3 | U | 118 | ASN |
| 3 | V | 63 | GLN |
| 3 | W | 11 | GLN |
| 3 | W | 72 | ASN |
| 3 | W | 76 | HIS |
| 3 | X | 72 | ASN |
| 3 | Y | 72 | ASN |
| 2 | a | 49 | GLN |
| 2 | a | 146 | GLN |
| 2 | b | 49 | GLN |
| 2 | b | 79 | ASN |
| 2 | c | 58 | GLN |
| 2 | d | 58 | GLN |
| 3 | h | 72 | ASN |
| 3 | i | 11 | GLN |
| 3 | j | 72 | ASN |
| 3 | k | 11 | GLN |
| 3 | k | 72 | ASN |
| 3 | l | 72 | ASN |
| 3 | l | 118 | ASN |

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry

54 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or 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 length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 5 | CYC | k | 200 | - | 42,46,46 | 6.49 | 25 (59%) | 50,67,67 | 4.40 | 11 (22%) |
| 5 | CYC | j | 201 | - | 42,46,46 | 6.53 | 24 (57%) | 50,67,67 | 4.64 | 11 (22%) |
| 5 | CYC | k | 201 | - | 42,46,46 | 6.60 | 24 (57%) | 50,67,67 | 4.34 | 12 (24%) |
| 5 | CYC | h | 201 | - | 42,46,46 | 6.52 | 24 (57%) | 50,67,67 | 4.70 | 11 (22%) |
| 5 | CYC | U | 201 | - | 42,46,46 | 6.52 | 25 (59%) | 50,67,67 | 4.70 | 11 (22%) |
| 5 | CYC | W | 200 | - | 42,46,46 | 6.45 | 23 (54%) | 50,67,67 | 4.40 | 13 (26%) |
| 5 | CYC | L | 201 | - | 42,46,46 | 6.51 | 24 (57%) | 50,67,67 | 4.58 | 15 (30%) |
| 5 | CYC | d | 200 | - | 42,46,46 | 6.56 | 23 (54%) | 50,67,67 | 4.27 | 10 (20%) |
| 5 | CYC | W | 201 | - | 42,46,46 | 6.48 | 24 (57%) | 50,67,67 | 4.60 | 11 (22%) |
| 5 | CYC | U | 200 | - | 42,46,46 | 6.57 | 25 (59%) | 50,67,67 | 4.28 | 12 (24%) |
| 5 | CYC | I | 201 | - | 42,46,46 | 6.47 | 23 (54%) | 50,67,67 | 4.50 | 12 (24%) |
| 5 | CYC | A | 200 | - | 42,46,46 | 6.44 | 23 (54%) | 50,67,67 | 4.44 | 10 (20%) |
| 5 | CYC | O | 200 | - | 42,46,46 | 6.55 | 25 (59%) | 50,67,67 | 4.69 | 13 (26%) |
| 5 | CYC | V | 201 | - | 42,46,46 | 6.54 | 25 (59%) | 50,67,67 | 4.57 | 9 (18%) |
| 5 | CYC | Y | 201 | - | 42,46,46 | 6.52 | 25 (59%) | 50,67,67 | 4.39 | 13 (26%) |
| 5 | CYC | X | 200 | - | 42,46,46 | 6.52 | 23 (54%) | 50,67,67 | 4.52 | 13 (26%) |
| 5 | CYC | X | 201 | - | 42,46,46 | 6.55 | 24 (57%) | 50,67,67 | 4.41 | 11 (22%) |
| 5 | CYC | K | 201 | - | 42,46,46 | 6.43 | 23 (54%) | 50,67,67 | 4.62 | 12 (24%) |
| 5 | CYC | I | 200 | - | 42,46,46 | 6.46 | 24 (57%) | 50,67,67 | 4.37 | 10 (20%) |
| 5 | CYC | G | 201 | - | 42,46,46 | 6.57 | 25 (59%) | 50,67,67 | 4.43 | 13 (26%) |
| 5 | CYC | i | 200 | - | 42,46,46 | 6.60 | 25 (59%) | 50,67,67 | 4.22 | 12 (24%) |
| 5 | CYC | S | 200 | - | 42,46,46 | 6.49 | 23 (54%) | 50,67,67 | 4.53 | 13 (26%) |
| 5 | CYC | E | 200 | - | 42,46,46 | 6.46 | 23 (54%) | 50,67,67 | 4.23 | 12 (24%) |
| 5 | CYC | T | 200 | - | 42,46,46 | 6.63 | 24 (57%) | 50,67,67 | 4.28 | 11 (22%) |
| 5 | CYC | h | 200 | - | 42,46,46 | 6.56 | 24 (57%) | 50,67,67 | 4.32 | 10 (20%) |
| 5 | CYC | 5 | 1202 | - | 42,46,46 | 6.53 | 25 (59%) | 50,67,67 | 4.49 | 12 (24%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 5 | CYC | Q | 200 | - | 42,46,46 | 6.52 | 24 (57%) | 50,67,67 | 4.42 | 11 (22%) |
| 5 | CYC | C | 200 | - | 42,46,46 | 6.46 | 23 (54%) | 50,67,67 | 4.38 | 10 (20%) |
| 5 | CYC | Y | 200 | - | 42,46,46 | 6.47 | 23 (54%) | 50,67,67 | 4.30 | 10 (20%) |
| 5 | CYC | l | 201 | - | 42,46,46 | 6.59 | 25 (59%) | 50,67,67 | 4.48 | 13 (26%) |
| 5 | CYC | D | 200 | - | 42,46,46 | 6.38 | 23 (54%) | 50,67,67 | 4.55 | 10 (20%) |
| 5 | CYC | R | 200 | - | 42,46,46 | 6.56 | 24 (57%) | 50,67,67 | 4.55 | 13 (26%) |
| 5 | CYC | J | 201 | - | 42,46,46 | 6.45 | 23 (54%) | 50,67,67 | 4.65 | 12 (24%) |
| 5 | CYC | j | 200 | - | 42,46,46 | 6.49 | 24 (57%) | 50,67,67 | 4.44 | 14 (28%) |
| 5 | CYC | G | 200 | - | 42,46,46 | 6.56 | 24 (57%) | 50,67,67 | 4.29 | 10 (20%) |
| 5 | CYC | f | 200 | - | 42,46,46 | 6.46 | 24 (57%) | 50,67,67 | 4.78 | 10 (20%) |
| 5 | CYC | V | 200 | - | 42,46,46 | 6.56 | 24 (57%) | 50,67,67 | 4.49 | 9 (18%) |
| 5 | CYC | H | 201 | - | 42,46,46 | 6.49 | 24 (57%) | 50,67,67 | 4.54 | 8 (16%) |
| 5 | CYC | P | 200 | - | 42,46,46 | 6.57 | 25 (59%) | 50,67,67 | 4.14 | 9 (18%) |
| 5 | CYC | e | 200 | - | 42,46,46 | 6.56 | 24 (57%) | 50,67,67 | 4.50 | 10 (20%) |
| 5 | CYC | g | 201 | - | 42,46,46 | 6.47 | 24 (57%) | 50,67,67 | 4.67 | 12 (24%) |
| 5 | CYC | F | 200 | - | 42,46,46 | 6.39 | 23 (54%) | 50,67,67 | 4.41 | 12 (24%) |
| 5 | CYC | 5 | 1201 | - | 42,46,46 | 6.40 | 23 (54%) | 50,67,67 | 4.32 | 12 (24%) |
| 5 | CYC | H | 200 | - | 42,46,46 | 6.51 | 24 (57%) | 50,67,67 | 4.41 | 12 (24%) |
| 5 | CYC | a | 200 | - | 42,46,46 | 6.58 | 25 (59%) | 50,67,67 | 4.58 | 13 (26%) |
| 5 | CYC | K | 200 | - | 42,46,46 | 6.47 | 23 (54%) | 50,67,67 | 4.50 | 13 (26%) |
| 5 | CYC | N | 200 | - | 42,46,46 | 6.46 | 25 (59%) | 50,67,67 | 4.33 | 12 (24%) |
| 5 | CYC | c | 200 | - | 42,46,46 | 6.60 | 25 (59%) | 50,67,67 | 4.45 | 12 (24%) |
| 5 | CYC | J | 200 | - | 42,46,46 | 6.48 | 23 (54%) | 50,67,67 | 4.47 | 13 (26%) |
| 5 | CYC | b | 200 | - | 42,46,46 | 6.56 | 24 (57%) | 50,67,67 | 4.45 | 10 (20%) |
| 5 | CYC | i | 201 | - | 42,46,46 | 6.60 | 24 (57%) | 50,67,67 | 4.54 | 11 (22%) |
| 5 | CYC | B | 200 | - | 42,46,46 | 6.56 | 24 (57%) | 50,67,67 | 4.61 | 13 (26%) |
| 5 | CYC | T | 201 | - | 42,46,46 | 6.50 | 25 (59%) | 50,67,67 | 4.55 | 12 (24%) |
| 5 | CYC | g | 200 | - | 42,46,46 | 6.63 | 25 (59%) | 50,67,67 | 4.26 | 11 (22%) |

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 |
|-----|------|-------|-----|------|---------|-------------|---------|
| 5 | CYC | k | 200 | - | - | 11/25/74/74 | 0/4/4/4 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|-------------|---------|
| 5 | CYC | j | 201 | - | - | 9/25/74/74 | 0/4/4/4 |
| 5 | CYC | k | 201 | - | - | 7/25/74/74 | 0/4/4/4 |
| 5 | CYC | h | 201 | - | - | 11/25/74/74 | 0/4/4/4 |
| 5 | CYC | U | 201 | - | - | 16/25/74/74 | 0/4/4/4 |
| 5 | CYC | W | 200 | - | - | 13/25/74/74 | 0/4/4/4 |
| 5 | CYC | L | 201 | - | - | 13/25/74/74 | 0/4/4/4 |
| 5 | CYC | d | 200 | - | - | 16/25/74/74 | 0/4/4/4 |
| 5 | CYC | W | 201 | - | - | 12/25/74/74 | 0/4/4/4 |
| 5 | CYC | U | 200 | - | - | 6/25/74/74 | 0/4/4/4 |
| 5 | CYC | I | 201 | - | - | 11/25/74/74 | 0/4/4/4 |
| 5 | CYC | A | 200 | - | - | 16/25/74/74 | 0/4/4/4 |
| 5 | CYC | O | 200 | - | - | 16/25/74/74 | 0/4/4/4 |
| 5 | CYC | V | 201 | - | - | 11/25/74/74 | 0/4/4/4 |
| 5 | CYC | Y | 201 | - | - | 18/25/74/74 | 0/4/4/4 |
| 5 | CYC | X | 200 | - | - | 14/25/74/74 | 0/4/4/4 |
| 5 | CYC | X | 201 | - | - | 13/25/74/74 | 0/4/4/4 |
| 5 | CYC | K | 201 | - | - | 15/25/74/74 | 0/4/4/4 |
| 5 | CYC | I | 200 | - | - | 11/25/74/74 | 0/4/4/4 |
| 5 | CYC | G | 201 | - | - | 14/25/74/74 | 0/4/4/4 |
| 5 | CYC | i | 200 | - | - | 14/25/74/74 | 0/4/4/4 |
| 5 | CYC | S | 200 | - | - | 16/25/74/74 | 0/4/4/4 |
| 5 | CYC | E | 200 | - | - | 14/25/74/74 | 0/4/4/4 |
| 5 | CYC | T | 200 | - | - | 9/25/74/74 | 0/4/4/4 |
| 5 | CYC | h | 200 | - | - | 12/25/74/74 | 0/4/4/4 |
| 5 | CYC | 5 | 1202 | - | - | 11/25/74/74 | 0/4/4/4 |
| 5 | CYC | Q | 200 | - | - | 12/25/74/74 | 0/4/4/4 |
| 5 | CYC | C | 200 | - | - | 16/25/74/74 | 0/4/4/4 |
| 5 | CYC | Y | 200 | - | - | 10/25/74/74 | 0/4/4/4 |
| 5 | CYC | l | 201 | - | - | 16/25/74/74 | 0/4/4/4 |
| 5 | CYC | D | 200 | - | - | 13/25/74/74 | 0/4/4/4 |
| 5 | CYC | R | 200 | - | - | 14/25/74/74 | 0/4/4/4 |
| 5 | CYC | J | 201 | - | - | 18/25/74/74 | 0/4/4/4 |
| 5 | CYC | j | 200 | - | - | 10/25/74/74 | 0/4/4/4 |
| 5 | CYC | G | 200 | - | - | 12/25/74/74 | 0/4/4/4 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|-------------|---------|
| 5 | CYC | f | 200 | - | - | 16/25/74/74 | 0/4/4/4 |
| 5 | CYC | V | 200 | - | - | 11/25/74/74 | 0/4/4/4 |
| 5 | CYC | H | 201 | - | - | 18/25/74/74 | 0/4/4/4 |
| 5 | CYC | P | 200 | - | - | 11/25/74/74 | 0/4/4/4 |
| 5 | CYC | e | 200 | - | - | 17/25/74/74 | 0/4/4/4 |
| 5 | CYC | g | 201 | - | - | 15/25/74/74 | 0/4/4/4 |
| 5 | CYC | F | 200 | - | - | 14/25/74/74 | 0/4/4/4 |
| 5 | CYC | 5 | 1201 | - | - | 7/25/74/74 | 0/4/4/4 |
| 5 | CYC | H | 200 | - | - | 11/25/74/74 | 0/4/4/4 |
| 5 | CYC | a | 200 | - | - | 20/25/74/74 | 0/4/4/4 |
| 5 | CYC | K | 200 | - | - | 13/25/74/74 | 0/4/4/4 |
| 5 | CYC | N | 200 | - | - | 12/25/74/74 | 0/4/4/4 |
| 5 | CYC | c | 200 | - | - | 17/25/74/74 | 0/4/4/4 |
| 5 | CYC | J | 200 | - | - | 8/25/74/74 | 0/4/4/4 |
| 5 | CYC | b | 200 | - | - | 9/25/74/74 | 0/4/4/4 |
| 5 | CYC | i | 201 | - | - | 16/25/74/74 | 0/4/4/4 |
| 5 | CYC | B | 200 | - | - | 17/25/74/74 | 0/4/4/4 |
| 5 | CYC | T | 201 | - | - | 14/25/74/74 | 0/4/4/4 |
| 5 | CYC | g | 200 | - | - | 7/25/74/74 | 0/4/4/4 |

All (1296) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 5 | T | 200 | CYC | CHA-C1A | 27.21 | 1.57 | 1.35 |
| 5 | g | 200 | CYC | CHA-C1A | 26.85 | 1.57 | 1.35 |
| 5 | V | 200 | CYC | CHA-C1A | 26.85 | 1.57 | 1.35 |
| 5 | i | 201 | CYC | CHA-C1A | 26.79 | 1.57 | 1.35 |
| 5 | O | 200 | CYC | CHA-C1A | 26.76 | 1.57 | 1.35 |
| 5 | i | 200 | CYC | CHA-C1A | 26.70 | 1.57 | 1.35 |
| 5 | S | 200 | CYC | CHA-C1A | 26.67 | 1.57 | 1.35 |
| 5 | B | 200 | CYC | CHA-C1A | 26.65 | 1.57 | 1.35 |
| 5 | l | 201 | CYC | CHA-C1A | 26.62 | 1.57 | 1.35 |
| 5 | G | 200 | CYC | CHA-C1A | 26.62 | 1.57 | 1.35 |
| 5 | k | 201 | CYC | CHA-C1A | 26.62 | 1.57 | 1.35 |
| 5 | c | 200 | CYC | CHA-C1A | 26.57 | 1.57 | 1.35 |
| 5 | G | 201 | CYC | CHA-C1A | 26.53 | 1.57 | 1.35 |
| 5 | a | 200 | CYC | CHA-C1A | 26.49 | 1.57 | 1.35 |
| 5 | e | 200 | CYC | CHA-C1A | 26.49 | 1.57 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 5 | Y | 200 | CYC | CHA-C1A | 26.45 | 1.57 | 1.35 |
| 5 | j | 201 | CYC | CHA-C1A | 26.45 | 1.57 | 1.35 |
| 5 | X | 201 | CYC | CHA-C1A | 26.41 | 1.57 | 1.35 |
| 5 | b | 200 | CYC | CHA-C1A | 26.40 | 1.57 | 1.35 |
| 5 | U | 200 | CYC | CHA-C1A | 26.39 | 1.57 | 1.35 |
| 5 | h | 200 | CYC | CHA-C1A | 26.35 | 1.57 | 1.35 |
| 5 | L | 201 | CYC | CHA-C1A | 26.33 | 1.57 | 1.35 |
| 5 | V | 201 | CYC | CHA-C1A | 26.32 | 1.57 | 1.35 |
| 5 | P | 200 | CYC | CHA-C1A | 26.32 | 1.57 | 1.35 |
| 5 | U | 201 | CYC | CHA-C1A | 26.29 | 1.57 | 1.35 |
| 5 | Q | 200 | CYC | CHA-C1A | 26.25 | 1.57 | 1.35 |
| 5 | W | 201 | CYC | CHA-C1A | 26.24 | 1.57 | 1.35 |
| 5 | Y | 201 | CYC | CHA-C1A | 26.24 | 1.57 | 1.35 |
| 5 | X | 200 | CYC | CHA-C1A | 26.24 | 1.57 | 1.35 |
| 5 | 5 | 1202 | CYC | CHA-C1A | 26.22 | 1.57 | 1.35 |
| 5 | H | 200 | CYC | CHA-C1A | 26.21 | 1.57 | 1.35 |
| 5 | W | 200 | CYC | CHA-C1A | 26.19 | 1.57 | 1.35 |
| 5 | d | 200 | CYC | CHA-C1A | 26.15 | 1.57 | 1.35 |
| 5 | I | 201 | CYC | CHA-C1A | 26.14 | 1.57 | 1.35 |
| 5 | j | 200 | CYC | CHA-C1A | 26.08 | 1.56 | 1.35 |
| 5 | h | 201 | CYC | CHA-C1A | 26.08 | 1.56 | 1.35 |
| 5 | T | 201 | CYC | CHA-C1A | 26.07 | 1.56 | 1.35 |
| 5 | K | 200 | CYC | CHA-C1A | 26.06 | 1.56 | 1.35 |
| 5 | k | 200 | CYC | CHA-C1A | 26.05 | 1.56 | 1.35 |
| 5 | R | 200 | CYC | CHA-C1A | 26.00 | 1.56 | 1.35 |
| 5 | J | 200 | CYC | CHA-C1A | 25.95 | 1.56 | 1.35 |
| 5 | I | 200 | CYC | CHA-C1A | 25.89 | 1.56 | 1.35 |
| 5 | H | 201 | CYC | CHA-C1A | 25.87 | 1.56 | 1.35 |
| 5 | J | 201 | CYC | CHA-C1A | 25.81 | 1.56 | 1.35 |
| 5 | N | 200 | CYC | CHA-C1A | 25.79 | 1.56 | 1.35 |
| 5 | E | 200 | CYC | CHA-C1A | 25.78 | 1.56 | 1.35 |
| 5 | A | 200 | CYC | CHA-C1A | 25.76 | 1.56 | 1.35 |
| 5 | K | 201 | CYC | CHA-C1A | 25.76 | 1.56 | 1.35 |
| 5 | g | 201 | CYC | CHA-C1A | 25.71 | 1.56 | 1.35 |
| 5 | f | 200 | CYC | CHA-C1A | 25.63 | 1.56 | 1.35 |
| 5 | 5 | 1201 | CYC | CHA-C1A | 25.61 | 1.56 | 1.35 |
| 5 | C | 200 | CYC | CHA-C1A | 25.56 | 1.56 | 1.35 |
| 5 | D | 200 | CYC | CHA-C1A | 25.55 | 1.56 | 1.35 |
| 5 | F | 200 | CYC | CHA-C1A | 25.52 | 1.56 | 1.35 |
| 5 | c | 200 | CYC | C2C-C1C | 13.78 | 1.64 | 1.52 |
| 5 | a | 200 | CYC | C2C-C1C | 13.68 | 1.64 | 1.52 |
| 5 | f | 200 | CYC | C2C-C1C | 13.62 | 1.64 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 5 | R | 200 | CYC | C2C-C1C | 13.61 | 1.64 | 1.52 |
| 5 | b | 200 | CYC | C2C-C1C | 13.55 | 1.64 | 1.52 |
| 5 | H | 201 | CYC | C2C-C1C | 13.52 | 1.64 | 1.52 |
| 5 | i | 201 | CYC | C2C-C1C | 13.48 | 1.64 | 1.52 |
| 5 | h | 201 | CYC | C2C-C1C | 13.46 | 1.64 | 1.52 |
| 5 | k | 201 | CYC | C2C-C1C | 13.45 | 1.64 | 1.52 |
| 5 | h | 200 | CYC | C2C-C1C | 13.33 | 1.64 | 1.52 |
| 5 | Q | 200 | CYC | C2C-C1C | 13.32 | 1.64 | 1.52 |
| 5 | g | 200 | CYC | C2C-C1C | 13.29 | 1.63 | 1.52 |
| 5 | k | 200 | CYC | C2C-C1C | 13.28 | 1.63 | 1.52 |
| 5 | P | 200 | CYC | C2C-C1C | 13.23 | 1.63 | 1.52 |
| 5 | V | 201 | CYC | C2C-C1C | 13.21 | 1.63 | 1.52 |
| 5 | P | 200 | CYC | C3C-C4C | 13.20 | 1.70 | 1.50 |
| 5 | e | 200 | CYC | C2C-C1C | 13.20 | 1.63 | 1.52 |
| 5 | B | 200 | CYC | C2C-C1C | 13.19 | 1.63 | 1.52 |
| 5 | C | 200 | CYC | C2C-C1C | 13.17 | 1.63 | 1.52 |
| 5 | i | 200 | CYC | C2C-C1C | 13.17 | 1.63 | 1.52 |
| 5 | g | 200 | CYC | C3C-C4C | 13.16 | 1.70 | 1.50 |
| 5 | I | 201 | CYC | C3C-C4C | 13.15 | 1.70 | 1.50 |
| 5 | l | 201 | CYC | C2C-C1C | 13.15 | 1.63 | 1.52 |
| 5 | Y | 201 | CYC | C2C-C1C | 13.12 | 1.63 | 1.52 |
| 5 | T | 200 | CYC | C3C-C4C | 13.12 | 1.69 | 1.50 |
| 5 | k | 201 | CYC | C3C-C4C | 13.11 | 1.69 | 1.50 |
| 5 | d | 200 | CYC | C3C-C4C | 13.09 | 1.69 | 1.50 |
| 5 | g | 201 | CYC | C2C-C1C | 13.03 | 1.63 | 1.52 |
| 5 | U | 201 | CYC | C3C-C4C | 13.03 | 1.69 | 1.50 |
| 5 | j | 201 | CYC | C3C-C4C | 13.00 | 1.69 | 1.50 |
| 5 | X | 201 | CYC | C3C-C4C | 13.00 | 1.69 | 1.50 |
| 5 | X | 201 | CYC | C2C-C1C | 12.99 | 1.63 | 1.52 |
| 5 | W | 200 | CYC | C3C-C4C | 12.98 | 1.69 | 1.50 |
| 5 | O | 200 | CYC | C3C-C4C | 12.98 | 1.69 | 1.50 |
| 5 | d | 200 | CYC | C2C-C1C | 12.96 | 1.63 | 1.52 |
| 5 | i | 200 | CYC | C3C-C4C | 12.96 | 1.69 | 1.50 |
| 5 | L | 201 | CYC | C3C-C4C | 12.96 | 1.69 | 1.50 |
| 5 | U | 200 | CYC | C2C-C1C | 12.96 | 1.63 | 1.52 |
| 5 | H | 200 | CYC | C2C-C1C | 12.96 | 1.63 | 1.52 |
| 5 | T | 201 | CYC | C3C-C4C | 12.95 | 1.69 | 1.50 |
| 5 | G | 200 | CYC | C3C-C4C | 12.94 | 1.69 | 1.50 |
| 5 | G | 201 | CYC | C3C-C4C | 12.94 | 1.69 | 1.50 |
| 5 | U | 200 | CYC | C3C-C4C | 12.94 | 1.69 | 1.50 |
| 5 | R | 200 | CYC | C3C-C4C | 12.93 | 1.69 | 1.50 |
| 5 | C | 200 | CYC | C3C-C4C | 12.93 | 1.69 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 5 | V | 201 | CYC | C3C-C4C | 12.93 | 1.69 | 1.50 |
| 5 | 5 | 1202 | CYC | C3C-C4C | 12.93 | 1.69 | 1.50 |
| 5 | T | 201 | CYC | C2C-C1C | 12.92 | 1.63 | 1.52 |
| 5 | j | 200 | CYC | C2C-C1C | 12.92 | 1.63 | 1.52 |
| 5 | i | 201 | CYC | C3C-C4C | 12.89 | 1.69 | 1.50 |
| 5 | N | 200 | CYC | C3C-C4C | 12.88 | 1.69 | 1.50 |
| 5 | j | 201 | CYC | C2C-C1C | 12.86 | 1.63 | 1.52 |
| 5 | X | 200 | CYC | C3C-C4C | 12.86 | 1.69 | 1.50 |
| 5 | J | 201 | CYC | C2C-C1C | 12.83 | 1.63 | 1.52 |
| 5 | V | 200 | CYC | C2C-C1C | 12.83 | 1.63 | 1.52 |
| 5 | E | 200 | CYC | C3C-C4C | 12.82 | 1.69 | 1.50 |
| 5 | l | 201 | CYC | C3C-C4C | 12.81 | 1.69 | 1.50 |
| 5 | S | 200 | CYC | C2C-C1C | 12.80 | 1.63 | 1.52 |
| 5 | W | 201 | CYC | C3C-C4C | 12.79 | 1.69 | 1.50 |
| 5 | Y | 201 | CYC | C3C-C4C | 12.78 | 1.69 | 1.50 |
| 5 | G | 201 | CYC | C2C-C1C | 12.78 | 1.63 | 1.52 |
| 5 | E | 200 | CYC | C2C-C1C | 12.76 | 1.63 | 1.52 |
| 5 | g | 201 | CYC | C3C-C4C | 12.76 | 1.69 | 1.50 |
| 5 | f | 200 | CYC | C3C-C4C | 12.75 | 1.69 | 1.50 |
| 5 | J | 201 | CYC | C3C-C4C | 12.75 | 1.69 | 1.50 |
| 5 | V | 200 | CYC | C3C-C4C | 12.75 | 1.69 | 1.50 |
| 5 | K | 200 | CYC | C3C-C4C | 12.74 | 1.69 | 1.50 |
| 5 | K | 201 | CYC | C3C-C4C | 12.73 | 1.69 | 1.50 |
| 5 | e | 200 | CYC | C3C-C4C | 12.71 | 1.69 | 1.50 |
| 5 | h | 200 | CYC | C3C-C4C | 12.71 | 1.69 | 1.50 |
| 5 | c | 200 | CYC | C3C-C4C | 12.71 | 1.69 | 1.50 |
| 5 | T | 200 | CYC | C2C-C1C | 12.71 | 1.63 | 1.52 |
| 5 | A | 200 | CYC | C2C-C1C | 12.70 | 1.63 | 1.52 |
| 5 | D | 200 | CYC | C3C-C4C | 12.70 | 1.69 | 1.50 |
| 5 | h | 201 | CYC | C3C-C4C | 12.68 | 1.69 | 1.50 |
| 5 | A | 200 | CYC | C3C-C4C | 12.67 | 1.69 | 1.50 |
| 5 | b | 200 | CYC | C3C-C4C | 12.67 | 1.69 | 1.50 |
| 5 | I | 200 | CYC | C2C-C1C | 12.65 | 1.63 | 1.52 |
| 5 | G | 200 | CYC | C2C-C1C | 12.64 | 1.63 | 1.52 |
| 5 | 5 | 1202 | CYC | C2C-C1C | 12.64 | 1.63 | 1.52 |
| 5 | L | 201 | CYC | C2C-C1C | 12.63 | 1.63 | 1.52 |
| 5 | B | 200 | CYC | C3C-C4C | 12.61 | 1.69 | 1.50 |
| 5 | J | 200 | CYC | C3C-C4C | 12.60 | 1.69 | 1.50 |
| 5 | k | 200 | CYC | C3C-C4C | 12.57 | 1.69 | 1.50 |
| 5 | 5 | 1201 | CYC | C2C-C1C | 12.56 | 1.63 | 1.52 |
| 5 | j | 200 | CYC | C3C-C4C | 12.54 | 1.69 | 1.50 |
| 5 | N | 200 | CYC | C2C-C1C | 12.52 | 1.63 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 5 | F | 200 | CYC | C2C-C1C | 12.52 | 1.63 | 1.52 |
| 5 | U | 201 | CYC | C2C-C1C | 12.51 | 1.63 | 1.52 |
| 5 | I | 200 | CYC | C3C-C4C | 12.49 | 1.69 | 1.50 |
| 5 | Q | 200 | CYC | C3C-C4C | 12.49 | 1.69 | 1.50 |
| 5 | Y | 200 | CYC | C3C-C4C | 12.47 | 1.69 | 1.50 |
| 5 | O | 200 | CYC | C2C-C1C | 12.47 | 1.63 | 1.52 |
| 5 | X | 200 | CYC | C2C-C1C | 12.46 | 1.63 | 1.52 |
| 5 | S | 200 | CYC | C3C-C4C | 12.40 | 1.68 | 1.50 |
| 5 | F | 200 | CYC | C3C-C4C | 12.37 | 1.68 | 1.50 |
| 5 | d | 200 | CYC | C1C-NC | 12.37 | 1.53 | 1.37 |
| 5 | H | 201 | CYC | C3C-C4C | 12.36 | 1.68 | 1.50 |
| 5 | K | 200 | CYC | C2C-C1C | 12.34 | 1.63 | 1.52 |
| 5 | J | 200 | CYC | C2C-C1C | 12.34 | 1.63 | 1.52 |
| 5 | g | 200 | CYC | C1C-NC | 12.30 | 1.53 | 1.37 |
| 5 | e | 200 | CYC | C1C-NC | 12.29 | 1.53 | 1.37 |
| 5 | H | 201 | CYC | C1C-NC | 12.28 | 1.53 | 1.37 |
| 5 | a | 200 | CYC | C1C-NC | 12.28 | 1.53 | 1.37 |
| 5 | W | 201 | CYC | C2C-C1C | 12.25 | 1.63 | 1.52 |
| 5 | X | 201 | CYC | C1C-NC | 12.23 | 1.53 | 1.37 |
| 5 | U | 200 | CYC | C1C-NC | 12.23 | 1.53 | 1.37 |
| 5 | R | 200 | CYC | C1C-NC | 12.22 | 1.53 | 1.37 |
| 5 | i | 200 | CYC | C1C-NC | 12.21 | 1.53 | 1.37 |
| 5 | H | 200 | CYC | C3C-C4C | 12.20 | 1.68 | 1.50 |
| 5 | i | 201 | CYC | C1C-NC | 12.17 | 1.53 | 1.37 |
| 5 | l | 201 | CYC | C1C-NC | 12.16 | 1.53 | 1.37 |
| 5 | c | 200 | CYC | C1C-NC | 12.16 | 1.53 | 1.37 |
| 5 | a | 200 | CYC | C3C-C4C | 12.15 | 1.68 | 1.50 |
| 5 | P | 200 | CYC | C1C-NC | 12.15 | 1.53 | 1.37 |
| 5 | I | 201 | CYC | C2C-C1C | 12.14 | 1.62 | 1.52 |
| 5 | U | 201 | CYC | C1C-NC | 12.12 | 1.53 | 1.37 |
| 5 | h | 200 | CYC | C1C-NC | 12.12 | 1.53 | 1.37 |
| 5 | k | 201 | CYC | C1C-NC | 12.11 | 1.53 | 1.37 |
| 5 | j | 200 | CYC | C1C-NC | 12.09 | 1.53 | 1.37 |
| 5 | G | 200 | CYC | C1C-NC | 12.08 | 1.53 | 1.37 |
| 5 | I | 200 | CYC | C1C-NC | 12.07 | 1.53 | 1.37 |
| 5 | b | 200 | CYC | C1C-NC | 12.06 | 1.53 | 1.37 |
| 5 | X | 200 | CYC | C1C-NC | 12.05 | 1.53 | 1.37 |
| 5 | 5 | 1202 | CYC | C1C-NC | 12.05 | 1.53 | 1.37 |
| 5 | h | 201 | CYC | C1C-NC | 12.05 | 1.53 | 1.37 |
| 5 | g | 201 | CYC | C1C-NC | 12.04 | 1.53 | 1.37 |
| 5 | G | 201 | CYC | C1C-NC | 12.01 | 1.53 | 1.37 |
| 5 | T | 200 | CYC | C1C-NC | 11.99 | 1.53 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 5 | K | 201 | CYC | C2C-C1C | 11.99 | 1.62 | 1.52 |
| 5 | J | 200 | CYC | C1C-NC | 11.99 | 1.53 | 1.37 |
| 5 | W | 201 | CYC | C1C-NC | 11.97 | 1.53 | 1.37 |
| 5 | D | 200 | CYC | C2C-C1C | 11.96 | 1.62 | 1.52 |
| 5 | 5 | 1201 | CYC | C3C-C4C | 11.96 | 1.68 | 1.50 |
| 5 | T | 201 | CYC | C1C-NC | 11.95 | 1.53 | 1.37 |
| 5 | C | 200 | CYC | C1C-NC | 11.94 | 1.53 | 1.37 |
| 5 | V | 201 | CYC | C1C-NC | 11.89 | 1.53 | 1.37 |
| 5 | j | 201 | CYC | C1C-NC | 11.87 | 1.53 | 1.37 |
| 5 | H | 200 | CYC | C1C-NC | 11.85 | 1.53 | 1.37 |
| 5 | 5 | 1201 | CYC | C1C-NC | 11.85 | 1.53 | 1.37 |
| 5 | k | 200 | CYC | C1C-NC | 11.85 | 1.52 | 1.37 |
| 5 | K | 200 | CYC | C1C-NC | 11.79 | 1.52 | 1.37 |
| 5 | V | 200 | CYC | C1C-NC | 11.79 | 1.52 | 1.37 |
| 5 | f | 200 | CYC | C1C-NC | 11.78 | 1.52 | 1.37 |
| 5 | E | 200 | CYC | C1C-NC | 11.77 | 1.52 | 1.37 |
| 5 | Y | 201 | CYC | C1C-NC | 11.77 | 1.52 | 1.37 |
| 5 | Y | 200 | CYC | C2C-C1C | 11.77 | 1.62 | 1.52 |
| 5 | Y | 200 | CYC | C1C-NC | 11.75 | 1.52 | 1.37 |
| 5 | L | 201 | CYC | C1C-NC | 11.74 | 1.52 | 1.37 |
| 5 | K | 201 | CYC | C1C-NC | 11.73 | 1.52 | 1.37 |
| 5 | B | 200 | CYC | C1C-NC | 11.71 | 1.52 | 1.37 |
| 5 | F | 200 | CYC | C1C-NC | 11.69 | 1.52 | 1.37 |
| 5 | J | 201 | CYC | C1C-NC | 11.61 | 1.52 | 1.37 |
| 5 | Q | 200 | CYC | C1C-NC | 11.57 | 1.52 | 1.37 |
| 5 | A | 200 | CYC | C1C-NC | 11.49 | 1.52 | 1.37 |
| 5 | O | 200 | CYC | C1C-NC | 11.48 | 1.52 | 1.37 |
| 5 | S | 200 | CYC | C1C-NC | 11.47 | 1.52 | 1.37 |
| 5 | N | 200 | CYC | C1C-NC | 11.46 | 1.52 | 1.37 |
| 5 | W | 200 | CYC | C2C-C1C | 11.46 | 1.62 | 1.52 |
| 5 | I | 201 | CYC | C1C-NC | 11.45 | 1.52 | 1.37 |
| 5 | V | 201 | CYC | OB-C4B | 11.41 | 1.45 | 1.23 |
| 5 | V | 200 | CYC | OB-C4B | 11.39 | 1.45 | 1.23 |
| 5 | c | 200 | CYC | OB-C4B | 11.39 | 1.45 | 1.23 |
| 5 | J | 200 | CYC | OB-C4B | 11.38 | 1.45 | 1.23 |
| 5 | k | 200 | CYC | OB-C4B | 11.38 | 1.45 | 1.23 |
| 5 | g | 201 | CYC | OB-C4B | 11.38 | 1.45 | 1.23 |
| 5 | P | 200 | CYC | OB-C4B | 11.38 | 1.45 | 1.23 |
| 5 | H | 200 | CYC | OB-C4B | 11.37 | 1.45 | 1.23 |
| 5 | X | 200 | CYC | OB-C4B | 11.37 | 1.45 | 1.23 |
| 5 | i | 200 | CYC | OB-C4B | 11.37 | 1.45 | 1.23 |
| 5 | R | 200 | CYC | OB-C4B | 11.36 | 1.45 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 5 | b | 200 | CYC | OB-C4B | 11.36 | 1.45 | 1.23 |
| 5 | 5 | 1202 | CYC | OB-C4B | 11.35 | 1.45 | 1.23 |
| 5 | h | 201 | CYC | OB-C4B | 11.35 | 1.45 | 1.23 |
| 5 | T | 200 | CYC | OB-C4B | 11.34 | 1.45 | 1.23 |
| 5 | h | 200 | CYC | OB-C4B | 11.34 | 1.45 | 1.23 |
| 5 | e | 200 | CYC | OB-C4B | 11.34 | 1.45 | 1.23 |
| 5 | N | 200 | CYC | OB-C4B | 11.32 | 1.45 | 1.23 |
| 5 | W | 200 | CYC | C1C-NC | 11.32 | 1.52 | 1.37 |
| 5 | l | 201 | CYC | OB-C4B | 11.31 | 1.45 | 1.23 |
| 5 | g | 200 | CYC | OB-C4B | 11.31 | 1.45 | 1.23 |
| 5 | G | 200 | CYC | OB-C4B | 11.31 | 1.45 | 1.23 |
| 5 | H | 201 | CYC | OB-C4B | 11.31 | 1.45 | 1.23 |
| 5 | a | 200 | CYC | OB-C4B | 11.30 | 1.45 | 1.23 |
| 5 | Q | 200 | CYC | OB-C4B | 11.30 | 1.45 | 1.23 |
| 5 | i | 201 | CYC | OB-C4B | 11.30 | 1.45 | 1.23 |
| 5 | D | 200 | CYC | C1C-NC | 11.29 | 1.52 | 1.37 |
| 5 | k | 201 | CYC | OB-C4B | 11.29 | 1.45 | 1.23 |
| 5 | E | 200 | CYC | OB-C4B | 11.29 | 1.45 | 1.23 |
| 5 | Y | 201 | CYC | OB-C4B | 11.29 | 1.45 | 1.23 |
| 5 | Y | 200 | CYC | OB-C4B | 11.28 | 1.45 | 1.23 |
| 5 | C | 200 | CYC | OB-C4B | 11.28 | 1.45 | 1.23 |
| 5 | U | 200 | CYC | OB-C4B | 11.28 | 1.45 | 1.23 |
| 5 | j | 200 | CYC | OB-C4B | 11.27 | 1.45 | 1.23 |
| 5 | O | 200 | CYC | OB-C4B | 11.27 | 1.45 | 1.23 |
| 5 | I | 200 | CYC | OB-C4B | 11.26 | 1.45 | 1.23 |
| 5 | F | 200 | CYC | OB-C4B | 11.26 | 1.45 | 1.23 |
| 5 | A | 200 | CYC | OB-C4B | 11.25 | 1.45 | 1.23 |
| 5 | K | 201 | CYC | OB-C4B | 11.25 | 1.45 | 1.23 |
| 5 | T | 201 | CYC | OB-C4B | 11.23 | 1.45 | 1.23 |
| 5 | K | 200 | CYC | OB-C4B | 11.23 | 1.44 | 1.23 |
| 5 | j | 201 | CYC | OB-C4B | 11.23 | 1.44 | 1.23 |
| 5 | I | 201 | CYC | OB-C4B | 11.22 | 1.44 | 1.23 |
| 5 | d | 200 | CYC | OB-C4B | 11.22 | 1.44 | 1.23 |
| 5 | 5 | 1201 | CYC | OB-C4B | 11.21 | 1.44 | 1.23 |
| 5 | U | 201 | CYC | OB-C4B | 11.20 | 1.44 | 1.23 |
| 5 | W | 201 | CYC | OB-C4B | 11.20 | 1.44 | 1.23 |
| 5 | W | 200 | CYC | OB-C4B | 11.19 | 1.44 | 1.23 |
| 5 | f | 200 | CYC | OB-C4B | 11.19 | 1.44 | 1.23 |
| 5 | X | 201 | CYC | OB-C4B | 11.16 | 1.44 | 1.23 |
| 5 | G | 201 | CYC | OB-C4B | 11.15 | 1.44 | 1.23 |
| 5 | B | 200 | CYC | OB-C4B | 11.14 | 1.44 | 1.23 |
| 5 | D | 200 | CYC | OB-C4B | 11.14 | 1.44 | 1.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 5 | J | 201 | CYC | OB-C4B | 11.12 | 1.44 | 1.23 |
| 5 | S | 200 | CYC | OB-C4B | 11.10 | 1.44 | 1.23 |
| 5 | L | 201 | CYC | OB-C4B | 11.05 | 1.44 | 1.23 |
| 5 | Y | 200 | CYC | C2C-C3C | -10.32 | 1.25 | 1.54 |
| 5 | j | 200 | CYC | C2C-C3C | -10.15 | 1.26 | 1.54 |
| 5 | J | 200 | CYC | C2C-C3C | -10.11 | 1.26 | 1.54 |
| 5 | W | 200 | CYC | C2C-C3C | -10.11 | 1.26 | 1.54 |
| 5 | I | 200 | CYC | C2C-C3C | -10.10 | 1.26 | 1.54 |
| 5 | 5 | 1201 | CYC | C2C-C3C | -10.10 | 1.26 | 1.54 |
| 5 | l | 201 | CYC | CHB-C4A | 10.07 | 1.64 | 1.40 |
| 5 | K | 200 | CYC | C2C-C3C | -10.04 | 1.26 | 1.54 |
| 5 | U | 201 | CYC | C2C-C3C | -10.03 | 1.26 | 1.54 |
| 5 | F | 200 | CYC | C2C-C3C | -10.03 | 1.26 | 1.54 |
| 5 | X | 200 | CYC | C2C-C3C | -9.99 | 1.26 | 1.54 |
| 5 | G | 201 | CYC | CHB-C4A | 9.99 | 1.63 | 1.40 |
| 5 | W | 201 | CYC | C2C-C3C | -9.97 | 1.26 | 1.54 |
| 5 | K | 201 | CYC | C2C-C3C | -9.97 | 1.26 | 1.54 |
| 5 | G | 201 | CYC | C2C-C3C | -9.96 | 1.26 | 1.54 |
| 5 | O | 200 | CYC | CHB-C4A | 9.95 | 1.63 | 1.40 |
| 5 | i | 200 | CYC | CHB-C4A | 9.95 | 1.63 | 1.40 |
| 5 | S | 200 | CYC | C2C-C3C | -9.94 | 1.26 | 1.54 |
| 5 | 5 | 1202 | CYC | C2C-C3C | -9.94 | 1.26 | 1.54 |
| 5 | a | 200 | CYC | C2C-C3C | -9.92 | 1.26 | 1.54 |
| 5 | I | 201 | CYC | C2C-C3C | -9.90 | 1.26 | 1.54 |
| 5 | D | 200 | CYC | C2C-C3C | -9.90 | 1.26 | 1.54 |
| 5 | X | 200 | CYC | CHB-C4A | 9.89 | 1.63 | 1.40 |
| 5 | d | 200 | CYC | C2C-C3C | -9.88 | 1.26 | 1.54 |
| 5 | H | 201 | CYC | C2C-C3C | -9.88 | 1.26 | 1.54 |
| 5 | N | 200 | CYC | C2C-C3C | -9.88 | 1.26 | 1.54 |
| 5 | X | 201 | CYC | C2C-C3C | -9.86 | 1.26 | 1.54 |
| 5 | U | 200 | CYC | C2C-C3C | -9.86 | 1.26 | 1.54 |
| 5 | G | 200 | CYC | C2C-C3C | -9.86 | 1.26 | 1.54 |
| 5 | J | 201 | CYC | C2C-C3C | -9.86 | 1.26 | 1.54 |
| 5 | A | 200 | CYC | C2C-C3C | -9.85 | 1.27 | 1.54 |
| 5 | H | 200 | CYC | C2C-C3C | -9.85 | 1.27 | 1.54 |
| 5 | k | 200 | CYC | C2C-C3C | -9.85 | 1.27 | 1.54 |
| 5 | l | 201 | CYC | C2C-C3C | -9.84 | 1.27 | 1.54 |
| 5 | j | 201 | CYC | C2C-C3C | -9.84 | 1.27 | 1.54 |
| 5 | Q | 200 | CYC | C2C-C3C | -9.84 | 1.27 | 1.54 |
| 5 | h | 200 | CYC | C2C-C3C | -9.83 | 1.27 | 1.54 |
| 5 | U | 200 | CYC | CHB-C4A | 9.83 | 1.63 | 1.40 |
| 5 | f | 200 | CYC | C2C-C3C | -9.83 | 1.27 | 1.54 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 5 | K | 200 | CYC | CHB-C4A | 9.82 | 1.63 | 1.40 |
| 5 | T | 200 | CYC | CHB-C4A | 9.82 | 1.63 | 1.40 |
| 5 | e | 200 | CYC | C2C-C3C | -9.81 | 1.27 | 1.54 |
| 5 | H | 200 | CYC | CHB-C4A | 9.80 | 1.63 | 1.40 |
| 5 | K | 201 | CYC | CHB-C4A | 9.80 | 1.63 | 1.40 |
| 5 | i | 201 | CYC | C2C-C3C | -9.79 | 1.27 | 1.54 |
| 5 | T | 200 | CYC | C2C-C3C | -9.79 | 1.27 | 1.54 |
| 5 | Y | 201 | CYC | C2C-C3C | -9.78 | 1.27 | 1.54 |
| 5 | L | 201 | CYC | C2C-C3C | -9.78 | 1.27 | 1.54 |
| 5 | B | 200 | CYC | C2C-C3C | -9.78 | 1.27 | 1.54 |
| 5 | C | 200 | CYC | C2C-C3C | -9.78 | 1.27 | 1.54 |
| 5 | T | 201 | CYC | C2C-C3C | -9.77 | 1.27 | 1.54 |
| 5 | h | 201 | CYC | C2C-C3C | -9.77 | 1.27 | 1.54 |
| 5 | R | 200 | CYC | C2C-C3C | -9.77 | 1.27 | 1.54 |
| 5 | c | 200 | CYC | C2C-C3C | -9.75 | 1.27 | 1.54 |
| 5 | V | 201 | CYC | C2C-C3C | -9.75 | 1.27 | 1.54 |
| 5 | G | 200 | CYC | CHB-C4A | 9.74 | 1.63 | 1.40 |
| 5 | a | 200 | CYC | CHB-C4A | 9.74 | 1.63 | 1.40 |
| 5 | J | 200 | CYC | CHB-C4A | 9.74 | 1.63 | 1.40 |
| 5 | W | 200 | CYC | CHB-C4A | 9.74 | 1.63 | 1.40 |
| 5 | i | 200 | CYC | C2C-C3C | -9.74 | 1.27 | 1.54 |
| 5 | g | 200 | CYC | C2C-C3C | -9.73 | 1.27 | 1.54 |
| 5 | b | 200 | CYC | C2C-C3C | -9.72 | 1.27 | 1.54 |
| 5 | k | 201 | CYC | C2C-C3C | -9.72 | 1.27 | 1.54 |
| 5 | R | 200 | CYC | CHB-C4A | 9.72 | 1.63 | 1.40 |
| 5 | V | 200 | CYC | C2C-C3C | -9.71 | 1.27 | 1.54 |
| 5 | N | 200 | CYC | CHB-C4A | 9.71 | 1.63 | 1.40 |
| 5 | d | 200 | CYC | CHB-C4A | 9.70 | 1.63 | 1.40 |
| 5 | Y | 200 | CYC | CHB-C4A | 9.70 | 1.63 | 1.40 |
| 5 | g | 201 | CYC | C2C-C3C | -9.70 | 1.27 | 1.54 |
| 5 | E | 200 | CYC | C2C-C3C | -9.68 | 1.27 | 1.54 |
| 5 | B | 200 | CYC | CHB-C4A | 9.68 | 1.63 | 1.40 |
| 5 | O | 200 | CYC | C2C-C3C | -9.66 | 1.27 | 1.54 |
| 5 | W | 201 | CYC | CHB-C4A | 9.64 | 1.63 | 1.40 |
| 5 | h | 200 | CYC | CHB-C4A | 9.64 | 1.63 | 1.40 |
| 5 | Y | 201 | CYC | CHB-C4A | 9.63 | 1.63 | 1.40 |
| 5 | i | 201 | CYC | CHB-C4A | 9.63 | 1.62 | 1.40 |
| 5 | g | 200 | CYC | CHB-C4A | 9.62 | 1.62 | 1.40 |
| 5 | 5 | 1202 | CYC | CHB-C4A | 9.61 | 1.62 | 1.40 |
| 5 | P | 200 | CYC | C2C-C3C | -9.60 | 1.27 | 1.54 |
| 5 | b | 200 | CYC | CHB-C4A | 9.57 | 1.62 | 1.40 |
| 5 | E | 200 | CYC | CHB-C4A | 9.56 | 1.62 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 5 | A | 200 | CYC | CHB-C4A | 9.56 | 1.62 | 1.40 |
| 5 | Q | 200 | CYC | CHB-C4A | 9.54 | 1.62 | 1.40 |
| 5 | I | 201 | CYC | CHB-C4A | 9.54 | 1.62 | 1.40 |
| 5 | D | 200 | CYC | CHB-C4A | 9.53 | 1.62 | 1.40 |
| 5 | k | 201 | CYC | CHB-C4A | 9.52 | 1.62 | 1.40 |
| 5 | j | 200 | CYC | CHB-C4A | 9.51 | 1.62 | 1.40 |
| 5 | T | 201 | CYC | CHB-C4A | 9.51 | 1.62 | 1.40 |
| 5 | e | 200 | CYC | CHB-C4A | 9.51 | 1.62 | 1.40 |
| 5 | L | 201 | CYC | CHB-C4A | 9.50 | 1.62 | 1.40 |
| 5 | c | 200 | CYC | CHB-C4A | 9.49 | 1.62 | 1.40 |
| 5 | g | 201 | CYC | CHB-C4A | 9.47 | 1.62 | 1.40 |
| 5 | P | 200 | CYC | CHB-C4A | 9.47 | 1.62 | 1.40 |
| 5 | X | 201 | CYC | CHB-C4A | 9.44 | 1.62 | 1.40 |
| 5 | 5 | 1201 | CYC | CHB-C4A | 9.44 | 1.62 | 1.40 |
| 5 | j | 201 | CYC | CHB-C4A | 9.42 | 1.62 | 1.40 |
| 5 | J | 201 | CYC | CHB-C4A | 9.40 | 1.62 | 1.40 |
| 5 | V | 200 | CYC | CHB-C4A | 9.40 | 1.62 | 1.40 |
| 5 | F | 200 | CYC | CHB-C4A | 9.38 | 1.62 | 1.40 |
| 5 | U | 201 | CYC | CHB-C4A | 9.37 | 1.62 | 1.40 |
| 5 | C | 200 | CYC | CHB-C4A | 9.36 | 1.62 | 1.40 |
| 5 | S | 200 | CYC | CHB-C4A | 9.36 | 1.62 | 1.40 |
| 5 | k | 200 | CYC | CHB-C4A | 9.35 | 1.62 | 1.40 |
| 5 | V | 201 | CYC | CHB-C4A | 9.29 | 1.62 | 1.40 |
| 5 | h | 201 | CYC | CHB-C4A | 9.26 | 1.62 | 1.40 |
| 5 | I | 200 | CYC | CHB-C4A | 9.25 | 1.62 | 1.40 |
| 5 | H | 201 | CYC | CHB-C4A | 9.14 | 1.61 | 1.40 |
| 5 | f | 200 | CYC | CHB-C4A | 9.14 | 1.61 | 1.40 |
| 5 | l | 201 | CYC | CHB-C1B | 6.31 | 1.53 | 1.38 |
| 5 | L | 201 | CYC | C4B-C3B | -6.31 | 1.36 | 1.48 |
| 5 | U | 200 | CYC | CHB-C1B | 6.27 | 1.53 | 1.38 |
| 5 | H | 200 | CYC | CHB-C1B | 6.25 | 1.52 | 1.38 |
| 5 | X | 200 | CYC | CHB-C1B | 6.24 | 1.52 | 1.38 |
| 5 | G | 201 | CYC | C4B-C3B | -6.23 | 1.36 | 1.48 |
| 5 | K | 201 | CYC | C4B-C3B | -6.22 | 1.36 | 1.48 |
| 5 | G | 201 | CYC | CHB-C1B | 6.18 | 1.52 | 1.38 |
| 5 | i | 200 | CYC | CHB-C1B | 6.18 | 1.52 | 1.38 |
| 5 | 5 | 1201 | CYC | C4B-C3B | -6.16 | 1.36 | 1.48 |
| 5 | W | 200 | CYC | C4B-C3B | -6.15 | 1.36 | 1.48 |
| 5 | T | 200 | CYC | CHB-C1B | 6.14 | 1.52 | 1.38 |
| 5 | J | 200 | CYC | C4B-C3B | -6.13 | 1.36 | 1.48 |
| 5 | Y | 200 | CYC | C4B-C3B | -6.13 | 1.36 | 1.48 |
| 5 | E | 200 | CYC | C4B-C3B | -6.13 | 1.36 | 1.48 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 5 | G | 200 | CYC | CHB-C1B | 6.12 | 1.52 | 1.38 |
| 5 | K | 200 | CYC | C4B-C3B | -6.12 | 1.36 | 1.48 |
| 5 | X | 200 | CYC | C4B-C3B | -6.11 | 1.36 | 1.48 |
| 5 | Q | 200 | CYC | CHB-C1B | 6.10 | 1.52 | 1.38 |
| 5 | h | 200 | CYC | CHB-C1B | 6.10 | 1.52 | 1.38 |
| 5 | U | 200 | CYC | C4B-C3B | -6.09 | 1.36 | 1.48 |
| 5 | j | 200 | CYC | C4B-C3B | -6.09 | 1.36 | 1.48 |
| 5 | K | 200 | CYC | CHB-C1B | 6.08 | 1.52 | 1.38 |
| 5 | O | 200 | CYC | CHB-C1B | 6.08 | 1.52 | 1.38 |
| 5 | E | 200 | CYC | CHB-C1B | 6.07 | 1.52 | 1.38 |
| 5 | d | 200 | CYC | CHB-C1B | 6.07 | 1.52 | 1.38 |
| 5 | k | 201 | CYC | CHB-C1B | 6.07 | 1.52 | 1.38 |
| 5 | D | 200 | CYC | C4B-C3B | -6.07 | 1.36 | 1.48 |
| 5 | J | 200 | CYC | CHB-C1B | 6.06 | 1.52 | 1.38 |
| 5 | K | 201 | CYC | CHB-C1B | 6.06 | 1.52 | 1.38 |
| 5 | N | 200 | CYC | CHB-C1B | 6.06 | 1.52 | 1.38 |
| 5 | j | 200 | CYC | CHB-C1B | 6.06 | 1.52 | 1.38 |
| 5 | J | 201 | CYC | C4B-C3B | -6.06 | 1.36 | 1.48 |
| 5 | X | 201 | CYC | CHB-C1B | 6.05 | 1.52 | 1.38 |
| 5 | H | 200 | CYC | C4B-C3B | -6.05 | 1.36 | 1.48 |
| 5 | 5 | 1202 | CYC | CHB-C1B | 6.04 | 1.52 | 1.38 |
| 5 | P | 200 | CYC | CHB-C1B | 6.04 | 1.52 | 1.38 |
| 5 | B | 200 | CYC | C4B-C3B | -6.02 | 1.36 | 1.48 |
| 5 | g | 200 | CYC | CHB-C1B | 6.02 | 1.52 | 1.38 |
| 5 | b | 200 | CYC | CHB-C1B | 6.01 | 1.52 | 1.38 |
| 5 | A | 200 | CYC | CHB-C1B | 6.01 | 1.52 | 1.38 |
| 5 | W | 200 | CYC | CHB-C1B | 6.01 | 1.52 | 1.38 |
| 5 | W | 201 | CYC | C4B-C3B | -6.00 | 1.36 | 1.48 |
| 5 | T | 200 | CYC | C4B-C3B | -6.00 | 1.36 | 1.48 |
| 5 | T | 201 | CYC | CHB-C1B | 5.99 | 1.52 | 1.38 |
| 5 | 5 | 1202 | CYC | C4B-C3B | -5.99 | 1.36 | 1.48 |
| 5 | i | 201 | CYC | CHB-C1B | 5.99 | 1.52 | 1.38 |
| 5 | g | 201 | CYC | CHB-C1B | 5.99 | 1.52 | 1.38 |
| 5 | c | 200 | CYC | CHB-C1B | 5.98 | 1.52 | 1.38 |
| 5 | I | 201 | CYC | CHB-C1B | 5.98 | 1.52 | 1.38 |
| 5 | a | 200 | CYC | CHB-C1B | 5.98 | 1.52 | 1.38 |
| 5 | Y | 200 | CYC | CHB-C1B | 5.97 | 1.52 | 1.38 |
| 5 | V | 200 | CYC | CHB-C1B | 5.97 | 1.52 | 1.38 |
| 5 | e | 200 | CYC | CHB-C1B | 5.97 | 1.52 | 1.38 |
| 5 | I | 201 | CYC | C4B-C3B | -5.96 | 1.36 | 1.48 |
| 5 | L | 201 | CYC | CHB-C1B | 5.96 | 1.52 | 1.38 |
| 5 | d | 200 | CYC | C4B-C3B | -5.96 | 1.36 | 1.48 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 5 | I | 200 | CYC | C4B-C3B | -5.96 | 1.36 | 1.48 |
| 5 | G | 200 | CYC | C4B-C3B | -5.95 | 1.36 | 1.48 |
| 5 | a | 200 | CYC | C4B-C3B | -5.94 | 1.36 | 1.48 |
| 5 | T | 201 | CYC | C4B-C3B | -5.94 | 1.36 | 1.48 |
| 5 | I | 200 | CYC | CHB-C1B | 5.94 | 1.52 | 1.38 |
| 5 | R | 200 | CYC | C4B-C3B | -5.93 | 1.36 | 1.48 |
| 5 | R | 200 | CYC | CHB-C1B | 5.93 | 1.52 | 1.38 |
| 5 | g | 201 | CYC | C4B-C3B | -5.92 | 1.37 | 1.48 |
| 5 | S | 200 | CYC | CHB-C1B | 5.92 | 1.52 | 1.38 |
| 5 | 5 | 1201 | CYC | CHB-C1B | 5.91 | 1.52 | 1.38 |
| 5 | B | 200 | CYC | CHB-C1B | 5.91 | 1.52 | 1.38 |
| 5 | h | 200 | CYC | C4B-C3B | -5.91 | 1.37 | 1.48 |
| 5 | X | 201 | CYC | C4B-C3B | -5.90 | 1.37 | 1.48 |
| 5 | V | 201 | CYC | CHB-C1B | 5.90 | 1.52 | 1.38 |
| 5 | Y | 201 | CYC | C4B-C3B | -5.89 | 1.37 | 1.48 |
| 5 | k | 201 | CYC | C4B-C3B | -5.88 | 1.37 | 1.48 |
| 5 | Y | 201 | CYC | CHB-C1B | 5.87 | 1.52 | 1.38 |
| 5 | F | 200 | CYC | CHB-C1B | 5.87 | 1.52 | 1.38 |
| 5 | f | 200 | CYC | C4B-C3B | -5.87 | 1.37 | 1.48 |
| 5 | h | 201 | CYC | CHB-C1B | 5.86 | 1.52 | 1.38 |
| 5 | C | 200 | CYC | CHB-C1B | 5.84 | 1.51 | 1.38 |
| 5 | Q | 200 | CYC | C4B-C3B | -5.84 | 1.37 | 1.48 |
| 5 | k | 200 | CYC | C4B-C3B | -5.83 | 1.37 | 1.48 |
| 5 | e | 200 | CYC | C4B-C3B | -5.82 | 1.37 | 1.48 |
| 5 | j | 201 | CYC | C4B-C3B | -5.81 | 1.37 | 1.48 |
| 5 | i | 200 | CYC | C4B-C3B | -5.80 | 1.37 | 1.48 |
| 5 | O | 200 | CYC | C4B-C3B | -5.79 | 1.37 | 1.48 |
| 5 | W | 201 | CYC | CHB-C1B | 5.79 | 1.51 | 1.38 |
| 5 | k | 200 | CYC | CHB-C1B | 5.79 | 1.51 | 1.38 |
| 5 | A | 200 | CYC | C4B-C3B | -5.78 | 1.37 | 1.48 |
| 5 | g | 200 | CYC | C4B-C3B | -5.78 | 1.37 | 1.48 |
| 5 | h | 201 | CYC | C4B-C3B | -5.77 | 1.37 | 1.48 |
| 5 | V | 200 | CYC | C4B-C3B | -5.77 | 1.37 | 1.48 |
| 5 | C | 200 | CYC | C4B-C3B | -5.77 | 1.37 | 1.48 |
| 5 | j | 201 | CYC | CHB-C1B | 5.76 | 1.51 | 1.38 |
| 5 | N | 200 | CYC | C4B-C3B | -5.76 | 1.37 | 1.48 |
| 5 | P | 200 | CYC | C4B-C3B | -5.76 | 1.37 | 1.48 |
| 5 | J | 201 | CYC | CHB-C1B | 5.76 | 1.51 | 1.38 |
| 5 | D | 200 | CYC | CHB-C1B | 5.75 | 1.51 | 1.38 |
| 5 | c | 200 | CYC | C4B-C3B | -5.74 | 1.37 | 1.48 |
| 5 | b | 200 | CYC | C4B-C3B | -5.74 | 1.37 | 1.48 |
| 5 | f | 200 | CYC | CHB-C1B | 5.72 | 1.51 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 5 | V | 201 | CYC | C4B-C3B | -5.71 | 1.37 | 1.48 |
| 5 | i | 201 | CYC | C4B-C3B | -5.69 | 1.37 | 1.48 |
| 5 | U | 201 | CYC | CHB-C1B | 5.68 | 1.51 | 1.38 |
| 5 | U | 201 | CYC | C4B-C3B | -5.68 | 1.37 | 1.48 |
| 5 | l | 201 | CYC | C4B-C3B | -5.63 | 1.37 | 1.48 |
| 5 | H | 201 | CYC | C4B-C3B | -5.61 | 1.37 | 1.48 |
| 5 | F | 200 | CYC | C4B-C3B | -5.60 | 1.37 | 1.48 |
| 5 | S | 200 | CYC | C4B-C3B | -5.54 | 1.37 | 1.48 |
| 5 | H | 201 | CYC | CHB-C1B | 5.49 | 1.51 | 1.38 |
| 5 | P | 200 | CYC | CHD-C4C | 5.48 | 1.52 | 1.38 |
| 5 | U | 201 | CYC | CHD-C4C | 5.42 | 1.51 | 1.38 |
| 5 | B | 200 | CYC | C4D-CHA | 5.36 | 1.62 | 1.41 |
| 5 | d | 200 | CYC | CHD-C4C | 5.36 | 1.51 | 1.38 |
| 5 | R | 200 | CYC | CHD-C4C | 5.34 | 1.51 | 1.38 |
| 5 | P | 200 | CYC | C4D-CHA | 5.33 | 1.61 | 1.41 |
| 5 | i | 200 | CYC | CHD-C4C | 5.33 | 1.51 | 1.38 |
| 5 | T | 200 | CYC | C4D-CHA | 5.32 | 1.61 | 1.41 |
| 5 | O | 200 | CYC | CHD-C4C | 5.32 | 1.51 | 1.38 |
| 5 | S | 200 | CYC | C4D-CHA | 5.30 | 1.61 | 1.41 |
| 5 | U | 200 | CYC | CHD-C4C | 5.30 | 1.51 | 1.38 |
| 5 | b | 200 | CYC | CHD-C4C | 5.29 | 1.51 | 1.38 |
| 5 | h | 201 | CYC | CHD-C4C | 5.29 | 1.51 | 1.38 |
| 5 | k | 200 | CYC | CHD-C4C | 5.29 | 1.51 | 1.38 |
| 5 | G | 200 | CYC | C4D-CHA | 5.28 | 1.61 | 1.41 |
| 5 | U | 201 | CYC | C4D-CHA | 5.28 | 1.61 | 1.41 |
| 5 | k | 201 | CYC | CHD-C4C | 5.28 | 1.51 | 1.38 |
| 5 | i | 201 | CYC | C4D-CHA | 5.25 | 1.61 | 1.41 |
| 5 | k | 201 | CYC | C4D-CHA | 5.25 | 1.61 | 1.41 |
| 5 | b | 200 | CYC | C4D-CHA | 5.25 | 1.61 | 1.41 |
| 5 | e | 200 | CYC | CHD-C4C | 5.25 | 1.51 | 1.38 |
| 5 | g | 200 | CYC | CHD-C4C | 5.24 | 1.51 | 1.38 |
| 5 | Q | 200 | CYC | C4D-CHA | 5.24 | 1.61 | 1.41 |
| 5 | V | 200 | CYC | C4D-CHA | 5.24 | 1.61 | 1.41 |
| 5 | V | 201 | CYC | C4D-CHA | 5.24 | 1.61 | 1.41 |
| 5 | W | 200 | CYC | CHD-C4C | 5.24 | 1.51 | 1.38 |
| 5 | c | 200 | CYC | C4D-CHA | 5.23 | 1.61 | 1.41 |
| 5 | V | 200 | CYC | CHD-C4C | 5.23 | 1.51 | 1.38 |
| 5 | R | 200 | CYC | C4D-CHA | 5.23 | 1.61 | 1.41 |
| 5 | g | 200 | CYC | C4D-CHA | 5.23 | 1.61 | 1.41 |
| 5 | I | 201 | CYC | CHD-C4C | 5.22 | 1.51 | 1.38 |
| 5 | E | 200 | CYC | CHD-C4C | 5.21 | 1.51 | 1.38 |
| 5 | G | 201 | CYC | C4D-CHA | 5.21 | 1.61 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 5 | j | 201 | CYC | C4D-CHA | 5.21 | 1.61 | 1.41 |
| 5 | a | 200 | CYC | C4D-CHA | 5.21 | 1.61 | 1.41 |
| 5 | i | 200 | CYC | C4D-CHA | 5.21 | 1.61 | 1.41 |
| 5 | H | 200 | CYC | CHD-C4C | 5.20 | 1.51 | 1.38 |
| 5 | N | 200 | CYC | CHD-C4C | 5.20 | 1.51 | 1.38 |
| 5 | Y | 200 | CYC | C4D-CHA | 5.20 | 1.61 | 1.41 |
| 5 | i | 201 | CYC | CHD-C4C | 5.20 | 1.51 | 1.38 |
| 5 | e | 200 | CYC | C4D-CHA | 5.20 | 1.61 | 1.41 |
| 5 | W | 200 | CYC | C4D-CHA | 5.20 | 1.61 | 1.41 |
| 5 | H | 201 | CYC | CHD-C4C | 5.20 | 1.51 | 1.38 |
| 5 | F | 200 | CYC | C4D-CHA | 5.19 | 1.61 | 1.41 |
| 5 | I | 201 | CYC | C4D-CHA | 5.19 | 1.61 | 1.41 |
| 5 | U | 200 | CYC | C4D-CHA | 5.19 | 1.61 | 1.41 |
| 5 | O | 200 | CYC | C4D-CHA | 5.19 | 1.61 | 1.41 |
| 5 | h | 200 | CYC | CHD-C4C | 5.18 | 1.51 | 1.38 |
| 5 | N | 200 | CYC | C4D-CHA | 5.18 | 1.61 | 1.41 |
| 5 | X | 201 | CYC | C4D-CHA | 5.18 | 1.61 | 1.41 |
| 5 | 5 | 1201 | CYC | C1A-C2A | -5.17 | 1.37 | 1.45 |
| 5 | L | 201 | CYC | CHD-C4C | 5.17 | 1.51 | 1.38 |
| 5 | E | 200 | CYC | C4D-CHA | 5.17 | 1.61 | 1.41 |
| 5 | 5 | 1202 | CYC | C4D-CHA | 5.17 | 1.61 | 1.41 |
| 5 | J | 201 | CYC | C4D-CHA | 5.17 | 1.61 | 1.41 |
| 5 | I | 200 | CYC | CHD-C4C | 5.17 | 1.51 | 1.38 |
| 5 | c | 200 | CYC | CHD-C4C | 5.16 | 1.51 | 1.38 |
| 5 | C | 200 | CYC | CHD-C4C | 5.16 | 1.51 | 1.38 |
| 5 | A | 200 | CYC | CHD-C4C | 5.16 | 1.51 | 1.38 |
| 5 | H | 200 | CYC | C4D-CHA | 5.16 | 1.61 | 1.41 |
| 5 | L | 201 | CYC | C4D-CHA | 5.15 | 1.61 | 1.41 |
| 5 | H | 201 | CYC | C4D-CHA | 5.14 | 1.61 | 1.41 |
| 5 | Y | 201 | CYC | C4D-CHA | 5.14 | 1.61 | 1.41 |
| 5 | 5 | 1201 | CYC | CHD-C4C | 5.14 | 1.51 | 1.38 |
| 5 | X | 200 | CYC | CHD-C4C | 5.13 | 1.51 | 1.38 |
| 5 | I | 200 | CYC | C4D-CHA | 5.13 | 1.61 | 1.41 |
| 5 | 5 | 1202 | CYC | CHD-C4C | 5.13 | 1.51 | 1.38 |
| 5 | B | 200 | CYC | CHD-C4C | 5.13 | 1.51 | 1.38 |
| 5 | V | 200 | CYC | C1D-CHD | 5.13 | 1.61 | 1.41 |
| 5 | h | 200 | CYC | C4D-CHA | 5.13 | 1.61 | 1.41 |
| 5 | j | 200 | CYC | C4D-CHA | 5.13 | 1.61 | 1.41 |
| 5 | Q | 200 | CYC | CHD-C4C | 5.13 | 1.51 | 1.38 |
| 5 | g | 201 | CYC | C4D-CHA | 5.13 | 1.61 | 1.41 |
| 5 | l | 201 | CYC | CHD-C4C | 5.12 | 1.51 | 1.38 |
| 5 | K | 200 | CYC | C4D-CHA | 5.12 | 1.61 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 5 | T | 201 | CYC | CHD-C4C | 5.11 | 1.51 | 1.38 |
| 5 | f | 200 | CYC | CHD-C4C | 5.11 | 1.51 | 1.38 |
| 5 | V | 201 | CYC | CHD-C4C | 5.11 | 1.51 | 1.38 |
| 5 | d | 200 | CYC | C4D-CHA | 5.11 | 1.61 | 1.41 |
| 5 | g | 201 | CYC | CHD-C4C | 5.11 | 1.51 | 1.38 |
| 5 | W | 201 | CYC | C4D-CHA | 5.10 | 1.61 | 1.41 |
| 5 | h | 201 | CYC | C4D-CHA | 5.10 | 1.61 | 1.41 |
| 5 | X | 201 | CYC | CHD-C4C | 5.10 | 1.51 | 1.38 |
| 5 | X | 200 | CYC | C4D-CHA | 5.10 | 1.61 | 1.41 |
| 5 | J | 200 | CYC | C4D-CHA | 5.10 | 1.61 | 1.41 |
| 5 | J | 201 | CYC | CHD-C4C | 5.09 | 1.51 | 1.38 |
| 5 | T | 200 | CYC | CHD-C4C | 5.09 | 1.51 | 1.38 |
| 5 | C | 200 | CYC | C4D-CHA | 5.09 | 1.60 | 1.41 |
| 5 | Y | 201 | CYC | CHD-C4C | 5.09 | 1.51 | 1.38 |
| 5 | h | 201 | CYC | C1D-CHD | 5.09 | 1.60 | 1.41 |
| 5 | k | 200 | CYC | C4D-CHA | 5.09 | 1.60 | 1.41 |
| 5 | G | 201 | CYC | CHD-C4C | 5.08 | 1.51 | 1.38 |
| 5 | G | 200 | CYC | CHD-C4C | 5.08 | 1.51 | 1.38 |
| 5 | l | 201 | CYC | C4D-CHA | 5.08 | 1.60 | 1.41 |
| 5 | K | 200 | CYC | CHD-C4C | 5.08 | 1.51 | 1.38 |
| 5 | P | 200 | CYC | C1D-CHD | 5.08 | 1.60 | 1.41 |
| 5 | D | 200 | CYC | C4D-CHA | 5.07 | 1.60 | 1.41 |
| 5 | U | 201 | CYC | C1D-CHD | 5.06 | 1.60 | 1.41 |
| 5 | A | 200 | CYC | C4D-CHA | 5.06 | 1.60 | 1.41 |
| 5 | T | 201 | CYC | C4D-CHA | 5.05 | 1.60 | 1.41 |
| 5 | f | 200 | CYC | C4D-CHA | 5.04 | 1.60 | 1.41 |
| 5 | a | 200 | CYC | CHD-C4C | 5.04 | 1.50 | 1.38 |
| 5 | K | 201 | CYC | C4D-CHA | 5.04 | 1.60 | 1.41 |
| 5 | Q | 200 | CYC | C1D-CHD | 5.04 | 1.60 | 1.41 |
| 5 | D | 200 | CYC | CHD-C4C | 5.03 | 1.50 | 1.38 |
| 5 | W | 201 | CYC | CHD-C4C | 5.02 | 1.50 | 1.38 |
| 5 | J | 200 | CYC | CHD-C4C | 5.02 | 1.50 | 1.38 |
| 5 | k | 200 | CYC | C1D-CHD | 5.01 | 1.60 | 1.41 |
| 5 | j | 201 | CYC | CHD-C4C | 5.00 | 1.50 | 1.38 |
| 5 | K | 201 | CYC | CHD-C4C | 4.99 | 1.50 | 1.38 |
| 5 | H | 201 | CYC | C1D-CHD | 4.99 | 1.60 | 1.41 |
| 5 | b | 200 | CYC | C1D-CHD | 4.98 | 1.60 | 1.41 |
| 5 | H | 200 | CYC | C1D-CHD | 4.98 | 1.60 | 1.41 |
| 5 | B | 200 | CYC | C1D-CHD | 4.98 | 1.60 | 1.41 |
| 5 | A | 200 | CYC | C1D-CHD | 4.96 | 1.60 | 1.41 |
| 5 | D | 200 | CYC | C1D-CHD | 4.96 | 1.60 | 1.41 |
| 5 | j | 200 | CYC | CHD-C4C | 4.95 | 1.50 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 5 | Y | 200 | CYC | CHD-C4C | 4.95 | 1.50 | 1.38 |
| 5 | C | 200 | CYC | C1D-CHD | 4.94 | 1.60 | 1.41 |
| 5 | W | 200 | CYC | C1D-CHD | 4.94 | 1.60 | 1.41 |
| 5 | 5 | 1201 | CYC | C4D-CHA | 4.93 | 1.60 | 1.41 |
| 5 | O | 200 | CYC | C1D-CHD | 4.91 | 1.60 | 1.41 |
| 5 | I | 201 | CYC | C1D-CHD | 4.91 | 1.60 | 1.41 |
| 5 | N | 200 | CYC | C1D-CHD | 4.91 | 1.60 | 1.41 |
| 5 | d | 200 | CYC | C1D-CHD | 4.91 | 1.60 | 1.41 |
| 5 | T | 200 | CYC | C1D-CHD | 4.90 | 1.60 | 1.41 |
| 5 | g | 200 | CYC | C1D-CHD | 4.90 | 1.60 | 1.41 |
| 5 | E | 200 | CYC | C1D-CHD | 4.90 | 1.60 | 1.41 |
| 5 | D | 200 | CYC | C1A-C2A | -4.90 | 1.37 | 1.45 |
| 5 | S | 200 | CYC | C1B-C2B | -4.89 | 1.36 | 1.45 |
| 5 | i | 200 | CYC | C1D-CHD | 4.87 | 1.60 | 1.41 |
| 5 | A | 200 | CYC | C1A-C2A | -4.87 | 1.38 | 1.45 |
| 5 | U | 200 | CYC | C1D-CHD | 4.86 | 1.60 | 1.41 |
| 5 | h | 200 | CYC | C1D-CHD | 4.85 | 1.60 | 1.41 |
| 5 | e | 200 | CYC | C1D-CHD | 4.85 | 1.60 | 1.41 |
| 5 | G | 200 | CYC | C1D-CHD | 4.84 | 1.60 | 1.41 |
| 5 | V | 201 | CYC | C1D-CHD | 4.84 | 1.59 | 1.41 |
| 5 | g | 201 | CYC | C1D-CHD | 4.83 | 1.59 | 1.41 |
| 5 | I | 200 | CYC | C1D-CHD | 4.83 | 1.59 | 1.41 |
| 5 | X | 201 | CYC | C1D-CHD | 4.82 | 1.59 | 1.41 |
| 5 | k | 201 | CYC | C1D-CHD | 4.82 | 1.59 | 1.41 |
| 5 | R | 200 | CYC | C1D-CHD | 4.82 | 1.59 | 1.41 |
| 5 | 5 | 1202 | CYC | C1D-CHD | 4.81 | 1.59 | 1.41 |
| 5 | i | 201 | CYC | C1D-CHD | 4.80 | 1.59 | 1.41 |
| 5 | F | 200 | CYC | C1B-C2B | -4.80 | 1.36 | 1.45 |
| 5 | D | 200 | CYC | C1B-C2B | -4.80 | 1.36 | 1.45 |
| 5 | F | 200 | CYC | CHD-C4C | 4.79 | 1.50 | 1.38 |
| 5 | c | 200 | CYC | C1D-CHD | 4.78 | 1.59 | 1.41 |
| 5 | K | 200 | CYC | C1D-CHD | 4.78 | 1.59 | 1.41 |
| 5 | j | 201 | CYC | C1D-CHD | 4.78 | 1.59 | 1.41 |
| 5 | f | 200 | CYC | C1D-CHD | 4.77 | 1.59 | 1.41 |
| 5 | j | 200 | CYC | C1D-CHD | 4.77 | 1.59 | 1.41 |
| 5 | F | 200 | CYC | C1A-C2A | -4.77 | 1.38 | 1.45 |
| 5 | l | 201 | CYC | C1D-CHD | 4.76 | 1.59 | 1.41 |
| 5 | T | 201 | CYC | C1D-CHD | 4.76 | 1.59 | 1.41 |
| 5 | Y | 200 | CYC | C1D-CHD | 4.76 | 1.59 | 1.41 |
| 5 | J | 200 | CYC | C1A-C2A | -4.75 | 1.38 | 1.45 |
| 5 | K | 201 | CYC | C1D-CHD | 4.75 | 1.59 | 1.41 |
| 5 | Y | 201 | CYC | C1D-CHD | 4.75 | 1.59 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 5 | L | 201 | CYC | C1D-CHD | 4.75 | 1.59 | 1.41 |
| 5 | G | 201 | CYC | C1D-CHD | 4.74 | 1.59 | 1.41 |
| 5 | J | 200 | CYC | C1D-CHD | 4.74 | 1.59 | 1.41 |
| 5 | E | 200 | CYC | C1A-C2A | -4.72 | 1.38 | 1.45 |
| 5 | X | 200 | CYC | C1D-CHD | 4.72 | 1.59 | 1.41 |
| 5 | J | 201 | CYC | C1D-CHD | 4.71 | 1.59 | 1.41 |
| 5 | W | 201 | CYC | C1D-CHD | 4.70 | 1.59 | 1.41 |
| 5 | J | 201 | CYC | C1B-C2B | -4.68 | 1.36 | 1.45 |
| 5 | a | 200 | CYC | C1D-CHD | 4.68 | 1.59 | 1.41 |
| 5 | Y | 201 | CYC | C1B-C2B | -4.65 | 1.36 | 1.45 |
| 5 | 5 | 1201 | CYC | C1B-C2B | -4.64 | 1.36 | 1.45 |
| 5 | F | 200 | CYC | C1D-CHD | 4.63 | 1.59 | 1.41 |
| 5 | S | 200 | CYC | CHD-C4C | 4.62 | 1.49 | 1.38 |
| 5 | N | 200 | CYC | C1A-C2A | -4.59 | 1.38 | 1.45 |
| 5 | C | 200 | CYC | C1B-C2B | -4.59 | 1.36 | 1.45 |
| 5 | W | 201 | CYC | C1B-C2B | -4.56 | 1.36 | 1.45 |
| 5 | 5 | 1201 | CYC | C1D-CHD | 4.55 | 1.58 | 1.41 |
| 5 | Q | 200 | CYC | C1B-C2B | -4.55 | 1.36 | 1.45 |
| 5 | N | 200 | CYC | C1B-C2B | -4.55 | 1.36 | 1.45 |
| 5 | S | 200 | CYC | C1D-CHD | 4.53 | 1.58 | 1.41 |
| 5 | k | 200 | CYC | C1B-C2B | -4.53 | 1.37 | 1.45 |
| 5 | Q | 200 | CYC | C1A-C2A | -4.52 | 1.38 | 1.45 |
| 5 | K | 201 | CYC | C1A-C2A | -4.50 | 1.38 | 1.45 |
| 5 | f | 200 | CYC | C1B-C2B | -4.49 | 1.37 | 1.45 |
| 5 | X | 200 | CYC | C1A-C2A | -4.49 | 1.38 | 1.45 |
| 5 | S | 200 | CYC | C1A-C2A | -4.48 | 1.38 | 1.45 |
| 5 | W | 200 | CYC | C1A-C2A | -4.48 | 1.38 | 1.45 |
| 5 | E | 200 | CYC | C1B-C2B | -4.48 | 1.37 | 1.45 |
| 5 | l | 201 | CYC | C1A-C2A | -4.47 | 1.38 | 1.45 |
| 5 | U | 200 | CYC | C1A-C2A | -4.47 | 1.38 | 1.45 |
| 5 | A | 200 | CYC | C1B-C2B | -4.47 | 1.37 | 1.45 |
| 5 | H | 200 | CYC | C1A-C2A | -4.46 | 1.38 | 1.45 |
| 5 | Y | 201 | CYC | C1A-C2A | -4.46 | 1.38 | 1.45 |
| 5 | j | 200 | CYC | C1A-C2A | -4.45 | 1.38 | 1.45 |
| 5 | G | 201 | CYC | C1A-C2A | -4.45 | 1.38 | 1.45 |
| 5 | d | 200 | CYC | C1A-C2A | -4.44 | 1.38 | 1.45 |
| 5 | B | 200 | CYC | C1B-C2B | -4.43 | 1.37 | 1.45 |
| 5 | J | 200 | CYC | C1B-C2B | -4.42 | 1.37 | 1.45 |
| 5 | C | 200 | CYC | C1A-C2A | -4.40 | 1.38 | 1.45 |
| 5 | H | 201 | CYC | C1B-C2B | -4.39 | 1.37 | 1.45 |
| 5 | h | 200 | CYC | C1A-C2A | -4.38 | 1.38 | 1.45 |
| 5 | Y | 200 | CYC | C1A-C2A | -4.37 | 1.38 | 1.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 5 | X | 200 | CYC | C1B-C2B | -4.37 | 1.37 | 1.45 |
| 5 | J | 201 | CYC | C1A-C2A | -4.37 | 1.38 | 1.45 |
| 5 | V | 201 | CYC | C1B-C2B | -4.37 | 1.37 | 1.45 |
| 5 | R | 200 | CYC | C1B-C2B | -4.37 | 1.37 | 1.45 |
| 5 | D | 200 | CYC | C1B-NB | -4.36 | 1.30 | 1.37 |
| 5 | a | 200 | CYC | C1B-C2B | -4.36 | 1.37 | 1.45 |
| 5 | K | 200 | CYC | C1A-C2A | -4.35 | 1.38 | 1.45 |
| 5 | Y | 200 | CYC | C1B-C2B | -4.35 | 1.37 | 1.45 |
| 5 | G | 200 | CYC | C1A-C2A | -4.34 | 1.38 | 1.45 |
| 5 | W | 200 | CYC | C1B-NB | -4.33 | 1.30 | 1.37 |
| 5 | h | 201 | CYC | C1B-C2B | -4.33 | 1.37 | 1.45 |
| 5 | K | 200 | CYC | C1B-C2B | -4.33 | 1.37 | 1.45 |
| 5 | O | 200 | CYC | C1B-NB | -4.32 | 1.30 | 1.37 |
| 5 | W | 201 | CYC | C1A-C2A | -4.32 | 1.38 | 1.45 |
| 5 | L | 201 | CYC | C1B-C2B | -4.32 | 1.37 | 1.45 |
| 5 | 5 | 1202 | CYC | CBA-CGA | 4.31 | 1.60 | 1.50 |
| 5 | K | 201 | CYC | C1B-C2B | -4.31 | 1.37 | 1.45 |
| 5 | j | 201 | CYC | C1B-C2B | -4.30 | 1.37 | 1.45 |
| 5 | e | 200 | CYC | C1B-C2B | -4.28 | 1.37 | 1.45 |
| 5 | T | 200 | CYC | C1A-C2A | -4.27 | 1.38 | 1.45 |
| 5 | I | 200 | CYC | C1B-C2B | -4.27 | 1.37 | 1.45 |
| 5 | P | 200 | CYC | C1B-C2B | -4.27 | 1.37 | 1.45 |
| 5 | c | 200 | CYC | C1B-C2B | -4.26 | 1.37 | 1.45 |
| 5 | I | 200 | CYC | C1A-C2A | -4.25 | 1.38 | 1.45 |
| 5 | G | 200 | CYC | C1B-C2B | -4.25 | 1.37 | 1.45 |
| 5 | X | 201 | CYC | C1B-C2B | -4.25 | 1.37 | 1.45 |
| 5 | c | 200 | CYC | C1A-C2A | -4.24 | 1.39 | 1.45 |
| 5 | J | 200 | CYC | C1B-NB | -4.23 | 1.30 | 1.37 |
| 5 | f | 200 | CYC | C1A-C2A | -4.23 | 1.39 | 1.45 |
| 5 | S | 200 | CYC | C1B-NB | -4.23 | 1.30 | 1.37 |
| 5 | W | 200 | CYC | C1B-C2B | -4.22 | 1.37 | 1.45 |
| 5 | g | 201 | CYC | C1A-C2A | -4.22 | 1.39 | 1.45 |
| 5 | I | 201 | CYC | C1A-C2A | -4.21 | 1.39 | 1.45 |
| 5 | V | 200 | CYC | C1B-C2B | -4.21 | 1.37 | 1.45 |
| 5 | O | 200 | CYC | C1B-C2B | -4.21 | 1.37 | 1.45 |
| 5 | k | 201 | CYC | C1B-C2B | -4.20 | 1.37 | 1.45 |
| 5 | V | 200 | CYC | C1A-C2A | -4.20 | 1.39 | 1.45 |
| 5 | a | 200 | CYC | C1A-C2A | -4.20 | 1.39 | 1.45 |
| 5 | U | 201 | CYC | C1B-C2B | -4.19 | 1.37 | 1.45 |
| 5 | R | 200 | CYC | C1A-C2A | -4.18 | 1.39 | 1.45 |
| 5 | T | 201 | CYC | C1B-C2B | -4.18 | 1.37 | 1.45 |
| 5 | i | 201 | CYC | C1B-C2B | -4.18 | 1.37 | 1.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 5 | 5 | 1202 | CYC | C1B-C2B | -4.17 | 1.37 | 1.45 |
| 5 | g | 200 | CYC | C1A-C2A | -4.17 | 1.39 | 1.45 |
| 5 | j | 200 | CYC | C1B-C2B | -4.17 | 1.37 | 1.45 |
| 5 | h | 200 | CYC | C1B-C2B | -4.17 | 1.37 | 1.45 |
| 5 | F | 200 | CYC | C1B-NB | -4.17 | 1.30 | 1.37 |
| 5 | b | 200 | CYC | C1B-C2B | -4.17 | 1.37 | 1.45 |
| 5 | j | 201 | CYC | C1A-C2A | -4.17 | 1.39 | 1.45 |
| 5 | i | 200 | CYC | C1A-C2A | -4.17 | 1.39 | 1.45 |
| 5 | B | 200 | CYC | C1B-NB | -4.16 | 1.30 | 1.37 |
| 5 | d | 200 | CYC | C1B-C2B | -4.16 | 1.37 | 1.45 |
| 5 | O | 200 | CYC | C1A-C2A | -4.16 | 1.39 | 1.45 |
| 5 | H | 201 | CYC | C1A-C2A | -4.15 | 1.39 | 1.45 |
| 5 | K | 200 | CYC | C1B-NB | -4.15 | 1.30 | 1.37 |
| 5 | L | 201 | CYC | C1A-C2A | -4.15 | 1.39 | 1.45 |
| 5 | G | 201 | CYC | C1B-C2B | -4.15 | 1.37 | 1.45 |
| 5 | I | 201 | CYC | C1B-C2B | -4.15 | 1.37 | 1.45 |
| 5 | N | 200 | CYC | C1B-NB | -4.14 | 1.30 | 1.37 |
| 5 | T | 201 | CYC | C1A-C2A | -4.13 | 1.39 | 1.45 |
| 5 | X | 201 | CYC | C1A-C2A | -4.13 | 1.39 | 1.45 |
| 5 | H | 201 | CYC | C1B-NB | -4.13 | 1.30 | 1.37 |
| 5 | K | 201 | CYC | C1B-NB | -4.13 | 1.30 | 1.37 |
| 5 | g | 201 | CYC | C1B-C2B | -4.13 | 1.37 | 1.45 |
| 5 | J | 201 | CYC | C1B-NB | -4.12 | 1.30 | 1.37 |
| 5 | Y | 200 | CYC | C1B-NB | -4.12 | 1.30 | 1.37 |
| 5 | b | 200 | CYC | C1A-C2A | -4.12 | 1.39 | 1.45 |
| 5 | T | 200 | CYC | C1B-C2B | -4.11 | 1.37 | 1.45 |
| 5 | G | 201 | CYC | C1B-NB | -4.11 | 1.30 | 1.37 |
| 5 | 5 | 1201 | CYC | C1B-NB | -4.11 | 1.30 | 1.37 |
| 5 | B | 200 | CYC | C1A-C2A | -4.11 | 1.39 | 1.45 |
| 5 | g | 200 | CYC | C1B-C2B | -4.11 | 1.37 | 1.45 |
| 5 | 5 | 1202 | CYC | C1A-C2A | -4.10 | 1.39 | 1.45 |
| 5 | H | 200 | CYC | C1B-C2B | -4.10 | 1.37 | 1.45 |
| 5 | i | 200 | CYC | C1B-C2B | -4.08 | 1.37 | 1.45 |
| 5 | T | 201 | CYC | C1B-NB | -4.06 | 1.31 | 1.37 |
| 5 | U | 200 | CYC | C1B-C2B | -4.05 | 1.37 | 1.45 |
| 5 | U | 201 | CYC | C1B-NB | -4.04 | 1.31 | 1.37 |
| 5 | g | 201 | CYC | C1B-NB | -4.03 | 1.31 | 1.37 |
| 5 | d | 200 | CYC | C1B-NB | -4.02 | 1.31 | 1.37 |
| 5 | I | 201 | CYC | C1B-NB | -4.02 | 1.31 | 1.37 |
| 5 | f | 200 | CYC | C1B-NB | -4.01 | 1.31 | 1.37 |
| 5 | U | 201 | CYC | CBA-CGA | 4.01 | 1.59 | 1.50 |
| 5 | E | 200 | CYC | C1B-NB | -4.01 | 1.31 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 5 | P | 200 | CYC | C1A-C2A | -4.00 | 1.39 | 1.45 |
| 5 | Q | 200 | CYC | C1B-NB | -3.99 | 1.31 | 1.37 |
| 5 | l | 201 | CYC | C1B-C2B | -3.99 | 1.37 | 1.45 |
| 5 | U | 200 | CYC | CBA-CGA | 3.98 | 1.59 | 1.50 |
| 5 | k | 201 | CYC | C1A-C2A | -3.98 | 1.39 | 1.45 |
| 5 | H | 200 | CYC | C1B-NB | -3.98 | 1.31 | 1.37 |
| 5 | R | 200 | CYC | C1B-NB | -3.98 | 1.31 | 1.37 |
| 5 | L | 201 | CYC | C1B-NB | -3.98 | 1.31 | 1.37 |
| 5 | h | 201 | CYC | C1A-C2A | -3.97 | 1.39 | 1.45 |
| 5 | A | 200 | CYC | CBA-CGA | 3.97 | 1.59 | 1.50 |
| 5 | Y | 201 | CYC | C1B-NB | -3.97 | 1.31 | 1.37 |
| 5 | W | 201 | CYC | C1B-NB | -3.96 | 1.31 | 1.37 |
| 5 | g | 200 | CYC | C1B-NB | -3.96 | 1.31 | 1.37 |
| 5 | h | 200 | CYC | CBA-CGA | 3.96 | 1.59 | 1.50 |
| 5 | R | 200 | CYC | CBA-CGA | 3.96 | 1.59 | 1.50 |
| 5 | V | 201 | CYC | CBA-CGA | 3.95 | 1.59 | 1.50 |
| 5 | N | 200 | CYC | CBA-CGA | 3.95 | 1.59 | 1.50 |
| 5 | G | 200 | CYC | C1B-NB | -3.95 | 1.31 | 1.37 |
| 5 | X | 200 | CYC | C1B-NB | -3.95 | 1.31 | 1.37 |
| 5 | T | 200 | CYC | C1B-NB | -3.94 | 1.31 | 1.37 |
| 5 | c | 200 | CYC | CBA-CGA | 3.94 | 1.59 | 1.50 |
| 5 | j | 201 | CYC | C1B-NB | -3.93 | 1.31 | 1.37 |
| 5 | h | 201 | CYC | CBA-CGA | 3.93 | 1.59 | 1.50 |
| 5 | W | 201 | CYC | CBA-CGA | 3.93 | 1.59 | 1.50 |
| 5 | l | 201 | CYC | C1B-NB | -3.93 | 1.31 | 1.37 |
| 5 | e | 200 | CYC | CBA-CGA | 3.93 | 1.59 | 1.50 |
| 5 | I | 200 | CYC | C1B-NB | -3.92 | 1.31 | 1.37 |
| 5 | a | 200 | CYC | CBA-CGA | 3.92 | 1.59 | 1.50 |
| 5 | U | 201 | CYC | C1A-C2A | -3.92 | 1.39 | 1.45 |
| 5 | k | 200 | CYC | C1B-NB | -3.91 | 1.31 | 1.37 |
| 5 | j | 201 | CYC | CBA-CGA | 3.91 | 1.59 | 1.50 |
| 5 | L | 201 | CYC | CBA-CGA | 3.91 | 1.59 | 1.50 |
| 5 | O | 200 | CYC | CBA-CGA | 3.91 | 1.59 | 1.50 |
| 5 | J | 201 | CYC | CBA-CGA | 3.90 | 1.59 | 1.50 |
| 5 | i | 201 | CYC | C1A-C2A | -3.90 | 1.39 | 1.45 |
| 5 | k | 200 | CYC | C1A-C2A | -3.90 | 1.39 | 1.45 |
| 5 | Y | 201 | CYC | CBA-CGA | 3.90 | 1.59 | 1.50 |
| 5 | A | 200 | CYC | C1B-NB | -3.90 | 1.31 | 1.37 |
| 5 | V | 201 | CYC | C1A-C2A | -3.90 | 1.39 | 1.45 |
| 5 | b | 200 | CYC | CBA-CGA | 3.90 | 1.59 | 1.50 |
| 5 | l | 201 | CYC | CBA-CGA | 3.89 | 1.59 | 1.50 |
| 5 | B | 200 | CYC | CBA-CGA | 3.89 | 1.59 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 5 | I | 201 | CYC | CBA-CGA | 3.89 | 1.59 | 1.50 |
| 5 | f | 200 | CYC | CBA-CGA | 3.89 | 1.59 | 1.50 |
| 5 | i | 201 | CYC | CBA-CGA | 3.89 | 1.59 | 1.50 |
| 5 | P | 200 | CYC | CBA-CGA | 3.88 | 1.59 | 1.50 |
| 5 | V | 201 | CYC | C1B-NB | -3.87 | 1.31 | 1.37 |
| 5 | X | 201 | CYC | CBA-CGA | 3.87 | 1.59 | 1.50 |
| 5 | K | 201 | CYC | CBA-CGA | 3.86 | 1.59 | 1.50 |
| 5 | G | 201 | CYC | CBA-CGA | 3.86 | 1.59 | 1.50 |
| 5 | 5 | 1202 | CYC | C1B-NB | -3.86 | 1.31 | 1.37 |
| 5 | C | 200 | CYC | C1B-NB | -3.86 | 1.31 | 1.37 |
| 5 | T | 201 | CYC | CBA-CGA | 3.86 | 1.59 | 1.50 |
| 5 | j | 200 | CYC | C1B-NB | -3.85 | 1.31 | 1.37 |
| 5 | R | 200 | CYC | CMC-C2C | 3.85 | 1.61 | 1.53 |
| 5 | X | 201 | CYC | C1B-NB | -3.85 | 1.31 | 1.37 |
| 5 | g | 200 | CYC | CBA-CGA | 3.84 | 1.59 | 1.50 |
| 5 | e | 200 | CYC | C1A-C2A | -3.84 | 1.39 | 1.45 |
| 5 | d | 200 | CYC | CBA-CGA | 3.84 | 1.59 | 1.50 |
| 5 | j | 200 | CYC | CBA-CGA | 3.83 | 1.59 | 1.50 |
| 5 | H | 201 | CYC | CBA-CGA | 3.83 | 1.59 | 1.50 |
| 5 | V | 200 | CYC | C1B-NB | -3.83 | 1.31 | 1.37 |
| 5 | T | 200 | CYC | CBA-CGA | 3.83 | 1.59 | 1.50 |
| 5 | i | 201 | CYC | C1B-NB | -3.83 | 1.31 | 1.37 |
| 5 | h | 201 | CYC | C1B-NB | -3.82 | 1.31 | 1.37 |
| 5 | g | 201 | CYC | CBA-CGA | 3.82 | 1.59 | 1.50 |
| 5 | h | 200 | CYC | C1B-NB | -3.82 | 1.31 | 1.37 |
| 5 | k | 201 | CYC | CBA-CGA | 3.82 | 1.59 | 1.50 |
| 5 | G | 200 | CYC | CBA-CGA | 3.82 | 1.59 | 1.50 |
| 5 | a | 200 | CYC | C1B-NB | -3.81 | 1.31 | 1.37 |
| 5 | H | 200 | CYC | CBA-CGA | 3.81 | 1.59 | 1.50 |
| 5 | g | 200 | CYC | CMC-C2C | 3.81 | 1.61 | 1.53 |
| 5 | i | 200 | CYC | CBA-CGA | 3.81 | 1.59 | 1.50 |
| 5 | k | 201 | CYC | C1B-NB | -3.80 | 1.31 | 1.37 |
| 5 | k | 200 | CYC | CBA-CGA | 3.79 | 1.59 | 1.50 |
| 5 | P | 200 | CYC | C1B-NB | -3.79 | 1.31 | 1.37 |
| 5 | P | 200 | CYC | CMC-C2C | 3.79 | 1.61 | 1.53 |
| 5 | I | 200 | CYC | CBA-CGA | 3.77 | 1.59 | 1.50 |
| 5 | C | 200 | CYC | CBA-CGA | 3.77 | 1.59 | 1.50 |
| 5 | e | 200 | CYC | C1B-NB | -3.77 | 1.31 | 1.37 |
| 5 | b | 200 | CYC | C1B-NB | -3.76 | 1.31 | 1.37 |
| 5 | U | 200 | CYC | C1B-NB | -3.75 | 1.31 | 1.37 |
| 5 | J | 200 | CYC | CBA-CGA | 3.75 | 1.59 | 1.50 |
| 5 | d | 200 | CYC | CMC-C2C | 3.75 | 1.61 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 5 | c | 200 | CYC | C1B-NB | -3.75 | 1.31 | 1.37 |
| 5 | e | 200 | CYC | CMC-C2C | 3.74 | 1.61 | 1.53 |
| 5 | c | 200 | CYC | CMC-C2C | 3.74 | 1.61 | 1.53 |
| 5 | U | 200 | CYC | CMC-C2C | 3.73 | 1.61 | 1.53 |
| 5 | j | 201 | CYC | CMC-C2C | 3.73 | 1.61 | 1.53 |
| 5 | a | 200 | CYC | CMC-C2C | 3.72 | 1.61 | 1.53 |
| 5 | k | 201 | CYC | CMC-C2C | 3.72 | 1.61 | 1.53 |
| 5 | g | 201 | CYC | CMC-C2C | 3.72 | 1.61 | 1.53 |
| 5 | 5 | 1201 | CYC | CBA-CGA | 3.71 | 1.59 | 1.50 |
| 5 | i | 200 | CYC | C1B-NB | -3.71 | 1.31 | 1.37 |
| 5 | T | 201 | CYC | CMC-C2C | 3.71 | 1.61 | 1.53 |
| 5 | W | 200 | CYC | CBA-CGA | 3.71 | 1.59 | 1.50 |
| 5 | D | 200 | CYC | CBA-CGA | 3.71 | 1.59 | 1.50 |
| 5 | V | 200 | CYC | CBA-CGA | 3.70 | 1.59 | 1.50 |
| 5 | V | 201 | CYC | CMC-C2C | 3.70 | 1.61 | 1.53 |
| 5 | X | 201 | CYC | CMC-C2C | 3.70 | 1.61 | 1.53 |
| 5 | V | 200 | CYC | CMC-C2C | 3.70 | 1.61 | 1.53 |
| 5 | 5 | 1202 | CYC | CMC-C2C | 3.69 | 1.61 | 1.53 |
| 5 | i | 200 | CYC | CMC-C2C | 3.69 | 1.61 | 1.53 |
| 5 | f | 200 | CYC | CMC-C2C | 3.68 | 1.61 | 1.53 |
| 5 | i | 201 | CYC | CMC-C2C | 3.68 | 1.61 | 1.53 |
| 5 | H | 201 | CYC | CMC-C2C | 3.68 | 1.61 | 1.53 |
| 5 | L | 201 | CYC | CMC-C2C | 3.68 | 1.61 | 1.53 |
| 5 | E | 200 | CYC | CBA-CGA | 3.67 | 1.59 | 1.50 |
| 5 | X | 200 | CYC | CMC-C2C | 3.67 | 1.61 | 1.53 |
| 5 | h | 200 | CYC | CMC-C2C | 3.66 | 1.61 | 1.53 |
| 5 | T | 200 | CYC | CMC-C2C | 3.66 | 1.61 | 1.53 |
| 5 | U | 201 | CYC | CMC-C2C | 3.65 | 1.61 | 1.53 |
| 5 | Y | 200 | CYC | CBA-CGA | 3.65 | 1.59 | 1.50 |
| 5 | Q | 200 | CYC | CBA-CGA | 3.65 | 1.59 | 1.50 |
| 5 | O | 200 | CYC | CMC-C2C | 3.64 | 1.61 | 1.53 |
| 5 | h | 201 | CYC | CMC-C2C | 3.64 | 1.61 | 1.53 |
| 5 | G | 201 | CYC | CMC-C2C | 3.63 | 1.61 | 1.53 |
| 5 | X | 200 | CYC | CBA-CGA | 3.62 | 1.59 | 1.50 |
| 5 | K | 200 | CYC | CBA-CGA | 3.61 | 1.59 | 1.50 |
| 5 | 5 | 1201 | CYC | CMC-C2C | 3.61 | 1.61 | 1.53 |
| 5 | Y | 201 | CYC | CMC-C2C | 3.61 | 1.61 | 1.53 |
| 5 | H | 200 | CYC | CMC-C2C | 3.60 | 1.60 | 1.53 |
| 5 | F | 200 | CYC | CBA-CGA | 3.59 | 1.58 | 1.50 |
| 5 | l | 201 | CYC | CMC-C2C | 3.59 | 1.60 | 1.53 |
| 5 | K | 200 | CYC | CMC-C2C | 3.58 | 1.60 | 1.53 |
| 5 | E | 200 | CYC | CMC-C2C | 3.58 | 1.60 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 5 | G | 200 | CYC | CMC-C2C | 3.58 | 1.60 | 1.53 |
| 5 | J | 201 | CYC | CMC-C2C | 3.57 | 1.60 | 1.53 |
| 5 | F | 200 | CYC | CMC-C2C | 3.57 | 1.60 | 1.53 |
| 5 | B | 200 | CYC | CMC-C2C | 3.57 | 1.60 | 1.53 |
| 5 | k | 200 | CYC | CMC-C2C | 3.57 | 1.60 | 1.53 |
| 5 | I | 201 | CYC | CMC-C2C | 3.57 | 1.60 | 1.53 |
| 5 | S | 200 | CYC | CMC-C2C | 3.57 | 1.60 | 1.53 |
| 5 | b | 200 | CYC | CMC-C2C | 3.56 | 1.60 | 1.53 |
| 5 | S | 200 | CYC | CBA-CGA | 3.55 | 1.58 | 1.50 |
| 5 | j | 200 | CYC | CMC-C2C | 3.55 | 1.60 | 1.53 |
| 5 | D | 200 | CYC | CMC-C2C | 3.55 | 1.60 | 1.53 |
| 5 | N | 200 | CYC | CMC-C2C | 3.54 | 1.60 | 1.53 |
| 5 | W | 200 | CYC | CMC-C2C | 3.53 | 1.60 | 1.53 |
| 5 | I | 200 | CYC | CMC-C2C | 3.52 | 1.60 | 1.53 |
| 5 | C | 200 | CYC | CMC-C2C | 3.52 | 1.60 | 1.53 |
| 5 | A | 200 | CYC | CMC-C2C | 3.51 | 1.60 | 1.53 |
| 5 | Q | 200 | CYC | CMC-C2C | 3.49 | 1.60 | 1.53 |
| 5 | W | 201 | CYC | CMC-C2C | 3.48 | 1.60 | 1.53 |
| 5 | K | 201 | CYC | CMC-C2C | 3.47 | 1.60 | 1.53 |
| 5 | J | 200 | CYC | CMC-C2C | 3.46 | 1.60 | 1.53 |
| 5 | Y | 200 | CYC | CMC-C2C | 3.36 | 1.60 | 1.53 |
| 5 | l | 201 | CYC | CAB-C3B | 3.18 | 1.59 | 1.51 |
| 5 | V | 201 | CYC | C4A-C3A | -3.08 | 1.39 | 1.45 |
| 5 | H | 201 | CYC | C4A-C3A | -3.08 | 1.39 | 1.45 |
| 5 | S | 200 | CYC | CAB-C3B | 3.06 | 1.59 | 1.51 |
| 5 | V | 200 | CYC | CAB-C3B | 3.05 | 1.58 | 1.51 |
| 5 | P | 200 | CYC | CAB-C3B | 3.05 | 1.58 | 1.51 |
| 5 | J | 201 | CYC | C1A-NA | -3.05 | 1.32 | 1.38 |
| 5 | i | 200 | CYC | CAB-C3B | 3.05 | 1.58 | 1.51 |
| 5 | f | 200 | CYC | C4A-C3A | -3.04 | 1.39 | 1.45 |
| 5 | X | 200 | CYC | CAB-C3B | 3.03 | 1.58 | 1.51 |
| 5 | c | 200 | CYC | CAB-C3B | 3.01 | 1.58 | 1.51 |
| 5 | T | 200 | CYC | CAB-C3B | 3.01 | 1.58 | 1.51 |
| 5 | g | 200 | CYC | CAB-C3B | 3.01 | 1.58 | 1.51 |
| 5 | S | 200 | CYC | C4A-C3A | -3.01 | 1.39 | 1.45 |
| 5 | F | 200 | CYC | CAB-C3B | 3.00 | 1.58 | 1.51 |
| 5 | Y | 201 | CYC | CAB-C3B | 3.00 | 1.58 | 1.51 |
| 5 | X | 201 | CYC | CAB-C3B | 2.99 | 1.58 | 1.51 |
| 5 | U | 200 | CYC | CAB-C3B | 2.99 | 1.58 | 1.51 |
| 5 | O | 200 | CYC | CAB-C3B | 2.99 | 1.58 | 1.51 |
| 5 | W | 200 | CYC | C4B-NB | -2.98 | 1.31 | 1.38 |
| 5 | i | 201 | CYC | CAB-C3B | 2.97 | 1.58 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 5 | N | 200 | CYC | CAB-C3B | 2.97 | 1.58 | 1.51 |
| 5 | b | 200 | CYC | CAB-C3B | 2.97 | 1.58 | 1.51 |
| 5 | j | 201 | CYC | CAB-C3B | 2.97 | 1.58 | 1.51 |
| 5 | d | 200 | CYC | CAB-C3B | 2.97 | 1.58 | 1.51 |
| 5 | G | 200 | CYC | CAB-C3B | 2.97 | 1.58 | 1.51 |
| 5 | H | 200 | CYC | CAB-C3B | 2.96 | 1.58 | 1.51 |
| 5 | D | 200 | CYC | C1A-NA | -2.96 | 1.32 | 1.38 |
| 5 | W | 200 | CYC | C1A-NA | -2.95 | 1.32 | 1.38 |
| 5 | C | 200 | CYC | C4A-C3A | -2.95 | 1.39 | 1.45 |
| 5 | e | 200 | CYC | CAB-C3B | 2.95 | 1.58 | 1.51 |
| 5 | h | 200 | CYC | CAB-C3B | 2.95 | 1.58 | 1.51 |
| 5 | A | 200 | CYC | CAB-C3B | 2.95 | 1.58 | 1.51 |
| 5 | J | 200 | CYC | CAB-C3B | 2.94 | 1.58 | 1.51 |
| 5 | I | 201 | CYC | CAB-C3B | 2.94 | 1.58 | 1.51 |
| 5 | K | 201 | CYC | C1A-NA | -2.94 | 1.32 | 1.38 |
| 5 | F | 200 | CYC | C1A-NA | -2.93 | 1.32 | 1.38 |
| 5 | h | 201 | CYC | CAB-C3B | 2.93 | 1.58 | 1.51 |
| 5 | V | 201 | CYC | CAB-C3B | 2.93 | 1.58 | 1.51 |
| 5 | B | 200 | CYC | CAB-C3B | 2.92 | 1.58 | 1.51 |
| 5 | k | 200 | CYC | CAB-C3B | 2.91 | 1.58 | 1.51 |
| 5 | Y | 200 | CYC | CAB-C3B | 2.91 | 1.58 | 1.51 |
| 5 | V | 200 | CYC | C4A-C3A | -2.91 | 1.39 | 1.45 |
| 5 | I | 200 | CYC | C1A-NA | -2.90 | 1.32 | 1.38 |
| 5 | J | 200 | CYC | C1A-NA | -2.90 | 1.32 | 1.38 |
| 5 | W | 200 | CYC | CAB-C3B | 2.90 | 1.58 | 1.51 |
| 5 | U | 201 | CYC | CAB-C3B | 2.90 | 1.58 | 1.51 |
| 5 | g | 201 | CYC | C1A-NA | -2.90 | 1.32 | 1.38 |
| 5 | D | 200 | CYC | C4B-NB | -2.89 | 1.31 | 1.38 |
| 5 | C | 200 | CYC | CAB-C3B | 2.89 | 1.58 | 1.51 |
| 5 | k | 201 | CYC | CAB-C3B | 2.89 | 1.58 | 1.51 |
| 5 | X | 201 | CYC | C4A-C3A | -2.89 | 1.39 | 1.45 |
| 5 | G | 201 | CYC | CAB-C3B | 2.89 | 1.58 | 1.51 |
| 5 | I | 200 | CYC | CAB-C3B | 2.89 | 1.58 | 1.51 |
| 5 | R | 200 | CYC | C1A-NA | -2.88 | 1.32 | 1.38 |
| 5 | K | 200 | CYC | CAB-C3B | 2.88 | 1.58 | 1.51 |
| 5 | O | 200 | CYC | C4B-NB | -2.87 | 1.31 | 1.38 |
| 5 | A | 200 | CYC | C4A-C3A | -2.87 | 1.39 | 1.45 |
| 5 | I | 200 | CYC | C4A-C3A | -2.87 | 1.39 | 1.45 |
| 5 | L | 201 | CYC | CAB-C3B | 2.87 | 1.58 | 1.51 |
| 5 | W | 201 | CYC | C1A-NA | -2.87 | 1.32 | 1.38 |
| 5 | Q | 200 | CYC | CAB-C3B | 2.87 | 1.58 | 1.51 |
| 5 | f | 200 | CYC | CAB-C3B | 2.87 | 1.58 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 5 | X | 201 | CYC | CAC-C3C | 2.86 | 1.59 | 1.54 |
| 5 | O | 200 | CYC | C1A-NA | -2.86 | 1.32 | 1.38 |
| 5 | R | 200 | CYC | CAB-C3B | 2.86 | 1.58 | 1.51 |
| 5 | j | 200 | CYC | CAB-C3B | 2.86 | 1.58 | 1.51 |
| 5 | K | 200 | CYC | C1A-NA | -2.86 | 1.32 | 1.38 |
| 5 | S | 200 | CYC | C4B-NB | -2.86 | 1.31 | 1.38 |
| 5 | U | 201 | CYC | C4A-C3A | -2.85 | 1.39 | 1.45 |
| 5 | T | 201 | CYC | CAB-C3B | 2.85 | 1.58 | 1.51 |
| 5 | a | 200 | CYC | CAB-C3B | 2.85 | 1.58 | 1.51 |
| 5 | H | 201 | CYC | C4B-NB | -2.85 | 1.31 | 1.38 |
| 5 | g | 201 | CYC | CAB-C3B | 2.85 | 1.58 | 1.51 |
| 5 | E | 200 | CYC | C4B-NB | -2.84 | 1.32 | 1.38 |
| 5 | h | 201 | CYC | C4A-C3A | -2.84 | 1.39 | 1.45 |
| 5 | B | 200 | CYC | C4B-NB | -2.84 | 1.32 | 1.38 |
| 5 | 5 | 1201 | CYC | CAB-C3B | 2.83 | 1.58 | 1.51 |
| 5 | 5 | 1202 | CYC | CAB-C3B | 2.83 | 1.58 | 1.51 |
| 5 | B | 200 | CYC | C1A-NA | -2.82 | 1.32 | 1.38 |
| 5 | H | 201 | CYC | CAB-C3B | 2.82 | 1.58 | 1.51 |
| 5 | Y | 201 | CYC | C1A-NA | -2.81 | 1.32 | 1.38 |
| 5 | 5 | 1201 | CYC | C4B-NB | -2.81 | 1.32 | 1.38 |
| 5 | U | 201 | CYC | C4B-NB | -2.81 | 1.32 | 1.38 |
| 5 | F | 200 | CYC | C4A-C3A | -2.80 | 1.39 | 1.45 |
| 5 | N | 200 | CYC | C1A-NA | -2.79 | 1.32 | 1.38 |
| 5 | C | 200 | CYC | C1A-NA | -2.78 | 1.32 | 1.38 |
| 5 | D | 200 | CYC | CAB-C3B | 2.78 | 1.58 | 1.51 |
| 5 | T | 201 | CYC | C1A-NA | -2.77 | 1.32 | 1.38 |
| 5 | g | 201 | CYC | C4B-NB | -2.77 | 1.32 | 1.38 |
| 5 | K | 201 | CYC | C4B-NB | -2.77 | 1.32 | 1.38 |
| 5 | I | 201 | CYC | C4A-C3A | -2.76 | 1.39 | 1.45 |
| 5 | K | 201 | CYC | CAB-C3B | 2.76 | 1.58 | 1.51 |
| 5 | c | 200 | CYC | CAC-C3C | 2.76 | 1.59 | 1.54 |
| 5 | 5 | 1201 | CYC | C1A-NA | -2.76 | 1.32 | 1.38 |
| 5 | X | 200 | CYC | C1A-NA | -2.76 | 1.32 | 1.38 |
| 5 | c | 200 | CYC | C4A-C3A | -2.76 | 1.39 | 1.45 |
| 5 | e | 200 | CYC | C4A-C3A | -2.75 | 1.39 | 1.45 |
| 5 | E | 200 | CYC | C1A-NA | -2.75 | 1.32 | 1.38 |
| 5 | k | 201 | CYC | CAC-C3C | 2.75 | 1.59 | 1.54 |
| 5 | N | 200 | CYC | C4B-NB | -2.75 | 1.32 | 1.38 |
| 5 | Q | 200 | CYC | C4B-NB | -2.74 | 1.32 | 1.38 |
| 5 | L | 201 | CYC | C1A-NA | -2.74 | 1.32 | 1.38 |
| 5 | I | 201 | CYC | C4B-NB | -2.74 | 1.32 | 1.38 |
| 5 | Q | 200 | CYC | C1A-NA | -2.74 | 1.32 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 5 | G | 201 | CYC | C4B-NB | -2.73 | 1.32 | 1.38 |
| 5 | F | 200 | CYC | C4B-NB | -2.73 | 1.32 | 1.38 |
| 5 | a | 200 | CYC | C1A-NA | -2.73 | 1.32 | 1.38 |
| 5 | P | 200 | CYC | C4A-C3A | -2.73 | 1.39 | 1.45 |
| 5 | E | 200 | CYC | CAB-C3B | 2.73 | 1.58 | 1.51 |
| 5 | H | 200 | CYC | C4B-NB | -2.73 | 1.32 | 1.38 |
| 5 | j | 200 | CYC | C4A-C3A | -2.72 | 1.40 | 1.45 |
| 5 | G | 201 | CYC | C1A-NA | -2.72 | 1.32 | 1.38 |
| 5 | G | 200 | CYC | C4B-NB | -2.72 | 1.32 | 1.38 |
| 5 | W | 201 | CYC | C4B-NB | -2.72 | 1.32 | 1.38 |
| 5 | T | 200 | CYC | C4B-NB | -2.72 | 1.32 | 1.38 |
| 5 | J | 200 | CYC | C4B-NB | -2.71 | 1.32 | 1.38 |
| 5 | E | 200 | CYC | C4A-C3A | -2.71 | 1.40 | 1.45 |
| 5 | Q | 200 | CYC | CMD-C2D | 2.71 | 1.57 | 1.51 |
| 5 | f | 200 | CYC | C1A-NA | -2.71 | 1.32 | 1.38 |
| 5 | J | 201 | CYC | CAB-C3B | 2.71 | 1.58 | 1.51 |
| 5 | f | 200 | CYC | C4B-NB | -2.71 | 1.32 | 1.38 |
| 5 | H | 200 | CYC | C1A-NA | -2.71 | 1.32 | 1.38 |
| 5 | L | 201 | CYC | CAC-C3C | 2.70 | 1.59 | 1.54 |
| 5 | K | 200 | CYC | C4B-NB | -2.70 | 1.32 | 1.38 |
| 5 | W | 201 | CYC | CAB-C3B | 2.70 | 1.58 | 1.51 |
| 5 | H | 201 | CYC | CAC-C3C | 2.70 | 1.59 | 1.54 |
| 5 | Y | 201 | CYC | C4A-C3A | -2.69 | 1.40 | 1.45 |
| 5 | S | 200 | CYC | C1A-NA | -2.69 | 1.32 | 1.38 |
| 5 | g | 201 | CYC | CAC-C3C | 2.69 | 1.59 | 1.54 |
| 5 | k | 201 | CYC | C4A-C3A | -2.68 | 1.40 | 1.45 |
| 5 | R | 200 | CYC | C4B-NB | -2.68 | 1.32 | 1.38 |
| 5 | b | 200 | CYC | C4A-C3A | -2.68 | 1.40 | 1.45 |
| 5 | Y | 201 | CYC | CAC-C3C | 2.68 | 1.59 | 1.54 |
| 5 | G | 200 | CYC | C1A-NA | -2.68 | 1.32 | 1.38 |
| 5 | Y | 200 | CYC | C4B-NB | -2.68 | 1.32 | 1.38 |
| 5 | F | 200 | CYC | CAC-C3C | 2.67 | 1.59 | 1.54 |
| 5 | U | 201 | CYC | CAC-C3C | 2.67 | 1.59 | 1.54 |
| 5 | k | 200 | CYC | C1A-NA | -2.67 | 1.32 | 1.38 |
| 5 | C | 200 | CYC | C4B-NB | -2.67 | 1.32 | 1.38 |
| 5 | T | 200 | CYC | CAC-C3C | 2.67 | 1.59 | 1.54 |
| 5 | j | 201 | CYC | C1A-NA | -2.67 | 1.32 | 1.38 |
| 5 | T | 201 | CYC | C4B-NB | -2.66 | 1.32 | 1.38 |
| 5 | V | 201 | CYC | C4B-NB | -2.66 | 1.32 | 1.38 |
| 5 | A | 200 | CYC | C4B-NB | -2.66 | 1.32 | 1.38 |
| 5 | i | 201 | CYC | C4A-C3A | -2.66 | 1.40 | 1.45 |
| 5 | U | 200 | CYC | C4B-NB | -2.66 | 1.32 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 5 | h | 201 | CYC | C4B-NB | -2.66 | 1.32 | 1.38 |
| 5 | d | 200 | CYC | C1A-NA | -2.66 | 1.32 | 1.38 |
| 5 | h | 201 | CYC | C1A-NA | -2.65 | 1.32 | 1.38 |
| 5 | b | 200 | CYC | CAC-C3C | 2.65 | 1.59 | 1.54 |
| 5 | V | 201 | CYC | C1A-NA | -2.65 | 1.32 | 1.38 |
| 5 | I | 201 | CYC | C1A-NA | -2.65 | 1.32 | 1.38 |
| 5 | H | 201 | CYC | CMD-C2D | 2.65 | 1.57 | 1.51 |
| 5 | k | 200 | CYC | C4A-C3A | -2.65 | 1.40 | 1.45 |
| 5 | j | 201 | CYC | C4A-C3A | -2.65 | 1.40 | 1.45 |
| 5 | g | 200 | CYC | C4A-C3A | -2.65 | 1.40 | 1.45 |
| 5 | d | 200 | CYC | C4B-NB | -2.64 | 1.32 | 1.38 |
| 5 | 5 | 1201 | CYC | C4A-C3A | -2.64 | 1.40 | 1.45 |
| 5 | J | 201 | CYC | C4A-C3A | -2.64 | 1.40 | 1.45 |
| 5 | A | 200 | CYC | C1A-NA | -2.63 | 1.32 | 1.38 |
| 5 | g | 200 | CYC | CAC-C3C | 2.63 | 1.59 | 1.54 |
| 5 | H | 200 | CYC | CMD-C2D | 2.62 | 1.57 | 1.51 |
| 5 | G | 200 | CYC | C4A-C3A | -2.62 | 1.40 | 1.45 |
| 5 | 5 | 1202 | CYC | C4B-NB | -2.62 | 1.32 | 1.38 |
| 5 | h | 200 | CYC | C4B-NB | -2.62 | 1.32 | 1.38 |
| 5 | j | 200 | CYC | C1A-NA | -2.61 | 1.33 | 1.38 |
| 5 | J | 201 | CYC | C4B-NB | -2.61 | 1.32 | 1.38 |
| 5 | G | 200 | CYC | CAC-C3C | 2.61 | 1.59 | 1.54 |
| 5 | X | 200 | CYC | C4A-C3A | -2.60 | 1.40 | 1.45 |
| 5 | P | 200 | CYC | CAC-C3C | 2.60 | 1.59 | 1.54 |
| 5 | X | 201 | CYC | C4B-NB | -2.60 | 1.32 | 1.38 |
| 5 | l | 201 | CYC | C4B-NB | -2.60 | 1.32 | 1.38 |
| 5 | T | 201 | CYC | CAC-C3C | 2.60 | 1.59 | 1.54 |
| 5 | h | 200 | CYC | C1A-NA | -2.60 | 1.33 | 1.38 |
| 5 | j | 201 | CYC | C4B-NB | -2.60 | 1.32 | 1.38 |
| 5 | d | 200 | CYC | CAC-C3C | 2.60 | 1.59 | 1.54 |
| 5 | H | 200 | CYC | CAC-C3C | 2.59 | 1.59 | 1.54 |
| 5 | i | 200 | CYC | C1A-NA | -2.59 | 1.33 | 1.38 |
| 5 | H | 201 | CYC | C1A-NA | -2.59 | 1.33 | 1.38 |
| 5 | j | 200 | CYC | C4B-NB | -2.59 | 1.32 | 1.38 |
| 5 | U | 201 | CYC | C1A-NA | -2.59 | 1.33 | 1.38 |
| 5 | a | 200 | CYC | C4B-NB | -2.59 | 1.32 | 1.38 |
| 5 | g | 200 | CYC | C4B-NB | -2.59 | 1.32 | 1.38 |
| 5 | 5 | 1202 | CYC | C1A-NA | -2.59 | 1.33 | 1.38 |
| 5 | j | 201 | CYC | CAC-C3C | 2.58 | 1.59 | 1.54 |
| 5 | B | 200 | CYC | CMD-C2D | 2.58 | 1.57 | 1.51 |
| 5 | V | 200 | CYC | CAC-C3C | 2.58 | 1.59 | 1.54 |
| 5 | L | 201 | CYC | C4B-NB | -2.58 | 1.32 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 5 | Y | 200 | CYC | C1A-NA | -2.58 | 1.33 | 1.38 |
| 5 | e | 200 | CYC | C1A-NA | -2.58 | 1.33 | 1.38 |
| 5 | L | 201 | CYC | C4A-C3A | -2.57 | 1.40 | 1.45 |
| 5 | k | 201 | CYC | C4B-NB | -2.57 | 1.32 | 1.38 |
| 5 | V | 200 | CYC | C1A-NA | -2.57 | 1.33 | 1.38 |
| 5 | I | 200 | CYC | C4B-NB | -2.56 | 1.32 | 1.38 |
| 5 | V | 200 | CYC | C4B-NB | -2.56 | 1.32 | 1.38 |
| 5 | X | 200 | CYC | CAC-C3C | 2.56 | 1.59 | 1.54 |
| 5 | T | 200 | CYC | C1A-NA | -2.56 | 1.33 | 1.38 |
| 5 | j | 201 | CYC | CMD-C2D | 2.56 | 1.57 | 1.51 |
| 5 | 5 | 1202 | CYC | C4A-C3A | -2.56 | 1.40 | 1.45 |
| 5 | i | 201 | CYC | C4B-NB | -2.56 | 1.32 | 1.38 |
| 5 | a | 200 | CYC | CAC-C3C | 2.56 | 1.59 | 1.54 |
| 5 | c | 200 | CYC | C4B-NB | -2.55 | 1.32 | 1.38 |
| 5 | k | 201 | CYC | C1A-NA | -2.55 | 1.33 | 1.38 |
| 5 | X | 200 | CYC | C4B-NB | -2.55 | 1.32 | 1.38 |
| 5 | S | 200 | CYC | CMD-C2D | 2.55 | 1.56 | 1.51 |
| 5 | l | 201 | CYC | C1A-NA | -2.54 | 1.33 | 1.38 |
| 5 | i | 201 | CYC | C1A-NA | -2.54 | 1.33 | 1.38 |
| 5 | V | 201 | CYC | CAC-C3C | 2.54 | 1.59 | 1.54 |
| 5 | e | 200 | CYC | CAC-C3C | 2.54 | 1.59 | 1.54 |
| 5 | X | 201 | CYC | C1A-NA | -2.54 | 1.33 | 1.38 |
| 5 | U | 200 | CYC | C1A-NA | -2.54 | 1.33 | 1.38 |
| 5 | Y | 201 | CYC | C4B-NB | -2.54 | 1.32 | 1.38 |
| 5 | b | 200 | CYC | C4B-NB | -2.54 | 1.32 | 1.38 |
| 5 | l | 201 | CYC | CAC-C3C | 2.54 | 1.59 | 1.54 |
| 5 | h | 201 | CYC | CAC-C3C | 2.54 | 1.59 | 1.54 |
| 5 | i | 200 | CYC | C4B-NB | -2.53 | 1.32 | 1.38 |
| 5 | K | 201 | CYC | CAC-C3C | 2.53 | 1.59 | 1.54 |
| 5 | c | 200 | CYC | C1A-NA | -2.53 | 1.33 | 1.38 |
| 5 | V | 200 | CYC | CMD-C2D | 2.53 | 1.56 | 1.51 |
| 5 | b | 200 | CYC | C1A-NA | -2.52 | 1.33 | 1.38 |
| 5 | J | 200 | CYC | CAC-C3C | 2.52 | 1.58 | 1.54 |
| 5 | P | 200 | CYC | C1A-NA | -2.52 | 1.33 | 1.38 |
| 5 | R | 200 | CYC | CAC-C3C | 2.51 | 1.58 | 1.54 |
| 5 | Y | 200 | CYC | C4A-C3A | -2.51 | 1.40 | 1.45 |
| 5 | J | 201 | CYC | CMD-C2D | 2.51 | 1.56 | 1.51 |
| 5 | T | 201 | CYC | C4A-C3A | -2.51 | 1.40 | 1.45 |
| 5 | k | 200 | CYC | CAC-C3C | 2.51 | 1.58 | 1.54 |
| 5 | X | 201 | CYC | CMD-C2D | 2.51 | 1.56 | 1.51 |
| 5 | b | 200 | CYC | CMD-C2D | 2.50 | 1.56 | 1.51 |
| 5 | i | 201 | CYC | CMD-C2D | 2.50 | 1.56 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 5 | V | 201 | CYC | CMD-C2D | 2.50 | 1.56 | 1.51 |
| 5 | D | 200 | CYC | CMD-C2D | 2.49 | 1.56 | 1.51 |
| 5 | W | 200 | CYC | CAC-C3C | 2.49 | 1.58 | 1.54 |
| 5 | E | 200 | CYC | CMD-C2D | 2.49 | 1.56 | 1.51 |
| 5 | W | 200 | CYC | C4A-C3A | -2.49 | 1.40 | 1.45 |
| 5 | D | 200 | CYC | C4A-C3A | -2.49 | 1.40 | 1.45 |
| 5 | d | 200 | CYC | C4A-C3A | -2.49 | 1.40 | 1.45 |
| 5 | U | 201 | CYC | CMD-C2D | 2.48 | 1.56 | 1.51 |
| 5 | P | 200 | CYC | C4B-NB | -2.48 | 1.32 | 1.38 |
| 5 | G | 201 | CYC | CAC-C3C | 2.48 | 1.58 | 1.54 |
| 5 | c | 200 | CYC | CMD-C2D | 2.47 | 1.56 | 1.51 |
| 5 | I | 201 | CYC | CAC-C3C | 2.46 | 1.58 | 1.54 |
| 5 | f | 200 | CYC | CAC-C3C | 2.46 | 1.58 | 1.54 |
| 5 | Q | 200 | CYC | C4A-C3A | -2.46 | 1.40 | 1.45 |
| 5 | L | 201 | CYC | CMD-C2D | 2.46 | 1.56 | 1.51 |
| 5 | e | 200 | CYC | C4B-NB | -2.46 | 1.32 | 1.38 |
| 5 | C | 200 | CYC | CMD-C2D | 2.46 | 1.56 | 1.51 |
| 5 | i | 201 | CYC | CAC-C3C | 2.46 | 1.58 | 1.54 |
| 5 | h | 200 | CYC | CAC-C3C | 2.45 | 1.58 | 1.54 |
| 5 | O | 200 | CYC | CAC-C3C | 2.45 | 1.58 | 1.54 |
| 5 | k | 201 | CYC | CMD-C2D | 2.45 | 1.56 | 1.51 |
| 5 | K | 200 | CYC | C4A-C3A | -2.45 | 1.40 | 1.45 |
| 5 | k | 200 | CYC | C4B-NB | -2.45 | 1.32 | 1.38 |
| 5 | K | 200 | CYC | CAC-C3C | 2.45 | 1.58 | 1.54 |
| 5 | T | 200 | CYC | C4A-C3A | -2.44 | 1.40 | 1.45 |
| 5 | B | 200 | CYC | C4A-C3A | -2.44 | 1.40 | 1.45 |
| 5 | Q | 200 | CYC | CAC-C3C | 2.44 | 1.58 | 1.54 |
| 5 | W | 201 | CYC | CAC-C3C | 2.44 | 1.58 | 1.54 |
| 5 | E | 200 | CYC | CAC-C3C | 2.43 | 1.58 | 1.54 |
| 5 | 5 | 1202 | CYC | CAC-C3C | 2.43 | 1.58 | 1.54 |
| 5 | f | 200 | CYC | CMD-C2D | 2.43 | 1.56 | 1.51 |
| 5 | g | 201 | CYC | C4A-C3A | -2.43 | 1.40 | 1.45 |
| 5 | C | 200 | CYC | CAC-C3C | 2.42 | 1.58 | 1.54 |
| 5 | h | 200 | CYC | C4A-C3A | -2.42 | 1.40 | 1.45 |
| 5 | U | 200 | CYC | C4A-C3A | -2.42 | 1.40 | 1.45 |
| 5 | P | 200 | CYC | CMD-C2D | 2.42 | 1.56 | 1.51 |
| 5 | G | 200 | CYC | CMD-C2D | 2.42 | 1.56 | 1.51 |
| 5 | I | 200 | CYC | CAC-C3C | 2.42 | 1.58 | 1.54 |
| 5 | g | 200 | CYC | C1A-NA | -2.41 | 1.33 | 1.38 |
| 5 | B | 200 | CYC | CAC-C3C | 2.41 | 1.58 | 1.54 |
| 5 | Y | 200 | CYC | CMD-C2D | 2.41 | 1.56 | 1.51 |
| 5 | I | 200 | CYC | CMD-C2D | 2.40 | 1.56 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 5 | h | 201 | CYC | CMD-C2D | 2.40 | 1.56 | 1.51 |
| 5 | N | 200 | CYC | C4A-C3A | -2.40 | 1.40 | 1.45 |
| 5 | O | 200 | CYC | CMD-C2D | 2.40 | 1.56 | 1.51 |
| 5 | A | 200 | CYC | CMD-C2D | 2.39 | 1.56 | 1.51 |
| 5 | U | 200 | CYC | CAC-C3C | 2.39 | 1.58 | 1.54 |
| 5 | J | 201 | CYC | CAC-C3C | 2.39 | 1.58 | 1.54 |
| 5 | S | 200 | CYC | CAC-C3C | 2.38 | 1.58 | 1.54 |
| 5 | I | 201 | CYC | CMD-C2D | 2.38 | 1.56 | 1.51 |
| 5 | g | 201 | CYC | CMD-C2D | 2.37 | 1.56 | 1.51 |
| 5 | j | 200 | CYC | CAC-C3C | 2.37 | 1.58 | 1.54 |
| 5 | N | 200 | CYC | CAC-C3C | 2.36 | 1.58 | 1.54 |
| 5 | l | 201 | CYC | CMD-C2D | 2.36 | 1.56 | 1.51 |
| 5 | R | 200 | CYC | C4A-C3A | -2.35 | 1.40 | 1.45 |
| 5 | G | 201 | CYC | CMD-C2D | 2.35 | 1.56 | 1.51 |
| 5 | T | 201 | CYC | CMD-C2D | 2.35 | 1.56 | 1.51 |
| 5 | Y | 201 | CYC | CMD-C2D | 2.35 | 1.56 | 1.51 |
| 5 | W | 201 | CYC | C4A-C3A | -2.34 | 1.40 | 1.45 |
| 5 | e | 200 | CYC | CMD-C2D | 2.34 | 1.56 | 1.51 |
| 5 | T | 200 | CYC | CMD-C2D | 2.34 | 1.56 | 1.51 |
| 5 | Y | 200 | CYC | CAC-C3C | 2.34 | 1.58 | 1.54 |
| 5 | a | 200 | CYC | CMD-C2D | 2.33 | 1.56 | 1.51 |
| 5 | J | 200 | CYC | C4A-C3A | -2.33 | 1.40 | 1.45 |
| 5 | d | 200 | CYC | CMD-C2D | 2.33 | 1.56 | 1.51 |
| 5 | A | 200 | CYC | CAC-C3C | 2.33 | 1.58 | 1.54 |
| 5 | g | 200 | CYC | CMA-C3A | 2.32 | 1.55 | 1.50 |
| 5 | W | 200 | CYC | CMD-C2D | 2.32 | 1.56 | 1.51 |
| 5 | k | 200 | CYC | CMD-C2D | 2.32 | 1.56 | 1.51 |
| 5 | a | 200 | CYC | CMA-C3A | 2.32 | 1.55 | 1.50 |
| 5 | K | 201 | CYC | CMD-C2D | 2.32 | 1.56 | 1.51 |
| 5 | W | 201 | CYC | CMD-C2D | 2.31 | 1.56 | 1.51 |
| 5 | g | 200 | CYC | CMD-C2D | 2.30 | 1.56 | 1.51 |
| 5 | i | 200 | CYC | C4A-C3A | -2.28 | 1.40 | 1.45 |
| 5 | K | 201 | CYC | C4A-C3A | -2.27 | 1.40 | 1.45 |
| 5 | a | 200 | CYC | C4A-C3A | -2.27 | 1.40 | 1.45 |
| 5 | 5 | 1202 | CYC | CMA-C3A | 2.26 | 1.55 | 1.50 |
| 5 | h | 200 | CYC | CMD-C2D | 2.25 | 1.56 | 1.51 |
| 5 | i | 200 | CYC | CAC-C3C | 2.25 | 1.58 | 1.54 |
| 5 | H | 200 | CYC | C4A-C3A | -2.25 | 1.41 | 1.45 |
| 5 | D | 200 | CYC | CAC-C3C | 2.25 | 1.58 | 1.54 |
| 5 | N | 200 | CYC | CMD-C2D | 2.23 | 1.56 | 1.51 |
| 5 | 5 | 1202 | CYC | CMD-C2D | 2.23 | 1.56 | 1.51 |
| 5 | l | 201 | CYC | C4A-C3A | -2.22 | 1.41 | 1.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 5 | P | 200 | CYC | CMA-C3A | 2.21 | 1.55 | 1.50 |
| 5 | W | 201 | CYC | CMA-C3A | 2.21 | 1.55 | 1.50 |
| 5 | b | 200 | CYC | CMA-C3A | 2.20 | 1.55 | 1.50 |
| 5 | K | 200 | CYC | CMD-C2D | 2.20 | 1.56 | 1.51 |
| 5 | U | 201 | CYC | CMA-C3A | 2.20 | 1.55 | 1.50 |
| 5 | X | 200 | CYC | CMD-C2D | 2.20 | 1.56 | 1.51 |
| 5 | j | 200 | CYC | CMD-C2D | 2.19 | 1.56 | 1.51 |
| 5 | g | 201 | CYC | CMA-C3A | 2.19 | 1.55 | 1.50 |
| 5 | O | 200 | CYC | CMA-C3A | 2.19 | 1.55 | 1.50 |
| 5 | R | 200 | CYC | CMD-C2D | 2.19 | 1.56 | 1.51 |
| 5 | k | 201 | CYC | CMA-C3A | 2.18 | 1.55 | 1.50 |
| 5 | J | 200 | CYC | CMD-C2D | 2.18 | 1.56 | 1.51 |
| 5 | F | 200 | CYC | CMD-C2D | 2.18 | 1.56 | 1.51 |
| 5 | T | 200 | CYC | CMA-C3A | 2.18 | 1.55 | 1.50 |
| 5 | h | 200 | CYC | CMA-C3A | 2.18 | 1.55 | 1.50 |
| 5 | i | 200 | CYC | CMA-C3A | 2.17 | 1.55 | 1.50 |
| 5 | Q | 200 | CYC | CMA-C3A | 2.17 | 1.55 | 1.50 |
| 5 | k | 200 | CYC | CMA-C3A | 2.17 | 1.55 | 1.50 |
| 5 | 5 | 1202 | CYC | CBA-CAA | 2.16 | 1.58 | 1.52 |
| 5 | U | 200 | CYC | CMA-C3A | 2.16 | 1.55 | 1.50 |
| 5 | G | 200 | CYC | CMA-C3A | 2.15 | 1.55 | 1.50 |
| 5 | U | 200 | CYC | CMD-C2D | 2.15 | 1.56 | 1.51 |
| 5 | V | 200 | CYC | CMA-C3A | 2.14 | 1.55 | 1.50 |
| 5 | j | 201 | CYC | CMA-C3A | 2.14 | 1.55 | 1.50 |
| 5 | h | 201 | CYC | CMA-C3A | 2.14 | 1.55 | 1.50 |
| 5 | f | 200 | CYC | CMA-C3A | 2.14 | 1.55 | 1.50 |
| 5 | e | 200 | CYC | CMA-C3A | 2.14 | 1.55 | 1.50 |
| 5 | 5 | 1201 | CYC | C4C-NC | -2.14 | 1.32 | 1.37 |
| 5 | X | 201 | CYC | CMA-C3A | 2.13 | 1.55 | 1.50 |
| 5 | c | 200 | CYC | CMA-C3A | 2.13 | 1.55 | 1.50 |
| 5 | i | 200 | CYC | CMD-C2D | 2.13 | 1.56 | 1.51 |
| 5 | T | 201 | CYC | CMA-C3A | 2.13 | 1.55 | 1.50 |
| 5 | i | 201 | CYC | CMA-C3A | 2.12 | 1.55 | 1.50 |
| 5 | B | 200 | CYC | CMA-C3A | 2.12 | 1.55 | 1.50 |
| 5 | G | 201 | CYC | C4A-C3A | -2.12 | 1.41 | 1.45 |
| 5 | j | 200 | CYC | CMA-C3A | 2.11 | 1.55 | 1.50 |
| 5 | O | 200 | CYC | C4A-C3A | -2.10 | 1.41 | 1.45 |
| 5 | G | 201 | CYC | CMA-C3A | 2.09 | 1.55 | 1.50 |
| 5 | N | 200 | CYC | CBA-CAA | 2.09 | 1.58 | 1.52 |
| 5 | I | 200 | CYC | CMA-C3A | 2.08 | 1.55 | 1.50 |
| 5 | O | 200 | CYC | CBA-CAA | 2.08 | 1.58 | 1.52 |
| 5 | g | 200 | CYC | CBA-CAA | 2.08 | 1.58 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 5 | U | 200 | CYC | CBA-CAA | 2.07 | 1.58 | 1.52 |
| 5 | L | 201 | CYC | CMA-C3A | 2.07 | 1.55 | 1.50 |
| 5 | i | 200 | CYC | CBA-CAA | 2.07 | 1.58 | 1.52 |
| 5 | G | 201 | CYC | CBA-CAA | 2.06 | 1.58 | 1.52 |
| 5 | l | 201 | CYC | CMA-C3A | 2.06 | 1.55 | 1.50 |
| 5 | U | 201 | CYC | CBA-CAA | 2.06 | 1.58 | 1.52 |
| 5 | R | 200 | CYC | CMA-C3A | 2.06 | 1.55 | 1.50 |
| 5 | N | 200 | CYC | CMA-C3A | 2.05 | 1.55 | 1.50 |
| 5 | P | 200 | CYC | CBA-CAA | 2.05 | 1.58 | 1.52 |
| 5 | H | 200 | CYC | CMA-C3A | 2.04 | 1.55 | 1.50 |
| 5 | a | 200 | CYC | CBA-CAA | 2.04 | 1.58 | 1.52 |
| 5 | k | 200 | CYC | CBA-CAA | 2.04 | 1.58 | 1.52 |
| 5 | l | 201 | CYC | CBA-CAA | 2.04 | 1.58 | 1.52 |
| 5 | V | 201 | CYC | CBA-CAA | 2.03 | 1.58 | 1.52 |
| 5 | H | 201 | CYC | CMA-C3A | 2.03 | 1.55 | 1.50 |
| 5 | c | 200 | CYC | CAD-C3D | 2.02 | 1.55 | 1.52 |
| 5 | Y | 201 | CYC | CBA-CAA | 2.02 | 1.58 | 1.52 |
| 5 | 5 | 1201 | CYC | CMD-C2D | 2.02 | 1.55 | 1.51 |
| 5 | V | 201 | CYC | CMA-C3A | 2.01 | 1.55 | 1.50 |
| 5 | T | 201 | CYC | CBA-CAA | 2.00 | 1.58 | 1.52 |
| 5 | Y | 201 | CYC | CMA-C3A | 2.00 | 1.55 | 1.50 |

All (620) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 5 | X | 200 | CYC | OC-C1C-C2C | -22.17 | 108.55 | 126.17 |
| 5 | J | 200 | CYC | OC-C1C-C2C | -22.07 | 108.62 | 126.17 |
| 5 | K | 200 | CYC | OC-C1C-C2C | -21.85 | 108.80 | 126.17 |
| 5 | I | 201 | CYC | OC-C1C-C2C | -21.84 | 108.81 | 126.17 |
| 5 | e | 200 | CYC | OC-C1C-C2C | -21.31 | 109.23 | 126.17 |
| 5 | W | 200 | CYC | OC-C1C-C2C | -21.30 | 109.24 | 126.17 |
| 5 | Y | 200 | CYC | OC-C1C-C2C | -21.14 | 109.36 | 126.17 |
| 5 | K | 201 | CYC | OC-C1C-C2C | -21.12 | 109.38 | 126.17 |
| 5 | j | 200 | CYC | OC-C1C-C2C | -20.98 | 109.49 | 126.17 |
| 5 | l | 201 | CYC | OC-C1C-C2C | -20.97 | 109.50 | 126.17 |
| 5 | G | 200 | CYC | OC-C1C-C2C | -20.93 | 109.53 | 126.17 |
| 5 | 5 | 1202 | CYC | OC-C1C-C2C | -20.88 | 109.57 | 126.17 |
| 5 | J | 201 | CYC | OC-C1C-C2C | -20.86 | 109.59 | 126.17 |
| 5 | H | 200 | CYC | OC-C1C-C2C | -20.75 | 109.67 | 126.17 |
| 5 | I | 200 | CYC | OC-C1C-C2C | -20.75 | 109.67 | 126.17 |
| 5 | 5 | 1201 | CYC | OC-C1C-C2C | -20.75 | 109.67 | 126.17 |
| 5 | U | 200 | CYC | OC-C1C-C2C | -20.60 | 109.80 | 126.17 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 5 | X | 201 | CYC | OC-C1C-C2C | -20.56 | 109.82 | 126.17 |
| 5 | H | 201 | CYC | OC-C1C-C2C | -20.56 | 109.82 | 126.17 |
| 5 | W | 201 | CYC | OC-C1C-C2C | -20.56 | 109.83 | 126.17 |
| 5 | T | 201 | CYC | OC-C1C-C2C | -20.52 | 109.86 | 126.17 |
| 5 | T | 200 | CYC | OC-C1C-C2C | -20.51 | 109.86 | 126.17 |
| 5 | V | 200 | CYC | OC-C1C-C2C | -20.51 | 109.87 | 126.17 |
| 5 | Q | 200 | CYC | OC-C1C-C2C | -20.36 | 109.98 | 126.17 |
| 5 | U | 201 | CYC | OC-C1C-C2C | -20.34 | 110.00 | 126.17 |
| 5 | b | 200 | CYC | OC-C1C-C2C | -20.28 | 110.05 | 126.17 |
| 5 | f | 200 | CYC | OC-C1C-C2C | -20.26 | 110.06 | 126.17 |
| 5 | g | 200 | CYC | OC-C1C-C2C | -20.26 | 110.06 | 126.17 |
| 5 | k | 201 | CYC | OC-C1C-C2C | -20.24 | 110.08 | 126.17 |
| 5 | F | 200 | CYC | OC-C1C-C2C | -20.24 | 110.08 | 126.17 |
| 5 | P | 200 | CYC | OC-C1C-C2C | -20.23 | 110.09 | 126.17 |
| 5 | j | 201 | CYC | OC-C1C-C2C | -20.22 | 110.10 | 126.17 |
| 5 | Y | 201 | CYC | OC-C1C-C2C | -20.17 | 110.14 | 126.17 |
| 5 | D | 200 | CYC | OC-C1C-C2C | -20.16 | 110.14 | 126.17 |
| 5 | i | 201 | CYC | OC-C1C-C2C | -20.16 | 110.14 | 126.17 |
| 5 | O | 200 | CYC | OC-C1C-C2C | -20.07 | 110.22 | 126.17 |
| 5 | V | 201 | CYC | OC-C1C-C2C | -20.06 | 110.22 | 126.17 |
| 5 | a | 200 | CYC | OC-C1C-C2C | -20.03 | 110.25 | 126.17 |
| 5 | h | 200 | CYC | OC-C1C-C2C | -20.01 | 110.27 | 126.17 |
| 5 | C | 200 | CYC | OC-C1C-C2C | -19.89 | 110.36 | 126.17 |
| 5 | k | 200 | CYC | OC-C1C-C2C | -19.87 | 110.38 | 126.17 |
| 5 | g | 201 | CYC | OC-C1C-C2C | -19.78 | 110.44 | 126.17 |
| 5 | S | 200 | CYC | OC-C1C-C2C | -19.76 | 110.46 | 126.17 |
| 5 | h | 201 | CYC | OC-C1C-C2C | -19.75 | 110.47 | 126.17 |
| 5 | L | 201 | CYC | OC-C1C-C2C | -19.75 | 110.47 | 126.17 |
| 5 | E | 200 | CYC | OC-C1C-C2C | -19.70 | 110.51 | 126.17 |
| 5 | A | 200 | CYC | OC-C1C-C2C | -19.66 | 110.54 | 126.17 |
| 5 | d | 200 | CYC | OC-C1C-C2C | -19.59 | 110.59 | 126.17 |
| 5 | N | 200 | CYC | OC-C1C-C2C | -19.56 | 110.62 | 126.17 |
| 5 | c | 200 | CYC | OC-C1C-C2C | -19.55 | 110.63 | 126.17 |
| 5 | R | 200 | CYC | OC-C1C-C2C | -19.52 | 110.65 | 126.17 |
| 5 | B | 200 | CYC | OC-C1C-C2C | -19.38 | 110.76 | 126.17 |
| 5 | i | 200 | CYC | OC-C1C-C2C | -19.13 | 110.97 | 126.17 |
| 5 | G | 201 | CYC | OC-C1C-C2C | -18.89 | 111.15 | 126.17 |
| 5 | g | 201 | CYC | C4D-CHA-C1A | -16.43 | 109.18 | 128.81 |
| 5 | R | 200 | CYC | C4D-CHA-C1A | -15.87 | 109.85 | 128.81 |
| 5 | h | 201 | CYC | C4D-CHA-C1A | -15.46 | 110.34 | 128.81 |
| 5 | L | 201 | CYC | C4D-CHA-C1A | -14.67 | 111.28 | 128.81 |
| 5 | J | 201 | CYC | C4D-CHA-C1A | -14.35 | 111.66 | 128.81 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 5 | B | 200 | CYC | C4D-CHA-C1A | -14.30 | 111.73 | 128.81 |
| 5 | a | 200 | CYC | C4D-CHA-C1A | -14.28 | 111.75 | 128.81 |
| 5 | f | 200 | CYC | C4D-CHA-C1A | -14.13 | 111.92 | 128.81 |
| 5 | j | 201 | CYC | C4D-CHA-C1A | -13.80 | 112.32 | 128.81 |
| 5 | A | 200 | CYC | CHD-C4C-NC | -13.73 | 108.88 | 125.20 |
| 5 | O | 200 | CYC | CHD-C4C-NC | -13.72 | 108.89 | 125.20 |
| 5 | U | 201 | CYC | CHD-C4C-NC | -13.65 | 108.97 | 125.20 |
| 5 | S | 200 | CYC | CHD-C4C-NC | -13.59 | 109.05 | 125.20 |
| 5 | T | 201 | CYC | C4D-CHA-C1A | -13.58 | 112.59 | 128.81 |
| 5 | W | 201 | CYC | C4D-CHA-C1A | -13.48 | 112.71 | 128.81 |
| 5 | H | 200 | CYC | CHD-C4C-NC | -13.48 | 109.18 | 125.20 |
| 5 | j | 201 | CYC | CHD-C4C-NC | -13.45 | 109.21 | 125.20 |
| 5 | O | 200 | CYC | C4D-CHA-C1A | -13.34 | 112.88 | 128.81 |
| 5 | B | 200 | CYC | CHD-C4C-NC | -13.28 | 109.42 | 125.20 |
| 5 | k | 200 | CYC | CHD-C4C-NC | -13.23 | 109.47 | 125.20 |
| 5 | a | 200 | CYC | CHD-C4C-NC | -13.19 | 109.52 | 125.20 |
| 5 | U | 201 | CYC | C4D-CHA-C1A | -13.16 | 113.09 | 128.81 |
| 5 | b | 200 | CYC | CHD-C4C-NC | -13.09 | 109.64 | 125.20 |
| 5 | i | 201 | CYC | C4D-CHA-C1A | -13.09 | 113.17 | 128.81 |
| 5 | Y | 200 | CYC | OC-C1C-NC | -13.07 | 109.11 | 124.94 |
| 5 | V | 200 | CYC | CHD-C4C-NC | -13.05 | 109.69 | 125.20 |
| 5 | D | 200 | CYC | CHD-C4C-NC | -13.05 | 109.69 | 125.20 |
| 5 | h | 201 | CYC | CHD-C4C-NC | -13.03 | 109.71 | 125.20 |
| 5 | V | 201 | CYC | CHD-C4C-NC | -13.03 | 109.72 | 125.20 |
| 5 | G | 201 | CYC | C4D-CHA-C1A | -13.02 | 113.25 | 128.81 |
| 5 | Q | 200 | CYC | CHD-C4C-NC | -12.96 | 109.79 | 125.20 |
| 5 | K | 200 | CYC | OC-C1C-NC | -12.93 | 109.28 | 124.94 |
| 5 | S | 200 | CYC | OC-C1C-NC | -12.90 | 109.32 | 124.94 |
| 5 | c | 200 | CYC | CHD-C4C-NC | -12.85 | 109.93 | 125.20 |
| 5 | H | 200 | CYC | OC-C1C-NC | -12.83 | 109.41 | 124.94 |
| 5 | f | 200 | CYC | OC-C1C-NC | -12.77 | 109.48 | 124.94 |
| 5 | K | 201 | CYC | C4D-CHA-C1A | -12.74 | 113.59 | 128.81 |
| 5 | J | 201 | CYC | OC-C1C-NC | -12.67 | 109.59 | 124.94 |
| 5 | l | 201 | CYC | CHD-C4C-NC | -12.67 | 110.14 | 125.20 |
| 5 | Q | 200 | CYC | OC-C1C-NC | -12.65 | 109.63 | 124.94 |
| 5 | i | 201 | CYC | CHD-C4C-NC | -12.61 | 110.21 | 125.20 |
| 5 | G | 201 | CYC | CHD-C4C-NC | -12.61 | 110.21 | 125.20 |
| 5 | J | 200 | CYC | OC-C1C-NC | -12.59 | 109.69 | 124.94 |
| 5 | d | 200 | CYC | C4D-CHA-C1A | -12.59 | 113.77 | 128.81 |
| 5 | f | 200 | CYC | CHD-C4C-NC | -12.58 | 110.25 | 125.20 |
| 5 | K | 201 | CYC | CHD-C4C-NC | -12.54 | 110.29 | 125.20 |
| 5 | 5 | 1202 | CYC | OC-C1C-NC | -12.53 | 109.77 | 124.94 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 5 | V | 201 | CYC | C4D-CHA-C1A | -12.50 | 113.88 | 128.81 |
| 5 | W | 201 | CYC | CHD-C4C-NC | -12.50 | 110.34 | 125.20 |
| 5 | I | 201 | CYC | OC-C1C-NC | -12.47 | 109.83 | 124.94 |
| 5 | j | 200 | CYC | OC-C1C-NC | -12.46 | 109.86 | 124.94 |
| 5 | g | 201 | CYC | CHD-C4C-NC | -12.42 | 110.44 | 125.20 |
| 5 | X | 201 | CYC | CHD-C4C-NC | -12.39 | 110.48 | 125.20 |
| 5 | k | 200 | CYC | OC-C1C-NC | -12.38 | 109.94 | 124.94 |
| 5 | F | 200 | CYC | OC-C1C-NC | -12.38 | 109.95 | 124.94 |
| 5 | b | 200 | CYC | OC-C1C-NC | -12.36 | 109.98 | 124.94 |
| 5 | Y | 200 | CYC | CHD-C4C-NC | -12.33 | 110.54 | 125.20 |
| 5 | N | 200 | CYC | CHD-C4C-NC | -12.33 | 110.55 | 125.20 |
| 5 | U | 200 | CYC | CHD-C4C-NC | -12.30 | 110.58 | 125.20 |
| 5 | L | 201 | CYC | CHD-C4C-NC | -12.27 | 110.61 | 125.20 |
| 5 | H | 201 | CYC | OC-C1C-NC | -12.27 | 110.08 | 124.94 |
| 5 | h | 200 | CYC | OC-C1C-NC | -12.26 | 110.09 | 124.94 |
| 5 | a | 200 | CYC | OC-C1C-NC | -12.26 | 110.09 | 124.94 |
| 5 | e | 200 | CYC | C4D-CHA-C1A | -12.25 | 114.17 | 128.81 |
| 5 | U | 201 | CYC | OC-C1C-NC | -12.25 | 110.11 | 124.94 |
| 5 | j | 200 | CYC | CHD-C4C-NC | -12.25 | 110.64 | 125.20 |
| 5 | H | 201 | CYC | C4D-CHA-C1A | -12.23 | 114.20 | 128.81 |
| 5 | c | 200 | CYC | C4D-CHA-C1A | -12.21 | 114.22 | 128.81 |
| 5 | T | 201 | CYC | CHD-C4C-NC | -12.21 | 110.69 | 125.20 |
| 5 | e | 200 | CYC | CHD-C4C-NC | -12.19 | 110.71 | 125.20 |
| 5 | V | 200 | CYC | OC-C1C-NC | -12.19 | 110.18 | 124.94 |
| 5 | Y | 201 | CYC | CHD-C4C-NC | -12.18 | 110.73 | 125.20 |
| 5 | i | 200 | CYC | CHD-C4C-NC | -12.17 | 110.74 | 125.20 |
| 5 | k | 201 | CYC | CHD-C4C-NC | -12.16 | 110.75 | 125.20 |
| 5 | I | 200 | CYC | OC-C1C-NC | -12.16 | 110.22 | 124.94 |
| 5 | J | 201 | CYC | CHD-C4C-NC | -12.13 | 110.78 | 125.20 |
| 5 | h | 201 | CYC | OC-C1C-NC | -12.11 | 110.27 | 124.94 |
| 5 | D | 200 | CYC | OC-C1C-NC | -12.09 | 110.30 | 124.94 |
| 5 | K | 201 | CYC | OC-C1C-NC | -12.06 | 110.34 | 124.94 |
| 5 | C | 200 | CYC | C4D-CHA-C1A | -12.05 | 114.42 | 128.81 |
| 5 | G | 201 | CYC | OC-C1C-NC | -12.05 | 110.35 | 124.94 |
| 5 | A | 200 | CYC | OC-C1C-NC | -12.03 | 110.37 | 124.94 |
| 5 | X | 200 | CYC | OC-C1C-NC | -12.03 | 110.38 | 124.94 |
| 5 | C | 200 | CYC | CHD-C4C-NC | -12.01 | 110.92 | 125.20 |
| 5 | R | 200 | CYC | CHD-C4C-NC | -12.01 | 110.93 | 125.20 |
| 5 | J | 200 | CYC | CHD-C4C-NC | -11.99 | 110.95 | 125.20 |
| 5 | X | 200 | CYC | CHD-C4C-NC | -11.99 | 110.95 | 125.20 |
| 5 | d | 200 | CYC | CHD-C4C-NC | -11.95 | 111.00 | 125.20 |
| 5 | O | 200 | CYC | OC-C1C-NC | -11.95 | 110.47 | 124.94 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 5 | i | 201 | CYC | OC-C1C-NC | -11.94 | 110.49 | 124.94 |
| 5 | N | 200 | CYC | OC-C1C-NC | -11.90 | 110.53 | 124.94 |
| 5 | k | 201 | CYC | OC-C1C-NC | -11.90 | 110.53 | 124.94 |
| 5 | Y | 201 | CYC | C4D-CHA-C1A | -11.87 | 114.62 | 128.81 |
| 5 | E | 200 | CYC | CHD-C4C-NC | -11.87 | 111.09 | 125.20 |
| 5 | h | 200 | CYC | CHD-C4C-NC | -11.87 | 111.10 | 125.20 |
| 5 | H | 201 | CYC | CHD-C4C-NC | -11.85 | 111.12 | 125.20 |
| 5 | L | 201 | CYC | OC-C1C-NC | -11.84 | 110.61 | 124.94 |
| 5 | T | 200 | CYC | OC-C1C-NC | -11.82 | 110.62 | 124.94 |
| 5 | W | 201 | CYC | OC-C1C-NC | -11.81 | 110.64 | 124.94 |
| 5 | T | 201 | CYC | OC-C1C-NC | -11.79 | 110.67 | 124.94 |
| 5 | X | 201 | CYC | OC-C1C-NC | -11.78 | 110.67 | 124.94 |
| 5 | j | 201 | CYC | OC-C1C-NC | -11.78 | 110.68 | 124.94 |
| 5 | I | 201 | CYC | CHD-C4C-NC | -11.76 | 111.23 | 125.20 |
| 5 | V | 201 | CYC | OC-C1C-NC | -11.75 | 110.72 | 124.94 |
| 5 | W | 200 | CYC | OC-C1C-NC | -11.74 | 110.73 | 124.94 |
| 5 | c | 200 | CYC | OC-C1C-NC | -11.73 | 110.74 | 124.94 |
| 5 | G | 200 | CYC | OC-C1C-NC | -11.68 | 110.80 | 124.94 |
| 5 | 5 | 1202 | CYC | CHD-C4C-NC | -11.66 | 111.34 | 125.20 |
| 5 | B | 200 | CYC | OC-C1C-NC | -11.59 | 110.91 | 124.94 |
| 5 | F | 200 | CYC | CHD-C4C-NC | -11.44 | 111.60 | 125.20 |
| 5 | I | 200 | CYC | CHD-C4C-NC | -11.43 | 111.61 | 125.20 |
| 5 | l | 201 | CYC | OC-C1C-NC | -11.42 | 111.12 | 124.94 |
| 5 | 5 | 1201 | CYC | OC-C1C-NC | -11.40 | 111.13 | 124.94 |
| 5 | P | 200 | CYC | OC-C1C-NC | -11.39 | 111.15 | 124.94 |
| 5 | 5 | 1202 | CYC | C4D-CHA-C1A | -11.37 | 115.22 | 128.81 |
| 5 | F | 200 | CYC | C4D-CHA-C1A | -11.36 | 115.23 | 128.81 |
| 5 | R | 200 | CYC | OC-C1C-NC | -11.36 | 111.18 | 124.94 |
| 5 | Y | 201 | CYC | OC-C1C-NC | -11.34 | 111.21 | 124.94 |
| 5 | I | 200 | CYC | C4D-CHA-C1A | -11.33 | 115.27 | 128.81 |
| 5 | g | 201 | CYC | OC-C1C-NC | -11.31 | 111.25 | 124.94 |
| 5 | b | 200 | CYC | C4D-CHA-C1A | -11.25 | 115.37 | 128.81 |
| 5 | g | 200 | CYC | CHD-C4C-NC | -11.25 | 111.83 | 125.20 |
| 5 | g | 200 | CYC | OC-C1C-NC | -11.23 | 111.34 | 124.94 |
| 5 | W | 200 | CYC | CHD-C4C-NC | -11.23 | 111.85 | 125.20 |
| 5 | C | 200 | CYC | OC-C1C-NC | -11.22 | 111.36 | 124.94 |
| 5 | 5 | 1201 | CYC | C4D-CHA-C1A | -11.22 | 115.41 | 128.81 |
| 5 | T | 200 | CYC | CHD-C4C-NC | -11.20 | 111.89 | 125.20 |
| 5 | K | 200 | CYC | CHD-C4C-NC | -11.19 | 111.91 | 125.20 |
| 5 | e | 200 | CYC | OC-C1C-NC | -11.17 | 111.42 | 124.94 |
| 5 | i | 200 | CYC | OC-C1C-NC | -11.14 | 111.45 | 124.94 |
| 5 | U | 200 | CYC | OC-C1C-NC | -11.14 | 111.45 | 124.94 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 5 | E | 200 | CYC | OC-C1C-NC | -11.13 | 111.46 | 124.94 |
| 5 | d | 200 | CYC | OC-C1C-NC | -11.02 | 111.59 | 124.94 |
| 5 | l | 201 | CYC | C4D-CHA-C1A | -11.02 | 115.64 | 128.81 |
| 5 | G | 200 | CYC | CHD-C4C-NC | -11.02 | 112.10 | 125.20 |
| 5 | X | 200 | CYC | C4D-CHA-C1A | -10.96 | 115.72 | 128.81 |
| 5 | P | 200 | CYC | CHD-C4C-NC | -10.91 | 112.23 | 125.20 |
| 5 | X | 201 | CYC | C4D-CHA-C1A | -10.91 | 115.78 | 128.81 |
| 5 | k | 201 | CYC | C4D-CHA-C1A | -10.89 | 115.80 | 128.81 |
| 5 | i | 200 | CYC | C4D-CHA-C1A | -10.77 | 115.95 | 128.81 |
| 5 | k | 200 | CYC | C4D-CHA-C1A | -10.72 | 116.00 | 128.81 |
| 5 | V | 200 | CYC | C4D-CHA-C1A | -10.64 | 116.10 | 128.81 |
| 5 | Q | 200 | CYC | C4D-CHA-C1A | -10.56 | 116.20 | 128.81 |
| 5 | j | 200 | CYC | C4D-CHA-C1A | -10.54 | 116.22 | 128.81 |
| 5 | h | 200 | CYC | C4D-CHA-C1A | -10.40 | 116.39 | 128.81 |
| 5 | S | 200 | CYC | C4D-CHA-C1A | -10.06 | 116.79 | 128.81 |
| 5 | T | 200 | CYC | C4D-CHA-C1A | -9.96 | 116.92 | 128.81 |
| 5 | D | 200 | CYC | C4D-CHA-C1A | -9.85 | 117.04 | 128.81 |
| 5 | U | 200 | CYC | C4D-CHA-C1A | -9.81 | 117.09 | 128.81 |
| 5 | G | 200 | CYC | C4D-CHA-C1A | -9.81 | 117.09 | 128.81 |
| 5 | K | 200 | CYC | C4D-CHA-C1A | -9.67 | 117.25 | 128.81 |
| 5 | g | 200 | CYC | C4D-CHA-C1A | -9.48 | 117.49 | 128.81 |
| 5 | H | 201 | CYC | C1B-CHB-C4A | -9.47 | 104.95 | 128.08 |
| 5 | J | 200 | CYC | C4D-CHA-C1A | -9.43 | 117.55 | 128.81 |
| 5 | A | 200 | CYC | C4D-CHA-C1A | -9.39 | 117.59 | 128.81 |
| 5 | f | 200 | CYC | C1B-CHB-C4A | -9.37 | 105.19 | 128.08 |
| 5 | D | 200 | CYC | C2C-C1C-NC | -9.36 | 100.20 | 108.27 |
| 5 | 5 | 1201 | CYC | CHD-C4C-NC | -9.10 | 114.39 | 125.20 |
| 5 | E | 200 | CYC | C4D-CHA-C1A | -9.07 | 117.97 | 128.81 |
| 5 | U | 201 | CYC | C1B-CHB-C4A | -8.91 | 106.30 | 128.08 |
| 5 | H | 200 | CYC | C4D-CHA-C1A | -8.89 | 118.19 | 128.81 |
| 5 | I | 201 | CYC | C4D-CHA-C1A | -8.86 | 118.22 | 128.81 |
| 5 | N | 200 | CYC | C4D-CHA-C1A | -8.68 | 118.44 | 128.81 |
| 5 | W | 200 | CYC | C4D-CHA-C1A | -8.40 | 118.78 | 128.81 |
| 5 | V | 201 | CYC | C1B-CHB-C4A | -8.26 | 107.89 | 128.08 |
| 5 | h | 201 | CYC | C1B-CHB-C4A | -8.25 | 107.92 | 128.08 |
| 5 | N | 200 | CYC | C2C-C1C-NC | -8.07 | 101.32 | 108.27 |
| 5 | c | 200 | CYC | C1B-CHB-C4A | -8.06 | 108.39 | 128.08 |
| 5 | A | 200 | CYC | C2C-C1C-NC | -7.66 | 101.67 | 108.27 |
| 5 | g | 200 | CYC | C1B-CHB-C4A | -7.45 | 109.88 | 128.08 |
| 5 | X | 201 | CYC | C1B-CHB-C4A | -7.44 | 109.90 | 128.08 |
| 5 | W | 200 | CYC | C2C-C1C-NC | -7.44 | 101.86 | 108.27 |
| 5 | P | 200 | CYC | C4D-CHA-C1A | -7.29 | 120.10 | 128.81 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 5 | V | 200 | CYC | C1B-CHB-C4A | -7.28 | 110.30 | 128.08 |
| 5 | O | 200 | CYC | C2C-C1C-NC | -7.27 | 102.01 | 108.27 |
| 5 | C | 200 | CYC | C1B-CHB-C4A | -6.92 | 111.16 | 128.08 |
| 5 | P | 200 | CYC | C1B-CHB-C4A | -6.89 | 111.24 | 128.08 |
| 5 | b | 200 | CYC | C1B-CHB-C4A | -6.87 | 111.29 | 128.08 |
| 5 | I | 201 | CYC | C2C-C1C-NC | -6.77 | 102.44 | 108.27 |
| 5 | i | 201 | CYC | C1B-CHB-C4A | -6.74 | 111.62 | 128.08 |
| 5 | 5 | 1202 | CYC | C1B-CHB-C4A | -6.72 | 111.67 | 128.08 |
| 5 | e | 200 | CYC | C1B-CHB-C4A | -6.70 | 111.72 | 128.08 |
| 5 | j | 200 | CYC | C1B-CHB-C4A | -6.62 | 111.92 | 128.08 |
| 5 | Y | 200 | CYC | C4D-CHA-C1A | -6.40 | 121.16 | 128.81 |
| 5 | E | 200 | CYC | C1B-CHB-C4A | -6.35 | 112.58 | 128.08 |
| 5 | j | 201 | CYC | C2C-C1C-NC | -6.15 | 102.97 | 108.27 |
| 5 | B | 200 | CYC | C2C-C1C-NC | -6.14 | 102.98 | 108.27 |
| 5 | S | 200 | CYC | C1B-CHB-C4A | -6.14 | 113.09 | 128.08 |
| 5 | K | 201 | CYC | C2C-C1C-NC | -5.98 | 103.11 | 108.27 |
| 5 | S | 200 | CYC | CAB-C3B-C4B | 5.97 | 130.81 | 121.38 |
| 5 | Y | 201 | CYC | C2C-C1C-NC | -5.92 | 103.17 | 108.27 |
| 5 | W | 201 | CYC | C2C-C1C-NC | -5.85 | 103.23 | 108.27 |
| 5 | A | 200 | CYC | C1B-CHB-C4A | -5.83 | 113.85 | 128.08 |
| 5 | F | 200 | CYC | C1B-CHB-C4A | -5.81 | 113.89 | 128.08 |
| 5 | j | 201 | CYC | C1B-CHB-C4A | -5.80 | 113.90 | 128.08 |
| 5 | I | 200 | CYC | C1B-CHB-C4A | -5.80 | 113.90 | 128.08 |
| 5 | I | 201 | CYC | C1B-CHB-C4A | -5.80 | 113.91 | 128.08 |
| 5 | V | 201 | CYC | C2C-C1C-NC | -5.78 | 103.29 | 108.27 |
| 5 | k | 200 | CYC | C1B-CHB-C4A | -5.73 | 114.08 | 128.08 |
| 5 | G | 201 | CYC | C2C-C1C-NC | -5.63 | 103.42 | 108.27 |
| 5 | 5 | 1201 | CYC | C1B-CHB-C4A | -5.49 | 114.68 | 128.08 |
| 5 | D | 200 | CYC | C1B-CHB-C4A | -5.45 | 114.76 | 128.08 |
| 5 | k | 201 | CYC | C1B-CHB-C4A | -5.38 | 114.94 | 128.08 |
| 5 | K | 200 | CYC | C2C-C3C-C4C | 5.33 | 109.32 | 101.34 |
| 5 | 5 | 1201 | CYC | C2C-C1C-NC | -5.28 | 103.72 | 108.27 |
| 5 | F | 200 | CYC | CAB-C3B-C4B | 5.28 | 129.71 | 121.38 |
| 5 | f | 200 | CYC | C2C-C1C-NC | -5.25 | 103.75 | 108.27 |
| 5 | T | 200 | CYC | C2C-C3C-C4C | 5.24 | 109.19 | 101.34 |
| 5 | g | 201 | CYC | C1B-CHB-C4A | -5.22 | 115.32 | 128.08 |
| 5 | 5 | 1202 | CYC | C2C-C3C-C4C | 5.20 | 109.14 | 101.34 |
| 5 | G | 200 | CYC | C1B-CHB-C4A | -5.19 | 115.39 | 128.08 |
| 5 | S | 200 | CYC | C2C-C1C-NC | -5.18 | 103.81 | 108.27 |
| 5 | l | 201 | CYC | CAB-C3B-C4B | 5.15 | 129.51 | 121.38 |
| 5 | L | 201 | CYC | C2C-C1C-NC | -5.11 | 103.87 | 108.27 |
| 5 | G | 200 | CYC | C2C-C3C-C4C | 5.08 | 108.95 | 101.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 5 | E | 200 | CYC | C2C-C1C-NC | -5.04 | 103.93 | 108.27 |
| 5 | 5 | 1201 | CYC | C2C-C3C-C4C | 4.99 | 108.81 | 101.34 |
| 5 | i | 200 | CYC | C2C-C3C-C4C | 4.96 | 108.76 | 101.34 |
| 5 | V | 200 | CYC | C2C-C1C-NC | -4.93 | 104.03 | 108.27 |
| 5 | Y | 200 | CYC | C1B-CHB-C4A | -4.92 | 116.05 | 128.08 |
| 5 | i | 201 | CYC | C2C-C3C-C4C | 4.91 | 108.69 | 101.34 |
| 5 | l | 201 | CYC | C2C-C3C-C4C | 4.89 | 108.66 | 101.34 |
| 5 | a | 200 | CYC | C1B-CHB-C4A | -4.87 | 116.18 | 128.08 |
| 5 | g | 201 | CYC | C2C-C3C-C4C | 4.85 | 108.60 | 101.34 |
| 5 | k | 201 | CYC | C2C-C3C-C4C | 4.83 | 108.57 | 101.34 |
| 5 | h | 200 | CYC | C1B-CHB-C4A | -4.81 | 116.33 | 128.08 |
| 5 | g | 200 | CYC | C2C-C3C-C4C | 4.80 | 108.53 | 101.34 |
| 5 | U | 200 | CYC | C1B-CHB-C4A | -4.77 | 116.42 | 128.08 |
| 5 | T | 201 | CYC | C2C-C3C-C4C | 4.75 | 108.45 | 101.34 |
| 5 | J | 201 | CYC | C2C-C3C-C4C | 4.72 | 108.42 | 101.34 |
| 5 | U | 200 | CYC | C2C-C3C-C4C | 4.72 | 108.41 | 101.34 |
| 5 | Q | 200 | CYC | C1B-CHB-C4A | -4.65 | 116.72 | 128.08 |
| 5 | P | 200 | CYC | C2C-C3C-C4C | 4.65 | 108.30 | 101.34 |
| 5 | J | 201 | CYC | CAB-C3B-C4B | 4.61 | 128.67 | 121.38 |
| 5 | T | 201 | CYC | C1B-CHB-C4A | -4.61 | 116.81 | 128.08 |
| 5 | h | 200 | CYC | C2C-C3C-C4C | 4.61 | 108.24 | 101.34 |
| 5 | X | 200 | CYC | C2C-C3C-C4C | 4.58 | 108.20 | 101.34 |
| 5 | E | 200 | CYC | C2C-C3C-C4C | 4.55 | 108.15 | 101.34 |
| 5 | g | 201 | CYC | C2C-C1C-NC | -4.53 | 104.37 | 108.27 |
| 5 | T | 200 | CYC | C1B-CHB-C4A | -4.51 | 117.06 | 128.08 |
| 5 | O | 200 | CYC | C2C-C3C-C4C | 4.47 | 108.04 | 101.34 |
| 5 | N | 200 | CYC | CAB-C3B-C4B | 4.45 | 128.40 | 121.38 |
| 5 | C | 200 | CYC | C2C-C3C-C4C | 4.39 | 107.91 | 101.34 |
| 5 | h | 201 | CYC | C2C-C1C-NC | -4.38 | 104.50 | 108.27 |
| 5 | f | 200 | CYC | C2C-C3C-C4C | 4.37 | 107.88 | 101.34 |
| 5 | Q | 200 | CYC | C2C-C1C-NC | -4.36 | 104.51 | 108.27 |
| 5 | i | 200 | CYC | C2C-C1C-NC | -4.36 | 104.52 | 108.27 |
| 5 | V | 201 | CYC | C2C-C3C-C4C | 4.34 | 107.84 | 101.34 |
| 5 | F | 200 | CYC | C2C-C3C-C4C | 4.30 | 107.78 | 101.34 |
| 5 | W | 201 | CYC | C1B-CHB-C4A | -4.30 | 117.59 | 128.08 |
| 5 | N | 200 | CYC | C1B-CHB-C4A | -4.27 | 117.64 | 128.08 |
| 5 | C | 200 | CYC | C2C-C1C-NC | -4.25 | 104.61 | 108.27 |
| 5 | S | 200 | CYC | C2C-C3C-C4C | 4.25 | 107.71 | 101.34 |
| 5 | N | 200 | CYC | C2C-C3C-C4C | 4.23 | 107.67 | 101.34 |
| 5 | W | 200 | CYC | C2C-C3C-C4C | 4.21 | 107.64 | 101.34 |
| 5 | U | 201 | CYC | CAB-C3B-C4B | 4.21 | 128.03 | 121.38 |
| 5 | D | 200 | CYC | C2C-C3C-C4C | 4.19 | 107.61 | 101.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 5 | l | 201 | CYC | CMA-C3A-C4A | 4.18 | 131.49 | 125.06 |
| 5 | K | 200 | CYC | CMA-C3A-C4A | 4.17 | 131.49 | 125.06 |
| 5 | T | 201 | CYC | C2C-C1C-NC | -4.17 | 104.67 | 108.27 |
| 5 | R | 200 | CYC | C2C-C3C-C4C | 4.16 | 107.57 | 101.34 |
| 5 | K | 201 | CYC | C2C-C3C-C4C | 4.16 | 107.56 | 101.34 |
| 5 | A | 200 | CYC | C2C-C3C-C4C | 4.15 | 107.56 | 101.34 |
| 5 | O | 200 | CYC | CMA-C3A-C4A | 4.15 | 131.45 | 125.06 |
| 5 | D | 200 | CYC | CAB-C3B-C4B | 4.14 | 127.92 | 121.38 |
| 5 | L | 201 | CYC | C2C-C3C-C4C | 4.11 | 107.49 | 101.34 |
| 5 | V | 200 | CYC | C2C-C3C-C4C | 4.09 | 107.47 | 101.34 |
| 5 | d | 200 | CYC | C2C-C1C-NC | -4.09 | 104.75 | 108.27 |
| 5 | 5 | 1201 | CYC | CMA-C3A-C4A | 4.06 | 131.32 | 125.06 |
| 5 | Y | 201 | CYC | C2C-C3C-C4C | 4.06 | 107.42 | 101.34 |
| 5 | Q | 200 | CYC | CAB-C3B-C4B | 4.06 | 127.79 | 121.38 |
| 5 | J | 200 | CYC | CMA-C3A-C4A | 4.05 | 131.29 | 125.06 |
| 5 | B | 200 | CYC | C2C-C3C-C4C | 4.02 | 107.36 | 101.34 |
| 5 | O | 200 | CYC | CAB-C3B-C4B | 4.02 | 127.72 | 121.38 |
| 5 | d | 200 | CYC | C1B-CHB-C4A | -4.01 | 118.29 | 128.08 |
| 5 | C | 200 | CYC | CAB-C3B-C4B | 3.99 | 127.68 | 121.38 |
| 5 | W | 201 | CYC | C2C-C3C-C4C | 3.98 | 107.29 | 101.34 |
| 5 | U | 201 | CYC | C2C-C1C-NC | -3.96 | 104.86 | 108.27 |
| 5 | k | 200 | CYC | C2C-C1C-NC | -3.94 | 104.88 | 108.27 |
| 5 | A | 200 | CYC | CAB-C3B-C4B | 3.94 | 127.59 | 121.38 |
| 5 | j | 201 | CYC | C2C-C3C-C4C | 3.91 | 107.19 | 101.34 |
| 5 | W | 200 | CYC | C1B-CHB-C4A | -3.91 | 118.53 | 128.08 |
| 5 | b | 200 | CYC | C2C-C1C-NC | -3.90 | 104.91 | 108.27 |
| 5 | h | 200 | CYC | C2C-C1C-NC | -3.88 | 104.92 | 108.27 |
| 5 | G | 201 | CYC | CMA-C3A-C4A | 3.88 | 131.04 | 125.06 |
| 5 | H | 200 | CYC | CMA-C3A-C4A | 3.88 | 131.03 | 125.06 |
| 5 | H | 201 | CYC | CAB-C3B-C4B | 3.87 | 127.49 | 121.38 |
| 5 | I | 201 | CYC | C2C-C3C-C4C | 3.86 | 107.12 | 101.34 |
| 5 | K | 201 | CYC | CMA-C3A-C4A | 3.86 | 131.01 | 125.06 |
| 5 | X | 201 | CYC | C2C-C3C-C4C | 3.86 | 107.12 | 101.34 |
| 5 | P | 200 | CYC | CAB-C3B-C4B | 3.85 | 127.46 | 121.38 |
| 5 | I | 200 | CYC | C2C-C1C-NC | -3.83 | 104.97 | 108.27 |
| 5 | H | 201 | CYC | C2C-C1C-NC | -3.81 | 104.99 | 108.27 |
| 5 | W | 200 | CYC | CMA-C3A-C4A | 3.78 | 130.89 | 125.06 |
| 5 | B | 200 | CYC | CAB-C3B-C4B | 3.78 | 127.35 | 121.38 |
| 5 | R | 200 | CYC | CAB-C3B-C4B | 3.75 | 127.30 | 121.38 |
| 5 | W | 201 | CYC | CAB-C3B-C4B | 3.75 | 127.30 | 121.38 |
| 5 | h | 201 | CYC | CAB-C3B-C4B | 3.72 | 127.26 | 121.38 |
| 5 | P | 200 | CYC | C2C-C1C-NC | -3.72 | 105.06 | 108.27 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 5 | b | 200 | CYC | CAB-C3B-C4B | 3.72 | 127.25 | 121.38 |
| 5 | T | 201 | CYC | CAB-C3B-C4B | 3.70 | 127.23 | 121.38 |
| 5 | G | 201 | CYC | C2C-C3C-C4C | 3.67 | 106.84 | 101.34 |
| 5 | i | 201 | CYC | CAB-C3B-C4B | 3.66 | 127.17 | 121.38 |
| 5 | Y | 200 | CYC | C2C-C1C-NC | -3.66 | 105.12 | 108.27 |
| 5 | i | 200 | CYC | CAB-C3B-C4B | 3.66 | 127.15 | 121.38 |
| 5 | f | 200 | CYC | CAB-C3B-C4B | 3.65 | 127.14 | 121.38 |
| 5 | j | 200 | CYC | C2C-C3C-C4C | 3.65 | 106.80 | 101.34 |
| 5 | k | 200 | CYC | CAB-C3B-C4B | 3.61 | 127.08 | 121.38 |
| 5 | X | 201 | CYC | CAB-C3B-C4B | 3.61 | 127.08 | 121.38 |
| 5 | e | 200 | CYC | C2C-C3C-C4C | 3.61 | 106.74 | 101.34 |
| 5 | D | 200 | CYC | CMA-C3A-C4A | 3.60 | 130.62 | 125.06 |
| 5 | i | 200 | CYC | C1B-CHB-C4A | -3.57 | 119.36 | 128.08 |
| 5 | I | 201 | CYC | CAB-C3B-C4B | 3.57 | 127.01 | 121.38 |
| 5 | H | 200 | CYC | C2C-C1C-NC | -3.56 | 105.20 | 108.27 |
| 5 | E | 200 | CYC | CAB-C3B-C4B | 3.55 | 126.99 | 121.38 |
| 5 | c | 200 | CYC | CAB-C3B-C4B | 3.55 | 126.98 | 121.38 |
| 5 | G | 200 | CYC | CAB-C3B-C4B | 3.55 | 126.98 | 121.38 |
| 5 | V | 201 | CYC | CAB-C3B-C4B | 3.54 | 126.97 | 121.38 |
| 5 | J | 200 | CYC | CAB-C3B-C4B | 3.53 | 126.95 | 121.38 |
| 5 | J | 200 | CYC | C2C-C3C-C4C | 3.52 | 106.61 | 101.34 |
| 5 | H | 200 | CYC | C2C-C3C-C4C | 3.51 | 106.60 | 101.34 |
| 5 | G | 201 | CYC | CAB-C3B-C4B | 3.51 | 126.92 | 121.38 |
| 5 | 5 | 1202 | CYC | CAB-C3B-C4B | 3.50 | 126.91 | 121.38 |
| 5 | a | 200 | CYC | C2C-C1C-NC | -3.50 | 105.26 | 108.27 |
| 5 | j | 201 | CYC | CAB-C3B-C4B | 3.50 | 126.90 | 121.38 |
| 5 | W | 201 | CYC | CMA-C3A-C4A | 3.49 | 130.44 | 125.06 |
| 5 | W | 200 | CYC | CAB-C3B-C4B | 3.48 | 126.88 | 121.38 |
| 5 | L | 201 | CYC | CAB-C3B-C4B | 3.48 | 126.87 | 121.38 |
| 5 | K | 200 | CYC | CAB-C3B-C4B | 3.48 | 126.87 | 121.38 |
| 5 | V | 200 | CYC | CAB-C3B-C4B | 3.48 | 126.87 | 121.38 |
| 5 | e | 200 | CYC | CAB-C3B-C4B | 3.46 | 126.84 | 121.38 |
| 5 | g | 200 | CYC | CAB-C3B-C4B | 3.45 | 126.83 | 121.38 |
| 5 | Y | 201 | CYC | CAB-C3B-C4B | 3.45 | 126.82 | 121.38 |
| 5 | k | 201 | CYC | CAB-C3B-C4B | 3.44 | 126.81 | 121.38 |
| 5 | X | 200 | CYC | CMA-C3A-C4A | 3.41 | 130.31 | 125.06 |
| 5 | G | 201 | CYC | CHB-C4A-C3A | 3.39 | 133.63 | 124.90 |
| 5 | O | 200 | CYC | CHB-C4A-C3A | 3.39 | 133.62 | 124.90 |
| 5 | X | 200 | CYC | CAB-C3B-C4B | 3.38 | 126.71 | 121.38 |
| 5 | R | 200 | CYC | C2C-C1C-NC | -3.32 | 105.41 | 108.27 |
| 5 | R | 200 | CYC | C1B-CHB-C4A | -3.31 | 119.99 | 128.08 |
| 5 | f | 200 | CYC | CBD-CAD-C3D | 3.31 | 118.27 | 112.62 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 5 | B | 200 | CYC | C1B-CHB-C4A | -3.31 | 120.00 | 128.08 |
| 5 | h | 200 | CYC | CMA-C3A-C4A | 3.30 | 130.15 | 125.06 |
| 5 | g | 200 | CYC | C2C-C1C-NC | -3.29 | 105.44 | 108.27 |
| 5 | L | 201 | CYC | OB-C4B-C3B | -3.29 | 124.47 | 128.04 |
| 5 | I | 200 | CYC | CAB-C3B-C4B | 3.29 | 126.57 | 121.38 |
| 5 | i | 201 | CYC | C2C-C1C-NC | -3.28 | 105.44 | 108.27 |
| 5 | Y | 200 | CYC | CMA-C3A-C4A | 3.28 | 130.12 | 125.06 |
| 5 | l | 201 | CYC | C2C-C1C-NC | -3.25 | 105.47 | 108.27 |
| 5 | k | 200 | CYC | C2C-C3C-C4C | 3.24 | 106.19 | 101.34 |
| 5 | h | 201 | CYC | C2C-C3C-C4C | 3.23 | 106.17 | 101.34 |
| 5 | H | 200 | CYC | CAB-C3B-C4B | 3.22 | 126.46 | 121.38 |
| 5 | a | 200 | CYC | CAB-C3B-C4B | 3.21 | 126.45 | 121.38 |
| 5 | d | 200 | CYC | CAB-C3B-C4B | 3.21 | 126.45 | 121.38 |
| 5 | J | 200 | CYC | CHB-C4A-C3A | 3.21 | 133.15 | 124.90 |
| 5 | Y | 201 | CYC | C1B-CHB-C4A | -3.19 | 120.29 | 128.08 |
| 5 | h | 200 | CYC | CAB-C3B-C4B | 3.18 | 126.40 | 121.38 |
| 5 | N | 200 | CYC | CMA-C3A-C4A | 3.17 | 129.94 | 125.06 |
| 5 | i | 200 | CYC | CMA-C3A-C4A | 3.17 | 129.94 | 125.06 |
| 5 | T | 200 | CYC | CAB-C3B-C4B | 3.15 | 126.36 | 121.38 |
| 5 | K | 201 | CYC | CAB-C3B-C4B | 3.14 | 126.34 | 121.38 |
| 5 | j | 200 | CYC | CAB-C3B-C4B | 3.13 | 126.33 | 121.38 |
| 5 | Q | 200 | CYC | C2C-C3C-C4C | 3.11 | 105.99 | 101.34 |
| 5 | E | 200 | CYC | CMA-C3A-C4A | 3.10 | 129.84 | 125.06 |
| 5 | G | 201 | CYC | C1A-NA-C4A | 3.10 | 112.35 | 106.51 |
| 5 | B | 200 | CYC | CMA-C3A-C4A | 3.09 | 129.82 | 125.06 |
| 5 | g | 201 | CYC | CMA-C3A-C4A | 3.09 | 129.82 | 125.06 |
| 5 | O | 200 | CYC | C1A-NA-C4A | 3.09 | 112.32 | 106.51 |
| 5 | K | 200 | CYC | CHB-C4A-C3A | 3.07 | 132.78 | 124.90 |
| 5 | e | 200 | CYC | C2C-C1C-NC | -3.06 | 105.64 | 108.27 |
| 5 | U | 200 | CYC | CMA-C3A-C4A | 3.05 | 129.76 | 125.06 |
| 5 | c | 200 | CYC | C2C-C3C-C4C | 3.05 | 105.90 | 101.34 |
| 5 | T | 200 | CYC | CMA-C3A-C4A | 3.03 | 129.73 | 125.06 |
| 5 | a | 200 | CYC | CMA-C3A-C4A | 3.02 | 129.72 | 125.06 |
| 5 | g | 201 | CYC | CAB-C3B-C4B | 2.96 | 126.06 | 121.38 |
| 5 | J | 201 | CYC | C1B-CHB-C4A | -2.94 | 120.89 | 128.08 |
| 5 | U | 201 | CYC | CMB-C2B-C1B | 2.93 | 127.82 | 124.17 |
| 5 | K | 201 | CYC | C1B-CHB-C4A | -2.89 | 121.01 | 128.08 |
| 5 | K | 200 | CYC | C1A-NA-C4A | 2.89 | 111.95 | 106.51 |
| 5 | R | 200 | CYC | CMA-C3A-C4A | 2.88 | 129.50 | 125.06 |
| 5 | K | 201 | CYC | CHB-C4A-C3A | 2.88 | 132.31 | 124.90 |
| 5 | l | 201 | CYC | CMB-C2B-C1B | 2.88 | 127.76 | 124.17 |
| 5 | T | 200 | CYC | C2C-C1C-NC | -2.87 | 105.80 | 108.27 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 5 | U | 201 | CYC | C2C-C3C-C4C | 2.86 | 105.62 | 101.34 |
| 5 | G | 200 | CYC | C2C-C1C-NC | -2.86 | 105.81 | 108.27 |
| 5 | F | 200 | CYC | CMC-C2C-C1C | -2.86 | 106.25 | 112.40 |
| 5 | X | 200 | CYC | C1A-NA-C4A | 2.85 | 111.88 | 106.51 |
| 5 | L | 201 | CYC | CMA-C3A-C4A | 2.85 | 129.45 | 125.06 |
| 5 | B | 200 | CYC | C1A-NA-C4A | 2.85 | 111.87 | 106.51 |
| 5 | l | 201 | CYC | C1B-CHB-C4A | -2.84 | 121.14 | 128.08 |
| 5 | Q | 200 | CYC | CMA-C3A-C4A | 2.83 | 129.43 | 125.06 |
| 5 | 5 | 1201 | CYC | CAC-C3C-C4C | -2.83 | 105.40 | 112.67 |
| 5 | c | 200 | CYC | C2C-C1C-NC | -2.83 | 105.83 | 108.27 |
| 5 | T | 200 | CYC | C1A-NA-C4A | 2.83 | 111.84 | 106.51 |
| 5 | k | 201 | CYC | C2C-C1C-NC | -2.82 | 105.84 | 108.27 |
| 5 | c | 200 | CYC | CBD-CAD-C3D | 2.82 | 117.43 | 112.62 |
| 5 | d | 200 | CYC | C2C-C3C-C4C | 2.81 | 105.55 | 101.34 |
| 5 | 5 | 1201 | CYC | CAB-C3B-C4B | 2.81 | 125.82 | 121.38 |
| 5 | i | 200 | CYC | C1A-NA-C4A | 2.79 | 111.77 | 106.51 |
| 5 | Y | 200 | CYC | CAB-C3B-C4B | 2.78 | 125.77 | 121.38 |
| 5 | T | 201 | CYC | CMA-C3A-C4A | 2.78 | 129.34 | 125.06 |
| 5 | j | 200 | CYC | C2C-C1C-NC | -2.78 | 105.88 | 108.27 |
| 5 | K | 201 | CYC | C1A-NA-C4A | 2.78 | 111.74 | 106.51 |
| 5 | l | 201 | CYC | C1A-NA-C4A | 2.76 | 111.71 | 106.51 |
| 5 | W | 201 | CYC | C1A-NA-C4A | 2.75 | 111.70 | 106.51 |
| 5 | a | 200 | CYC | C1A-NA-C4A | 2.75 | 111.70 | 106.51 |
| 5 | W | 200 | CYC | C1A-NA-C4A | 2.75 | 111.69 | 106.51 |
| 5 | R | 200 | CYC | C1A-NA-C4A | 2.74 | 111.67 | 106.51 |
| 5 | L | 201 | CYC | C1A-NA-C4A | 2.73 | 111.66 | 106.51 |
| 5 | J | 201 | CYC | CMA-C3A-C4A | 2.72 | 129.26 | 125.06 |
| 5 | B | 200 | CYC | CBD-CAD-C3D | 2.72 | 117.26 | 112.62 |
| 5 | J | 201 | CYC | C2C-C1C-NC | -2.71 | 105.94 | 108.27 |
| 5 | U | 201 | CYC | CAC-C3C-C2C | -2.71 | 107.49 | 114.26 |
| 5 | J | 201 | CYC | C1A-NA-C4A | 2.70 | 111.59 | 106.51 |
| 5 | J | 200 | CYC | C1A-NA-C4A | 2.68 | 111.57 | 106.51 |
| 5 | d | 200 | CYC | CMA-C3A-C4A | 2.68 | 129.20 | 125.06 |
| 5 | H | 200 | CYC | CHB-C4A-C3A | 2.67 | 131.75 | 124.90 |
| 5 | Y | 201 | CYC | C1A-NA-C4A | 2.65 | 111.50 | 106.51 |
| 5 | U | 200 | CYC | CAB-C3B-C4B | 2.65 | 125.56 | 121.38 |
| 5 | g | 200 | CYC | CMB-C2B-C1B | 2.64 | 127.47 | 124.17 |
| 5 | H | 200 | CYC | C1B-CHB-C4A | -2.64 | 121.63 | 128.08 |
| 5 | F | 200 | CYC | C2C-C1C-NC | -2.64 | 106.00 | 108.27 |
| 5 | b | 200 | CYC | C2C-C3C-C4C | 2.63 | 105.28 | 101.34 |
| 5 | X | 200 | CYC | CHB-C4A-C3A | 2.63 | 131.66 | 124.90 |
| 5 | X | 201 | CYC | C2C-C1C-NC | -2.63 | 106.01 | 108.27 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 5 | R | 200 | CYC | CHB-C4A-C3A | 2.61 | 131.62 | 124.90 |
| 5 | H | 201 | CYC | CMB-C2B-C1B | 2.61 | 127.43 | 124.17 |
| 5 | S | 200 | CYC | CAC-C3C-C4C | -2.61 | 105.97 | 112.67 |
| 5 | l | 201 | CYC | CHB-C4A-C3A | 2.61 | 131.61 | 124.90 |
| 5 | j | 200 | CYC | CMB-C2B-C1B | 2.61 | 127.42 | 124.17 |
| 5 | 5 | 1202 | CYC | CMB-C2B-C1B | 2.60 | 127.41 | 124.17 |
| 5 | U | 200 | CYC | OB-C4B-C3B | -2.59 | 125.23 | 128.04 |
| 5 | H | 200 | CYC | C1A-NA-C4A | 2.56 | 111.34 | 106.51 |
| 5 | g | 201 | CYC | C1A-NA-C4A | 2.56 | 111.34 | 106.51 |
| 5 | L | 201 | CYC | CMB-C2B-C1B | 2.56 | 127.36 | 124.17 |
| 5 | d | 200 | CYC | C1A-NA-C4A | 2.56 | 111.33 | 106.51 |
| 5 | j | 201 | CYC | C1A-NA-C4A | 2.56 | 111.33 | 106.51 |
| 5 | a | 200 | CYC | CBD-CAD-C3D | 2.56 | 116.98 | 112.62 |
| 5 | G | 200 | CYC | C1A-NA-C4A | 2.55 | 111.32 | 106.51 |
| 5 | L | 201 | CYC | CHB-C4A-C3A | 2.55 | 131.46 | 124.90 |
| 5 | I | 200 | CYC | C2C-C3C-C4C | 2.55 | 105.15 | 101.34 |
| 5 | B | 200 | CYC | CHB-C4A-C3A | 2.54 | 131.43 | 124.90 |
| 5 | J | 201 | CYC | CHB-C1B-C2B | -2.53 | 121.93 | 126.95 |
| 5 | Y | 201 | CYC | CMA-C3A-C4A | 2.53 | 128.97 | 125.06 |
| 5 | T | 201 | CYC | C1A-NA-C4A | 2.52 | 111.26 | 106.51 |
| 5 | F | 200 | CYC | CMA-C3A-C4A | 2.52 | 128.95 | 125.06 |
| 5 | F | 200 | CYC | CAC-C3C-C4C | -2.51 | 106.23 | 112.67 |
| 5 | 5 | 1202 | CYC | O2A-CGA-CBA | 2.50 | 122.07 | 114.03 |
| 5 | W | 201 | CYC | CHB-C4A-C3A | 2.49 | 131.31 | 124.90 |
| 5 | j | 200 | CYC | OB-C4B-C3B | -2.48 | 125.35 | 128.04 |
| 5 | i | 201 | CYC | C1A-NA-C4A | 2.47 | 111.17 | 106.51 |
| 5 | R | 200 | CYC | CHA-C1A-NA | -2.47 | 125.40 | 128.83 |
| 5 | X | 201 | CYC | OB-C4B-C3B | -2.47 | 125.36 | 128.04 |
| 5 | J | 201 | CYC | CHB-C4A-C3A | 2.45 | 131.19 | 124.90 |
| 5 | G | 200 | CYC | CMA-C3A-C4A | 2.44 | 128.82 | 125.06 |
| 5 | e | 200 | CYC | C1A-NA-C4A | 2.44 | 111.11 | 106.51 |
| 5 | O | 200 | CYC | CHB-C4A-NA | -2.44 | 119.84 | 124.93 |
| 5 | I | 201 | CYC | CMB-C2B-C1B | 2.43 | 127.19 | 124.17 |
| 5 | U | 200 | CYC | C1A-NA-C4A | 2.42 | 111.07 | 106.51 |
| 5 | X | 201 | CYC | CMB-C2B-C1B | 2.42 | 127.18 | 124.17 |
| 5 | G | 201 | CYC | CHB-C4A-NA | -2.41 | 119.90 | 124.93 |
| 5 | W | 200 | CYC | CHB-C4A-C3A | 2.40 | 131.06 | 124.90 |
| 5 | j | 200 | CYC | CMA-C3A-C4A | 2.39 | 128.75 | 125.06 |
| 5 | E | 200 | CYC | CMB-C2B-C1B | 2.38 | 127.14 | 124.17 |
| 5 | N | 200 | CYC | C1A-NA-C4A | 2.38 | 110.99 | 106.51 |
| 5 | J | 200 | CYC | C2C-C1C-NC | -2.38 | 106.22 | 108.27 |
| 5 | k | 201 | CYC | C1A-NA-C4A | 2.38 | 110.98 | 106.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 5 | E | 200 | CYC | CMC-C2C-C1C | -2.37 | 107.29 | 112.40 |
| 5 | J | 200 | CYC | CHB-C4A-NA | -2.37 | 119.97 | 124.93 |
| 5 | c | 200 | CYC | C1A-NA-C4A | 2.36 | 110.96 | 106.51 |
| 5 | K | 200 | CYC | C1B-CHB-C4A | -2.36 | 122.32 | 128.08 |
| 5 | T | 201 | CYC | CMB-C2B-C1B | 2.35 | 127.11 | 124.17 |
| 5 | L | 201 | CYC | CMC-C2C-C1C | -2.34 | 107.35 | 112.40 |
| 5 | O | 200 | CYC | C1B-CHB-C4A | -2.34 | 122.37 | 128.08 |
| 5 | I | 201 | CYC | C1A-NA-C4A | 2.33 | 110.91 | 106.51 |
| 5 | h | 200 | CYC | C1A-NA-C4A | 2.33 | 110.91 | 106.51 |
| 5 | Y | 200 | CYC | C1A-NA-C4A | 2.33 | 110.90 | 106.51 |
| 5 | D | 200 | CYC | C1A-NA-C4A | 2.32 | 110.88 | 106.51 |
| 5 | S | 200 | CYC | C1A-NA-C4A | 2.31 | 110.87 | 106.51 |
| 5 | V | 200 | CYC | C1A-NA-C4A | 2.31 | 110.87 | 106.51 |
| 5 | k | 201 | CYC | CMB-C2B-C1B | 2.31 | 127.05 | 124.17 |
| 5 | 5 | 1201 | CYC | CAC-C3C-C2C | -2.31 | 108.49 | 114.26 |
| 5 | i | 200 | CYC | CHB-C4A-C3A | 2.30 | 130.82 | 124.90 |
| 5 | k | 200 | CYC | C1A-NA-C4A | 2.30 | 110.84 | 106.51 |
| 5 | I | 201 | CYC | CMA-C3A-C4A | 2.30 | 128.60 | 125.06 |
| 5 | L | 201 | CYC | C1B-CHB-C4A | -2.29 | 122.48 | 128.08 |
| 5 | Q | 200 | CYC | CMD-C2D-C3D | -2.29 | 120.62 | 124.94 |
| 5 | g | 200 | CYC | C1A-NA-C4A | 2.29 | 110.82 | 106.51 |
| 5 | k | 201 | CYC | OB-C4B-C3B | -2.28 | 125.56 | 128.04 |
| 5 | 5 | 1202 | CYC | C1A-NA-C4A | 2.28 | 110.80 | 106.51 |
| 5 | h | 201 | CYC | CHA-C1A-NA | -2.28 | 125.67 | 128.83 |
| 5 | a | 200 | CYC | CHB-C4A-C3A | 2.28 | 130.75 | 124.90 |
| 5 | b | 200 | CYC | C1A-NA-C4A | 2.27 | 110.79 | 106.51 |
| 5 | Y | 201 | CYC | OB-C4B-C3B | -2.27 | 125.58 | 128.04 |
| 5 | I | 200 | CYC | C1A-NA-C4A | 2.27 | 110.78 | 106.51 |
| 5 | i | 201 | CYC | CMB-C2B-C1B | 2.26 | 126.99 | 124.17 |
| 5 | j | 201 | CYC | CMA-C3A-C4A | 2.26 | 128.55 | 125.06 |
| 5 | O | 200 | CYC | CMC-C2C-C1C | -2.26 | 107.53 | 112.40 |
| 5 | E | 200 | CYC | C1A-NA-C4A | 2.25 | 110.76 | 106.51 |
| 5 | b | 200 | CYC | CMB-C2B-C1B | 2.25 | 126.98 | 124.17 |
| 5 | S | 200 | CYC | CAB-C3B-C2B | -2.24 | 123.70 | 127.53 |
| 5 | X | 200 | CYC | C1B-CHB-C4A | -2.24 | 122.61 | 128.08 |
| 5 | j | 201 | CYC | OB-C4B-C3B | -2.24 | 125.61 | 128.04 |
| 5 | B | 200 | CYC | CHA-C1A-NA | -2.24 | 125.72 | 128.83 |
| 5 | h | 201 | CYC | C1A-NA-C4A | 2.24 | 110.72 | 106.51 |
| 5 | T | 200 | CYC | CMB-C2B-C1B | 2.23 | 126.95 | 124.17 |
| 5 | g | 201 | CYC | CMB-C2B-C1B | 2.22 | 126.94 | 124.17 |
| 5 | V | 201 | CYC | C1A-NA-C4A | 2.22 | 110.70 | 106.51 |
| 5 | Q | 200 | CYC | C1A-NA-C4A | 2.22 | 110.69 | 106.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 5 | T | 201 | CYC | OB-C4B-C3B | -2.22 | 125.64 | 128.04 |
| 5 | X | 200 | CYC | OB-C4B-C3B | -2.21 | 125.64 | 128.04 |
| 5 | F | 200 | CYC | C1A-NA-C4A | 2.21 | 110.67 | 106.51 |
| 5 | L | 201 | CYC | CHB-C1B-C2B | -2.19 | 122.60 | 126.95 |
| 5 | Y | 201 | CYC | CHB-C4A-C3A | 2.19 | 130.53 | 124.90 |
| 5 | Y | 200 | CYC | C2C-C3C-C4C | 2.19 | 104.62 | 101.34 |
| 5 | i | 200 | CYC | CMB-C2B-C1B | 2.19 | 126.90 | 124.17 |
| 5 | k | 200 | CYC | OB-C4B-C3B | -2.18 | 125.67 | 128.04 |
| 5 | I | 200 | CYC | OB-C4B-C3B | -2.18 | 125.68 | 128.04 |
| 5 | N | 200 | CYC | O2A-CGA-CBA | 2.18 | 121.02 | 114.03 |
| 5 | g | 201 | CYC | CHA-C1A-NA | -2.17 | 125.81 | 128.83 |
| 5 | e | 200 | CYC | OB-C4B-C3B | -2.15 | 125.71 | 128.04 |
| 5 | j | 200 | CYC | C1A-NA-C4A | 2.14 | 110.55 | 106.51 |
| 5 | G | 201 | CYC | CMB-C2B-C1B | 2.14 | 126.83 | 124.17 |
| 5 | S | 200 | CYC | CMA-C3A-C4A | 2.14 | 128.35 | 125.06 |
| 5 | P | 200 | CYC | C1A-NA-C4A | 2.13 | 110.52 | 106.51 |
| 5 | f | 200 | CYC | CMB-C2B-C1B | 2.13 | 126.82 | 124.17 |
| 5 | S | 200 | CYC | CBD-CAD-C3D | 2.12 | 116.23 | 112.62 |
| 5 | c | 200 | CYC | CAC-C3C-C4C | -2.11 | 107.25 | 112.67 |
| 5 | U | 201 | CYC | C1A-NA-C4A | 2.11 | 110.49 | 106.51 |
| 5 | l | 201 | CYC | CAC-C3C-C2C | -2.11 | 108.99 | 114.26 |
| 5 | k | 201 | CYC | CMA-C3A-C4A | 2.11 | 128.31 | 125.06 |
| 5 | H | 200 | CYC | CMB-C2B-C1B | 2.11 | 126.80 | 124.17 |
| 5 | 5 | 1201 | CYC | C1A-NA-C4A | 2.10 | 110.47 | 106.51 |
| 5 | U | 200 | CYC | C2C-C1C-NC | -2.10 | 106.46 | 108.27 |
| 5 | K | 200 | CYC | CAA-C2A-C1A | 2.10 | 128.73 | 125.01 |
| 5 | k | 200 | CYC | CMA-C3A-C4A | 2.10 | 128.30 | 125.06 |
| 5 | Y | 201 | CYC | CHB-C1B-C2B | -2.10 | 122.79 | 126.95 |
| 5 | A | 200 | CYC | O2A-CGA-CBA | 2.10 | 120.76 | 114.03 |
| 5 | X | 201 | CYC | C1A-NA-C4A | 2.09 | 110.45 | 106.51 |
| 5 | A | 200 | CYC | C1A-NA-C4A | 2.09 | 110.44 | 106.51 |
| 5 | h | 201 | CYC | CMB-C2B-C1B | 2.09 | 126.77 | 124.17 |
| 5 | i | 201 | CYC | CAC-C3C-C2C | -2.08 | 109.06 | 114.26 |
| 5 | C | 200 | CYC | C1A-NA-C4A | 2.08 | 110.43 | 106.51 |
| 5 | K | 201 | CYC | OB-C4B-C3B | -2.08 | 125.79 | 128.04 |
| 5 | 5 | 1202 | CYC | CAC-C3C-C2C | -2.07 | 109.09 | 114.26 |
| 5 | I | 201 | CYC | OB-C4B-C3B | -2.06 | 125.81 | 128.04 |
| 5 | X | 200 | CYC | CHB-C1B-C2B | -2.05 | 122.88 | 126.95 |
| 5 | a | 200 | CYC | OB-C4B-C3B | -2.05 | 125.82 | 128.04 |
| 5 | g | 200 | CYC | CMA-C3A-C4A | 2.05 | 128.22 | 125.06 |
| 5 | X | 200 | CYC | CAC-C3C-C2C | -2.05 | 109.14 | 114.26 |
| 5 | J | 200 | CYC | CMC-C2C-C1C | -2.05 | 107.99 | 112.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 5 | W | 200 | CYC | CBD-CAD-C3D | -2.05 | 109.13 | 112.62 |
| 5 | c | 200 | CYC | CMB-C2B-C1B | 2.05 | 126.72 | 124.17 |
| 5 | j | 200 | CYC | CAC-C3C-C2C | -2.04 | 109.17 | 114.26 |
| 5 | N | 200 | CYC | CHB-C4A-C3A | 2.04 | 130.14 | 124.90 |
| 5 | R | 200 | CYC | CMB-C2B-C1B | 2.03 | 126.71 | 124.17 |
| 5 | K | 200 | CYC | CHB-C4A-NA | -2.03 | 120.69 | 124.93 |
| 5 | a | 200 | CYC | O2A-CGA-CBA | 2.03 | 120.54 | 114.03 |
| 5 | W | 200 | CYC | CMB-C2B-C1B | 2.02 | 126.69 | 124.17 |
| 5 | j | 200 | CYC | O2A-CGA-CBA | 2.02 | 120.51 | 114.03 |
| 5 | U | 200 | CYC | CMC-C2C-C1C | -2.01 | 108.06 | 112.40 |
| 5 | G | 201 | CYC | C1B-CHB-C4A | -2.01 | 123.16 | 128.08 |
| 5 | C | 200 | CYC | CMB-C2B-C1B | 2.01 | 126.68 | 124.17 |
| 5 | K | 200 | CYC | C2C-C1C-NC | -2.01 | 106.54 | 108.27 |
| 5 | 5 | 1202 | CYC | C2C-C1C-NC | -2.01 | 106.54 | 108.27 |
| 5 | J | 200 | CYC | C1B-CHB-C4A | -2.00 | 123.19 | 128.08 |

There are no chirality outliers.

All (703) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 5 | 5 | 1201 | CYC | NA-C4A-CHB-C1B |
| 5 | 5 | 1201 | CYC | C3A-C4A-CHB-C1B |
| 5 | 5 | 1201 | CYC | C4C-C3C-CAC-CBC |
| 5 | 5 | 1201 | CYC | NC-C4C-CHD-C1D |
| 5 | 5 | 1201 | CYC | C2D-C1D-CHD-C4C |
| 5 | 5 | 1202 | CYC | NA-C4A-CHB-C1B |
| 5 | 5 | 1202 | CYC | C3A-C4A-CHB-C1B |
| 5 | 5 | 1202 | CYC | NC-C4C-CHD-C1D |
| 5 | 5 | 1202 | CYC | ND-C1D-CHD-C4C |
| 5 | 5 | 1202 | CYC | C2D-C1D-CHD-C4C |
| 5 | 5 | 1202 | CYC | C3D-CAD-CBD-CGD |
| 5 | A | 200 | CYC | ND-C4D-CHA-C1A |
| 5 | A | 200 | CYC | C3D-C4D-CHA-C1A |
| 5 | A | 200 | CYC | NA-C4A-CHB-C1B |
| 5 | A | 200 | CYC | C3A-C4A-CHB-C1B |
| 5 | A | 200 | CYC | NC-C4C-CHD-C1D |
| 5 | A | 200 | CYC | C2D-C1D-CHD-C4C |
| 5 | B | 200 | CYC | NA-C1A-CHA-C4D |
| 5 | B | 200 | CYC | C2A-C1A-CHA-C4D |
| 5 | B | 200 | CYC | ND-C4D-CHA-C1A |
| 5 | B | 200 | CYC | C3D-C4D-CHA-C1A |
| 5 | B | 200 | CYC | NA-C4A-CHB-C1B |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 5 | B | 200 | CYC | C3A-C4A-CHB-C1B |
| 5 | B | 200 | CYC | NC-C4C-CHD-C1D |
| 5 | B | 200 | CYC | ND-C1D-CHD-C4C |
| 5 | B | 200 | CYC | C2D-C1D-CHD-C4C |
| 5 | B | 200 | CYC | C2D-C3D-CAD-CBD |
| 5 | B | 200 | CYC | C4D-C3D-CAD-CBD |
| 5 | C | 200 | CYC | NA-C1A-CHA-C4D |
| 5 | C | 200 | CYC | C2A-C1A-CHA-C4D |
| 5 | C | 200 | CYC | ND-C4D-CHA-C1A |
| 5 | C | 200 | CYC | C3D-C4D-CHA-C1A |
| 5 | C | 200 | CYC | NA-C4A-CHB-C1B |
| 5 | C | 200 | CYC | C3A-C4A-CHB-C1B |
| 5 | C | 200 | CYC | C4C-C3C-CAC-CBC |
| 5 | C | 200 | CYC | NC-C4C-CHD-C1D |
| 5 | C | 200 | CYC | ND-C1D-CHD-C4C |
| 5 | C | 200 | CYC | C2D-C1D-CHD-C4C |
| 5 | D | 200 | CYC | NA-C4A-CHB-C1B |
| 5 | D | 200 | CYC | C3A-C4A-CHB-C1B |
| 5 | D | 200 | CYC | NC-C4C-CHD-C1D |
| 5 | D | 200 | CYC | C2D-C1D-CHD-C4C |
| 5 | E | 200 | CYC | ND-C4D-CHA-C1A |
| 5 | E | 200 | CYC | C3D-C4D-CHA-C1A |
| 5 | E | 200 | CYC | NA-C4A-CHB-C1B |
| 5 | E | 200 | CYC | C3A-C4A-CHB-C1B |
| 5 | E | 200 | CYC | C2A-CAA-CBA-CGA |
| 5 | E | 200 | CYC | NC-C4C-CHD-C1D |
| 5 | E | 200 | CYC | ND-C1D-CHD-C4C |
| 5 | E | 200 | CYC | C2D-C1D-CHD-C4C |
| 5 | F | 200 | CYC | NA-C1A-CHA-C4D |
| 5 | F | 200 | CYC | C2A-C1A-CHA-C4D |
| 5 | F | 200 | CYC | NA-C4A-CHB-C1B |
| 5 | F | 200 | CYC | C3A-C4A-CHB-C1B |
| 5 | F | 200 | CYC | C2B-C3B-CAB-CBB |
| 5 | F | 200 | CYC | NC-C4C-CHD-C1D |
| 5 | F | 200 | CYC | ND-C1D-CHD-C4C |
| 5 | F | 200 | CYC | C2D-C1D-CHD-C4C |
| 5 | G | 200 | CYC | NA-C4A-CHB-C1B |
| 5 | G | 200 | CYC | C3A-C4A-CHB-C1B |
| 5 | G | 200 | CYC | NC-C4C-CHD-C1D |
| 5 | G | 200 | CYC | ND-C1D-CHD-C4C |
| 5 | G | 200 | CYC | C2D-C1D-CHD-C4C |
| 5 | G | 201 | CYC | NA-C1A-CHA-C4D |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 5 | G | 201 | CYC | ND-C4D-CHA-C1A |
| 5 | G | 201 | CYC | C3D-C4D-CHA-C1A |
| 5 | G | 201 | CYC | NA-C4A-CHB-C1B |
| 5 | G | 201 | CYC | C3A-C4A-CHB-C1B |
| 5 | G | 201 | CYC | C2C-C3C-CAC-CBC |
| 5 | G | 201 | CYC | C4C-C3C-CAC-CBC |
| 5 | G | 201 | CYC | NC-C4C-CHD-C1D |
| 5 | G | 201 | CYC | ND-C1D-CHD-C4C |
| 5 | G | 201 | CYC | C2D-C1D-CHD-C4C |
| 5 | H | 200 | CYC | NA-C4A-CHB-C1B |
| 5 | H | 200 | CYC | C2C-C3C-CAC-CBC |
| 5 | H | 200 | CYC | C4C-C3C-CAC-CBC |
| 5 | H | 200 | CYC | NC-C4C-CHD-C1D |
| 5 | H | 200 | CYC | ND-C1D-CHD-C4C |
| 5 | H | 201 | CYC | ND-C4D-CHA-C1A |
| 5 | H | 201 | CYC | C3D-C4D-CHA-C1A |
| 5 | H | 201 | CYC | NA-C4A-CHB-C1B |
| 5 | H | 201 | CYC | C3A-C4A-CHB-C1B |
| 5 | H | 201 | CYC | C2C-C3C-CAC-CBC |
| 5 | H | 201 | CYC | NC-C4C-CHD-C1D |
| 5 | H | 201 | CYC | ND-C1D-CHD-C4C |
| 5 | H | 201 | CYC | C2D-C1D-CHD-C4C |
| 5 | I | 200 | CYC | NA-C4A-CHB-C1B |
| 5 | I | 200 | CYC | C3A-C4A-CHB-C1B |
| 5 | I | 200 | CYC | C4C-C3C-CAC-CBC |
| 5 | I | 200 | CYC | NC-C4C-CHD-C1D |
| 5 | I | 200 | CYC | ND-C1D-CHD-C4C |
| 5 | I | 200 | CYC | C2D-C1D-CHD-C4C |
| 5 | I | 201 | CYC | NA-C4A-CHB-C1B |
| 5 | I | 201 | CYC | C3A-C4A-CHB-C1B |
| 5 | I | 201 | CYC | C2C-C3C-CAC-CBC |
| 5 | I | 201 | CYC | C4C-C3C-CAC-CBC |
| 5 | I | 201 | CYC | NC-C4C-CHD-C1D |
| 5 | I | 201 | CYC | ND-C1D-CHD-C4C |
| 5 | I | 201 | CYC | C2D-C1D-CHD-C4C |
| 5 | J | 200 | CYC | NA-C4A-CHB-C1B |
| 5 | J | 200 | CYC | C3A-C4A-CHB-C1B |
| 5 | J | 200 | CYC | C2C-C3C-CAC-CBC |
| 5 | J | 200 | CYC | C4C-C3C-CAC-CBC |
| 5 | J | 200 | CYC | NC-C4C-CHD-C1D |
| 5 | J | 200 | CYC | ND-C1D-CHD-C4C |
| 5 | J | 200 | CYC | C2D-C1D-CHD-C4C |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 5 | J | 201 | CYC | NA-C1A-CHA-C4D |
| 5 | J | 201 | CYC | C2A-C1A-CHA-C4D |
| 5 | J | 201 | CYC | ND-C4D-CHA-C1A |
| 5 | J | 201 | CYC | C3D-C4D-CHA-C1A |
| 5 | J | 201 | CYC | NA-C4A-CHB-C1B |
| 5 | J | 201 | CYC | C3A-C4A-CHB-C1B |
| 5 | J | 201 | CYC | C4B-C3B-CAB-CBB |
| 5 | J | 201 | CYC | C2C-C3C-CAC-CBC |
| 5 | J | 201 | CYC | NC-C4C-CHD-C1D |
| 5 | J | 201 | CYC | ND-C1D-CHD-C4C |
| 5 | J | 201 | CYC | C2D-C1D-CHD-C4C |
| 5 | K | 200 | CYC | ND-C4D-CHA-C1A |
| 5 | K | 200 | CYC | C3D-C4D-CHA-C1A |
| 5 | K | 200 | CYC | C3A-C4A-CHB-C1B |
| 5 | K | 200 | CYC | C2A-CAA-CBA-CGA |
| 5 | K | 200 | CYC | NC-C4C-CHD-C1D |
| 5 | K | 200 | CYC | ND-C1D-CHD-C4C |
| 5 | K | 200 | CYC | C2D-C1D-CHD-C4C |
| 5 | K | 201 | CYC | ND-C4D-CHA-C1A |
| 5 | K | 201 | CYC | NA-C4A-CHB-C1B |
| 5 | K | 201 | CYC | C2C-C3C-CAC-CBC |
| 5 | K | 201 | CYC | NC-C4C-CHD-C1D |
| 5 | K | 201 | CYC | ND-C1D-CHD-C4C |
| 5 | K | 201 | CYC | C2D-C1D-CHD-C4C |
| 5 | L | 201 | CYC | NA-C1A-CHA-C4D |
| 5 | L | 201 | CYC | C2A-C1A-CHA-C4D |
| 5 | L | 201 | CYC | ND-C4D-CHA-C1A |
| 5 | L | 201 | CYC | C3D-C4D-CHA-C1A |
| 5 | L | 201 | CYC | NA-C4A-CHB-C1B |
| 5 | L | 201 | CYC | NC-C4C-CHD-C1D |
| 5 | L | 201 | CYC | ND-C1D-CHD-C4C |
| 5 | L | 201 | CYC | C2D-C1D-CHD-C4C |
| 5 | L | 201 | CYC | C3D-CAD-CBD-CGD |
| 5 | N | 200 | CYC | NA-C4A-CHB-C1B |
| 5 | N | 200 | CYC | C3A-C4A-CHB-C1B |
| 5 | N | 200 | CYC | C4B-C3B-CAB-CBB |
| 5 | N | 200 | CYC | NC-C4C-CHD-C1D |
| 5 | N | 200 | CYC | ND-C1D-CHD-C4C |
| 5 | N | 200 | CYC | C2D-C1D-CHD-C4C |
| 5 | O | 200 | CYC | NA-C1A-CHA-C4D |
| 5 | O | 200 | CYC | C2A-C1A-CHA-C4D |
| 5 | O | 200 | CYC | ND-C4D-CHA-C1A |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 5 | O | 200 | CYC | C3D-C4D-CHA-C1A |
| 5 | O | 200 | CYC | C4B-C3B-CAB-CBB |
| 5 | O | 200 | CYC | NC-C4C-CHD-C1D |
| 5 | O | 200 | CYC | ND-C1D-CHD-C4C |
| 5 | O | 200 | CYC | C2D-C1D-CHD-C4C |
| 5 | P | 200 | CYC | NA-C4A-CHB-C1B |
| 5 | P | 200 | CYC | C3A-C4A-CHB-C1B |
| 5 | P | 200 | CYC | NC-C4C-CHD-C1D |
| 5 | P | 200 | CYC | ND-C1D-CHD-C4C |
| 5 | P | 200 | CYC | C2D-C1D-CHD-C4C |
| 5 | Q | 200 | CYC | NA-C4A-CHB-C1B |
| 5 | Q | 200 | CYC | C3A-C4A-CHB-C1B |
| 5 | Q | 200 | CYC | NC-C4C-CHD-C1D |
| 5 | Q | 200 | CYC | ND-C1D-CHD-C4C |
| 5 | Q | 200 | CYC | C2D-C1D-CHD-C4C |
| 5 | R | 200 | CYC | NA-C1A-CHA-C4D |
| 5 | R | 200 | CYC | C2A-C1A-CHA-C4D |
| 5 | R | 200 | CYC | ND-C4D-CHA-C1A |
| 5 | R | 200 | CYC | C3D-C4D-CHA-C1A |
| 5 | R | 200 | CYC | NA-C4A-CHB-C1B |
| 5 | R | 200 | CYC | NC-C4C-CHD-C1D |
| 5 | R | 200 | CYC | ND-C1D-CHD-C4C |
| 5 | R | 200 | CYC | C2D-C1D-CHD-C4C |
| 5 | S | 200 | CYC | NA-C1A-CHA-C4D |
| 5 | S | 200 | CYC | C2A-C1A-CHA-C4D |
| 5 | S | 200 | CYC | ND-C4D-CHA-C1A |
| 5 | S | 200 | CYC | C3D-C4D-CHA-C1A |
| 5 | S | 200 | CYC | NA-C4A-CHB-C1B |
| 5 | S | 200 | CYC | C3A-C4A-CHB-C1B |
| 5 | S | 200 | CYC | C2B-C3B-CAB-CBB |
| 5 | S | 200 | CYC | C4B-C3B-CAB-CBB |
| 5 | S | 200 | CYC | NC-C4C-CHD-C1D |
| 5 | S | 200 | CYC | ND-C1D-CHD-C4C |
| 5 | S | 200 | CYC | C2D-C1D-CHD-C4C |
| 5 | S | 200 | CYC | C2D-C3D-CAD-CBD |
| 5 | S | 200 | CYC | C4D-C3D-CAD-CBD |
| 5 | T | 200 | CYC | NA-C4A-CHB-C1B |
| 5 | T | 200 | CYC | C3A-C4A-CHB-C1B |
| 5 | T | 200 | CYC | NC-C4C-CHD-C1D |
| 5 | T | 200 | CYC | ND-C1D-CHD-C4C |
| 5 | T | 200 | CYC | C2D-C1D-CHD-C4C |
| 5 | T | 201 | CYC | NA-C1A-CHA-C4D |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 5 | T | 201 | CYC | C2A-C1A-CHA-C4D |
| 5 | T | 201 | CYC | ND-C4D-CHA-C1A |
| 5 | T | 201 | CYC | C3D-C4D-CHA-C1A |
| 5 | T | 201 | CYC | NA-C4A-CHB-C1B |
| 5 | T | 201 | CYC | C3A-C4A-CHB-C1B |
| 5 | T | 201 | CYC | NC-C4C-CHD-C1D |
| 5 | T | 201 | CYC | ND-C1D-CHD-C4C |
| 5 | T | 201 | CYC | C2D-C1D-CHD-C4C |
| 5 | U | 200 | CYC | NA-C4A-CHB-C1B |
| 5 | U | 200 | CYC | C3A-C4A-CHB-C1B |
| 5 | U | 200 | CYC | NC-C4C-CHD-C1D |
| 5 | U | 200 | CYC | ND-C1D-CHD-C4C |
| 5 | U | 200 | CYC | C2D-C1D-CHD-C4C |
| 5 | U | 201 | CYC | NA-C1A-CHA-C4D |
| 5 | U | 201 | CYC | C2A-C1A-CHA-C4D |
| 5 | U | 201 | CYC | ND-C4D-CHA-C1A |
| 5 | U | 201 | CYC | C3D-C4D-CHA-C1A |
| 5 | U | 201 | CYC | NA-C4A-CHB-C1B |
| 5 | U | 201 | CYC | C3A-C4A-CHB-C1B |
| 5 | U | 201 | CYC | C2C-C3C-CAC-CBC |
| 5 | U | 201 | CYC | C4C-C3C-CAC-CBC |
| 5 | U | 201 | CYC | NC-C4C-CHD-C1D |
| 5 | U | 201 | CYC | ND-C1D-CHD-C4C |
| 5 | V | 200 | CYC | NA-C1A-CHA-C4D |
| 5 | V | 200 | CYC | C2A-C1A-CHA-C4D |
| 5 | V | 200 | CYC | NA-C4A-CHB-C1B |
| 5 | V | 200 | CYC | C3A-C4A-CHB-C1B |
| 5 | V | 200 | CYC | NC-C4C-CHD-C1D |
| 5 | V | 200 | CYC | ND-C1D-CHD-C4C |
| 5 | V | 200 | CYC | C2D-C1D-CHD-C4C |
| 5 | V | 201 | CYC | NA-C4A-CHB-C1B |
| 5 | V | 201 | CYC | C3A-C4A-CHB-C1B |
| 5 | V | 201 | CYC | NC-C4C-CHD-C1D |
| 5 | V | 201 | CYC | ND-C1D-CHD-C4C |
| 5 | V | 201 | CYC | C2D-C1D-CHD-C4C |
| 5 | W | 200 | CYC | NA-C1A-CHA-C4D |
| 5 | W | 200 | CYC | ND-C4D-CHA-C1A |
| 5 | W | 200 | CYC | C3D-C4D-CHA-C1A |
| 5 | W | 200 | CYC | NA-C4A-CHB-C1B |
| 5 | W | 200 | CYC | C3A-C4A-CHB-C1B |
| 5 | W | 200 | CYC | C2C-C3C-CAC-CBC |
| 5 | W | 200 | CYC | C4C-C3C-CAC-CBC |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 5 | W | 200 | CYC | NC-C4C-CHD-C1D |
| 5 | W | 201 | CYC | ND-C4D-CHA-C1A |
| 5 | W | 201 | CYC | C3D-C4D-CHA-C1A |
| 5 | W | 201 | CYC | NC-C4C-CHD-C1D |
| 5 | W | 201 | CYC | ND-C1D-CHD-C4C |
| 5 | W | 201 | CYC | C2D-C1D-CHD-C4C |
| 5 | W | 201 | CYC | C3D-CAD-CBD-CGD |
| 5 | X | 200 | CYC | ND-C4D-CHA-C1A |
| 5 | X | 200 | CYC | C3D-C4D-CHA-C1A |
| 5 | X | 200 | CYC | C4C-C3C-CAC-CBC |
| 5 | X | 200 | CYC | NC-C4C-CHD-C1D |
| 5 | X | 200 | CYC | ND-C1D-CHD-C4C |
| 5 | X | 200 | CYC | C2D-C1D-CHD-C4C |
| 5 | X | 201 | CYC | NA-C4A-CHB-C1B |
| 5 | X | 201 | CYC | C3A-C4A-CHB-C1B |
| 5 | X | 201 | CYC | C2C-C3C-CAC-CBC |
| 5 | X | 201 | CYC | C4C-C3C-CAC-CBC |
| 5 | X | 201 | CYC | NC-C4C-CHD-C1D |
| 5 | X | 201 | CYC | ND-C1D-CHD-C4C |
| 5 | X | 201 | CYC | C2D-C1D-CHD-C4C |
| 5 | X | 201 | CYC | C3D-CAD-CBD-CGD |
| 5 | Y | 200 | CYC | NA-C4A-CHB-C1B |
| 5 | Y | 200 | CYC | C3A-C4A-CHB-C1B |
| 5 | Y | 200 | CYC | C2C-C3C-CAC-CBC |
| 5 | Y | 200 | CYC | C4C-C3C-CAC-CBC |
| 5 | Y | 200 | CYC | NC-C4C-CHD-C1D |
| 5 | Y | 200 | CYC | ND-C1D-CHD-C4C |
| 5 | Y | 200 | CYC | C2D-C1D-CHD-C4C |
| 5 | Y | 201 | CYC | NA-C1A-CHA-C4D |
| 5 | Y | 201 | CYC | C2A-C1A-CHA-C4D |
| 5 | Y | 201 | CYC | ND-C4D-CHA-C1A |
| 5 | Y | 201 | CYC | C3D-C4D-CHA-C1A |
| 5 | Y | 201 | CYC | C2C-C3C-CAC-CBC |
| 5 | Y | 201 | CYC | C4C-C3C-CAC-CBC |
| 5 | Y | 201 | CYC | NC-C4C-CHD-C1D |
| 5 | Y | 201 | CYC | ND-C1D-CHD-C4C |
| 5 | Y | 201 | CYC | C2D-C1D-CHD-C4C |
| 5 | a | 200 | CYC | NA-C1A-CHA-C4D |
| 5 | a | 200 | CYC | ND-C4D-CHA-C1A |
| 5 | a | 200 | CYC | C3D-C4D-CHA-C1A |
| 5 | a | 200 | CYC | C2B-C1B-CHB-C4A |
| 5 | a | 200 | CYC | C2C-C3C-CAC-CBC |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 5 | a | 200 | CYC | C4C-C3C-CAC-CBC |
| 5 | a | 200 | CYC | NC-C4C-CHD-C1D |
| 5 | a | 200 | CYC | ND-C1D-CHD-C4C |
| 5 | a | 200 | CYC | C2D-C1D-CHD-C4C |
| 5 | a | 200 | CYC | C2D-C3D-CAD-CBD |
| 5 | a | 200 | CYC | C4D-C3D-CAD-CBD |
| 5 | a | 200 | CYC | C3D-CAD-CBD-CGD |
| 5 | b | 200 | CYC | NA-C4A-CHB-C1B |
| 5 | b | 200 | CYC | C3A-C4A-CHB-C1B |
| 5 | b | 200 | CYC | C2C-C3C-CAC-CBC |
| 5 | b | 200 | CYC | C4C-C3C-CAC-CBC |
| 5 | b | 200 | CYC | NC-C4C-CHD-C1D |
| 5 | c | 200 | CYC | NA-C4A-CHB-C1B |
| 5 | c | 200 | CYC | C3A-C4A-CHB-C1B |
| 5 | c | 200 | CYC | NC-C4C-CHD-C1D |
| 5 | c | 200 | CYC | ND-C1D-CHD-C4C |
| 5 | c | 200 | CYC | C2D-C1D-CHD-C4C |
| 5 | c | 200 | CYC | C2D-C3D-CAD-CBD |
| 5 | c | 200 | CYC | C4D-C3D-CAD-CBD |
| 5 | d | 200 | CYC | NA-C1A-CHA-C4D |
| 5 | d | 200 | CYC | NA-C4A-CHB-C1B |
| 5 | d | 200 | CYC | C3A-C4A-CHB-C1B |
| 5 | d | 200 | CYC | C2C-C3C-CAC-CBC |
| 5 | d | 200 | CYC | C4C-C3C-CAC-CBC |
| 5 | d | 200 | CYC | NC-C4C-CHD-C1D |
| 5 | d | 200 | CYC | ND-C1D-CHD-C4C |
| 5 | d | 200 | CYC | C2D-C1D-CHD-C4C |
| 5 | e | 200 | CYC | NA-C1A-CHA-C4D |
| 5 | e | 200 | CYC | C2A-C1A-CHA-C4D |
| 5 | e | 200 | CYC | NA-C4A-CHB-C1B |
| 5 | e | 200 | CYC | C3A-C4A-CHB-C1B |
| 5 | e | 200 | CYC | C2B-C1B-CHB-C4A |
| 5 | e | 200 | CYC | C2C-C3C-CAC-CBC |
| 5 | e | 200 | CYC | C4C-C3C-CAC-CBC |
| 5 | e | 200 | CYC | NC-C4C-CHD-C1D |
| 5 | e | 200 | CYC | ND-C1D-CHD-C4C |
| 5 | e | 200 | CYC | C2D-C1D-CHD-C4C |
| 5 | f | 200 | CYC | NA-C1A-CHA-C4D |
| 5 | f | 200 | CYC | C2A-C1A-CHA-C4D |
| 5 | f | 200 | CYC | ND-C4D-CHA-C1A |
| 5 | f | 200 | CYC | C3D-C4D-CHA-C1A |
| 5 | f | 200 | CYC | NA-C4A-CHB-C1B |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 5 | f | 200 | CYC | C3A-C4A-CHB-C1B |
| 5 | f | 200 | CYC | C4C-C3C-CAC-CBC |
| 5 | f | 200 | CYC | NC-C4C-CHD-C1D |
| 5 | f | 200 | CYC | ND-C1D-CHD-C4C |
| 5 | f | 200 | CYC | C2D-C1D-CHD-C4C |
| 5 | f | 200 | CYC | C2D-C3D-CAD-CBD |
| 5 | f | 200 | CYC | C4D-C3D-CAD-CBD |
| 5 | f | 200 | CYC | C3D-CAD-CBD-CGD |
| 5 | g | 200 | CYC | NA-C4A-CHB-C1B |
| 5 | g | 200 | CYC | C3A-C4A-CHB-C1B |
| 5 | g | 200 | CYC | NB-C1B-CHB-C4A |
| 5 | g | 200 | CYC | C2B-C1B-CHB-C4A |
| 5 | g | 200 | CYC | NC-C4C-CHD-C1D |
| 5 | g | 200 | CYC | ND-C1D-CHD-C4C |
| 5 | g | 200 | CYC | C2D-C1D-CHD-C4C |
| 5 | g | 201 | CYC | NA-C1A-CHA-C4D |
| 5 | g | 201 | CYC | C2A-C1A-CHA-C4D |
| 5 | g | 201 | CYC | ND-C4D-CHA-C1A |
| 5 | g | 201 | CYC | C3D-C4D-CHA-C1A |
| 5 | g | 201 | CYC | NA-C4A-CHB-C1B |
| 5 | g | 201 | CYC | C3A-C4A-CHB-C1B |
| 5 | g | 201 | CYC | C2C-C3C-CAC-CBC |
| 5 | g | 201 | CYC | NC-C4C-CHD-C1D |
| 5 | g | 201 | CYC | ND-C1D-CHD-C4C |
| 5 | g | 201 | CYC | C2D-C1D-CHD-C4C |
| 5 | h | 200 | CYC | NA-C4A-CHB-C1B |
| 5 | h | 200 | CYC | C3A-C4A-CHB-C1B |
| 5 | h | 200 | CYC | C2C-C3C-CAC-CBC |
| 5 | h | 200 | CYC | C4C-C3C-CAC-CBC |
| 5 | h | 200 | CYC | NC-C4C-CHD-C1D |
| 5 | h | 200 | CYC | ND-C1D-CHD-C4C |
| 5 | h | 200 | CYC | C2D-C1D-CHD-C4C |
| 5 | h | 201 | CYC | NA-C1A-CHA-C4D |
| 5 | h | 201 | CYC | C2A-C1A-CHA-C4D |
| 5 | h | 201 | CYC | ND-C4D-CHA-C1A |
| 5 | h | 201 | CYC | C3D-C4D-CHA-C1A |
| 5 | h | 201 | CYC | NA-C4A-CHB-C1B |
| 5 | h | 201 | CYC | NC-C4C-CHD-C1D |
| 5 | h | 201 | CYC | C3D-CAD-CBD-CGD |
| 5 | i | 200 | CYC | NA-C1A-CHA-C4D |
| 5 | i | 200 | CYC | C2A-C1A-CHA-C4D |
| 5 | i | 200 | CYC | ND-C4D-CHA-C1A |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 5 | i | 200 | CYC | C3D-C4D-CHA-C1A |
| 5 | i | 200 | CYC | C3A-C4A-CHB-C1B |
| 5 | i | 200 | CYC | NB-C1B-CHB-C4A |
| 5 | i | 200 | CYC | C2B-C1B-CHB-C4A |
| 5 | i | 200 | CYC | NC-C4C-CHD-C1D |
| 5 | i | 200 | CYC | ND-C1D-CHD-C4C |
| 5 | i | 200 | CYC | C2D-C1D-CHD-C4C |
| 5 | i | 201 | CYC | NA-C4A-CHB-C1B |
| 5 | i | 201 | CYC | C3A-C4A-CHB-C1B |
| 5 | i | 201 | CYC | C4C-C3C-CAC-CBC |
| 5 | i | 201 | CYC | NC-C4C-CHD-C1D |
| 5 | i | 201 | CYC | ND-C1D-CHD-C4C |
| 5 | i | 201 | CYC | C2D-C1D-CHD-C4C |
| 5 | j | 200 | CYC | NA-C4A-CHB-C1B |
| 5 | j | 200 | CYC | C3A-C4A-CHB-C1B |
| 5 | j | 200 | CYC | C4C-C3C-CAC-CBC |
| 5 | j | 200 | CYC | NC-C4C-CHD-C1D |
| 5 | j | 200 | CYC | ND-C1D-CHD-C4C |
| 5 | j | 200 | CYC | C2D-C1D-CHD-C4C |
| 5 | j | 201 | CYC | NA-C4A-CHB-C1B |
| 5 | j | 201 | CYC | C3A-C4A-CHB-C1B |
| 5 | j | 201 | CYC | NC-C4C-CHD-C1D |
| 5 | j | 201 | CYC | ND-C1D-CHD-C4C |
| 5 | j | 201 | CYC | C2D-C1D-CHD-C4C |
| 5 | j | 201 | CYC | C3D-CAD-CBD-CGD |
| 5 | k | 200 | CYC | ND-C4D-CHA-C1A |
| 5 | k | 200 | CYC | C3D-C4D-CHA-C1A |
| 5 | k | 200 | CYC | NA-C4A-CHB-C1B |
| 5 | k | 200 | CYC | C3A-C4A-CHB-C1B |
| 5 | k | 200 | CYC | C2C-C3C-CAC-CBC |
| 5 | k | 200 | CYC | NC-C4C-CHD-C1D |
| 5 | k | 201 | CYC | NA-C4A-CHB-C1B |
| 5 | k | 201 | CYC | C3A-C4A-CHB-C1B |
| 5 | k | 201 | CYC | NC-C4C-CHD-C1D |
| 5 | k | 201 | CYC | ND-C1D-CHD-C4C |
| 5 | k | 201 | CYC | C2D-C1D-CHD-C4C |
| 5 | l | 201 | CYC | C2B-C1B-CHB-C4A |
| 5 | l | 201 | CYC | C2B-C3B-CAB-CBB |
| 5 | l | 201 | CYC | C4B-C3B-CAB-CBB |
| 5 | l | 201 | CYC | C2C-C3C-CAC-CBC |
| 5 | l | 201 | CYC | C4C-C3C-CAC-CBC |
| 5 | l | 201 | CYC | NC-C4C-CHD-C1D |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 5 | l | 201 | CYC | ND-C1D-CHD-C4C |
| 5 | l | 201 | CYC | C2D-C1D-CHD-C4C |
| 5 | l | 201 | CYC | C3D-CAD-CBD-CGD |
| 5 | J | 201 | CYC | C2B-C3B-CAB-CBB |
| 5 | N | 200 | CYC | C2B-C3B-CAB-CBB |
| 5 | O | 200 | CYC | C2B-C3B-CAB-CBB |
| 5 | W | 200 | CYC | C2B-C3B-CAB-CBB |
| 5 | H | 201 | CYC | C2B-C3B-CAB-CBB |
| 5 | e | 200 | CYC | NB-C1B-CHB-C4A |
| 5 | G | 200 | CYC | C2B-C3B-CAB-CBB |
| 5 | B | 200 | CYC | C2A-CAA-CBA-CGA |
| 5 | T | 200 | CYC | C2A-CAA-CBA-CGA |
| 5 | X | 201 | CYC | C2A-CAA-CBA-CGA |
| 5 | Y | 200 | CYC | C2A-CAA-CBA-CGA |
| 5 | a | 200 | CYC | C2A-CAA-CBA-CGA |
| 5 | c | 200 | CYC | C2A-CAA-CBA-CGA |
| 5 | j | 200 | CYC | C2A-CAA-CBA-CGA |
| 5 | H | 200 | CYC | C3A-C4A-CHB-C1B |
| 5 | K | 201 | CYC | C3A-C4A-CHB-C1B |
| 5 | R | 200 | CYC | C3A-C4A-CHB-C1B |
| 5 | h | 201 | CYC | C3A-C4A-CHB-C1B |
| 5 | A | 200 | CYC | C2B-C3B-CAB-CBB |
| 5 | W | 201 | CYC | NB-C1B-CHB-C4A |
| 5 | a | 200 | CYC | NB-C1B-CHB-C4A |
| 5 | l | 201 | CYC | NB-C1B-CHB-C4A |
| 5 | W | 201 | CYC | C2B-C1B-CHB-C4A |
| 5 | h | 200 | CYC | C2B-C3B-CAB-CBB |
| 5 | A | 200 | CYC | C3D-CAD-CBD-CGD |
| 5 | C | 200 | CYC | C3D-CAD-CBD-CGD |
| 5 | G | 200 | CYC | C3D-CAD-CBD-CGD |
| 5 | I | 201 | CYC | C3D-CAD-CBD-CGD |
| 5 | J | 201 | CYC | C3D-CAD-CBD-CGD |
| 5 | Q | 200 | CYC | C3D-CAD-CBD-CGD |
| 5 | R | 200 | CYC | C3D-CAD-CBD-CGD |
| 5 | T | 201 | CYC | C3D-CAD-CBD-CGD |
| 5 | i | 201 | CYC | C3D-CAD-CBD-CGD |
| 5 | k | 201 | CYC | C3D-CAD-CBD-CGD |
| 5 | D | 200 | CYC | NA-C1A-CHA-C4D |
| 5 | E | 200 | CYC | NA-C1A-CHA-C4D |
| 5 | G | 200 | CYC | NA-C1A-CHA-C4D |
| 5 | H | 201 | CYC | NA-C1A-CHA-C4D |
| 5 | K | 201 | CYC | NA-C1A-CHA-C4D |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 5 | c | 200 | CYC | NA-C1A-CHA-C4D |
| 5 | i | 201 | CYC | NA-C1A-CHA-C4D |
| 5 | l | 201 | CYC | NA-C1A-CHA-C4D |
| 5 | F | 200 | CYC | C4B-C3B-CAB-CBB |
| 5 | H | 201 | CYC | C4B-C3B-CAB-CBB |
| 5 | W | 200 | CYC | C4B-C3B-CAB-CBB |
| 5 | B | 200 | CYC | C2B-C3B-CAB-CBB |
| 5 | H | 200 | CYC | NB-C1B-CHB-C4A |
| 5 | V | 200 | CYC | NB-C1B-CHB-C4A |
| 5 | Y | 201 | CYC | NB-C1B-CHB-C4A |
| 5 | i | 201 | CYC | NB-C1B-CHB-C4A |
| 5 | H | 200 | CYC | C2B-C1B-CHB-C4A |
| 5 | c | 200 | CYC | C2B-C3B-CAB-CBB |
| 5 | A | 200 | CYC | C2A-CAA-CBA-CGA |
| 5 | I | 200 | CYC | C2A-CAA-CBA-CGA |
| 5 | J | 201 | CYC | C2A-CAA-CBA-CGA |
| 5 | K | 200 | CYC | NA-C4A-CHB-C1B |
| 5 | S | 200 | CYC | C2A-CAA-CBA-CGA |
| 5 | X | 200 | CYC | C2A-CAA-CBA-CGA |
| 5 | f | 200 | CYC | C2A-CAA-CBA-CGA |
| 5 | h | 201 | CYC | C2A-CAA-CBA-CGA |
| 5 | O | 200 | CYC | C3A-C4A-CHB-C1B |
| 5 | D | 200 | CYC | C2B-C3B-CAB-CBB |
| 5 | C | 200 | CYC | C2B-C3B-CAB-CBB |
| 5 | P | 200 | CYC | C2B-C3B-CAB-CBB |
| 5 | O | 200 | CYC | NA-C4A-CHB-C1B |
| 5 | W | 201 | CYC | NA-C4A-CHB-C1B |
| 5 | X | 200 | CYC | NA-C4A-CHB-C1B |
| 5 | Y | 201 | CYC | NA-C4A-CHB-C1B |
| 5 | a | 200 | CYC | NA-C4A-CHB-C1B |
| 5 | e | 200 | CYC | C2A-CAA-CBA-CGA |
| 5 | i | 200 | CYC | NA-C4A-CHB-C1B |
| 5 | l | 201 | CYC | NA-C4A-CHB-C1B |
| 5 | J | 200 | CYC | C2B-C3B-CAB-CBB |
| 5 | L | 201 | CYC | C2B-C3B-CAB-CBB |
| 5 | L | 201 | CYC | C3A-C4A-CHB-C1B |
| 5 | W | 201 | CYC | C3A-C4A-CHB-C1B |
| 5 | X | 200 | CYC | C3A-C4A-CHB-C1B |
| 5 | Y | 201 | CYC | C3A-C4A-CHB-C1B |
| 5 | a | 200 | CYC | C3A-C4A-CHB-C1B |
| 5 | l | 201 | CYC | C3A-C4A-CHB-C1B |
| 5 | V | 200 | CYC | C2B-C1B-CHB-C4A |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 5 | Y | 201 | CYC | C2B-C1B-CHB-C4A |
| 5 | i | 201 | CYC | C2B-C1B-CHB-C4A |
| 5 | a | 200 | CYC | C2B-C3B-CAB-CBB |
| 5 | X | 201 | CYC | NB-C1B-CHB-C4A |
| 5 | N | 200 | CYC | C2A-CAA-CBA-CGA |
| 5 | P | 200 | CYC | C2A-CAA-CBA-CGA |
| 5 | b | 200 | CYC | C2A-CAA-CBA-CGA |
| 5 | h | 200 | CYC | C2A-CAA-CBA-CGA |
| 5 | D | 200 | CYC | C2A-C1A-CHA-C4D |
| 5 | G | 201 | CYC | C2A-C1A-CHA-C4D |
| 5 | W | 200 | CYC | C2A-C1A-CHA-C4D |
| 5 | a | 200 | CYC | C2A-C1A-CHA-C4D |
| 5 | d | 200 | CYC | C2A-C1A-CHA-C4D |
| 5 | 5 | 1201 | CYC | C2C-C3C-CAC-CBC |
| 5 | B | 200 | CYC | C3D-CAD-CBD-CGD |
| 5 | I | 200 | CYC | C2C-C3C-CAC-CBC |
| 5 | V | 201 | CYC | C3D-CAD-CBD-CGD |
| 5 | i | 201 | CYC | C2C-C3C-CAC-CBC |
| 5 | j | 200 | CYC | C2C-C3C-CAC-CBC |
| 5 | A | 200 | CYC | NA-C1A-CHA-C4D |
| 5 | G | 200 | CYC | C4B-C3B-CAB-CBB |
| 5 | H | 200 | CYC | C2B-C3B-CAB-CBB |
| 5 | U | 201 | CYC | C2A-CAA-CBA-CGA |
| 5 | K | 200 | CYC | NB-C1B-CHB-C4A |
| 5 | E | 200 | CYC | C2A-C1A-CHA-C4D |
| 5 | H | 201 | CYC | C2A-C1A-CHA-C4D |
| 5 | K | 201 | CYC | C2A-C1A-CHA-C4D |
| 5 | c | 200 | CYC | C2A-C1A-CHA-C4D |
| 5 | i | 201 | CYC | C2A-C1A-CHA-C4D |
| 5 | l | 201 | CYC | C2A-C1A-CHA-C4D |
| 5 | d | 200 | CYC | NB-C1B-CHB-C4A |
| 5 | F | 200 | CYC | C2A-CAA-CBA-CGA |
| 5 | i | 200 | CYC | C2A-CAA-CBA-CGA |
| 5 | k | 200 | CYC | C2A-CAA-CBA-CGA |
| 5 | 5 | 1201 | CYC | NA-C1A-CHA-C4D |
| 5 | X | 200 | CYC | NA-C1A-CHA-C4D |
| 5 | A | 200 | CYC | C4B-C3B-CAB-CBB |
| 5 | Y | 201 | CYC | C4B-C3B-CAB-CBB |
| 5 | X | 201 | CYC | C2B-C1B-CHB-C4A |
| 5 | U | 200 | CYC | C4C-C3C-CAC-CBC |
| 5 | k | 200 | CYC | C4C-C3C-CAC-CBC |
| 5 | X | 200 | CYC | NB-C1B-CHB-C4A |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 5 | K | 200 | CYC | C3D-CAD-CBD-CGD |
| 5 | h | 200 | CYC | C4B-C3B-CAB-CBB |
| 5 | X | 200 | CYC | C2C-C3C-CAC-CBC |
| 5 | k | 200 | CYC | C3D-CAD-CBD-CGD |
| 5 | g | 201 | CYC | NB-C1B-CHB-C4A |
| 5 | T | 200 | CYC | NA-C1A-CHA-C4D |
| 5 | A | 200 | CYC | C2D-C3D-CAD-CBD |
| 5 | P | 200 | CYC | C2D-C3D-CAD-CBD |
| 5 | P | 200 | CYC | C4D-C3D-CAD-CBD |
| 5 | B | 200 | CYC | C4B-C3B-CAB-CBB |
| 5 | Y | 201 | CYC | C2B-C3B-CAB-CBB |
| 5 | C | 200 | CYC | C2A-CAA-CBA-CGA |
| 5 | G | 200 | CYC | C2A-C1A-CHA-C4D |
| 5 | H | 201 | CYC | C2A-CAA-CBA-CGA |
| 5 | c | 200 | CYC | C4B-C3B-CAB-CBB |
| 5 | V | 201 | CYC | C2B-C3B-CAB-CBB |
| 5 | A | 200 | CYC | CAA-CBA-CGA-O2A |
| 5 | C | 200 | CYC | CAA-CBA-CGA-O2A |
| 5 | J | 201 | CYC | CAD-CBD-CGD-O2D |
| 5 | a | 200 | CYC | CAA-CBA-CGA-O2A |
| 5 | l | 201 | CYC | CAA-CBA-CGA-O2A |
| 5 | I | 200 | CYC | CAA-CBA-CGA-O1A |
| 5 | P | 200 | CYC | CAA-CBA-CGA-O2A |
| 5 | V | 201 | CYC | CAD-CBD-CGD-O1D |
| 5 | Y | 201 | CYC | CAA-CBA-CGA-O2A |
| 5 | c | 200 | CYC | CAA-CBA-CGA-O2A |
| 5 | I | 201 | CYC | CAA-CBA-CGA-O1A |
| 5 | i | 201 | CYC | CAD-CBD-CGD-O2D |
| 5 | j | 200 | CYC | CAA-CBA-CGA-O1A |
| 5 | D | 200 | CYC | CAA-CBA-CGA-O1A |
| 5 | L | 201 | CYC | CAA-CBA-CGA-O1A |
| 5 | S | 200 | CYC | CAA-CBA-CGA-O1A |
| 5 | Y | 200 | CYC | CAA-CBA-CGA-O1A |
| 5 | b | 200 | CYC | CAD-CBD-CGD-O1D |
| 5 | d | 200 | CYC | CAD-CBD-CGD-O1D |
| 5 | H | 201 | CYC | CAD-CBD-CGD-O1D |
| 5 | N | 200 | CYC | CAA-CBA-CGA-O1A |
| 5 | e | 200 | CYC | CAD-CBD-CGD-O2D |
| 5 | g | 201 | CYC | CAD-CBD-CGD-O1D |
| 5 | N | 200 | CYC | C3D-CAD-CBD-CGD |
| 5 | 5 | 1202 | CYC | CAA-CBA-CGA-O2A |
| 5 | A | 200 | CYC | CAA-CBA-CGA-O1A |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 5 | D | 200 | CYC | CAA-CBA-CGA-O2A |
| 5 | V | 201 | CYC | CAA-CBA-CGA-O2A |
| 5 | Q | 200 | CYC | CAA-CBA-CGA-O2A |
| 5 | Y | 201 | CYC | CAA-CBA-CGA-O1A |
| 5 | 5 | 1202 | CYC | C2A-CAA-CBA-CGA |
| 5 | W | 200 | CYC | CAA-CBA-CGA-O1A |
| 5 | c | 200 | CYC | CAD-CBD-CGD-O1D |
| 5 | e | 200 | CYC | CAA-CBA-CGA-O1A |
| 5 | F | 200 | CYC | CAA-CBA-CGA-O1A |
| 5 | G | 201 | CYC | CAD-CBD-CGD-O2D |
| 5 | N | 200 | CYC | CAA-CBA-CGA-O2A |
| 5 | O | 200 | CYC | CAD-CBD-CGD-O1D |
| 5 | R | 200 | CYC | CAA-CBA-CGA-O1A |
| 5 | a | 200 | CYC | CAA-CBA-CGA-O1A |
| 5 | k | 201 | CYC | NB-C1B-CHB-C4A |
| 5 | L | 201 | CYC | CAA-CBA-CGA-O2A |
| 5 | W | 201 | CYC | CAD-CBD-CGD-O1D |
| 5 | Y | 200 | CYC | CAA-CBA-CGA-O2A |
| 5 | d | 200 | CYC | CAD-CBD-CGD-O2D |
| 5 | i | 201 | CYC | CAA-CBA-CGA-O1A |
| 5 | j | 200 | CYC | CAA-CBA-CGA-O2A |
| 5 | A | 200 | CYC | CAD-CBD-CGD-O1D |
| 5 | Q | 200 | CYC | CAA-CBA-CGA-O1A |
| 5 | T | 201 | CYC | CAA-CBA-CGA-O2A |
| 5 | H | 201 | CYC | CAD-CBD-CGD-O2D |
| 5 | T | 201 | CYC | CAA-CBA-CGA-O1A |
| 5 | U | 201 | CYC | CAA-CBA-CGA-O2A |
| 5 | h | 201 | CYC | CAD-CBD-CGD-O1D |
| 5 | i | 200 | CYC | CAA-CBA-CGA-O1A |
| 5 | J | 201 | CYC | CAA-CBA-CGA-O2A |
| 5 | J | 201 | CYC | CAD-CBD-CGD-O1D |
| 5 | i | 200 | CYC | CAA-CBA-CGA-O2A |
| 5 | C | 200 | CYC | CAA-CBA-CGA-O1A |
| 5 | E | 200 | CYC | CAA-CBA-CGA-O1A |
| 5 | I | 201 | CYC | CAA-CBA-CGA-O2A |
| 5 | J | 201 | CYC | CAA-CBA-CGA-O1A |
| 5 | U | 201 | CYC | CAA-CBA-CGA-O1A |
| 5 | b | 200 | CYC | CAD-CBD-CGD-O2D |
| 5 | e | 200 | CYC | CAD-CBD-CGD-O1D |
| 5 | g | 201 | CYC | CAD-CBD-CGD-O2D |
| 5 | G | 201 | CYC | CAD-CBD-CGD-O1D |
| 5 | V | 201 | CYC | CAA-CBA-CGA-O1A |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 5 | e | 200 | CYC | CAA-CBA-CGA-O2A |
| 5 | O | 200 | CYC | C2A-CAA-CBA-CGA |
| 5 | g | 201 | CYC | C2A-CAA-CBA-CGA |
| 5 | j | 201 | CYC | C2A-CAA-CBA-CGA |
| 5 | G | 200 | CYC | CAA-CBA-CGA-O1A |
| 5 | I | 200 | CYC | CAA-CBA-CGA-O2A |
| 5 | K | 201 | CYC | CAA-CBA-CGA-O1A |
| 5 | V | 201 | CYC | CAD-CBD-CGD-O2D |
| 5 | I | 200 | CYC | C2B-C3B-CAB-CBB |
| 5 | c | 200 | CYC | CAD-CBD-CGD-O2D |
| 5 | h | 200 | CYC | CAA-CBA-CGA-O2A |
| 5 | Q | 200 | CYC | CAD-CBD-CGD-O2D |
| 5 | S | 200 | CYC | CAA-CBA-CGA-O2A |
| 5 | W | 201 | CYC | CAD-CBD-CGD-O2D |
| 5 | d | 200 | CYC | CAA-CBA-CGA-O2A |
| 5 | i | 201 | CYC | CAA-CBA-CGA-O2A |
| 5 | X | 201 | CYC | CAD-CBD-CGD-O2D |
| 5 | Q | 200 | CYC | C1A-C2A-CAA-CBA |
| 5 | d | 200 | CYC | C2B-C1B-CHB-C4A |
| 5 | A | 200 | CYC | CAD-CBD-CGD-O2D |
| 5 | P | 200 | CYC | CAA-CBA-CGA-O1A |
| 5 | c | 200 | CYC | CAA-CBA-CGA-O1A |
| 5 | h | 200 | CYC | CAA-CBA-CGA-O1A |
| 5 | i | 201 | CYC | CAD-CBD-CGD-O1D |
| 5 | j | 201 | CYC | CAD-CBD-CGD-O2D |
| 5 | l | 201 | CYC | CAA-CBA-CGA-O1A |
| 5 | G | 200 | CYC | CAA-CBA-CGA-O2A |
| 5 | W | 200 | CYC | CAA-CBA-CGA-O2A |
| 5 | k | 200 | CYC | C3A-C2A-CAA-CBA |
| 5 | F | 200 | CYC | CAA-CBA-CGA-O2A |
| 5 | K | 201 | CYC | CAA-CBA-CGA-O2A |
| 5 | O | 200 | CYC | CAA-CBA-CGA-O2A |
| 5 | d | 200 | CYC | CAA-CBA-CGA-O1A |
| 5 | E | 200 | CYC | CAD-CBD-CGD-O1D |
| 5 | H | 201 | CYC | C4C-C3C-CAC-CBC |
| 5 | K | 201 | CYC | C2A-CAA-CBA-CGA |
| 5 | T | 201 | CYC | CAD-CBD-CGD-O2D |
| 5 | X | 201 | CYC | CAD-CBD-CGD-O1D |
| 5 | Q | 200 | CYC | C3A-C2A-CAA-CBA |
| 5 | V | 200 | CYC | CAA-CBA-CGA-O2A |
| 5 | j | 201 | CYC | CAD-CBD-CGD-O1D |
| 5 | F | 200 | CYC | CAD-CBD-CGD-O2D |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 5 | Q | 200 | CYC | CAD-CBD-CGD-O1D |
| 5 | T | 200 | CYC | CAA-CBA-CGA-O2A |
| 5 | O | 200 | CYC | CAD-CBD-CGD-O2D |
| 5 | k | 200 | CYC | C1A-C2A-CAA-CBA |
| 5 | O | 200 | CYC | CAA-CBA-CGA-O1A |
| 5 | 5 | 1202 | CYC | CAA-CBA-CGA-O1A |
| 5 | 5 | 1202 | CYC | CAD-CBD-CGD-O2D |
| 5 | T | 201 | CYC | CAD-CBD-CGD-O1D |
| 5 | U | 201 | CYC | CAD-CBD-CGD-O1D |
| 5 | X | 200 | CYC | CAA-CBA-CGA-O2A |
| 5 | D | 200 | CYC | CAD-CBD-CGD-O1D |
| 5 | F | 200 | CYC | CAD-CBD-CGD-O1D |
| 5 | K | 201 | CYC | CAD-CBD-CGD-O2D |
| 5 | R | 200 | CYC | CAA-CBA-CGA-O2A |
| 5 | T | 200 | CYC | CAA-CBA-CGA-O1A |
| 5 | V | 200 | CYC | CAA-CBA-CGA-O1A |
| 5 | K | 200 | CYC | C2B-C1B-CHB-C4A |
| 5 | b | 200 | CYC | NA-C1A-CHA-C4D |
| 5 | K | 201 | CYC | CAD-CBD-CGD-O1D |
| 5 | X | 200 | CYC | CAA-CBA-CGA-O1A |
| 5 | D | 200 | CYC | CAD-CBD-CGD-O2D |
| 5 | E | 200 | CYC | CAA-CBA-CGA-O2A |
| 5 | H | 201 | CYC | CAA-CBA-CGA-O1A |
| 5 | h | 201 | CYC | CAD-CBD-CGD-O2D |
| 5 | U | 201 | CYC | CAD-CBD-CGD-O2D |
| 5 | f | 200 | CYC | CAA-CBA-CGA-O2A |
| 5 | B | 200 | CYC | CAD-CBD-CGD-O2D |
| 5 | H | 200 | CYC | CAA-CBA-CGA-O2A |
| 5 | g | 201 | CYC | C2B-C1B-CHB-C4A |
| 5 | 5 | 1202 | CYC | CAD-CBD-CGD-O1D |
| 5 | Y | 201 | CYC | C2A-CAA-CBA-CGA |
| 5 | E | 200 | CYC | CAD-CBD-CGD-O2D |
| 5 | C | 200 | CYC | C4B-C3B-CAB-CBB |
| 5 | D | 200 | CYC | C4B-C3B-CAB-CBB |
| 5 | H | 200 | CYC | CAA-CBA-CGA-O1A |
| 5 | H | 201 | CYC | CAA-CBA-CGA-O2A |
| 5 | f | 200 | CYC | CAA-CBA-CGA-O1A |
| 5 | K | 200 | CYC | CAA-CBA-CGA-O2A |
| 5 | R | 200 | CYC | CAD-CBD-CGD-O2D |
| 5 | e | 200 | CYC | C2B-C3B-CAB-CBB |
| 5 | K | 200 | CYC | CAA-CBA-CGA-O1A |
| 5 | R | 200 | CYC | CAD-CBD-CGD-O1D |

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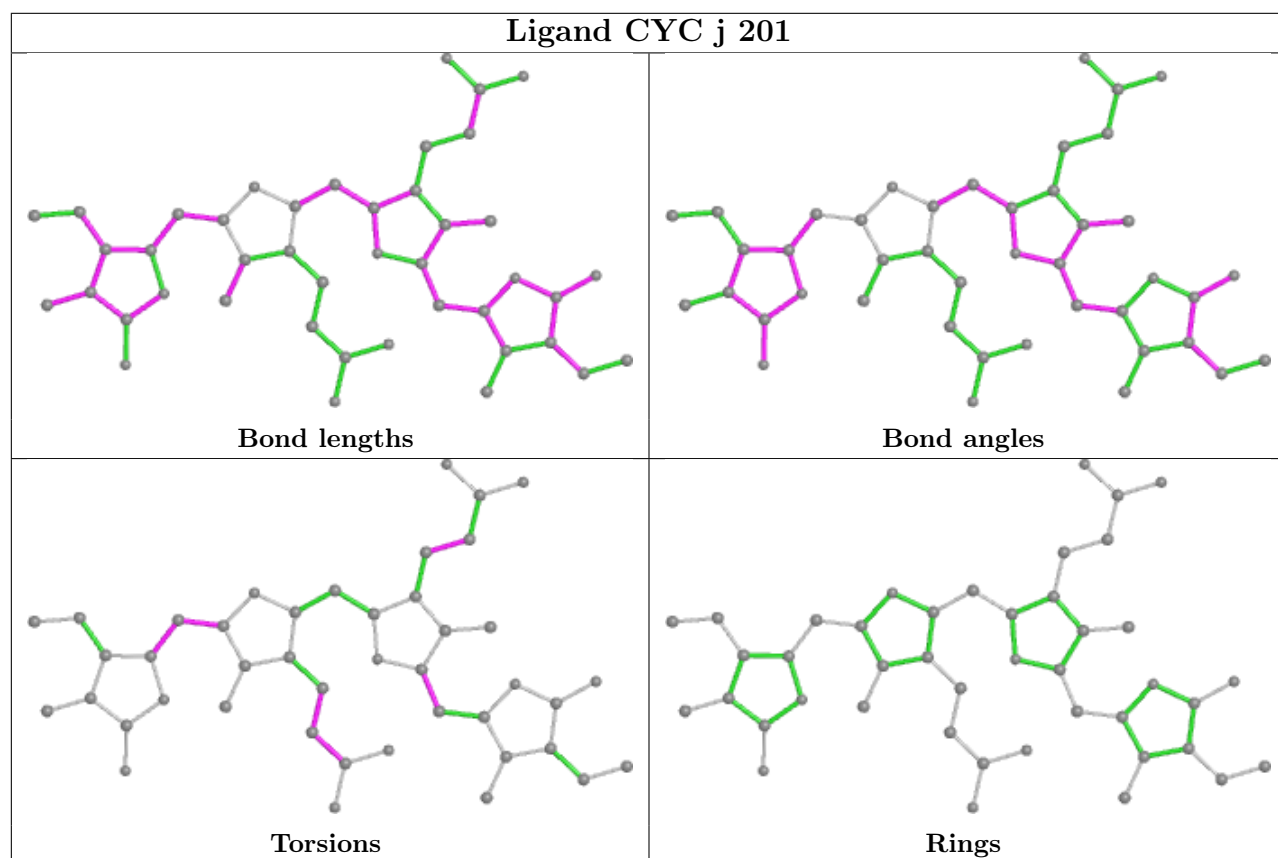
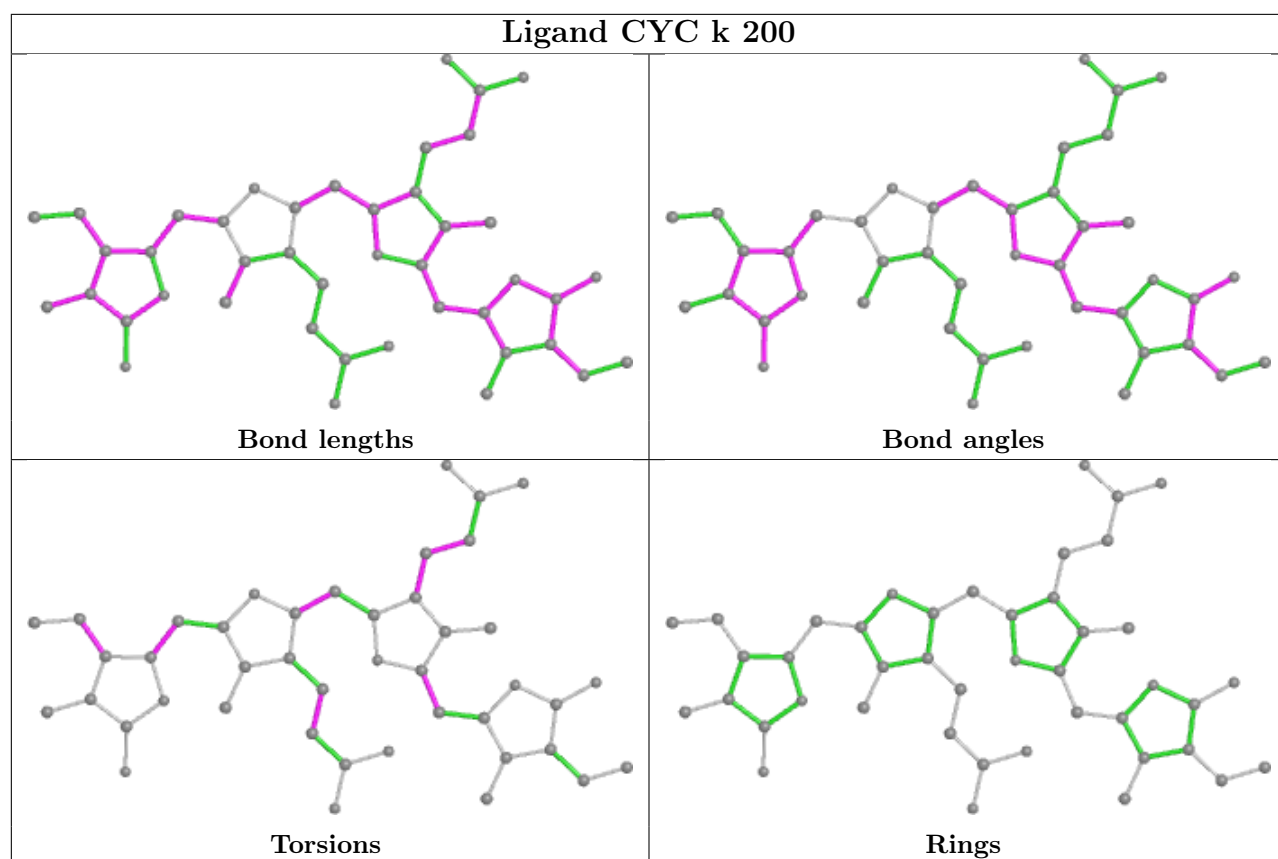
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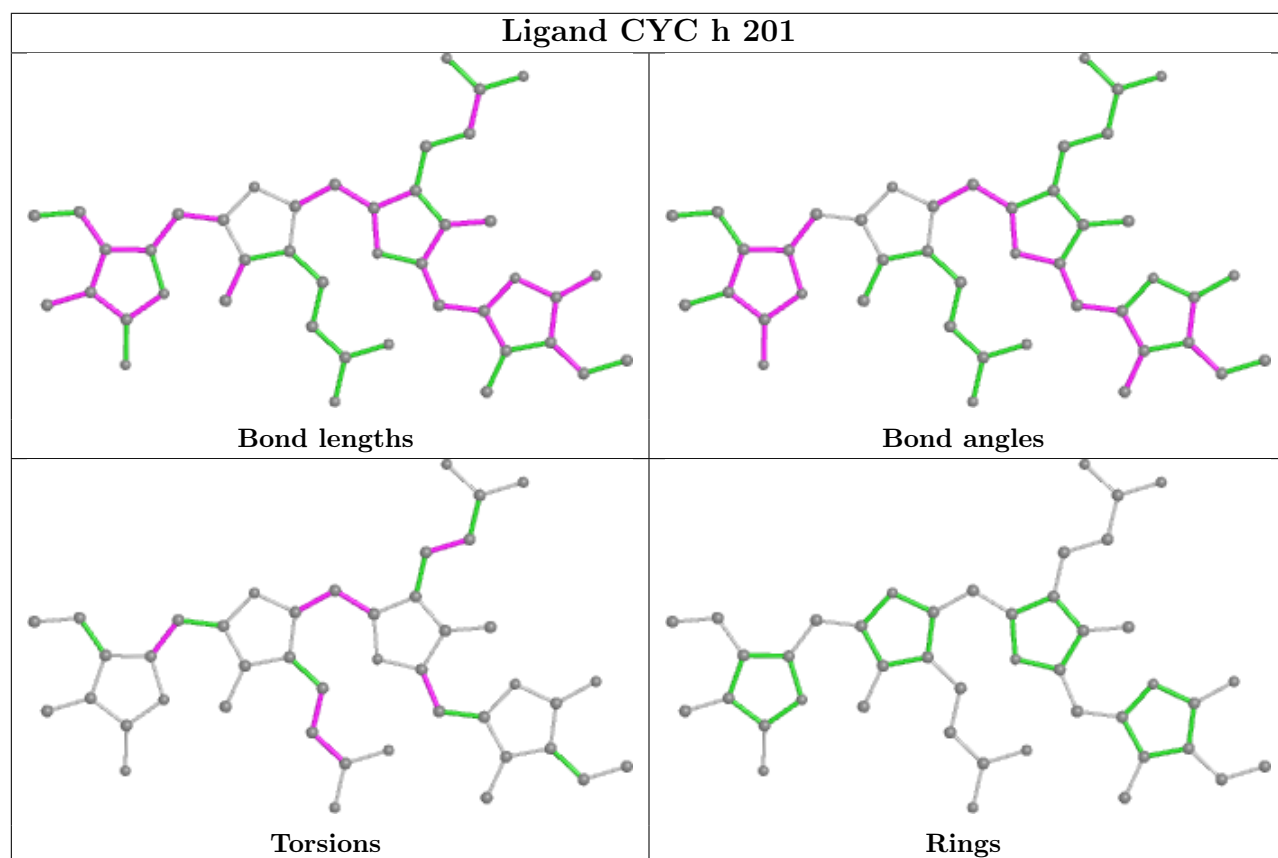
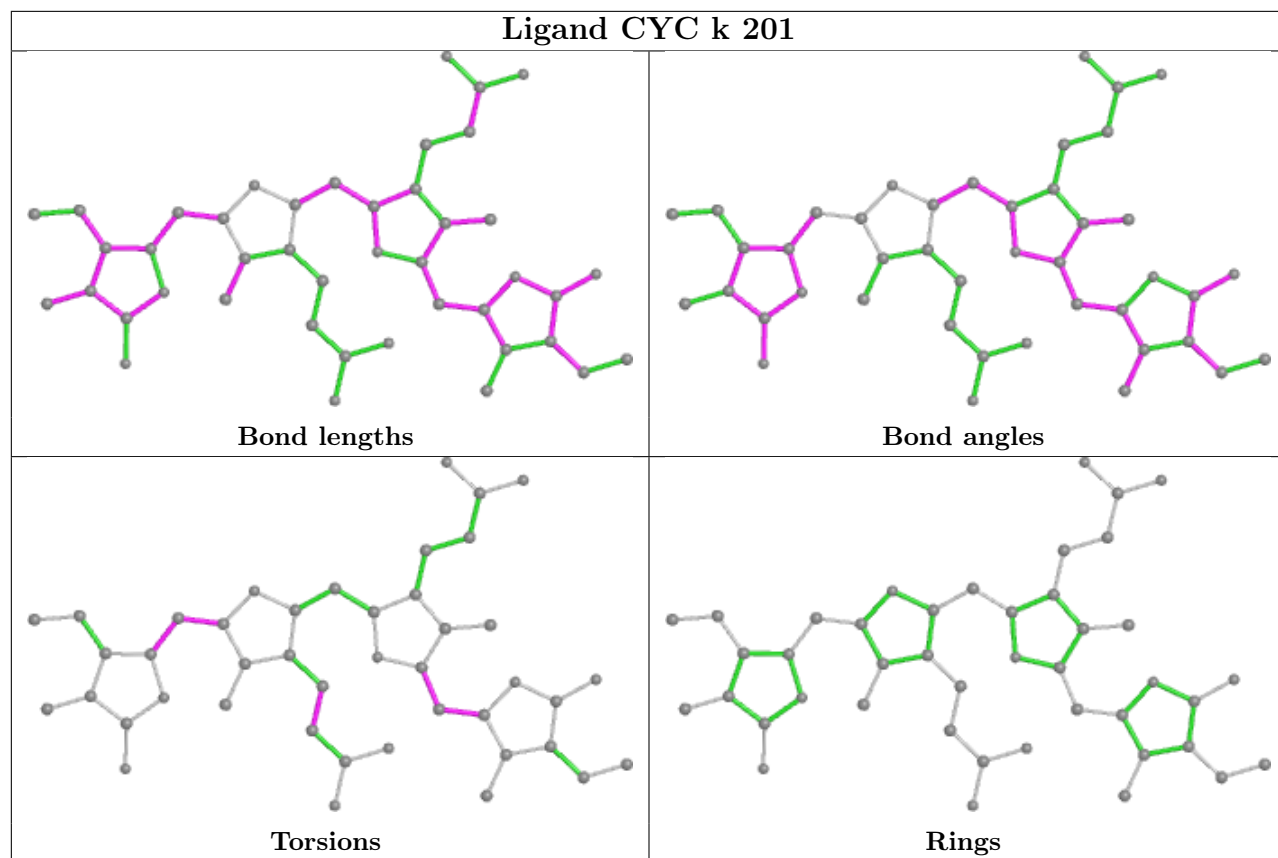
| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 5 | c | 200 | CYC | NB-C1B-CHB-C4A |
| 5 | B | 200 | CYC | CAD-CBD-CGD-O1D |
| 5 | G | 201 | CYC | C2B-C3B-CAB-CBB |
| 5 | U | 201 | CYC | C3D-CAD-CBD-CGD |
| 5 | d | 200 | CYC | C3D-CAD-CBD-CGD |
| 5 | K | 201 | CYC | C2B-C3B-CAB-CBB |
| 5 | I | 201 | CYC | CAD-CBD-CGD-O1D |
| 5 | D | 200 | CYC | C2A-CAA-CBA-CGA |
| 5 | N | 200 | CYC | CAD-CBD-CGD-O2D |

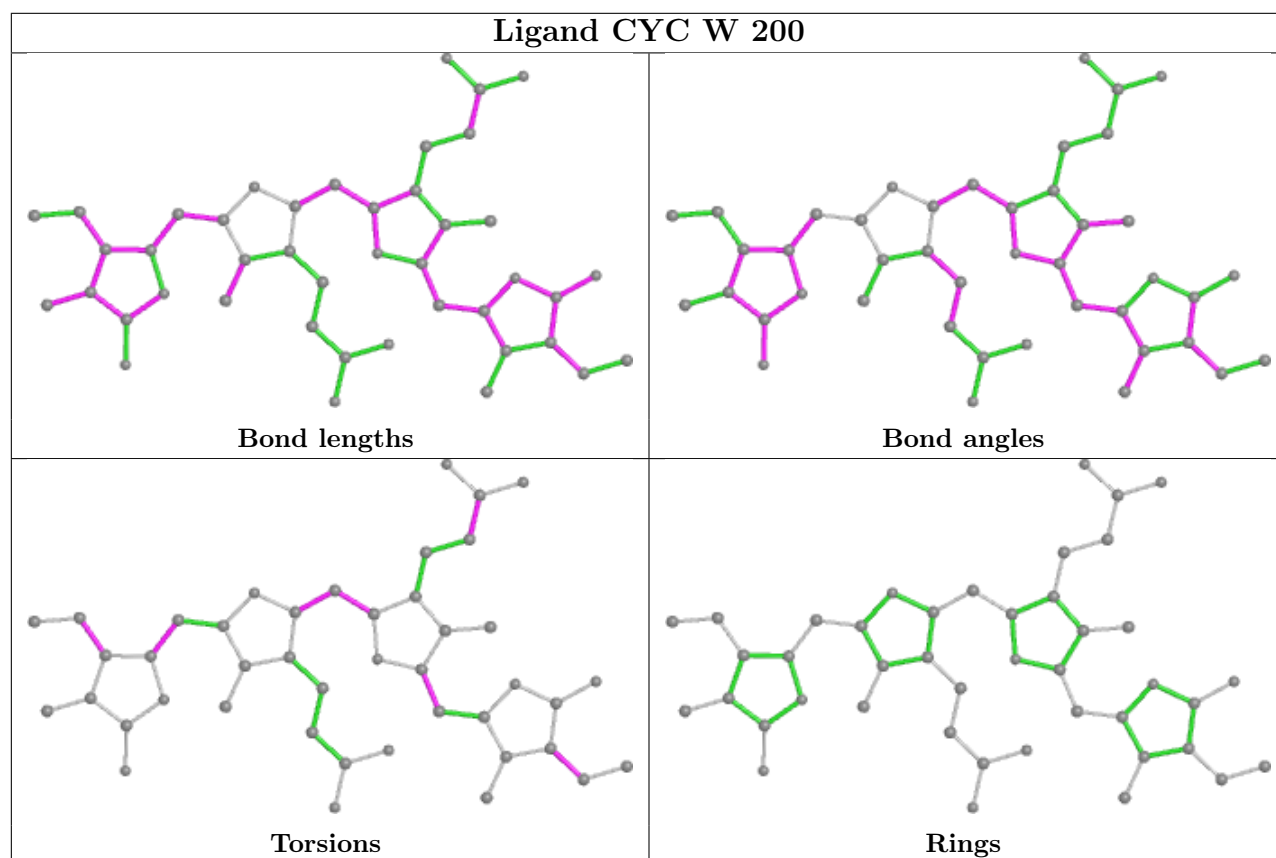
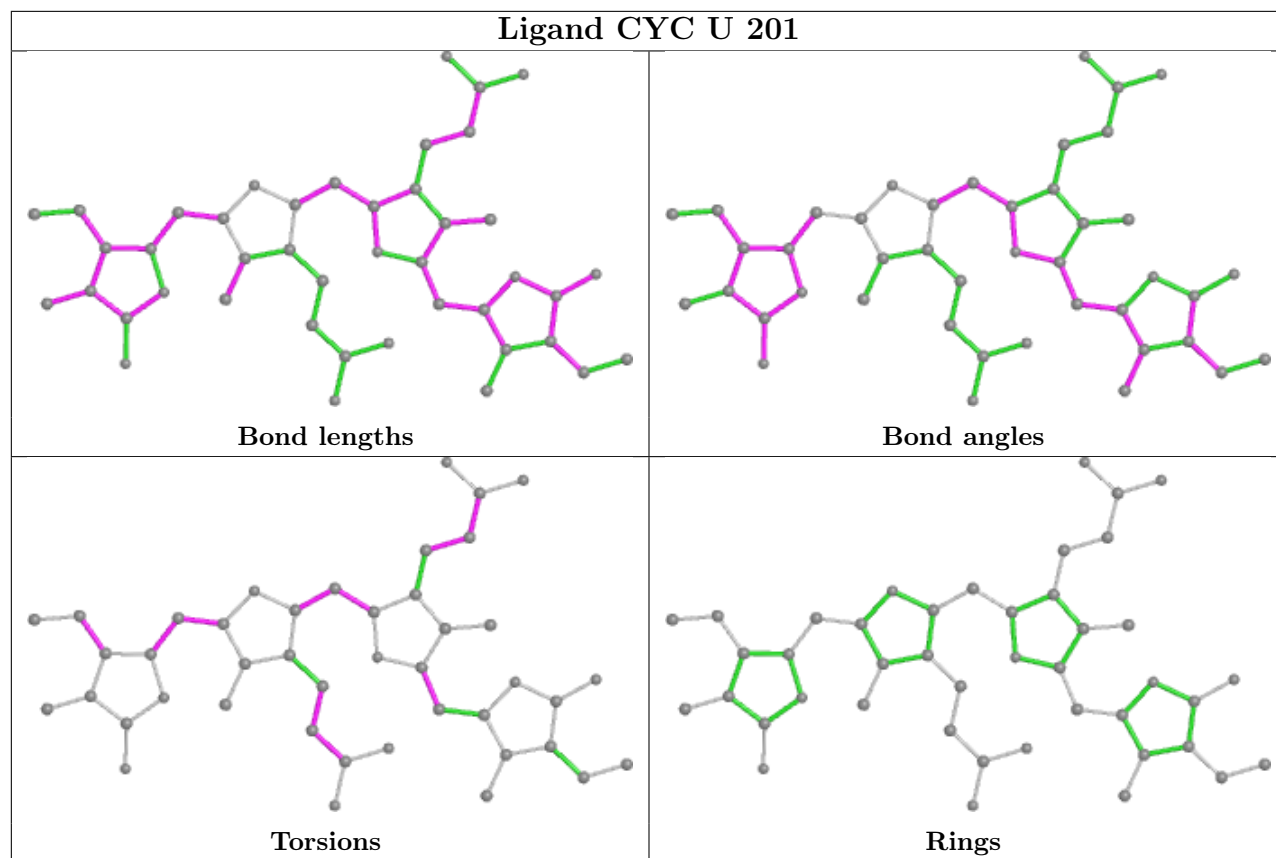
There are no ring outliers.

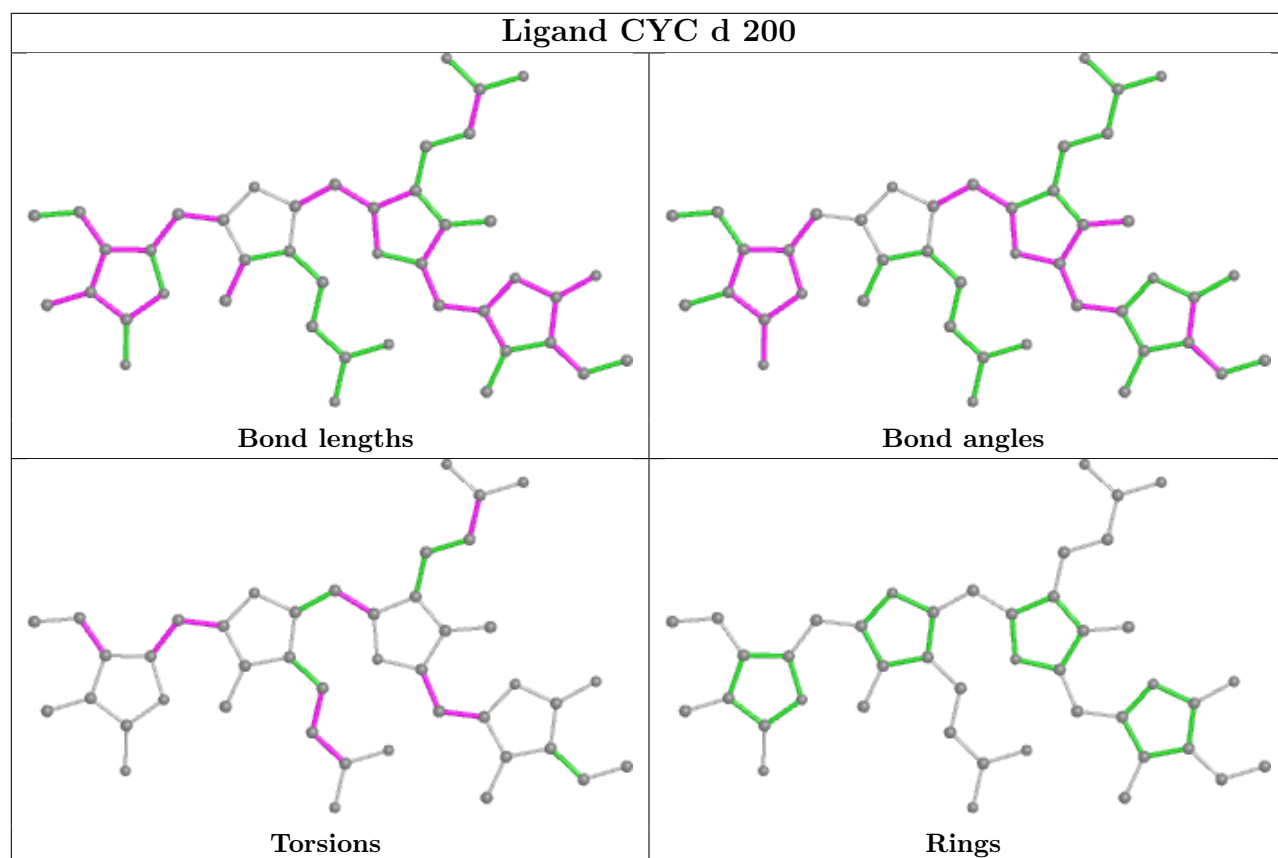
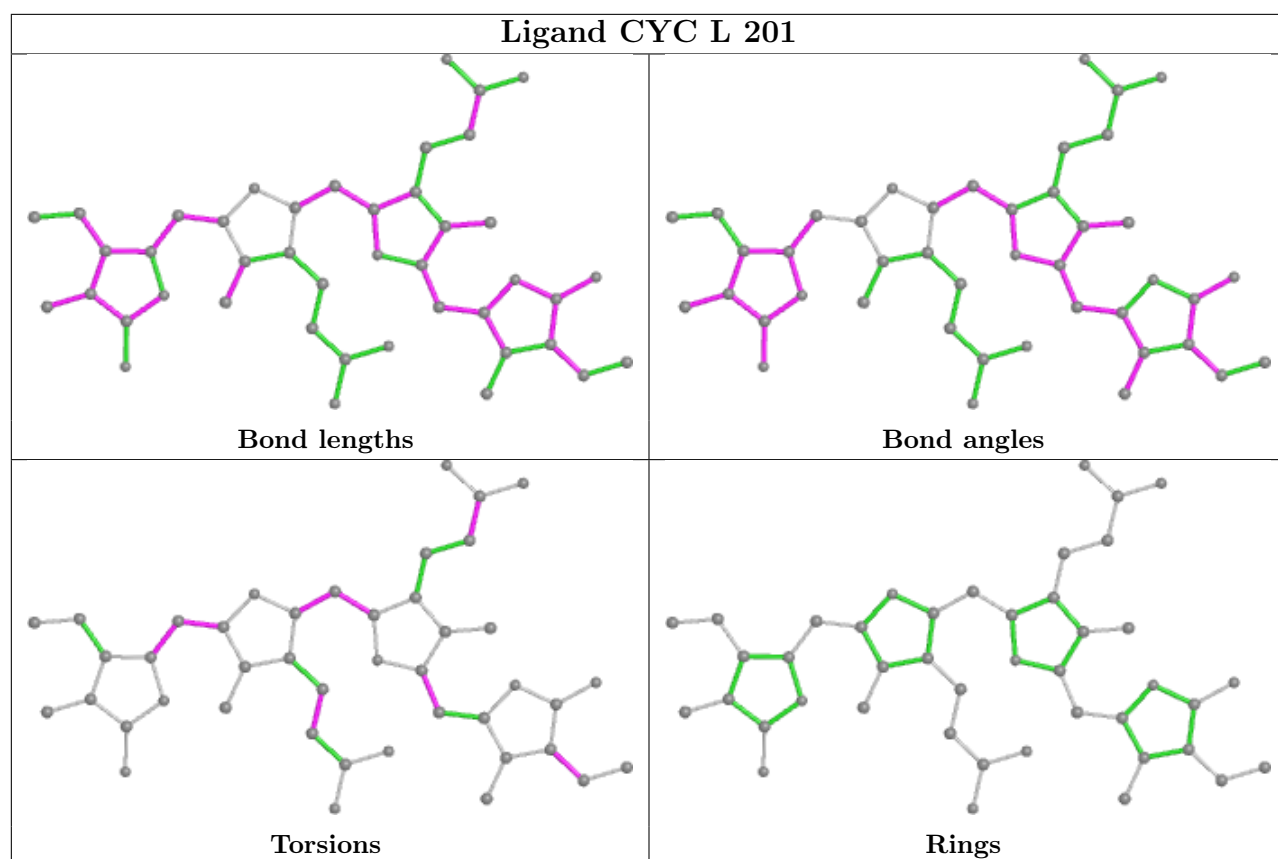
No monomer is involved in short contacts.

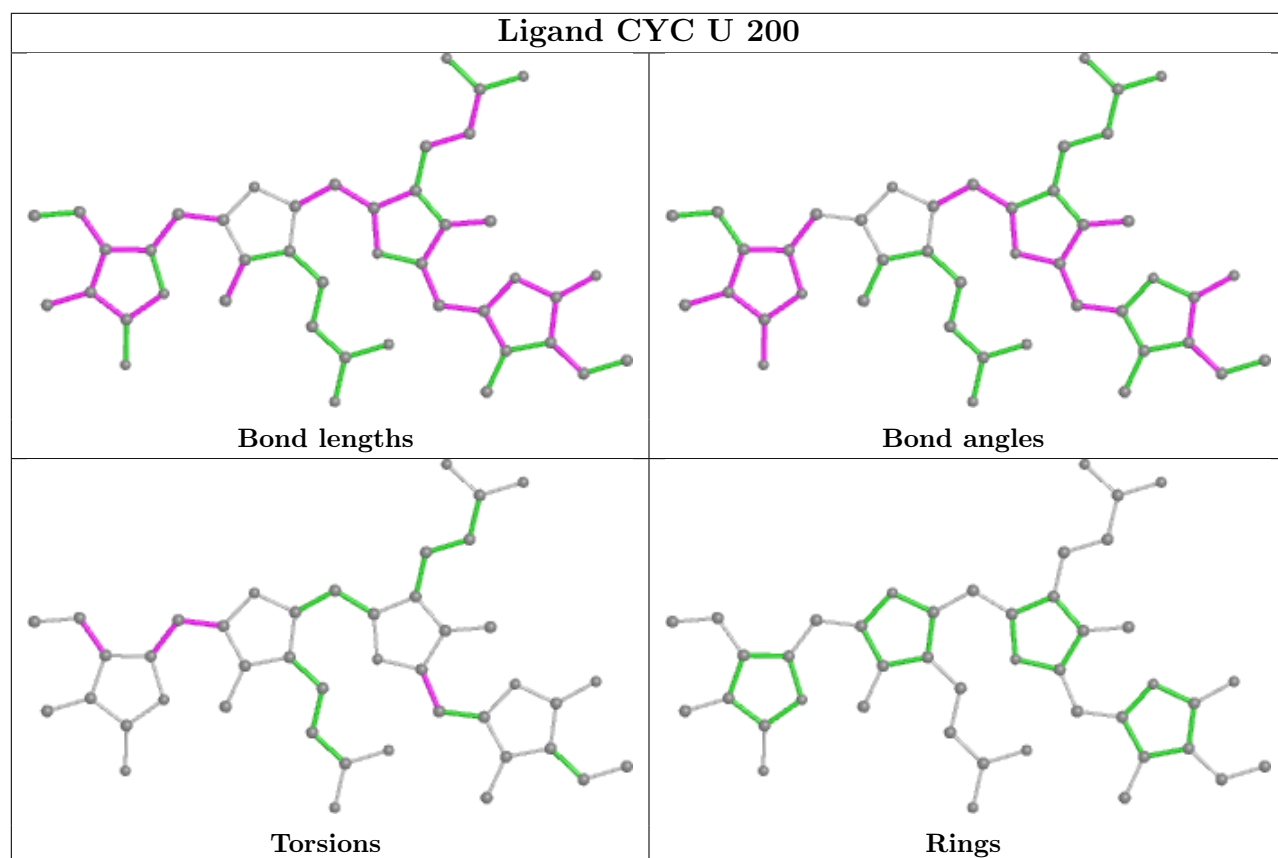
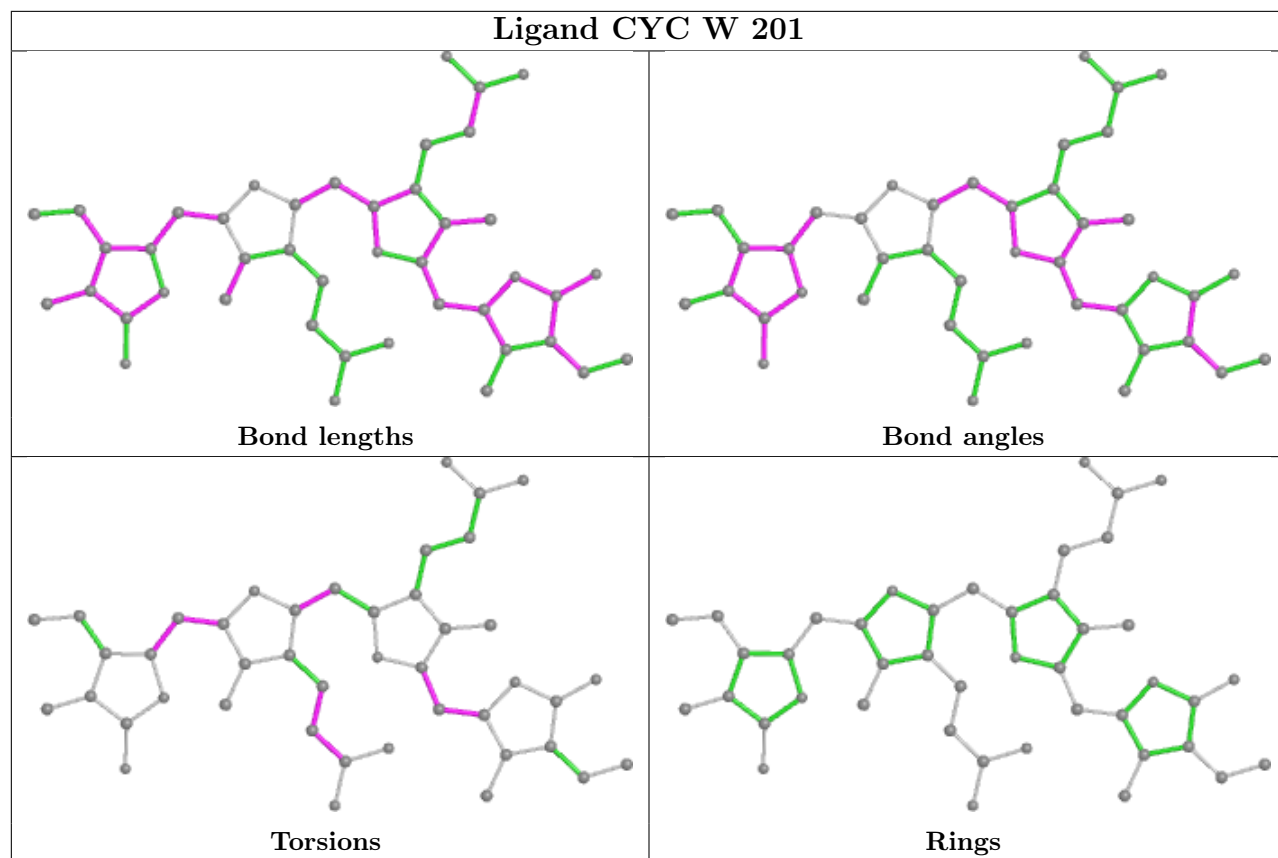
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

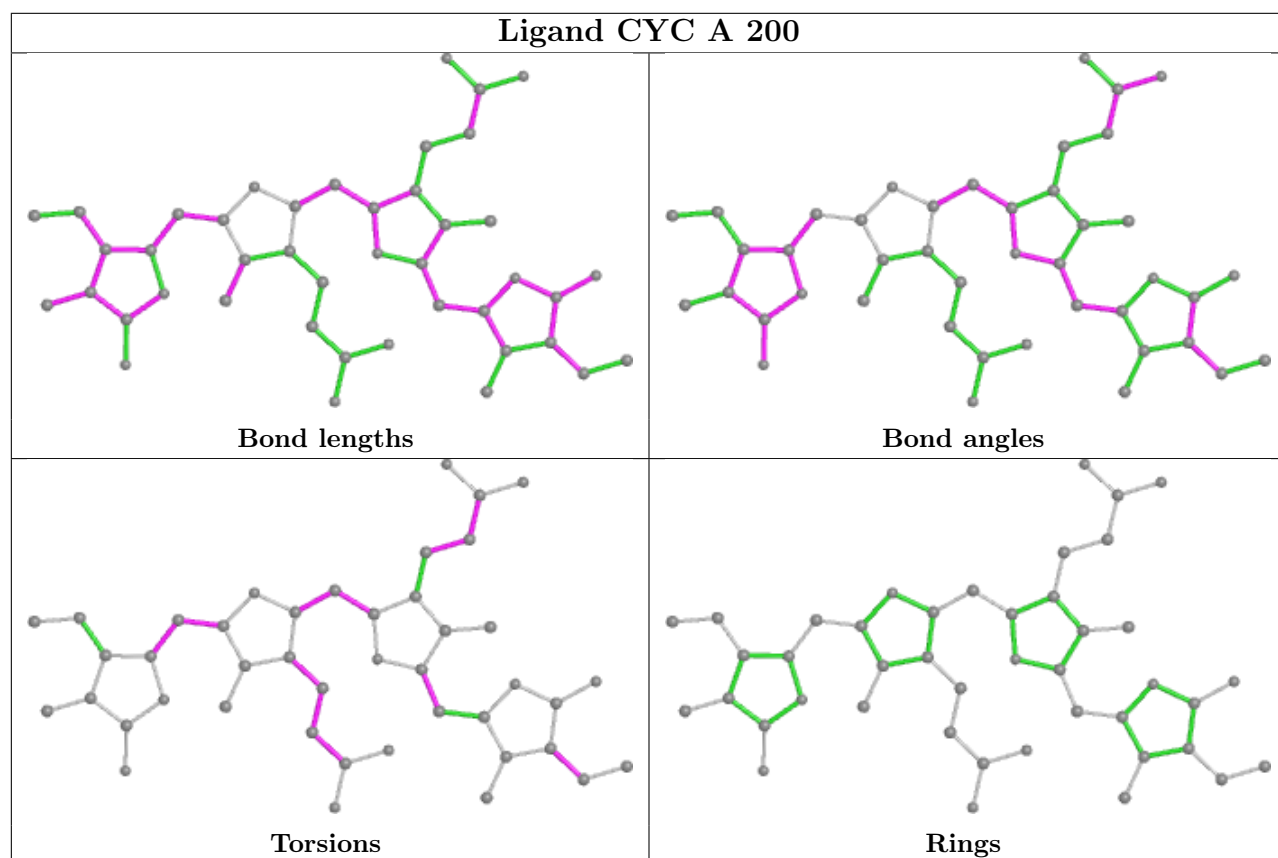
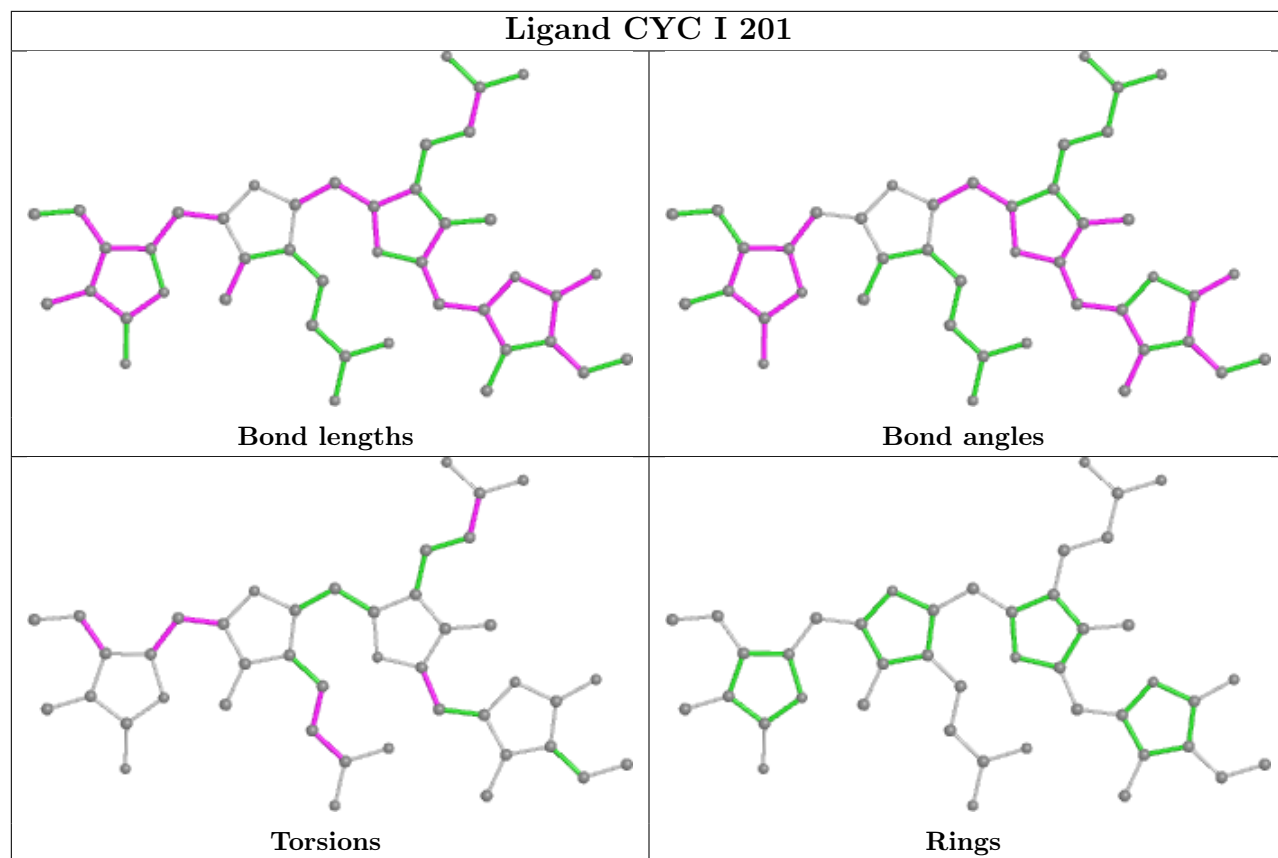


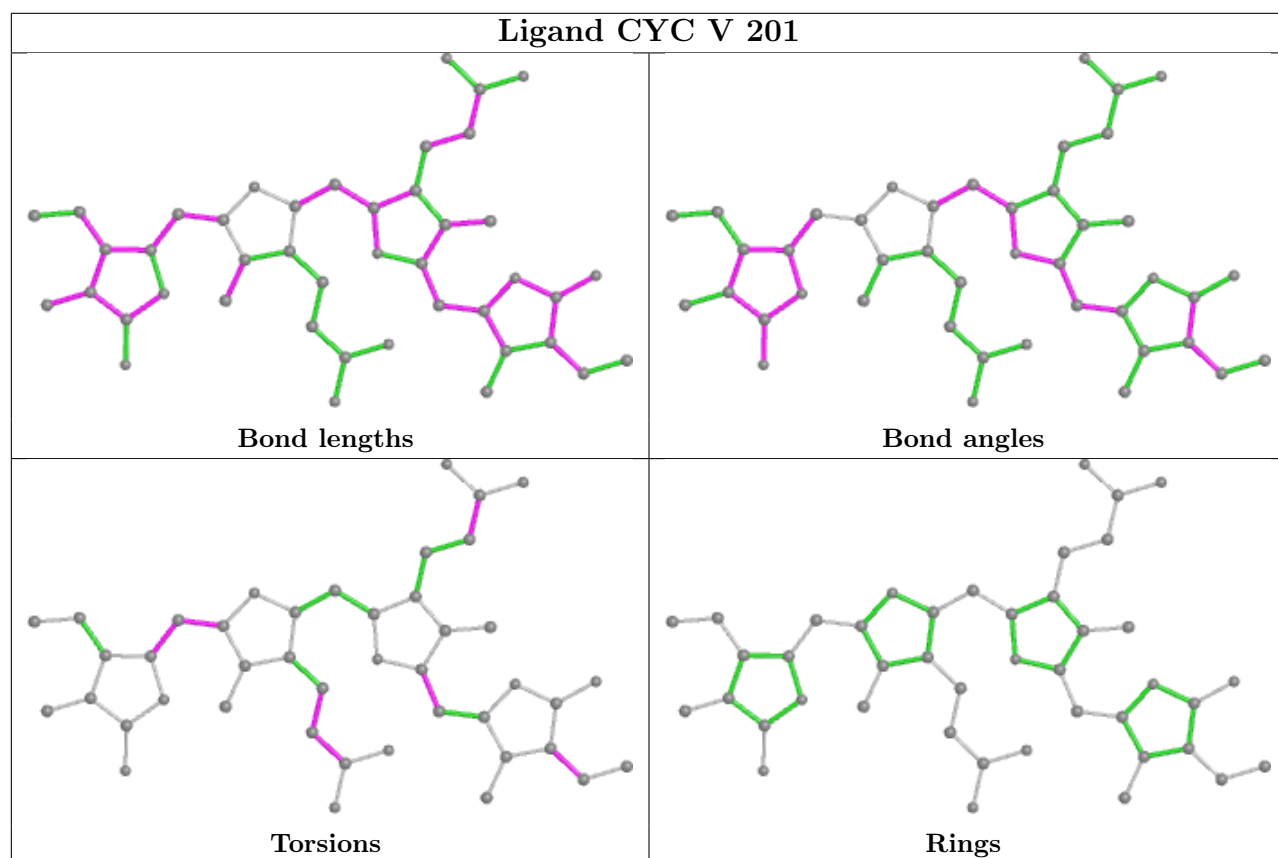
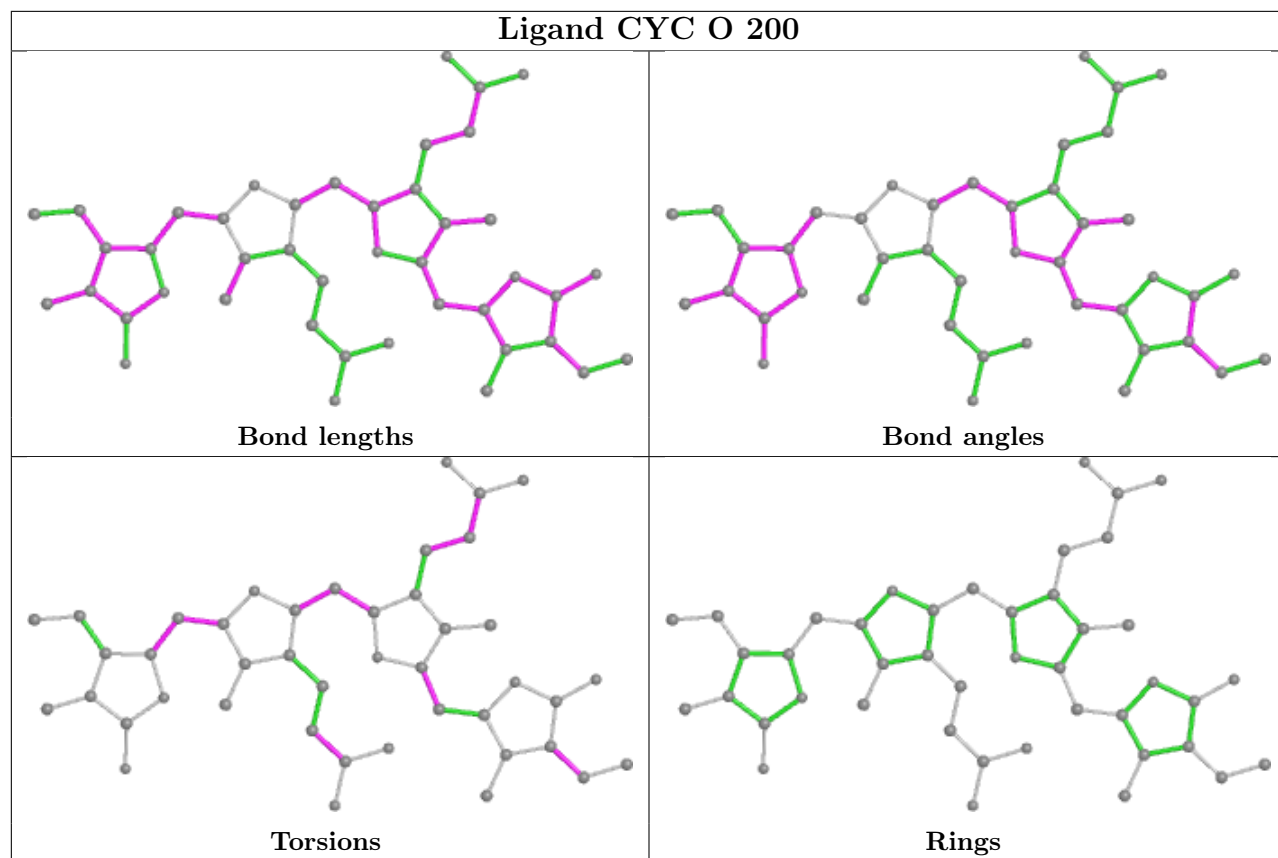


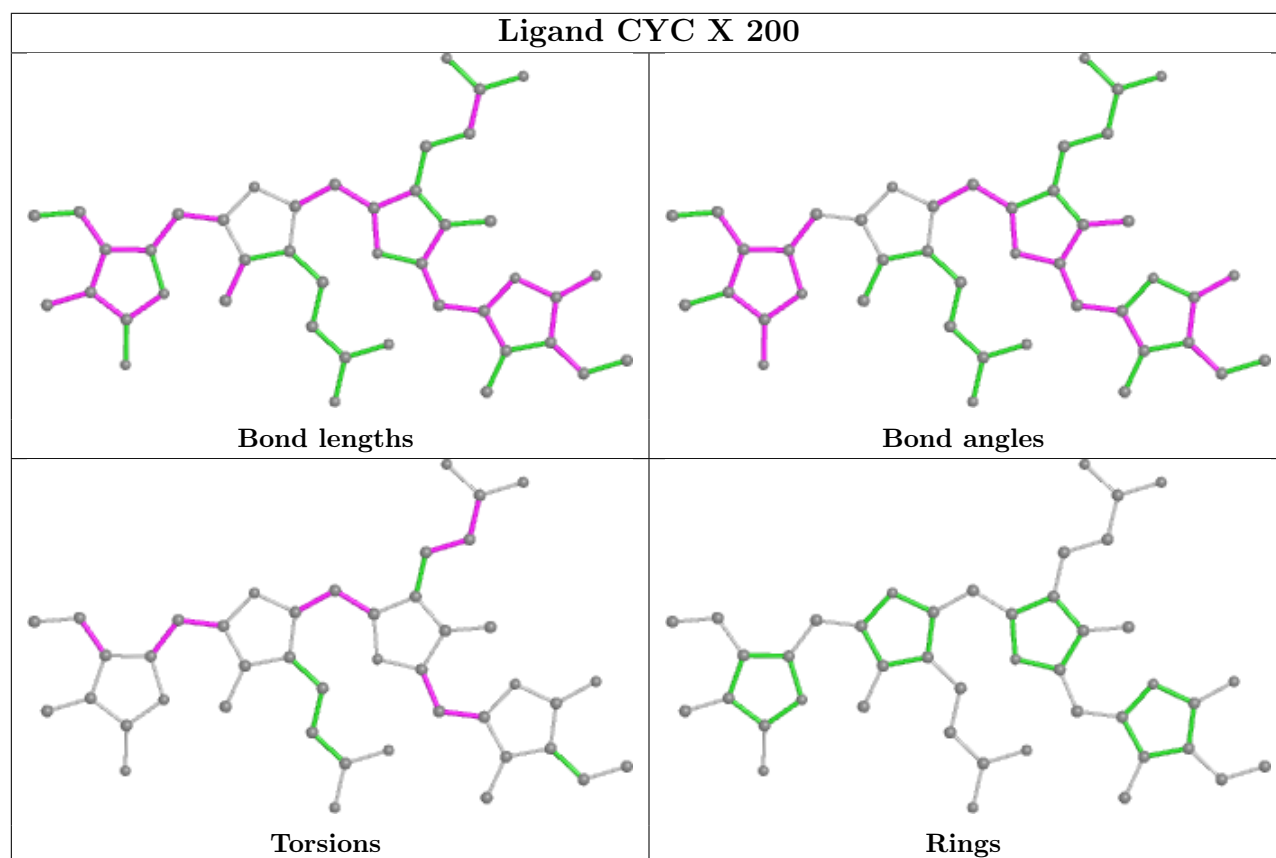
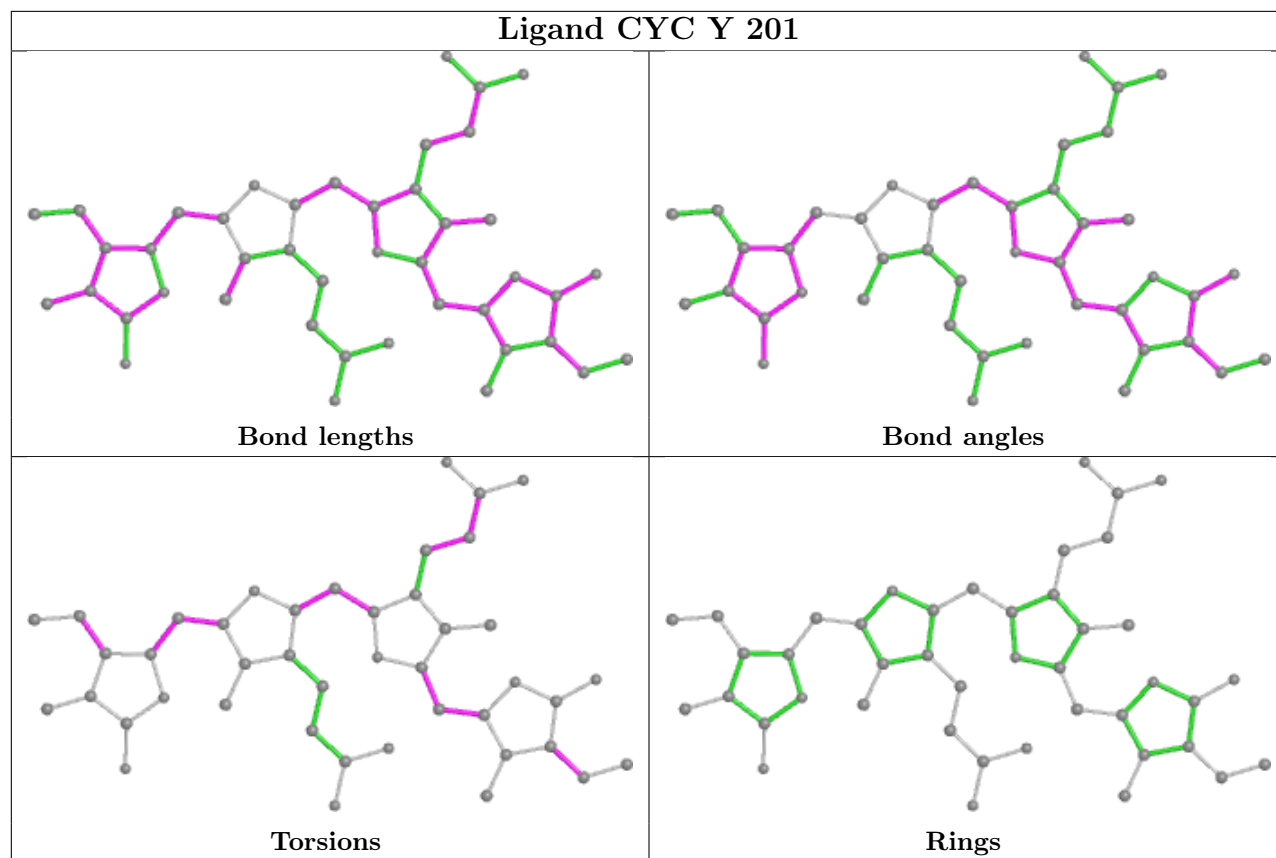


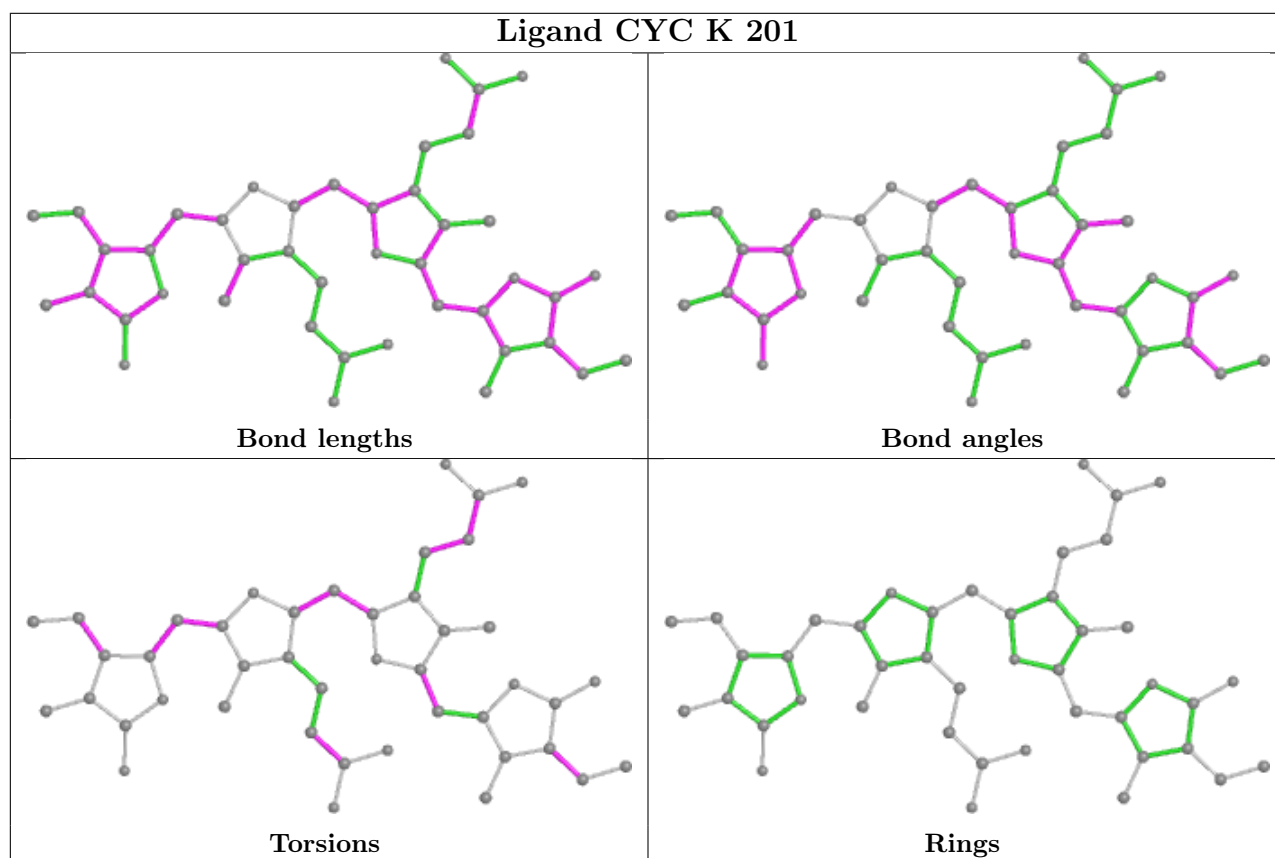
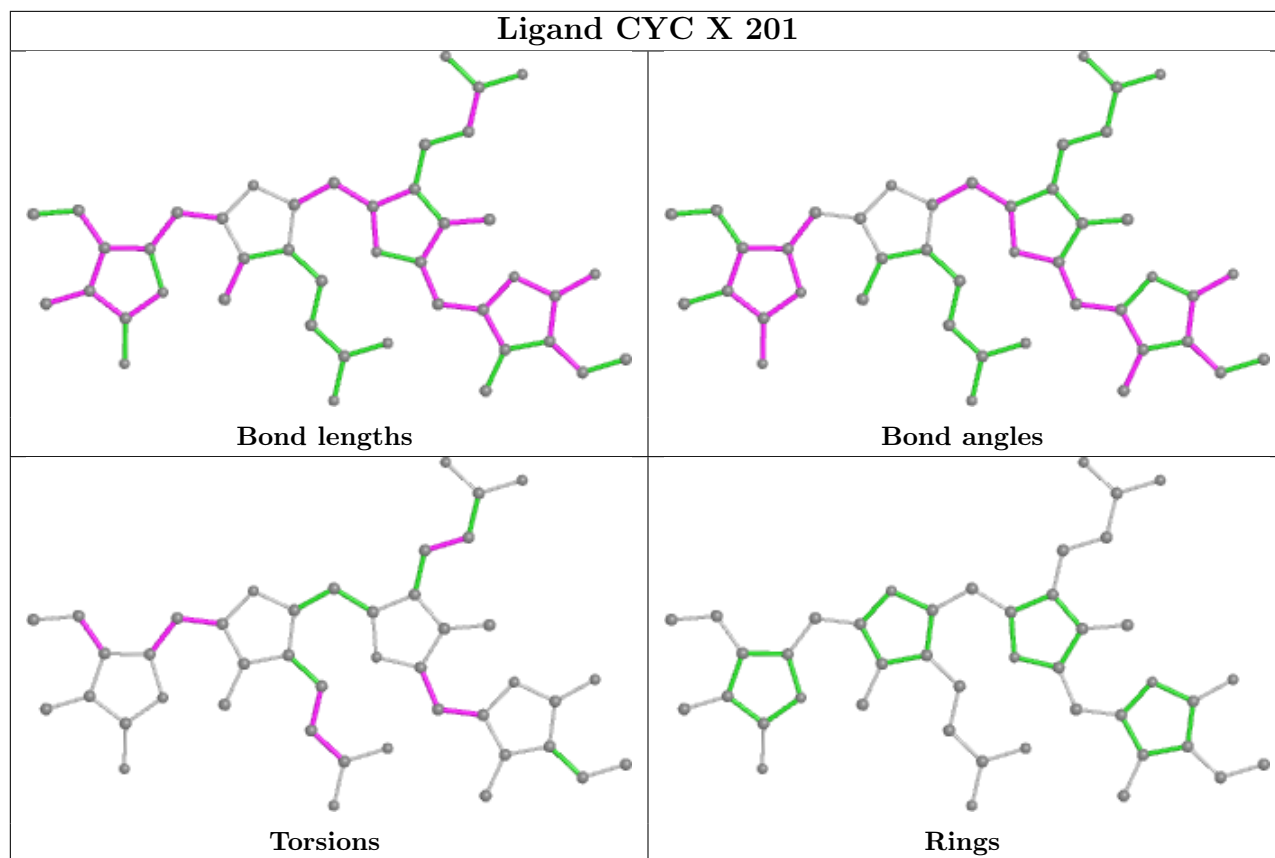


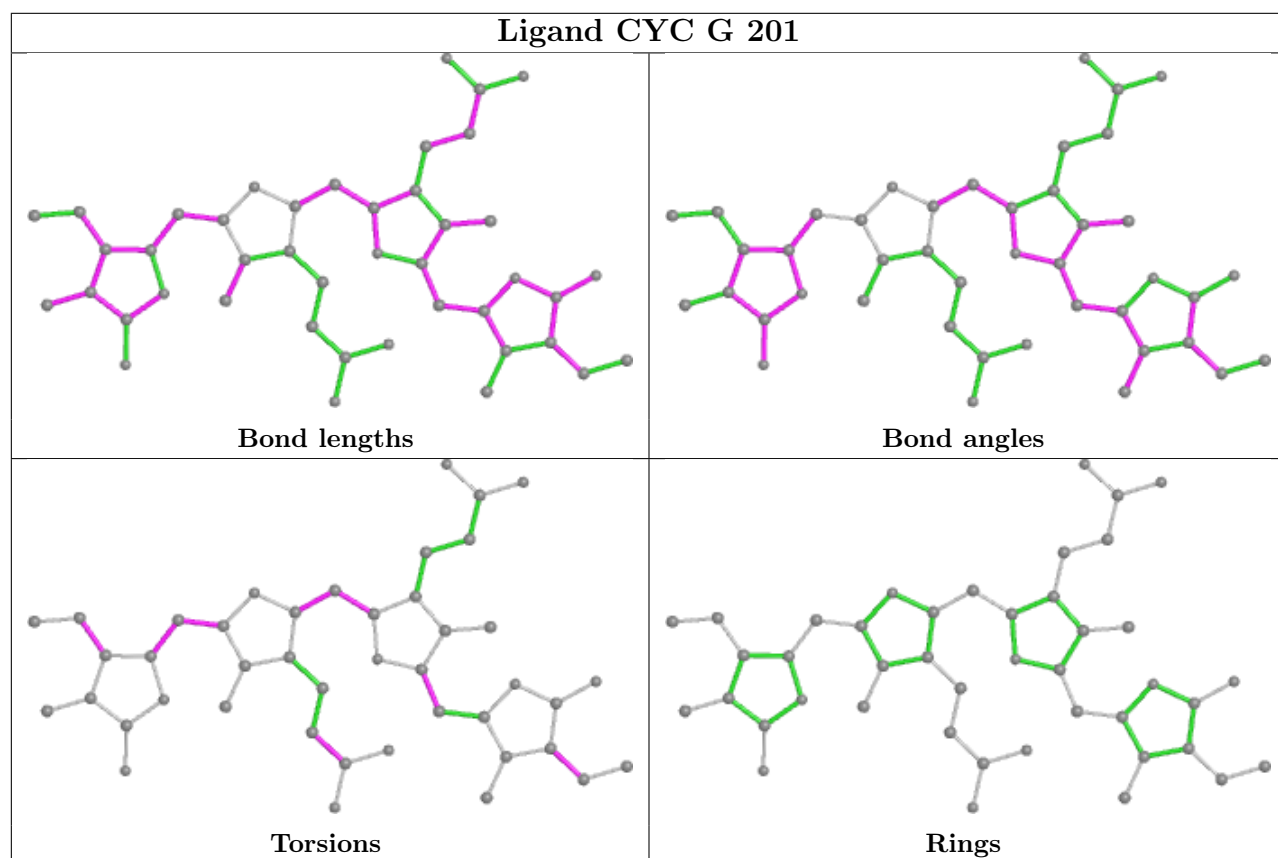
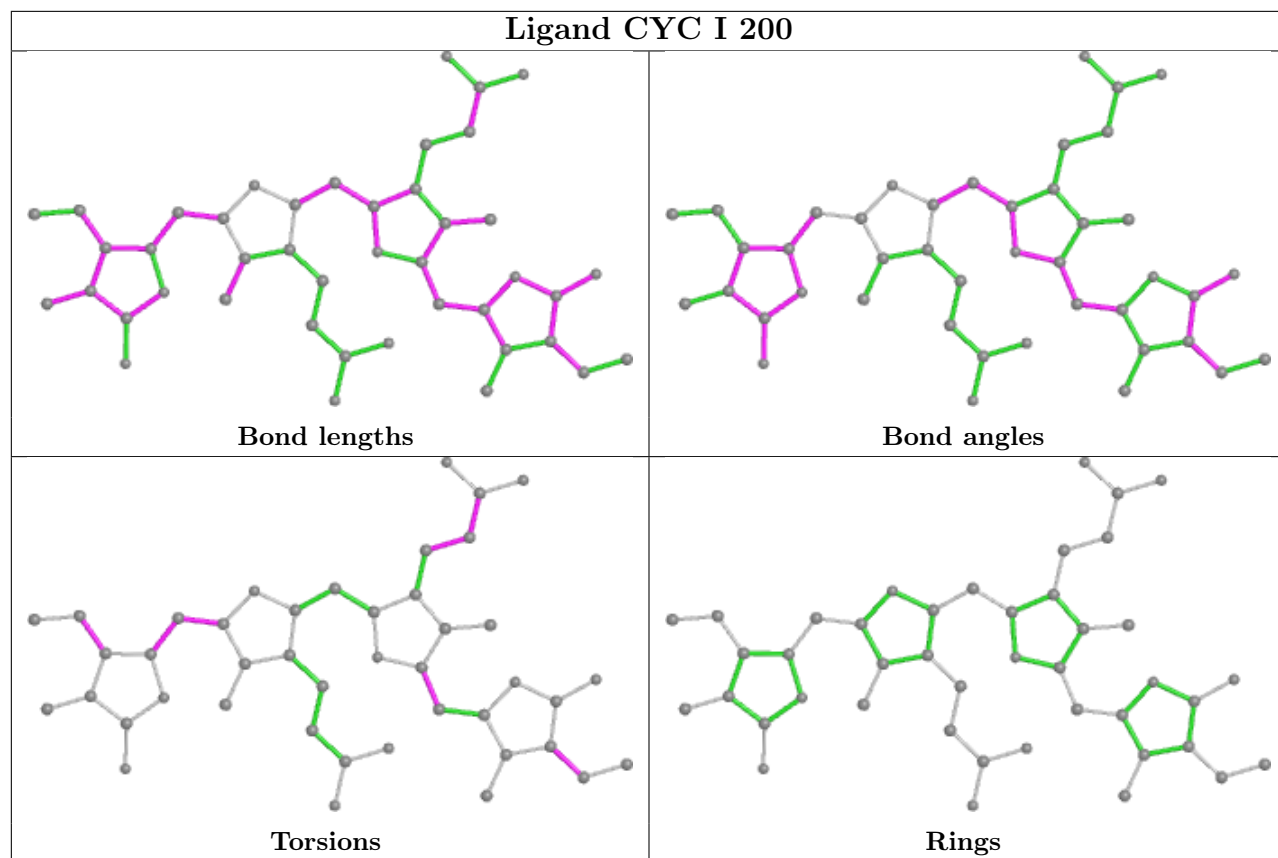


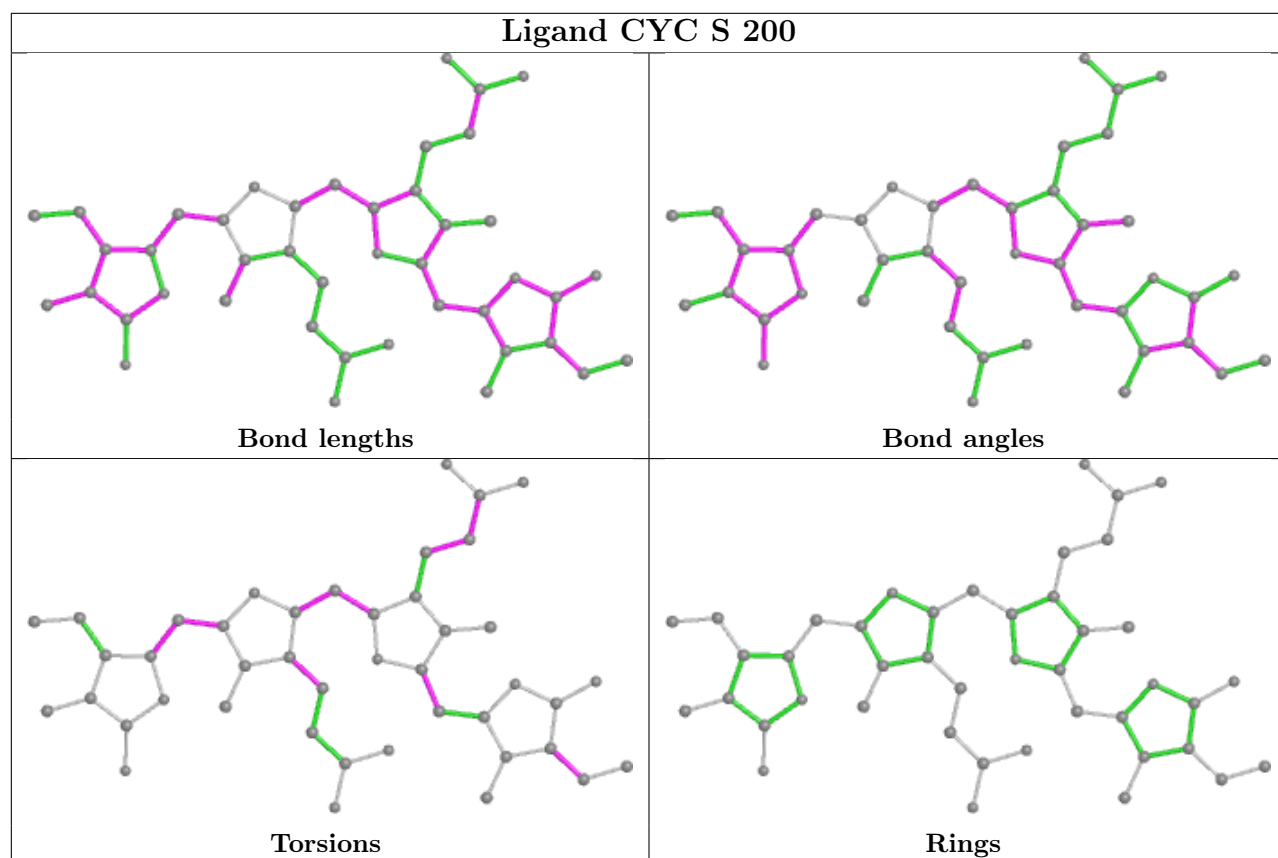
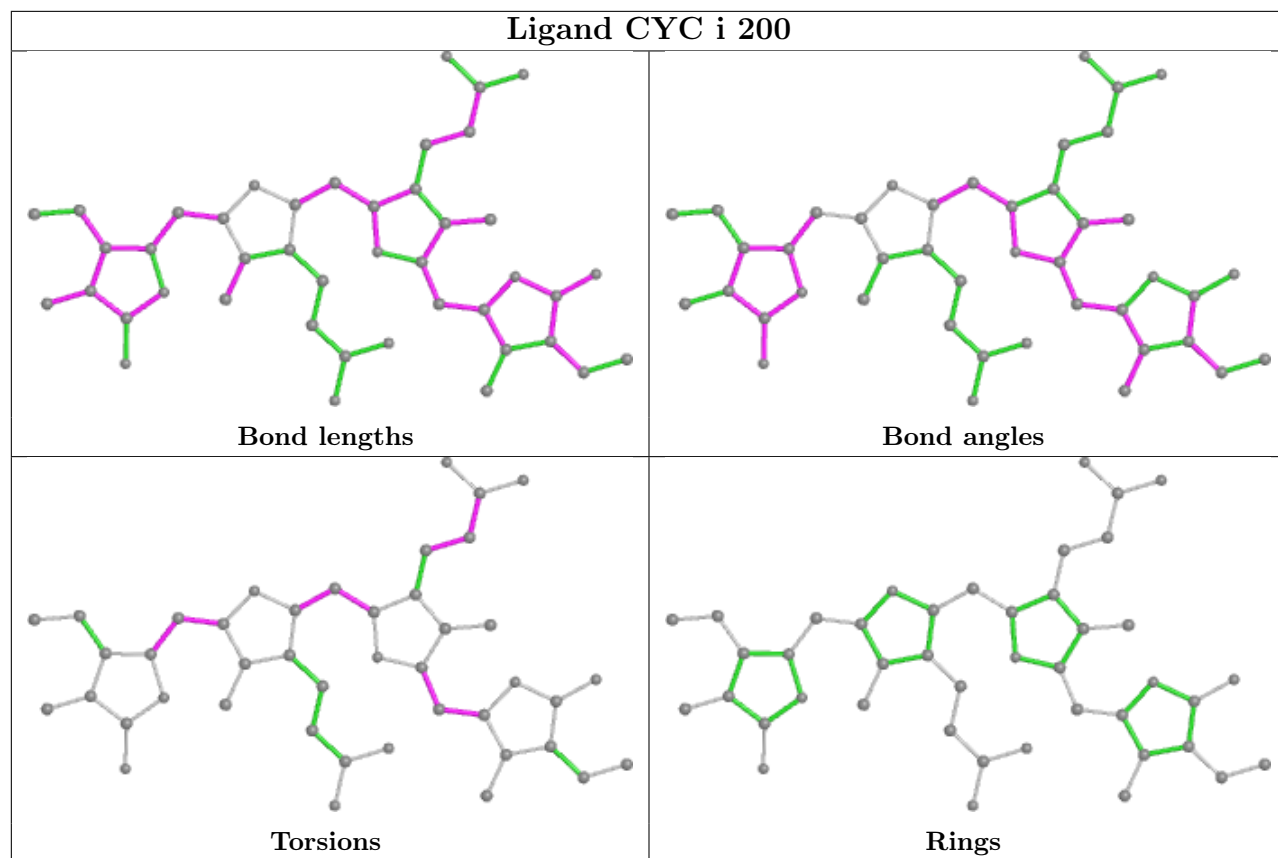


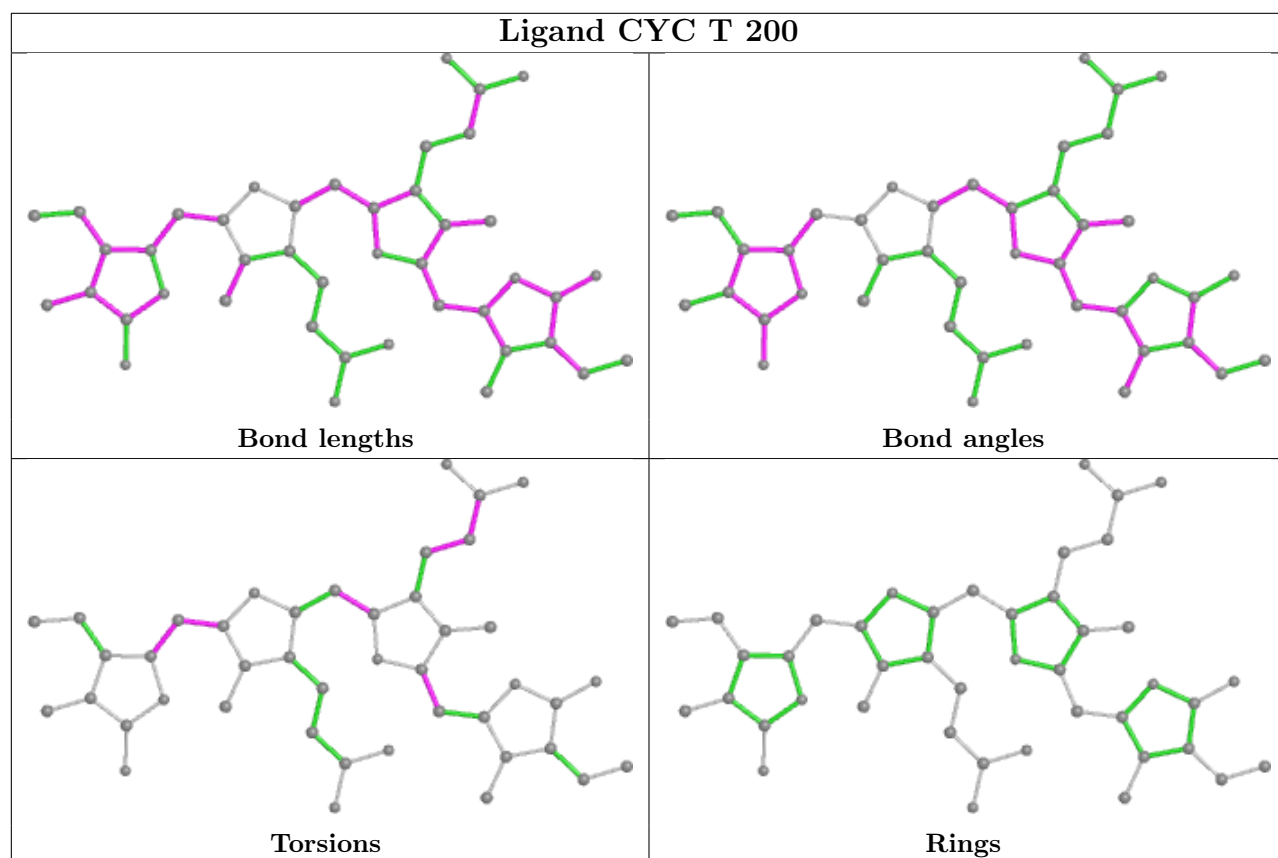
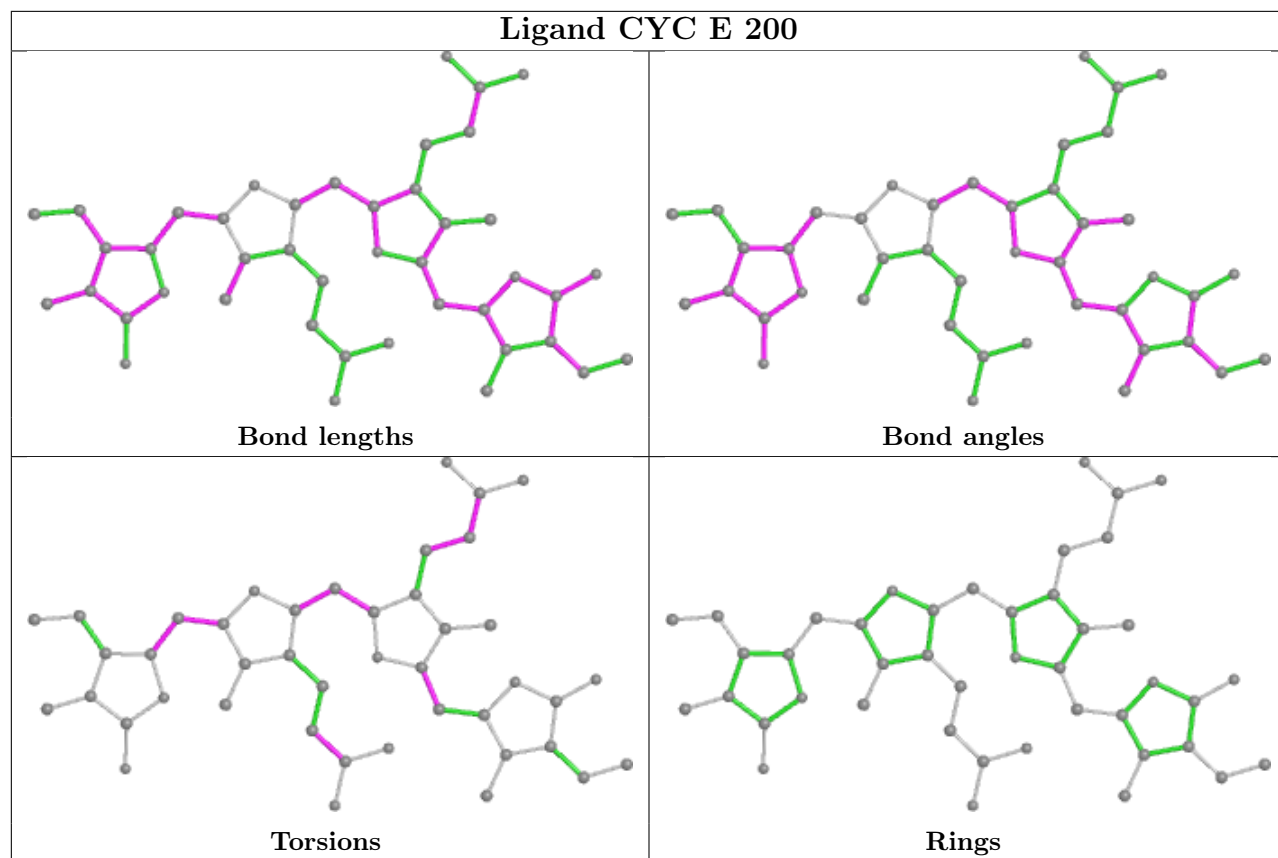


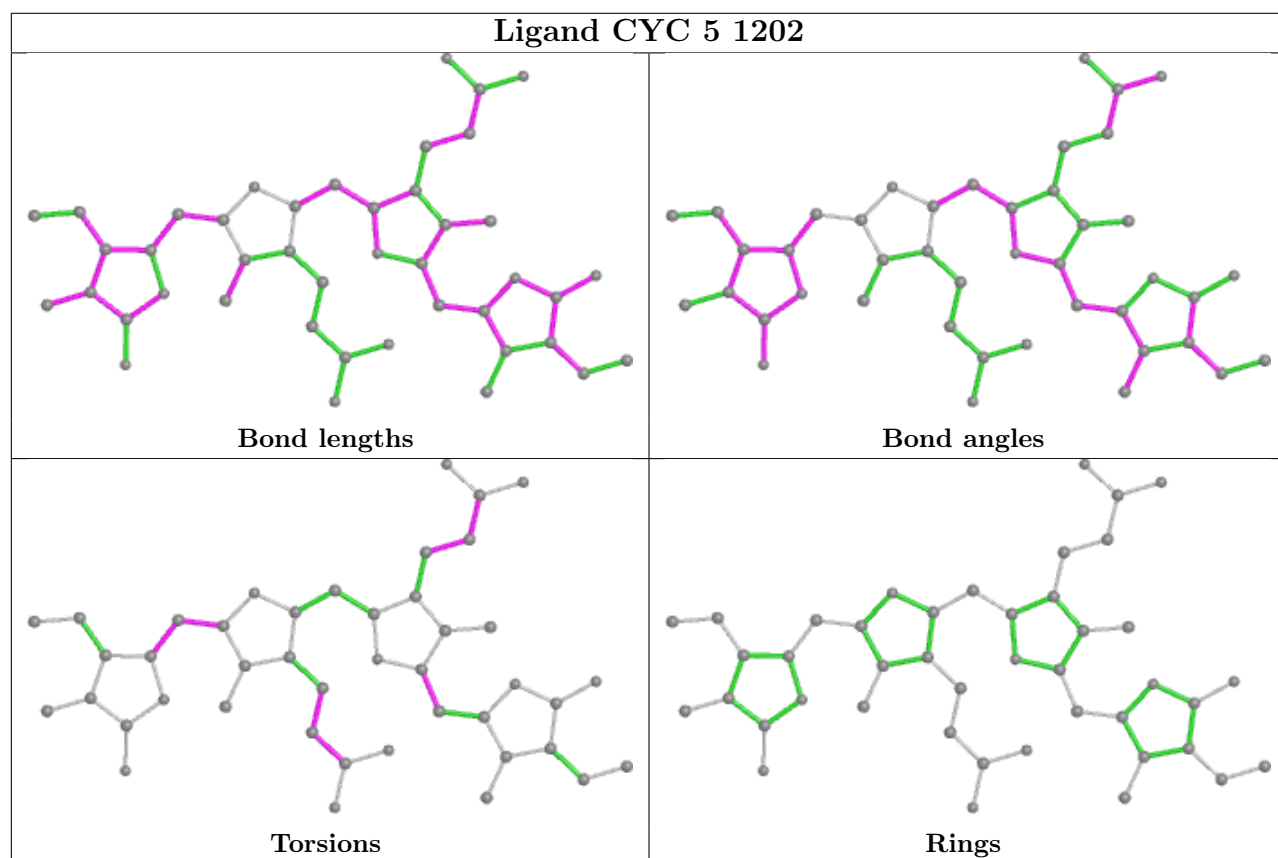
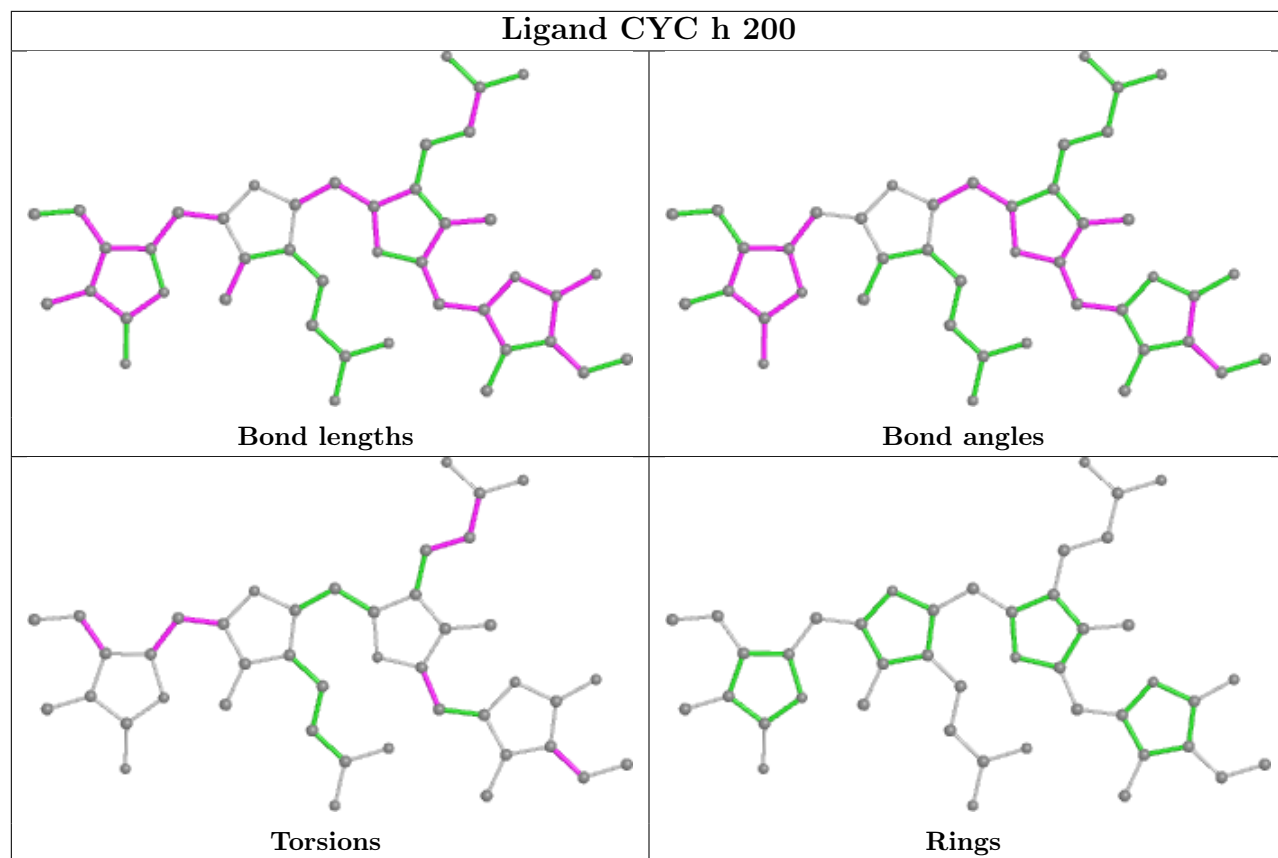


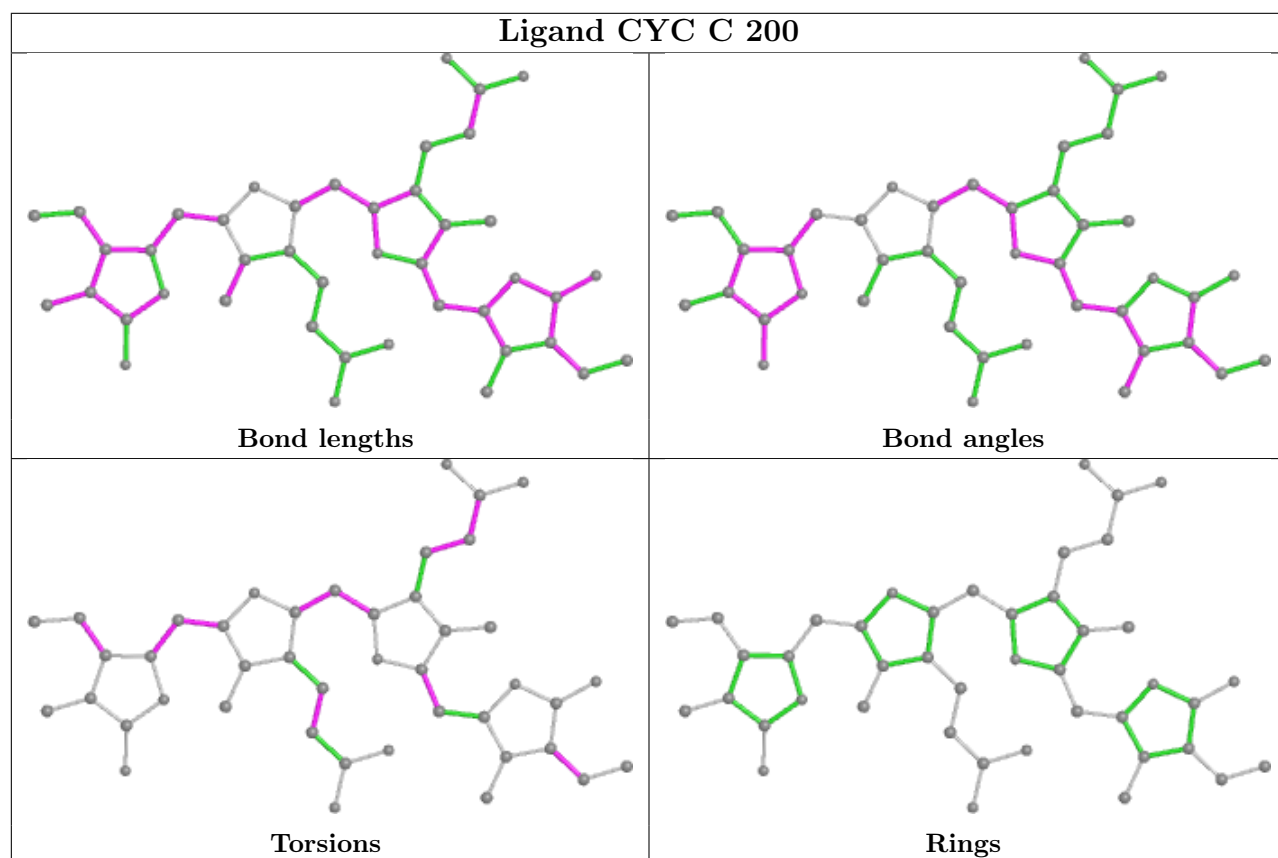
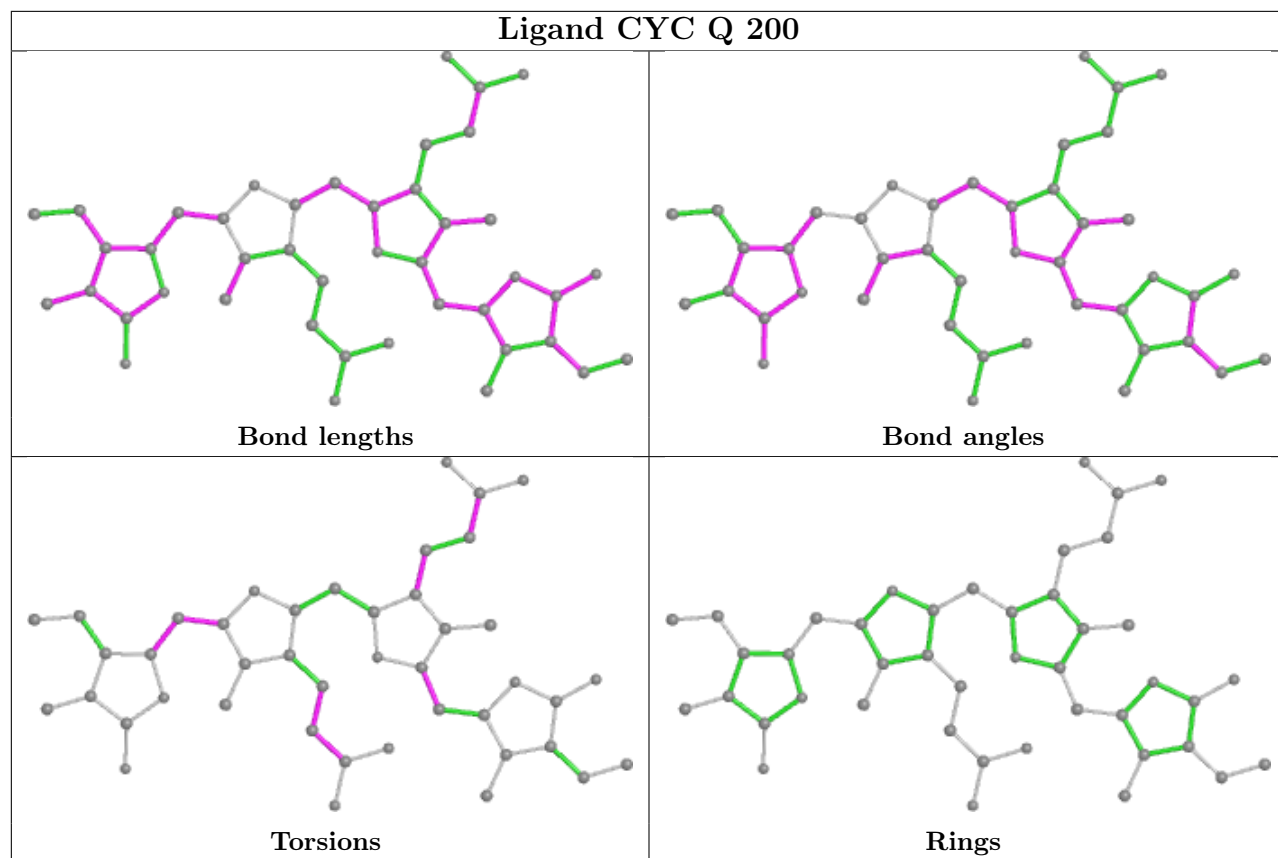


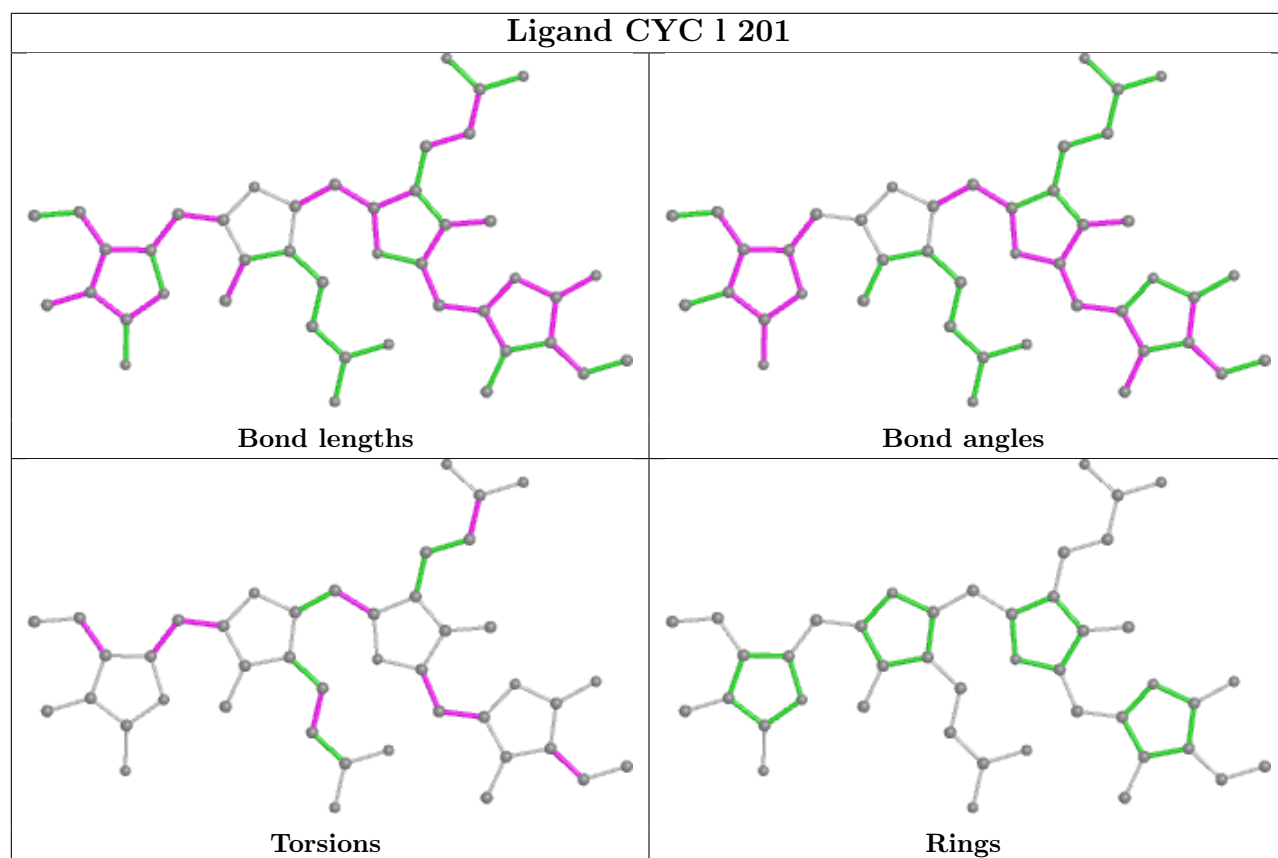
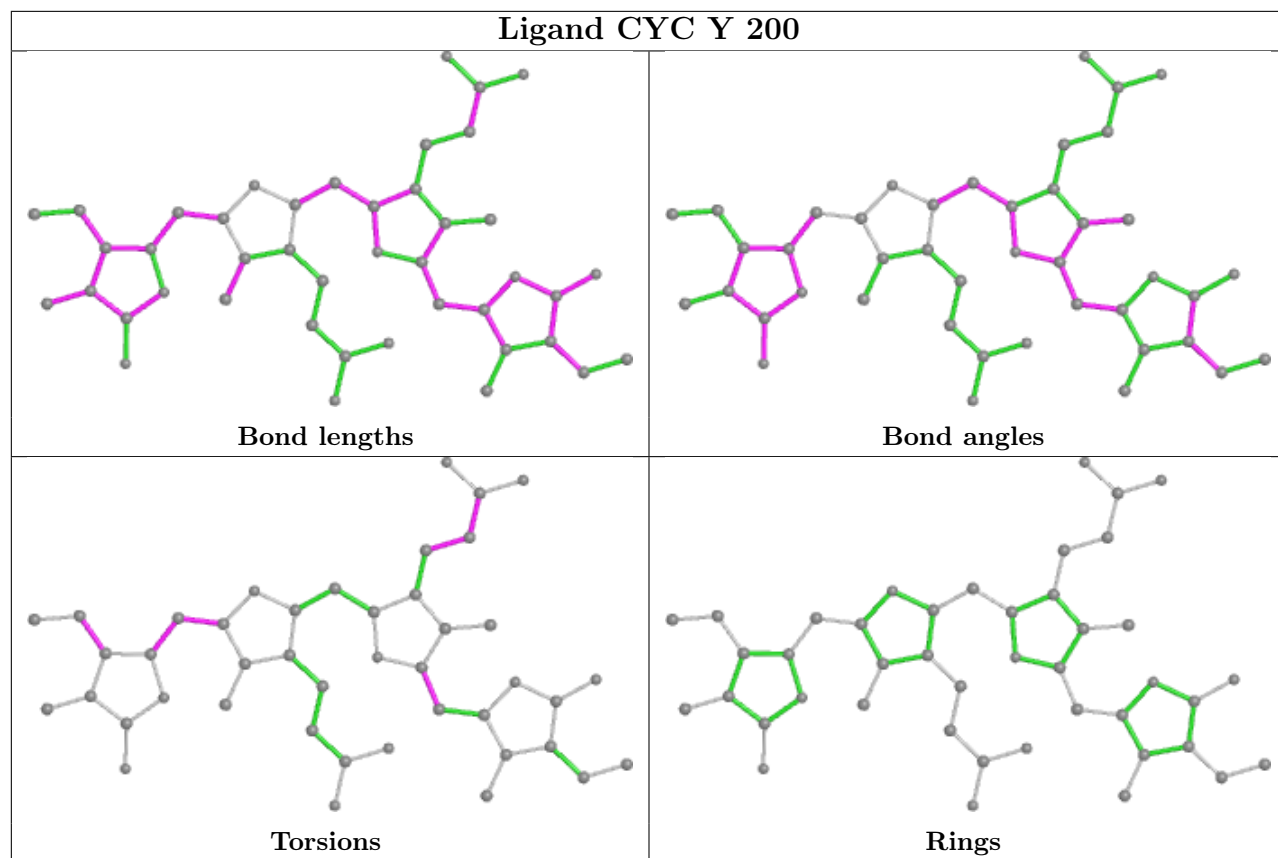


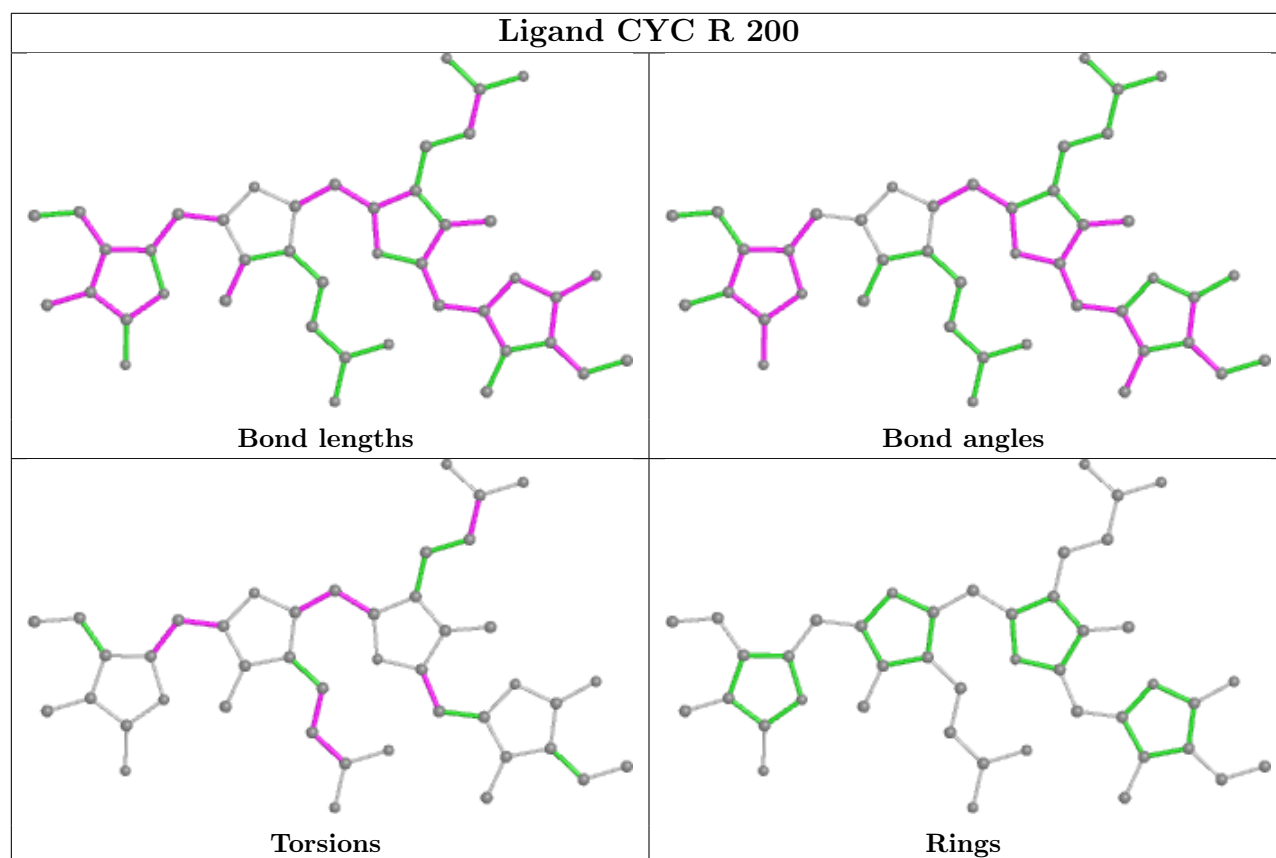
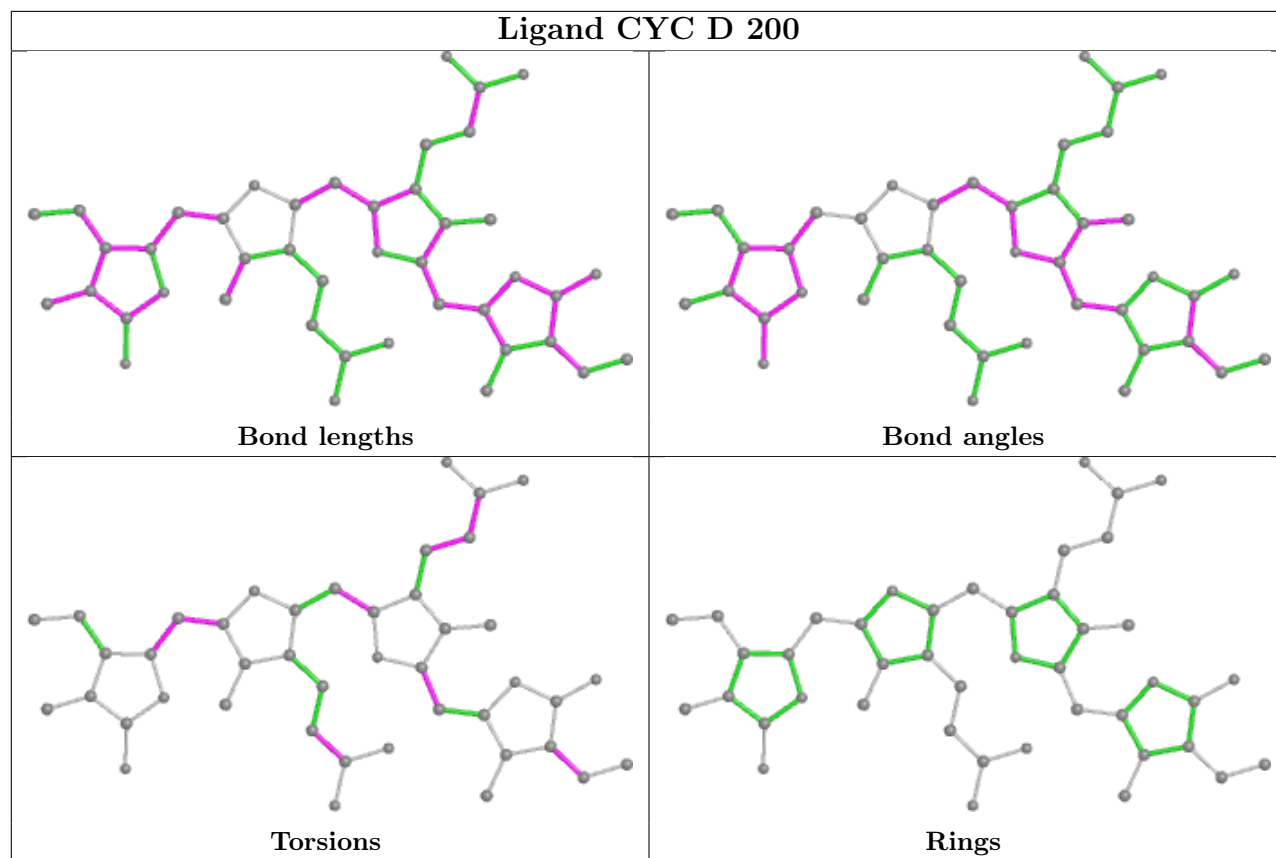


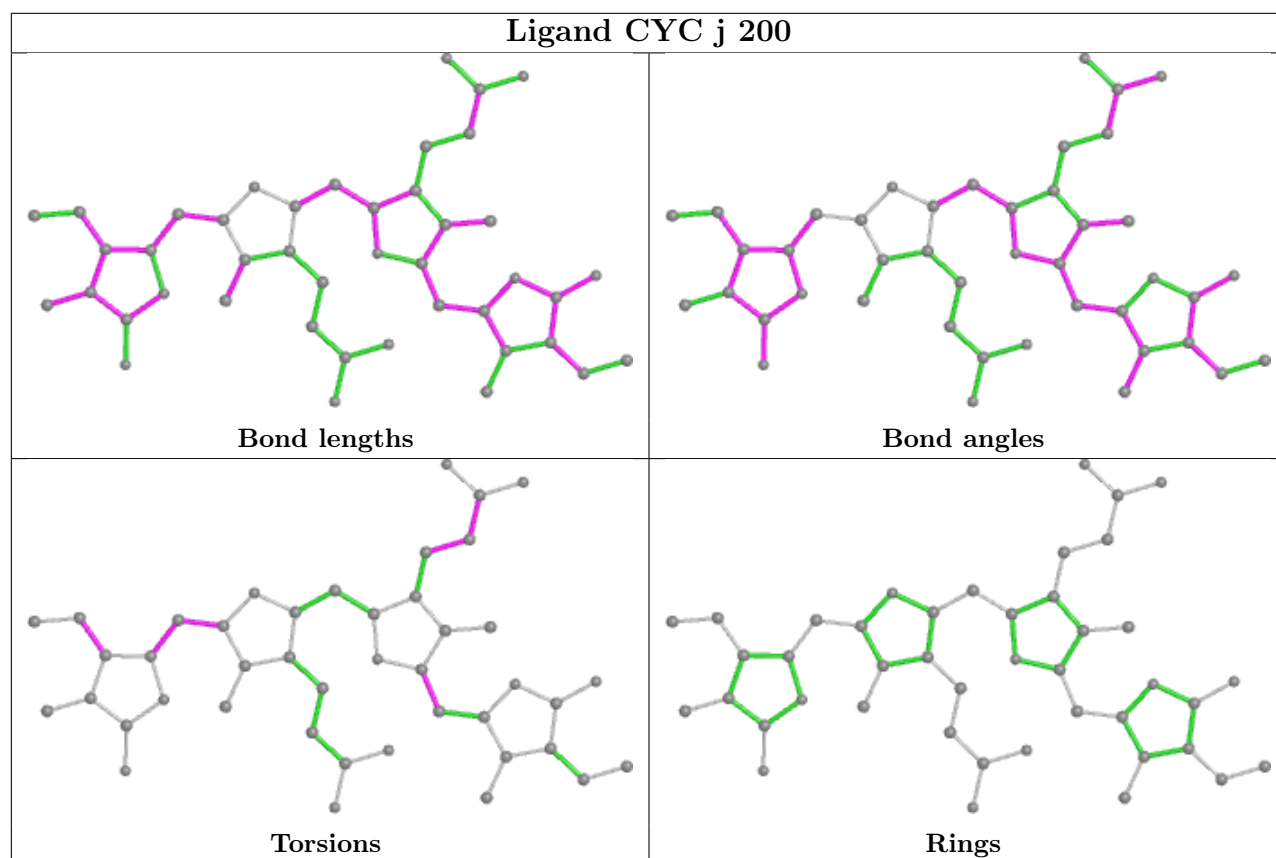
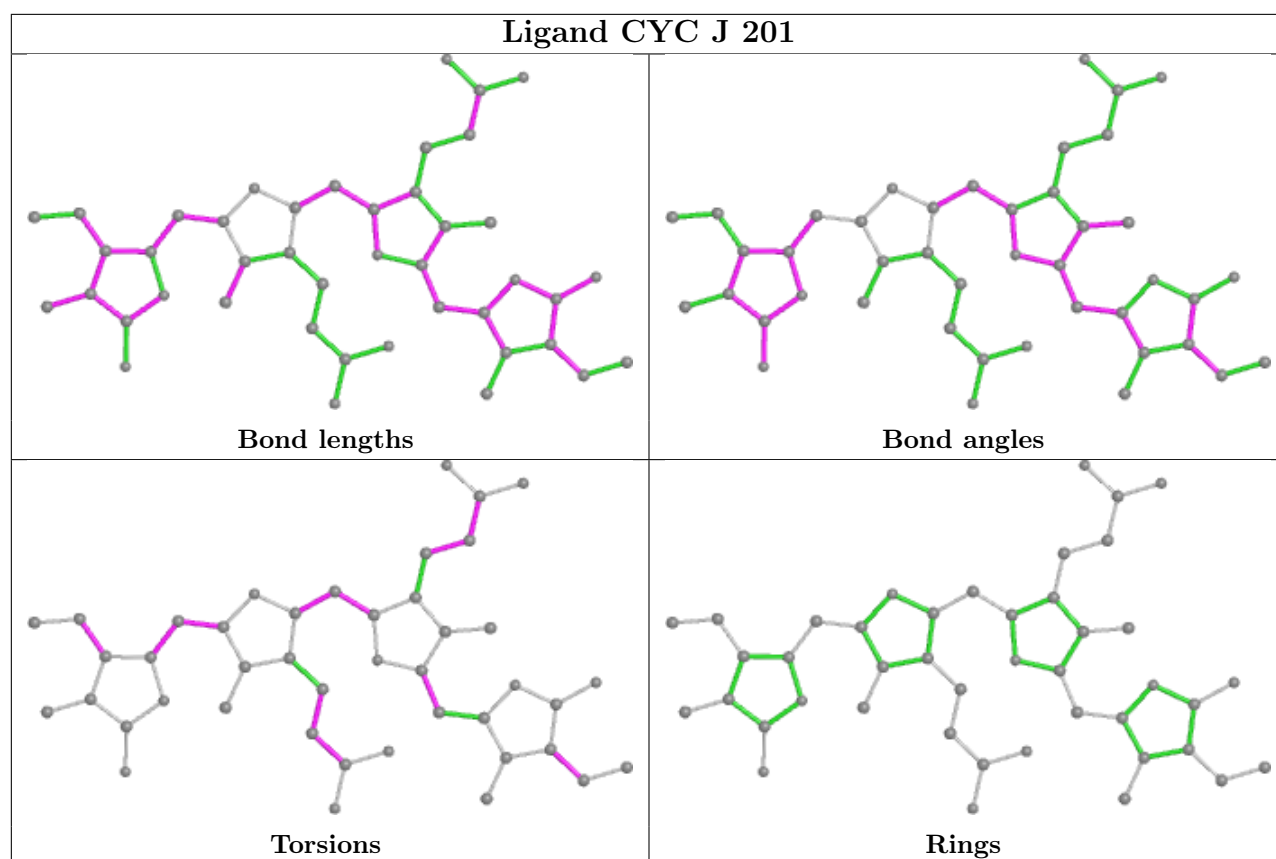


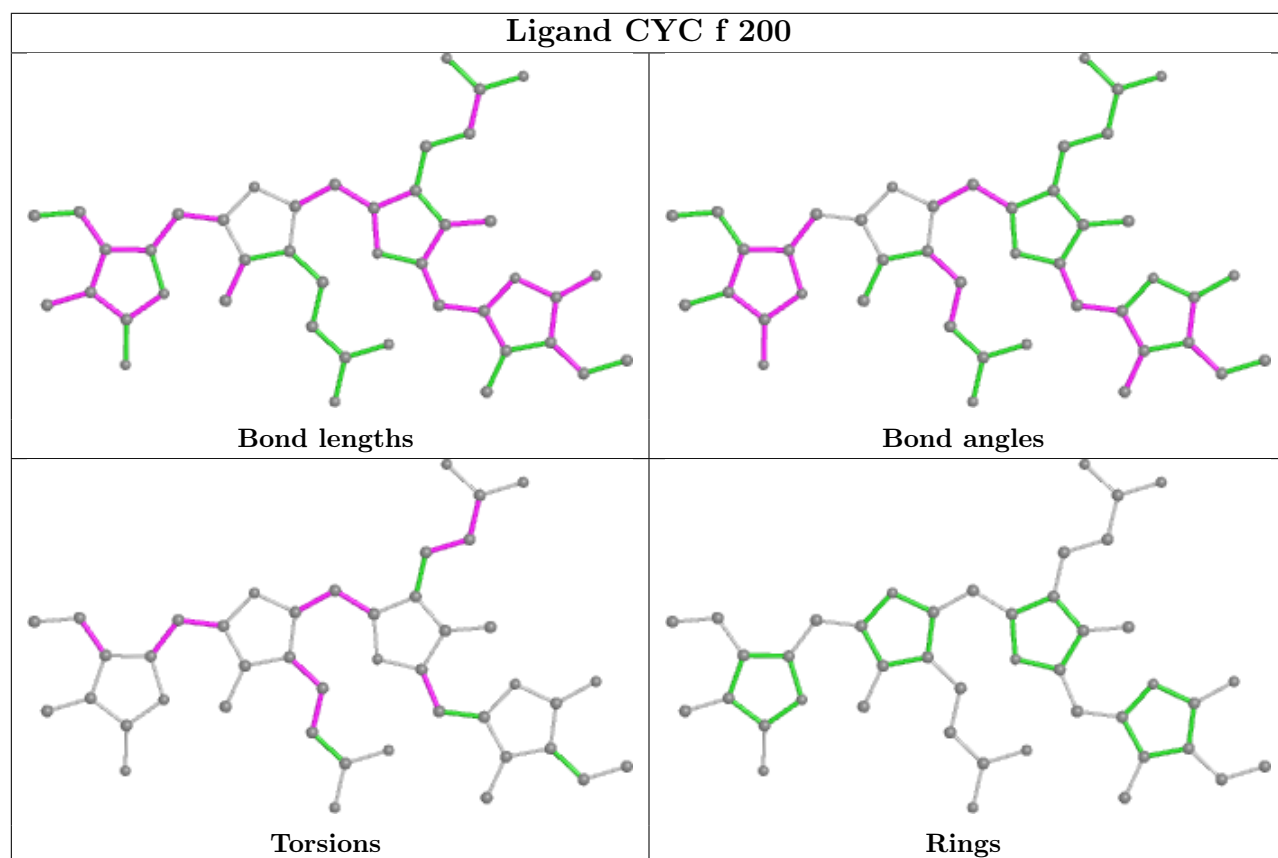
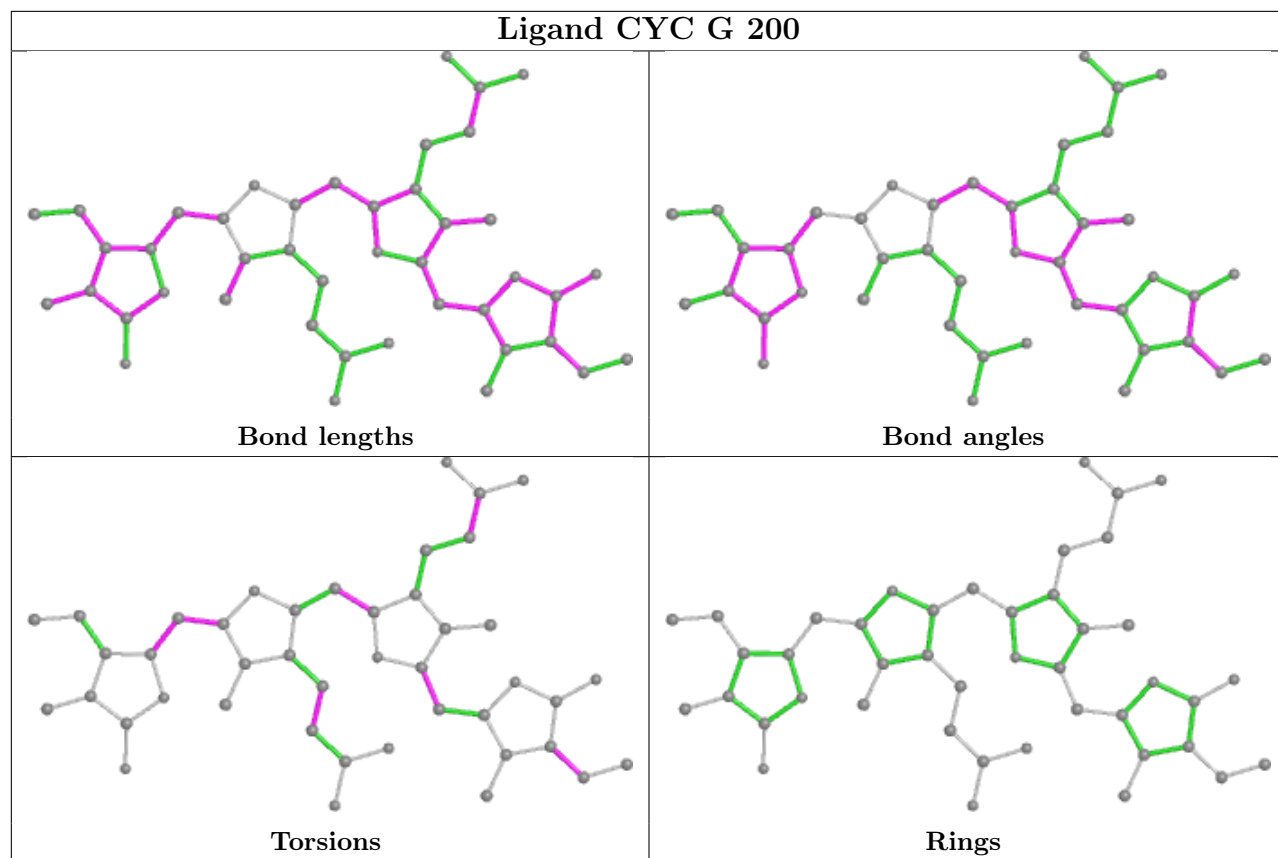


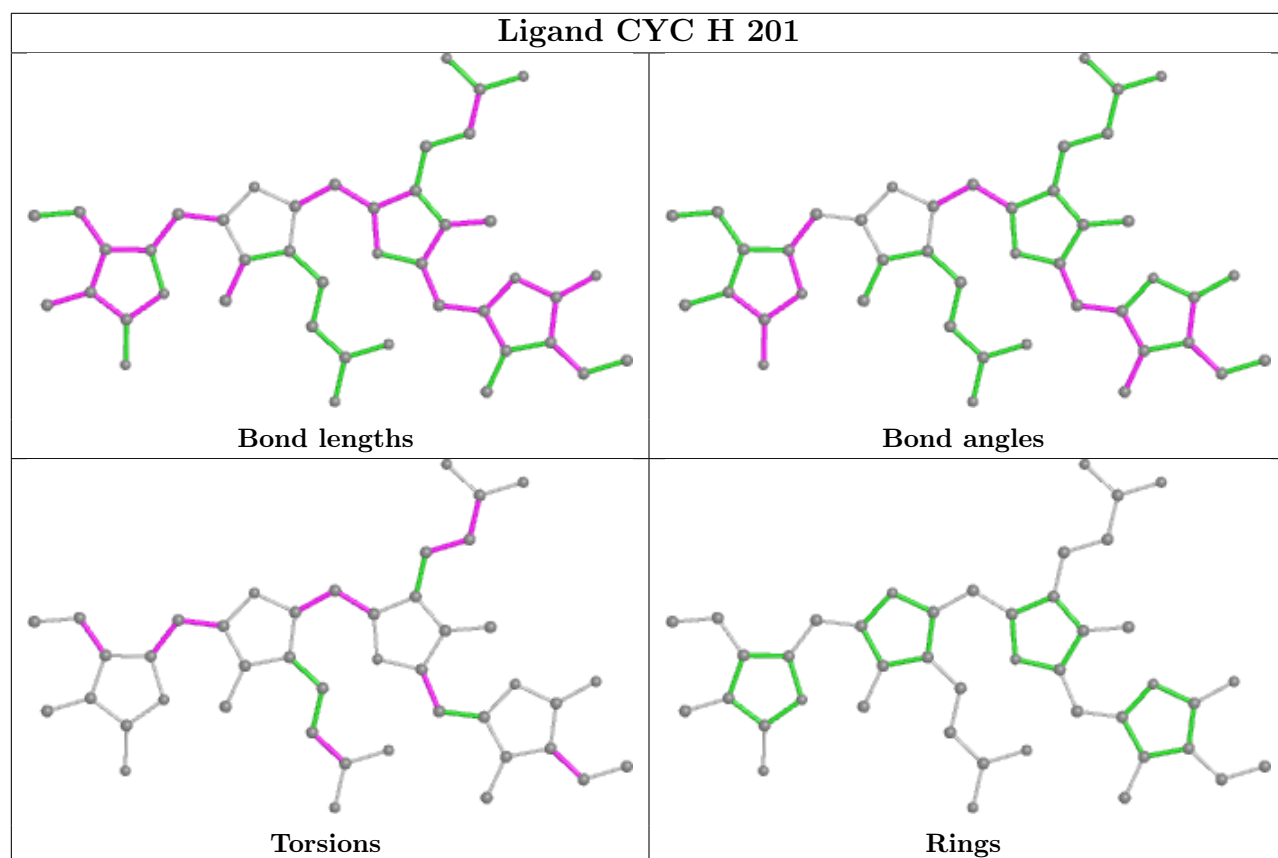
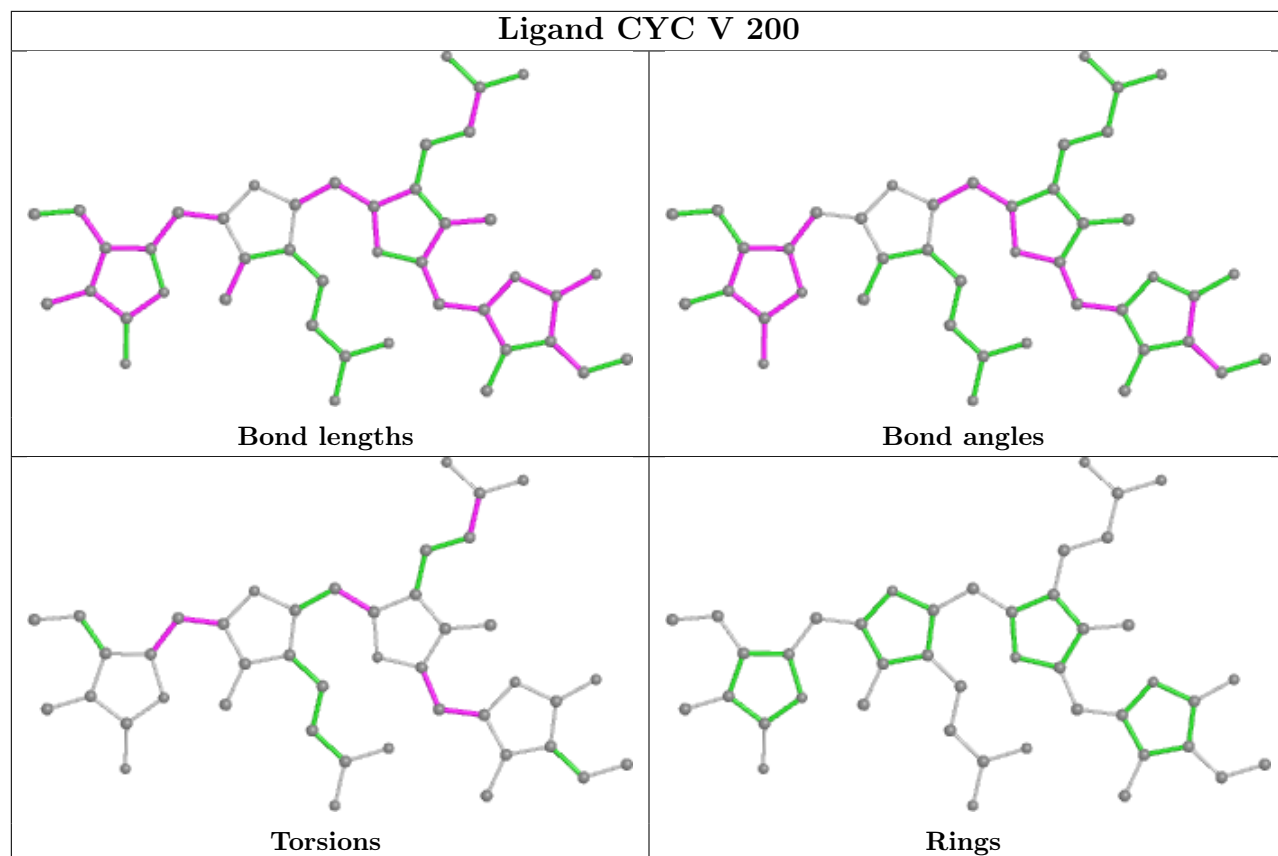


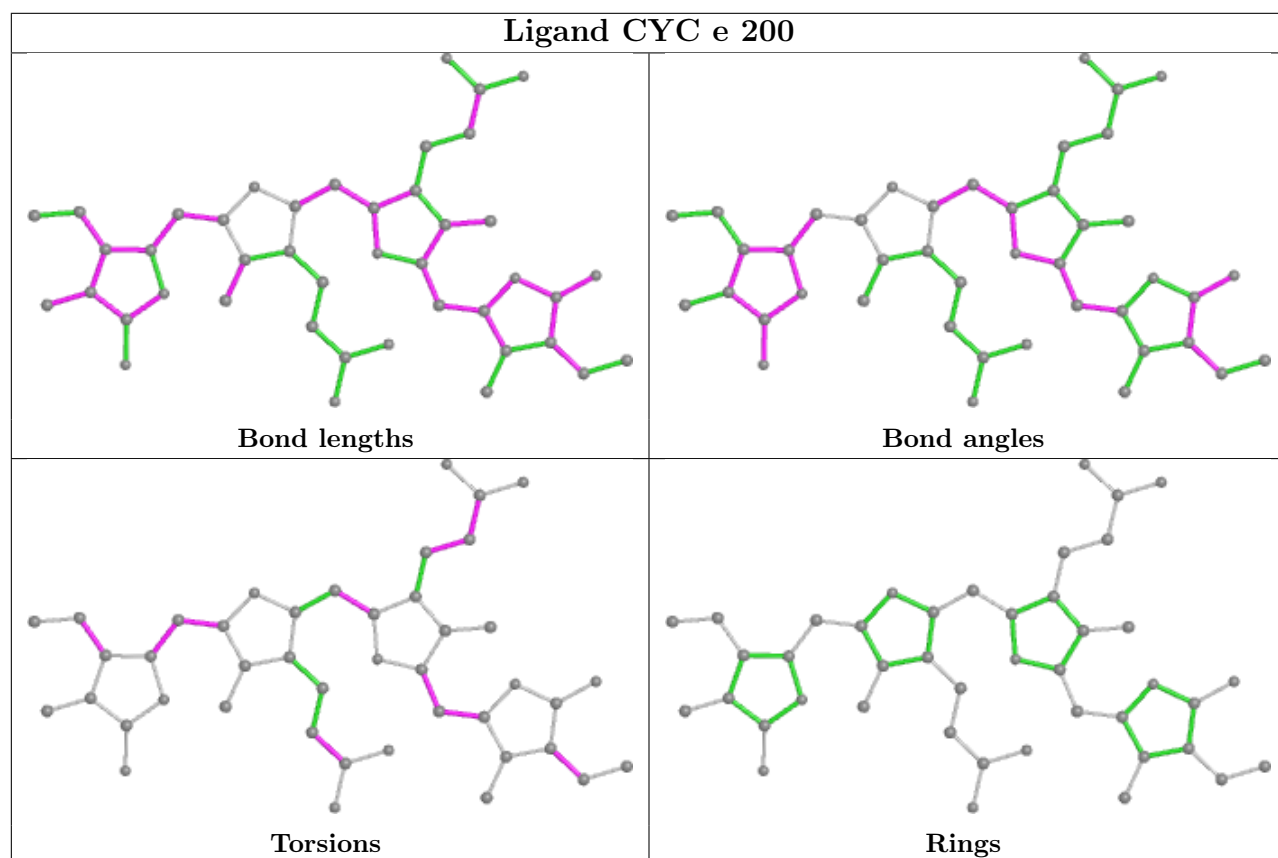
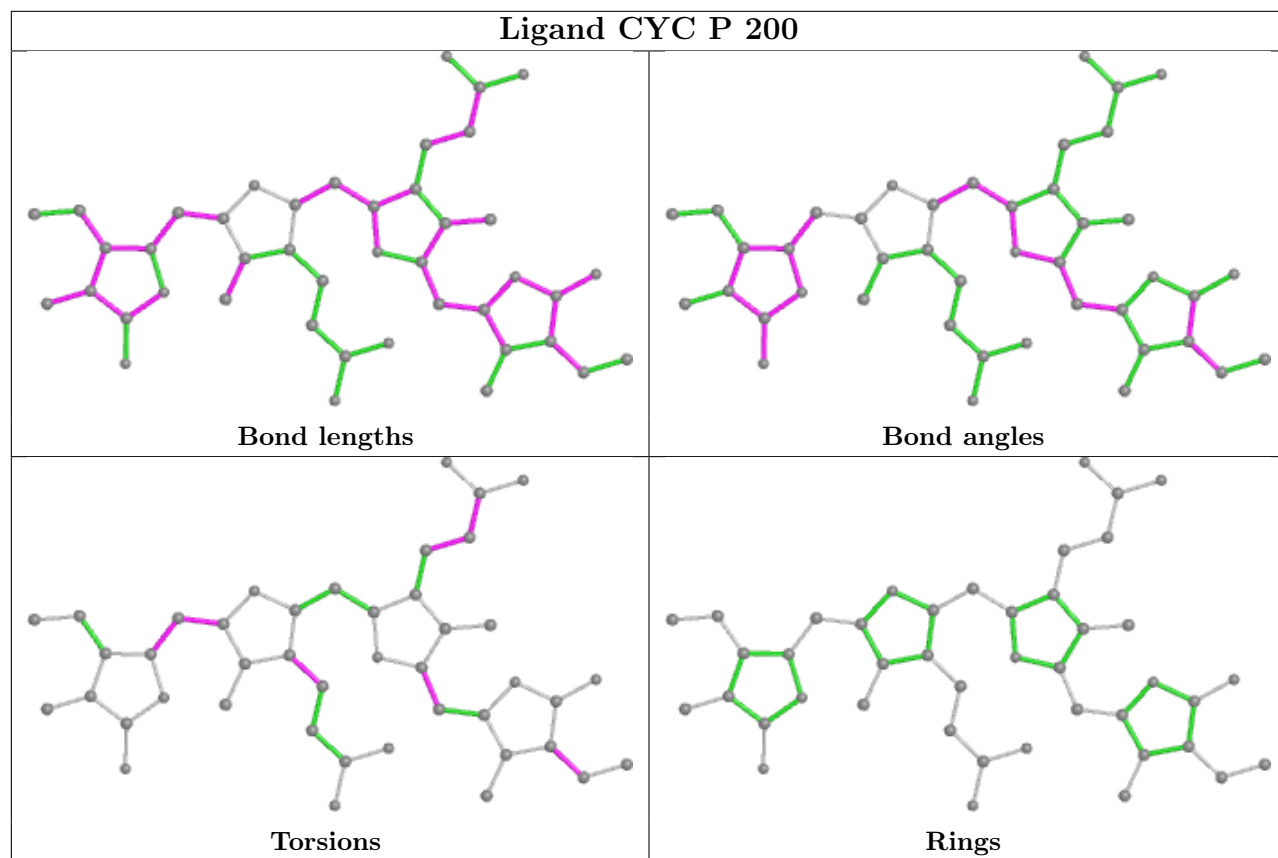


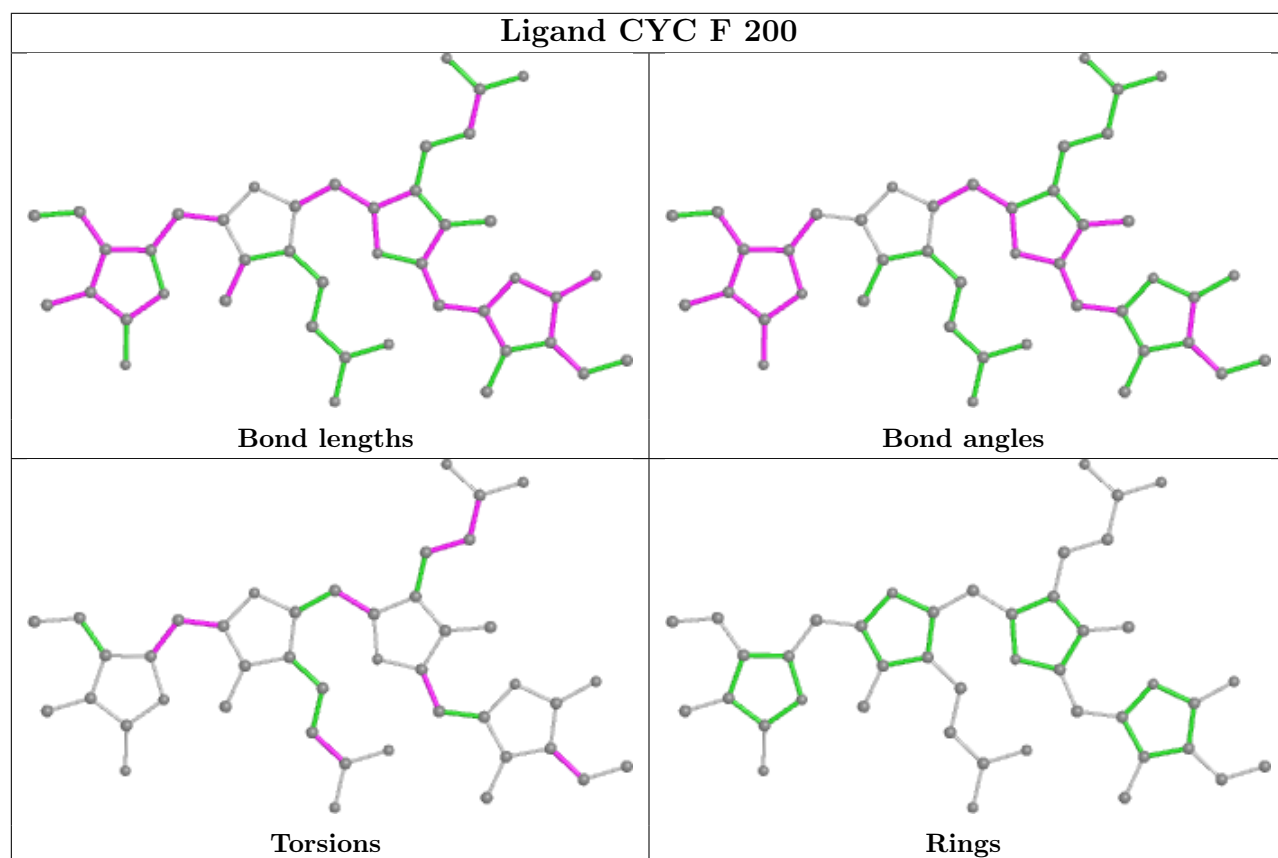
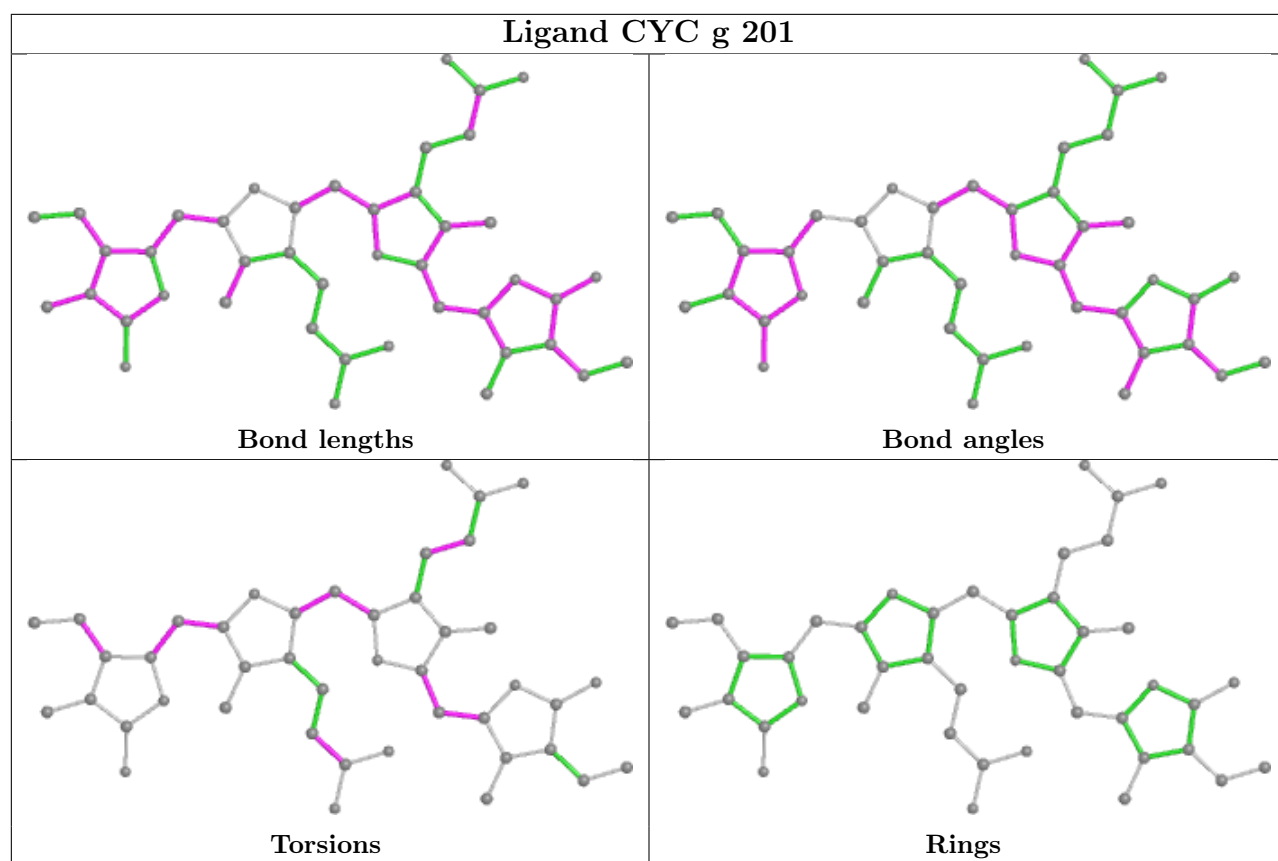


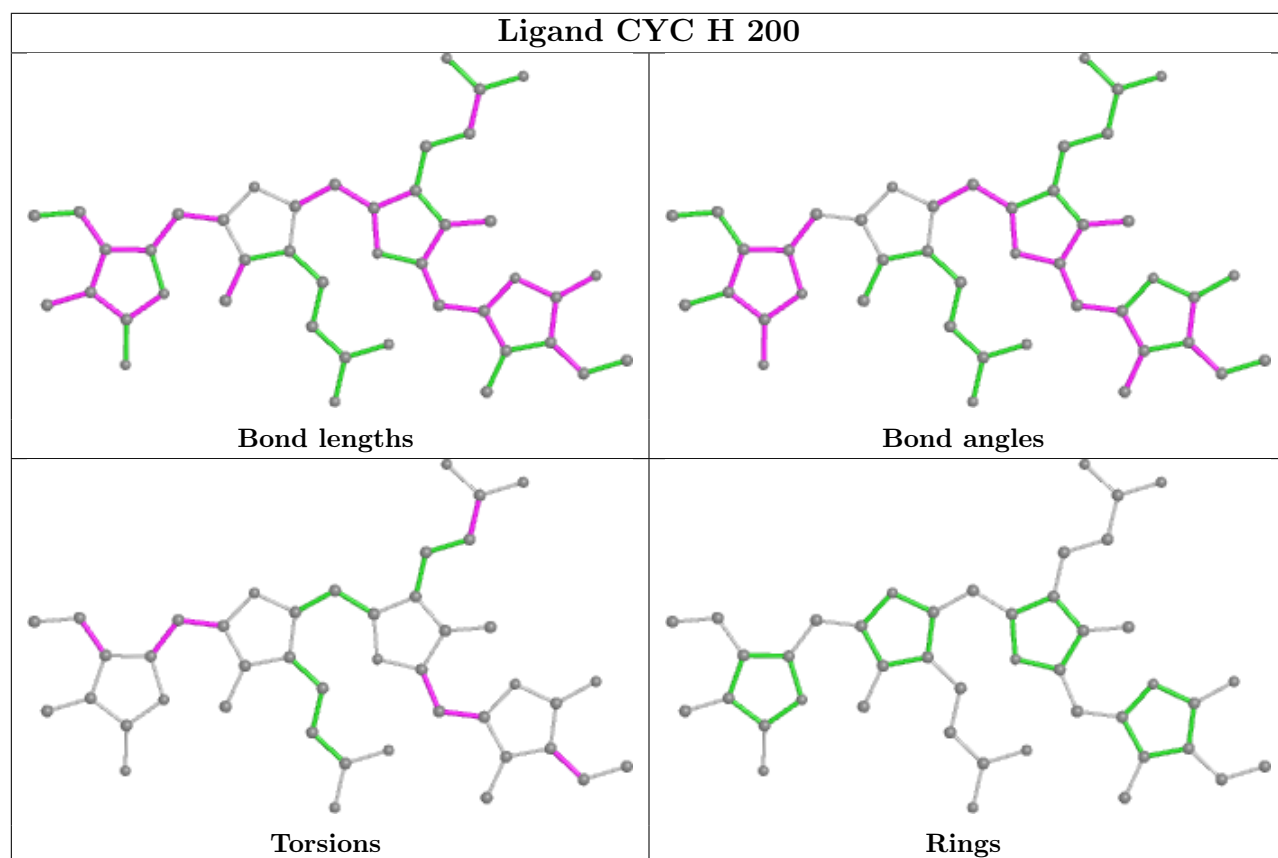
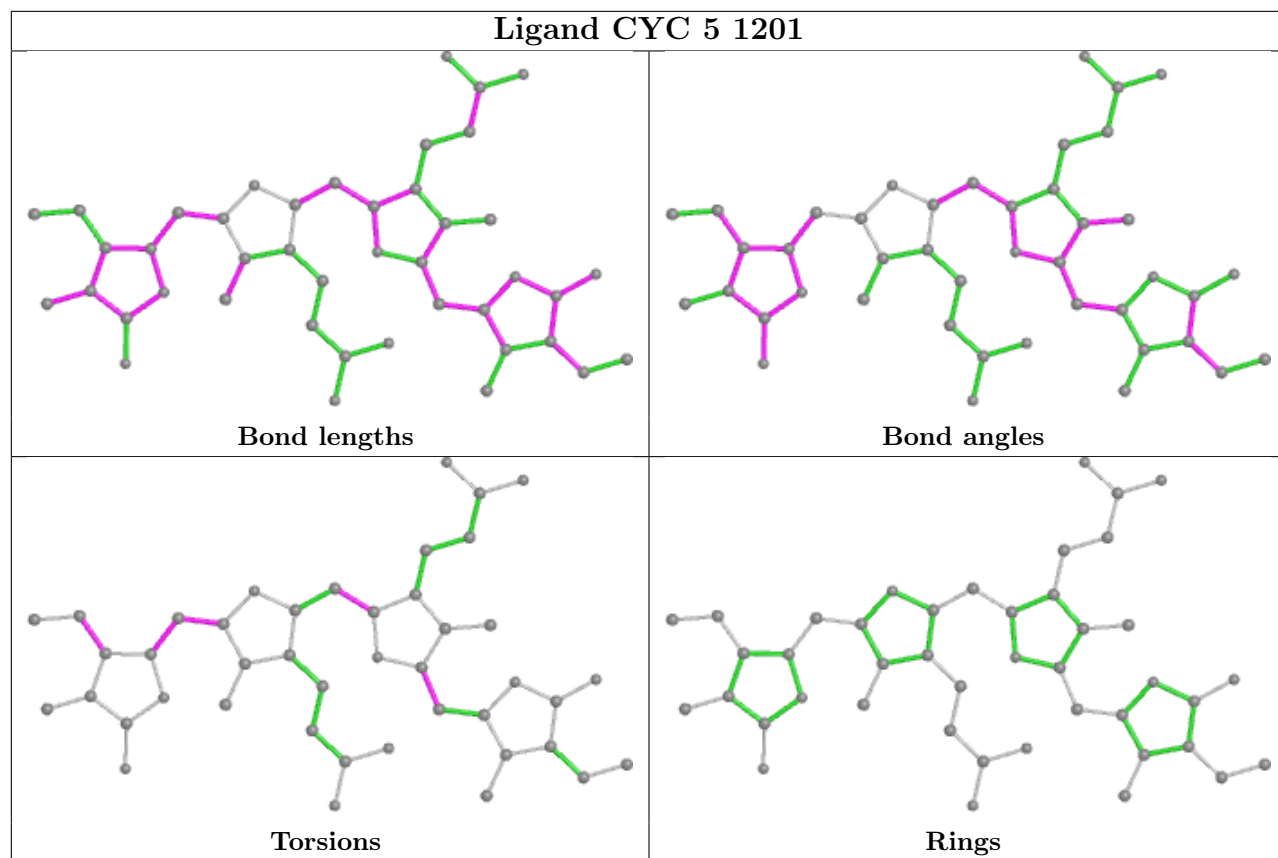


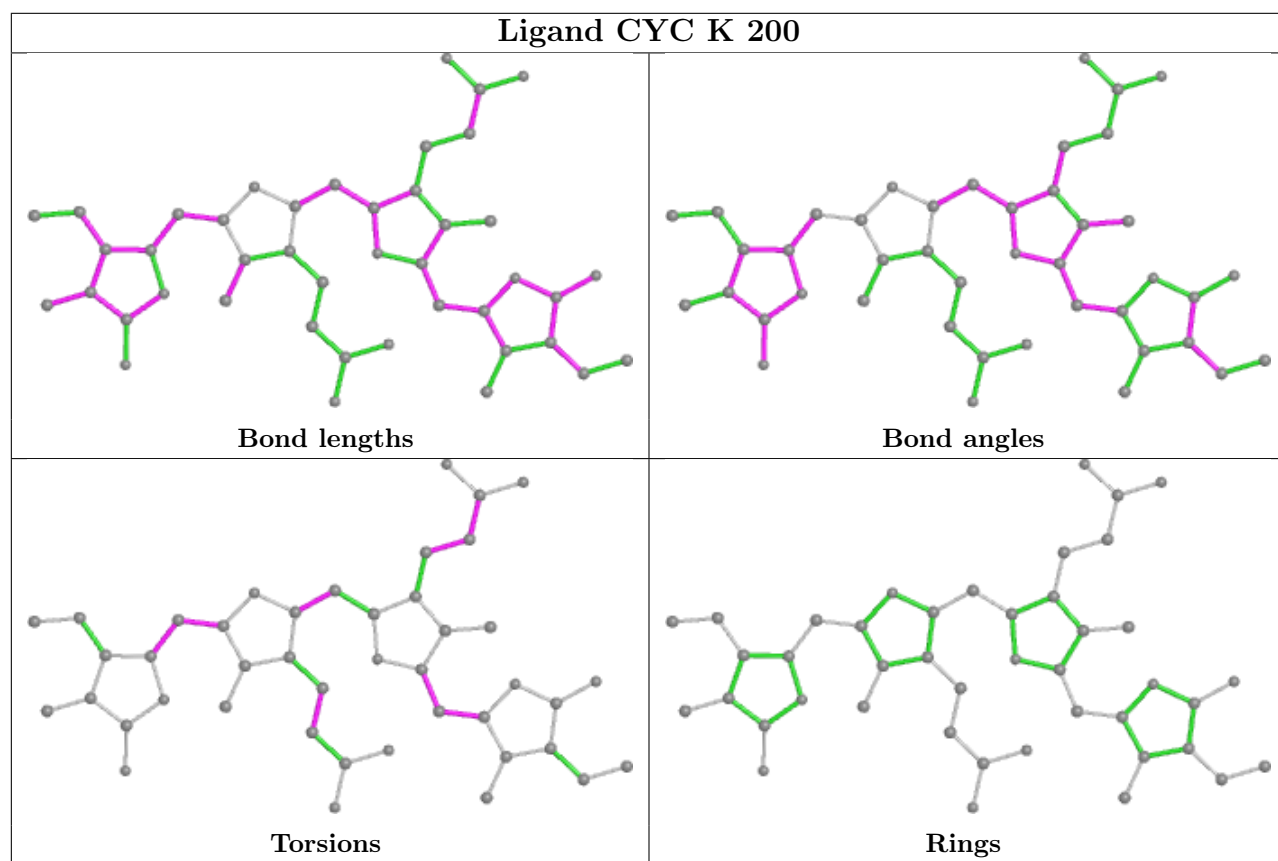
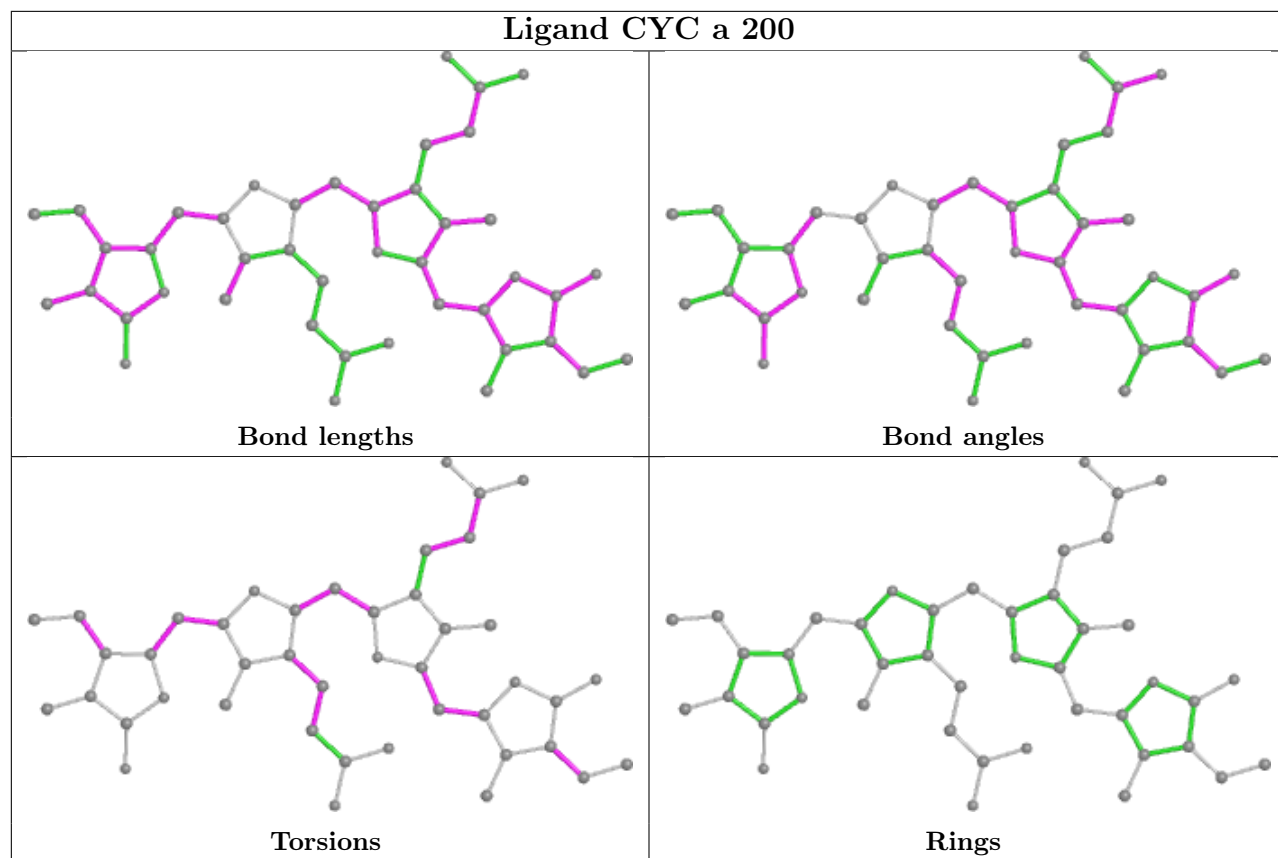


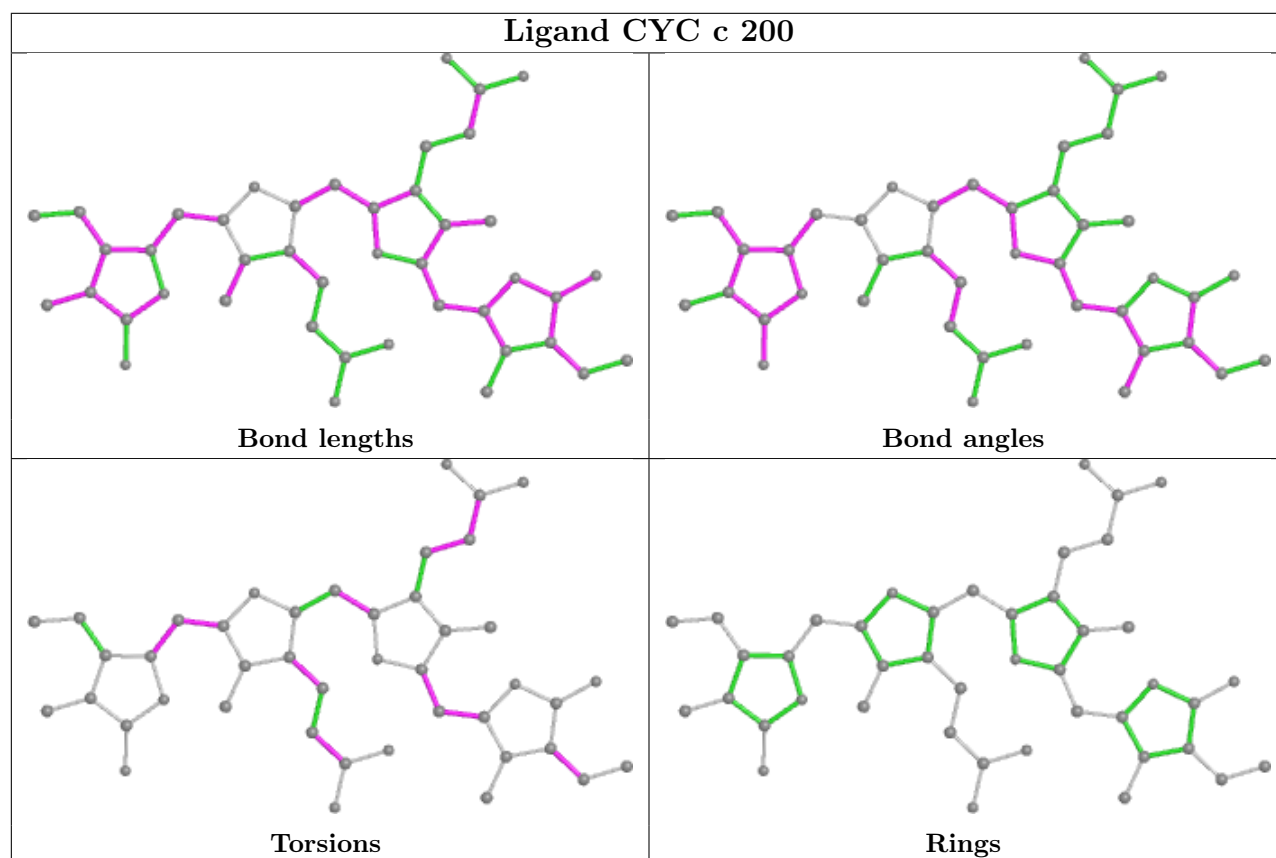
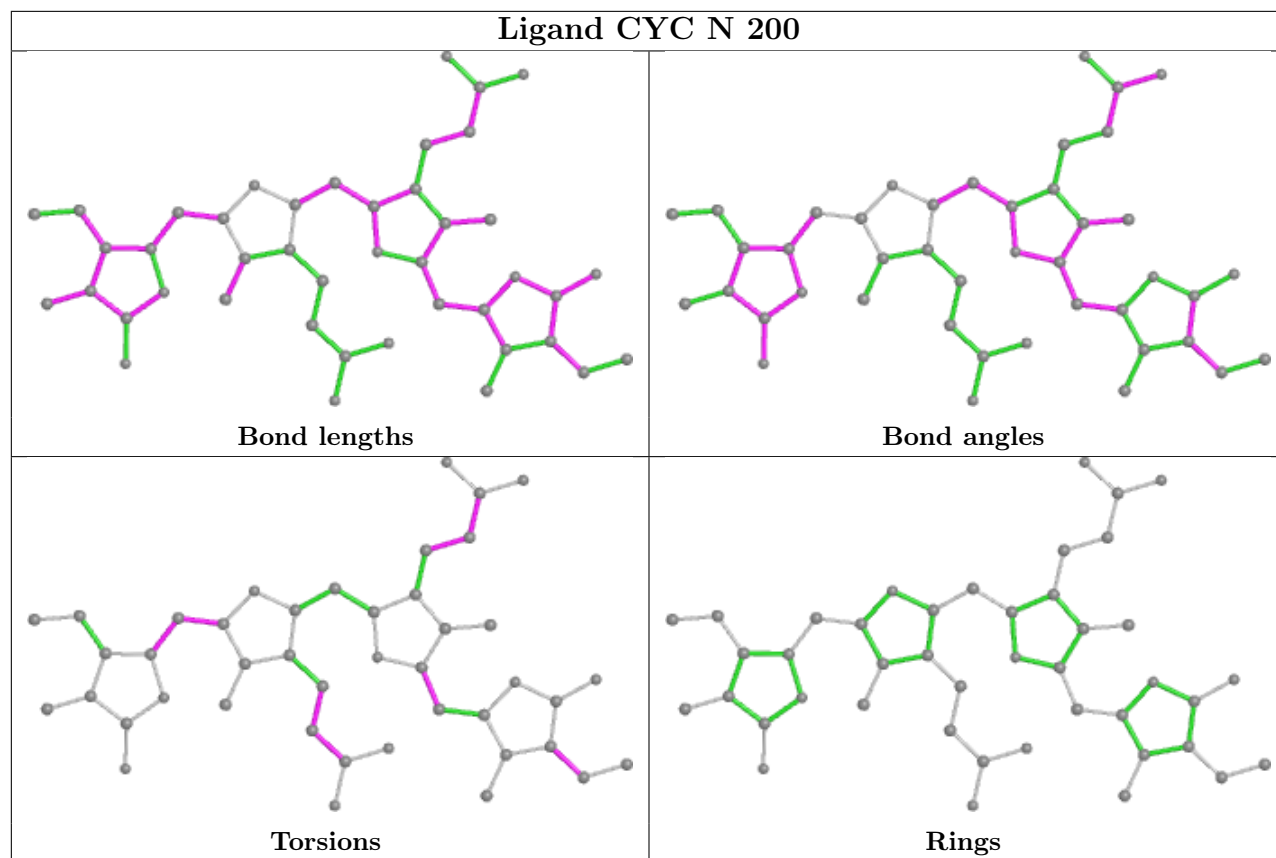


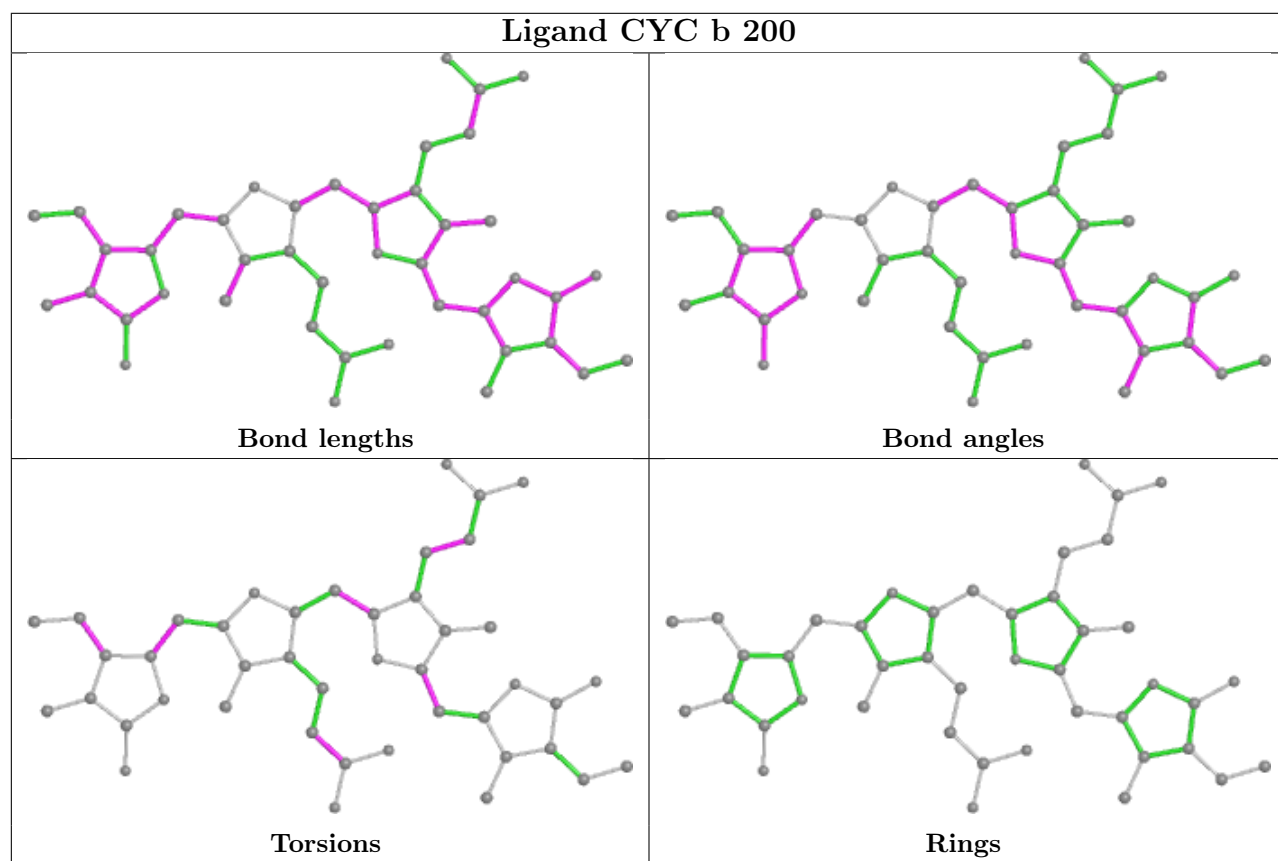
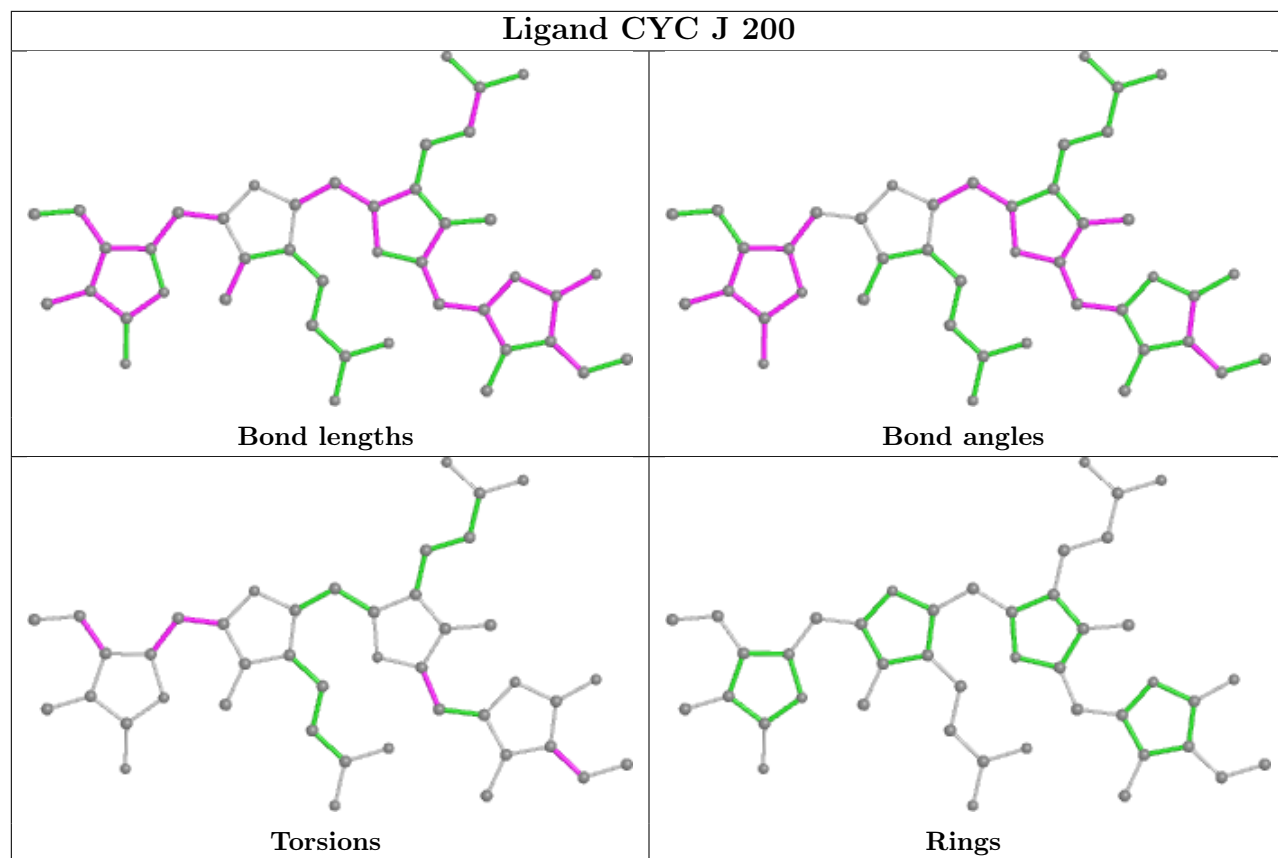


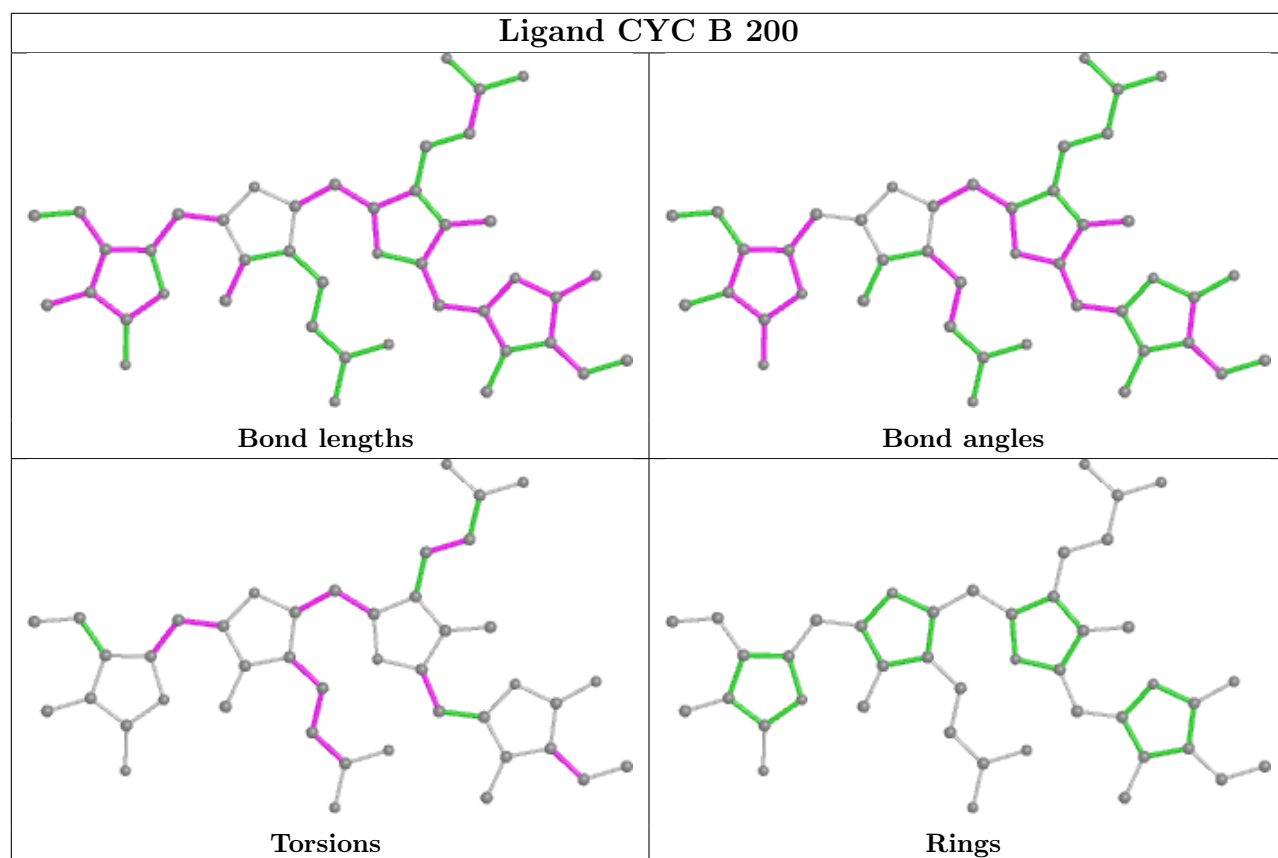
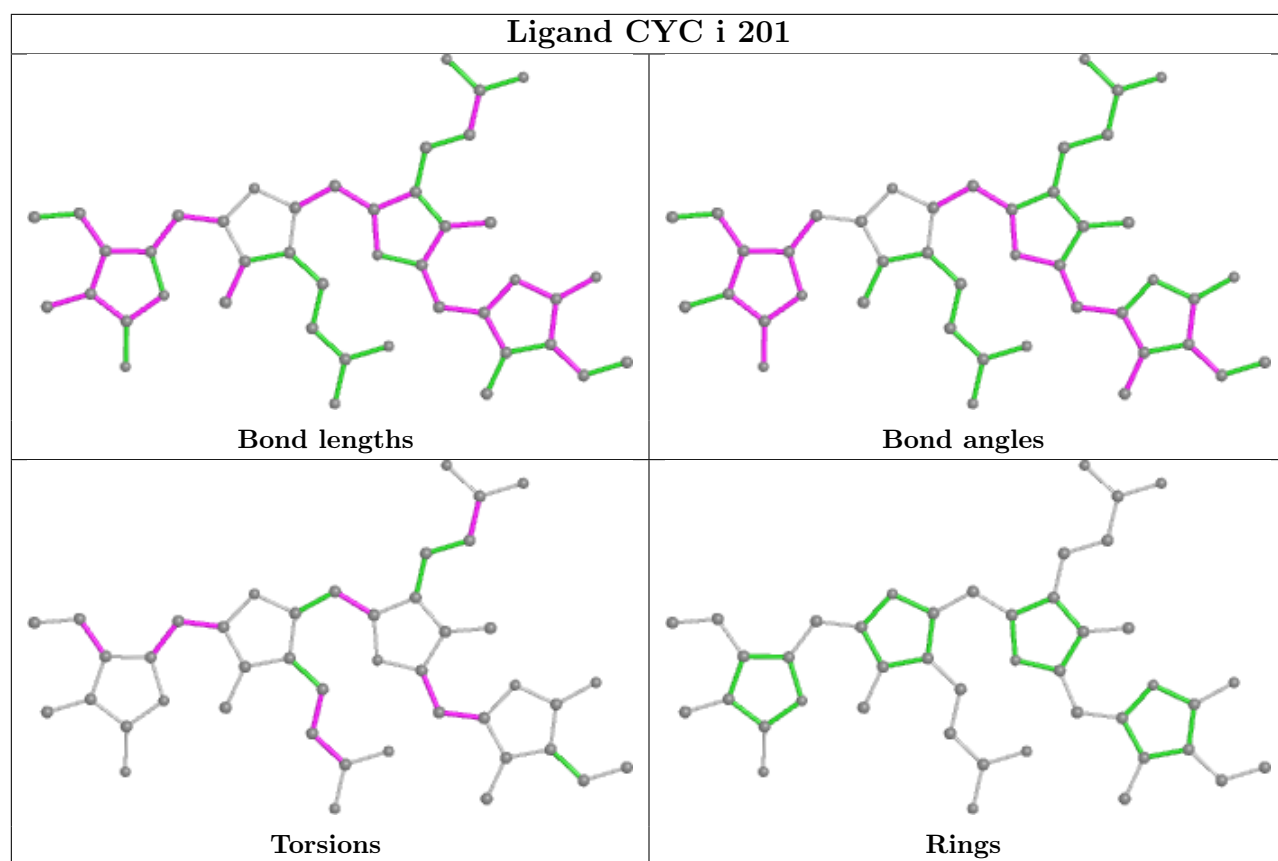


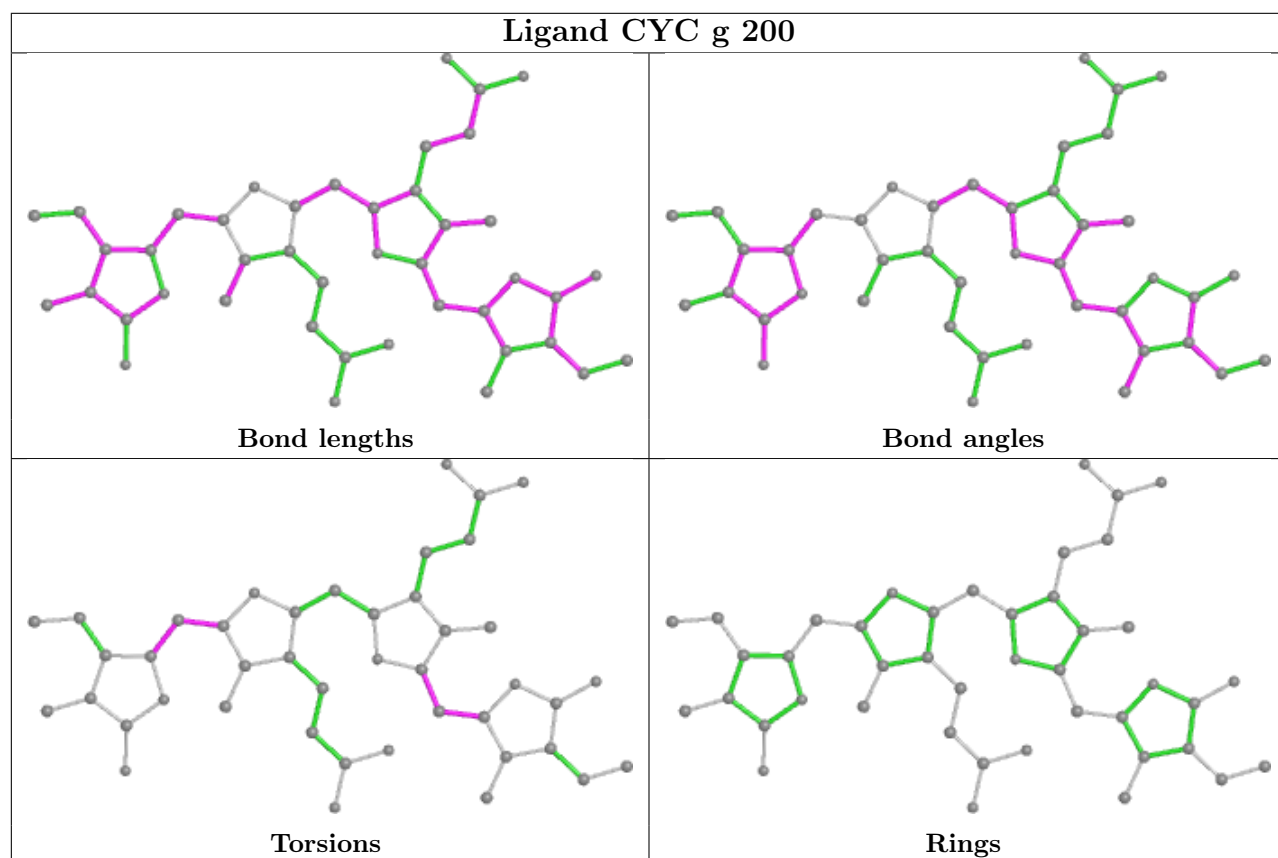
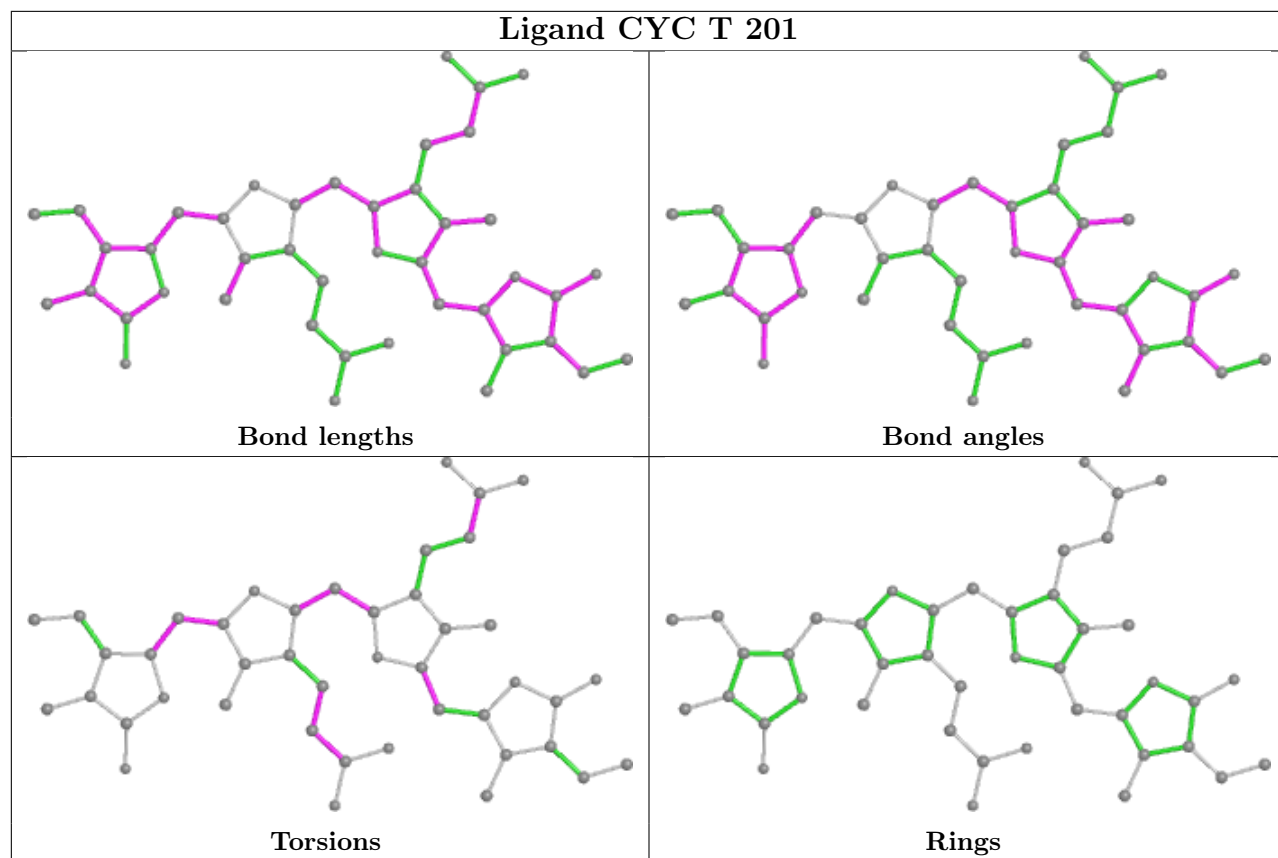












5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35570. These allow visual inspection of the internal detail of the map and identification of artifacts.

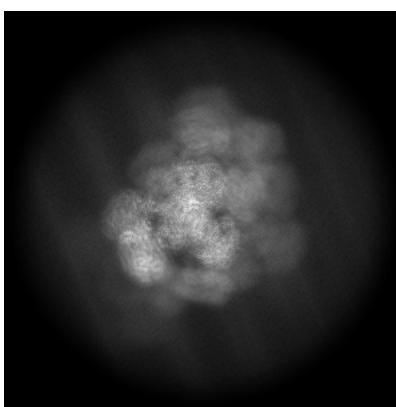
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

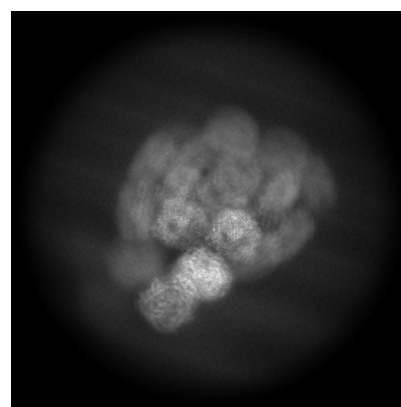
6.1.1 Primary map



X



Y

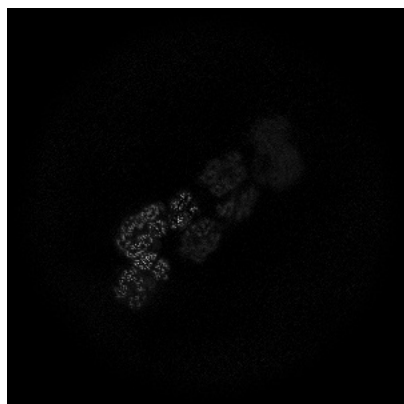


Z

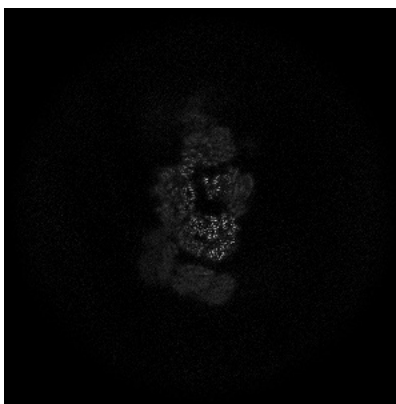
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

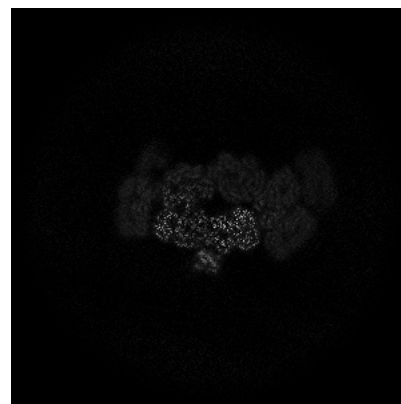
6.2.1 Primary map



X Index: 340



Y Index: 340

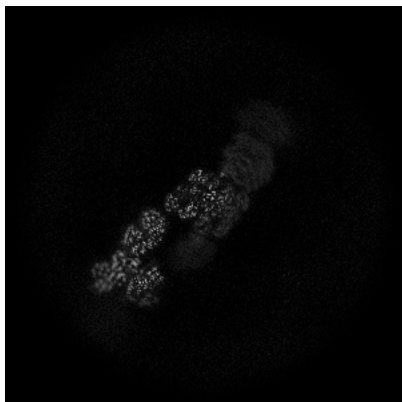


Z Index: 340

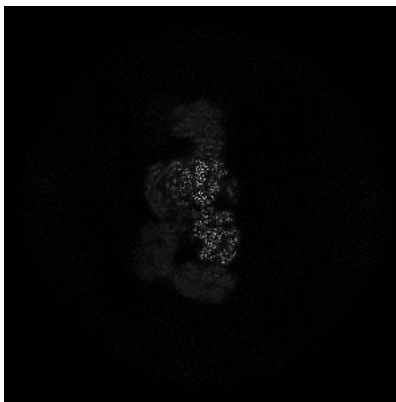
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

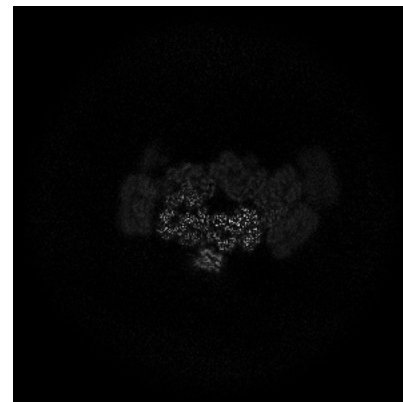
6.3.1 Primary map



X Index: 298



Y Index: 320



Z Index: 337

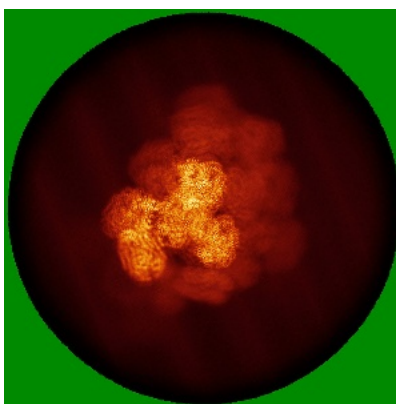
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

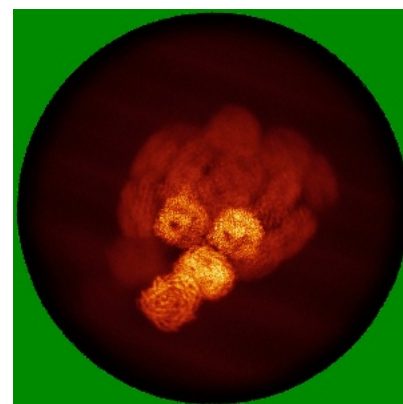
6.4.1 Primary map



X



Y



Z

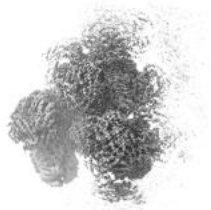
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.8. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

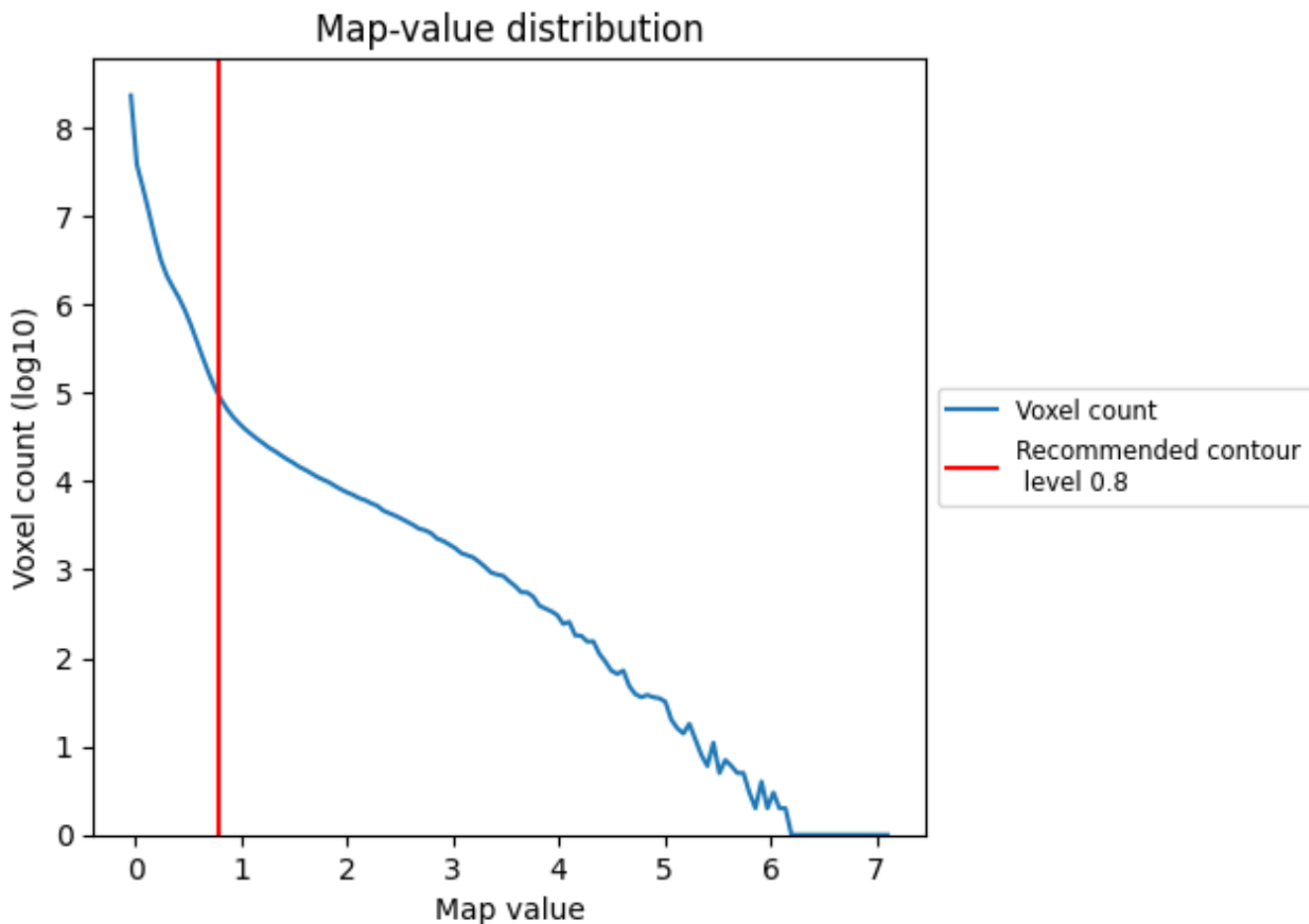
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

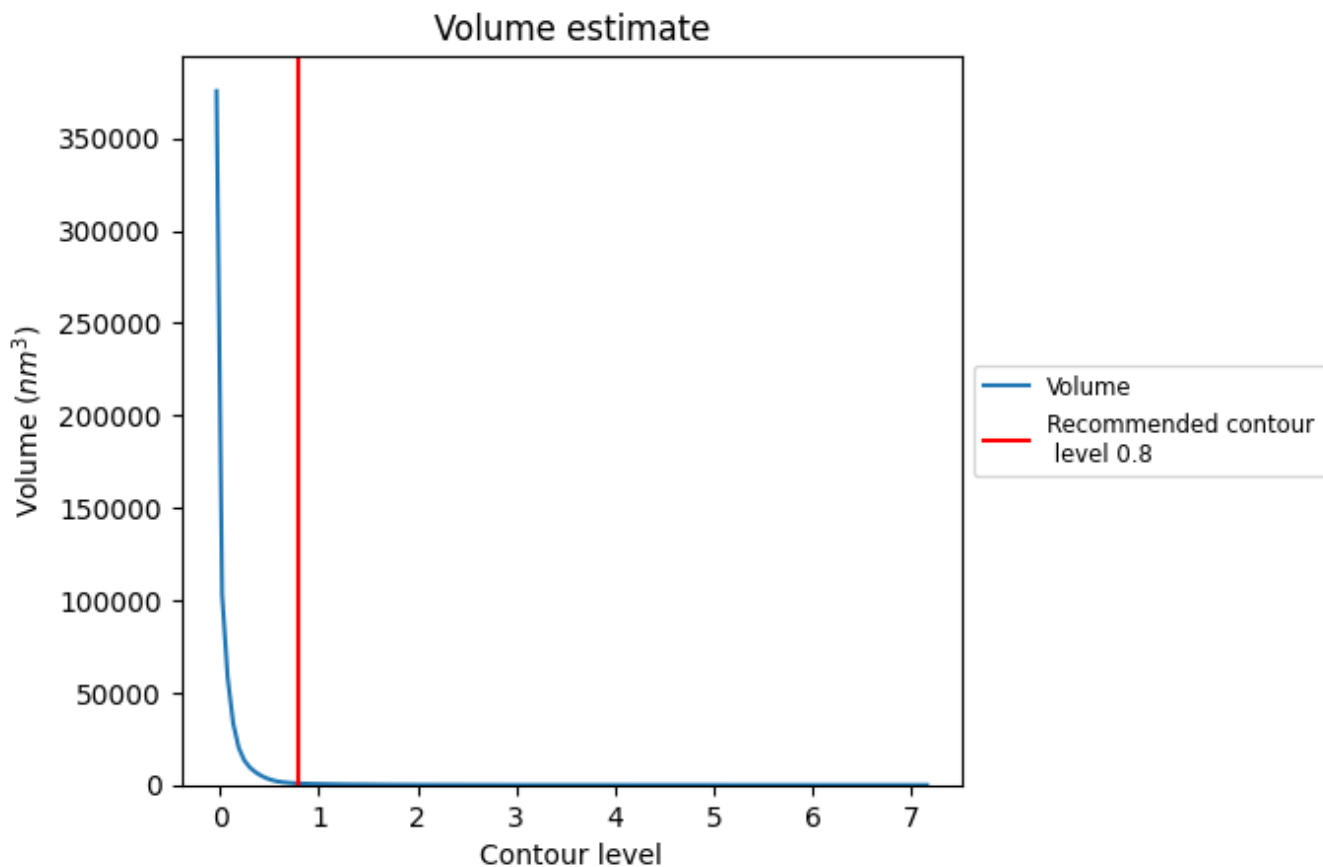
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

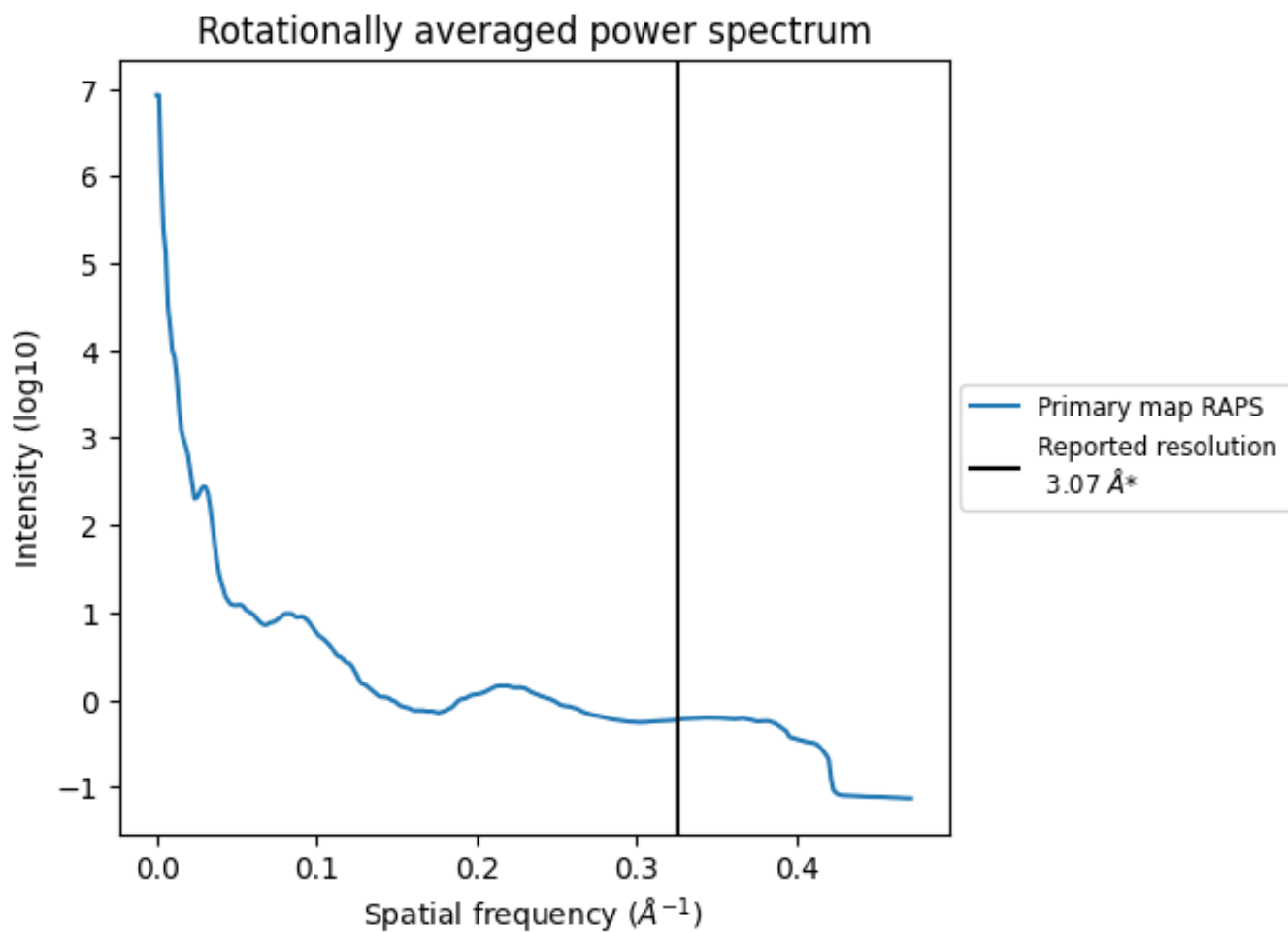
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 815 nm^3 ; this corresponds to an approximate mass of 736 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)



*Reported resolution corresponds to spatial frequency of 0.326 \AA^{-1}

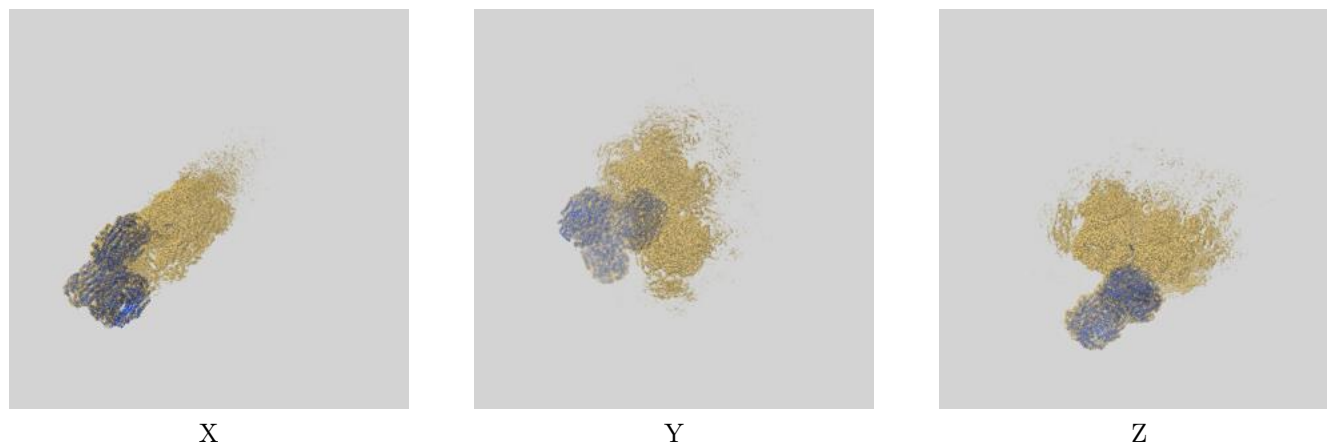
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

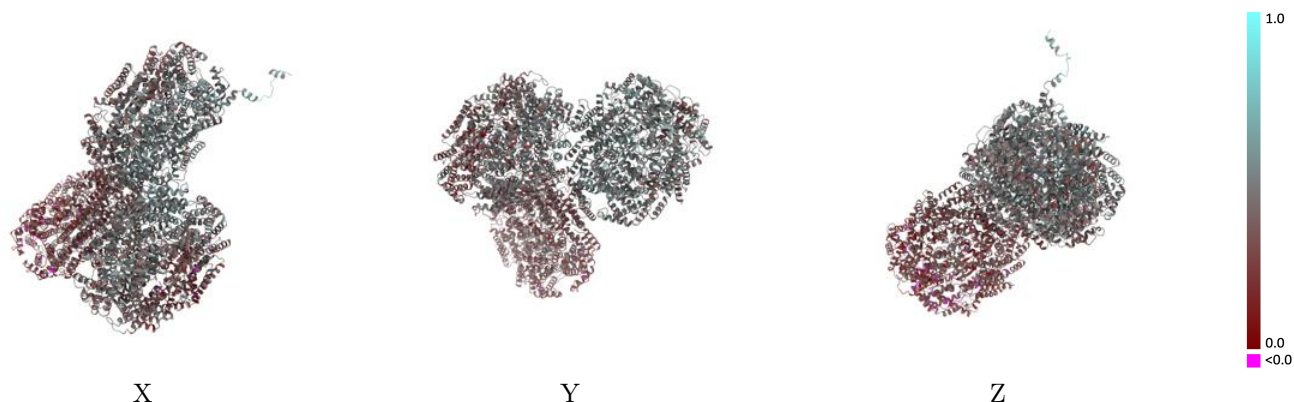
This section contains information regarding the fit between EMDB map EMD-35570 and PDB model 8IMN. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



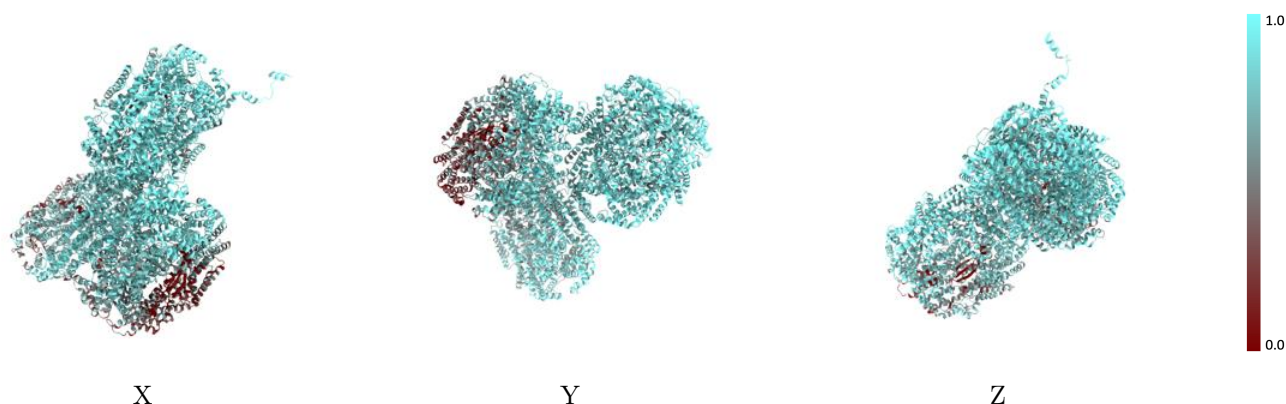
The images above show the 3D surface view of the map at the recommended contour level 0.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



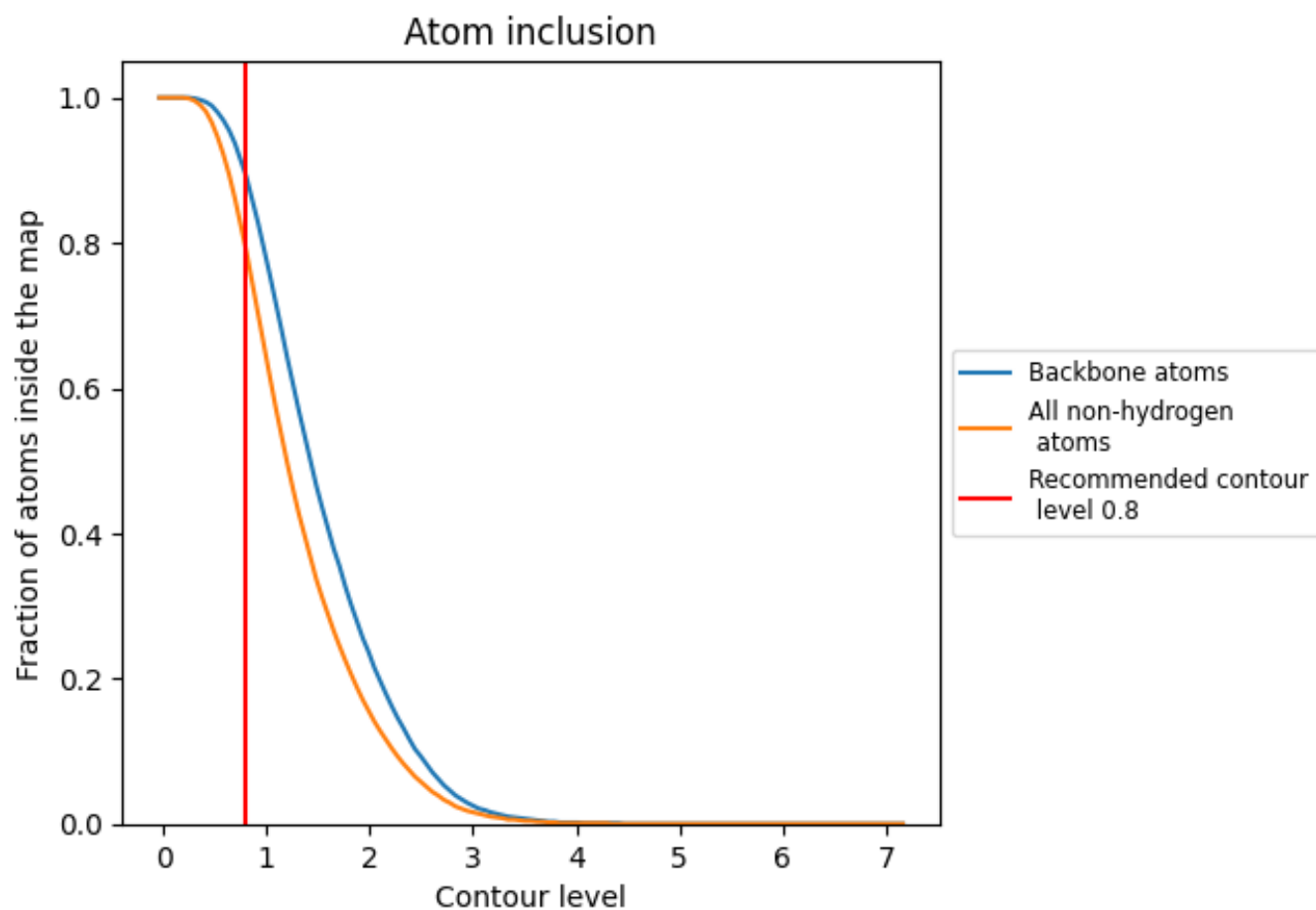
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.8).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 79% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary













The table lists the average atom inclusion at the recommended contour level (0.8) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|-------|--|--|
| All |  0.7910 |  0.3970 |
| 5 |  0.8500 |  0.4540 |
| A |  0.9390 |  0.4340 |
| B |  0.9400 |  0.4870 |
| C |  0.8590 |  0.4420 |
| D |  0.9220 |  0.5150 |
| E |  0.9220 |  0.4720 |
| F |  0.9100 |  0.5040 |
| G |  0.9210 |  0.4320 |
| H |  0.8160 |  0.4020 |
| I |  0.8720 |  0.4500 |
| J |  0.9170 |  0.5150 |
| K |  0.9180 |  0.5200 |
| L |  0.8680 |  0.5080 |
| M |  0.5730 |  0.3850 |
| N |  0.7860 |  0.4440 |
| O |  0.7730 |  0.4600 |
| P |  0.2910 |  0.3400 |
| Q |  0.7440 |  0.4660 |
| R |  0.6520 |  0.4330 |
| S |  0.9270 |  0.5170 |
| T |  0.7730 |  0.4070 |
| U |  0.4110 |  0.3550 |
| V |  0.4600 |  0.3910 |
| W |  0.9250 |  0.5130 |
| X |  0.7780 |  0.4660 |
| Y |  0.8300 |  0.4950 |
| Z |  0.0700 |  0.3000 |
| a |  0.8620 |  0.2810 |
| b |  0.8270 |  0.2670 |
| c |  0.6320 |  0.2060 |
| d |  0.8700 |  0.2620 |
| e |  0.8890 |  0.2670 |
| f |  0.9300 |  0.3340 |
| g |  0.8680 |  0.2740 |



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| Chain | Atom inclusion | Q-score |
|-------|--|--|
| h |  0.6360 |  0.2190 |
| i |  0.6710 |  0.2130 |
| j |  0.7710 |  0.2990 |
| k |  0.8330 |  0.2670 |
| l |  0.8970 |  0.3290 |
| m |  0.2480 |  0.1930 |