



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:18 PM UTC

PDB ID : 6TGE / pdb\_00006tge  
Title : NADP dependent methylene-tetrahydromethanopterin dehydrogenase-NADP  
+/-methenyl-H4MPT+ complex  
Authors : Ermler, U.; Shima, S.  
Deposited on : 2019-11-15  
Resolution : 1.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

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>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

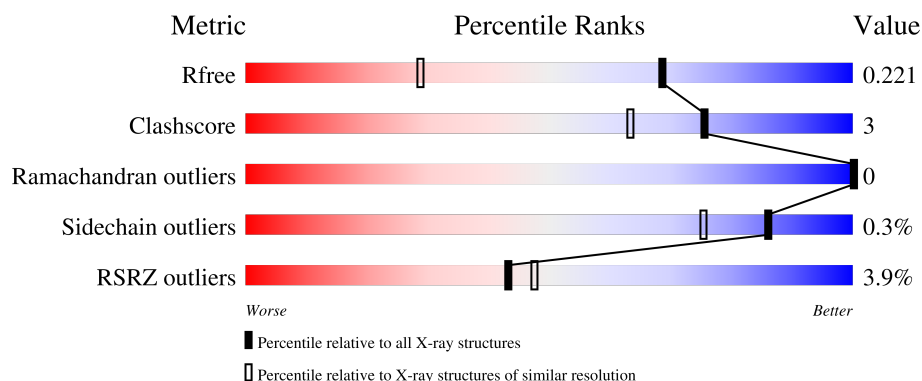
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.50 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.



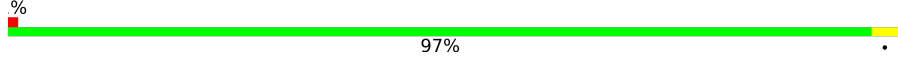
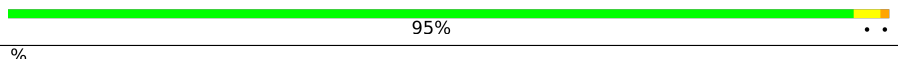
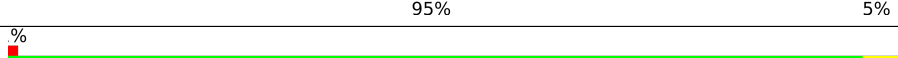
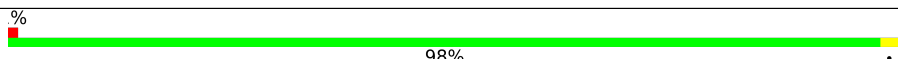
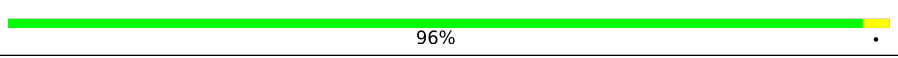
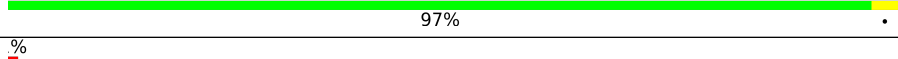
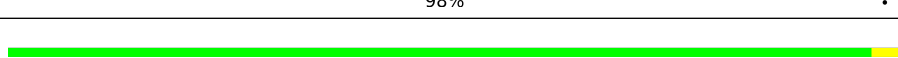
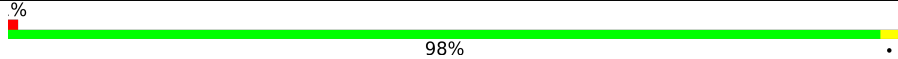
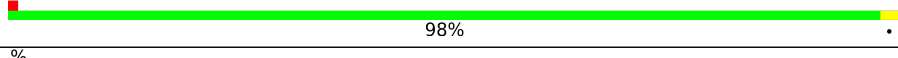
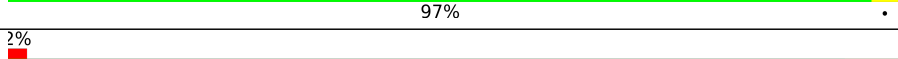
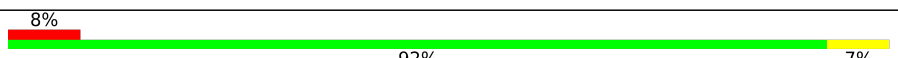
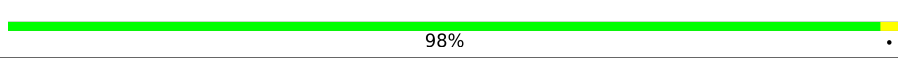
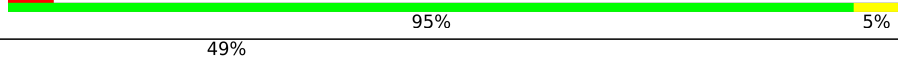
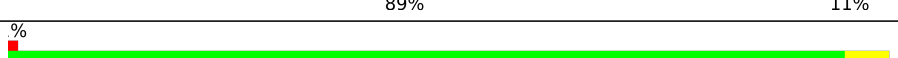
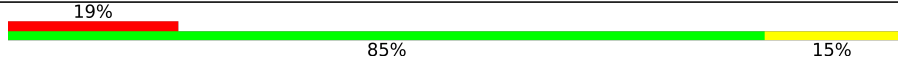
| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 4037 (1.50-1.50)                                      |
| Clashscore            | 190562                      | 4235 (1.50-1.50)                                      |
| Ramachandran outliers | 187476                      | 4153 (1.50-1.50)                                      |
| Sidechain outliers    | 187428                      | 4150 (1.50-1.50)                                      |
| RSRZ outliers         | 180081                      | 4039 (1.50-1.50)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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 electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 288    | 98%              |
| 1   | B     | 288    | 97%              |
| 1   | C     | 288    | 96%              |
| 1   | D     | 288    | 96%              |
| 1   | E     | 288    | 96%              |

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| Mol | Chain | Length | Quality of chain                                                                                 |
|-----|-------|--------|--------------------------------------------------------------------------------------------------|
| 1   | F     | 288    |  97% .         |
| 1   | G     | 288    |  95% . .       |
| 1   | H     | 288    |  95% 5%        |
| 1   | I     | 288    |  96% .         |
| 1   | J     | 288    |  98% .         |
| 1   | K     | 288    |  96% .         |
| 1   | L     | 288    |  97% .         |
| 1   | M     | 288    |  98% .         |
| 1   | N     | 288    |  97% .         |
| 1   | O     | 288    |  98% .        |
| 1   | P     | 288    |  98% .       |
| 1   | Q     | 288    |  97% .       |
| 1   | R     | 288    |  94% 6%      |
| 1   | S     | 288    |  92% 7%      |
| 1   | T     | 288    |  98% .       |
| 1   | U     | 288    |  95% 5%      |
| 1   | V     | 288    |  49% 89% 11% |
| 1   | W     | 288    |  94% 5%      |
| 1   | X     | 288    |  19% 85% 15% |

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 60219 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Bifunctional NADP-dependent methylenetetrahydromethano pterin dehydrogenase/methylenetetrahydrofolate dehydrogenase.

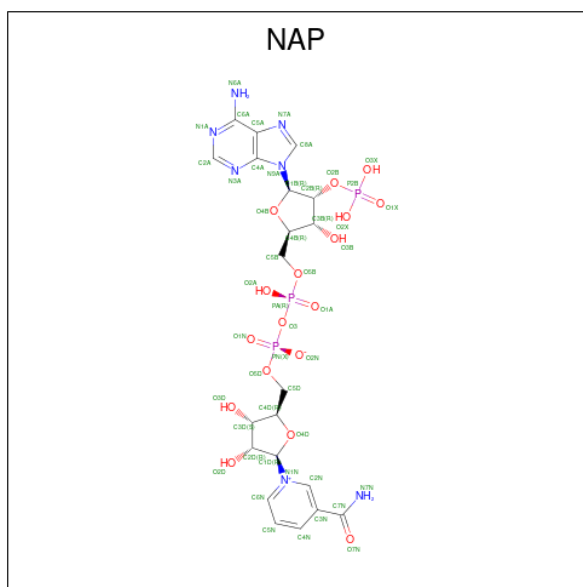
| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | A     | 287      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2084  | 1313 | 361 | 403 | 7 |         |         |       |
| 1   | B     | 287      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2084  | 1313 | 361 | 403 | 7 |         |         |       |
| 1   | C     | 287      | Total | C    | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 2091  | 1317 | 362 | 405 | 7 |         |         |       |
| 1   | D     | 287      | Total | C    | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 2092  | 1317 | 363 | 405 | 7 |         |         |       |
| 1   | E     | 287      | Total | C    | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 2091  | 1317 | 362 | 405 | 7 |         |         |       |
| 1   | F     | 287      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2084  | 1313 | 361 | 403 | 7 |         |         |       |
| 1   | G     | 287      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2084  | 1313 | 361 | 403 | 7 |         |         |       |
| 1   | H     | 287      | Total | C    | N   | O   | S | 0       | 4       | 0     |
|     |       |          | 2113  | 1328 | 365 | 413 | 7 |         |         |       |
| 1   | I     | 287      | Total | C    | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 2091  | 1317 | 362 | 405 | 7 |         |         |       |
| 1   | J     | 287      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2084  | 1313 | 361 | 403 | 7 |         |         |       |
| 1   | K     | 287      | Total | C    | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 2090  | 1316 | 362 | 405 | 7 |         |         |       |
| 1   | L     | 287      | Total | C    | N   | O   | S | 0       | 3       | 0     |
|     |       |          | 2105  | 1324 | 364 | 410 | 7 |         |         |       |
| 1   | M     | 287      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2084  | 1313 | 361 | 403 | 7 |         |         |       |
| 1   | N     | 287      | Total | C    | N   | O   | S | 0       | 3       | 0     |
|     |       |          | 2105  | 1325 | 365 | 408 | 7 |         |         |       |
| 1   | O     | 287      | Total | C    | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 2093  | 1319 | 363 | 404 | 7 |         |         |       |
| 1   | P     | 287      | Total | C    | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 2090  | 1316 | 362 | 405 | 7 |         |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | Q     | 287      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2084  | 1313 | 361 | 403 | 7 |         |         |       |
| 1   | R     | 287      | Total | C    | N   | O   | S | 0       | 3       | 0     |
|     |       |          | 2104  | 1323 | 364 | 410 | 7 |         |         |       |
| 1   | S     | 287      | Total | C    | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 2093  | 1319 | 363 | 404 | 7 |         |         |       |
| 1   | T     | 287      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2084  | 1313 | 361 | 403 | 7 |         |         |       |
| 1   | U     | 287      | Total | C    | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 2095  | 1319 | 365 | 404 | 7 |         |         |       |
| 1   | V     | 287      | Total | C    | N   | O   | S | 0       | 2       | 0     |
|     |       |          | 2099  | 1321 | 363 | 408 | 7 |         |         |       |
| 1   | W     | 287      | Total | C    | N   | O   | S | 0       | 2       | 0     |
|     |       |          | 2096  | 1319 | 363 | 407 | 7 |         |         |       |
| 1   | X     | 287      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2084  | 1313 | 361 | 403 | 7 |         |         |       |

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula:  $C_{21}H_{28}N_7O_{17}P_3$ ) (labeled as "Ligand of Interest" by depositor).



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| Mol | Chain | Residues | Atoms       |         |        |         |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|--------|---------|---------|
| 2   | D     | 1        | Total<br>48 | C<br>21 | N<br>7 | O<br>17 | P<br>3 | 0       | 0       |
| 2   | E     | 1        | Total<br>48 | C<br>21 | N<br>7 | O<br>17 | P<br>3 | 0       | 0       |
| 2   | F     | 1        | Total<br>48 | C<br>21 | N<br>7 | O<br>17 | P<br>3 | 0       | 0       |
| 2   | G     | 1        | Total<br>48 | C<br>21 | N<br>7 | O<br>17 | P<br>3 | 0       | 0       |
| 2   | H     | 1        | Total<br>48 | C<br>21 | N<br>7 | O<br>17 | P<br>3 | 0       | 0       |
| 2   | I     | 1        | Total<br>48 | C<br>21 | N<br>7 | O<br>17 | P<br>3 | 0       | 0       |
| 2   | J     | 1        | Total<br>48 | C<br>21 | N<br>7 | O<br>17 | P<br>3 | 0       | 0       |
| 2   | K     | 1        | Total<br>48 | C<br>21 | N<br>7 | O<br>17 | P<br>3 | 0       | 0       |
| 2   | L     | 1        | Total<br>48 | C<br>21 | N<br>7 | O<br>17 | P<br>3 | 0       | 0       |
| 2   | M     | 1        | Total<br>48 | C<br>21 | N<br>7 | O<br>17 | P<br>3 | 0       | 0       |
| 2   | N     | 1        | Total<br>48 | C<br>21 | N<br>7 | O<br>17 | P<br>3 | 0       | 0       |
| 2   | O     | 1        | Total<br>48 | C<br>21 | N<br>7 | O<br>17 | P<br>3 | 0       | 0       |
| 2   | P     | 1        | Total<br>48 | C<br>21 | N<br>7 | O<br>17 | P<br>3 | 0       | 0       |
| 2   | Q     | 1        | Total<br>48 | C<br>21 | N<br>7 | O<br>17 | P<br>3 | 0       | 0       |
| 2   | R     | 1        | Total<br>48 | C<br>21 | N<br>7 | O<br>17 | P<br>3 | 0       | 0       |
| 2   | S     | 1        | Total<br>48 | C<br>21 | N<br>7 | O<br>17 | P<br>3 | 0       | 0       |
| 2   | T     | 1        | Total<br>48 | C<br>21 | N<br>7 | O<br>17 | P<br>3 | 0       | 0       |
| 2   | U     | 1        | Total<br>48 | C<br>21 | N<br>7 | O<br>17 | P<br>3 | 0       | 0       |
| 2   | V     | 1        | Total<br>48 | C<br>21 | N<br>7 | O<br>17 | P<br>3 | 0       | 0       |
| 2   | W     | 1        | Total<br>48 | C<br>21 | N<br>7 | O<br>17 | P<br>3 | 0       | 0       |
| 2   | X     | 1        | Total<br>48 | C<br>21 | N<br>7 | O<br>17 | P<br>3 | 0       | 0       |

- # H4M

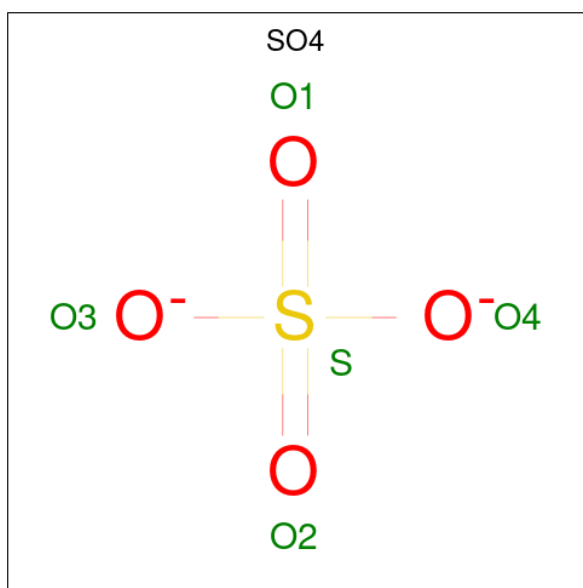
| Mol | Chain | Residues | Atoms       |         |        |         |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|--------|---------|---------|
| 3   | A     | 1        | Total<br>45 | C<br>26 | N<br>6 | O<br>12 | P<br>1 | 0       | 0       |
| 3   | B     | 1        | Total<br>45 | C<br>26 | N<br>6 | O<br>12 | P<br>1 | 14      | 0       |
| 3   | C     | 1        | Total<br>45 | C<br>26 | N<br>6 | O<br>12 | P<br>1 | 0       | 0       |
| 3   | D     | 1        | Total<br>45 | C<br>26 | N<br>6 | O<br>12 | P<br>1 | 0       | 0       |
| 3   | E     | 1        | Total<br>45 | C<br>26 | N<br>6 | O<br>12 | P<br>1 | 14      | 0       |
| 3   | F     | 1        | Total<br>45 | C<br>26 | N<br>6 | O<br>12 | P<br>1 | 14      | 0       |
| 3   | G     | 1        | Total<br>45 | C<br>26 | N<br>6 | O<br>12 | P<br>1 | 0       | 0       |
| 3   | H     | 1        | Total<br>45 | C<br>26 | N<br>6 | O<br>12 | P<br>1 | 14      | 0       |
| 3   | I     | 1        | Total<br>45 | C<br>26 | N<br>6 | O<br>12 | P<br>1 | 13      | 0       |
| 3   | J     | 1        | Total<br>45 | C<br>26 | N<br>6 | O<br>12 | P<br>1 | 0       | 0       |
| 3   | K     | 1        | Total<br>45 | C<br>26 | N<br>6 | O<br>12 | P<br>1 | 13      | 0       |
| 3   | L     | 1        | Total<br>45 | C<br>26 | N<br>6 | O<br>12 | P<br>1 | 13      | 0       |

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| Mol | Chain | Residues | Atoms |    |   |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| 3   | M     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 45    | 26 | 6 | 12 | 1 |         |         |
| 3   | N     | 1        | Total | C  | N | O  | P | 13      | 0       |
|     |       |          | 45    | 26 | 6 | 12 | 1 |         |         |
| 3   | O     | 1        | Total | C  | N | O  | P | 13      | 0       |
|     |       |          | 45    | 26 | 6 | 12 | 1 |         |         |
| 3   | P     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 45    | 26 | 6 | 12 | 1 |         |         |
| 3   | Q     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 45    | 26 | 6 | 12 | 1 |         |         |
| 3   | R     | 1        | Total | C  | N | O  | P | 13      | 0       |
|     |       |          | 45    | 26 | 6 | 12 | 1 |         |         |
| 3   | S     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 45    | 26 | 6 | 12 | 1 |         |         |
| 3   | T     | 1        | Total | C  | N | O  | P | 13      | 0       |
|     |       |          | 45    | 26 | 6 | 12 | 1 |         |         |
| 3   | U     | 1        | Total | C  | N | O  | P | 13      | 0       |
|     |       |          | 45    | 26 | 6 | 12 | 1 |         |         |
| 3   | V     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 45    | 26 | 6 | 12 | 1 |         |         |
| 3   | W     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 45    | 26 | 6 | 12 | 1 |         |         |
| 3   | X     | 1        | Total | C  | N | O  | P | 13      | 0       |
|     |       |          | 45    | 26 | 6 | 12 | 1 |         |         |

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



| Mol | Chain | Residues | Atoms              | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 4   | A     | 1        | Total O S<br>5 4 1 | 0       | 0       |
| 4   | D     | 1        | Total O S<br>5 4 1 | 0       | 0       |
| 4   | H     | 1        | Total O S<br>5 4 1 | 0       | 0       |
| 4   | J     | 1        | Total O S<br>5 4 1 | 0       | 0       |
| 4   | M     | 1        | Total O S<br>5 4 1 | 0       | 0       |
| 4   | P     | 1        | Total O S<br>5 4 1 | 0       | 0       |
| 4   | S     | 1        | Total O S<br>5 4 1 | 0       | 0       |
| 4   | V     | 1        | Total O S<br>5 4 1 | 0       | 0       |

- Molecule 5 is water.

| Mol | Chain | Residues | Atoms              | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 5   | A     | 386      | Total O<br>387 387 | 0       | 1       |
| 5   | B     | 349      | Total O<br>354 354 | 0       | 5       |
| 5   | C     | 339      | Total O<br>341 341 | 0       | 2       |
| 5   | D     | 329      | Total O<br>331 331 | 0       | 2       |
| 5   | E     | 387      | Total O<br>390 390 | 0       | 3       |
| 5   | F     | 365      | Total O<br>368 368 | 0       | 3       |
| 5   | G     | 379      | Total O<br>385 385 | 0       | 6       |
| 5   | H     | 401      | Total O<br>404 404 | 0       | 3       |
| 5   | I     | 347      | Total O<br>350 350 | 0       | 3       |
| 5   | J     | 349      | Total O<br>352 352 | 0       | 3       |
| 5   | K     | 348      | Total O<br>352 352 | 0       | 4       |
| 5   | L     | 308      | Total O<br>309 309 | 0       | 1       |

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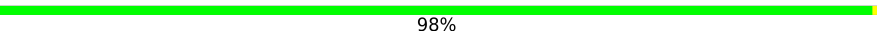
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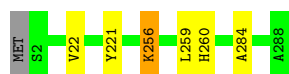
| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 5   | M     | 381      | Total<br>382 | O<br>382 | 0       | 1       |
| 5   | N     | 362      | Total<br>363 | O<br>363 | 0       | 1       |
| 5   | O     | 331      | Total<br>334 | O<br>334 | 0       | 3       |
| 5   | P     | 310      | Total<br>310 | O<br>310 | 0       | 0       |
| 5   | Q     | 378      | Total<br>381 | O<br>381 | 0       | 3       |
| 5   | R     | 227      | Total<br>232 | O<br>232 | 0       | 5       |
| 5   | S     | 253      | Total<br>257 | O<br>257 | 0       | 4       |
| 5   | T     | 328      | Total<br>330 | O<br>330 | 0       | 2       |
| 5   | U     | 194      | Total<br>194 | O<br>194 | 0       | 0       |
| 5   | V     | 197      | Total<br>197 | O<br>197 | 0       | 0       |
| 5   | W     | 320      | Total<br>323 | O<br>323 | 0       | 3       |
| 5   | X     | 116      | Total<br>117 | O<br>117 | 0       | 1       |

### 3 Residue-property plots [i](#)

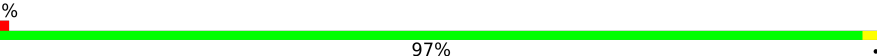
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

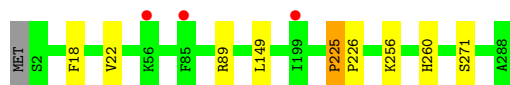
- Molecule 1: Bifunctional NADP-dependent methylenetetrahydromethanopterin dehydrogenase /methylenetetrahydrofolate dehydrogenase

Chain A:  98%

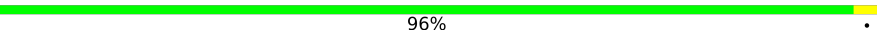


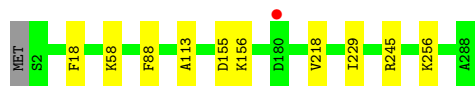
- Molecule 1: Bifunctional NADP-dependent methylenetetrahydromethanopterin dehydrogenase /methylenetetrahydrofolate dehydrogenase

Chain B:  97%

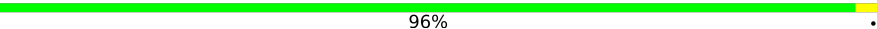


- Molecule 1: Bifunctional NADP-dependent methylenetetrahydromethanopterin dehydrogenase /methylenetetrahydrofolate dehydrogenase

Chain C:  96%

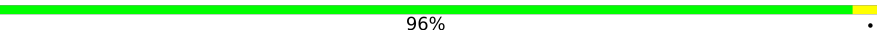


- Molecule 1: Bifunctional NADP-dependent methylenetetrahydromethanopterin dehydrogenase /methylenetetrahydrofolate dehydrogenase

Chain D:  96%

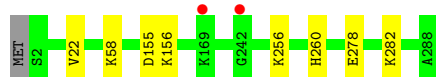


- Molecule 1: Bifunctional NADP-dependent methylenetetrahydromethanopterin dehydrogenase /methylenetetrahydrofolate dehydrogenase

Chain E:  96%



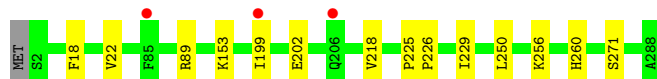
- Molecule 1: Bifunctional NADP-dependent methylenetetrahydromethanopterin dehydrogenase /methylenetetrahydrofolate dehydrogenase



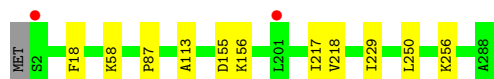
- Molecule 1: Bifunctional NADP-dependent methylenetetrahydromethanopterin dehydrogenase /methylenetetrahydrofolate dehydrogenase



- Molecule 1: Bifunctional NADP-dependent methylenetetrahydromethanopterin dehydrogenase /methylenetetrahydrofolate dehydrogenase



- Molecule 1: Bifunctional NADP-dependent methylenetetrahydromethanopterin dehydrogenase /methylenetetrahydrofolate dehydrogenase

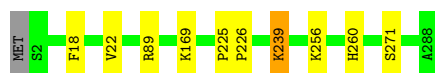


- Molecule 1: Bifunctional NADP-dependent methylenetetrahydromethanopterin dehydrogenase /methylenetetrahydrofolate dehydrogenase

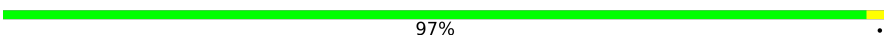


- Molecule 1: Bifunctional NADP-dependent methylenetetrahydromethanopterin dehydrogenase /methylenetetrahydrofolate dehydrogenase



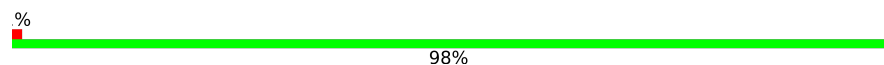


- Molecule 1: Bifunctional NADP-dependent methylenetetrahydromethanopterin dehydrogenase /methylenetetrahydrofolate dehydrogenase

Chain L:  97%

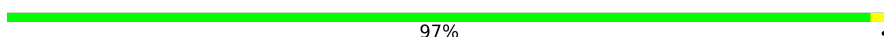


- Molecule 1: Bifunctional NADP-dependent methylenetetrahydromethanopterin dehydrogenase /methylenetetrahydrofolate dehydrogenase

Chain M:  98%

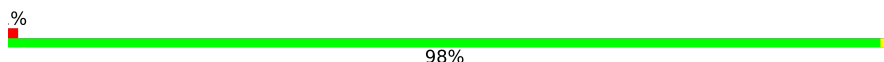


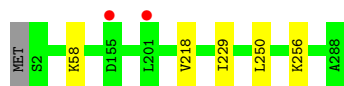
- Molecule 1: Bifunctional NADP-dependent methylenetetrahydromethanopterin dehydrogenase /methylenetetrahydrofolate dehydrogenase

Chain N:  97%

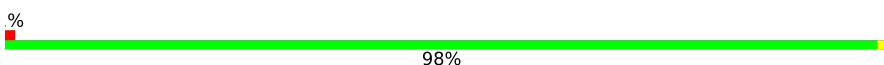


- Molecule 1: Bifunctional NADP-dependent methylenetetrahydromethanopterin dehydrogenase /methylenetetrahydrofolate dehydrogenase

Chain O:  98%

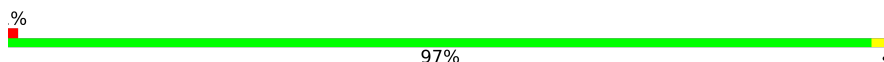


- Molecule 1: Bifunctional NADP-dependent methylenetetrahydromethanopterin dehydrogenase /methylenetetrahydrofolate dehydrogenase

Chain P:  98%

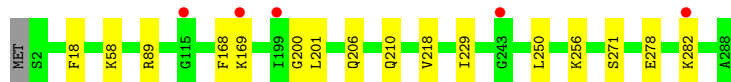


- Molecule 1: Bifunctional NADP-dependent methylenetetrahydromethanopterin dehydrogenase /methylenetetrahydrofolate dehydrogenase

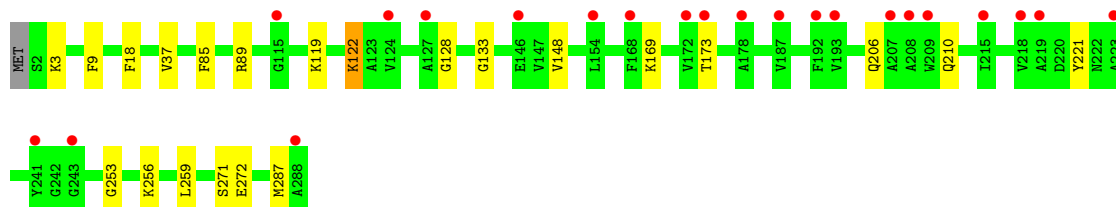
Chain Q:  97%



- Molecule 1: Bifunctional NADP-dependent methylenetetrahydromethanopterin dehydrogenase /methylenetetrahydrofolate dehydrogenase



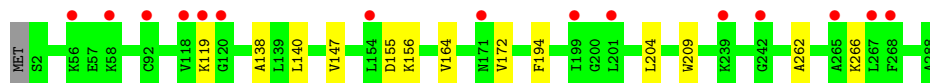
- Molecule 1: Bifunctional NADP-dependent methylenetetrahydromethanopterin dehydrogenase /methylenetetrahydrofolate dehydrogenase



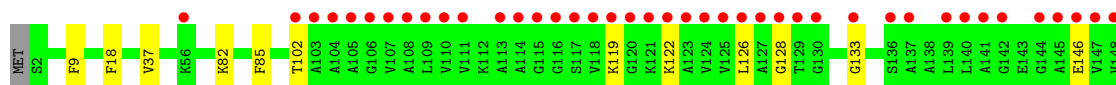
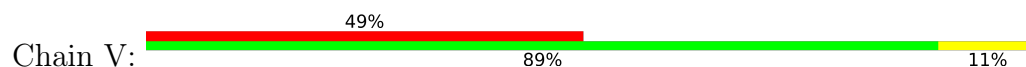
- Molecule 1: Bifunctional NADP-dependent methylenetetrahydromethanopterin dehydrogenase /methylenetetrahydrofolate dehydrogenase

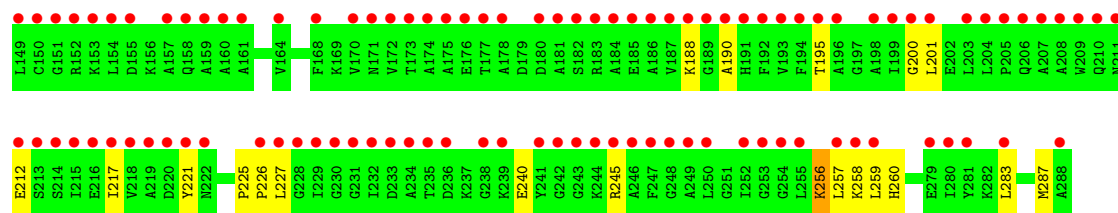


- Molecule 1: Bifunctional NADP-dependent methylenetetrahydromethanopterin dehydrogenase /methylenetetrahydrofolate dehydrogenase



- Molecule 1: Bifunctional NADP-dependent methylenetetrahydromethanopterin dehydrogenase /methylenetetrahydrofolate dehydrogenase

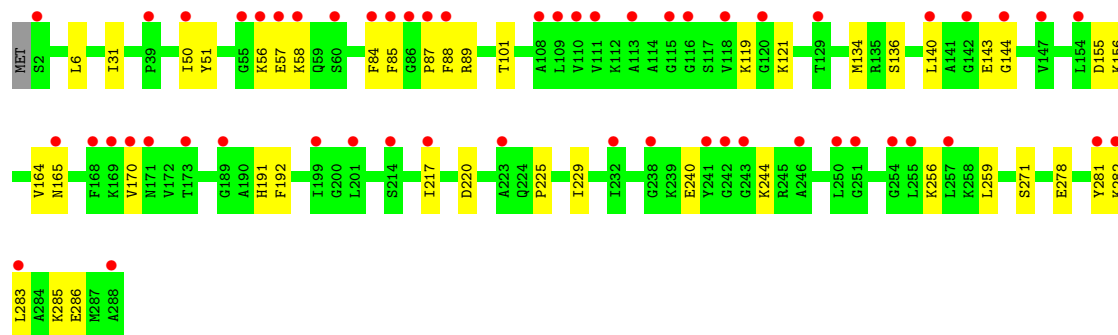
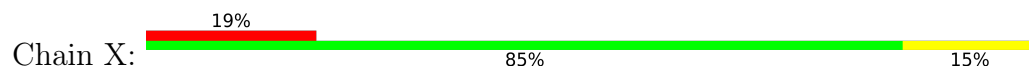




- Molecule 1: Bifunctional NADP-dependent methylenetetrahydromethanopterin dehydrogenase /methylenetetrahydrofolate dehydrogenase



- Molecule 1: Bifunctional NADP-dependent methylenetetrahydromethanopterin dehydrogenase /methylenetetrahydrofolate dehydrogenase



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 1                                                         | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 98.64Å 123.50Å 167.30Å<br>94.79° 100.39° 108.97°            | Depositor        |
| Resolution (Å)                                                          | 48.76 – 1.50<br>48.76 – 1.50                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 95.4 (48.76-1.50)<br>95.5 (48.76-1.50)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.00 (at 1.50Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX 1.14_3260                                            | Depositor        |
| R, $R_{free}$                                                           | 0.186 , 0.216<br>0.192 , 0.221                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 55363 reflections (4.76%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 19.9                                                        | Xtriage          |
| Anisotropy                                                              | 0.514                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.36 , 48.0                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.97                                                        | EDS              |
| Total number of atoms                                                   | 60219                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 31.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.59 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.7090e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 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: SO4, NAP, H4M

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   | A     | 0.35         | 1/2116 (0.0%)  | 0.50        | 0/2850         |
| 1   | B     | 0.45         | 1/2116 (0.0%)  | 0.53        | 1/2850 (0.0%)  |
| 1   | C     | 0.25         | 0/2123         | 0.43        | 0/2860         |
| 1   | D     | 0.30         | 0/2124         | 0.48        | 0/2861         |
| 1   | E     | 0.29         | 0/2123         | 0.46        | 0/2860         |
| 1   | F     | 0.29         | 0/2116         | 0.46        | 0/2850         |
| 1   | G     | 0.44         | 2/2116 (0.1%)  | 0.53        | 1/2850 (0.0%)  |
| 1   | H     | 0.33         | 0/2145         | 0.50        | 0/2889         |
| 1   | I     | 0.27         | 0/2123         | 0.46        | 0/2860         |
| 1   | J     | 0.25         | 0/2116         | 0.46        | 0/2850         |
| 1   | K     | 0.24         | 0/2122         | 0.43        | 0/2858         |
| 1   | L     | 0.26         | 0/2137         | 0.44        | 1/2878 (0.0%)  |
| 1   | M     | 0.33         | 0/2116         | 0.53        | 0/2850         |
| 1   | N     | 0.32         | 0/2137         | 0.47        | 0/2877         |
| 1   | O     | 0.24         | 0/2125         | 0.43        | 0/2861         |
| 1   | P     | 0.30         | 0/2122         | 0.47        | 0/2858         |
| 1   | Q     | 0.28         | 0/2116         | 0.46        | 0/2850         |
| 1   | R     | 0.26         | 0/2136         | 0.43        | 0/2877         |
| 1   | S     | 0.24         | 0/2125         | 0.43        | 0/2861         |
| 1   | T     | 0.24         | 0/2116         | 0.43        | 0/2850         |
| 1   | U     | 0.25         | 0/2127         | 0.41        | 0/2864         |
| 1   | V     | 0.30         | 0/2131         | 0.48        | 0/2870         |
| 1   | W     | 0.23         | 0/2128         | 0.41        | 0/2866         |
| 1   | X     | 0.36         | 1/2116 (0.0%)  | 0.46        | 1/2850 (0.0%)  |
| All | All   | 0.30         | 5/50972 (0.0%) | 0.46        | 4/68650 (0.0%) |

All (5) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 1   | B     | 225 | PRO  | CA-C  | -16.04 | 1.43        | 1.51     |
| 1   | X     | 225 | PRO  | CA-C  | 13.38  | 1.59        | 1.51     |

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| Mol | Chain | Res | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 1   | G     | 225 | PRO  | CA-C  | -13.06 | 1.44        | 1.51     |
| 1   | A     | 256 | LYS  | C-O   | -6.02  | 1.17        | 1.24     |
| 1   | G     | 256 | LYS  | C-O   | -5.56  | 1.17        | 1.24     |

All (4) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1   | B     | 225 | PRO  | O-C-N   | -13.78 | 114.97      | 121.31   |
| 1   | X     | 225 | PRO  | O-C-N   | 10.20  | 126.00      | 121.31   |
| 1   | G     | 225 | PRO  | O-C-N   | -9.80  | 116.80      | 121.31   |
| 1   | L     | 179 | ASP  | CB-CA-C | -6.93  | 97.15       | 113.02   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 2084  | 0        | 2086     | 3       | 0            |
| 1   | B     | 2084  | 0        | 2086     | 7       | 0            |
| 1   | C     | 2091  | 0        | 2092     | 8       | 0            |
| 1   | D     | 2092  | 0        | 2091     | 11      | 0            |
| 1   | E     | 2091  | 0        | 2092     | 12      | 0            |
| 1   | F     | 2084  | 0        | 2086     | 9       | 0            |
| 1   | G     | 2084  | 0        | 2086     | 8       | 0            |
| 1   | H     | 2113  | 0        | 2102     | 13      | 0            |
| 1   | I     | 2091  | 0        | 2092     | 8       | 0            |
| 1   | J     | 2084  | 0        | 2086     | 6       | 0            |
| 1   | K     | 2090  | 0        | 2090     | 8       | 0            |
| 1   | L     | 2105  | 0        | 2099     | 6       | 0            |
| 1   | M     | 2084  | 0        | 2086     | 6       | 0            |
| 1   | N     | 2105  | 0        | 2106     | 4       | 0            |
| 1   | O     | 2093  | 0        | 2098     | 6       | 0            |
| 1   | P     | 2090  | 0        | 2090     | 4       | 0            |
| 1   | Q     | 2084  | 0        | 2086     | 9       | 0            |
| 1   | R     | 2104  | 0        | 2097     | 11      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | S     | 2093  | 0        | 2098     | 21      | 0            |
| 1   | T     | 2084  | 0        | 2086     | 6       | 0            |
| 1   | U     | 2095  | 0        | 2098     | 7       | 0            |
| 1   | V     | 2099  | 0        | 2095     | 36      | 0            |
| 1   | W     | 2096  | 0        | 2094     | 14      | 0            |
| 1   | X     | 2084  | 0        | 2086     | 30      | 0            |
| 2   | A     | 48    | 0        | 25       | 8       | 0            |
| 2   | B     | 48    | 0        | 25       | 1       | 0            |
| 2   | C     | 48    | 0        | 25       | 1       | 0            |
| 2   | D     | 48    | 0        | 25       | 5       | 0            |
| 2   | E     | 48    | 0        | 25       | 1       | 0            |
| 2   | F     | 48    | 0        | 25       | 2       | 0            |
| 2   | G     | 48    | 0        | 25       | 6       | 0            |
| 2   | H     | 48    | 0        | 25       | 1       | 0            |
| 2   | I     | 48    | 0        | 25       | 1       | 0            |
| 2   | J     | 48    | 0        | 25       | 5       | 0            |
| 2   | K     | 48    | 0        | 25       | 1       | 0            |
| 2   | L     | 48    | 0        | 25       | 2       | 0            |
| 2   | M     | 48    | 0        | 25       | 6       | 0            |
| 2   | N     | 48    | 0        | 25       | 1       | 0            |
| 2   | O     | 48    | 0        | 25       | 1       | 0            |
| 2   | P     | 48    | 0        | 25       | 4       | 0            |
| 2   | Q     | 48    | 0        | 25       | 1       | 0            |
| 2   | R     | 48    | 0        | 25       | 1       | 0            |
| 2   | S     | 48    | 0        | 25       | 7       | 0            |
| 2   | T     | 48    | 0        | 25       | 1       | 0            |
| 2   | U     | 48    | 0        | 25       | 2       | 0            |
| 2   | V     | 48    | 0        | 25       | 3       | 0            |
| 2   | W     | 48    | 0        | 25       | 1       | 0            |
| 2   | X     | 48    | 0        | 25       | 1       | 0            |
| 3   | A     | 45    | 0        | 37       | 8       | 0            |
| 3   | B     | 45    | 0        | 37       | 4       | 0            |
| 3   | C     | 45    | 0        | 37       | 4       | 0            |
| 3   | D     | 45    | 0        | 37       | 6       | 0            |
| 3   | E     | 45    | 0        | 37       | 3       | 0            |
| 3   | F     | 45    | 0        | 37       | 3       | 0            |
| 3   | G     | 45    | 0        | 37       | 7       | 0            |
| 3   | H     | 45    | 0        | 37       | 6       | 0            |
| 3   | I     | 45    | 0        | 37       | 3       | 0            |
| 3   | J     | 45    | 0        | 37       | 7       | 0            |
| 3   | K     | 45    | 0        | 37       | 5       | 0            |
| 3   | L     | 45    | 0        | 37       | 4       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3   | M     | 45    | 0        | 37       | 5       | 0            |
| 3   | N     | 45    | 0        | 37       | 3       | 0            |
| 3   | O     | 45    | 0        | 37       | 4       | 0            |
| 3   | P     | 45    | 0        | 37       | 8       | 0            |
| 3   | Q     | 45    | 0        | 37       | 3       | 0            |
| 3   | R     | 45    | 0        | 37       | 7       | 0            |
| 3   | S     | 45    | 0        | 37       | 8       | 0            |
| 3   | T     | 45    | 0        | 37       | 3       | 0            |
| 3   | U     | 45    | 0        | 37       | 3       | 0            |
| 3   | V     | 45    | 0        | 37       | 7       | 0            |
| 3   | W     | 45    | 0        | 37       | 3       | 0            |
| 3   | X     | 45    | 0        | 37       | 4       | 0            |
| 4   | A     | 5     | 0        | 0        | 0       | 0            |
| 4   | D     | 5     | 0        | 0        | 0       | 0            |
| 4   | H     | 5     | 0        | 0        | 0       | 0            |
| 4   | J     | 5     | 0        | 0        | 0       | 0            |
| 4   | M     | 5     | 0        | 0        | 0       | 0            |
| 4   | P     | 5     | 0        | 0        | 0       | 0            |
| 4   | S     | 5     | 0        | 0        | 0       | 0            |
| 4   | V     | 5     | 0        | 0        | 0       | 0            |
| 5   | A     | 387   | 0        | 0        | 0       | 0            |
| 5   | B     | 354   | 0        | 0        | 0       | 0            |
| 5   | C     | 341   | 0        | 0        | 2       | 0            |
| 5   | D     | 331   | 0        | 0        | 2       | 0            |
| 5   | E     | 390   | 0        | 0        | 5       | 0            |
| 5   | F     | 368   | 0        | 0        | 3       | 0            |
| 5   | G     | 385   | 0        | 0        | 3       | 0            |
| 5   | H     | 404   | 0        | 0        | 3       | 0            |
| 5   | I     | 350   | 0        | 0        | 0       | 0            |
| 5   | J     | 352   | 0        | 0        | 0       | 0            |
| 5   | K     | 352   | 0        | 0        | 1       | 0            |
| 5   | L     | 309   | 0        | 0        | 1       | 0            |
| 5   | M     | 382   | 0        | 0        | 1       | 0            |
| 5   | N     | 363   | 0        | 0        | 0       | 0            |
| 5   | O     | 334   | 0        | 0        | 0       | 0            |
| 5   | P     | 310   | 0        | 0        | 1       | 0            |
| 5   | Q     | 381   | 0        | 0        | 1       | 0            |
| 5   | R     | 232   | 0        | 0        | 0       | 0            |
| 5   | S     | 257   | 0        | 0        | 3       | 0            |
| 5   | T     | 330   | 0        | 0        | 2       | 0            |
| 5   | U     | 194   | 0        | 0        | 0       | 0            |
| 5   | V     | 197   | 0        | 0        | 6       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 5   | W     | 323   | 0        | 0        | 2       | 0            |
| 5   | X     | 117   | 0        | 0        | 2       | 0            |
| All | All   | 60219 | 0        | 51696    | 316     | 0            |

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

All (316) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 2:A:301:NAP:C4N | 3:A:302:H4M:H16 | 1.36                     | 1.51              |
| 2:M:301:NAP:C4N | 3:M:302:H4M:H16 | 1.54                     | 1.38              |
| 2:G:301:NAP:C4N | 3:G:302:H4M:H16 | 1.61                     | 1.29              |
| 2:P:301:NAP:C4N | 3:P:302:H4M:H16 | 1.72                     | 1.19              |
| 2:S:301:NAP:C4N | 3:S:302:H4M:H16 | 1.73                     | 1.17              |
| 3:D:301:H4M:H16 | 2:D:302:NAP:C4N | 1.75                     | 1.17              |
| 2:J:301:NAP:C4N | 3:J:302:H4M:H16 | 1.78                     | 1.12              |
| 2:A:301:NAP:C4N | 3:A:302:H4M:C10 | 2.28                     | 1.10              |
| 2:M:301:NAP:H4N | 3:M:302:H4M:H16 | 1.30                     | 1.09              |
| 2:P:301:NAP:H4N | 3:P:302:H4M:H16 | 1.34                     | 1.08              |
| 2:S:301:NAP:H4N | 3:S:302:H4M:H16 | 1.35                     | 1.04              |
| 2:G:301:NAP:H4N | 3:G:302:H4M:H16 | 1.36                     | 1.03              |
| 2:A:301:NAP:H4N | 3:A:302:H4M:H16 | 1.03                     | 1.02              |
| 3:D:301:H4M:H16 | 2:D:302:NAP:H4N | 1.45                     | 0.95              |
| 2:M:301:NAP:C4N | 3:M:302:H4M:C10 | 2.45                     | 0.94              |
| 2:A:301:NAP:H4N | 3:A:302:H4M:C10 | 1.95                     | 0.93              |
| 2:J:301:NAP:H4N | 3:J:302:H4M:H16 | 1.49                     | 0.93              |
| 1:T:153:LYS:HE3 | 5:T:490:HOH:O   | 1.70                     | 0.91              |
| 2:G:301:NAP:C4N | 3:G:302:H4M:C10 | 2.49                     | 0.89              |
| 2:S:301:NAP:C4N | 3:S:302:H4M:C10 | 2.53                     | 0.87              |
| 2:P:301:NAP:C4N | 3:P:302:H4M:C10 | 2.56                     | 0.84              |
| 1:J:256:LYS:HE3 | 1:J:256:LYS:O   | 1.82                     | 0.80              |
| 1:V:256:LYS:NZ  | 1:V:260:HIS:ND1 | 2.31                     | 0.79              |
| 2:J:301:NAP:C4N | 3:J:302:H4M:C10 | 2.61                     | 0.79              |
| 3:D:301:H4M:C10 | 2:D:302:NAP:C4N | 2.60                     | 0.78              |
| 1:R:168:PHE:O   | 1:R:169:LYS:HG2 | 1.83                     | 0.77              |
| 3:K:302:H4M:OX4 | 3:K:302:H4M:OX2 | 1.99                     | 0.74              |
| 2:H:301:NAP:O7N | 3:H:302:H4M:H16 | 1.88                     | 0.72              |
| 2:N:301:NAP:O7N | 3:N:302:H4M:H16 | 1.89                     | 0.72              |
| 3:N:302:H4M:OX4 | 3:N:302:H4M:OX2 | 2.07                     | 0.72              |
| 2:A:301:NAP:C3N | 3:A:302:H4M:H16 | 2.16                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:K:301:NAP:O7N  | 3:K:302:H4M:H16  | 1.91                     | 0.70              |
| 1:E:119:LYS:NZ   | 5:E:401:HOH:O    | 2.24                     | 0.70              |
| 1:S:3:LYS:NZ     | 5:S:401:HOH:O    | 2.25                     | 0.69              |
| 2:B:301:NAP:O7N  | 3:B:302:H4M:H16  | 1.93                     | 0.69              |
| 2:F:301:NAP:N7N  | 3:F:302:H4M:H16  | 2.08                     | 0.69              |
| 1:H:199:ILE:HD11 | 5:H:567[B]:HOH:O | 1.94                     | 0.68              |
| 2:C:301:NAP:O7N  | 3:C:302:H4M:H16  | 1.94                     | 0.68              |
| 1:U:155:ASP:OD1  | 1:U:156:LYS:N    | 2.25                     | 0.67              |
| 1:F:58:LYS:HG3   | 5:F:522:HOH:O    | 1.95                     | 0.67              |
| 3:L:302:H4M:H18  | 3:L:302:H4M:H12  | 1.77                     | 0.67              |
| 1:X:119:LYS:HD3  | 1:X:144:GLY:HA3  | 1.76                     | 0.67              |
| 1:C:155:ASP:OD1  | 1:C:156:LYS:N    | 2.29                     | 0.66              |
| 2:T:301:NAP:O7N  | 3:T:302:H4M:H16  | 1.97                     | 0.65              |
| 1:S:221:TYR:O    | 2:S:301:NAP:H2N  | 1.95                     | 0.65              |
| 1:M:256:LYS:HE3  | 1:M:256:LYS:O    | 1.96                     | 0.64              |
| 2:Q:301:NAP:N7N  | 3:Q:302:H4M:H16  | 2.12                     | 0.64              |
| 2:V:301:NAP:C4N  | 3:V:302:H4M:H16  | 2.27                     | 0.64              |
| 2:L:301:NAP:N7N  | 3:L:302:H4M:H16  | 2.13                     | 0.64              |
| 1:S:122:LYS:NZ   | 5:S:403:HOH:O    | 2.30                     | 0.64              |
| 3:B:302:H4M:OX4  | 3:B:302:H4M:OX2  | 2.13                     | 0.64              |
| 2:R:301:NAP:O7N  | 3:R:302:H4M:H16  | 1.98                     | 0.63              |
| 1:A:259:LEU:HD11 | 1:A:284:ALA:HB2  | 1.80                     | 0.63              |
| 2:I:301:NAP:O7N  | 3:I:302:H4M:H16  | 1.98                     | 0.63              |
| 1:X:56:LYS:H     | 1:X:56:LYS:HD3   | 1.64                     | 0.62              |
| 1:X:220:ASP:HB2  | 1:X:229:ILE:HD12 | 1.82                     | 0.62              |
| 1:I:155:ASP:OD1  | 1:I:156:LYS:N    | 2.33                     | 0.62              |
| 1:W:153:LYS:HE3  | 5:W:622:HOH:O    | 2.00                     | 0.62              |
| 3:R:302:H4M:OX2  | 3:R:302:H4M:H17  | 1.99                     | 0.61              |
| 1:S:253:GLY:HA2  | 2:S:301:NAP:H72N | 1.65                     | 0.61              |
| 2:M:301:NAP:C3N  | 3:M:302:H4M:H16  | 2.29                     | 0.60              |
| 1:V:256:LYS:HE2  | 3:V:302:H4M:OH4  | 2.00                     | 0.60              |
| 2:U:301:NAP:N7N  | 3:U:302:H4M:H16  | 2.17                     | 0.60              |
| 1:V:258:LYS:CD   | 5:V:417:HOH:O    | 2.50                     | 0.60              |
| 1:H:18:PHE:CE2   | 3:H:302:H4M:H15  | 2.36                     | 0.60              |
| 1:S:256:LYS:HE2  | 3:S:302:H4M:OH4  | 2.02                     | 0.59              |
| 1:E:153:LYS:HD2  | 5:E:427:HOH:O    | 2.01                     | 0.59              |
| 2:E:301:NAP:O7N  | 3:E:302:H4M:H16  | 2.02                     | 0.59              |
| 2:O:301:NAP:O7N  | 3:O:302:H4M:H16  | 2.03                     | 0.59              |
| 1:W:88:PHE:CZ    | 3:X:302:H4M:H25  | 2.38                     | 0.58              |
| 1:P:221:TYR:O    | 2:P:301:NAP:H2N  | 2.02                     | 0.58              |
| 1:V:18:PHE:CZ    | 3:V:302:H4M:H15  | 2.37                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Q:256:LYS:HE2  | 3:Q:302:H4M:OH4  | 2.04                     | 0.57              |
| 2:W:301:NAP:O7N  | 3:W:302:H4M:H16  | 2.05                     | 0.57              |
| 1:L:250:LEU:O    | 3:L:302:H4M:OX3  | 2.23                     | 0.57              |
| 1:V:122:LYS:HA   | 1:V:146:GLU:HB2  | 1.87                     | 0.56              |
| 1:L:171:ASN:ND2  | 5:L:401:HOH:O    | 2.38                     | 0.56              |
| 1:B:256:LYS:HE2  | 3:B:302:H4M:OH4  | 2.06                     | 0.56              |
| 1:W:279:GLU:HA   | 1:W:282:LYS:HD2  | 1.87                     | 0.56              |
| 1:R:282:LYS:HD3  | 1:R:282:LYS:N    | 2.20                     | 0.56              |
| 1:D:221:TYR:O    | 2:D:302:NAP:H2N  | 2.05                     | 0.55              |
| 1:C:58:LYS:HE2   | 5:C:403:HOH:O    | 2.05                     | 0.55              |
| 1:V:221:TYR:O    | 2:V:301:NAP:H2N  | 2.07                     | 0.55              |
| 1:H:256:LYS:HE2  | 3:H:302:H4M:OH4  | 2.06                     | 0.55              |
| 1:B:18:PHE:CE2   | 3:B:302:H4M:H15  | 2.42                     | 0.55              |
| 1:R:278:GLU:O    | 1:R:282:LYS:HD3  | 2.07                     | 0.55              |
| 1:T:256:LYS:HE2  | 3:T:302:H4M:OH4  | 2.07                     | 0.54              |
| 1:A:221:TYR:O    | 2:A:301:NAP:H2N  | 2.06                     | 0.54              |
| 2:G:301:NAP:C3N  | 3:G:302:H4M:H16  | 2.30                     | 0.54              |
| 2:S:301:NAP:C2N  | 3:S:302:H4M:H13  | 2.38                     | 0.54              |
| 1:W:22:VAL:HG11  | 1:W:260:HIS:CG   | 2.42                     | 0.54              |
| 1:J:221:TYR:O    | 2:J:301:NAP:H2N  | 2.08                     | 0.54              |
| 2:A:301:NAP:C2N  | 3:A:302:H4M:H13  | 2.37                     | 0.54              |
| 1:H:256:LYS:CE   | 3:H:302:H4M:OH4  | 2.55                     | 0.54              |
| 1:N:18:PHE:CE2   | 3:N:302:H4M:H15  | 2.43                     | 0.54              |
| 1:V:256:LYS:HG3  | 1:V:257:LEU:N    | 2.18                     | 0.54              |
| 1:M:221:TYR:O    | 2:M:301:NAP:H2N  | 2.08                     | 0.53              |
| 1:D:162:ASP:O    | 1:D:166:LYS:HE3  | 2.08                     | 0.53              |
| 1:F:58:LYS:CG    | 5:F:522:HOH:O    | 2.55                     | 0.53              |
| 1:H:202:GLU:HG2  | 5:H:445:HOH:O    | 2.07                     | 0.53              |
| 1:N:22:VAL:HG11  | 1:N:260:HIS:CG   | 2.44                     | 0.53              |
| 1:V:257:LEU:HD13 | 3:V:302:H4M:H20  | 1.89                     | 0.53              |
| 1:W:256:LYS:NZ   | 3:W:302:H4M:OH4  | 2.30                     | 0.53              |
| 1:X:165:ASN:HA   | 1:X:170:VAL:HG23 | 1.89                     | 0.53              |
| 1:N:89:ARG:HG3   | 1:N:271:SER:O    | 2.09                     | 0.53              |
| 3:P:302:H4M:H18  | 3:P:302:H4M:H12  | 1.90                     | 0.53              |
| 1:V:200:GLY:C    | 1:V:201:LEU:HD23 | 2.33                     | 0.53              |
| 1:E:82:LYS:HE3   | 5:E:481:HOH:O    | 2.09                     | 0.53              |
| 1:H:250:LEU:HB3  | 3:H:302:H4M:H26  | 1.91                     | 0.52              |
| 1:P:18:PHE:CZ    | 3:P:302:H4M:H15  | 2.43                     | 0.52              |
| 1:O:250:LEU:HB3  | 3:O:302:H4M:H27  | 1.90                     | 0.52              |
| 1:U:119:LYS:HD3  | 1:U:119:LYS:C    | 2.34                     | 0.52              |
| 1:R:18:PHE:CE2   | 3:R:302:H4M:H15  | 2.45                     | 0.52              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:W:56:LYS:HD3    | 1:W:56:LYS:H     | 1.75                     | 0.52              |
| 1:E:119:LYS:NZ    | 5:E:404:HOH:O    | 2.42                     | 0.52              |
| 1:D:18:PHE:CZ     | 3:D:301:H4M:H15  | 2.44                     | 0.52              |
| 1:O:218:VAL:HB    | 1:O:229:ILE:HD13 | 1.92                     | 0.52              |
| 1:S:259:LEU:HA    | 1:S:287:MET:HE1  | 1.90                     | 0.51              |
| 1:V:18:PHE:CE2    | 3:V:302:H4M:H15  | 2.45                     | 0.51              |
| 1:G:82:LYS:NZ     | 5:G:405:HOH:O    | 2.43                     | 0.51              |
| 1:R:218:VAL:HB    | 1:R:229:ILE:HD13 | 1.93                     | 0.51              |
| 3:S:302:H4M:H12   | 3:S:302:H4M:H18  | 1.93                     | 0.51              |
| 1:L:185[A]:GLU:HA | 1:L:188:LYS:HD2  | 1.94                     | 0.51              |
| 1:S:85:PHE:CD2    | 1:V:119:LYS:HG3  | 2.46                     | 0.50              |
| 1:F:278:GLU:HG2   | 5:F:482:HOH:O    | 2.11                     | 0.50              |
| 1:K:22:VAL:HG11   | 1:K:260:HIS:CG   | 2.47                     | 0.50              |
| 1:V:259:LEU:HB2   | 1:V:287:MET:HE1  | 1.93                     | 0.50              |
| 1:D:89:ARG:HG3    | 1:D:271:SER:O    | 2.12                     | 0.50              |
| 1:W:57:GLU:OE2    | 1:W:57:GLU:HA    | 2.12                     | 0.50              |
| 1:B:256:LYS:HD3   | 1:B:256:LYS:C    | 2.37                     | 0.50              |
| 1:S:119:LYS:HD3   | 1:V:85:PHE:CZ    | 2.47                     | 0.50              |
| 1:S:169:LYS:O     | 1:V:82:LYS:HE3   | 2.12                     | 0.50              |
| 1:G:221:TYR:O     | 2:G:301:NAP:H2N  | 2.10                     | 0.49              |
| 1:V:188:LYS:HG2   | 1:V:212:GLU:OE1  | 2.12                     | 0.49              |
| 1:V:200:GLY:O     | 1:V:201:LEU:HD23 | 2.12                     | 0.49              |
| 1:V:126:LEU:HD12  | 1:V:195:THR:HG22 | 1.93                     | 0.49              |
| 1:C:18:PHE:CZ     | 3:C:302:H4M:H15  | 2.47                     | 0.49              |
| 1:Q:22:VAL:HG11   | 1:Q:260:HIS:CG   | 2.47                     | 0.49              |
| 1:E:156:LYS:NZ    | 5:E:406:HOH:O    | 2.45                     | 0.49              |
| 1:X:101:THR:OG1   | 1:X:256:LYS:HE2  | 2.13                     | 0.49              |
| 1:X:155:ASP:OD1   | 1:X:156:LYS:N    | 2.46                     | 0.49              |
| 1:C:113:ALA:O     | 1:C:245:ARG:NH2  | 2.46                     | 0.48              |
| 1:K:256:LYS:HE3   | 3:K:302:H4M:OH4  | 2.13                     | 0.48              |
| 1:L:185[B]:GLU:HA | 1:L:188:LYS:HD2  | 1.96                     | 0.48              |
| 1:V:259:LEU:HA    | 1:V:287:MET:HE1  | 1.96                     | 0.48              |
| 1:X:259:LEU:HD12  | 1:X:283:LEU:HD23 | 1.95                     | 0.48              |
| 1:D:162:ASP:C     | 1:D:166:LYS:HE3  | 2.39                     | 0.48              |
| 3:V:302:H4M:H12   | 3:V:302:H4M:H18  | 1.95                     | 0.48              |
| 1:V:258:LYS:HD3   | 5:V:417:HOH:O    | 2.14                     | 0.48              |
| 1:X:165:ASN:HA    | 1:X:170:VAL:CG2  | 2.44                     | 0.48              |
| 1:W:56:LYS:H      | 1:W:56:LYS:CD    | 2.27                     | 0.48              |
| 1:S:85:PHE:CE2    | 1:V:119:LYS:HG3  | 2.48                     | 0.47              |
| 1:Q:256:LYS:HD3   | 1:Q:256:LYS:C    | 2.40                     | 0.47              |
| 1:S:256:LYS:HD3   | 1:S:256:LYS:C    | 2.40                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:256:LYS:HD3  | 1:F:256:LYS:C    | 2.39                     | 0.47              |
| 1:K:18:PHE:CE2   | 3:K:302:H4M:H15  | 2.50                     | 0.47              |
| 1:M:256:LYS:C    | 1:M:256:LYS:CD   | 2.86                     | 0.47              |
| 1:X:192:PHE:CD1  | 1:X:217:ILE:HD12 | 2.50                     | 0.47              |
| 1:J:18:PHE:CZ    | 3:J:302:H4M:H15  | 2.50                     | 0.47              |
| 5:T:524:HOH:O    | 3:U:302:H4M:H8   | 2.14                     | 0.47              |
| 1:H:250:LEU:HD22 | 3:H:302:H4M:H21  | 1.96                     | 0.47              |
| 1:Q:112:LYS:NZ   | 5:Q:407:HOH:O    | 2.47                     | 0.47              |
| 1:C:88:PHE:HA    | 5:C:403:HOH:O    | 2.14                     | 0.47              |
| 1:F:256:LYS:HE2  | 3:F:302:H4M:OH4  | 2.15                     | 0.47              |
| 2:M:301:NAP:C2N  | 3:M:302:H4M:H13  | 2.45                     | 0.47              |
| 1:V:227:LEU:HD12 | 5:V:563:HOH:O    | 2.15                     | 0.47              |
| 1:W:56:LYS:HD3   | 1:W:56:LYS:N     | 2.31                     | 0.47              |
| 1:W:82:LYS:NZ    | 5:W:413:HOH:O    | 2.48                     | 0.47              |
| 1:E:153:LYS:HD3  | 1:E:153:LYS:N    | 2.31                     | 0.46              |
| 1:S:89:ARG:HD2   | 1:S:272:GLU:HG2  | 1.97                     | 0.46              |
| 1:B:22:VAL:HG11  | 1:B:260:HIS:CG   | 2.50                     | 0.46              |
| 1:D:18:PHE:CE2   | 3:D:301:H4M:H15  | 2.51                     | 0.46              |
| 1:X:57:GLU:OE1   | 1:X:57:GLU:HA    | 2.15                     | 0.46              |
| 1:X:240:GLU:HA   | 1:X:244:LYS:O    | 2.16                     | 0.46              |
| 1:X:278:GLU:O    | 1:X:282:LYS:HG2  | 2.16                     | 0.46              |
| 1:F:282:LYS:HB3  | 1:F:282:LYS:HE3  | 1.71                     | 0.46              |
| 1:H:22:VAL:HG11  | 1:H:260:HIS:CG   | 2.50                     | 0.46              |
| 1:T:18:PHE:CZ    | 3:T:302:H4M:H15  | 2.50                     | 0.46              |
| 1:C:18:PHE:CE2   | 3:C:302:H4M:H15  | 2.51                     | 0.46              |
| 1:L:256:LYS:HD2  | 2:L:301:NAP:N7N  | 2.31                     | 0.46              |
| 1:W:180:ASP:OD1  | 1:W:180:ASP:N    | 2.47                     | 0.46              |
| 1:X:56:LYS:H     | 1:X:56:LYS:CD    | 2.27                     | 0.46              |
| 1:R:206:GLN:HG3  | 1:R:210:GLN:CD   | 2.39                     | 0.46              |
| 1:W:18:PHE:CZ    | 3:W:302:H4M:H15  | 2.50                     | 0.46              |
| 1:D:56:LYS:HE3   | 5:D:434:HOH:O    | 2.16                     | 0.46              |
| 1:I:218:VAL:HB   | 1:I:229:ILE:HD13 | 1.97                     | 0.46              |
| 1:S:206:GLN:HG3  | 1:S:210:GLN:CD   | 2.41                     | 0.46              |
| 1:D:166:LYS:NZ   | 5:D:407:HOH:O    | 2.49                     | 0.46              |
| 1:K:256:LYS:CE   | 3:K:302:H4M:OH4  | 2.64                     | 0.46              |
| 1:R:200:GLY:O    | 1:R:201:LEU:HD23 | 2.15                     | 0.46              |
| 1:S:206:GLN:HG3  | 1:S:210:GLN:NE2  | 2.30                     | 0.46              |
| 1:I:58:LYS:HE2   | 1:I:87:PRO:O     | 2.16                     | 0.46              |
| 1:V:102:THR:OG1  | 2:V:301:NAP:H4N  | 2.16                     | 0.46              |
| 1:V:225:PRO:HA   | 1:V:226:PRO:C    | 2.40                     | 0.46              |
| 1:S:89:ARG:HG3   | 1:S:271:SER:O    | 2.16                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:A:302:H4M:H18  | 3:A:302:H4M:H12  | 1.97                     | 0.45              |
| 1:P:18:PHE:CE2   | 3:P:302:H4M:H15  | 2.51                     | 0.45              |
| 1:R:18:PHE:HE1   | 1:R:256:LYS:HZ3  | 1.64                     | 0.45              |
| 1:B:89:ARG:HG3   | 1:B:271:SER:O    | 2.16                     | 0.45              |
| 1:M:256:LYS:C    | 1:M:256:LYS:HD3  | 2.42                     | 0.45              |
| 1:O:256:LYS:HE2  | 3:O:302:H4M:OH4  | 2.17                     | 0.45              |
| 1:S:9:PHE:HB3    | 1:S:37:VAL:HG11  | 1.99                     | 0.45              |
| 1:E:18:PHE:CZ    | 3:E:302:H4M:H15  | 2.51                     | 0.45              |
| 1:I:250:LEU:HD22 | 3:I:302:H4M:H22  | 1.99                     | 0.45              |
| 1:G:18:PHE:CZ    | 3:G:302:H4M:H15  | 2.52                     | 0.45              |
| 1:R:250:LEU:CD2  | 3:R:302:H4M:H23  | 2.47                     | 0.44              |
| 1:T:256:LYS:HD3  | 1:T:256:LYS:C    | 2.42                     | 0.44              |
| 1:X:136:SER:O    | 1:X:140:LEU:HG   | 2.17                     | 0.44              |
| 1:C:218:VAL:HB   | 1:C:229:ILE:HD13 | 1.99                     | 0.44              |
| 2:G:301:NAP:C2N  | 3:G:302:H4M:H13  | 2.46                     | 0.44              |
| 1:H:199:ILE:HG13 | 5:H:569:HOH:O    | 2.16                     | 0.44              |
| 3:J:302:H4M:H18  | 3:J:302:H4M:H12  | 1.98                     | 0.44              |
| 1:C:256:LYS:CE   | 3:C:302:H4M:OH4  | 2.65                     | 0.44              |
| 1:U:147:VAL:HB   | 1:U:172:VAL:HG22 | 2.00                     | 0.44              |
| 1:D:162:ASP:O    | 1:D:166:LYS:HG3  | 2.17                     | 0.44              |
| 1:K:169:LYS:N    | 1:K:169:LYS:HD2  | 2.33                     | 0.44              |
| 1:X:58:LYS:NZ    | 1:X:88:PHE:HA    | 2.32                     | 0.44              |
| 1:U:262:ALA:O    | 1:U:266:LYS:HG2  | 2.16                     | 0.44              |
| 1:G:155:ASP:OD1  | 1:G:156:LYS:N    | 2.51                     | 0.44              |
| 1:V:122:LYS:HZ3  | 1:V:190:ALA:HB2  | 1.82                     | 0.44              |
| 1:X:282:LYS:O    | 1:X:286:GLU:HG3  | 2.17                     | 0.44              |
| 1:B:149:LEU:C    | 1:B:149:LEU:HD23 | 2.42                     | 0.44              |
| 1:G:283:LEU:O    | 1:G:287:MET:HG3  | 2.18                     | 0.44              |
| 2:U:301:NAP:C3N  | 3:U:302:H4M:H13  | 2.48                     | 0.44              |
| 1:V:259:LEU:CB   | 1:V:287:MET:HE1  | 2.47                     | 0.44              |
| 1:I:58:LYS:NZ    | 1:I:58:LYS:HB3   | 2.33                     | 0.43              |
| 1:F:22:VAL:HG11  | 1:F:260:HIS:CG   | 2.53                     | 0.43              |
| 1:O:256:LYS:CE   | 3:O:302:H4M:OH4  | 2.65                     | 0.43              |
| 1:D:163:SER:HA   | 1:D:166:LYS:HE3  | 2.00                     | 0.43              |
| 1:Q:182:SER:HA   | 1:Q:185:GLU:CD   | 2.43                     | 0.43              |
| 1:W:51:TYR:HB3   | 3:X:302:H4M:C16  | 2.49                     | 0.43              |
| 1:A:22:VAL:HG11  | 1:A:260:HIS:CG   | 2.53                     | 0.43              |
| 3:P:302:H4M:H27  | 3:P:302:H4M:H23  | 1.69                     | 0.43              |
| 1:X:121:LYS:HD3  | 1:X:191:HIS:ND1  | 2.33                     | 0.43              |
| 1:E:152:ARG:C    | 1:E:153:LYS:HD3  | 2.44                     | 0.43              |
| 1:I:113:ALA:HB3  | 1:I:217:ILE:HD13 | 2.01                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:V:9:PHE:HB3    | 1:V:37:VAL:HG11  | 2.00                     | 0.43              |
| 1:V:240:GLU:HG2  | 5:V:543:HOH:O    | 2.18                     | 0.43              |
| 1:X:192:PHE:CE1  | 1:X:217:ILE:HD12 | 2.53                     | 0.43              |
| 1:J:18:PHE:CE2   | 3:J:302:H4M:H15  | 2.54                     | 0.43              |
| 1:P:22:VAL:HG11  | 1:P:260:HIS:CG   | 2.53                     | 0.43              |
| 3:P:302:H4M:OX3  | 5:P:401:HOH:O    | 2.21                     | 0.43              |
| 1:S:18:PHE:CZ    | 3:S:302:H4M:H15  | 2.54                     | 0.43              |
| 1:V:257:LEU:CD1  | 3:V:302:H4M:H20  | 2.48                     | 0.43              |
| 1:X:58:LYS:HE2   | 5:X:433:HOH:O    | 2.19                     | 0.43              |
| 1:X:134:MET:CE   | 5:X:466:HOH:O    | 2.66                     | 0.43              |
| 1:X:143:GLU:OE1  | 1:X:285:LYS:HE3  | 2.18                     | 0.43              |
| 1:S:128:GLY:HA2  | 1:S:133:GLY:HA3  | 2.01                     | 0.42              |
| 1:H:256:LYS:HD3  | 1:H:256:LYS:C    | 2.44                     | 0.42              |
| 1:S:18:PHE:CE2   | 3:S:302:H4M:H15  | 2.54                     | 0.42              |
| 1:X:85:PHE:O     | 1:X:88:PHE:HB2   | 2.20                     | 0.42              |
| 1:J:22:VAL:HG11  | 1:J:260:HIS:CG   | 2.55                     | 0.42              |
| 1:J:102:THR:HA   | 1:J:256:LYS:HG3  | 2.01                     | 0.42              |
| 1:Q:18:PHE:CZ    | 3:Q:302:H4M:H15  | 2.54                     | 0.42              |
| 1:V:259:LEU:HD12 | 1:V:283:LEU:HD23 | 2.01                     | 0.42              |
| 1:O:256:LYS:HD3  | 1:O:256:LYS:C    | 2.44                     | 0.42              |
| 1:R:89:ARG:HG3   | 1:R:271:SER:O    | 2.20                     | 0.42              |
| 1:E:22:VAL:HG11  | 1:E:260:HIS:CG   | 2.53                     | 0.42              |
| 1:F:58:LYS:HB2   | 1:F:58:LYS:HE3   | 1.79                     | 0.42              |
| 2:J:301:NAP:C2N  | 3:J:302:H4M:H13  | 2.50                     | 0.42              |
| 1:K:239:LYS:NZ   | 5:K:404:HOH:O    | 2.45                     | 0.42              |
| 1:N:218:VAL:HB   | 1:N:229:ILE:HD13 | 2.02                     | 0.42              |
| 1:Q:82:LYS:HA    | 1:Q:82:LYS:HD2   | 1.93                     | 0.42              |
| 1:S:119:LYS:HD3  | 1:V:85:PHE:CE2   | 2.54                     | 0.42              |
| 1:V:258:LYS:NZ   | 5:V:417:HOH:O    | 2.53                     | 0.42              |
| 1:X:6:LEU:HB3    | 1:X:31:ILE:HG12  | 2.01                     | 0.42              |
| 1:X:281:TYR:CD2  | 1:X:282:LYS:HE3  | 2.55                     | 0.42              |
| 1:O:58:LYS:HE2   | 1:O:58:LYS:HB2   | 1.80                     | 0.42              |
| 1:V:102:THR:OG1  | 1:V:256:LYS:HD3  | 2.20                     | 0.42              |
| 1:X:87:PRO:HG2   | 1:X:88:PHE:CD1   | 2.54                     | 0.42              |
| 1:V:258:LYS:CE   | 5:V:417:HOH:O    | 2.67                     | 0.42              |
| 1:W:185:GLU:HA   | 1:W:188:LYS:HD2  | 2.00                     | 0.42              |
| 2:X:301:NAP:O7N  | 3:X:302:H4M:H16  | 2.19                     | 0.42              |
| 1:E:256:LYS:CE   | 3:E:302:H4M:OH4  | 2.68                     | 0.41              |
| 1:H:218:VAL:HB   | 1:H:229:ILE:HD13 | 2.02                     | 0.41              |
| 1:X:51:TYR:HE1   | 1:X:88:PHE:CE2   | 2.38                     | 0.41              |
| 3:D:301:H4M:H13  | 2:D:302:NAP:C2N  | 2.51                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:225:PRO:HA   | 1:G:226:PRO:C    | 2.45                     | 0.41              |
| 1:H:89:ARG:HG3   | 1:H:271:SER:O    | 2.21                     | 0.41              |
| 1:H:225:PRO:HA   | 1:H:226:PRO:C    | 2.43                     | 0.41              |
| 2:S:301:NAP:H6N  | 5:S:488:HOH:O    | 2.20                     | 0.41              |
| 1:T:56:LYS:O     | 1:T:56:LYS:HD3   | 2.20                     | 0.41              |
| 1:L:218:VAL:HB   | 1:L:229:ILE:HD13 | 2.01                     | 0.41              |
| 1:R:250:LEU:HD22 | 3:R:302:H4M:H23  | 2.02                     | 0.41              |
| 3:L:302:H4M:H12  | 3:L:302:H4M:C13  | 2.49                     | 0.41              |
| 1:F:155:ASP:OD1  | 1:F:156:LYS:N    | 2.53                     | 0.41              |
| 2:A:301:NAP:C4N  | 3:A:302:H4M:N5   | 2.76                     | 0.41              |
| 1:I:58:LYS:HB3   | 1:I:58:LYS:HZ2   | 1.85                     | 0.41              |
| 1:S:148:VAL:HG22 | 1:S:173:THR:HG23 | 2.02                     | 0.41              |
| 3:X:302:H4M:H15  | 3:X:302:H4M:H19  | 1.81                     | 0.41              |
| 3:G:302:H4M:H18  | 3:G:302:H4M:H12  | 2.01                     | 0.41              |
| 1:K:225:PRO:HA   | 1:K:226:PRO:C    | 2.46                     | 0.41              |
| 1:M:84:PHE:O     | 5:M:401:HOH:O    | 2.22                     | 0.41              |
| 1:M:149:LEU:HD23 | 1:M:149:LEU:C    | 2.46                     | 0.41              |
| 1:U:204:LEU:HD21 | 1:U:209:TRP:HB3  | 2.03                     | 0.41              |
| 1:X:50:ILE:HD12  | 1:X:88:PHE:HB3   | 2.03                     | 0.41              |
| 1:X:89:ARG:HG3   | 1:X:271:SER:O    | 2.21                     | 0.41              |
| 1:T:22:VAL:HG11  | 1:T:260:HIS:CG   | 2.55                     | 0.41              |
| 1:V:128:GLY:HA2  | 1:V:133:GLY:HA3  | 2.03                     | 0.41              |
| 1:V:258:LYS:HD3  | 1:V:258:LYS:HA   | 1.91                     | 0.41              |
| 1:B:225:PRO:HA   | 1:B:226:PRO:C    | 2.45                     | 0.40              |
| 1:E:155:ASP:OD1  | 1:E:156:LYS:N    | 2.54                     | 0.40              |
| 1:I:18:PHE:CZ    | 3:I:302:H4M:H15  | 2.57                     | 0.40              |
| 1:K:89:ARG:HG3   | 1:K:271:SER:O    | 2.21                     | 0.40              |
| 1:Q:88:PHE:CE2   | 3:R:302:H4M:H24  | 2.56                     | 0.40              |
| 1:X:84:PHE:CD2   | 1:X:89:ARG:HB2   | 2.56                     | 0.40              |
| 1:U:140:LEU:HD11 | 1:U:194:PHE:CE1  | 2.56                     | 0.40              |
| 2:F:301:NAP:C7N  | 3:F:302:H4M:H13  | 2.52                     | 0.40              |
| 1:G:4:LYS:NZ     | 5:G:415:HOH:O    | 2.54                     | 0.40              |
| 1:G:122:LYS:NZ   | 5:G:414:HOH:O    | 2.53                     | 0.40              |
| 1:U:138:ALA:HB2  | 1:U:164:VAL:HG13 | 2.04                     | 0.40              |
| 1:X:164:VAL:HG12 | 1:X:170:VAL:HG21 | 2.02                     | 0.40              |
| 1:D:225:PRO:HA   | 1:D:226:PRO:C    | 2.46                     | 0.40              |
| 1:E:180:ASP:OD1  | 1:E:180:ASP:N    | 2.55                     | 0.40              |
| 1:Q:88:PHE:HE2   | 3:R:302:H4M:H24  | 1.87                     | 0.40              |
| 1:V:217:ILE:HG12 | 1:V:245:ARG:HB2  | 2.02                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1   | A     | 285/288 (99%)   | 280 (98%)  | 5 (2%)   | 0        | 100         | 100 |
| 1   | B     | 285/288 (99%)   | 281 (99%)  | 4 (1%)   | 0        | 100         | 100 |
| 1   | C     | 286/288 (99%)   | 281 (98%)  | 5 (2%)   | 0        | 100         | 100 |
| 1   | D     | 286/288 (99%)   | 281 (98%)  | 5 (2%)   | 0        | 100         | 100 |
| 1   | E     | 286/288 (99%)   | 281 (98%)  | 5 (2%)   | 0        | 100         | 100 |
| 1   | F     | 285/288 (99%)   | 281 (99%)  | 4 (1%)   | 0        | 100         | 100 |
| 1   | G     | 285/288 (99%)   | 279 (98%)  | 6 (2%)   | 0        | 100         | 100 |
| 1   | H     | 289/288 (100%)  | 285 (99%)  | 4 (1%)   | 0        | 100         | 100 |
| 1   | I     | 286/288 (99%)   | 282 (99%)  | 4 (1%)   | 0        | 100         | 100 |
| 1   | J     | 285/288 (99%)   | 279 (98%)  | 6 (2%)   | 0        | 100         | 100 |
| 1   | K     | 286/288 (99%)   | 282 (99%)  | 4 (1%)   | 0        | 100         | 100 |
| 1   | L     | 288/288 (100%)  | 284 (99%)  | 4 (1%)   | 0        | 100         | 100 |
| 1   | M     | 285/288 (99%)   | 279 (98%)  | 6 (2%)   | 0        | 100         | 100 |
| 1   | N     | 288/288 (100%)  | 284 (99%)  | 4 (1%)   | 0        | 100         | 100 |
| 1   | O     | 286/288 (99%)   | 281 (98%)  | 5 (2%)   | 0        | 100         | 100 |
| 1   | P     | 286/288 (99%)   | 279 (98%)  | 7 (2%)   | 0        | 100         | 100 |
| 1   | Q     | 285/288 (99%)   | 280 (98%)  | 5 (2%)   | 0        | 100         | 100 |
| 1   | R     | 288/288 (100%)  | 284 (99%)  | 4 (1%)   | 0        | 100         | 100 |
| 1   | S     | 286/288 (99%)   | 280 (98%)  | 6 (2%)   | 0        | 100         | 100 |
| 1   | T     | 285/288 (99%)   | 280 (98%)  | 5 (2%)   | 0        | 100         | 100 |
| 1   | U     | 286/288 (99%)   | 281 (98%)  | 5 (2%)   | 0        | 100         | 100 |
| 1   | V     | 287/288 (100%)  | 278 (97%)  | 9 (3%)   | 0        | 100         | 100 |
| 1   | W     | 287/288 (100%)  | 282 (98%)  | 5 (2%)   | 0        | 100         | 100 |
| 1   | X     | 285/288 (99%)   | 278 (98%)  | 7 (2%)   | 0        | 100         | 100 |
| All | All   | 6866/6912 (99%) | 6742 (98%) | 124 (2%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 1   | A     | 204/205 (100%) | 203 (100%) | 1 (0%)   | 81          | 66  |
| 1   | B     | 204/205 (100%) | 204 (100%) | 0        | 100         | 100 |
| 1   | C     | 205/205 (100%) | 205 (100%) | 0        | 100         | 100 |
| 1   | D     | 205/205 (100%) | 204 (100%) | 1 (0%)   | 81          | 66  |
| 1   | E     | 205/205 (100%) | 205 (100%) | 0        | 100         | 100 |
| 1   | F     | 204/205 (100%) | 204 (100%) | 0        | 100         | 100 |
| 1   | G     | 204/205 (100%) | 203 (100%) | 1 (0%)   | 81          | 66  |
| 1   | H     | 208/205 (102%) | 207 (100%) | 1 (0%)   | 81          | 66  |
| 1   | I     | 205/205 (100%) | 204 (100%) | 1 (0%)   | 81          | 66  |
| 1   | J     | 204/205 (100%) | 203 (100%) | 1 (0%)   | 81          | 66  |
| 1   | K     | 205/205 (100%) | 204 (100%) | 1 (0%)   | 81          | 66  |
| 1   | L     | 207/205 (101%) | 204 (99%)  | 3 (1%)   | 59          | 33  |
| 1   | M     | 204/205 (100%) | 203 (100%) | 1 (0%)   | 81          | 66  |
| 1   | N     | 207/205 (101%) | 206 (100%) | 1 (0%)   | 81          | 66  |
| 1   | O     | 205/205 (100%) | 205 (100%) | 0        | 100         | 100 |
| 1   | P     | 205/205 (100%) | 204 (100%) | 1 (0%)   | 81          | 66  |
| 1   | Q     | 204/205 (100%) | 204 (100%) | 0        | 100         | 100 |
| 1   | R     | 207/205 (101%) | 206 (100%) | 1 (0%)   | 81          | 66  |
| 1   | S     | 205/205 (100%) | 204 (100%) | 1 (0%)   | 81          | 66  |
| 1   | T     | 204/205 (100%) | 204 (100%) | 0        | 100         | 100 |
| 1   | U     | 205/205 (100%) | 205 (100%) | 0        | 100         | 100 |
| 1   | V     | 206/205 (100%) | 205 (100%) | 1 (0%)   | 81          | 66  |
| 1   | W     | 206/205 (100%) | 206 (100%) | 0        | 100         | 100 |
| 1   | X     | 204/205 (100%) | 204 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed         | Rotameric   | Outliers | Percentiles |
|-----|-------|------------------|-------------|----------|-------------|
| All | All   | 4922/4920 (100%) | 4906 (100%) | 16 (0%)  | 86 75       |

All (16) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | A     | 256    | LYS  |
| 1   | D     | 256    | LYS  |
| 1   | G     | 256    | LYS  |
| 1   | H     | 153    | LYS  |
| 1   | I     | 256    | LYS  |
| 1   | J     | 256    | LYS  |
| 1   | K     | 239    | LYS  |
| 1   | L     | 179    | ASP  |
| 1   | L     | 213[A] | SER  |
| 1   | L     | 213[B] | SER  |
| 1   | M     | 256    | LYS  |
| 1   | N     | 256    | LYS  |
| 1   | P     | 256    | LYS  |
| 1   | R     | 58     | LYS  |
| 1   | S     | 122    | LYS  |
| 1   | V     | 256    | LYS  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 210 | GLN  |
| 1   | C     | 224 | GLN  |
| 1   | E     | 206 | GLN  |
| 1   | E     | 211 | ASN  |
| 1   | F     | 206 | GLN  |
| 1   | H     | 210 | GLN  |
| 1   | H     | 211 | ASN  |
| 1   | J     | 59  | GLN  |
| 1   | K     | 97  | ASN  |
| 1   | L     | 171 | ASN  |
| 1   | N     | 158 | GLN  |
| 1   | O     | 158 | GLN  |
| 1   | P     | 158 | GLN  |
| 1   | P     | 206 | GLN  |
| 1   | Q     | 206 | GLN  |
| 1   | R     | 59  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | S     | 171 | ASN  |
| 1   | T     | 210 | GLN  |
| 1   | T     | 224 | GLN  |
| 1   | U     | 224 | GLN  |
| 1   | V     | 30  | HIS  |
| 1   | V     | 211 | ASN  |
| 1   | W     | 59  | GLN  |
| 1   | W     | 158 | GLN  |
| 1   | W     | 210 | GLN  |
| 1   | W     | 224 | GLN  |
| 1   | X     | 171 | ASN  |
| 1   | X     | 206 | GLN  |
| 1   | X     | 260 | HIS  |

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

56 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 | $\# Z  > 2$ |
| 3   | H4M  | C     | 302 | -    | 47,49,58     | 4.90 | 6 (12%)     | 58,74,86    | 1.48 | 8 (13%)     |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 2   | NAP  | V     | 301 | -    | 50,52,52     | 2.10 | 15 (30%) | 71,80,80    | 1.69 | 13 (18%) |
| 2   | NAP  | X     | 301 | -    | 50,52,52     | 2.09 | 15 (30%) | 71,80,80    | 1.70 | 13 (18%) |
| 4   | SO4  | A     | 303 | -    | 4,4,4        | 0.20 | 0        | 6,6,6       | 0.12 | 0        |
| 3   | H4M  | E     | 302 | -    | 47,49,58     | 4.92 | 6 (12%)  | 58,74,86    | 1.40 | 8 (13%)  |
| 4   | SO4  | V     | 303 | -    | 4,4,4        | 0.25 | 0        | 6,6,6       | 0.14 | 0        |
| 3   | H4M  | A     | 302 | -    | 47,49,58     | 4.86 | 7 (14%)  | 58,74,86    | 1.64 | 9 (15%)  |
| 3   | H4M  | U     | 302 | -    | 47,49,58     | 5.34 | 7 (14%)  | 58,74,86    | 1.69 | 11 (18%) |
| 4   | SO4  | H     | 303 | -    | 4,4,4        | 0.23 | 0        | 6,6,6       | 0.11 | 0        |
| 4   | SO4  | P     | 303 | -    | 4,4,4        | 0.24 | 0        | 6,6,6       | 0.16 | 0        |
| 2   | NAP  | U     | 301 | -    | 50,52,52     | 2.13 | 15 (30%) | 71,80,80    | 1.74 | 16 (22%) |
| 2   | NAP  | G     | 301 | -    | 50,52,52     | 2.08 | 14 (28%) | 71,80,80    | 1.66 | 15 (21%) |
| 3   | H4M  | O     | 302 | -    | 47,49,58     | 5.09 | 8 (17%)  | 58,74,86    | 1.63 | 9 (15%)  |
| 3   | H4M  | K     | 302 | -    | 47,49,58     | 5.10 | 7 (14%)  | 58,74,86    | 1.52 | 6 (10%)  |
| 4   | SO4  | S     | 303 | -    | 4,4,4        | 0.28 | 0        | 6,6,6       | 0.12 | 0        |
| 3   | H4M  | J     | 302 | -    | 47,49,58     | 4.96 | 8 (17%)  | 58,74,86    | 1.66 | 8 (13%)  |
| 3   | H4M  | P     | 302 | -    | 47,49,58     | 4.85 | 8 (17%)  | 58,74,86    | 1.80 | 8 (13%)  |
| 2   | NAP  | E     | 301 | -    | 50,52,52     | 2.15 | 16 (32%) | 71,80,80    | 1.74 | 16 (22%) |
| 2   | NAP  | A     | 301 | -    | 50,52,52     | 2.11 | 15 (30%) | 71,80,80    | 1.74 | 16 (22%) |
| 2   | NAP  | D     | 302 | -    | 50,52,52     | 1.99 | 13 (26%) | 71,80,80    | 1.73 | 16 (22%) |
| 2   | NAP  | T     | 301 | -    | 50,52,52     | 2.10 | 15 (30%) | 71,80,80    | 1.76 | 17 (23%) |
| 3   | H4M  | H     | 302 | -    | 47,49,58     | 5.07 | 8 (17%)  | 58,74,86    | 1.51 | 9 (15%)  |
| 2   | NAP  | S     | 301 | -    | 50,52,52     | 2.05 | 15 (30%) | 71,80,80    | 1.69 | 16 (22%) |
| 3   | H4M  | L     | 302 | -    | 47,49,58     | 5.14 | 7 (14%)  | 58,74,86    | 1.56 | 10 (17%) |
| 3   | H4M  | M     | 302 | -    | 47,49,58     | 4.95 | 7 (14%)  | 58,74,86    | 1.82 | 11 (18%) |
| 3   | H4M  | Q     | 302 | -    | 47,49,58     | 4.96 | 6 (12%)  | 58,74,86    | 1.42 | 6 (10%)  |
| 3   | H4M  | X     | 302 | -    | 47,49,58     | 5.09 | 8 (17%)  | 58,74,86    | 1.61 | 11 (18%) |
| 4   | SO4  | D     | 303 | -    | 4,4,4        | 0.28 | 0        | 6,6,6       | 0.10 | 0        |
| 4   | SO4  | J     | 303 | -    | 4,4,4        | 0.27 | 0        | 6,6,6       | 0.16 | 0        |
| 2   | NAP  | M     | 301 | -    | 50,52,52     | 1.97 | 12 (24%) | 71,80,80    | 1.57 | 9 (12%)  |
| 3   | H4M  | D     | 301 | -    | 47,49,58     | 4.84 | 8 (17%)  | 58,74,86    | 1.54 | 6 (10%)  |
| 2   | NAP  | R     | 301 | -    | 50,52,52     | 2.07 | 15 (30%) | 71,80,80    | 1.74 | 16 (22%) |
| 3   | H4M  | S     | 302 | -    | 47,49,58     | 5.04 | 8 (17%)  | 58,74,86    | 1.69 | 8 (13%)  |
| 3   | H4M  | I     | 302 | -    | 47,49,58     | 5.00 | 7 (14%)  | 58,74,86    | 1.47 | 6 (10%)  |
| 2   | NAP  | P     | 301 | -    | 50,52,52     | 2.04 | 12 (24%) | 71,80,80    | 1.65 | 14 (19%) |
| 3   | H4M  | F     | 302 | -    | 47,49,58     | 5.30 | 7 (14%)  | 58,74,86    | 1.67 | 12 (20%) |
| 2   | NAP  | K     | 301 | -    | 50,52,52     | 1.93 | 11 (22%) | 71,80,80    | 1.70 | 15 (21%) |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 2   | NAP  | I     | 301 | -    | 50,52,52     | 2.01 | 16 (32%) | 71,80,80    | 1.73 | 15 (21%) |
| 2   | NAP  | B     | 301 | -    | 50,52,52     | 1.96 | 13 (26%) | 71,80,80    | 1.60 | 14 (19%) |
| 2   | NAP  | O     | 301 | -    | 50,52,52     | 2.06 | 15 (30%) | 71,80,80    | 1.76 | 17 (23%) |
| 2   | NAP  | Q     | 301 | -    | 50,52,52     | 2.06 | 14 (28%) | 71,80,80    | 1.70 | 16 (22%) |
| 3   | H4M  | N     | 302 | -    | 47,49,58     | 5.20 | 7 (14%)  | 58,74,86    | 1.54 | 9 (15%)  |
| 3   | H4M  | W     | 302 | -    | 47,49,58     | 4.94 | 7 (14%)  | 58,74,86    | 1.39 | 7 (12%)  |
| 4   | SO4  | M     | 303 | -    | 4,4,4        | 0.28 | 0        | 6,6,6       | 0.24 | 0        |
| 3   | H4M  | V     | 302 | -    | 47,49,58     | 4.68 | 8 (17%)  | 58,74,86    | 1.85 | 10 (17%) |
| 2   | NAP  | J     | 301 | -    | 50,52,52     | 2.13 | 15 (30%) | 71,80,80    | 1.69 | 14 (19%) |
| 2   | NAP  | N     | 301 | -    | 50,52,52     | 2.00 | 14 (28%) | 71,80,80    | 1.69 | 12 (16%) |
| 3   | H4M  | R     | 302 | -    | 47,49,58     | 4.90 | 7 (14%)  | 58,74,86    | 1.62 | 8 (13%)  |
| 2   | NAP  | C     | 301 | -    | 50,52,52     | 2.02 | 12 (24%) | 71,80,80    | 1.75 | 14 (19%) |
| 2   | NAP  | F     | 301 | -    | 50,52,52     | 2.00 | 14 (28%) | 71,80,80    | 1.70 | 17 (23%) |
| 3   | H4M  | T     | 302 | -    | 47,49,58     | 4.93 | 6 (12%)  | 58,74,86    | 1.38 | 6 (10%)  |
| 2   | NAP  | L     | 301 | -    | 50,52,52     | 2.04 | 15 (30%) | 71,80,80    | 1.75 | 17 (23%) |
| 2   | NAP  | W     | 301 | -    | 50,52,52     | 2.15 | 15 (30%) | 71,80,80    | 1.74 | 17 (23%) |
| 2   | NAP  | H     | 301 | -    | 50,52,52     | 1.94 | 12 (24%) | 71,80,80    | 1.58 | 12 (16%) |
| 3   | H4M  | B     | 302 | -    | 47,49,58     | 5.05 | 8 (17%)  | 58,74,86    | 1.56 | 10 (17%) |
| 3   | H4M  | G     | 302 | -    | 47,49,58     | 5.05 | 9 (19%)  | 58,74,86    | 1.75 | 6 (10%)  |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions    | Rings   |
|-----|------|-------|-----|------|---------|-------------|---------|
| 3   | H4M  | C     | 302 | -    | -       | 9/27/71/85  | 0/5/5/5 |
| 2   | NAP  | V     | 301 | -    | -       | 7/35/67/67  | 0/5/5/5 |
| 2   | NAP  | X     | 301 | -    | -       | 4/35/67/67  | 0/5/5/5 |
| 3   | H4M  | E     | 302 | -    | -       | 10/27/71/85 | 0/5/5/5 |
| 3   | H4M  | A     | 302 | -    | -       | 7/27/71/85  | 0/5/5/5 |
| 3   | H4M  | U     | 302 | -    | -       | 13/27/71/85 | 0/5/5/5 |
| 2   | NAP  | U     | 301 | -    | -       | 5/35/67/67  | 0/5/5/5 |
| 2   | NAP  | G     | 301 | -    | -       | 7/35/67/67  | 0/5/5/5 |
| 3   | H4M  | O     | 302 | -    | -       | 17/27/71/85 | 0/5/5/5 |
| 3   | H4M  | K     | 302 | -    | -       | 17/27/71/85 | 0/5/5/5 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions    | Rings   |
|-----|------|-------|-----|------|---------|-------------|---------|
| 3   | H4M  | J     | 302 | -    | -       | 9/27/71/85  | 0/5/5/5 |
| 3   | H4M  | P     | 302 | -    | -       | 19/27/71/85 | 0/5/5/5 |
| 2   | NAP  | E     | 301 | -    | -       | 3/35/67/67  | 0/5/5/5 |
| 2   | NAP  | A     | 301 | -    | -       | 6/35/67/67  | 0/5/5/5 |
| 2   | NAP  | D     | 302 | -    | -       | 7/35/67/67  | 0/5/5/5 |
| 2   | NAP  | T     | 301 | -    | -       | 3/35/67/67  | 0/5/5/5 |
| 3   | H4M  | H     | 302 | -    | -       | 18/27/71/85 | 0/5/5/5 |
| 2   | NAP  | S     | 301 | -    | -       | 7/35/67/67  | 0/5/5/5 |
| 3   | H4M  | L     | 302 | -    | -       | 18/27/71/85 | 0/5/5/5 |
| 3   | H4M  | M     | 302 | -    | -       | 7/27/71/85  | 0/5/5/5 |
| 3   | H4M  | Q     | 302 | -    | -       | 8/27/71/85  | 0/5/5/5 |
| 3   | H4M  | X     | 302 | -    | -       | 20/27/71/85 | 0/5/5/5 |
| 2   | NAP  | M     | 301 | -    | -       | 8/35/67/67  | 0/5/5/5 |
| 3   | H4M  | D     | 301 | -    | -       | 9/27/71/85  | 0/5/5/5 |
| 2   | NAP  | R     | 301 | -    | -       | 4/35/67/67  | 0/5/5/5 |
| 3   | H4M  | S     | 302 | -    | -       | 10/27/71/85 | 0/5/5/5 |
| 3   | H4M  | I     | 302 | -    | -       | 14/27/71/85 | 0/5/5/5 |
| 2   | NAP  | P     | 301 | -    | -       | 6/35/67/67  | 0/5/5/5 |
| 3   | H4M  | F     | 302 | -    | -       | 15/27/71/85 | 0/5/5/5 |
| 2   | NAP  | K     | 301 | -    | -       | 3/35/67/67  | 0/5/5/5 |
| 2   | NAP  | I     | 301 | -    | -       | 2/35/67/67  | 0/5/5/5 |
| 2   | NAP  | B     | 301 | -    | -       | 5/35/67/67  | 0/5/5/5 |
| 2   | NAP  | O     | 301 | -    | -       | 5/35/67/67  | 0/5/5/5 |
| 2   | NAP  | Q     | 301 | -    | -       | 5/35/67/67  | 0/5/5/5 |
| 3   | H4M  | N     | 302 | -    | -       | 17/27/71/85 | 0/5/5/5 |
| 3   | H4M  | W     | 302 | -    | -       | 12/27/71/85 | 0/5/5/5 |
| 3   | H4M  | V     | 302 | -    | -       | 10/27/71/85 | 0/5/5/5 |
| 2   | NAP  | J     | 301 | -    | -       | 7/35/67/67  | 0/5/5/5 |
| 2   | NAP  | N     | 301 | -    | -       | 4/35/67/67  | 0/5/5/5 |
| 3   | H4M  | R     | 302 | -    | -       | 12/27/71/85 | 0/5/5/5 |
| 2   | NAP  | C     | 301 | -    | -       | 3/35/67/67  | 0/5/5/5 |
| 2   | NAP  | F     | 301 | -    | -       | 5/35/67/67  | 0/5/5/5 |
| 3   | H4M  | T     | 302 | -    | -       | 6/27/71/85  | 0/5/5/5 |
| 2   | NAP  | L     | 301 | -    | -       | 6/35/67/67  | 0/5/5/5 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions    | Rings   |
|-----|------|-------|-----|------|---------|-------------|---------|
| 2   | NAP  | W     | 301 | -    | -       | 6/35/67/67  | 0/5/5/5 |
| 2   | NAP  | H     | 301 | -    | -       | 4/35/67/67  | 0/5/5/5 |
| 3   | H4M  | B     | 302 | -    | -       | 15/27/71/85 | 0/5/5/5 |
| 3   | H4M  | G     | 302 | -    | -       | 16/27/71/85 | 0/5/5/5 |

All (513) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 3   | U     | 302 | H4M  | C10-N5  | -34.70 | 1.23        | 1.45     |
| 3   | F     | 302 | H4M  | C10-N5  | -34.39 | 1.23        | 1.45     |
| 3   | N     | 302 | H4M  | C10-N5  | -33.76 | 1.24        | 1.45     |
| 3   | L     | 302 | H4M  | C10-N5  | -33.36 | 1.24        | 1.45     |
| 3   | K     | 302 | H4M  | C10-N5  | -32.95 | 1.24        | 1.45     |
| 3   | O     | 302 | H4M  | C10-N5  | -32.86 | 1.24        | 1.45     |
| 3   | B     | 302 | H4M  | C10-N5  | -32.82 | 1.24        | 1.45     |
| 3   | X     | 302 | H4M  | C10-N5  | -32.76 | 1.24        | 1.45     |
| 3   | H     | 302 | H4M  | C10-N5  | -32.74 | 1.24        | 1.45     |
| 3   | S     | 302 | H4M  | C10-N5  | -32.58 | 1.24        | 1.45     |
| 3   | G     | 302 | H4M  | C10-N5  | -32.55 | 1.24        | 1.45     |
| 3   | I     | 302 | H4M  | C10-N5  | -32.20 | 1.25        | 1.45     |
| 3   | Q     | 302 | H4M  | C10-N5  | -32.18 | 1.25        | 1.45     |
| 3   | J     | 302 | H4M  | C10-N5  | -32.17 | 1.25        | 1.45     |
| 3   | W     | 302 | H4M  | C10-N5  | -31.99 | 1.25        | 1.45     |
| 3   | M     | 302 | H4M  | C10-N5  | -31.97 | 1.25        | 1.45     |
| 3   | E     | 302 | H4M  | C10-N5  | -31.92 | 1.25        | 1.45     |
| 3   | T     | 302 | H4M  | C10-N5  | -31.92 | 1.25        | 1.45     |
| 3   | C     | 302 | H4M  | C10-N5  | -31.64 | 1.25        | 1.45     |
| 3   | A     | 302 | H4M  | C10-N5  | -31.48 | 1.25        | 1.45     |
| 3   | R     | 302 | H4M  | C10-N5  | -31.42 | 1.25        | 1.45     |
| 3   | D     | 301 | H4M  | C10-N5  | -31.27 | 1.25        | 1.45     |
| 3   | P     | 302 | H4M  | C10-N5  | -31.23 | 1.25        | 1.45     |
| 3   | V     | 302 | H4M  | C10-N5  | -30.09 | 1.26        | 1.45     |
| 3   | X     | 302 | H4M  | C8A-N8  | 7.91   | 1.43        | 1.35     |
| 3   | I     | 302 | H4M  | C8A-N8  | 7.89   | 1.43        | 1.35     |
| 3   | R     | 302 | H4M  | C8A-N8  | 7.63   | 1.43        | 1.35     |
| 3   | U     | 302 | H4M  | C8A-N8  | 7.61   | 1.43        | 1.35     |
| 3   | K     | 302 | H4M  | C8A-N8  | 7.48   | 1.43        | 1.35     |
| 3   | O     | 302 | H4M  | C8A-N8  | 7.37   | 1.43        | 1.35     |
| 3   | F     | 302 | H4M  | C8A-N8  | 7.32   | 1.43        | 1.35     |
| 2   | J     | 301 | NAP  | C7N-N7N | 7.24   | 1.46        | 1.33     |
| 2   | P     | 301 | NAP  | C7N-N7N | 7.22   | 1.46        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | N     | 302 | H4M  | C8A-N8  | 7.20  | 1.43        | 1.35     |
| 3   | T     | 302 | H4M  | C8A-N8  | 7.18  | 1.43        | 1.35     |
| 3   | W     | 302 | H4M  | C8A-N8  | 7.07  | 1.42        | 1.35     |
| 2   | X     | 301 | NAP  | C7N-N7N | 7.06  | 1.46        | 1.33     |
| 2   | U     | 301 | NAP  | C7N-N7N | 7.06  | 1.46        | 1.33     |
| 3   | L     | 302 | H4M  | C8A-N8  | 7.04  | 1.42        | 1.35     |
| 2   | A     | 301 | NAP  | C7N-N7N | 7.03  | 1.45        | 1.33     |
| 3   | E     | 302 | H4M  | C8A-N8  | 7.03  | 1.42        | 1.35     |
| 2   | G     | 301 | NAP  | C7N-N7N | 7.01  | 1.45        | 1.33     |
| 2   | V     | 301 | NAP  | C7N-N7N | 6.99  | 1.45        | 1.33     |
| 2   | W     | 301 | NAP  | C7N-N7N | 6.94  | 1.45        | 1.33     |
| 3   | C     | 302 | H4M  | C8A-N8  | 6.92  | 1.42        | 1.35     |
| 2   | E     | 301 | NAP  | C7N-N7N | 6.92  | 1.45        | 1.33     |
| 2   | R     | 301 | NAP  | C7N-N7N | 6.85  | 1.45        | 1.33     |
| 3   | M     | 302 | H4M  | C8A-N8  | 6.83  | 1.42        | 1.35     |
| 2   | F     | 301 | NAP  | C7N-N7N | 6.82  | 1.45        | 1.33     |
| 2   | C     | 301 | NAP  | C7N-N7N | 6.79  | 1.45        | 1.33     |
| 2   | M     | 301 | NAP  | C7N-N7N | 6.79  | 1.45        | 1.33     |
| 2   | Q     | 301 | NAP  | C7N-N7N | 6.78  | 1.45        | 1.33     |
| 3   | Q     | 302 | H4M  | C8A-N8  | 6.78  | 1.42        | 1.35     |
| 2   | T     | 301 | NAP  | C7N-N7N | 6.78  | 1.45        | 1.33     |
| 2   | N     | 301 | NAP  | C7N-N7N | 6.77  | 1.45        | 1.33     |
| 2   | I     | 301 | NAP  | C7N-N7N | 6.75  | 1.45        | 1.33     |
| 3   | H     | 302 | H4M  | C8A-N8  | 6.75  | 1.42        | 1.35     |
| 2   | S     | 301 | NAP  | C7N-N7N | 6.70  | 1.45        | 1.33     |
| 2   | O     | 301 | NAP  | C7N-N7N | 6.70  | 1.45        | 1.33     |
| 3   | S     | 302 | H4M  | C8A-N8  | 6.64  | 1.42        | 1.35     |
| 2   | B     | 301 | NAP  | C7N-N7N | 6.60  | 1.45        | 1.33     |
| 3   | D     | 301 | H4M  | C8A-N8  | 6.53  | 1.42        | 1.35     |
| 2   | L     | 301 | NAP  | C7N-N7N | 6.53  | 1.45        | 1.33     |
| 2   | D     | 302 | NAP  | C7N-N7N | 6.49  | 1.44        | 1.33     |
| 3   | B     | 302 | H4M  | C8A-N8  | 6.47  | 1.42        | 1.35     |
| 2   | H     | 301 | NAP  | C7N-N7N | 6.34  | 1.44        | 1.33     |
| 3   | P     | 302 | H4M  | C8A-N8  | 6.32  | 1.42        | 1.35     |
| 2   | K     | 301 | NAP  | C7N-N7N | 6.28  | 1.44        | 1.33     |
| 2   | W     | 301 | NAP  | C5A-N7A | -6.24 | 1.27        | 1.39     |
| 3   | V     | 302 | H4M  | C8A-N8  | 6.22  | 1.42        | 1.35     |
| 3   | G     | 302 | H4M  | C8A-N8  | 6.21  | 1.42        | 1.35     |
| 2   | J     | 301 | NAP  | C5A-N7A | -6.20 | 1.27        | 1.39     |
| 2   | A     | 301 | NAP  | C5A-N7A | -6.18 | 1.27        | 1.39     |
| 2   | R     | 301 | NAP  | C5A-N7A | -6.15 | 1.27        | 1.39     |
| 2   | U     | 301 | NAP  | C5A-N7A | -6.09 | 1.28        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | S     | 301 | NAP  | C5A-N7A | -6.07 | 1.28        | 1.39     |
| 2   | C     | 301 | NAP  | C5A-N7A | -6.07 | 1.28        | 1.39     |
| 2   | X     | 301 | NAP  | C5A-N7A | -6.06 | 1.28        | 1.39     |
| 2   | B     | 301 | NAP  | C5A-N7A | -6.06 | 1.28        | 1.39     |
| 2   | D     | 302 | NAP  | C5A-N7A | -6.05 | 1.28        | 1.39     |
| 3   | J     | 302 | H4M  | C8A-N8  | 6.05  | 1.41        | 1.35     |
| 2   | L     | 301 | NAP  | C5A-N7A | -6.03 | 1.28        | 1.39     |
| 2   | M     | 301 | NAP  | C5A-N7A | -6.01 | 1.28        | 1.39     |
| 2   | K     | 301 | NAP  | C5A-N7A | -6.01 | 1.28        | 1.39     |
| 2   | T     | 301 | NAP  | C5A-N7A | -6.01 | 1.28        | 1.39     |
| 2   | Q     | 301 | NAP  | C5A-N7A | -5.98 | 1.28        | 1.39     |
| 2   | O     | 301 | NAP  | C5A-N7A | -5.97 | 1.28        | 1.39     |
| 2   | P     | 301 | NAP  | C5A-N7A | -5.97 | 1.28        | 1.39     |
| 3   | A     | 302 | H4M  | C8A-N8  | 5.95  | 1.41        | 1.35     |
| 2   | H     | 301 | NAP  | C5A-N7A | -5.92 | 1.28        | 1.39     |
| 2   | G     | 301 | NAP  | C5A-N7A | -5.91 | 1.28        | 1.39     |
| 2   | V     | 301 | NAP  | C5A-N7A | -5.89 | 1.28        | 1.39     |
| 2   | E     | 301 | NAP  | C5A-N7A | -5.81 | 1.28        | 1.39     |
| 2   | I     | 301 | NAP  | C5A-N7A | -5.79 | 1.28        | 1.39     |
| 2   | F     | 301 | NAP  | C5A-N7A | -5.69 | 1.28        | 1.39     |
| 2   | N     | 301 | NAP  | C5A-N7A | -5.66 | 1.28        | 1.39     |
| 3   | X     | 302 | H4M  | CX1-C11 | -5.34 | 1.38        | 1.51     |
| 3   | F     | 302 | H4M  | CX1-C11 | -5.14 | 1.39        | 1.51     |
| 3   | U     | 302 | H4M  | CX1-C11 | -5.08 | 1.39        | 1.51     |
| 3   | S     | 302 | H4M  | CX1-C11 | -4.99 | 1.39        | 1.51     |
| 3   | H     | 302 | H4M  | CX1-C11 | -4.89 | 1.39        | 1.51     |
| 3   | O     | 302 | H4M  | CX1-C11 | -4.88 | 1.39        | 1.51     |
| 3   | L     | 302 | H4M  | CX1-C11 | -4.83 | 1.39        | 1.51     |
| 3   | N     | 302 | H4M  | CX1-C11 | -4.77 | 1.40        | 1.51     |
| 3   | J     | 302 | H4M  | CX1-C11 | -4.75 | 1.40        | 1.51     |
| 3   | K     | 302 | H4M  | CX1-C11 | -4.68 | 1.40        | 1.51     |
| 3   | M     | 302 | H4M  | CX1-C11 | -4.66 | 1.40        | 1.51     |
| 3   | E     | 302 | H4M  | CX1-C11 | -4.62 | 1.40        | 1.51     |
| 3   | G     | 302 | H4M  | CX1-C11 | -4.61 | 1.40        | 1.51     |
| 3   | P     | 302 | H4M  | CX1-C11 | -4.57 | 1.40        | 1.51     |
| 3   | W     | 302 | H4M  | CX1-C11 | -4.54 | 1.40        | 1.51     |
| 3   | A     | 302 | H4M  | CX1-C11 | -4.54 | 1.40        | 1.51     |
| 3   | V     | 302 | H4M  | CX1-C11 | -4.52 | 1.40        | 1.51     |
| 3   | B     | 302 | H4M  | CX1-C11 | -4.49 | 1.40        | 1.51     |
| 3   | D     | 301 | H4M  | CX1-C11 | -4.48 | 1.40        | 1.51     |
| 3   | I     | 302 | H4M  | CX1-C11 | -4.47 | 1.40        | 1.51     |
| 3   | T     | 302 | H4M  | CX1-C11 | -4.46 | 1.40        | 1.51     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | R     | 302 | H4M  | CX1-C11 | -4.44 | 1.40        | 1.51     |
| 3   | C     | 302 | H4M  | CX1-C11 | -4.32 | 1.41        | 1.51     |
| 3   | Q     | 302 | H4M  | CX1-C11 | -4.17 | 1.41        | 1.51     |
| 3   | P     | 302 | H4M  | C7-N8   | -4.10 | 1.42        | 1.47     |
| 2   | Q     | 301 | NAP  | PA-O3   | -4.02 | 1.55        | 1.59     |
| 3   | H     | 302 | H4M  | C7-N8   | -3.84 | 1.43        | 1.47     |
| 2   | H     | 301 | NAP  | C4A-N9A | -3.80 | 1.29        | 1.37     |
| 2   | U     | 301 | NAP  | C4A-N9A | -3.75 | 1.29        | 1.37     |
| 2   | W     | 301 | NAP  | C8A-N9A | -3.75 | 1.31        | 1.37     |
| 3   | G     | 302 | H4M  | C7-N8   | -3.75 | 1.43        | 1.47     |
| 2   | G     | 301 | NAP  | C8A-N9A | -3.75 | 1.31        | 1.37     |
| 2   | M     | 301 | NAP  | C8A-N9A | -3.73 | 1.31        | 1.37     |
| 2   | J     | 301 | NAP  | C8A-N9A | -3.68 | 1.31        | 1.37     |
| 2   | Q     | 301 | NAP  | C8A-N9A | -3.67 | 1.31        | 1.37     |
| 2   | G     | 301 | NAP  | PA-O3   | -3.67 | 1.55        | 1.59     |
| 2   | T     | 301 | NAP  | C8A-N9A | -3.65 | 1.31        | 1.37     |
| 2   | U     | 301 | NAP  | C8A-N9A | -3.62 | 1.31        | 1.37     |
| 3   | V     | 302 | H4M  | C7-N8   | -3.61 | 1.43        | 1.47     |
| 2   | C     | 301 | NAP  | C8A-N9A | -3.60 | 1.31        | 1.37     |
| 3   | G     | 302 | H4M  | PA-O3A  | 3.59  | 1.68        | 1.54     |
| 2   | F     | 301 | NAP  | C8A-N9A | -3.59 | 1.31        | 1.37     |
| 3   | J     | 302 | H4M  | PA-O3A  | 3.57  | 1.68        | 1.54     |
| 2   | R     | 301 | NAP  | C8A-N9A | -3.56 | 1.31        | 1.37     |
| 3   | S     | 302 | H4M  | C7-N8   | -3.55 | 1.43        | 1.47     |
| 3   | P     | 302 | H4M  | PA-O3A  | 3.55  | 1.68        | 1.54     |
| 2   | S     | 301 | NAP  | C8A-N9A | -3.54 | 1.31        | 1.37     |
| 2   | O     | 301 | NAP  | C8A-N9A | -3.53 | 1.31        | 1.37     |
| 3   | M     | 302 | H4M  | PA-O3A  | 3.52  | 1.67        | 1.54     |
| 3   | V     | 302 | H4M  | PA-O3A  | 3.52  | 1.67        | 1.54     |
| 2   | K     | 301 | NAP  | C8A-N9A | -3.52 | 1.31        | 1.37     |
| 3   | W     | 302 | H4M  | PA-O3A  | 3.51  | 1.67        | 1.54     |
| 2   | I     | 301 | NAP  | C8A-N9A | -3.50 | 1.31        | 1.37     |
| 2   | A     | 301 | NAP  | PA-O3   | -3.48 | 1.55        | 1.59     |
| 3   | A     | 302 | H4M  | PA-O3A  | 3.48  | 1.67        | 1.54     |
| 2   | A     | 301 | NAP  | C8A-N9A | -3.48 | 1.31        | 1.37     |
| 3   | S     | 302 | H4M  | PA-O3A  | 3.48  | 1.67        | 1.54     |
| 2   | E     | 301 | NAP  | C8A-N9A | -3.45 | 1.31        | 1.37     |
| 2   | L     | 301 | NAP  | C8A-N9A | -3.44 | 1.31        | 1.37     |
| 3   | D     | 301 | H4M  | C7-N8   | -3.43 | 1.43        | 1.47     |
| 2   | D     | 302 | NAP  | C8A-N9A | -3.43 | 1.31        | 1.37     |
| 2   | L     | 301 | NAP  | C4A-N9A | -3.42 | 1.30        | 1.37     |
| 2   | X     | 301 | NAP  | C8A-N9A | -3.42 | 1.31        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | Q     | 302 | H4M  | PA-O3A  | 3.42  | 1.67        | 1.54     |
| 2   | V     | 301 | NAP  | C4A-N9A | -3.42 | 1.30        | 1.37     |
| 3   | C     | 302 | H4M  | PA-O3A  | 3.41  | 1.67        | 1.54     |
| 3   | D     | 301 | H4M  | PA-O3A  | 3.40  | 1.67        | 1.54     |
| 2   | R     | 301 | NAP  | C4A-N9A | -3.40 | 1.30        | 1.37     |
| 3   | R     | 302 | H4M  | PA-O3A  | 3.37  | 1.67        | 1.54     |
| 2   | P     | 301 | NAP  | C8A-N9A | -3.37 | 1.31        | 1.37     |
| 2   | H     | 301 | NAP  | C8A-N9A | -3.37 | 1.31        | 1.37     |
| 3   | N     | 302 | H4M  | PA-O3A  | 3.37  | 1.67        | 1.54     |
| 3   | H     | 302 | H4M  | PA-O3A  | 3.37  | 1.67        | 1.54     |
| 3   | B     | 302 | H4M  | PA-O3A  | 3.36  | 1.67        | 1.54     |
| 3   | O     | 302 | H4M  | PA-O3A  | 3.36  | 1.67        | 1.54     |
| 2   | V     | 301 | NAP  | C8A-N9A | -3.36 | 1.31        | 1.37     |
| 3   | E     | 302 | H4M  | PA-O3A  | 3.35  | 1.67        | 1.54     |
| 3   | L     | 302 | H4M  | PA-O3A  | 3.35  | 1.67        | 1.54     |
| 3   | F     | 302 | H4M  | PA-O3A  | 3.35  | 1.67        | 1.54     |
| 3   | I     | 302 | H4M  | PA-O3A  | 3.35  | 1.67        | 1.54     |
| 3   | X     | 302 | H4M  | PA-O3A  | 3.35  | 1.67        | 1.54     |
| 2   | X     | 301 | NAP  | C4A-N9A | -3.34 | 1.30        | 1.37     |
| 3   | T     | 302 | H4M  | PA-O3A  | 3.34  | 1.67        | 1.54     |
| 2   | X     | 301 | NAP  | P2B-O1X | -3.34 | 1.40        | 1.50     |
| 3   | U     | 302 | H4M  | PA-O3A  | 3.33  | 1.67        | 1.54     |
| 3   | K     | 302 | H4M  | PA-O3A  | 3.33  | 1.67        | 1.54     |
| 2   | J     | 301 | NAP  | P2B-O1X | -3.33 | 1.40        | 1.50     |
| 2   | V     | 301 | NAP  | C3N-C7N | 3.32  | 1.55        | 1.50     |
| 2   | Q     | 301 | NAP  | C4A-N9A | -3.29 | 1.30        | 1.37     |
| 2   | O     | 301 | NAP  | P2B-O1X | -3.29 | 1.40        | 1.50     |
| 2   | D     | 302 | NAP  | C4A-N9A | -3.28 | 1.30        | 1.37     |
| 2   | W     | 301 | NAP  | P2B-O1X | -3.27 | 1.40        | 1.50     |
| 2   | B     | 301 | NAP  | C4A-N9A | -3.27 | 1.30        | 1.37     |
| 2   | B     | 301 | NAP  | C8A-N9A | -3.26 | 1.32        | 1.37     |
| 2   | S     | 301 | NAP  | C4A-N9A | -3.25 | 1.30        | 1.37     |
| 2   | X     | 301 | NAP  | P2B-O2X | -3.25 | 1.42        | 1.54     |
| 2   | T     | 301 | NAP  | P2B-O1X | -3.24 | 1.40        | 1.50     |
| 2   | E     | 301 | NAP  | P2B-O1X | -3.24 | 1.40        | 1.50     |
| 2   | U     | 301 | NAP  | C3N-C7N | 3.23  | 1.55        | 1.50     |
| 2   | A     | 301 | NAP  | C4A-N9A | -3.23 | 1.31        | 1.37     |
| 2   | U     | 301 | NAP  | P2B-O1X | -3.23 | 1.40        | 1.50     |
| 2   | F     | 301 | NAP  | C3N-C7N | 3.23  | 1.55        | 1.50     |
| 2   | S     | 301 | NAP  | P2B-O1X | -3.23 | 1.40        | 1.50     |
| 2   | M     | 301 | NAP  | PA-O3   | -3.22 | 1.56        | 1.59     |
| 2   | N     | 301 | NAP  | C4A-N9A | -3.21 | 1.31        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | O     | 301 | NAP  | C4A-N9A | -3.21 | 1.31        | 1.37     |
| 3   | A     | 302 | H4M  | C6-C7   | -3.20 | 1.48        | 1.53     |
| 2   | W     | 301 | NAP  | C4A-N9A | -3.19 | 1.31        | 1.37     |
| 2   | O     | 301 | NAP  | C3N-C7N | 3.18  | 1.55        | 1.50     |
| 2   | C     | 301 | NAP  | C3N-C7N | 3.16  | 1.55        | 1.50     |
| 2   | E     | 301 | NAP  | C4A-N9A | -3.15 | 1.31        | 1.37     |
| 3   | A     | 302 | H4M  | C7-N8   | -3.15 | 1.43        | 1.47     |
| 3   | L     | 302 | H4M  | C7-N8   | -3.15 | 1.43        | 1.47     |
| 2   | P     | 301 | NAP  | C3N-C7N | 3.14  | 1.55        | 1.50     |
| 2   | L     | 301 | NAP  | P2B-O1X | -3.14 | 1.40        | 1.50     |
| 2   | N     | 301 | NAP  | C8A-N9A | -3.14 | 1.32        | 1.37     |
| 2   | M     | 301 | NAP  | C4A-N9A | -3.14 | 1.31        | 1.37     |
| 2   | C     | 301 | NAP  | C4A-N9A | -3.14 | 1.31        | 1.37     |
| 2   | G     | 301 | NAP  | C4A-N9A | -3.13 | 1.31        | 1.37     |
| 2   | I     | 301 | NAP  | C4A-N9A | -3.13 | 1.31        | 1.37     |
| 2   | F     | 301 | NAP  | C4A-N9A | -3.13 | 1.31        | 1.37     |
| 3   | J     | 302 | H4M  | C7-N8   | -3.13 | 1.43        | 1.47     |
| 2   | T     | 301 | NAP  | C3N-C7N | 3.13  | 1.55        | 1.50     |
| 2   | N     | 301 | NAP  | PA-O3   | -3.12 | 1.56        | 1.59     |
| 2   | E     | 301 | NAP  | PA-O3   | -3.12 | 1.56        | 1.59     |
| 2   | D     | 302 | NAP  | O4D-C1D | 3.12  | 1.45        | 1.40     |
| 2   | K     | 301 | NAP  | C4A-N9A | -3.11 | 1.31        | 1.37     |
| 2   | G     | 301 | NAP  | O4D-C1D | 3.11  | 1.45        | 1.40     |
| 2   | V     | 301 | NAP  | P2B-O1X | -3.11 | 1.40        | 1.50     |
| 2   | I     | 301 | NAP  | C3N-C7N | 3.10  | 1.55        | 1.50     |
| 2   | I     | 301 | NAP  | P2B-O1X | -3.08 | 1.40        | 1.50     |
| 2   | E     | 301 | NAP  | PA-O2A  | -3.06 | 1.41        | 1.55     |
| 2   | E     | 301 | NAP  | PN-O1N  | -3.02 | 1.40        | 1.50     |
| 2   | P     | 301 | NAP  | C4A-N9A | -3.01 | 1.31        | 1.37     |
| 2   | A     | 301 | NAP  | P2B-O1X | -3.00 | 1.41        | 1.50     |
| 3   | G     | 302 | H4M  | C6-C7   | -3.00 | 1.48        | 1.53     |
| 2   | W     | 301 | NAP  | P2B-O2X | -3.00 | 1.43        | 1.54     |
| 3   | K     | 302 | H4M  | C7-N8   | -2.99 | 1.43        | 1.47     |
| 3   | B     | 302 | H4M  | C7-N8   | -2.99 | 1.43        | 1.47     |
| 3   | X     | 302 | H4M  | C7-N8   | -2.98 | 1.43        | 1.47     |
| 2   | J     | 301 | NAP  | PA-O3   | -2.97 | 1.56        | 1.59     |
| 2   | E     | 301 | NAP  | O4D-C1D | 2.97  | 1.44        | 1.40     |
| 3   | M     | 302 | H4M  | C7-N8   | -2.96 | 1.44        | 1.47     |
| 3   | W     | 302 | H4M  | C7-N8   | -2.96 | 1.44        | 1.47     |
| 3   | O     | 302 | H4M  | C7-N8   | -2.95 | 1.44        | 1.47     |
| 2   | T     | 301 | NAP  | PN-O1N  | -2.95 | 1.40        | 1.50     |
| 2   | C     | 301 | NAP  | P2B-O1X | -2.95 | 1.41        | 1.50     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | X     | 301 | NAP  | C3N-C7N | 2.95  | 1.55        | 1.50     |
| 2   | E     | 301 | NAP  | PA-O1A  | -2.95 | 1.40        | 1.50     |
| 2   | N     | 301 | NAP  | O7N-C7N | -2.95 | 1.18        | 1.24     |
| 2   | W     | 301 | NAP  | PA-O1A  | -2.94 | 1.40        | 1.50     |
| 2   | J     | 301 | NAP  | C4A-N9A | -2.91 | 1.31        | 1.37     |
| 2   | T     | 301 | NAP  | C4A-N9A | -2.91 | 1.31        | 1.37     |
| 2   | W     | 301 | NAP  | PN-O1N  | -2.90 | 1.40        | 1.50     |
| 2   | A     | 301 | NAP  | O4D-C1D | 2.90  | 1.44        | 1.40     |
| 2   | N     | 301 | NAP  | PA-O2A  | -2.90 | 1.41        | 1.55     |
| 2   | N     | 301 | NAP  | C3N-C7N | 2.89  | 1.54        | 1.50     |
| 2   | E     | 301 | NAP  | C3N-C7N | 2.88  | 1.54        | 1.50     |
| 2   | R     | 301 | NAP  | C3N-C7N | 2.88  | 1.54        | 1.50     |
| 2   | J     | 301 | NAP  | O4D-C1D | 2.88  | 1.44        | 1.40     |
| 3   | U     | 302 | H4M  | C7-N8   | -2.88 | 1.44        | 1.47     |
| 2   | H     | 301 | NAP  | C3N-C7N | 2.87  | 1.54        | 1.50     |
| 2   | G     | 301 | NAP  | O7N-C7N | -2.86 | 1.18        | 1.24     |
| 2   | V     | 301 | NAP  | PA-O2A  | -2.86 | 1.42        | 1.55     |
| 2   | E     | 301 | NAP  | O4B-C4B | -2.85 | 1.38        | 1.45     |
| 2   | A     | 301 | NAP  | PA-O2A  | -2.84 | 1.42        | 1.55     |
| 2   | L     | 301 | NAP  | P2B-O2X | -2.82 | 1.44        | 1.54     |
| 2   | E     | 301 | NAP  | P2B-O2X | -2.81 | 1.44        | 1.54     |
| 2   | M     | 301 | NAP  | O4D-C1D | 2.81  | 1.44        | 1.40     |
| 2   | Q     | 301 | NAP  | C3N-C7N | 2.81  | 1.54        | 1.50     |
| 2   | U     | 301 | NAP  | PA-O2A  | -2.81 | 1.42        | 1.55     |
| 3   | F     | 302 | H4M  | C7-N8   | -2.80 | 1.44        | 1.47     |
| 3   | Q     | 302 | H4M  | C7-N8   | -2.80 | 1.44        | 1.47     |
| 2   | D     | 302 | NAP  | P2B-O2X | -2.79 | 1.44        | 1.54     |
| 3   | N     | 302 | H4M  | C7-N8   | -2.78 | 1.44        | 1.47     |
| 2   | J     | 301 | NAP  | C3N-C7N | 2.78  | 1.54        | 1.50     |
| 2   | W     | 301 | NAP  | O7N-C7N | -2.78 | 1.19        | 1.24     |
| 2   | J     | 301 | NAP  | P2B-O2X | -2.78 | 1.44        | 1.54     |
| 2   | T     | 301 | NAP  | O7N-C7N | -2.78 | 1.19        | 1.24     |
| 2   | K     | 301 | NAP  | O7N-C7N | -2.75 | 1.19        | 1.24     |
| 2   | P     | 301 | NAP  | PA-O2A  | -2.75 | 1.42        | 1.55     |
| 2   | R     | 301 | NAP  | P2B-O2X | -2.75 | 1.44        | 1.54     |
| 2   | F     | 301 | NAP  | P2B-O1X | -2.75 | 1.41        | 1.50     |
| 2   | W     | 301 | NAP  | C3N-C7N | 2.74  | 1.54        | 1.50     |
| 2   | O     | 301 | NAP  | PA-O1A  | -2.74 | 1.41        | 1.50     |
| 3   | I     | 302 | H4M  | C7-N8   | -2.74 | 1.44        | 1.47     |
| 2   | X     | 301 | NAP  | PA-O2A  | -2.72 | 1.42        | 1.55     |
| 2   | H     | 301 | NAP  | O7N-C7N | -2.71 | 1.19        | 1.24     |
| 2   | W     | 301 | NAP  | PA-O2A  | -2.70 | 1.42        | 1.55     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | D     | 302 | NAP  | PA-O1A  | -2.70 | 1.41        | 1.50     |
| 2   | S     | 301 | NAP  | P2B-O2X | -2.70 | 1.44        | 1.54     |
| 2   | G     | 301 | NAP  | PA-O2A  | -2.70 | 1.42        | 1.55     |
| 3   | O     | 302 | H4M  | OX5-C1J | 2.69  | 1.44        | 1.40     |
| 2   | S     | 301 | NAP  | O4B-C4B | -2.69 | 1.39        | 1.45     |
| 2   | C     | 301 | NAP  | O7N-C7N | -2.69 | 1.19        | 1.24     |
| 3   | G     | 302 | H4M  | OH4-C4  | -2.69 | 1.18        | 1.23     |
| 2   | G     | 301 | NAP  | C3N-C7N | 2.69  | 1.54        | 1.50     |
| 3   | S     | 302 | H4M  | OX5-C1J | 2.68  | 1.44        | 1.40     |
| 2   | L     | 301 | NAP  | C3N-C7N | 2.68  | 1.54        | 1.50     |
| 2   | L     | 301 | NAP  | PA-O2A  | -2.67 | 1.43        | 1.55     |
| 3   | G     | 302 | H4M  | OX5-C1J | 2.67  | 1.44        | 1.40     |
| 2   | Q     | 301 | NAP  | P2B-O1X | -2.66 | 1.42        | 1.50     |
| 3   | R     | 302 | H4M  | C7-N8   | -2.66 | 1.44        | 1.47     |
| 2   | U     | 301 | NAP  | PN-O1N  | -2.65 | 1.41        | 1.50     |
| 2   | A     | 301 | NAP  | C3N-C7N | 2.65  | 1.54        | 1.50     |
| 2   | T     | 301 | NAP  | O4B-C4B | -2.64 | 1.39        | 1.45     |
| 2   | Q     | 301 | NAP  | O4D-C1D | 2.64  | 1.44        | 1.40     |
| 2   | A     | 301 | NAP  | P2B-O2X | -2.63 | 1.45        | 1.54     |
| 3   | N     | 302 | H4M  | C6-N5   | -2.63 | 1.43        | 1.47     |
| 2   | S     | 301 | NAP  | PA-O1A  | -2.63 | 1.41        | 1.50     |
| 2   | V     | 301 | NAP  | PN-O1N  | -2.63 | 1.41        | 1.50     |
| 3   | N     | 302 | H4M  | OX5-C1J | 2.62  | 1.44        | 1.40     |
| 2   | T     | 301 | NAP  | PA-O1A  | -2.62 | 1.41        | 1.50     |
| 2   | Q     | 301 | NAP  | P2B-O2X | -2.61 | 1.45        | 1.54     |
| 3   | P     | 302 | H4M  | C6-N5   | -2.61 | 1.43        | 1.47     |
| 2   | X     | 301 | NAP  | PA-O1A  | -2.60 | 1.41        | 1.50     |
| 2   | F     | 301 | NAP  | O4D-C1D | 2.60  | 1.44        | 1.40     |
| 2   | S     | 301 | NAP  | PA-O2A  | -2.60 | 1.43        | 1.55     |
| 3   | R     | 302 | H4M  | OX5-C1J | 2.60  | 1.44        | 1.40     |
| 2   | P     | 301 | NAP  | P2B-O2X | -2.59 | 1.45        | 1.54     |
| 3   | C     | 302 | H4M  | OX5-C1J | 2.59  | 1.44        | 1.40     |
| 2   | R     | 301 | NAP  | P2B-O1X | -2.58 | 1.42        | 1.50     |
| 2   | W     | 301 | NAP  | O4B-C4B | -2.58 | 1.39        | 1.45     |
| 3   | S     | 302 | H4M  | C6-N5   | -2.58 | 1.43        | 1.47     |
| 2   | B     | 301 | NAP  | C3N-C7N | 2.58  | 1.54        | 1.50     |
| 2   | X     | 301 | NAP  | O4B-C4B | -2.58 | 1.39        | 1.45     |
| 2   | L     | 301 | NAP  | PA-O1A  | -2.58 | 1.41        | 1.50     |
| 2   | B     | 301 | NAP  | O7N-C7N | -2.58 | 1.19        | 1.24     |
| 2   | J     | 301 | NAP  | PA-O1A  | -2.58 | 1.41        | 1.50     |
| 2   | S     | 301 | NAP  | PN-O1N  | -2.57 | 1.41        | 1.50     |
| 3   | C     | 302 | H4M  | C7-N8   | -2.57 | 1.44        | 1.47     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | N     | 301 | NAP  | P2B-O1X | -2.57 | 1.42        | 1.50     |
| 3   | R     | 302 | H4M  | C6-N5   | -2.56 | 1.43        | 1.47     |
| 2   | F     | 301 | NAP  | PA-O1A  | -2.56 | 1.41        | 1.50     |
| 2   | D     | 302 | NAP  | PA-O2A  | -2.56 | 1.43        | 1.55     |
| 2   | B     | 301 | NAP  | PA-O2A  | -2.56 | 1.43        | 1.55     |
| 2   | U     | 301 | NAP  | PA-O1A  | -2.56 | 1.41        | 1.50     |
| 3   | B     | 302 | H4M  | OX5-C1J | 2.55  | 1.44        | 1.40     |
| 2   | K     | 301 | NAP  | C3N-C7N | 2.55  | 1.54        | 1.50     |
| 2   | K     | 301 | NAP  | PN-O1N  | -2.55 | 1.42        | 1.50     |
| 3   | P     | 302 | H4M  | C6-C7   | -2.55 | 1.49        | 1.53     |
| 2   | V     | 301 | NAP  | PA-O1A  | -2.55 | 1.42        | 1.50     |
| 2   | N     | 301 | NAP  | P2B-O2X | -2.55 | 1.45        | 1.54     |
| 2   | Q     | 301 | NAP  | PN-O1N  | -2.55 | 1.42        | 1.50     |
| 3   | H     | 302 | H4M  | C6-N5   | -2.54 | 1.43        | 1.47     |
| 2   | R     | 301 | NAP  | O7N-C7N | -2.54 | 1.19        | 1.24     |
| 2   | P     | 301 | NAP  | P2B-O1X | -2.54 | 1.42        | 1.50     |
| 2   | D     | 302 | NAP  | P2B-O1X | -2.53 | 1.42        | 1.50     |
| 2   | L     | 301 | NAP  | PN-O1N  | -2.53 | 1.42        | 1.50     |
| 3   | A     | 302 | H4M  | OX5-C1J | 2.53  | 1.44        | 1.40     |
| 3   | Q     | 302 | H4M  | OX5-C1J | 2.53  | 1.44        | 1.40     |
| 3   | V     | 302 | H4M  | C6-N5   | -2.53 | 1.43        | 1.47     |
| 2   | R     | 301 | NAP  | PA-O2A  | -2.53 | 1.43        | 1.55     |
| 2   | J     | 301 | NAP  | PA-O2A  | -2.52 | 1.43        | 1.55     |
| 2   | C     | 301 | NAP  | P2B-O2X | -2.52 | 1.45        | 1.54     |
| 2   | T     | 301 | NAP  | P2B-O2X | -2.52 | 1.45        | 1.54     |
| 2   | V     | 301 | NAP  | P2B-O2X | -2.52 | 1.45        | 1.54     |
| 2   | L     | 301 | NAP  | O7N-C7N | -2.52 | 1.19        | 1.24     |
| 2   | D     | 302 | NAP  | O7N-C7N | -2.51 | 1.19        | 1.24     |
| 2   | T     | 301 | NAP  | PA-O2A  | -2.50 | 1.43        | 1.55     |
| 2   | B     | 301 | NAP  | P2B-O1X | -2.50 | 1.42        | 1.50     |
| 2   | R     | 301 | NAP  | PA-O1A  | -2.50 | 1.42        | 1.50     |
| 3   | L     | 302 | H4M  | OX5-C1J | 2.50  | 1.44        | 1.40     |
| 3   | D     | 301 | H4M  | C6-N5   | -2.50 | 1.43        | 1.47     |
| 3   | I     | 302 | H4M  | OX5-C1J | 2.49  | 1.44        | 1.40     |
| 2   | U     | 301 | NAP  | P2B-O2X | -2.49 | 1.45        | 1.54     |
| 2   | O     | 301 | NAP  | PA-O2A  | -2.49 | 1.43        | 1.55     |
| 2   | P     | 301 | NAP  | O7N-C7N | -2.49 | 1.19        | 1.24     |
| 2   | I     | 301 | NAP  | PA-O1A  | -2.49 | 1.42        | 1.50     |
| 2   | I     | 301 | NAP  | O4B-C4B | -2.48 | 1.39        | 1.45     |
| 2   | J     | 301 | NAP  | O7N-C7N | -2.48 | 1.19        | 1.24     |
| 2   | H     | 301 | NAP  | PA-O1A  | -2.48 | 1.42        | 1.50     |
| 2   | N     | 301 | NAP  | PN-O1N  | -2.48 | 1.42        | 1.50     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | R     | 301 | NAP  | PN-O1N  | -2.48 | 1.42        | 1.50     |
| 2   | K     | 301 | NAP  | PA-O2A  | -2.48 | 1.43        | 1.55     |
| 2   | A     | 301 | NAP  | O7N-C7N | -2.48 | 1.19        | 1.24     |
| 2   | H     | 301 | NAP  | P2B-O1X | -2.47 | 1.42        | 1.50     |
| 3   | J     | 302 | H4M  | OX5-C1J | 2.47  | 1.44        | 1.40     |
| 3   | P     | 302 | H4M  | OX5-C1J | 2.47  | 1.44        | 1.40     |
| 2   | I     | 301 | NAP  | O7N-C7N | -2.46 | 1.19        | 1.24     |
| 2   | V     | 301 | NAP  | O4B-C4B | -2.46 | 1.39        | 1.45     |
| 3   | M     | 302 | H4M  | C6-C7   | -2.46 | 1.49        | 1.53     |
| 2   | I     | 301 | NAP  | PN-O1N  | -2.46 | 1.42        | 1.50     |
| 2   | U     | 301 | NAP  | O4B-C4B | -2.46 | 1.39        | 1.45     |
| 2   | S     | 301 | NAP  | PA-O3   | -2.45 | 1.56        | 1.59     |
| 2   | O     | 301 | NAP  | O4B-C4B | -2.45 | 1.39        | 1.45     |
| 2   | A     | 301 | NAP  | O4B-C4B | -2.45 | 1.39        | 1.45     |
| 2   | C     | 301 | NAP  | PA-O2A  | -2.44 | 1.44        | 1.55     |
| 2   | B     | 301 | NAP  | P2B-O2X | -2.44 | 1.45        | 1.54     |
| 2   | H     | 301 | NAP  | P2B-O2X | -2.43 | 1.45        | 1.54     |
| 3   | E     | 302 | H4M  | C7-N8   | -2.43 | 1.44        | 1.47     |
| 2   | F     | 301 | NAP  | PA-O2A  | -2.43 | 1.44        | 1.55     |
| 2   | L     | 301 | NAP  | PA-O3   | -2.42 | 1.56        | 1.59     |
| 2   | M     | 301 | NAP  | O7N-C7N | -2.42 | 1.19        | 1.24     |
| 2   | O     | 301 | NAP  | P2B-O2X | -2.42 | 1.45        | 1.54     |
| 3   | O     | 302 | H4M  | C6-N5   | -2.41 | 1.44        | 1.47     |
| 2   | F     | 301 | NAP  | PN-O1N  | -2.41 | 1.42        | 1.50     |
| 2   | K     | 301 | NAP  | O4B-C4B | -2.41 | 1.39        | 1.45     |
| 2   | O     | 301 | NAP  | O7N-C7N | -2.41 | 1.19        | 1.24     |
| 2   | O     | 301 | NAP  | PN-O1N  | -2.41 | 1.42        | 1.50     |
| 2   | K     | 301 | NAP  | P2B-O2X | -2.40 | 1.45        | 1.54     |
| 2   | P     | 301 | NAP  | O4D-C1D | 2.40  | 1.44        | 1.40     |
| 2   | X     | 301 | NAP  | O7N-C7N | -2.40 | 1.19        | 1.24     |
| 3   | J     | 302 | H4M  | C6-C7   | -2.39 | 1.49        | 1.53     |
| 2   | C     | 301 | NAP  | PN-O1N  | -2.39 | 1.42        | 1.50     |
| 3   | X     | 302 | H4M  | OX5-C1J | 2.39  | 1.44        | 1.40     |
| 3   | H     | 302 | H4M  | C6-C7   | -2.39 | 1.49        | 1.53     |
| 3   | F     | 302 | H4M  | OX5-C1J | 2.38  | 1.44        | 1.40     |
| 3   | V     | 302 | H4M  | OX5-C1J | 2.38  | 1.44        | 1.40     |
| 2   | W     | 301 | NAP  | PA-O3   | -2.38 | 1.56        | 1.59     |
| 2   | B     | 301 | NAP  | O4B-C4B | -2.38 | 1.39        | 1.45     |
| 2   | K     | 301 | NAP  | P2B-O1X | -2.37 | 1.43        | 1.50     |
| 2   | P     | 301 | NAP  | PA-O1A  | -2.37 | 1.42        | 1.50     |
| 2   | D     | 302 | NAP  | C3N-C7N | 2.37  | 1.54        | 1.50     |
| 2   | T     | 301 | NAP  | PA-O3   | -2.37 | 1.56        | 1.59     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | G     | 301 | NAP  | O4B-C4B | -2.37 | 1.39        | 1.45     |
| 3   | K     | 302 | H4M  | OX5-C1J | 2.36  | 1.44        | 1.40     |
| 2   | F     | 301 | NAP  | O4B-C4B | -2.36 | 1.39        | 1.45     |
| 2   | I     | 301 | NAP  | PA-O2A  | -2.36 | 1.44        | 1.55     |
| 2   | W     | 301 | NAP  | O5B-C5B | -2.36 | 1.35        | 1.44     |
| 2   | X     | 301 | NAP  | PN-O1N  | -2.35 | 1.42        | 1.50     |
| 2   | R     | 301 | NAP  | PA-O3   | -2.35 | 1.57        | 1.59     |
| 2   | L     | 301 | NAP  | O4B-C4B | -2.34 | 1.39        | 1.45     |
| 2   | R     | 301 | NAP  | O4D-C1D | 2.34  | 1.44        | 1.40     |
| 2   | A     | 301 | NAP  | PA-O1A  | -2.33 | 1.42        | 1.50     |
| 2   | C     | 301 | NAP  | O4B-C4B | -2.33 | 1.39        | 1.45     |
| 3   | W     | 302 | H4M  | OX5-C1J | 2.33  | 1.44        | 1.40     |
| 2   | F     | 301 | NAP  | O7N-C7N | -2.32 | 1.19        | 1.24     |
| 2   | I     | 301 | NAP  | O4D-C1D | 2.32  | 1.43        | 1.40     |
| 2   | G     | 301 | NAP  | P2B-O2X | -2.32 | 1.46        | 1.54     |
| 2   | J     | 301 | NAP  | O4B-C4B | -2.31 | 1.39        | 1.45     |
| 2   | M     | 301 | NAP  | C3N-C7N | 2.31  | 1.54        | 1.50     |
| 3   | B     | 302 | H4M  | C6-N5   | -2.31 | 1.44        | 1.47     |
| 3   | X     | 302 | H4M  | C6-N5   | -2.31 | 1.44        | 1.47     |
| 2   | Q     | 301 | NAP  | PA-O2A  | -2.31 | 1.44        | 1.55     |
| 3   | D     | 301 | H4M  | OX5-C1J | 2.30  | 1.44        | 1.40     |
| 3   | M     | 302 | H4M  | OX5-C1J | 2.30  | 1.44        | 1.40     |
| 2   | H     | 301 | NAP  | PA-O2A  | -2.30 | 1.44        | 1.55     |
| 2   | H     | 301 | NAP  | O4D-C1D | 2.29  | 1.43        | 1.40     |
| 3   | D     | 301 | H4M  | C6-C7   | -2.29 | 1.49        | 1.53     |
| 2   | B     | 301 | NAP  | O4D-C1D | 2.29  | 1.43        | 1.40     |
| 3   | G     | 302 | H4M  | C6-N5   | -2.29 | 1.44        | 1.47     |
| 3   | U     | 302 | H4M  | OX5-C1J | 2.28  | 1.44        | 1.40     |
| 2   | E     | 301 | NAP  | O5B-C5B | -2.28 | 1.36        | 1.44     |
| 3   | T     | 302 | H4M  | C7-N8   | -2.28 | 1.44        | 1.47     |
| 2   | S     | 301 | NAP  | O7N-C7N | -2.26 | 1.19        | 1.24     |
| 2   | G     | 301 | NAP  | P2B-O1X | -2.26 | 1.43        | 1.50     |
| 2   | D     | 302 | NAP  | O4B-C4B | -2.26 | 1.40        | 1.45     |
| 2   | V     | 301 | NAP  | O7N-C7N | -2.25 | 1.19        | 1.24     |
| 2   | X     | 301 | NAP  | PA-O3   | -2.25 | 1.57        | 1.59     |
| 2   | V     | 301 | NAP  | O4D-C1D | 2.24  | 1.43        | 1.40     |
| 2   | S     | 301 | NAP  | C3N-C7N | 2.24  | 1.53        | 1.50     |
| 2   | C     | 301 | NAP  | O4D-C1D | 2.24  | 1.43        | 1.40     |
| 2   | J     | 301 | NAP  | O5B-C5B | -2.23 | 1.36        | 1.44     |
| 2   | I     | 301 | NAP  | P2B-O2X | -2.23 | 1.46        | 1.54     |
| 2   | T     | 301 | NAP  | O5B-C5B | -2.23 | 1.36        | 1.44     |
| 3   | J     | 302 | H4M  | OH4-C4  | -2.23 | 1.19        | 1.23     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | G     | 301 | NAP  | PA-O1A  | -2.22 | 1.43        | 1.50     |
| 3   | T     | 302 | H4M  | OX5-C1J | 2.21  | 1.43        | 1.40     |
| 3   | K     | 302 | H4M  | C6-N5   | -2.21 | 1.44        | 1.47     |
| 2   | V     | 301 | NAP  | O5B-C5B | -2.20 | 1.36        | 1.44     |
| 2   | L     | 301 | NAP  | O5B-C5B | -2.19 | 1.36        | 1.44     |
| 2   | E     | 301 | NAP  | O7N-C7N | -2.18 | 1.20        | 1.24     |
| 3   | H     | 302 | H4M  | OX5-C1J | 2.18  | 1.43        | 1.40     |
| 2   | J     | 301 | NAP  | PN-O1N  | -2.17 | 1.43        | 1.50     |
| 3   | S     | 302 | H4M  | C6-C7   | -2.17 | 1.49        | 1.53     |
| 3   | E     | 302 | H4M  | OX5-C1J | 2.17  | 1.43        | 1.40     |
| 2   | P     | 301 | NAP  | O5B-C5B | -2.16 | 1.36        | 1.44     |
| 2   | U     | 301 | NAP  | O4D-C1D | 2.16  | 1.43        | 1.40     |
| 2   | H     | 301 | NAP  | PN-O1N  | -2.15 | 1.43        | 1.50     |
| 2   | F     | 301 | NAP  | P2B-O2X | -2.15 | 1.46        | 1.54     |
| 2   | Q     | 301 | NAP  | O7N-C7N | -2.15 | 1.20        | 1.24     |
| 2   | Q     | 301 | NAP  | PA-O1A  | -2.15 | 1.43        | 1.50     |
| 2   | B     | 301 | NAP  | PA-O3   | -2.15 | 1.57        | 1.59     |
| 2   | V     | 301 | NAP  | PA-O3   | -2.14 | 1.57        | 1.59     |
| 2   | U     | 301 | NAP  | O5B-C5B | -2.13 | 1.36        | 1.44     |
| 2   | U     | 301 | NAP  | PA-O3   | -2.13 | 1.57        | 1.59     |
| 3   | O     | 302 | H4M  | C6-C7   | -2.13 | 1.49        | 1.53     |
| 3   | W     | 302 | H4M  | C6-C7   | -2.13 | 1.49        | 1.53     |
| 3   | F     | 302 | H4M  | C6-C7   | -2.11 | 1.50        | 1.53     |
| 2   | S     | 301 | NAP  | O4D-C1D | 2.11  | 1.43        | 1.40     |
| 2   | N     | 301 | NAP  | O4B-C4B | -2.11 | 1.40        | 1.45     |
| 2   | M     | 301 | NAP  | PA-O2A  | -2.10 | 1.45        | 1.55     |
| 2   | I     | 301 | NAP  | PA-O3   | -2.10 | 1.57        | 1.59     |
| 2   | X     | 301 | NAP  | O4D-C1D | 2.10  | 1.43        | 1.40     |
| 3   | U     | 302 | H4M  | C6-C7   | -2.10 | 1.50        | 1.53     |
| 2   | U     | 301 | NAP  | O7N-C7N | -2.10 | 1.20        | 1.24     |
| 2   | X     | 301 | NAP  | O5B-C5B | -2.10 | 1.36        | 1.44     |
| 2   | F     | 301 | NAP  | O5B-C5B | -2.10 | 1.36        | 1.44     |
| 3   | B     | 302 | H4M  | C6-C7   | -2.09 | 1.50        | 1.53     |
| 2   | N     | 301 | NAP  | PA-O1A  | -2.09 | 1.43        | 1.50     |
| 2   | I     | 301 | NAP  | C6A-N1A | -2.09 | 1.29        | 1.35     |
| 2   | R     | 301 | NAP  | O5B-C5B | -2.09 | 1.36        | 1.44     |
| 2   | S     | 301 | NAP  | O5B-C5B | -2.09 | 1.36        | 1.44     |
| 2   | M     | 301 | NAP  | P2B-O2X | -2.09 | 1.47        | 1.54     |
| 2   | D     | 302 | NAP  | PN-O1N  | -2.09 | 1.43        | 1.50     |
| 3   | X     | 302 | H4M  | C6-C7   | -2.08 | 1.50        | 1.53     |
| 3   | L     | 302 | H4M  | C6-C7   | -2.08 | 1.50        | 1.53     |
| 3   | I     | 302 | H4M  | C6-C7   | -2.07 | 1.50        | 1.53     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | B     | 301 | NAP  | PN-O1N  | -2.07 | 1.43        | 1.50     |
| 2   | E     | 301 | NAP  | P2B-O3X | -2.06 | 1.47        | 1.54     |
| 2   | I     | 301 | NAP  | O5B-C5B | -2.05 | 1.36        | 1.44     |
| 2   | R     | 301 | NAP  | O4B-C4B | -2.05 | 1.40        | 1.45     |
| 2   | W     | 301 | NAP  | P2B-O3X | -2.05 | 1.47        | 1.54     |
| 2   | M     | 301 | NAP  | PN-O1N  | -2.04 | 1.43        | 1.50     |
| 2   | O     | 301 | NAP  | O5B-C5B | -2.04 | 1.36        | 1.44     |
| 2   | Q     | 301 | NAP  | P2B-O3X | -2.04 | 1.47        | 1.54     |
| 2   | O     | 301 | NAP  | O4D-C1D | 2.04  | 1.43        | 1.40     |
| 2   | T     | 301 | NAP  | PN-O3   | 2.04  | 1.61        | 1.59     |
| 2   | L     | 301 | NAP  | O4D-C1D | 2.03  | 1.43        | 1.40     |
| 2   | A     | 301 | NAP  | P2B-O3X | -2.03 | 1.47        | 1.54     |
| 2   | N     | 301 | NAP  | O4D-C1D | 2.02  | 1.43        | 1.40     |
| 3   | V     | 302 | H4M  | C6-C7   | -2.01 | 1.50        | 1.53     |
| 2   | A     | 301 | NAP  | O5B-C5B | -2.01 | 1.37        | 1.44     |
| 2   | O     | 301 | NAP  | P2B-O3X | -2.01 | 1.47        | 1.54     |
| 2   | M     | 301 | NAP  | P2B-O1X | -2.01 | 1.44        | 1.50     |
| 2   | G     | 301 | NAP  | PN-O1N  | -2.00 | 1.43        | 1.50     |

All (559) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | P     | 302 | H4M  | C7-C6-N5    | 6.48  | 115.07      | 108.61   |
| 3   | A     | 302 | H4M  | C7-C6-N5    | 6.47  | 115.06      | 108.61   |
| 2   | E     | 301 | NAP  | C5A-C4A-N3A | -6.38 | 117.94      | 126.72   |
| 2   | W     | 301 | NAP  | C5A-C4A-N3A | -6.33 | 118.00      | 126.72   |
| 3   | G     | 302 | H4M  | C7-C6-N5    | 6.31  | 114.89      | 108.61   |
| 3   | S     | 302 | H4M  | C7-C6-N5    | 6.29  | 114.88      | 108.61   |
| 2   | N     | 301 | NAP  | C5A-C4A-N3A | -6.28 | 118.06      | 126.72   |
| 2   | Q     | 301 | NAP  | C5A-C4A-N3A | -6.27 | 118.08      | 126.72   |
| 2   | J     | 301 | NAP  | C5A-C4A-N3A | -6.26 | 118.10      | 126.72   |
| 3   | V     | 302 | H4M  | C7-C6-N5    | 6.23  | 114.82      | 108.61   |
| 2   | C     | 301 | NAP  | C5A-C4A-N3A | -6.22 | 118.15      | 126.72   |
| 3   | M     | 302 | H4M  | C7-C6-N5    | 6.22  | 114.80      | 108.61   |
| 2   | A     | 301 | NAP  | C5A-C4A-N3A | -6.15 | 118.25      | 126.72   |
| 2   | T     | 301 | NAP  | C5A-C4A-N3A | -6.13 | 118.28      | 126.72   |
| 2   | K     | 301 | NAP  | C5A-C4A-N3A | -6.05 | 118.39      | 126.72   |
| 3   | G     | 302 | H4M  | C4A-C4-N3   | 6.01  | 121.52      | 110.94   |
| 2   | O     | 301 | NAP  | C5A-C4A-N3A | -6.00 | 118.45      | 126.72   |
| 2   | S     | 301 | NAP  | C5A-C4A-N3A | -6.00 | 118.45      | 126.72   |
| 2   | M     | 301 | NAP  | C5A-C4A-N3A | -6.00 | 118.46      | 126.72   |
| 2   | D     | 302 | NAP  | C5A-C4A-N3A | -5.96 | 118.51      | 126.72   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | I     | 301 | NAP  | C5A-C4A-N3A | -5.93 | 118.55      | 126.72   |
| 2   | X     | 301 | NAP  | C5A-C4A-N3A | -5.92 | 118.56      | 126.72   |
| 3   | P     | 302 | H4M  | C4A-C4-N3   | 5.89  | 121.31      | 110.94   |
| 2   | L     | 301 | NAP  | C5A-C4A-N3A | -5.87 | 118.64      | 126.72   |
| 2   | R     | 301 | NAP  | C5A-C4A-N3A | -5.85 | 118.66      | 126.72   |
| 3   | J     | 302 | H4M  | C4A-C4-N3   | 5.85  | 121.23      | 110.94   |
| 2   | B     | 301 | NAP  | C5A-C4A-N3A | -5.77 | 118.78      | 126.72   |
| 3   | D     | 301 | H4M  | C7-C6-N5    | 5.74  | 114.33      | 108.61   |
| 2   | P     | 301 | NAP  | C5A-C4A-N3A | -5.71 | 118.86      | 126.72   |
| 2   | Q     | 301 | NAP  | N3A-C4A-N9A | 5.71  | 136.87      | 127.17   |
| 2   | G     | 301 | NAP  | C5A-C4A-N3A | -5.59 | 119.02      | 126.72   |
| 2   | V     | 301 | NAP  | C5A-C4A-N3A | -5.58 | 119.04      | 126.72   |
| 2   | E     | 301 | NAP  | N3A-C4A-N9A | 5.56  | 136.62      | 127.17   |
| 2   | H     | 301 | NAP  | C5A-C4A-N3A | -5.54 | 119.09      | 126.72   |
| 2   | N     | 301 | NAP  | N3A-C4A-N9A | 5.40  | 136.35      | 127.17   |
| 3   | R     | 302 | H4M  | C6-C9-N10   | 5.39  | 106.50      | 102.55   |
| 2   | W     | 301 | NAP  | N3A-C4A-N9A | 5.37  | 136.30      | 127.17   |
| 3   | V     | 302 | H4M  | C2-N1-C8A   | 5.37  | 122.83      | 113.36   |
| 3   | K     | 302 | H4M  | C2-N1-C8A   | 5.36  | 122.82      | 113.36   |
| 3   | V     | 302 | H4M  | C4A-C4-N3   | 5.34  | 120.34      | 110.94   |
| 3   | O     | 302 | H4M  | C4A-C4-N3   | 5.32  | 120.31      | 110.94   |
| 2   | A     | 301 | NAP  | N3A-C4A-N9A | 5.29  | 136.17      | 127.17   |
| 3   | O     | 302 | H4M  | C2-N1-C8A   | 5.29  | 122.70      | 113.36   |
| 2   | J     | 301 | NAP  | N3A-C4A-N9A | 5.28  | 136.14      | 127.17   |
| 2   | U     | 301 | NAP  | C5A-C4A-N3A | -5.25 | 119.48      | 126.72   |
| 2   | T     | 301 | NAP  | N3A-C4A-N9A | 5.25  | 136.09      | 127.17   |
| 2   | F     | 301 | NAP  | C5A-C4A-N3A | -5.24 | 119.50      | 126.72   |
| 3   | C     | 302 | H4M  | C4A-C4-N3   | 5.23  | 120.15      | 110.94   |
| 3   | S     | 302 | H4M  | C4A-C4-N3   | 5.22  | 120.13      | 110.94   |
| 2   | K     | 301 | NAP  | N3A-C4A-N9A | 5.20  | 136.02      | 127.17   |
| 3   | L     | 302 | H4M  | C2-N1-C8A   | 5.20  | 122.54      | 113.36   |
| 3   | B     | 302 | H4M  | C2-N1-C8A   | 5.19  | 122.53      | 113.36   |
| 3   | I     | 302 | H4M  | C2-N1-C8A   | 5.19  | 122.52      | 113.36   |
| 2   | G     | 301 | NAP  | N3A-C4A-N9A | 5.19  | 135.99      | 127.17   |
| 3   | S     | 302 | H4M  | C2-N1-C8A   | 5.17  | 122.49      | 113.36   |
| 2   | M     | 301 | NAP  | N3A-C4A-N9A | 5.17  | 135.96      | 127.17   |
| 3   | T     | 302 | H4M  | C4A-C4-N3   | 5.14  | 119.99      | 110.94   |
| 3   | J     | 302 | H4M  | C7-C6-N5    | 5.12  | 113.71      | 108.61   |
| 2   | C     | 301 | NAP  | N3A-C4A-N9A | 5.08  | 135.81      | 127.17   |
| 3   | Q     | 302 | H4M  | C4A-C4-N3   | 5.07  | 119.86      | 110.94   |
| 3   | D     | 301 | H4M  | C2-N1-C8A   | 5.07  | 122.31      | 113.36   |
| 3   | B     | 302 | H4M  | C4A-C4-N3   | 5.06  | 119.84      | 110.94   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | P     | 301 | NAP  | N3A-C4A-N9A | 5.05  | 135.76      | 127.17   |
| 3   | T     | 302 | H4M  | C2-N1-C8A   | 5.05  | 122.27      | 113.36   |
| 2   | S     | 301 | NAP  | N3A-C4A-N9A | 5.04  | 135.74      | 127.17   |
| 3   | F     | 302 | H4M  | C2-N1-C8A   | 5.03  | 122.24      | 113.36   |
| 2   | B     | 301 | NAP  | N3A-C4A-N9A | 5.02  | 135.71      | 127.17   |
| 3   | U     | 302 | H4M  | C2-N1-C8A   | 5.01  | 122.20      | 113.36   |
| 2   | H     | 301 | NAP  | N3A-C4A-N9A | 4.97  | 135.62      | 127.17   |
| 3   | E     | 302 | H4M  | C4A-C4-N3   | 4.97  | 119.69      | 110.94   |
| 3   | G     | 302 | H4M  | C2-N1-C8A   | 4.97  | 122.12      | 113.36   |
| 3   | N     | 302 | H4M  | C6-C9-N10   | 4.96  | 106.19      | 102.55   |
| 3   | Q     | 302 | H4M  | C2-N1-C8A   | 4.94  | 122.08      | 113.36   |
| 3   | I     | 302 | H4M  | C4A-C4-N3   | 4.93  | 119.62      | 110.94   |
| 2   | D     | 302 | NAP  | N3A-C4A-N9A | 4.92  | 135.54      | 127.17   |
| 2   | O     | 301 | NAP  | N3A-C4A-N9A | 4.90  | 135.51      | 127.17   |
| 3   | N     | 302 | H4M  | C2-N1-C8A   | 4.90  | 122.00      | 113.36   |
| 3   | E     | 302 | H4M  | C2-N1-C8A   | 4.89  | 121.98      | 113.36   |
| 3   | W     | 302 | H4M  | C2-N1-C8A   | 4.88  | 121.97      | 113.36   |
| 3   | L     | 302 | H4M  | C4A-C4-N3   | 4.88  | 119.52      | 110.94   |
| 3   | C     | 302 | H4M  | C2-N1-C8A   | 4.85  | 121.92      | 113.36   |
| 3   | F     | 302 | H4M  | C4A-C4-N3   | 4.85  | 119.47      | 110.94   |
| 3   | K     | 302 | H4M  | C4A-C4-N3   | 4.84  | 119.46      | 110.94   |
| 3   | R     | 302 | H4M  | C2-N1-C8A   | 4.84  | 121.90      | 113.36   |
| 3   | X     | 302 | H4M  | C2-N1-C8A   | 4.83  | 121.88      | 113.36   |
| 3   | H     | 302 | H4M  | C2-N1-C8A   | 4.83  | 121.88      | 113.36   |
| 2   | I     | 301 | NAP  | N3A-C4A-N9A | 4.83  | 135.37      | 127.17   |
| 2   | R     | 301 | NAP  | N3A-C4A-N9A | 4.78  | 135.30      | 127.17   |
| 3   | D     | 301 | H4M  | C4A-C4-N3   | 4.77  | 119.33      | 110.94   |
| 2   | L     | 301 | NAP  | N3A-C4A-N9A | 4.73  | 135.22      | 127.17   |
| 3   | M     | 302 | H4M  | CX5-CX4-CX3 | -4.71 | 103.33      | 112.22   |
| 2   | X     | 301 | NAP  | N3A-C4A-N9A | 4.68  | 135.13      | 127.17   |
| 3   | R     | 302 | H4M  | C4A-C4-N3   | 4.64  | 119.10      | 110.94   |
| 3   | A     | 302 | H4M  | C2-N1-C8A   | 4.61  | 121.49      | 113.36   |
| 3   | W     | 302 | H4M  | C4A-C4-N3   | 4.58  | 119.00      | 110.94   |
| 2   | F     | 301 | NAP  | N3A-C4A-N9A | 4.51  | 134.83      | 127.17   |
| 3   | P     | 302 | H4M  | C2-N1-C8A   | 4.51  | 121.31      | 113.36   |
| 3   | U     | 302 | H4M  | C4A-C4-N3   | 4.49  | 118.84      | 110.94   |
| 3   | A     | 302 | H4M  | C4A-C4-N3   | 4.47  | 118.80      | 110.94   |
| 3   | N     | 302 | H4M  | C4A-C4-N3   | 4.44  | 118.75      | 110.94   |
| 2   | K     | 301 | NAP  | N3A-C2A-N1A | -4.38 | 121.95      | 128.58   |
| 3   | J     | 302 | H4M  | C2-N1-C8A   | 4.38  | 121.08      | 113.36   |
| 2   | V     | 301 | NAP  | N3A-C4A-N9A | 4.37  | 134.59      | 127.17   |
| 2   | N     | 301 | NAP  | N3A-C2A-N1A | -4.34 | 122.01      | 128.58   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | U     | 301 | NAP  | N3A-C2A-N1A | -4.31 | 122.06      | 128.58   |
| 3   | X     | 302 | H4M  | C4A-C4-N3   | 4.31  | 118.52      | 110.94   |
| 3   | H     | 302 | H4M  | C4A-C4-N3   | 4.29  | 118.49      | 110.94   |
| 2   | U     | 301 | NAP  | N3A-C4A-N9A | 4.28  | 134.44      | 127.17   |
| 3   | M     | 302 | H4M  | C2-N1-C8A   | 4.25  | 120.86      | 113.36   |
| 2   | N     | 301 | NAP  | C2A-N3A-C4A | 4.21  | 122.11      | 111.83   |
| 2   | R     | 301 | NAP  | N3A-C2A-N1A | -4.18 | 122.26      | 128.58   |
| 2   | K     | 301 | NAP  | C2A-N3A-C4A | 4.17  | 122.03      | 111.83   |
| 3   | V     | 302 | H4M  | C6-C9-N10   | 4.13  | 105.58      | 102.55   |
| 3   | K     | 302 | H4M  | C6-C9-N10   | 4.13  | 105.58      | 102.55   |
| 2   | X     | 301 | NAP  | N3A-C2A-N1A | -4.11 | 122.36      | 128.58   |
| 3   | M     | 302 | H4M  | C4A-C4-N3   | 4.07  | 118.10      | 110.94   |
| 2   | U     | 301 | NAP  | C4A-N9A-C1B | -4.05 | 117.15      | 126.63   |
| 2   | T     | 301 | NAP  | C2B-C1B-N9A | -4.02 | 107.13      | 113.75   |
| 3   | M     | 302 | H4M  | O4J-C1J-OX5 | -4.02 | 107.55      | 111.95   |
| 2   | R     | 301 | NAP  | C2A-N3A-C4A | 4.01  | 121.63      | 111.83   |
| 2   | X     | 301 | NAP  | C2A-N3A-C4A | 4.00  | 121.60      | 111.83   |
| 2   | W     | 301 | NAP  | C2A-N3A-C4A | 3.99  | 121.57      | 111.83   |
| 2   | P     | 301 | NAP  | N3A-C2A-N1A | -3.98 | 122.56      | 128.58   |
| 2   | E     | 301 | NAP  | C2A-N3A-C4A | 3.98  | 121.54      | 111.83   |
| 2   | V     | 301 | NAP  | C4A-N9A-C1B | -3.96 | 117.37      | 126.63   |
| 2   | F     | 301 | NAP  | N3A-C2A-N1A | -3.96 | 122.59      | 128.58   |
| 3   | X     | 302 | H4M  | C7M-C7-N8   | 3.96  | 113.23      | 109.44   |
| 2   | V     | 301 | NAP  | N3A-C2A-N1A | -3.96 | 122.59      | 128.58   |
| 2   | T     | 301 | NAP  | C2A-N3A-C4A | 3.95  | 121.48      | 111.83   |
| 2   | O     | 301 | NAP  | N3A-C2A-N1A | -3.94 | 122.61      | 128.58   |
| 2   | O     | 301 | NAP  | C2A-N3A-C4A | 3.94  | 121.46      | 111.83   |
| 2   | H     | 301 | NAP  | N3A-C2A-N1A | -3.94 | 122.62      | 128.58   |
| 2   | L     | 301 | NAP  | C2A-N3A-C4A | 3.92  | 121.40      | 111.83   |
| 2   | D     | 302 | NAP  | N3A-C2A-N1A | -3.92 | 122.65      | 128.58   |
| 2   | Q     | 301 | NAP  | C2A-N3A-C4A | 3.91  | 121.38      | 111.83   |
| 3   | O     | 302 | H4M  | C6-C9-N10   | 3.90  | 105.41      | 102.55   |
| 2   | T     | 301 | NAP  | N3A-C2A-N1A | -3.89 | 122.69      | 128.58   |
| 2   | L     | 301 | NAP  | N3A-C2A-N1A | -3.88 | 122.70      | 128.58   |
| 3   | U     | 302 | H4M  | C15-C14-N10 | -3.87 | 114.11      | 121.13   |
| 2   | C     | 301 | NAP  | C2A-N3A-C4A | 3.85  | 121.23      | 111.83   |
| 2   | J     | 301 | NAP  | C2A-N3A-C4A | 3.85  | 121.22      | 111.83   |
| 3   | R     | 302 | H4M  | CX4-CX3-CX2 | -3.84 | 107.18      | 113.57   |
| 2   | W     | 301 | NAP  | N3A-C2A-N1A | -3.83 | 122.78      | 128.58   |
| 2   | A     | 301 | NAP  | C2A-N3A-C4A | 3.83  | 121.18      | 111.83   |
| 2   | U     | 301 | NAP  | C2A-N3A-C4A | 3.83  | 121.18      | 111.83   |
| 2   | V     | 301 | NAP  | C2A-N3A-C4A | 3.82  | 121.15      | 111.83   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | S     | 301 | NAP  | C2A-N3A-C4A | 3.81  | 121.13      | 111.83   |
| 2   | D     | 302 | NAP  | C2A-N3A-C4A | 3.80  | 121.12      | 111.83   |
| 2   | G     | 301 | NAP  | N3A-C2A-N1A | -3.79 | 122.85      | 128.58   |
| 2   | P     | 301 | NAP  | C2A-N3A-C4A | 3.78  | 121.05      | 111.83   |
| 2   | J     | 301 | NAP  | N3A-C2A-N1A | -3.76 | 122.89      | 128.58   |
| 2   | A     | 301 | NAP  | N3A-C2A-N1A | -3.74 | 122.92      | 128.58   |
| 2   | I     | 301 | NAP  | N3A-C2A-N1A | -3.73 | 122.93      | 128.58   |
| 2   | I     | 301 | NAP  | C2A-N3A-C4A | 3.73  | 120.93      | 111.83   |
| 2   | R     | 301 | NAP  | C2B-C1B-N9A | -3.70 | 107.67      | 113.75   |
| 2   | D     | 302 | NAP  | C6N-N1N-C2N | -3.70 | 118.73      | 121.88   |
| 2   | F     | 301 | NAP  | C2A-N3A-C4A | 3.69  | 120.85      | 111.83   |
| 2   | E     | 301 | NAP  | C2B-C1B-N9A | -3.69 | 107.69      | 113.75   |
| 2   | E     | 301 | NAP  | N3A-C2A-N1A | -3.68 | 123.01      | 128.58   |
| 2   | S     | 301 | NAP  | N3A-C2A-N1A | -3.68 | 123.02      | 128.58   |
| 2   | L     | 301 | NAP  | N6A-C6A-N1A | -3.67 | 110.19      | 118.38   |
| 2   | C     | 301 | NAP  | N3A-C2A-N1A | -3.67 | 123.02      | 128.58   |
| 3   | F     | 302 | H4M  | C6-C9-N10   | -3.67 | 99.85       | 102.55   |
| 2   | Q     | 301 | NAP  | N3A-C2A-N1A | -3.65 | 123.06      | 128.58   |
| 3   | J     | 302 | H4M  | OH4-C4-C4A  | -3.64 | 118.68      | 127.62   |
| 3   | O     | 302 | H4M  | C7-C6-N5    | 3.60  | 112.19      | 108.61   |
| 2   | B     | 301 | NAP  | N3A-C2A-N1A | -3.59 | 123.15      | 128.58   |
| 2   | H     | 301 | NAP  | C2A-N3A-C4A | 3.59  | 120.59      | 111.83   |
| 2   | M     | 301 | NAP  | C6N-N1N-C2N | -3.56 | 118.85      | 121.88   |
| 3   | M     | 302 | H4M  | C6-C9-N10   | 3.55  | 105.15      | 102.55   |
| 2   | B     | 301 | NAP  | C2A-N3A-C4A | 3.54  | 120.47      | 111.83   |
| 3   | U     | 302 | H4M  | C7M-C7-N8   | 3.53  | 112.83      | 109.44   |
| 2   | G     | 301 | NAP  | C2A-N3A-C4A | 3.53  | 120.45      | 111.83   |
| 3   | B     | 302 | H4M  | C6-C9-N10   | 3.53  | 105.13      | 102.55   |
| 2   | F     | 301 | NAP  | C4A-N9A-C1B | -3.52 | 118.40      | 126.63   |
| 2   | C     | 301 | NAP  | N6A-C6A-N1A | -3.51 | 110.56      | 118.38   |
| 3   | X     | 302 | H4M  | C6-C9-N10   | 3.47  | 105.09      | 102.55   |
| 2   | V     | 301 | NAP  | C1B-N9A-C8A | 3.46  | 134.78      | 127.09   |
| 2   | O     | 301 | NAP  | N6A-C6A-N1A | -3.44 | 110.72      | 118.38   |
| 2   | M     | 301 | NAP  | C2A-N3A-C4A | 3.42  | 120.19      | 111.83   |
| 2   | I     | 301 | NAP  | N6A-C6A-N1A | -3.42 | 110.75      | 118.38   |
| 2   | V     | 301 | NAP  | N6A-C6A-N1A | -3.42 | 110.76      | 118.38   |
| 2   | U     | 301 | NAP  | C1B-N9A-C8A | 3.41  | 134.66      | 127.09   |
| 2   | L     | 301 | NAP  | C4A-N9A-C1B | -3.38 | 118.72      | 126.63   |
| 3   | U     | 302 | H4M  | C6-C9-N10   | -3.36 | 100.07      | 102.55   |
| 2   | U     | 301 | NAP  | N6A-C6A-N1A | -3.35 | 110.91      | 118.38   |
| 3   | L     | 302 | H4M  | C15-C14-N10 | -3.34 | 115.06      | 121.13   |
| 2   | S     | 301 | NAP  | N6A-C6A-N1A | -3.34 | 110.94      | 118.38   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | X     | 301 | NAP  | C4A-N9A-C1B | -3.32 | 118.88      | 126.63   |
| 2   | F     | 301 | NAP  | N6A-C6A-N1A | -3.30 | 111.03      | 118.38   |
| 2   | B     | 301 | NAP  | C2B-C1B-N9A | -3.28 | 108.36      | 113.75   |
| 3   | I     | 302 | H4M  | C2-N3-C4    | -3.27 | 119.18      | 125.11   |
| 3   | G     | 302 | H4M  | OH4-C4-C4A  | -3.26 | 119.63      | 127.62   |
| 2   | T     | 301 | NAP  | O7N-C7N-N7N | -3.25 | 117.91      | 122.62   |
| 2   | P     | 301 | NAP  | C4A-N9A-C1B | -3.25 | 119.03      | 126.63   |
| 2   | C     | 301 | NAP  | C5A-N7A-C8A | 3.24  | 108.55      | 103.45   |
| 2   | R     | 301 | NAP  | N6A-C6A-N1A | -3.23 | 111.18      | 118.38   |
| 3   | C     | 302 | H4M  | C6-C9-N10   | 3.23  | 104.92      | 102.55   |
| 3   | F     | 302 | H4M  | C15-C14-N10 | -3.23 | 115.27      | 121.13   |
| 3   | O     | 302 | H4M  | C2-N3-C4    | -3.23 | 119.26      | 125.11   |
| 2   | D     | 302 | NAP  | N6A-C6A-N1A | -3.22 | 111.21      | 118.38   |
| 3   | A     | 302 | H4M  | O4J-C1J-OX5 | -3.22 | 108.42      | 111.95   |
| 2   | M     | 301 | NAP  | N3A-C2A-N1A | -3.21 | 123.72      | 128.58   |
| 3   | P     | 302 | H4M  | C2-N3-C4    | -3.21 | 119.30      | 125.11   |
| 2   | W     | 301 | NAP  | C2B-C1B-N9A | -3.20 | 108.49      | 113.75   |
| 3   | J     | 302 | H4M  | C2-N3-C4    | -3.18 | 119.33      | 125.11   |
| 2   | C     | 301 | NAP  | O7N-C7N-N7N | -3.18 | 118.02      | 122.62   |
| 2   | O     | 301 | NAP  | C4A-N9A-C1B | -3.18 | 119.19      | 126.63   |
| 2   | O     | 301 | NAP  | C2B-C1B-N9A | -3.18 | 108.53      | 113.75   |
| 3   | P     | 302 | H4M  | OH4-C4-C4A  | -3.17 | 119.83      | 127.62   |
| 2   | X     | 301 | NAP  | N6A-C6A-N1A | -3.17 | 111.32      | 118.38   |
| 2   | G     | 301 | NAP  | C2B-C1B-N9A | -3.16 | 108.55      | 113.75   |
| 3   | X     | 302 | H4M  | C11-CX1-CX2 | -3.16 | 107.64      | 113.39   |
| 3   | F     | 302 | H4M  | C2-N3-C4    | -3.15 | 119.39      | 125.11   |
| 3   | G     | 302 | H4M  | C2-N3-C4    | -3.14 | 119.41      | 125.11   |
| 2   | J     | 301 | NAP  | C5A-N7A-C8A | 3.14  | 108.38      | 103.45   |
| 3   | U     | 302 | H4M  | C2-N3-C4    | -3.13 | 119.43      | 125.11   |
| 2   | G     | 301 | NAP  | C6N-N1N-C2N | -3.13 | 119.22      | 121.88   |
| 2   | O     | 301 | NAP  | C5A-N7A-C8A | 3.10  | 108.33      | 103.45   |
| 2   | C     | 301 | NAP  | C5A-C6A-N6A | 3.10  | 130.97      | 123.29   |
| 2   | A     | 301 | NAP  | C6N-N1N-C2N | -3.10 | 119.24      | 121.88   |
| 2   | L     | 301 | NAP  | C5A-C6A-N6A | 3.10  | 130.96      | 123.29   |
| 2   | K     | 301 | NAP  | O7N-C7N-N7N | -3.10 | 118.14      | 122.62   |
| 2   | K     | 301 | NAP  | N6A-C6A-N1A | -3.10 | 111.48      | 118.38   |
| 2   | R     | 301 | NAP  | C4A-N9A-C1B | -3.10 | 119.39      | 126.63   |
| 2   | S     | 301 | NAP  | C5A-N7A-C8A | 3.09  | 108.31      | 103.45   |
| 3   | H     | 302 | H4M  | C7M-C7-N8   | 3.09  | 112.40      | 109.44   |
| 2   | F     | 301 | NAP  | C3N-C7N-N7N | 3.09  | 121.55      | 117.74   |
| 3   | S     | 302 | H4M  | C2-N3-C4    | -3.09 | 119.51      | 125.11   |
| 3   | H     | 302 | H4M  | CX4-CX3-CX2 | -3.08 | 108.44      | 113.57   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | W     | 301 | NAP  | N6A-C6A-N1A | -3.08 | 111.51      | 118.38   |
| 3   | T     | 302 | H4M  | C2-N3-C4    | -3.08 | 119.53      | 125.11   |
| 2   | J     | 301 | NAP  | N6A-C6A-N1A | -3.08 | 111.52      | 118.38   |
| 3   | B     | 302 | H4M  | C2-N3-C4    | -3.05 | 119.59      | 125.11   |
| 3   | P     | 302 | H4M  | O4J-C1J-OX5 | -3.04 | 108.61      | 111.95   |
| 3   | L     | 302 | H4M  | C2-N3-C4    | -3.04 | 119.59      | 125.11   |
| 3   | X     | 302 | H4M  | C7-C6-N5    | 3.04  | 111.64      | 108.61   |
| 2   | L     | 301 | NAP  | C5A-N7A-C8A | 3.03  | 108.22      | 103.45   |
| 2   | T     | 301 | NAP  | N6A-C6A-N1A | -3.03 | 111.62      | 118.38   |
| 3   | B     | 302 | H4M  | C7-C6-N5    | 3.03  | 111.63      | 108.61   |
| 2   | N     | 301 | NAP  | O7N-C7N-N7N | -3.02 | 118.25      | 122.62   |
| 2   | H     | 301 | NAP  | O7N-C7N-N7N | -3.02 | 118.25      | 122.62   |
| 2   | N     | 301 | NAP  | C3N-C7N-N7N | 3.02  | 121.46      | 117.74   |
| 3   | Q     | 302 | H4M  | C2-N3-C4    | -3.01 | 119.64      | 125.11   |
| 2   | I     | 301 | NAP  | C5A-C6A-N6A | 3.01  | 130.73      | 123.29   |
| 2   | X     | 301 | NAP  | C5A-N7A-C8A | 3.00  | 108.16      | 103.45   |
| 3   | C     | 302 | H4M  | C2-N3-C4    | -3.00 | 119.68      | 125.11   |
| 3   | P     | 302 | H4M  | O4J-C1J-C2J | 3.00  | 108.79      | 104.98   |
| 2   | A     | 301 | NAP  | N6A-C6A-N1A | -2.99 | 111.72      | 118.38   |
| 2   | V     | 301 | NAP  | C5A-C6A-N6A | 2.99  | 130.69      | 123.29   |
| 2   | T     | 301 | NAP  | C5A-N7A-C8A | 2.98  | 108.14      | 103.45   |
| 2   | V     | 301 | NAP  | C5A-N7A-C8A | 2.98  | 108.14      | 103.45   |
| 3   | U     | 302 | H4M  | C13-C14-N10 | 2.98  | 126.54      | 121.13   |
| 2   | M     | 301 | NAP  | C5N-C4N-C3N | -2.98 | 117.43      | 120.36   |
| 2   | O     | 301 | NAP  | C5A-C6A-N6A | 2.98  | 130.66      | 123.29   |
| 2   | S     | 301 | NAP  | C4A-N9A-C1B | -2.97 | 119.69      | 126.63   |
| 2   | W     | 301 | NAP  | C5A-N7A-C8A | 2.96  | 108.11      | 103.45   |
| 2   | S     | 301 | NAP  | C5A-C6A-N6A | 2.96  | 130.61      | 123.29   |
| 2   | N     | 301 | NAP  | N6A-C6A-N1A | -2.96 | 111.79      | 118.38   |
| 2   | R     | 301 | NAP  | C5A-N7A-C8A | 2.95  | 108.09      | 103.45   |
| 2   | D     | 302 | NAP  | C5A-C6A-N6A | 2.95  | 130.59      | 123.29   |
| 3   | L     | 302 | H4M  | C13-C14-N10 | 2.95  | 126.48      | 121.13   |
| 2   | F     | 301 | NAP  | C5A-C6A-N6A | 2.95  | 130.58      | 123.29   |
| 3   | V     | 302 | H4M  | OH4-C4-C4A  | -2.95 | 120.39      | 127.62   |
| 2   | D     | 302 | NAP  | C5A-N7A-C8A | 2.95  | 108.08      | 103.45   |
| 2   | A     | 301 | NAP  | O2A-PA-O3   | 2.94  | 115.22      | 107.27   |
| 2   | U     | 301 | NAP  | C5A-C6A-N6A | 2.93  | 130.53      | 123.29   |
| 3   | W     | 302 | H4M  | C7-C6-N5    | 2.92  | 111.52      | 108.61   |
| 3   | X     | 302 | H4M  | C2-N3-C4    | -2.92 | 119.81      | 125.11   |
| 2   | I     | 301 | NAP  | O7N-C7N-N7N | -2.92 | 118.39      | 122.62   |
| 3   | E     | 302 | H4M  | C2-N3-C4    | -2.92 | 119.82      | 125.11   |
| 2   | P     | 301 | NAP  | N6A-C6A-N1A | -2.91 | 111.89      | 118.38   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | N     | 302 | H4M  | C2-N3-C4    | -2.91 | 119.83      | 125.11   |
| 2   | B     | 301 | NAP  | C5A-N7A-C8A | 2.91  | 108.03      | 103.45   |
| 2   | F     | 301 | NAP  | C1B-N9A-C8A | 2.91  | 133.55      | 127.09   |
| 2   | I     | 301 | NAP  | C5A-N7A-C8A | 2.91  | 108.02      | 103.45   |
| 3   | R     | 302 | H4M  | C2-N3-C4    | -2.89 | 119.86      | 125.11   |
| 2   | A     | 301 | NAP  | C2B-C1B-N9A | -2.88 | 109.01      | 113.75   |
| 3   | I     | 302 | H4M  | C7M-C7-N8   | 2.87  | 112.19      | 109.44   |
| 2   | I     | 301 | NAP  | C3N-C7N-N7N | 2.86  | 121.27      | 117.74   |
| 3   | T     | 302 | H4M  | OH4-C4-C4A  | -2.86 | 120.59      | 127.62   |
| 2   | C     | 301 | NAP  | C4A-C5A-N7A | -2.86 | 107.31      | 110.58   |
| 2   | K     | 301 | NAP  | C3N-C7N-N7N | 2.86  | 121.26      | 117.74   |
| 3   | P     | 302 | H4M  | C6-C9-N10   | 2.86  | 104.64      | 102.55   |
| 3   | W     | 302 | H4M  | CX5-CX4-CX3 | -2.85 | 106.85      | 112.22   |
| 2   | X     | 301 | NAP  | C1B-N9A-C8A | 2.84  | 133.40      | 127.09   |
| 2   | U     | 301 | NAP  | C6N-N1N-C2N | -2.84 | 119.46      | 121.88   |
| 3   | Q     | 302 | H4M  | C7-C6-N5    | 2.84  | 111.44      | 108.61   |
| 3   | G     | 302 | H4M  | C6-C9-N10   | 2.84  | 104.63      | 102.55   |
| 2   | V     | 301 | NAP  | C4A-C5A-N7A | -2.83 | 107.34      | 110.58   |
| 2   | I     | 301 | NAP  | C4A-N9A-C1B | -2.83 | 120.02      | 126.63   |
| 2   | L     | 301 | NAP  | C1B-N9A-C8A | 2.83  | 133.37      | 127.09   |
| 3   | E     | 302 | H4M  | OH4-C4-C4A  | -2.82 | 120.69      | 127.62   |
| 2   | L     | 301 | NAP  | C4A-C5A-N7A | -2.82 | 107.36      | 110.58   |
| 3   | A     | 302 | H4M  | C6-C9-N10   | 2.81  | 104.61      | 102.55   |
| 2   | O     | 301 | NAP  | C4A-C5A-N7A | -2.81 | 107.36      | 110.58   |
| 2   | I     | 301 | NAP  | C2B-C1B-N9A | -2.81 | 109.12      | 113.75   |
| 2   | J     | 301 | NAP  | C5A-C6A-N6A | 2.81  | 130.25      | 123.29   |
| 2   | C     | 301 | NAP  | C4A-N9A-C1B | -2.81 | 120.06      | 126.63   |
| 3   | D     | 301 | H4M  | OH4-C4-C4A  | -2.81 | 120.72      | 127.62   |
| 3   | S     | 302 | H4M  | OH4-C4-C4A  | -2.81 | 120.72      | 127.62   |
| 2   | U     | 301 | NAP  | C5A-N7A-C8A | 2.81  | 107.86      | 103.45   |
| 3   | S     | 302 | H4M  | CX5-CX4-CX3 | -2.79 | 106.95      | 112.22   |
| 3   | Q     | 302 | H4M  | OH4-C4-C4A  | -2.79 | 120.77      | 127.62   |
| 3   | D     | 301 | H4M  | C2-N3-C4    | -2.79 | 120.06      | 125.11   |
| 2   | A     | 301 | NAP  | C5N-C4N-C3N | -2.77 | 117.64      | 120.36   |
| 3   | U     | 302 | H4M  | CX4-CX3-CX2 | -2.77 | 108.96      | 113.57   |
| 3   | U     | 302 | H4M  | OH4-C4-C4A  | -2.77 | 120.83      | 127.62   |
| 2   | P     | 301 | NAP  | C6N-N1N-C2N | -2.76 | 119.53      | 121.88   |
| 3   | K     | 302 | H4M  | C2-N3-C4    | -2.76 | 120.10      | 125.11   |
| 2   | A     | 301 | NAP  | C4A-N9A-C1B | -2.76 | 120.17      | 126.63   |
| 2   | D     | 302 | NAP  | C4A-N9A-C1B | -2.76 | 120.18      | 126.63   |
| 2   | X     | 301 | NAP  | C4A-C5A-N7A | -2.75 | 107.44      | 110.58   |
| 2   | X     | 301 | NAP  | C5A-C6A-N6A | 2.74  | 130.07      | 123.29   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | F     | 301 | NAP  | C5A-N7A-C8A | 2.74  | 107.75      | 103.45   |
| 2   | J     | 301 | NAP  | C4A-C5A-N7A | -2.74 | 107.45      | 110.58   |
| 2   | A     | 301 | NAP  | C5A-N7A-C8A | 2.72  | 107.73      | 103.45   |
| 2   | R     | 301 | NAP  | C5A-C6A-N6A | 2.72  | 130.01      | 123.29   |
| 2   | I     | 301 | NAP  | C4A-C5A-N7A | -2.71 | 107.48      | 110.58   |
| 2   | E     | 301 | NAP  | N6A-C6A-N1A | -2.71 | 112.34      | 118.38   |
| 2   | S     | 301 | NAP  | C4A-C5A-N7A | -2.71 | 107.48      | 110.58   |
| 3   | F     | 302 | H4M  | O4J-C1J-OX5 | -2.71 | 108.98      | 111.95   |
| 3   | W     | 302 | H4M  | C2-N3-C4    | -2.70 | 120.21      | 125.11   |
| 2   | P     | 301 | NAP  | C5A-N7A-C8A | 2.70  | 107.69      | 103.45   |
| 2   | E     | 301 | NAP  | C6N-N1N-C2N | -2.70 | 119.58      | 121.88   |
| 2   | J     | 301 | NAP  | C2B-C1B-N9A | -2.70 | 109.31      | 113.75   |
| 3   | V     | 302 | H4M  | C2-N3-C4    | -2.70 | 120.22      | 125.11   |
| 2   | W     | 301 | NAP  | C4A-N9A-C1B | -2.70 | 120.33      | 126.63   |
| 2   | B     | 301 | NAP  | N6A-C6A-N1A | -2.69 | 112.39      | 118.38   |
| 3   | C     | 302 | H4M  | OH4-C4-C4A  | -2.68 | 121.03      | 127.62   |
| 2   | C     | 301 | NAP  | C2B-C1B-N9A | -2.68 | 109.34      | 113.75   |
| 2   | Q     | 301 | NAP  | N6A-C6A-N1A | -2.68 | 112.42      | 118.38   |
| 2   | Q     | 301 | NAP  | C2B-C1B-N9A | -2.67 | 109.36      | 113.75   |
| 3   | A     | 302 | H4M  | CX5-CX4-CX3 | -2.67 | 107.19      | 112.22   |
| 2   | O     | 301 | NAP  | C6N-N1N-C2N | -2.66 | 119.62      | 121.88   |
| 2   | E     | 301 | NAP  | C5A-N7A-C8A | 2.66  | 107.62      | 103.45   |
| 2   | R     | 301 | NAP  | N9A-C8A-N7A | -2.65 | 110.17      | 113.94   |
| 3   | V     | 302 | H4M  | C7M-C7-N8   | -2.64 | 106.91      | 109.44   |
| 2   | T     | 301 | NAP  | C4A-N9A-C1B | -2.64 | 120.45      | 126.63   |
| 2   | E     | 301 | NAP  | C4A-N9A-C1B | -2.64 | 120.47      | 126.63   |
| 2   | U     | 301 | NAP  | N9A-C8A-N7A | -2.64 | 110.20      | 113.94   |
| 2   | F     | 301 | NAP  | O7N-C7N-N7N | -2.63 | 118.81      | 122.62   |
| 2   | H     | 301 | NAP  | C4A-N9A-C8A | 2.63  | 108.50      | 105.74   |
| 2   | O     | 301 | NAP  | O7N-C7N-N7N | -2.63 | 118.82      | 122.62   |
| 2   | G     | 301 | NAP  | N6A-C6A-N1A | -2.63 | 112.53      | 118.38   |
| 3   | L     | 302 | H4M  | O4J-C1J-C2J | 2.62  | 108.32      | 104.98   |
| 2   | N     | 301 | NAP  | C2B-C1B-N9A | -2.62 | 109.44      | 113.75   |
| 3   | F     | 302 | H4M  | C13-C14-N10 | 2.62  | 125.88      | 121.13   |
| 2   | S     | 301 | NAP  | C2B-C1B-N9A | -2.61 | 109.45      | 113.75   |
| 3   | L     | 302 | H4M  | OH4-C4-C4A  | -2.61 | 121.22      | 127.62   |
| 2   | T     | 301 | NAP  | C3N-C7N-N7N | 2.61  | 120.95      | 117.74   |
| 2   | K     | 301 | NAP  | C5A-N7A-C8A | 2.60  | 107.54      | 103.45   |
| 3   | O     | 302 | H4M  | C7M-C7-N8   | 2.60  | 111.93      | 109.44   |
| 2   | K     | 301 | NAP  | C4A-N9A-C1B | -2.60 | 120.55      | 126.63   |
| 2   | W     | 301 | NAP  | C5A-C6A-N6A | 2.60  | 129.72      | 123.29   |
| 2   | H     | 301 | NAP  | C6N-N1N-C2N | -2.60 | 119.67      | 121.88   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | O     | 301 | NAP  | C1B-N9A-C8A | 2.59  | 132.85      | 127.09   |
| 2   | T     | 301 | NAP  | C5A-C6A-N6A | 2.59  | 129.71      | 123.29   |
| 3   | T     | 302 | H4M  | C10-N10-C14 | 2.59  | 128.64      | 120.41   |
| 2   | C     | 301 | NAP  | N9A-C8A-N7A | -2.58 | 110.27      | 113.94   |
| 3   | V     | 302 | H4M  | OX5-C1J-C2J | 2.58  | 111.93      | 107.81   |
| 3   | E     | 302 | H4M  | C10-N10-C14 | 2.57  | 128.56      | 120.41   |
| 2   | G     | 301 | NAP  | C4A-N9A-C8A | 2.57  | 108.43      | 105.74   |
| 2   | V     | 301 | NAP  | N9A-C8A-N7A | -2.56 | 110.30      | 113.94   |
| 3   | H     | 302 | H4M  | C9-C6-N5    | 2.56  | 104.76      | 102.36   |
| 2   | P     | 301 | NAP  | N9A-C8A-N7A | -2.56 | 110.30      | 113.94   |
| 3   | F     | 302 | H4M  | OH4-C4-C4A  | -2.56 | 121.33      | 127.62   |
| 3   | F     | 302 | H4M  | C10-N10-C9  | -2.56 | 98.25       | 108.56   |
| 2   | O     | 301 | NAP  | N9A-C8A-N7A | -2.56 | 110.31      | 113.94   |
| 2   | N     | 301 | NAP  | C6N-N1N-C2N | -2.55 | 119.70      | 121.88   |
| 2   | G     | 301 | NAP  | C4A-N9A-C1B | -2.55 | 120.66      | 126.63   |
| 3   | J     | 302 | H4M  | C1J-C2J-C3J | 2.55  | 105.46      | 102.29   |
| 3   | K     | 302 | H4M  | C9M-C9-N10  | -2.55 | 108.46      | 112.63   |
| 3   | C     | 302 | H4M  | C9M-C9-N10  | -2.54 | 108.46      | 112.63   |
| 2   | R     | 301 | NAP  | C4A-C5A-N7A | -2.54 | 107.67      | 110.58   |
| 2   | Q     | 301 | NAP  | C5A-N7A-C8A | 2.54  | 107.45      | 103.45   |
| 2   | B     | 301 | NAP  | N9A-C8A-N7A | -2.54 | 110.33      | 113.94   |
| 2   | K     | 301 | NAP  | C5A-C6A-N6A | 2.54  | 129.56      | 123.29   |
| 2   | U     | 301 | NAP  | C4A-C5A-N7A | -2.53 | 107.69      | 110.58   |
| 2   | K     | 301 | NAP  | C6N-N1N-C2N | -2.53 | 119.73      | 121.88   |
| 3   | W     | 302 | H4M  | C10-N10-C14 | 2.52  | 128.42      | 120.41   |
| 2   | J     | 301 | NAP  | C6N-N1N-C2N | -2.52 | 119.73      | 121.88   |
| 2   | A     | 301 | NAP  | C5A-C6A-N6A | 2.52  | 129.52      | 123.29   |
| 2   | P     | 301 | NAP  | C1B-N9A-C8A | 2.52  | 132.68      | 127.09   |
| 2   | L     | 301 | NAP  | N9A-C8A-N7A | -2.52 | 110.37      | 113.94   |
| 2   | D     | 302 | NAP  | C4A-C5A-N7A | -2.52 | 107.71      | 110.58   |
| 2   | X     | 301 | NAP  | N9A-C8A-N7A | -2.51 | 110.37      | 113.94   |
| 2   | S     | 301 | NAP  | N9A-C8A-N7A | -2.51 | 110.38      | 113.94   |
| 2   | B     | 301 | NAP  | C6N-N1N-C2N | -2.50 | 119.75      | 121.88   |
| 3   | F     | 302 | H4M  | O4J-C1J-C2J | 2.50  | 108.16      | 104.98   |
| 3   | X     | 302 | H4M  | O4J-C1J-OX5 | -2.50 | 109.21      | 111.95   |
| 2   | X     | 301 | NAP  | C6N-N1N-C2N | -2.49 | 119.76      | 121.88   |
| 3   | S     | 302 | H4M  | C6-C9-N10   | 2.49  | 104.37      | 102.55   |
| 2   | N     | 301 | NAP  | C5A-C6A-N6A | 2.48  | 129.43      | 123.29   |
| 2   | T     | 301 | NAP  | C4A-C5A-N7A | -2.48 | 107.75      | 110.58   |
| 2   | W     | 301 | NAP  | C4A-C5A-N7A | -2.48 | 107.75      | 110.58   |
| 2   | B     | 301 | NAP  | O7N-C7N-N7N | -2.48 | 119.03      | 122.62   |
| 2   | W     | 301 | NAP  | C6N-N1N-C2N | -2.48 | 119.77      | 121.88   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | R     | 301 | NAP  | C1B-N9A-C8A | 2.48  | 132.59      | 127.09   |
| 3   | Q     | 302 | H4M  | C10-N10-C14 | 2.47  | 128.25      | 120.41   |
| 3   | A     | 302 | H4M  | OH4-C4-C4A  | -2.47 | 121.57      | 127.62   |
| 2   | G     | 301 | NAP  | C5A-N7A-C8A | 2.46  | 107.32      | 103.45   |
| 2   | Q     | 301 | NAP  | C4A-N9A-C8A | 2.46  | 108.32      | 105.74   |
| 3   | V     | 302 | H4M  | C11-CX1-CX2 | 2.46  | 117.87      | 113.39   |
| 3   | N     | 302 | H4M  | C15-C14-N10 | -2.46 | 116.67      | 121.13   |
| 2   | W     | 301 | NAP  | O7N-C7N-N7N | -2.45 | 119.08      | 122.62   |
| 3   | W     | 302 | H4M  | OH4-C4-C4A  | -2.44 | 121.62      | 127.62   |
| 2   | E     | 301 | NAP  | O4B-C1B-N9A | 2.44  | 112.77      | 108.09   |
| 2   | U     | 301 | NAP  | C2B-C1B-N9A | -2.43 | 109.75      | 113.75   |
| 2   | D     | 302 | NAP  | N9A-C8A-N7A | -2.43 | 110.48      | 113.94   |
| 2   | L     | 301 | NAP  | C2B-C1B-N9A | -2.43 | 109.75      | 113.75   |
| 3   | M     | 302 | H4M  | OH4-C4-C4A  | -2.43 | 121.65      | 127.62   |
| 2   | P     | 301 | NAP  | C4A-N9A-C8A | 2.43  | 108.29      | 105.74   |
| 2   | R     | 301 | NAP  | C6N-N1N-C2N | -2.43 | 119.81      | 121.88   |
| 3   | F     | 302 | H4M  | C7M-C7-N8   | 2.43  | 111.76      | 109.44   |
| 2   | Q     | 301 | NAP  | C4A-N9A-C1B | -2.43 | 120.96      | 126.63   |
| 2   | F     | 301 | NAP  | C2B-C1B-N9A | -2.42 | 109.78      | 113.75   |
| 2   | F     | 301 | NAP  | C4A-C5A-N7A | -2.41 | 107.83      | 110.58   |
| 2   | U     | 301 | NAP  | C3N-C7N-N7N | 2.41  | 120.71      | 117.74   |
| 3   | O     | 302 | H4M  | C15-C14-N10 | -2.41 | 116.76      | 121.13   |
| 2   | F     | 301 | NAP  | O4B-C1B-N9A | 2.40  | 112.71      | 108.09   |
| 2   | P     | 301 | NAP  | C5A-C6A-N6A | 2.40  | 129.24      | 123.29   |
| 2   | L     | 301 | NAP  | O4B-C1B-N9A | 2.40  | 112.69      | 108.09   |
| 3   | I     | 302 | H4M  | C15-C14-N10 | -2.39 | 116.78      | 121.13   |
| 3   | H     | 302 | H4M  | C11-CX1-CX2 | 2.39  | 117.75      | 113.39   |
| 3   | O     | 302 | H4M  | OH4-C4-C4A  | -2.39 | 121.74      | 127.62   |
| 3   | N     | 302 | H4M  | OH4-C4-C4A  | -2.39 | 121.75      | 127.62   |
| 2   | T     | 301 | NAP  | N9A-C8A-N7A | -2.39 | 110.55      | 113.94   |
| 2   | W     | 301 | NAP  | N9A-C8A-N7A | -2.39 | 110.55      | 113.94   |
| 2   | G     | 301 | NAP  | O4B-C1B-N9A | 2.39  | 112.67      | 108.09   |
| 3   | J     | 302 | H4M  | C6-C9-N10   | 2.38  | 104.29      | 102.55   |
| 2   | H     | 301 | NAP  | N6A-C6A-N1A | -2.38 | 113.09      | 118.38   |
| 3   | X     | 302 | H4M  | O4J-C1J-C2J | 2.37  | 108.00      | 104.98   |
| 3   | A     | 302 | H4M  | C2-N3-C4    | -2.37 | 120.81      | 125.11   |
| 2   | M     | 301 | NAP  | C2B-C1B-N9A | -2.37 | 109.86      | 113.75   |
| 3   | X     | 302 | H4M  | C1J-C2J-C3J | 2.36  | 105.22      | 102.29   |
| 2   | M     | 301 | NAP  | C4A-N9A-C1B | -2.36 | 121.12      | 126.63   |
| 2   | J     | 301 | NAP  | C4A-N9A-C1B | -2.36 | 121.12      | 126.63   |
| 2   | B     | 301 | NAP  | C5A-C6A-N6A | 2.35  | 129.10      | 123.29   |
| 3   | A     | 302 | H4M  | NA2-C2-N3   | 2.35  | 121.71      | 116.76   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | I     | 301 | NAP  | C6N-N1N-C2N | -2.34 | 119.88      | 121.88   |
| 2   | L     | 301 | NAP  | O7N-C7N-N7N | -2.34 | 119.23      | 122.62   |
| 2   | S     | 301 | NAP  | C1B-N9A-C8A | 2.34  | 132.29      | 127.09   |
| 3   | V     | 302 | H4M  | C1J-C2J-C3J | 2.34  | 105.20      | 102.29   |
| 2   | M     | 301 | NAP  | C5A-N7A-C8A | 2.33  | 107.12      | 103.45   |
| 2   | I     | 301 | NAP  | C1B-N9A-C8A | 2.33  | 132.26      | 127.09   |
| 2   | O     | 301 | NAP  | O4B-C1B-N9A | 2.33  | 112.56      | 108.09   |
| 3   | S     | 302 | H4M  | O4J-C1J-OX5 | -2.33 | 109.40      | 111.95   |
| 2   | U     | 301 | NAP  | C4A-N9A-C8A | 2.32  | 108.18      | 105.74   |
| 2   | X     | 301 | NAP  | C2B-C1B-N9A | -2.32 | 109.93      | 113.75   |
| 2   | A     | 301 | NAP  | O4B-C1B-N9A | 2.32  | 112.54      | 108.09   |
| 2   | B     | 301 | NAP  | C4A-N9A-C8A | 2.31  | 108.17      | 105.74   |
| 3   | C     | 302 | H4M  | CX5-CX4-CX3 | -2.31 | 107.86      | 112.22   |
| 2   | B     | 301 | NAP  | C4A-N9A-C1B | -2.31 | 121.24      | 126.63   |
| 3   | X     | 302 | H4M  | OH4-C4-C4A  | -2.30 | 121.97      | 127.62   |
| 2   | L     | 301 | NAP  | C3N-C7N-N7N | 2.30  | 120.58      | 117.74   |
| 2   | D     | 302 | NAP  | C5N-C4N-C3N | -2.29 | 118.11      | 120.36   |
| 2   | B     | 301 | NAP  | C4A-C5A-N7A | -2.29 | 107.96      | 110.58   |
| 2   | E     | 301 | NAP  | C5A-C6A-N6A | 2.29  | 128.96      | 123.29   |
| 2   | Q     | 301 | NAP  | C3N-C7N-N7N | 2.29  | 120.56      | 117.74   |
| 2   | R     | 301 | NAP  | O7N-C7N-N7N | -2.29 | 119.31      | 122.62   |
| 2   | K     | 301 | NAP  | N9A-C8A-N7A | -2.29 | 110.69      | 113.94   |
| 2   | V     | 301 | NAP  | O7N-C7N-N7N | -2.29 | 119.31      | 122.62   |
| 2   | F     | 301 | NAP  | N9A-C8A-N7A | -2.29 | 110.69      | 113.94   |
| 2   | I     | 301 | NAP  | N9A-C8A-N7A | -2.28 | 110.70      | 113.94   |
| 2   | N     | 301 | NAP  | C4A-N9A-C1B | -2.28 | 121.30      | 126.63   |
| 2   | Q     | 301 | NAP  | O4B-C1B-N9A | 2.28  | 112.47      | 108.09   |
| 2   | A     | 301 | NAP  | C4A-C5A-N7A | -2.28 | 107.98      | 110.58   |
| 2   | J     | 301 | NAP  | C5N-C4N-C3N | -2.27 | 118.13      | 120.36   |
| 2   | Q     | 301 | NAP  | C6N-N1N-C2N | -2.27 | 119.94      | 121.88   |
| 3   | N     | 302 | H4M  | O4J-C1J-C2J | 2.27  | 107.86      | 104.98   |
| 2   | C     | 301 | NAP  | C3N-C7N-N7N | 2.27  | 120.53      | 117.74   |
| 2   | J     | 301 | NAP  | N9A-C8A-N7A | -2.26 | 110.73      | 113.94   |
| 2   | C     | 301 | NAP  | C1B-N9A-C8A | 2.26  | 132.11      | 127.09   |
| 2   | D     | 302 | NAP  | C2B-C1B-N9A | -2.26 | 110.04      | 113.75   |
| 2   | G     | 301 | NAP  | O2A-PA-O3   | 2.25  | 113.37      | 107.27   |
| 2   | P     | 301 | NAP  | C3N-C7N-N7N | 2.25  | 120.52      | 117.74   |
| 2   | L     | 301 | NAP  | C6N-N1N-C2N | -2.25 | 119.96      | 121.88   |
| 3   | D     | 301 | H4M  | C7M-C7-N8   | 2.25  | 111.60      | 109.44   |
| 2   | H     | 301 | NAP  | C2B-C1B-N9A | -2.25 | 110.05      | 113.75   |
| 2   | K     | 301 | NAP  | C2B-C1B-N9A | -2.25 | 110.05      | 113.75   |
| 3   | K     | 302 | H4M  | OX5-C1J-C2J | 2.25  | 111.40      | 107.81   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | H     | 301 | NAP  | C4A-N9A-C1B | -2.24 | 121.40      | 126.63   |
| 3   | R     | 302 | H4M  | C7M-C7-N8   | 2.23  | 111.58      | 109.44   |
| 2   | Q     | 301 | NAP  | C5A-C6A-N6A | 2.23  | 128.81      | 123.29   |
| 2   | D     | 302 | NAP  | C1B-N9A-C8A | 2.23  | 132.04      | 127.09   |
| 2   | J     | 301 | NAP  | O4B-C1B-N9A | 2.23  | 112.37      | 108.09   |
| 3   | B     | 302 | H4M  | C15-C14-N10 | -2.23 | 117.09      | 121.13   |
| 3   | N     | 302 | H4M  | C9M-C9-N10  | -2.22 | 108.99      | 112.63   |
| 2   | E     | 301 | NAP  | N9A-C8A-N7A | -2.21 | 110.80      | 113.94   |
| 2   | A     | 301 | NAP  | C1B-N9A-C8A | 2.21  | 132.00      | 127.09   |
| 2   | D     | 302 | NAP  | O4B-C1B-N9A | 2.20  | 112.32      | 108.09   |
| 2   | F     | 301 | NAP  | C4A-N9A-C8A | 2.20  | 108.05      | 105.74   |
| 2   | E     | 301 | NAP  | C4A-N9A-C8A | 2.20  | 108.05      | 105.74   |
| 2   | H     | 301 | NAP  | N9A-C8A-N7A | -2.20 | 110.81      | 113.94   |
| 2   | U     | 301 | NAP  | O7N-C7N-N7N | -2.20 | 119.44      | 122.62   |
| 2   | G     | 301 | NAP  | C5A-C6A-N6A | 2.20  | 128.72      | 123.29   |
| 2   | F     | 301 | NAP  | C6N-N1N-C2N | -2.19 | 120.01      | 121.88   |
| 2   | Q     | 301 | NAP  | O7N-C7N-N7N | -2.19 | 119.45      | 122.62   |
| 3   | R     | 302 | H4M  | OH4-C4-C4A  | -2.19 | 122.25      | 127.62   |
| 3   | F     | 302 | H4M  | CX4-CX3-CX2 | -2.18 | 109.94      | 113.57   |
| 2   | E     | 301 | NAP  | C4A-C5A-N7A | -2.18 | 108.08      | 110.58   |
| 3   | R     | 302 | H4M  | C9M-C9-N10  | -2.18 | 109.05      | 112.63   |
| 2   | W     | 301 | NAP  | O4B-C1B-N9A | 2.18  | 112.28      | 108.09   |
| 2   | G     | 301 | NAP  | O7N-C7N-N7N | -2.18 | 119.47      | 122.62   |
| 2   | G     | 301 | NAP  | N9A-C8A-N7A | -2.18 | 110.85      | 113.94   |
| 2   | R     | 301 | NAP  | C4A-N9A-C8A | 2.17  | 108.02      | 105.74   |
| 3   | H     | 302 | H4M  | CX1-C11-C12 | -2.17 | 116.86      | 120.90   |
| 2   | S     | 301 | NAP  | C4A-N9A-C8A | 2.17  | 108.02      | 105.74   |
| 3   | B     | 302 | H4M  | C7M-C7-N8   | 2.17  | 111.52      | 109.44   |
| 3   | C     | 302 | H4M  | C7-C6-N5    | 2.17  | 110.77      | 108.61   |
| 3   | E     | 302 | H4M  | CX5-CX4-CX3 | -2.16 | 108.13      | 112.22   |
| 2   | R     | 301 | NAP  | O2A-PA-O3   | 2.16  | 113.11      | 107.27   |
| 2   | A     | 301 | NAP  | N9A-C8A-N7A | -2.15 | 110.88      | 113.94   |
| 2   | S     | 301 | NAP  | C6N-N1N-C2N | -2.15 | 120.05      | 121.88   |
| 3   | M     | 302 | H4M  | C9M-C9-N10  | -2.15 | 109.10      | 112.63   |
| 3   | M     | 302 | H4M  | O4J-C1J-C2J | 2.14  | 107.71      | 104.98   |
| 3   | H     | 302 | H4M  | C6-C9-N10   | 2.13  | 104.11      | 102.55   |
| 3   | U     | 302 | H4M  | C10-N10-C9  | -2.13 | 99.99       | 108.56   |
| 2   | P     | 301 | NAP  | O7N-C7N-N7N | -2.13 | 119.54      | 122.62   |
| 2   | Q     | 301 | NAP  | N9A-C8A-N7A | -2.12 | 110.92      | 113.94   |
| 3   | B     | 302 | H4M  | O4J-C1J-C2J | 2.12  | 107.68      | 104.98   |
| 3   | L     | 302 | H4M  | O4J-C1J-OX5 | -2.12 | 109.62      | 111.95   |
| 3   | L     | 302 | H4M  | C9M-C9-N10  | 2.12  | 116.11      | 112.63   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | O     | 301 | NAP  | C4A-N9A-C8A | 2.11  | 107.95      | 105.74   |
| 2   | W     | 301 | NAP  | C1B-N9A-C8A | 2.11  | 131.77      | 127.09   |
| 3   | U     | 302 | H4M  | C11-CX1-CX2 | -2.10 | 109.56      | 113.39   |
| 3   | B     | 302 | H4M  | C9M-C9-N10  | -2.10 | 109.19      | 112.63   |
| 3   | T     | 302 | H4M  | C9M-C9-N10  | -2.10 | 109.19      | 112.63   |
| 3   | B     | 302 | H4M  | OH4-C4-C4A  | -2.10 | 122.48      | 127.62   |
| 3   | O     | 302 | H4M  | C1J-C2J-C3J | 2.09  | 104.90      | 102.29   |
| 2   | T     | 301 | NAP  | C4A-N9A-C8A | 2.09  | 107.93      | 105.74   |
| 3   | I     | 302 | H4M  | C1J-C2J-C3J | 2.09  | 104.89      | 102.29   |
| 3   | J     | 302 | H4M  | C15-C14-N10 | -2.08 | 117.35      | 121.13   |
| 2   | E     | 301 | NAP  | O7N-C7N-N7N | -2.08 | 119.61      | 122.62   |
| 3   | M     | 302 | H4M  | C11-CX1-CX2 | 2.08  | 117.18      | 113.39   |
| 2   | K     | 301 | NAP  | C4A-N9A-C8A | 2.08  | 107.92      | 105.74   |
| 3   | E     | 302 | H4M  | C7-C6-N5    | 2.07  | 110.67      | 108.61   |
| 3   | H     | 302 | H4M  | C2-N3-C4    | -2.07 | 121.36      | 125.11   |
| 2   | S     | 301 | NAP  | C5N-C4N-C3N | -2.07 | 118.33      | 120.36   |
| 2   | L     | 301 | NAP  | C4A-N9A-C8A | 2.07  | 107.91      | 105.74   |
| 2   | H     | 301 | NAP  | O7N-C7N-C3N | 2.07  | 122.12      | 119.60   |
| 2   | W     | 301 | NAP  | C4A-N9A-C8A | 2.06  | 107.90      | 105.74   |
| 3   | L     | 302 | H4M  | C1J-C2J-C3J | 2.06  | 104.85      | 102.29   |
| 2   | T     | 301 | NAP  | O4B-C1B-N9A | 2.05  | 112.03      | 108.09   |
| 3   | E     | 302 | H4M  | OX5-C1J-C2J | 2.04  | 111.07      | 107.81   |
| 3   | M     | 302 | H4M  | C2-N3-C4    | -2.04 | 121.41      | 125.11   |
| 2   | D     | 302 | NAP  | O7N-C7N-C3N | 2.04  | 122.09      | 119.60   |
| 2   | T     | 301 | NAP  | C6N-N1N-C2N | -2.03 | 120.15      | 121.88   |
| 2   | K     | 301 | NAP  | C4A-C5A-N7A | -2.03 | 108.26      | 110.58   |
| 2   | Q     | 301 | NAP  | C4A-C5A-N7A | -2.03 | 108.26      | 110.58   |
| 2   | W     | 301 | NAP  | C3N-C7N-N7N | 2.03  | 120.24      | 117.74   |
| 3   | N     | 302 | H4M  | C13-C14-N10 | 2.03  | 124.82      | 121.13   |
| 2   | T     | 301 | NAP  | C1B-N9A-C8A | 2.03  | 131.60      | 127.09   |
| 2   | N     | 301 | NAP  | C5A-N7A-C8A | 2.02  | 106.62      | 103.45   |
| 2   | V     | 301 | NAP  | C4A-N9A-C8A | 2.02  | 107.85      | 105.74   |
| 2   | O     | 301 | NAP  | C3N-C7N-N7N | 2.01  | 120.22      | 117.74   |
| 2   | E     | 301 | NAP  | O2A-PA-O3   | 2.01  | 112.71      | 107.27   |
| 2   | S     | 301 | NAP  | C4D-O4D-C1D | -2.00 | 108.09      | 109.92   |

There are no chirality outliers.

All (430) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | A     | 301 | NAP  | O4D-C1D-N1N-C2N |
| 2   | A     | 301 | NAP  | O4D-C1D-N1N-C6N |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | A     | 301 | NAP  | C2D-C1D-N1N-C2N |
| 2   | A     | 301 | NAP  | C2D-C1D-N1N-C6N |
| 2   | B     | 301 | NAP  | O4D-C1D-N1N-C6N |
| 2   | C     | 301 | NAP  | O4D-C1D-N1N-C6N |
| 2   | D     | 302 | NAP  | O4D-C1D-N1N-C2N |
| 2   | D     | 302 | NAP  | O4D-C1D-N1N-C6N |
| 2   | D     | 302 | NAP  | C2D-C1D-N1N-C2N |
| 2   | D     | 302 | NAP  | C2D-C1D-N1N-C6N |
| 2   | E     | 301 | NAP  | O4D-C1D-N1N-C6N |
| 2   | F     | 301 | NAP  | O4D-C1D-N1N-C2N |
| 2   | F     | 301 | NAP  | O4D-C1D-N1N-C6N |
| 2   | G     | 301 | NAP  | O4D-C1D-N1N-C2N |
| 2   | G     | 301 | NAP  | O4D-C1D-N1N-C6N |
| 2   | G     | 301 | NAP  | C2D-C1D-N1N-C2N |
| 2   | G     | 301 | NAP  | C2D-C1D-N1N-C6N |
| 2   | H     | 301 | NAP  | O4D-C1D-N1N-C6N |
| 2   | I     | 301 | NAP  | O4D-C1D-N1N-C6N |
| 2   | J     | 301 | NAP  | O4D-C1D-N1N-C2N |
| 2   | J     | 301 | NAP  | O4D-C1D-N1N-C6N |
| 2   | J     | 301 | NAP  | C2D-C1D-N1N-C2N |
| 2   | J     | 301 | NAP  | C2D-C1D-N1N-C6N |
| 2   | K     | 301 | NAP  | O4D-C1D-N1N-C6N |
| 2   | L     | 301 | NAP  | O4D-C1D-N1N-C2N |
| 2   | L     | 301 | NAP  | O4D-C1D-N1N-C6N |
| 2   | M     | 301 | NAP  | O4D-C1D-N1N-C2N |
| 2   | M     | 301 | NAP  | O4D-C1D-N1N-C6N |
| 2   | M     | 301 | NAP  | C2D-C1D-N1N-C2N |
| 2   | M     | 301 | NAP  | C2D-C1D-N1N-C6N |
| 2   | N     | 301 | NAP  | O4D-C1D-N1N-C6N |
| 2   | O     | 301 | NAP  | O4D-C1D-N1N-C6N |
| 2   | P     | 301 | NAP  | O4D-C1D-N1N-C2N |
| 2   | P     | 301 | NAP  | O4D-C1D-N1N-C6N |
| 2   | P     | 301 | NAP  | C2D-C1D-N1N-C2N |
| 2   | P     | 301 | NAP  | C2D-C1D-N1N-C6N |
| 2   | Q     | 301 | NAP  | O4D-C1D-N1N-C6N |
| 2   | R     | 301 | NAP  | O4D-C1D-N1N-C6N |
| 2   | S     | 301 | NAP  | O4D-C1D-N1N-C2N |
| 2   | S     | 301 | NAP  | O4D-C1D-N1N-C6N |
| 2   | S     | 301 | NAP  | C2D-C1D-N1N-C2N |
| 2   | S     | 301 | NAP  | C2D-C1D-N1N-C6N |
| 2   | T     | 301 | NAP  | O4D-C1D-N1N-C6N |
| 2   | U     | 301 | NAP  | O4D-C1D-N1N-C6N |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | V     | 301 | NAP  | O4D-C1D-N1N-C2N |
| 2   | V     | 301 | NAP  | O4D-C1D-N1N-C6N |
| 2   | V     | 301 | NAP  | C2D-C1D-N1N-C2N |
| 2   | V     | 301 | NAP  | C2D-C1D-N1N-C6N |
| 2   | W     | 301 | NAP  | O4D-C1D-N1N-C6N |
| 2   | X     | 301 | NAP  | O4D-C1D-N1N-C6N |
| 3   | A     | 302 | H4M  | C5J-O5J-PA-O1A  |
| 3   | A     | 302 | H4M  | C5J-O5J-PA-O2A  |
| 3   | A     | 302 | H4M  | C5J-O5J-PA-O3A  |
| 3   | B     | 302 | H4M  | CX1-CX2-CX3-CX4 |
| 3   | B     | 302 | H4M  | CX1-CX2-CX3-OX3 |
| 3   | B     | 302 | H4M  | OX2-CX2-CX3-CX4 |
| 3   | B     | 302 | H4M  | OX2-CX2-CX3-OX3 |
| 3   | B     | 302 | H4M  | CX3-CX4-CX5-OX5 |
| 3   | B     | 302 | H4M  | OX4-CX4-CX5-OX5 |
| 3   | B     | 302 | H4M  | C5J-O5J-PA-O1A  |
| 3   | B     | 302 | H4M  | C5J-O5J-PA-O2A  |
| 3   | B     | 302 | H4M  | C5J-O5J-PA-O3A  |
| 3   | C     | 302 | H4M  | C5J-O5J-PA-O1A  |
| 3   | C     | 302 | H4M  | C5J-O5J-PA-O2A  |
| 3   | C     | 302 | H4M  | C5J-O5J-PA-O3A  |
| 3   | C     | 302 | H4M  | O4J-C4J-C5J-O5J |
| 3   | D     | 301 | H4M  | O4J-C1J-OX5-CX5 |
| 3   | D     | 301 | H4M  | C2J-C1J-OX5-CX5 |
| 3   | D     | 301 | H4M  | O4J-C4J-C5J-O5J |
| 3   | E     | 302 | H4M  | CX3-CX4-CX5-OX5 |
| 3   | E     | 302 | H4M  | OX4-CX4-CX5-OX5 |
| 3   | E     | 302 | H4M  | O4J-C1J-OX5-CX5 |
| 3   | E     | 302 | H4M  | C2J-C1J-OX5-CX5 |
| 3   | E     | 302 | H4M  | C5J-O5J-PA-O2A  |
| 3   | E     | 302 | H4M  | C5J-O5J-PA-O3A  |
| 3   | F     | 302 | H4M  | CX1-CX2-CX3-CX4 |
| 3   | F     | 302 | H4M  | CX1-CX2-CX3-OX3 |
| 3   | F     | 302 | H4M  | OX2-CX2-CX3-CX4 |
| 3   | F     | 302 | H4M  | OX2-CX2-CX3-OX3 |
| 3   | F     | 302 | H4M  | CX3-CX4-CX5-OX5 |
| 3   | F     | 302 | H4M  | OX4-CX4-CX5-OX5 |
| 3   | F     | 302 | H4M  | O4J-C1J-OX5-CX5 |
| 3   | F     | 302 | H4M  | C2J-C1J-OX5-CX5 |
| 3   | G     | 302 | H4M  | CX1-CX2-CX3-CX4 |
| 3   | G     | 302 | H4M  | CX1-CX2-CX3-OX3 |
| 3   | G     | 302 | H4M  | OX2-CX2-CX3-CX4 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 3   | G     | 302 | H4M  | OX2-CX2-CX3-OX3 |
| 3   | G     | 302 | H4M  | CX3-CX4-CX5-OX5 |
| 3   | G     | 302 | H4M  | OX4-CX4-CX5-OX5 |
| 3   | H     | 302 | H4M  | CX1-CX2-CX3-CX4 |
| 3   | H     | 302 | H4M  | CX1-CX2-CX3-OX3 |
| 3   | H     | 302 | H4M  | OX2-CX2-CX3-CX4 |
| 3   | H     | 302 | H4M  | OX2-CX2-CX3-OX3 |
| 3   | H     | 302 | H4M  | CX3-CX4-CX5-OX5 |
| 3   | H     | 302 | H4M  | OX4-CX4-CX5-OX5 |
| 3   | H     | 302 | H4M  | O4J-C1J-OX5-CX5 |
| 3   | H     | 302 | H4M  | C2J-C1J-OX5-CX5 |
| 3   | H     | 302 | H4M  | C5J-O5J-PA-O1A  |
| 3   | H     | 302 | H4M  | C5J-O5J-PA-O2A  |
| 3   | H     | 302 | H4M  | C5J-O5J-PA-O3A  |
| 3   | I     | 302 | H4M  | CX1-CX2-CX3-CX4 |
| 3   | I     | 302 | H4M  | CX1-CX2-CX3-OX3 |
| 3   | I     | 302 | H4M  | OX2-CX2-CX3-CX4 |
| 3   | I     | 302 | H4M  | OX2-CX2-CX3-OX3 |
| 3   | I     | 302 | H4M  | CX2-CX3-CX4-OX4 |
| 3   | I     | 302 | H4M  | OX3-CX3-CX4-CX5 |
| 3   | I     | 302 | H4M  | OX3-CX3-CX4-OX4 |
| 3   | J     | 302 | H4M  | C5J-O5J-PA-O2A  |
| 3   | J     | 302 | H4M  | C5J-O5J-PA-O3A  |
| 3   | K     | 302 | H4M  | CX1-CX2-CX3-CX4 |
| 3   | K     | 302 | H4M  | CX1-CX2-CX3-OX3 |
| 3   | K     | 302 | H4M  | OX2-CX2-CX3-CX4 |
| 3   | K     | 302 | H4M  | OX2-CX2-CX3-OX3 |
| 3   | K     | 302 | H4M  | CX2-CX3-CX4-CX5 |
| 3   | K     | 302 | H4M  | CX2-CX3-CX4-OX4 |
| 3   | K     | 302 | H4M  | OX3-CX3-CX4-OX4 |
| 3   | K     | 302 | H4M  | O4J-C1J-OX5-CX5 |
| 3   | K     | 302 | H4M  | C2J-C1J-OX5-CX5 |
| 3   | K     | 302 | H4M  | C5J-O5J-PA-O1A  |
| 3   | K     | 302 | H4M  | C5J-O5J-PA-O2A  |
| 3   | K     | 302 | H4M  | C5J-O5J-PA-O3A  |
| 3   | L     | 302 | H4M  | CX3-CX4-CX5-OX5 |
| 3   | L     | 302 | H4M  | OX4-CX4-CX5-OX5 |
| 3   | M     | 302 | H4M  | O4J-C4J-C5J-O5J |
| 3   | N     | 302 | H4M  | CX1-CX2-CX3-CX4 |
| 3   | N     | 302 | H4M  | CX1-CX2-CX3-OX3 |
| 3   | N     | 302 | H4M  | OX2-CX2-CX3-CX4 |
| 3   | N     | 302 | H4M  | OX2-CX2-CX3-OX3 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 3   | N     | 302 | H4M  | CX2-CX3-CX4-CX5 |
| 3   | N     | 302 | H4M  | CX2-CX3-CX4-OX4 |
| 3   | N     | 302 | H4M  | O4J-C1J-OX5-CX5 |
| 3   | N     | 302 | H4M  | C2J-C1J-OX5-CX5 |
| 3   | N     | 302 | H4M  | C5J-O5J-PA-O1A  |
| 3   | N     | 302 | H4M  | C5J-O5J-PA-O2A  |
| 3   | N     | 302 | H4M  | C5J-O5J-PA-O3A  |
| 3   | N     | 302 | H4M  | O4J-C4J-C5J-O5J |
| 3   | N     | 302 | H4M  | C3J-C4J-C5J-O5J |
| 3   | O     | 302 | H4M  | CX1-CX2-CX3-CX4 |
| 3   | O     | 302 | H4M  | CX1-CX2-CX3-OX3 |
| 3   | O     | 302 | H4M  | OX2-CX2-CX3-CX4 |
| 3   | O     | 302 | H4M  | OX2-CX2-CX3-OX3 |
| 3   | O     | 302 | H4M  | CX3-CX4-CX5-OX5 |
| 3   | O     | 302 | H4M  | OX4-CX4-CX5-OX5 |
| 3   | O     | 302 | H4M  | C2J-C1J-OX5-CX5 |
| 3   | O     | 302 | H4M  | C5J-O5J-PA-O1A  |
| 3   | O     | 302 | H4M  | C5J-O5J-PA-O2A  |
| 3   | O     | 302 | H4M  | C5J-O5J-PA-O3A  |
| 3   | P     | 302 | H4M  | CX2-CX3-CX4-CX5 |
| 3   | P     | 302 | H4M  | OX3-CX3-CX4-CX5 |
| 3   | P     | 302 | H4M  | OX3-CX3-CX4-OX4 |
| 3   | P     | 302 | H4M  | O4J-C1J-OX5-CX5 |
| 3   | P     | 302 | H4M  | C2J-C1J-OX5-CX5 |
| 3   | Q     | 302 | H4M  | CX3-CX4-CX5-OX5 |
| 3   | Q     | 302 | H4M  | OX4-CX4-CX5-OX5 |
| 3   | Q     | 302 | H4M  | O4J-C1J-OX5-CX5 |
| 3   | Q     | 302 | H4M  | C2J-C1J-OX5-CX5 |
| 3   | Q     | 302 | H4M  | C3J-C4J-C5J-O5J |
| 3   | R     | 302 | H4M  | OX4-CX4-CX5-OX5 |
| 3   | R     | 302 | H4M  | C4J-C5J-O5J-PA  |
| 3   | R     | 302 | H4M  | C5J-O5J-PA-O2A  |
| 3   | S     | 302 | H4M  | O4J-C1J-OX5-CX5 |
| 3   | S     | 302 | H4M  | C2J-C1J-OX5-CX5 |
| 3   | T     | 302 | H4M  | O4J-C4J-C5J-O5J |
| 3   | U     | 302 | H4M  | CX3-CX4-CX5-OX5 |
| 3   | U     | 302 | H4M  | OX4-CX4-CX5-OX5 |
| 3   | U     | 302 | H4M  | O4J-C1J-OX5-CX5 |
| 3   | U     | 302 | H4M  | C2J-C1J-OX5-CX5 |
| 3   | U     | 302 | H4M  | O4J-C4J-C5J-O5J |
| 3   | U     | 302 | H4M  | C3J-C4J-C5J-O5J |
| 3   | V     | 302 | H4M  | CX3-CX4-CX5-OX5 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 3   | V     | 302 | H4M  | OX4-CX4-CX5-OX5 |
| 3   | V     | 302 | H4M  | O4J-C1J-OX5-CX5 |
| 3   | V     | 302 | H4M  | C2J-C1J-OX5-CX5 |
| 3   | V     | 302 | H4M  | C5J-O5J-PA-O1A  |
| 3   | V     | 302 | H4M  | C5J-O5J-PA-O2A  |
| 3   | V     | 302 | H4M  | C5J-O5J-PA-O3A  |
| 3   | V     | 302 | H4M  | O4J-C4J-C5J-O5J |
| 3   | V     | 302 | H4M  | C3J-C4J-C5J-O5J |
| 3   | W     | 302 | H4M  | CX3-CX4-CX5-OX5 |
| 3   | W     | 302 | H4M  | OX4-CX4-CX5-OX5 |
| 3   | W     | 302 | H4M  | O4J-C1J-OX5-CX5 |
| 3   | W     | 302 | H4M  | C2J-C1J-OX5-CX5 |
| 3   | W     | 302 | H4M  | C5J-O5J-PA-O1A  |
| 3   | W     | 302 | H4M  | C5J-O5J-PA-O2A  |
| 3   | W     | 302 | H4M  | C5J-O5J-PA-O3A  |
| 3   | W     | 302 | H4M  | O4J-C4J-C5J-O5J |
| 3   | X     | 302 | H4M  | C13-C14-N10-C9  |
| 3   | X     | 302 | H4M  | C15-C14-N10-C9  |
| 3   | X     | 302 | H4M  | CX1-CX2-CX3-CX4 |
| 3   | X     | 302 | H4M  | OX2-CX2-CX3-CX4 |
| 3   | X     | 302 | H4M  | CX2-CX3-CX4-CX5 |
| 3   | X     | 302 | H4M  | CX2-CX3-CX4-OX4 |
| 3   | X     | 302 | H4M  | OX3-CX3-CX4-OX4 |
| 3   | X     | 302 | H4M  | CX3-CX4-CX5-OX5 |
| 3   | X     | 302 | H4M  | OX4-CX4-CX5-OX5 |
| 3   | X     | 302 | H4M  | O4J-C1J-OX5-CX5 |
| 3   | X     | 302 | H4M  | C2J-C1J-OX5-CX5 |
| 3   | X     | 302 | H4M  | C5J-O5J-PA-O1A  |
| 3   | X     | 302 | H4M  | C5J-O5J-PA-O2A  |
| 3   | N     | 302 | H4M  | OX3-CX3-CX4-OX4 |
| 3   | X     | 302 | H4M  | OX2-CX2-CX3-OX3 |
| 3   | L     | 302 | H4M  | OX2-CX2-CX3-CX4 |
| 3   | D     | 301 | H4M  | C3J-C4J-C5J-O5J |
| 3   | H     | 302 | H4M  | O4J-C4J-C5J-O5J |
| 3   | H     | 302 | H4M  | C3J-C4J-C5J-O5J |
| 3   | I     | 302 | H4M  | O4J-C4J-C5J-O5J |
| 3   | I     | 302 | H4M  | C3J-C4J-C5J-O5J |
| 3   | L     | 302 | H4M  | C3J-C4J-C5J-O5J |
| 3   | M     | 302 | H4M  | C3J-C4J-C5J-O5J |
| 3   | K     | 302 | H4M  | OX3-CX3-CX4-CX5 |
| 3   | N     | 302 | H4M  | OX3-CX3-CX4-CX5 |
| 3   | X     | 302 | H4M  | OX3-CX3-CX4-CX5 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 3   | I     | 302 | H4M  | CX2-CX3-CX4-CX5 |
| 3   | L     | 302 | H4M  | OX2-CX2-CX3-OX3 |
| 3   | P     | 302 | H4M  | OX2-CX2-CX3-OX3 |
| 3   | P     | 302 | H4M  | OX2-CX2-CX3-CX4 |
| 3   | P     | 302 | H4M  | CX2-CX3-CX4-OX4 |
| 3   | A     | 302 | H4M  | O4J-C4J-C5J-O5J |
| 3   | F     | 302 | H4M  | O4J-C4J-C5J-O5J |
| 3   | G     | 302 | H4M  | O4J-C4J-C5J-O5J |
| 3   | K     | 302 | H4M  | O4J-C4J-C5J-O5J |
| 3   | L     | 302 | H4M  | O4J-C4J-C5J-O5J |
| 3   | P     | 302 | H4M  | O4J-C4J-C5J-O5J |
| 3   | Q     | 302 | H4M  | O4J-C4J-C5J-O5J |
| 3   | T     | 302 | H4M  | C3J-C4J-C5J-O5J |
| 3   | W     | 302 | H4M  | C3J-C4J-C5J-O5J |
| 3   | E     | 302 | H4M  | O4J-C4J-C5J-O5J |
| 3   | G     | 302 | H4M  | C3J-C4J-C5J-O5J |
| 3   | K     | 302 | H4M  | C3J-C4J-C5J-O5J |
| 3   | G     | 302 | H4M  | CX2-CX3-CX4-CX5 |
| 3   | C     | 302 | H4M  | C3J-C4J-C5J-O5J |
| 3   | R     | 302 | H4M  | C3J-C4J-C5J-O5J |
| 3   | G     | 302 | H4M  | OX3-CX3-CX4-CX5 |
| 3   | L     | 302 | H4M  | OX3-CX3-CX4-CX5 |
| 3   | D     | 301 | H4M  | OX2-CX2-CX3-OX3 |
| 3   | L     | 302 | H4M  | OX3-CX3-CX4-OX4 |
| 3   | G     | 302 | H4M  | CX2-CX3-CX4-OX4 |
| 3   | L     | 302 | H4M  | CX2-CX3-CX4-OX4 |
| 3   | I     | 302 | H4M  | C13-C14-N10-C9  |
| 3   | I     | 302 | H4M  | C15-C14-N10-C9  |
| 3   | D     | 301 | H4M  | OX2-CX2-CX3-CX4 |
| 3   | O     | 302 | H4M  | C11-CX1-CX2-OX2 |
| 3   | P     | 302 | H4M  | C11-CX1-CX2-OX2 |
| 3   | U     | 302 | H4M  | C11-CX1-CX2-OX2 |
| 3   | X     | 302 | H4M  | C11-CX1-CX2-OX2 |
| 3   | L     | 302 | H4M  | CX2-CX3-CX4-CX5 |
| 3   | H     | 302 | H4M  | C12-C11-CX1-CX2 |
| 3   | H     | 302 | H4M  | C16-C11-CX1-CX2 |
| 3   | I     | 302 | H4M  | CX3-CX4-CX5-OX5 |
| 3   | P     | 302 | H4M  | CX3-CX4-CX5-OX5 |
| 3   | R     | 302 | H4M  | CX3-CX4-CX5-OX5 |
| 3   | P     | 302 | H4M  | C3J-C4J-C5J-O5J |
| 3   | S     | 302 | H4M  | O4J-C4J-C5J-O5J |
| 3   | R     | 302 | H4M  | C12-C11-CX1-CX2 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 3   | C     | 302 | H4M  | O4J-C1J-OX5-CX5 |
| 3   | O     | 302 | H4M  | O4J-C1J-OX5-CX5 |
| 3   | G     | 302 | H4M  | C4J-C5J-O5J-PA  |
| 3   | L     | 302 | H4M  | C4J-C5J-O5J-PA  |
| 3   | U     | 302 | H4M  | OX2-CX2-CX3-CX4 |
| 3   | J     | 302 | H4M  | CX2-CX3-CX4-CX5 |
| 3   | R     | 302 | H4M  | C16-C11-CX1-CX2 |
| 3   | O     | 302 | H4M  | C4J-C5J-O5J-PA  |
| 3   | F     | 302 | H4M  | C3J-C4J-C5J-O5J |
| 3   | L     | 302 | H4M  | C13-C14-N10-C10 |
| 3   | I     | 302 | H4M  | OX4-CX4-CX5-OX5 |
| 3   | C     | 302 | H4M  | C12-C11-CX1-CX2 |
| 3   | G     | 302 | H4M  | C12-C11-CX1-CX2 |
| 3   | G     | 302 | H4M  | C16-C11-CX1-CX2 |
| 3   | J     | 302 | H4M  | C12-C11-CX1-CX2 |
| 3   | J     | 302 | H4M  | C16-C11-CX1-CX2 |
| 3   | M     | 302 | H4M  | C12-C11-CX1-CX2 |
| 3   | M     | 302 | H4M  | C16-C11-CX1-CX2 |
| 3   | Q     | 302 | H4M  | C12-C11-CX1-CX2 |
| 3   | S     | 302 | H4M  | C12-C11-CX1-CX2 |
| 3   | S     | 302 | H4M  | C16-C11-CX1-CX2 |
| 3   | T     | 302 | H4M  | C12-C11-CX1-CX2 |
| 3   | T     | 302 | H4M  | C16-C11-CX1-CX2 |
| 3   | A     | 302 | H4M  | C3J-C4J-C5J-O5J |
| 3   | B     | 302 | H4M  | CX4-CX5-OX5-C1J |
| 3   | P     | 302 | H4M  | CX4-CX5-OX5-C1J |
| 3   | R     | 302 | H4M  | C5J-O5J-PA-O3A  |
| 3   | C     | 302 | H4M  | C16-C11-CX1-CX2 |
| 3   | E     | 302 | H4M  | C12-C11-CX1-CX2 |
| 3   | Q     | 302 | H4M  | C16-C11-CX1-CX2 |
| 3   | J     | 302 | H4M  | CX2-CX3-CX4-OX4 |
| 3   | F     | 302 | H4M  | C15-C14-N10-C9  |
| 2   | S     | 301 | NAP  | PN-O3-PA-O2A    |
| 3   | E     | 302 | H4M  | C16-C11-CX1-CX2 |
| 3   | L     | 302 | H4M  | CX1-CX2-CX3-CX4 |
| 3   | P     | 302 | H4M  | CX1-CX2-CX3-CX4 |
| 3   | S     | 302 | H4M  | CX2-CX3-CX4-OX4 |
| 3   | U     | 302 | H4M  | OX2-CX2-CX3-OX3 |
| 3   | B     | 302 | H4M  | C4J-C5J-O5J-PA  |
| 3   | L     | 302 | H4M  | C2J-C1J-OX5-CX5 |
| 3   | S     | 302 | H4M  | OX3-CX3-CX4-CX5 |
| 3   | G     | 302 | H4M  | OX3-CX3-CX4-OX4 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 3   | S     | 302 | H4M  | OX3-CX3-CX4-OX4 |
| 3   | N     | 302 | H4M  | C11-CX1-CX2-OX2 |
| 2   | C     | 301 | NAP  | C5D-O5D-PN-O1N  |
| 2   | F     | 301 | NAP  | C5D-O5D-PN-O1N  |
| 2   | J     | 301 | NAP  | C5D-O5D-PN-O1N  |
| 2   | L     | 301 | NAP  | C5D-O5D-PN-O1N  |
| 2   | S     | 301 | NAP  | C5D-O5D-PN-O1N  |
| 2   | U     | 301 | NAP  | C5D-O5D-PN-O1N  |
| 2   | V     | 301 | NAP  | C5D-O5D-PN-O1N  |
| 2   | W     | 301 | NAP  | C5D-O5D-PN-O1N  |
| 2   | X     | 301 | NAP  | C5D-O5D-PN-O1N  |
| 3   | K     | 302 | H4M  | C11-CX1-CX2-CX3 |
| 3   | U     | 302 | H4M  | C11-CX1-CX2-CX3 |
| 3   | U     | 302 | H4M  | C4J-C5J-O5J-PA  |
| 3   | V     | 302 | H4M  | C4J-C5J-O5J-PA  |
| 3   | F     | 302 | H4M  | C13-C14-N10-C9  |
| 3   | R     | 302 | H4M  | C13-C14-N10-C9  |
| 3   | R     | 302 | H4M  | C5J-O5J-PA-O1A  |
| 3   | J     | 302 | H4M  | OX4-CX4-CX5-OX5 |
| 3   | P     | 302 | H4M  | OX4-CX4-CX5-OX5 |
| 2   | A     | 301 | NAP  | PN-O3-PA-O2A    |
| 2   | D     | 302 | NAP  | PN-O3-PA-O2A    |
| 2   | G     | 301 | NAP  | PN-O3-PA-O2A    |
| 2   | J     | 301 | NAP  | PN-O3-PA-O2A    |
| 2   | M     | 301 | NAP  | PN-O3-PA-O2A    |
| 2   | P     | 301 | NAP  | PN-O3-PA-O2A    |
| 2   | V     | 301 | NAP  | PN-O3-PA-O2A    |
| 3   | E     | 302 | H4M  | C3J-C4J-C5J-O5J |
| 3   | B     | 302 | H4M  | C16-C11-CX1-CX2 |
| 3   | L     | 302 | H4M  | O4J-C1J-OX5-CX5 |
| 3   | M     | 302 | H4M  | O4J-C1J-OX5-CX5 |
| 3   | N     | 302 | H4M  | C4J-C5J-O5J-PA  |
| 3   | B     | 302 | H4M  | C13-C14-N10-C9  |
| 3   | R     | 302 | H4M  | C15-C14-N10-C9  |
| 3   | A     | 302 | H4M  | C12-C11-CX1-CX2 |
| 3   | W     | 302 | H4M  | C16-C11-CX1-CX2 |
| 2   | L     | 301 | NAP  | C2D-C1D-N1N-C2N |
| 3   | B     | 302 | H4M  | C12-C11-CX1-CX2 |
| 3   | W     | 302 | H4M  | C12-C11-CX1-CX2 |
| 3   | O     | 302 | H4M  | O4J-C4J-C5J-O5J |
| 3   | S     | 302 | H4M  | CX2-CX3-CX4-CX5 |
| 3   | D     | 301 | H4M  | CX1-CX2-CX3-OX3 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 3   | L     | 302 | H4M  | CX1-CX2-CX3-OX3 |
| 3   | P     | 302 | H4M  | CX1-CX2-CX3-OX3 |
| 3   | X     | 302 | H4M  | CX1-CX2-CX3-OX3 |
| 3   | J     | 302 | H4M  | OX3-CX3-CX4-OX4 |
| 3   | A     | 302 | H4M  | C16-C11-CX1-CX2 |
| 2   | B     | 301 | NAP  | O4D-C1D-N1N-C2N |
| 2   | C     | 301 | NAP  | O4D-C1D-N1N-C2N |
| 2   | E     | 301 | NAP  | O4D-C1D-N1N-C2N |
| 2   | H     | 301 | NAP  | O4D-C1D-N1N-C2N |
| 2   | I     | 301 | NAP  | O4D-C1D-N1N-C2N |
| 2   | K     | 301 | NAP  | O4D-C1D-N1N-C2N |
| 2   | N     | 301 | NAP  | O4D-C1D-N1N-C2N |
| 2   | O     | 301 | NAP  | O4D-C1D-N1N-C2N |
| 2   | Q     | 301 | NAP  | O4D-C1D-N1N-C2N |
| 2   | R     | 301 | NAP  | O4D-C1D-N1N-C2N |
| 2   | T     | 301 | NAP  | O4D-C1D-N1N-C2N |
| 2   | U     | 301 | NAP  | O4D-C1D-N1N-C2N |
| 2   | W     | 301 | NAP  | O4D-C1D-N1N-C2N |
| 2   | X     | 301 | NAP  | O4D-C1D-N1N-C2N |
| 3   | H     | 302 | H4M  | C13-C14-N10-C10 |
| 3   | H     | 302 | H4M  | C15-C14-N10-C10 |
| 3   | L     | 302 | H4M  | C15-C14-N10-C10 |
| 3   | O     | 302 | H4M  | C13-C14-N10-C10 |
| 3   | O     | 302 | H4M  | C15-C14-N10-C10 |
| 3   | U     | 302 | H4M  | C13-C14-N10-C10 |
| 3   | U     | 302 | H4M  | C15-C14-N10-C10 |
| 2   | B     | 301 | NAP  | C2B-O2B-P2B-O1X |
| 2   | D     | 302 | NAP  | C2B-O2B-P2B-O1X |
| 2   | F     | 301 | NAP  | C2B-O2B-P2B-O1X |
| 2   | H     | 301 | NAP  | C2B-O2B-P2B-O1X |
| 2   | K     | 301 | NAP  | C2B-O2B-P2B-O1X |
| 2   | L     | 301 | NAP  | C2B-O2B-P2B-O1X |
| 2   | M     | 301 | NAP  | C2B-O2B-P2B-O1X |
| 2   | Q     | 301 | NAP  | C2B-O2B-P2B-O1X |
| 2   | R     | 301 | NAP  | C2B-O2B-P2B-O1X |
| 2   | S     | 301 | NAP  | C2B-O2B-P2B-O1X |
| 2   | U     | 301 | NAP  | C2B-O2B-P2B-O1X |
| 2   | W     | 301 | NAP  | C2B-O2B-P2B-O1X |
| 3   | X     | 302 | H4M  | C16-C11-CX1-CX2 |
| 2   | W     | 301 | NAP  | PN-O3-PA-O2A    |
| 3   | P     | 302 | H4M  | C4J-C5J-O5J-PA  |
| 3   | W     | 302 | H4M  | C4J-C5J-O5J-PA  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 3   | F     | 302 | H4M  | C16-C11-CX1-CX2 |
| 3   | H     | 302 | H4M  | C11-CX1-CX2-OX2 |
| 3   | L     | 302 | H4M  | C11-CX1-CX2-OX2 |
| 3   | B     | 302 | H4M  | C15-C14-N10-C9  |
| 3   | G     | 302 | H4M  | CX4-CX5-OX5-C1J |
| 3   | M     | 302 | H4M  | CX4-CX5-OX5-C1J |
| 3   | T     | 302 | H4M  | C5J-O5J-PA-O3A  |
| 3   | X     | 302 | H4M  | C5J-O5J-PA-O3A  |
| 3   | X     | 302 | H4M  | C12-C11-CX1-CX2 |
| 2   | D     | 302 | NAP  | PN-O3-PA-O1A    |
| 2   | E     | 301 | NAP  | PN-O3-PA-O2A    |
| 2   | F     | 301 | NAP  | PN-O3-PA-O2A    |
| 2   | H     | 301 | NAP  | PN-O3-PA-O2A    |
| 2   | J     | 301 | NAP  | PN-O3-PA-O1A    |
| 2   | L     | 301 | NAP  | PN-O3-PA-O2A    |
| 2   | N     | 301 | NAP  | PN-O3-PA-O2A    |
| 2   | O     | 301 | NAP  | PN-O3-PA-O2A    |
| 2   | P     | 301 | NAP  | PN-O3-PA-O1A    |
| 2   | Q     | 301 | NAP  | PN-O3-PA-O1A    |
| 2   | Q     | 301 | NAP  | PN-O3-PA-O2A    |
| 2   | R     | 301 | NAP  | PN-O3-PA-O2A    |
| 2   | T     | 301 | NAP  | PN-O3-PA-O2A    |
| 2   | X     | 301 | NAP  | PN-O3-PA-O2A    |
| 3   | F     | 302 | H4M  | C12-C11-CX1-CX2 |
| 3   | O     | 302 | H4M  | C3J-C4J-C5J-O5J |
| 3   | R     | 302 | H4M  | O4J-C4J-C5J-O5J |
| 3   | S     | 302 | H4M  | C3J-C4J-C5J-O5J |
| 2   | B     | 301 | NAP  | C2B-O2B-P2B-O3X |
| 2   | M     | 301 | NAP  | C2B-O2B-P2B-O3X |
| 2   | O     | 301 | NAP  | C2B-O2B-P2B-O2X |
| 2   | U     | 301 | NAP  | C2B-O2B-P2B-O3X |
| 3   | J     | 302 | H4M  | OX3-CX3-CX4-CX5 |
| 3   | T     | 302 | H4M  | C4J-C5J-O5J-PA  |
| 3   | D     | 301 | H4M  | C16-C11-CX1-CX2 |
| 3   | P     | 302 | H4M  | C16-C11-CX1-CX2 |
| 2   | A     | 301 | NAP  | C2B-O2B-P2B-O1X |
| 2   | G     | 301 | NAP  | C2B-O2B-P2B-O1X |
| 2   | N     | 301 | NAP  | C2B-O2B-P2B-O1X |
| 2   | V     | 301 | NAP  | C2B-O2B-P2B-O1X |
| 3   | C     | 302 | H4M  | C2J-C1J-OX5-CX5 |
| 3   | M     | 302 | H4M  | C2J-C1J-OX5-CX5 |
| 3   | F     | 302 | H4M  | C4J-C5J-O5J-PA  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 3   | K     | 302 | H4M  | C11-CX1-CX2-OX2 |
| 3   | D     | 301 | H4M  | C12-C11-CX1-CX2 |
| 3   | P     | 302 | H4M  | C12-C11-CX1-CX2 |
| 2   | B     | 301 | NAP  | PN-O3-PA-O2A    |
| 2   | G     | 301 | NAP  | PN-O3-PA-O1A    |
| 2   | M     | 301 | NAP  | PN-O3-PA-O1A    |
| 2   | O     | 301 | NAP  | PN-O3-PA-O1A    |
| 2   | W     | 301 | NAP  | PN-O3-PA-O1A    |

There are no ring outliers.

48 monomers are involved in 130 short contacts:

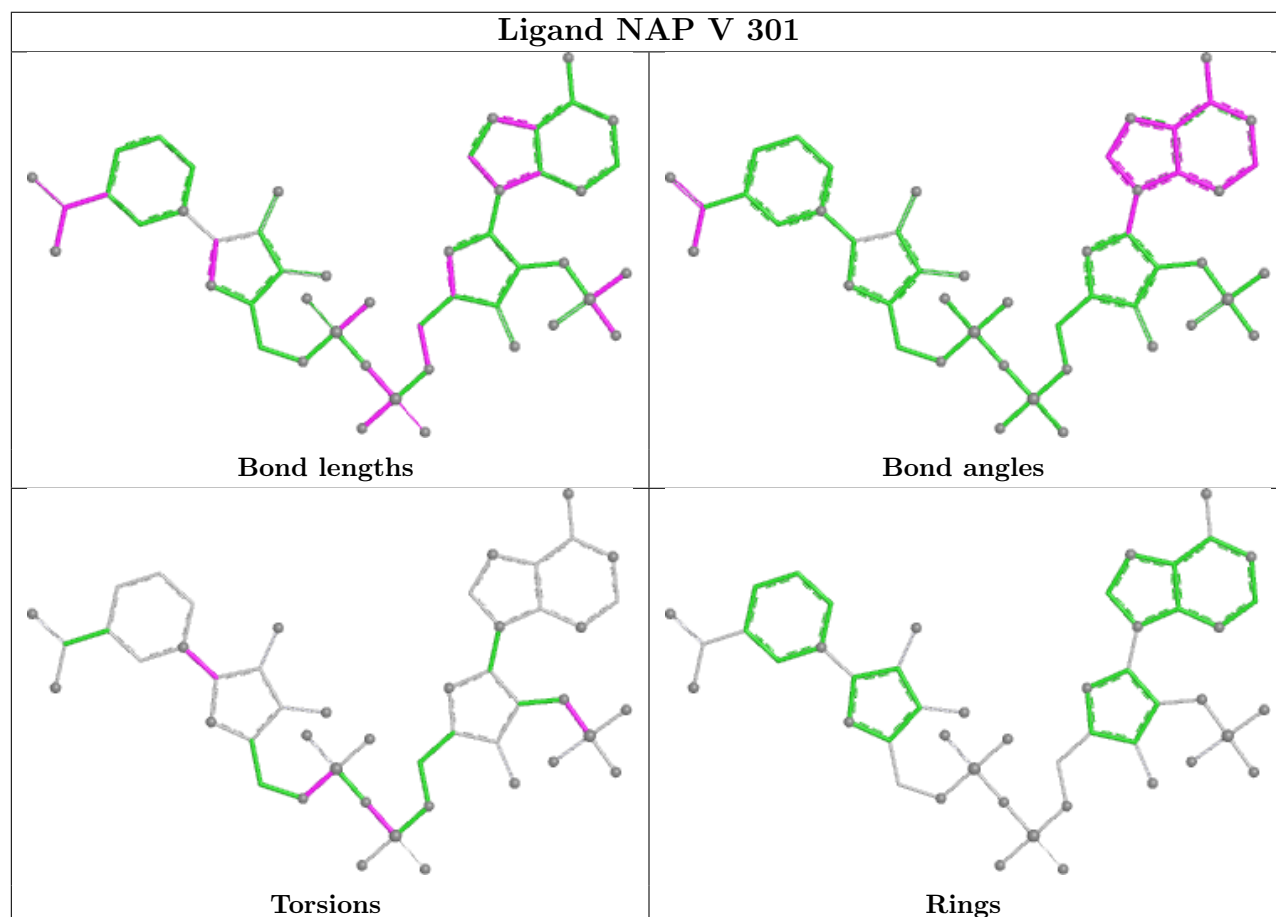
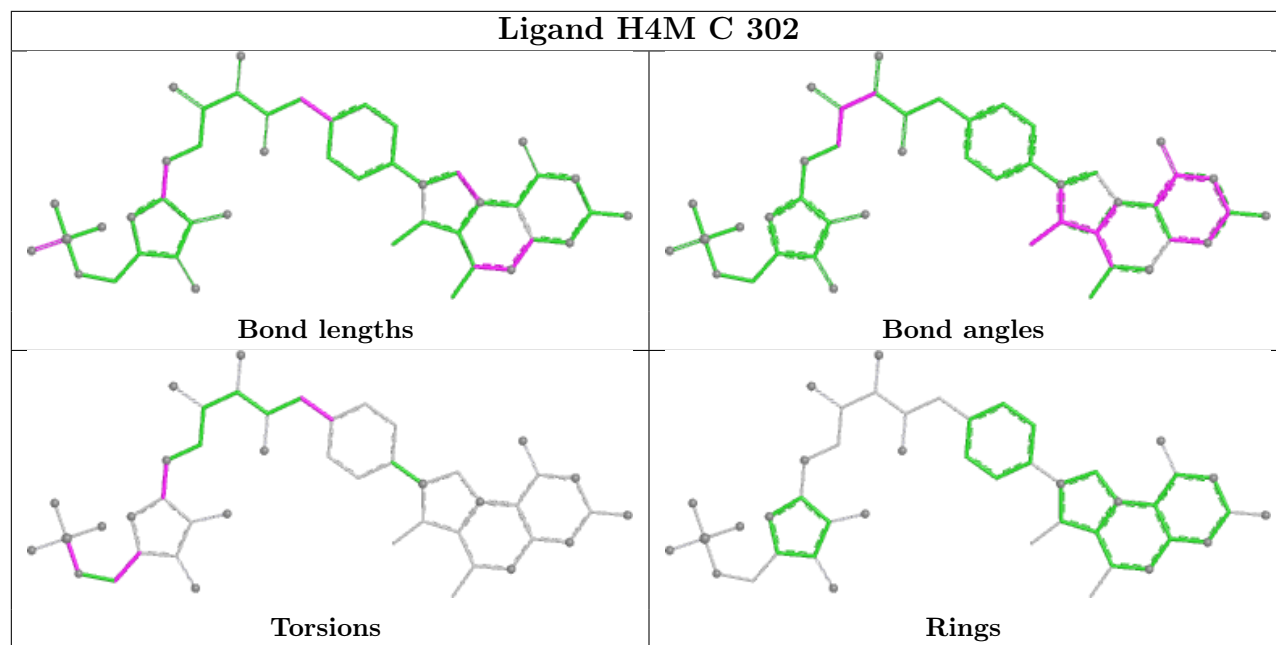
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3   | C     | 302 | H4M  | 4       | 0            |
| 2   | V     | 301 | NAP  | 3       | 0            |
| 2   | X     | 301 | NAP  | 1       | 0            |
| 3   | E     | 302 | H4M  | 3       | 0            |
| 3   | A     | 302 | H4M  | 8       | 0            |
| 3   | U     | 302 | H4M  | 3       | 0            |
| 2   | U     | 301 | NAP  | 2       | 0            |
| 2   | G     | 301 | NAP  | 6       | 0            |
| 3   | O     | 302 | H4M  | 4       | 0            |
| 3   | K     | 302 | H4M  | 5       | 0            |
| 3   | J     | 302 | H4M  | 7       | 0            |
| 3   | P     | 302 | H4M  | 8       | 0            |
| 2   | E     | 301 | NAP  | 1       | 0            |
| 2   | A     | 301 | NAP  | 8       | 0            |
| 2   | D     | 302 | NAP  | 5       | 0            |
| 2   | T     | 301 | NAP  | 1       | 0            |
| 3   | H     | 302 | H4M  | 6       | 0            |
| 2   | S     | 301 | NAP  | 7       | 0            |
| 3   | L     | 302 | H4M  | 4       | 0            |
| 3   | M     | 302 | H4M  | 5       | 0            |
| 3   | Q     | 302 | H4M  | 3       | 0            |
| 3   | X     | 302 | H4M  | 4       | 0            |
| 2   | M     | 301 | NAP  | 6       | 0            |
| 3   | D     | 301 | H4M  | 6       | 0            |
| 2   | R     | 301 | NAP  | 1       | 0            |
| 3   | S     | 302 | H4M  | 8       | 0            |
| 3   | I     | 302 | H4M  | 3       | 0            |
| 2   | P     | 301 | NAP  | 4       | 0            |
| 3   | F     | 302 | H4M  | 3       | 0            |

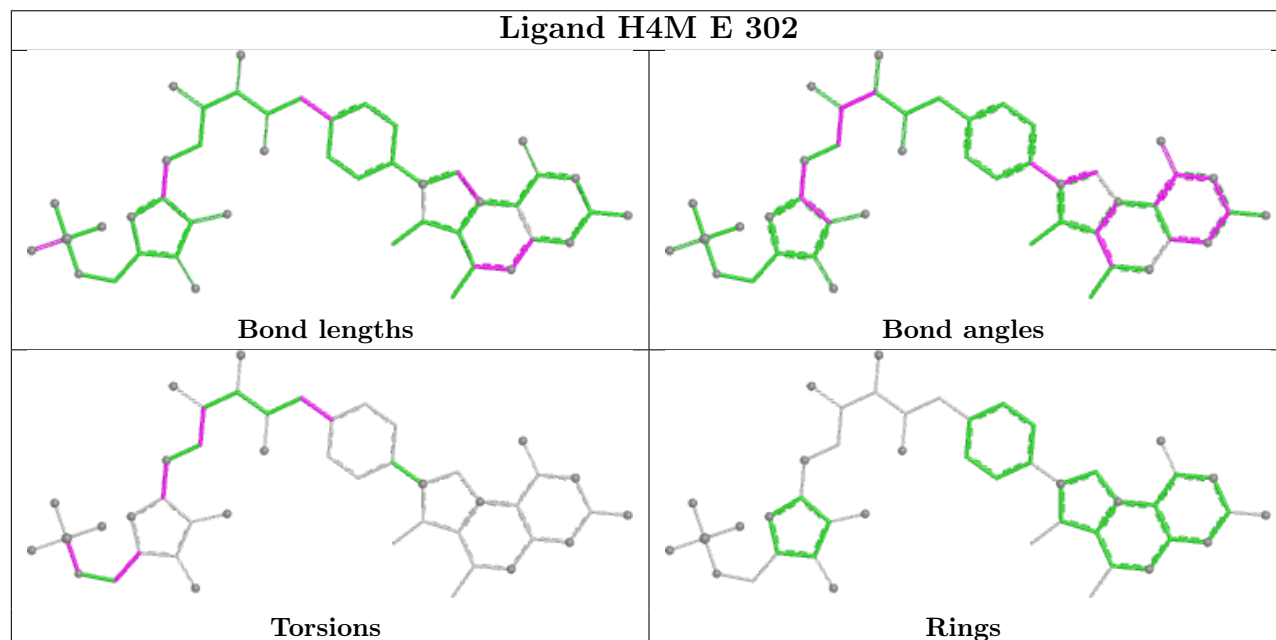
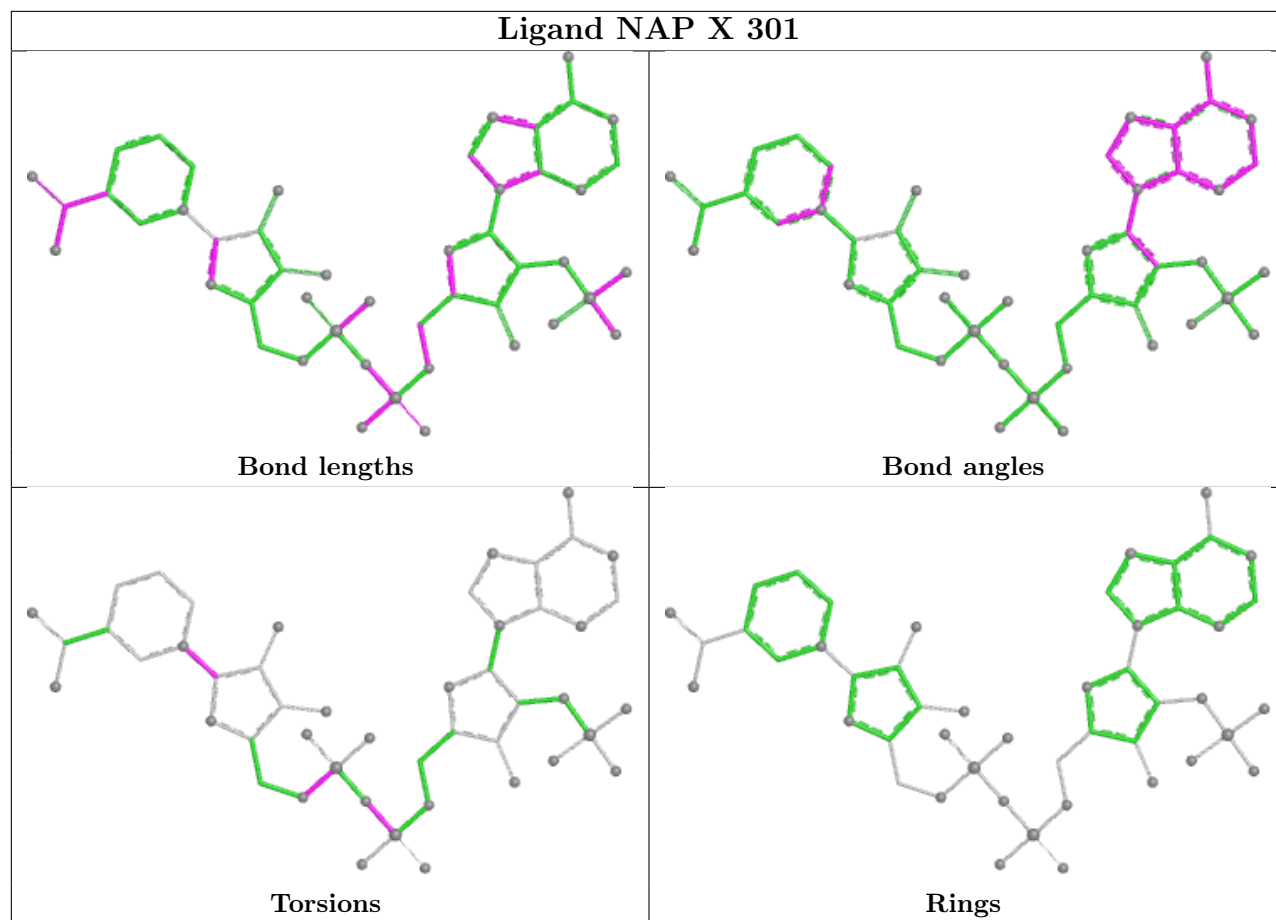
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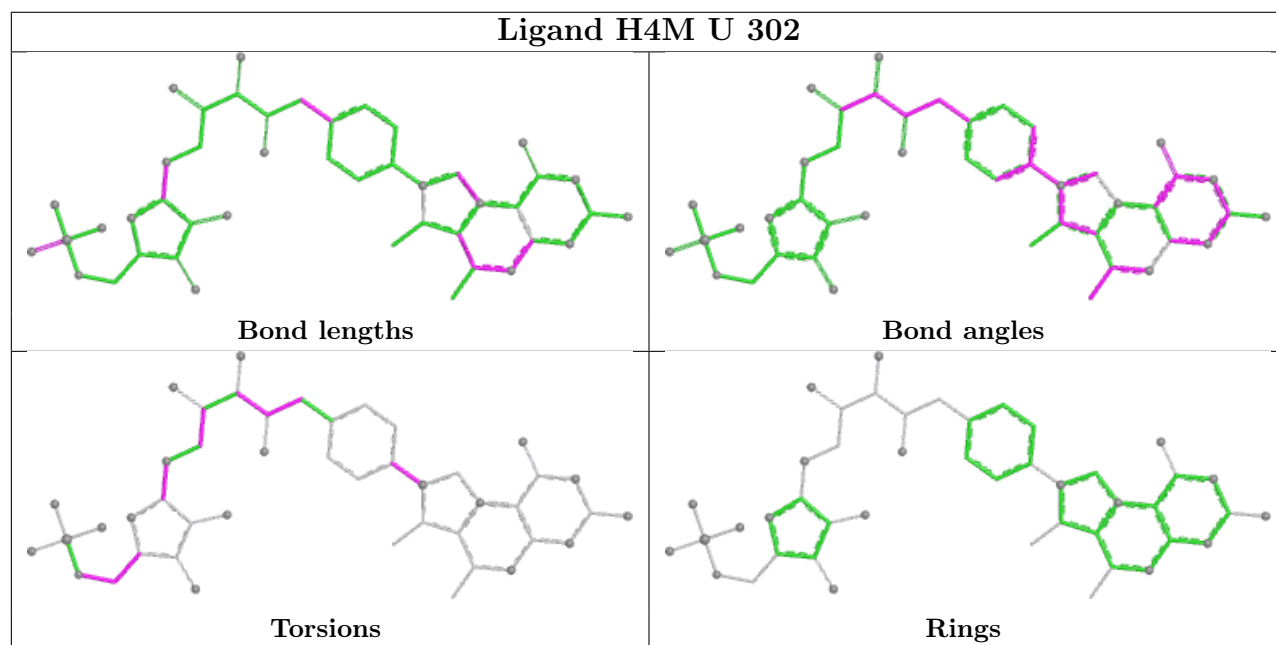
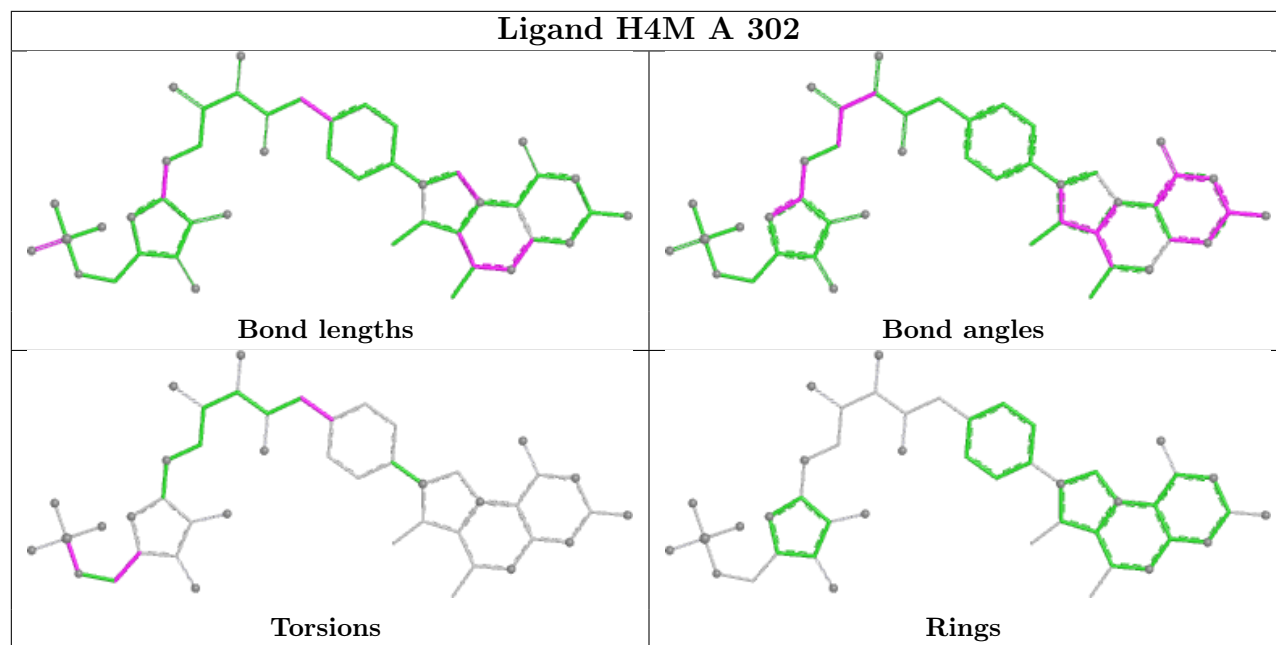
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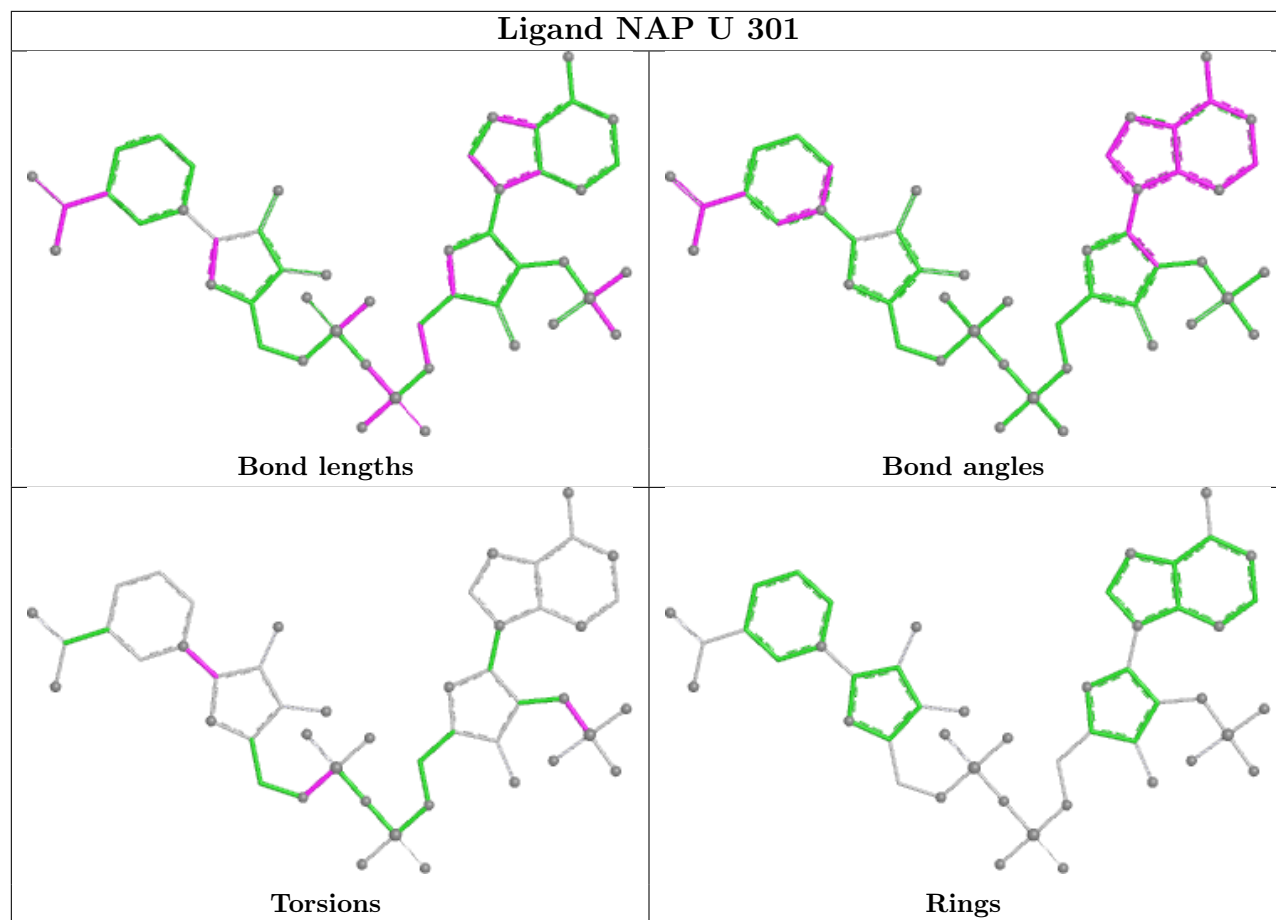
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2   | K     | 301 | NAP  | 1       | 0            |
| 2   | I     | 301 | NAP  | 1       | 0            |
| 2   | B     | 301 | NAP  | 1       | 0            |
| 2   | O     | 301 | NAP  | 1       | 0            |
| 2   | Q     | 301 | NAP  | 1       | 0            |
| 3   | N     | 302 | H4M  | 3       | 0            |
| 3   | W     | 302 | H4M  | 3       | 0            |
| 3   | V     | 302 | H4M  | 7       | 0            |
| 2   | J     | 301 | NAP  | 5       | 0            |
| 2   | N     | 301 | NAP  | 1       | 0            |
| 3   | R     | 302 | H4M  | 7       | 0            |
| 2   | C     | 301 | NAP  | 1       | 0            |
| 2   | F     | 301 | NAP  | 2       | 0            |
| 3   | T     | 302 | H4M  | 3       | 0            |
| 2   | L     | 301 | NAP  | 2       | 0            |
| 2   | W     | 301 | NAP  | 1       | 0            |
| 2   | H     | 301 | NAP  | 1       | 0            |
| 3   | B     | 302 | H4M  | 4       | 0            |
| 3   | G     | 302 | H4M  | 7       | 0            |

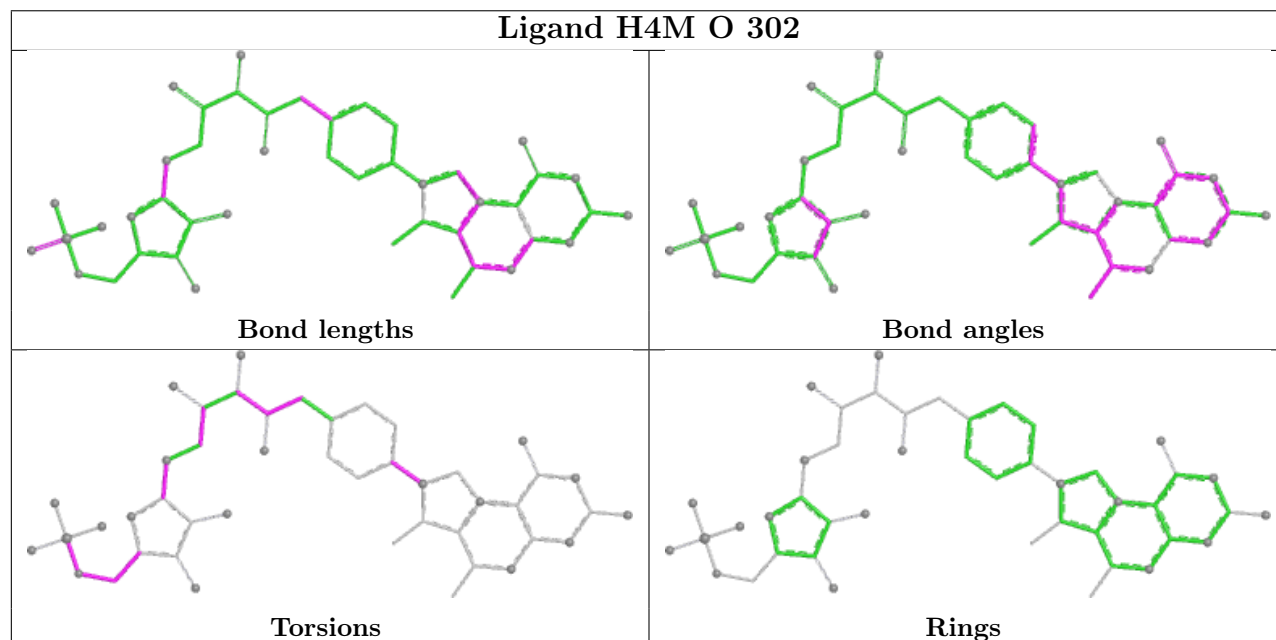
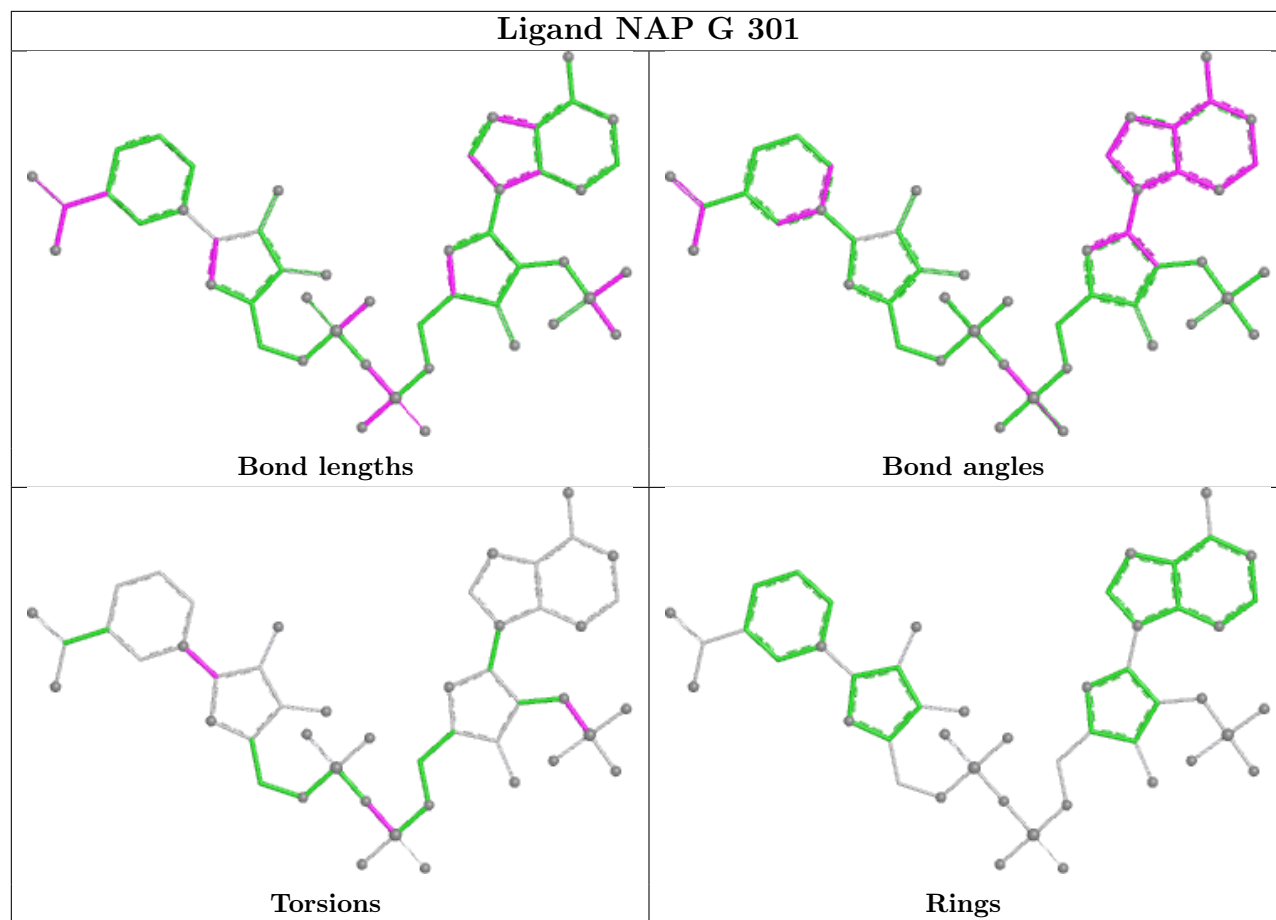
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

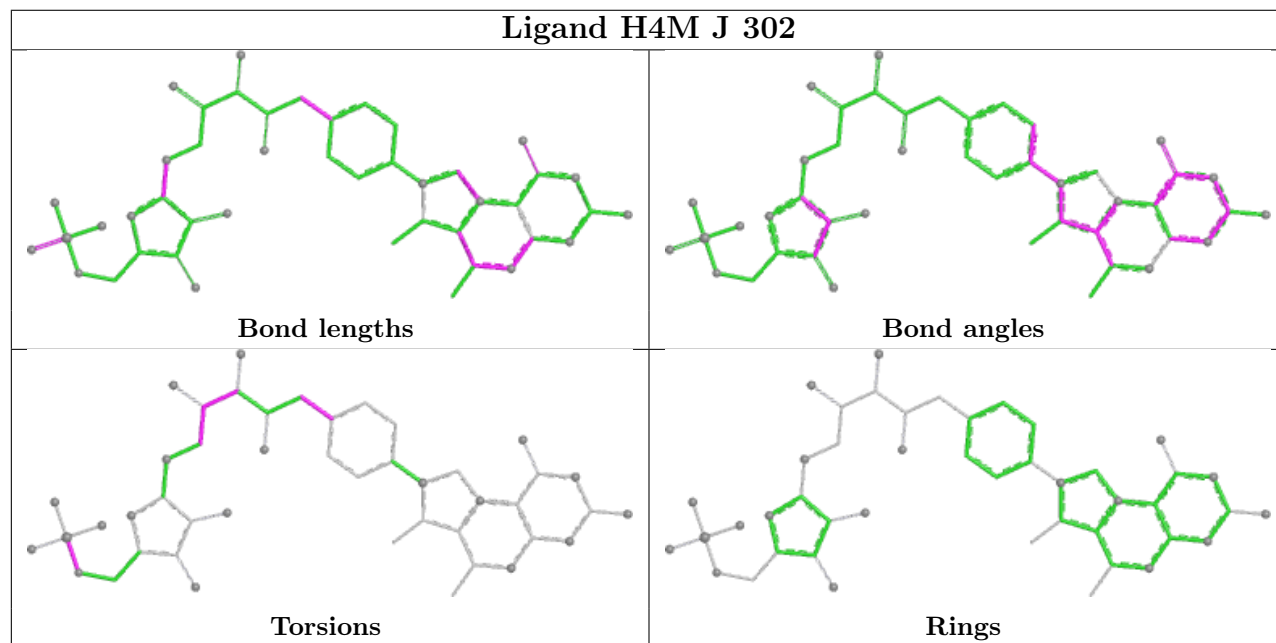
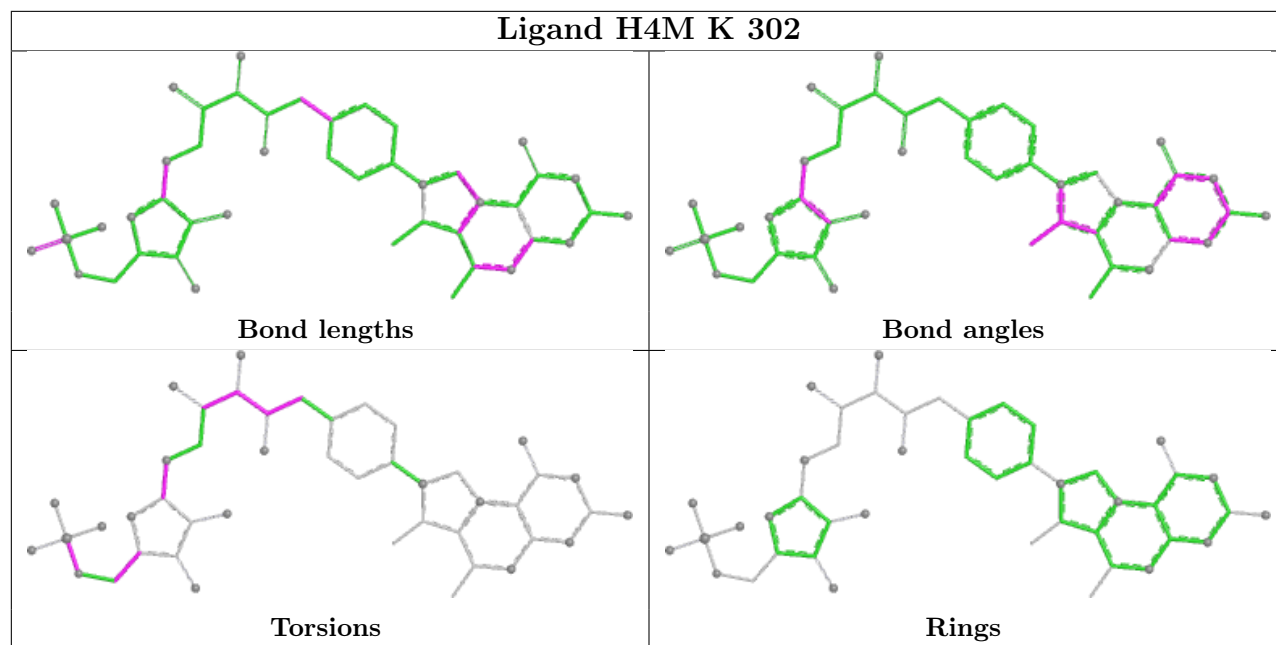




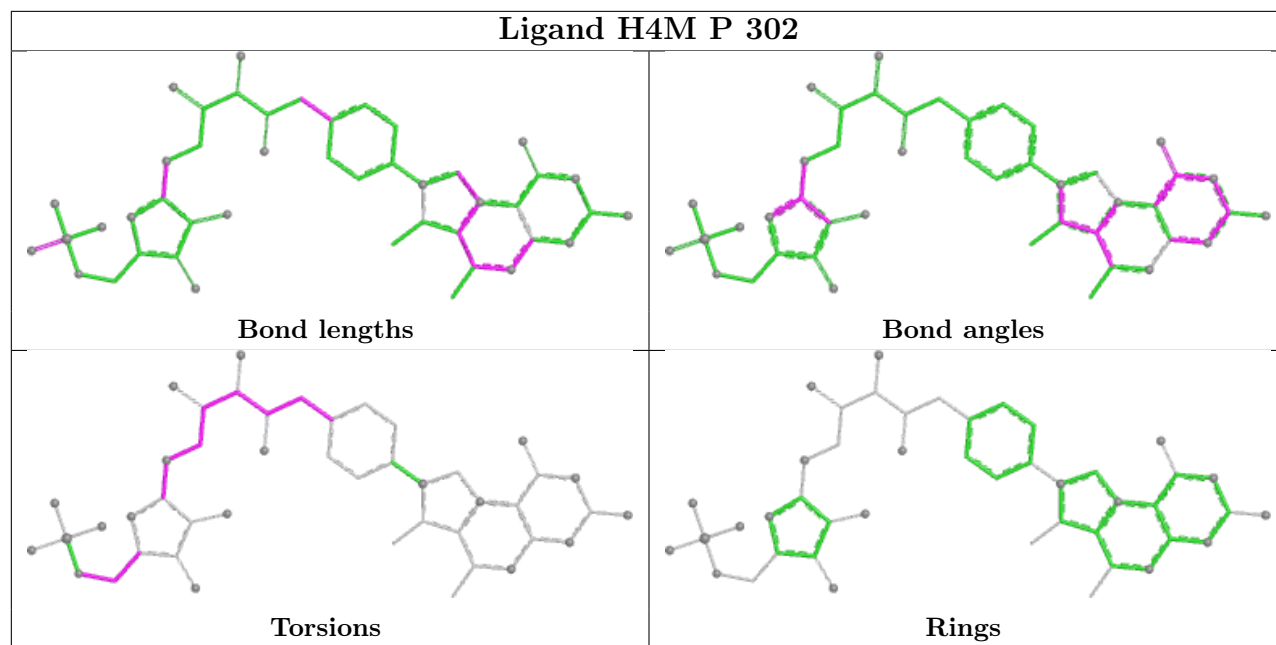




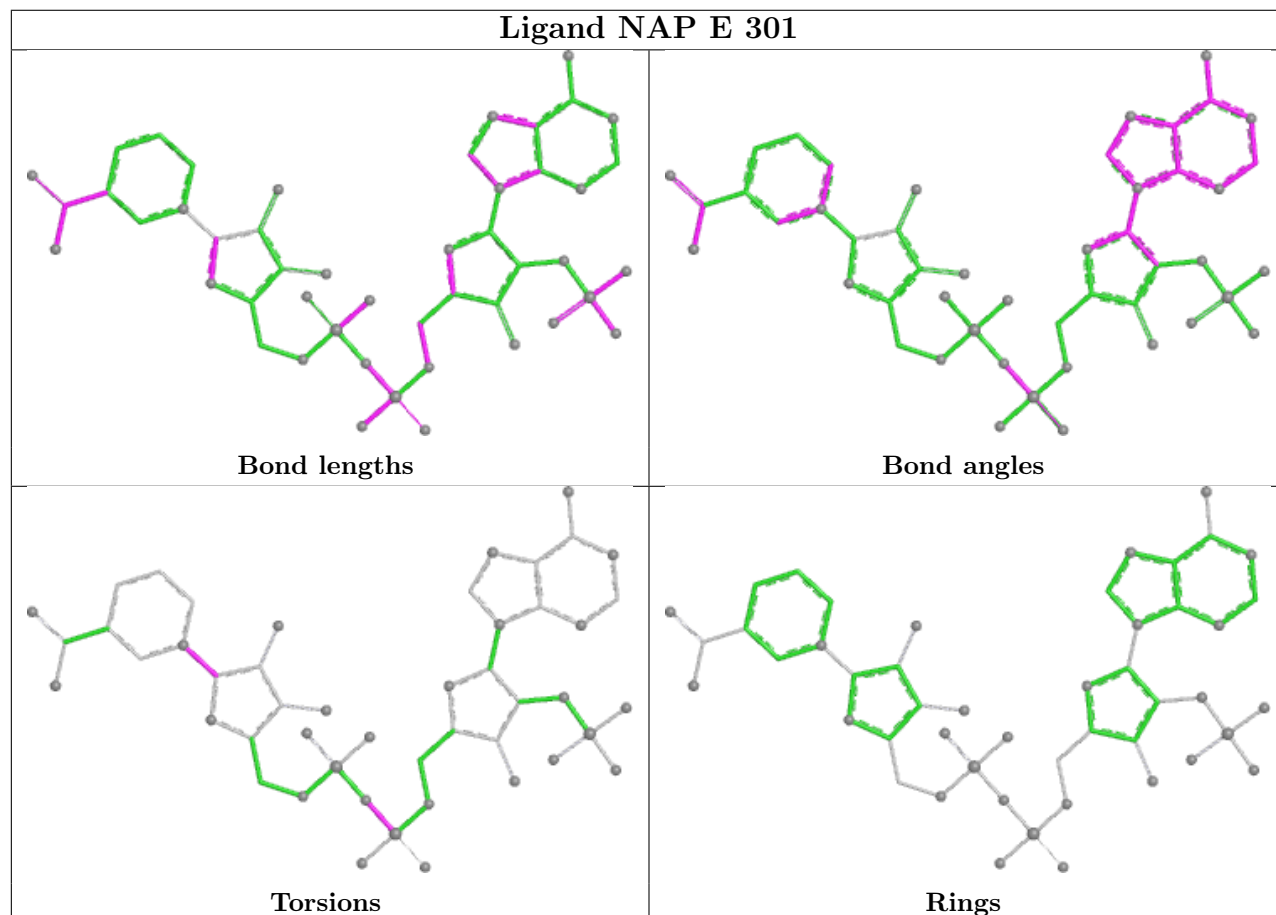


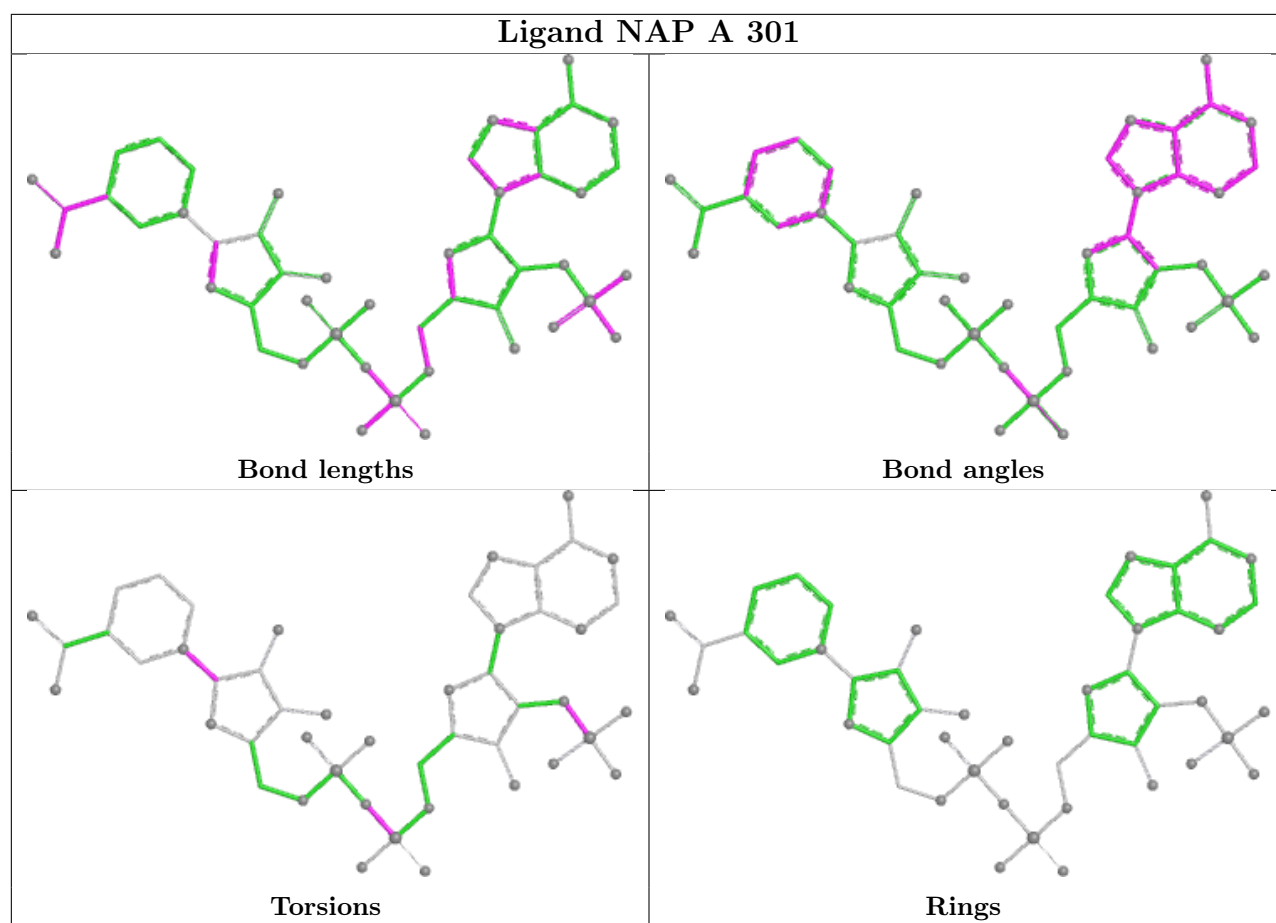


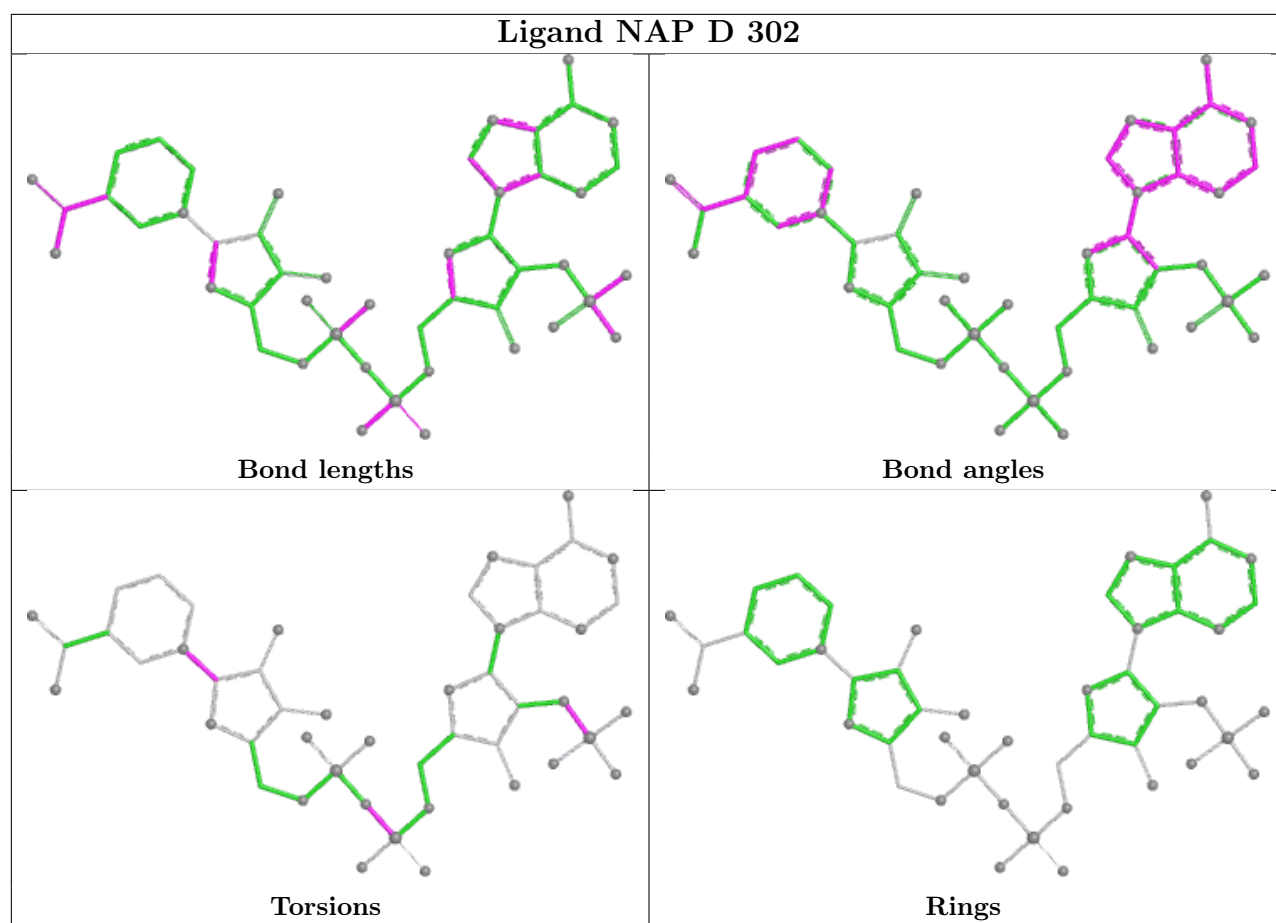
## Ligand H4M P 302

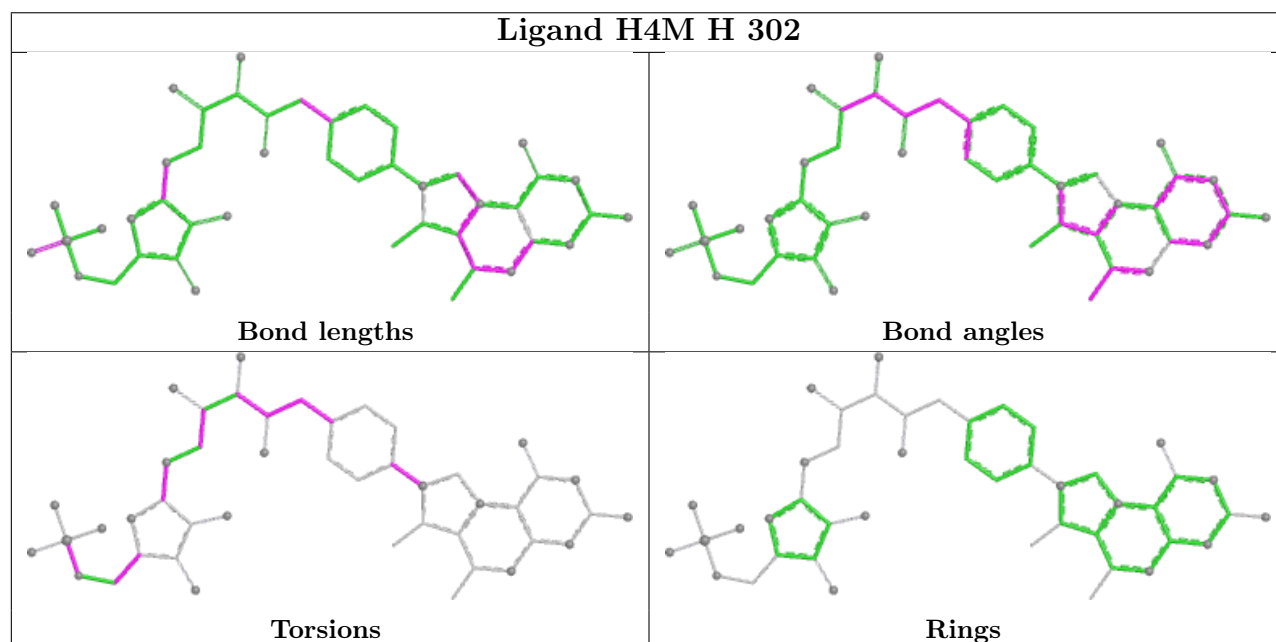
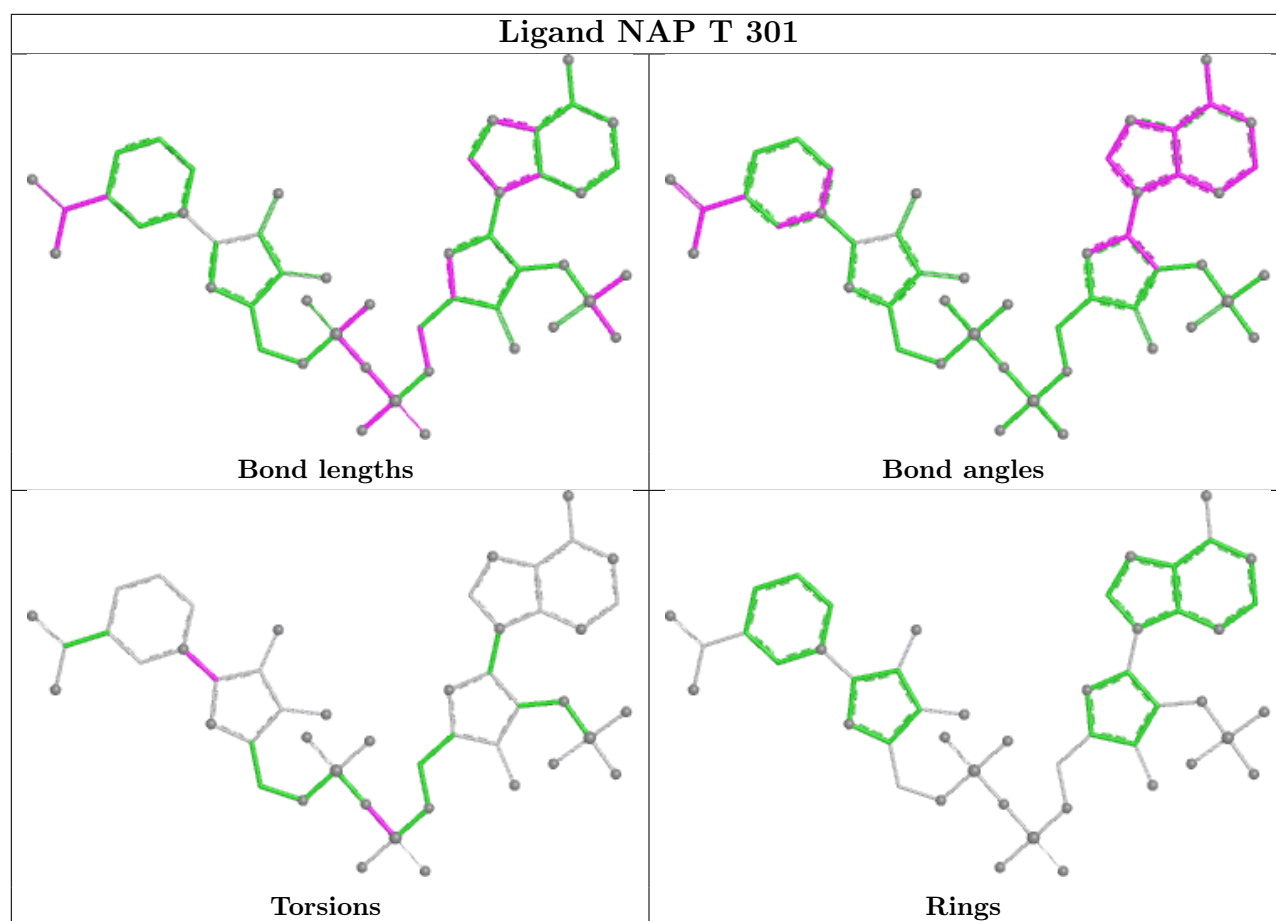


## Ligand NAP E 301

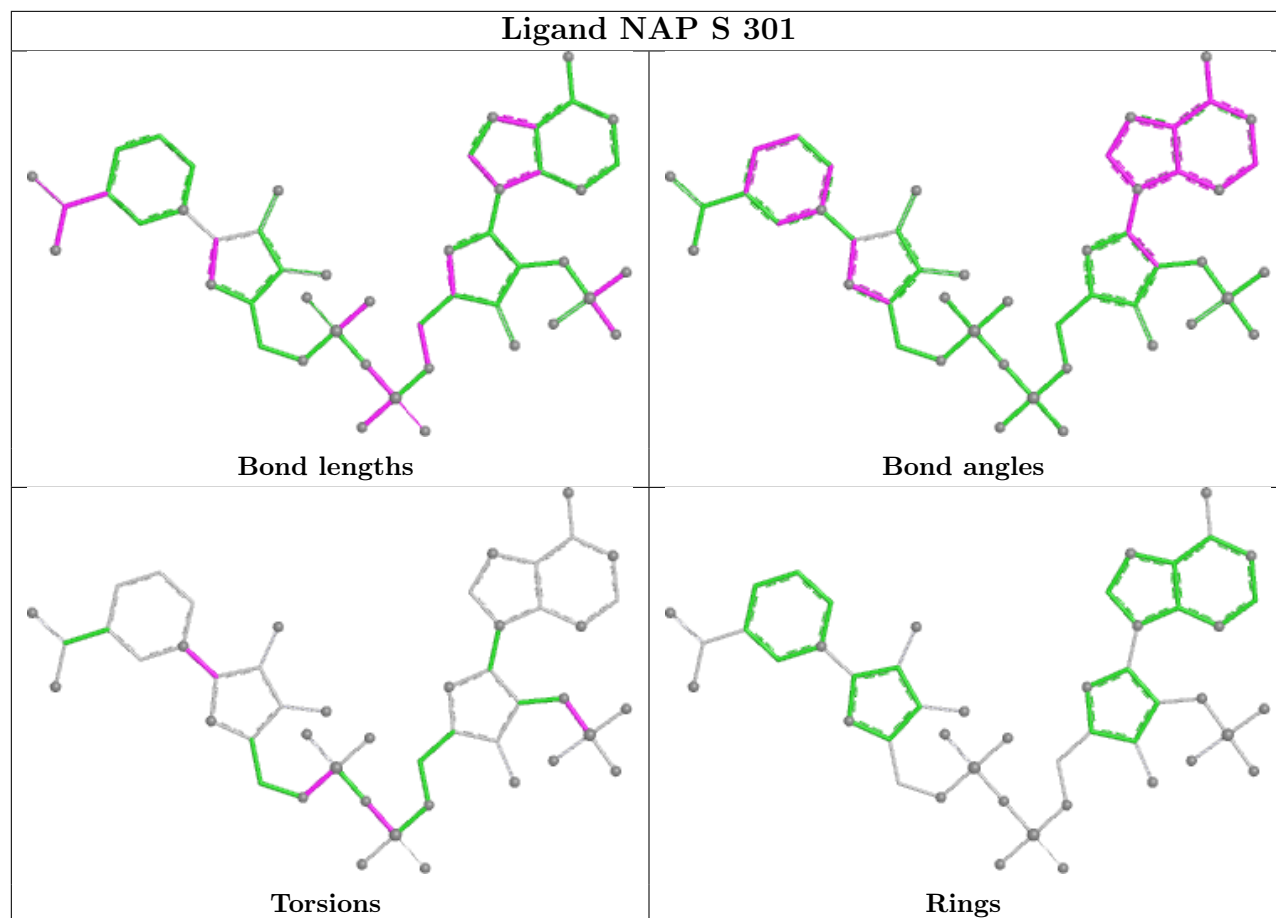




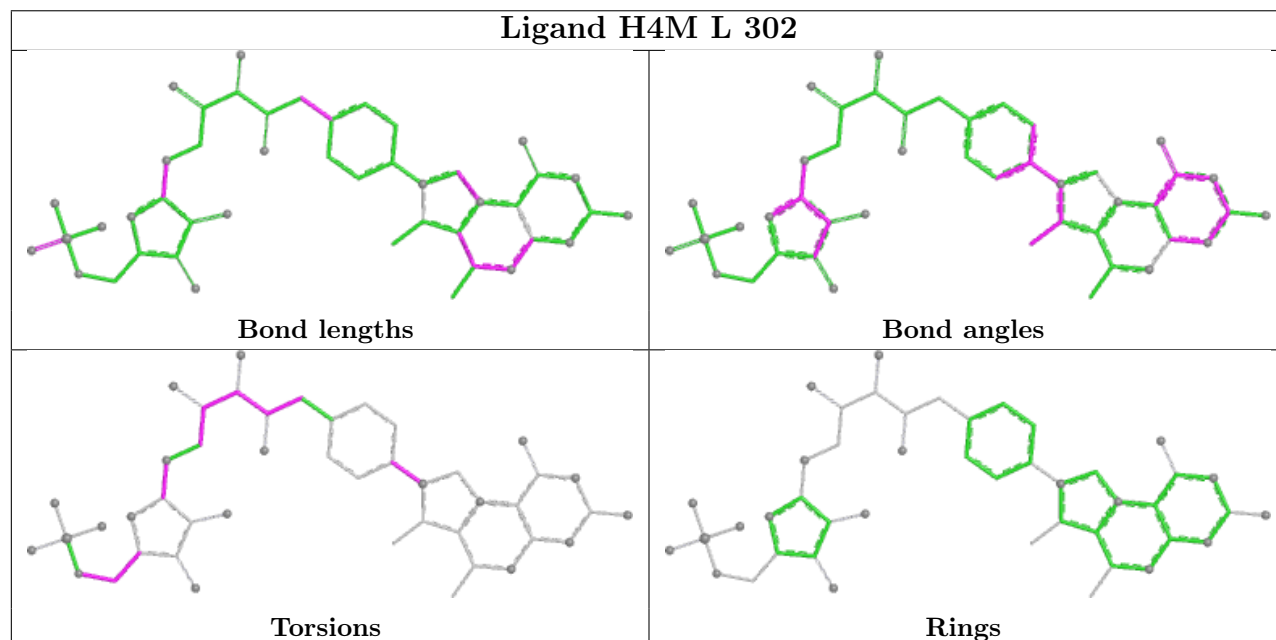


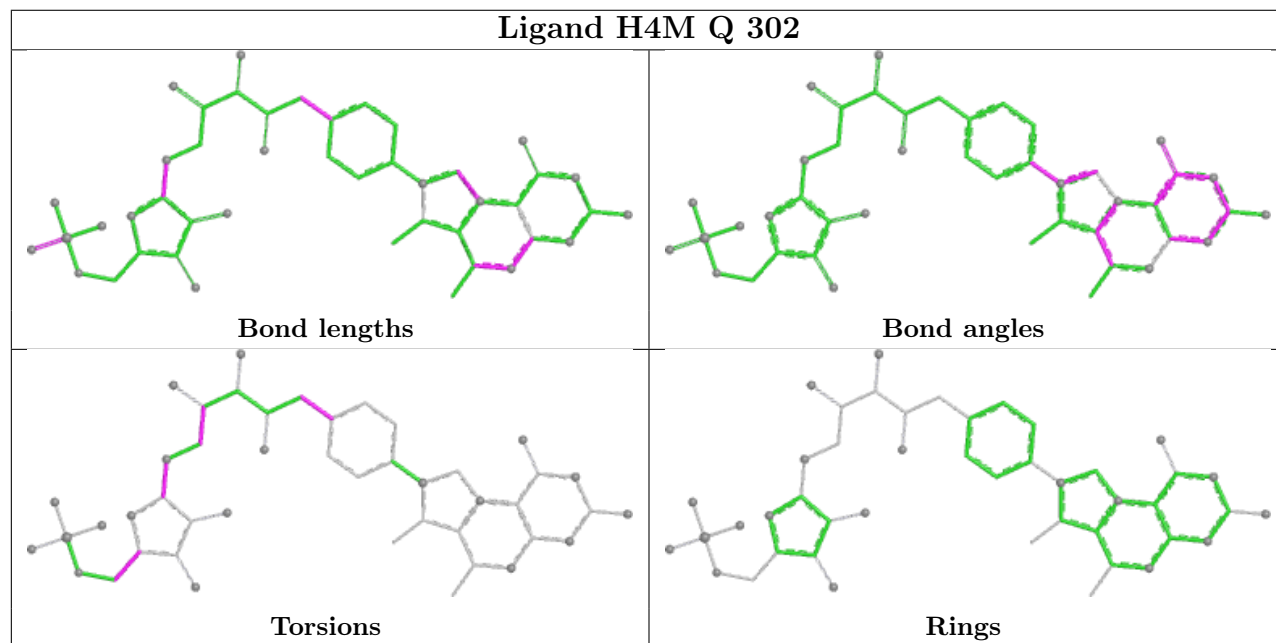
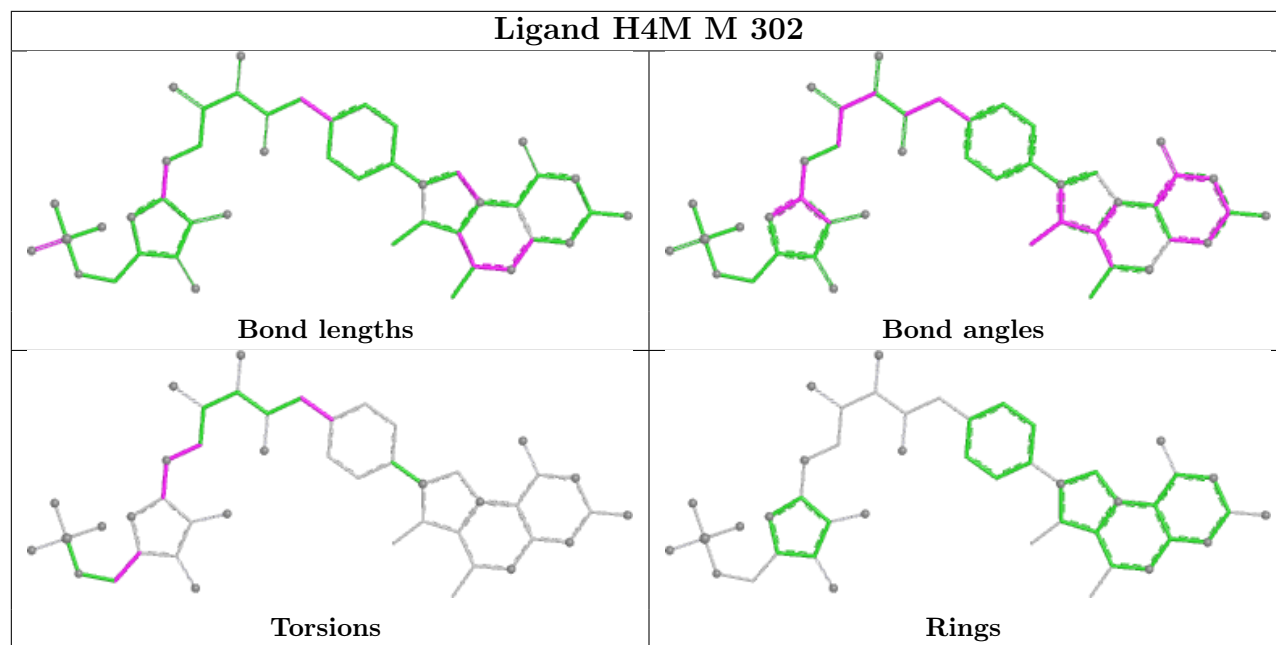


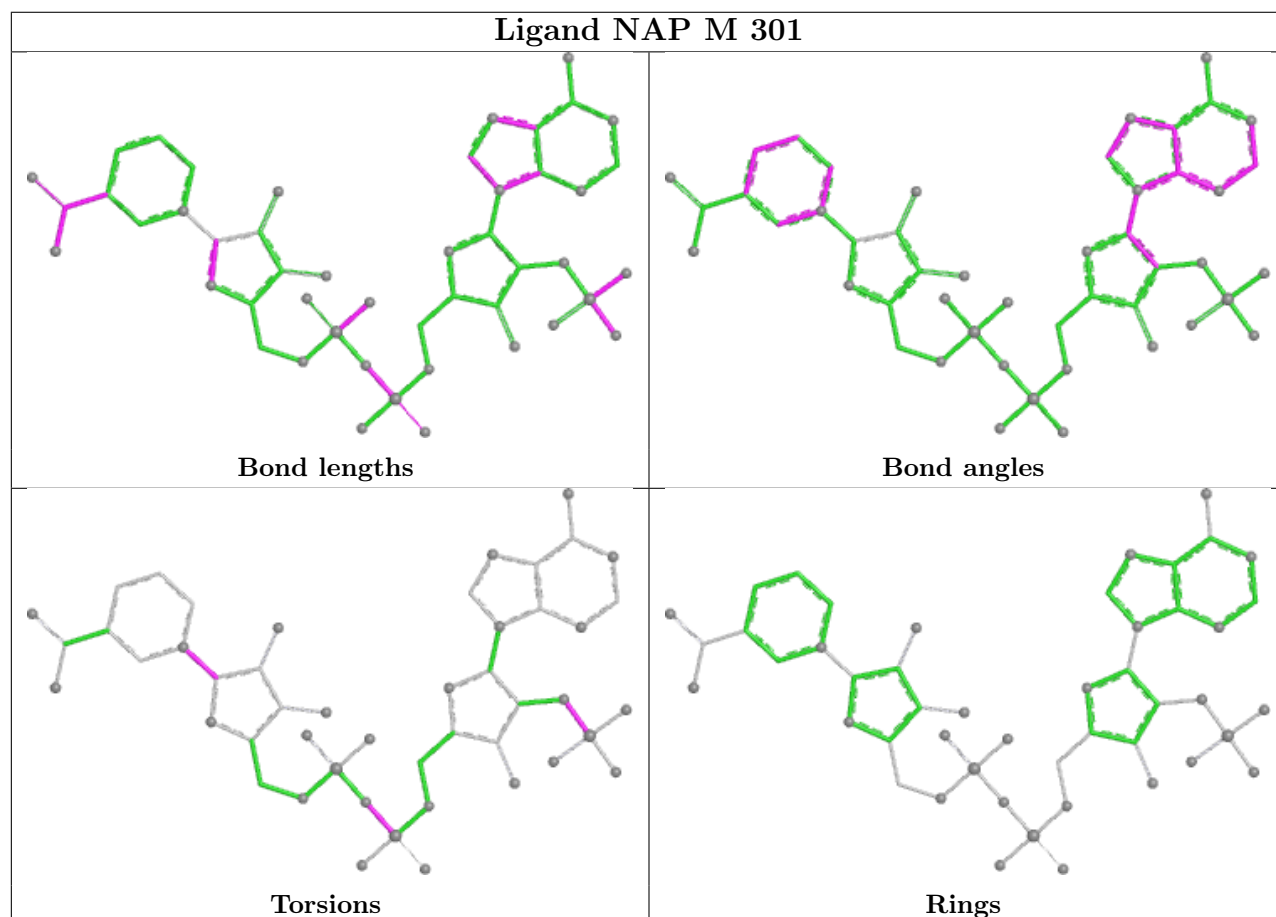
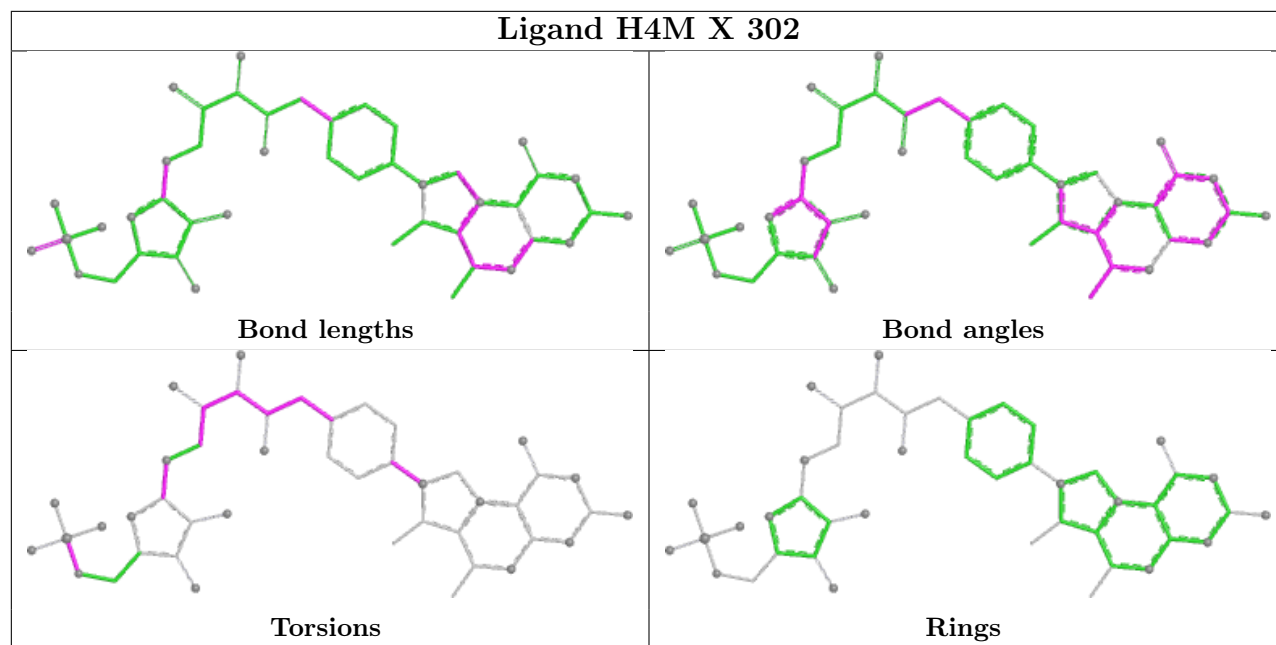
## Ligand NAP S 301

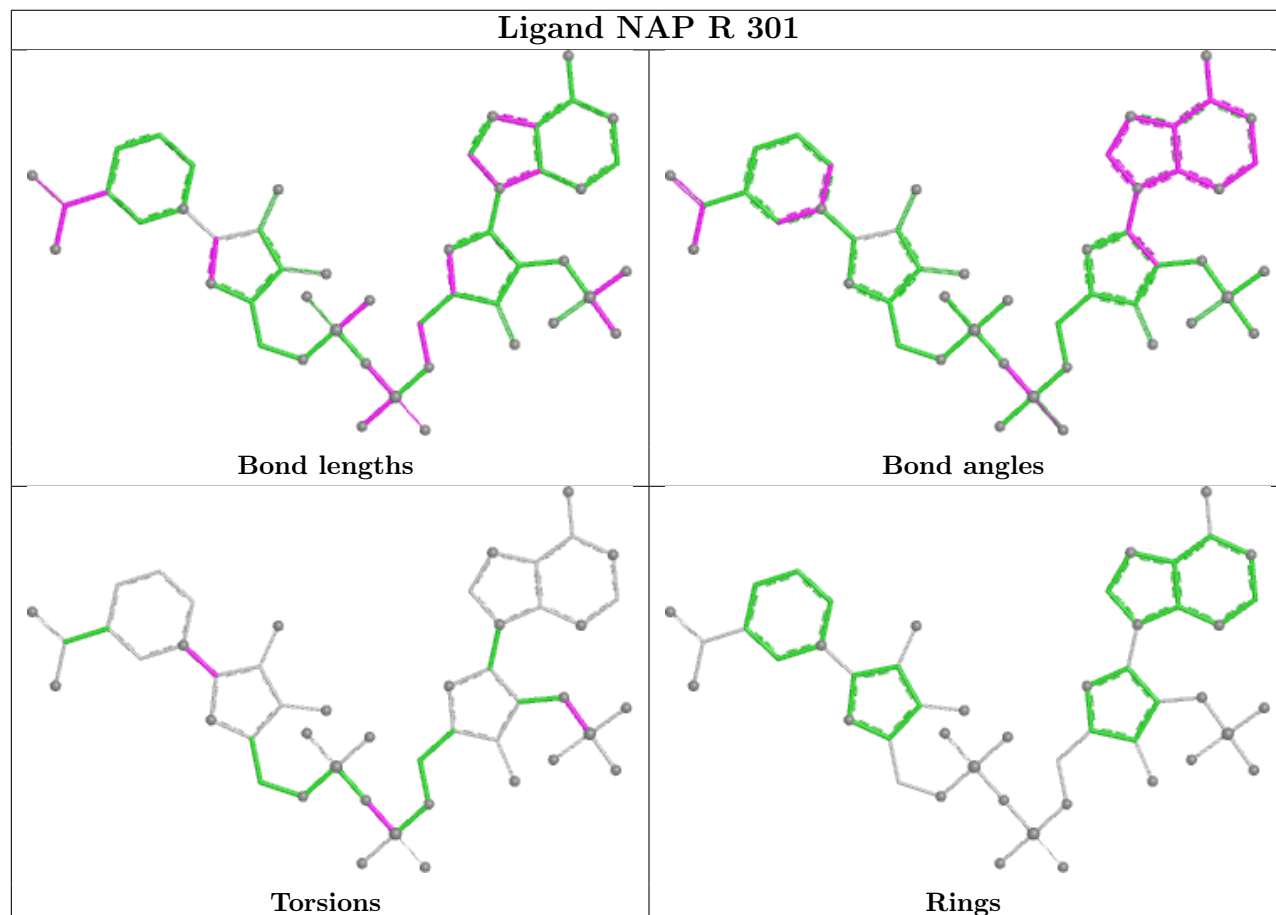
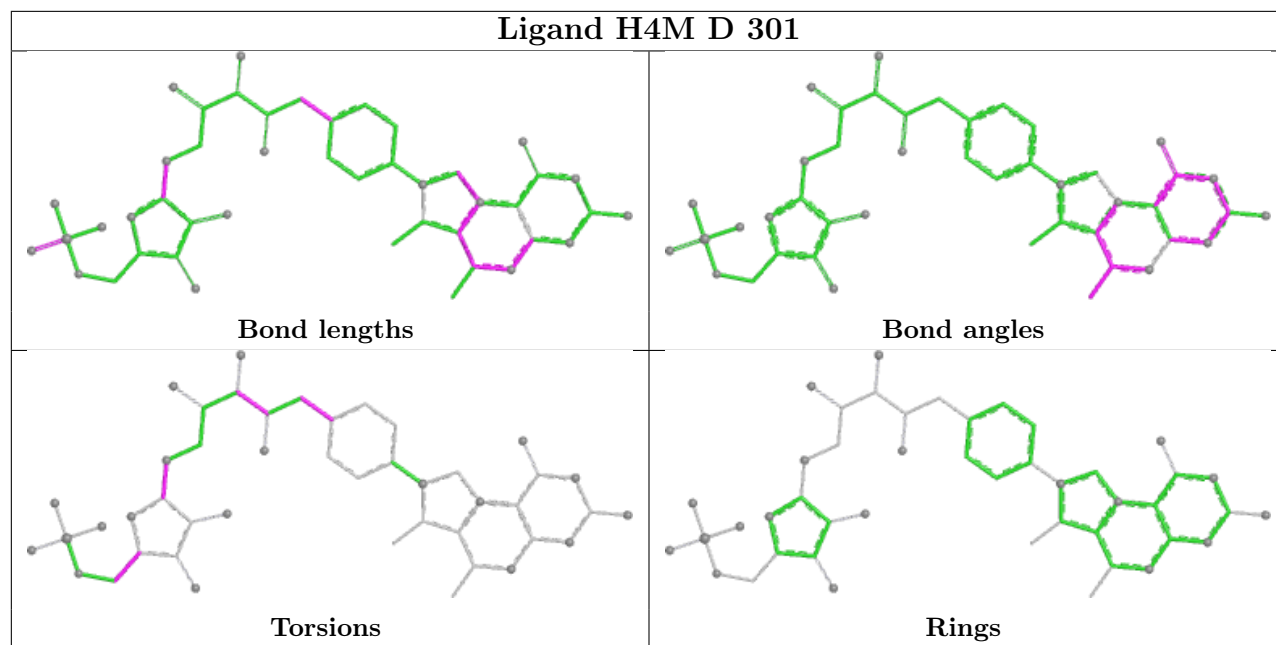


## Ligand H4M L 302

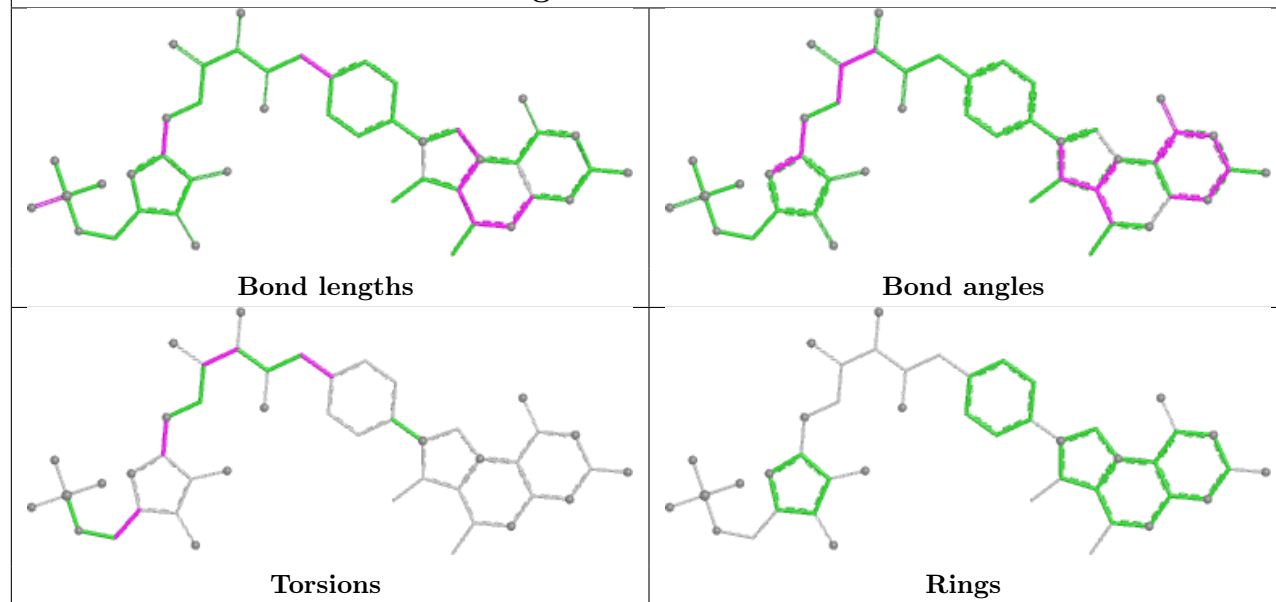




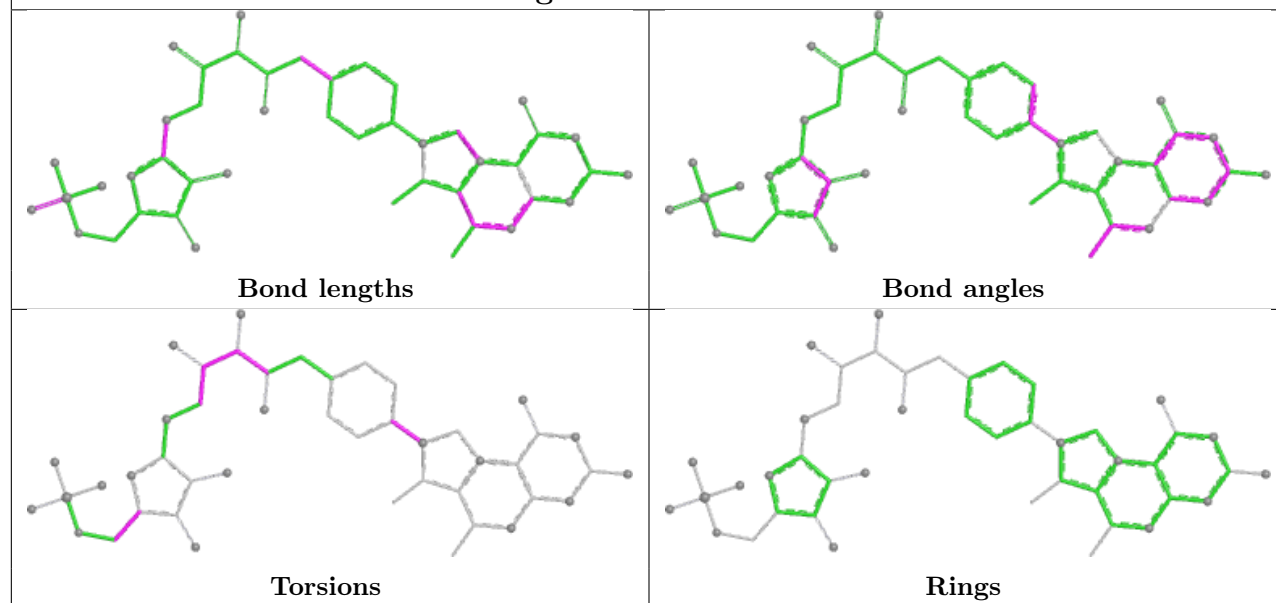




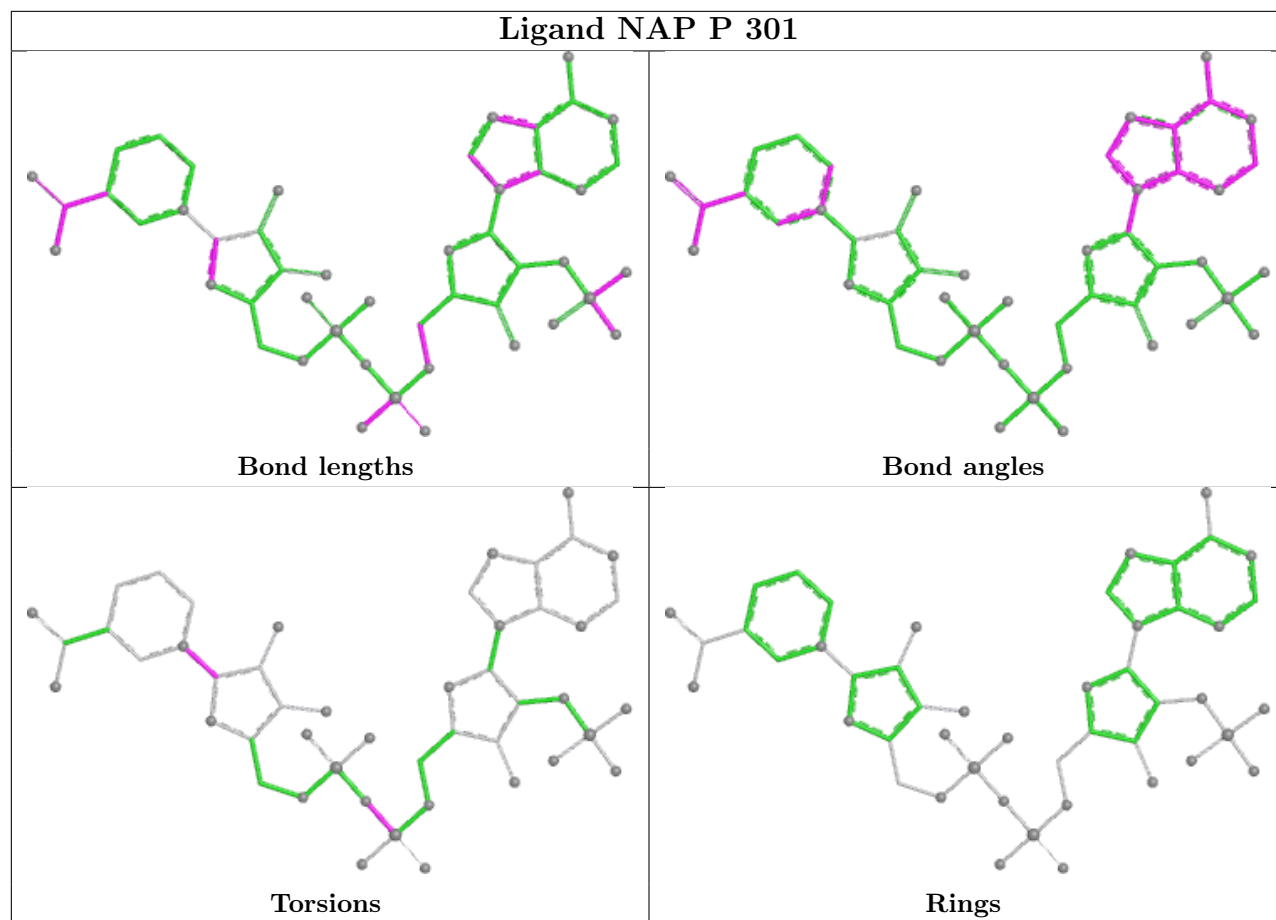
## Ligand H4M S 302



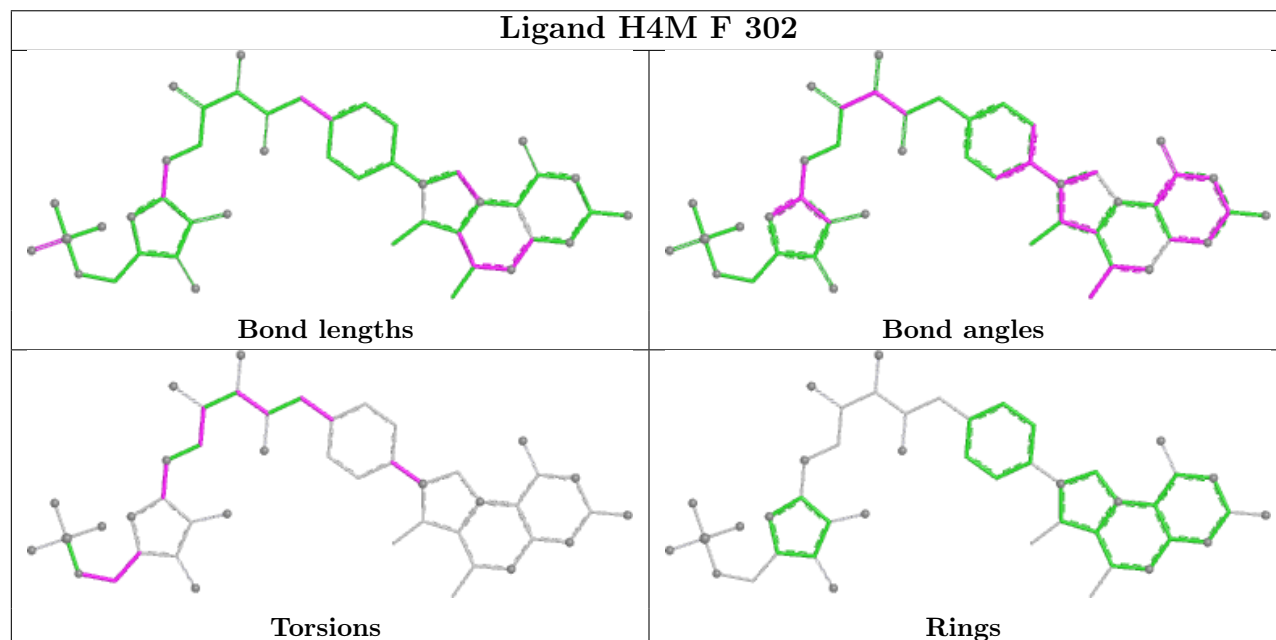
## Ligand H4M I 302

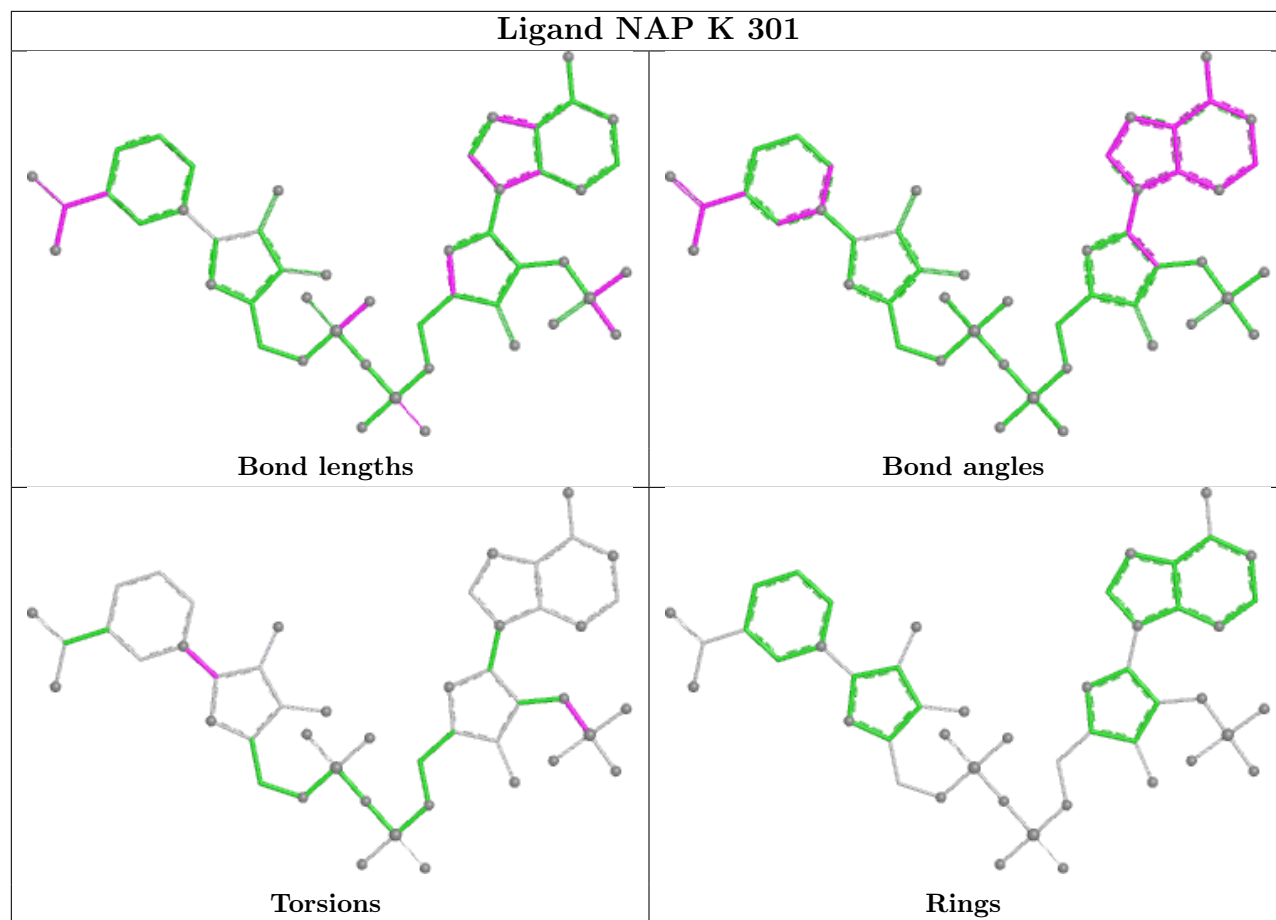


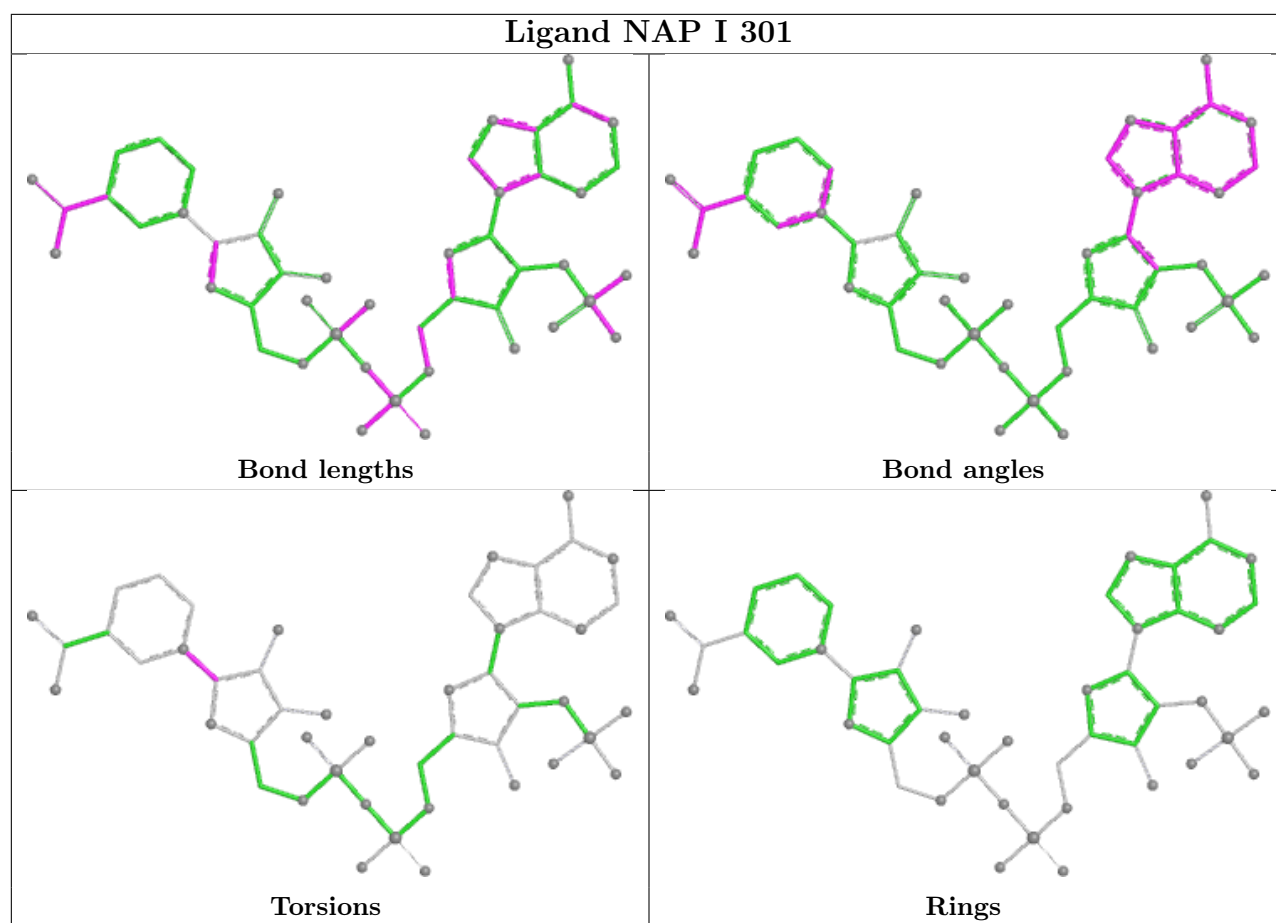
## Ligand NAP P 301

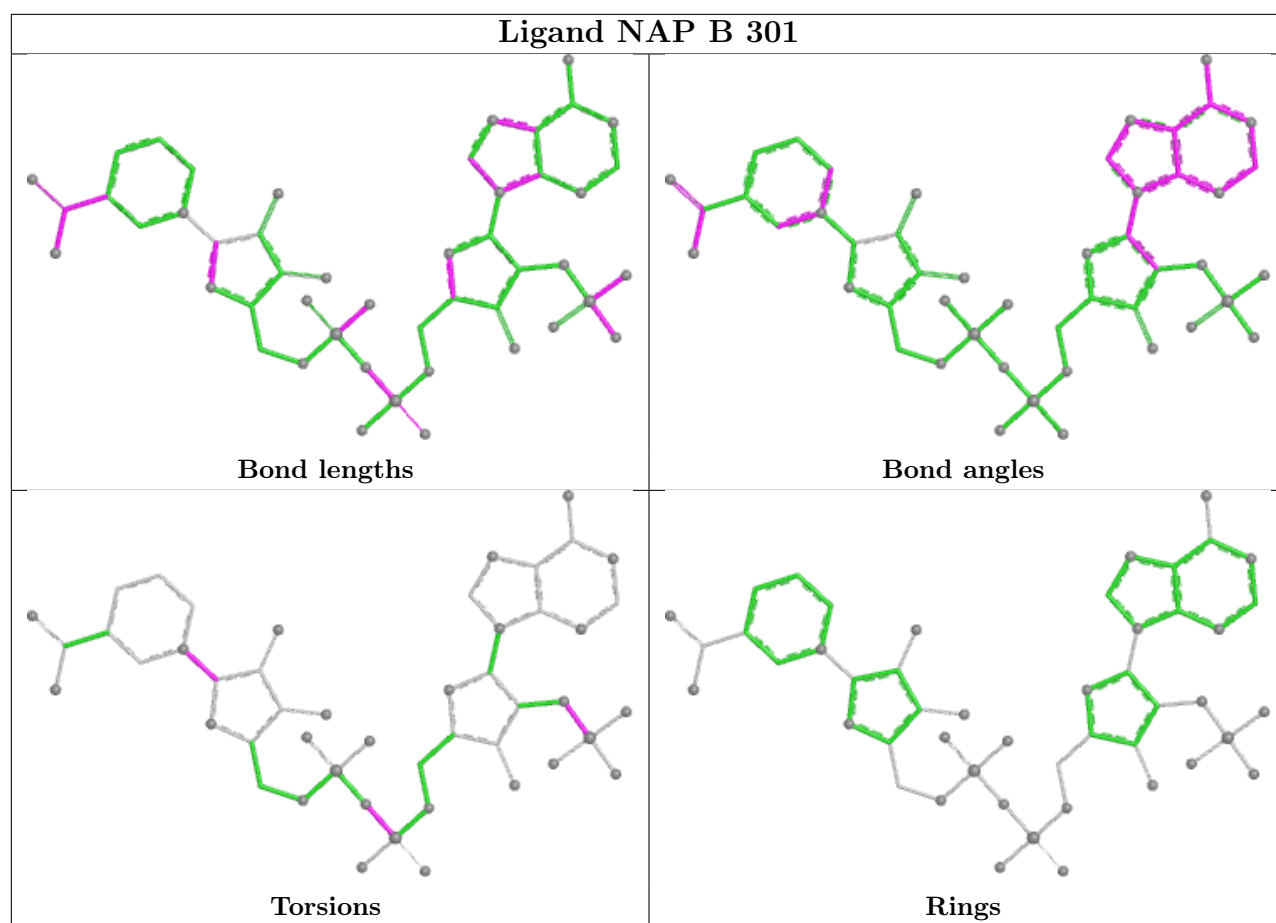


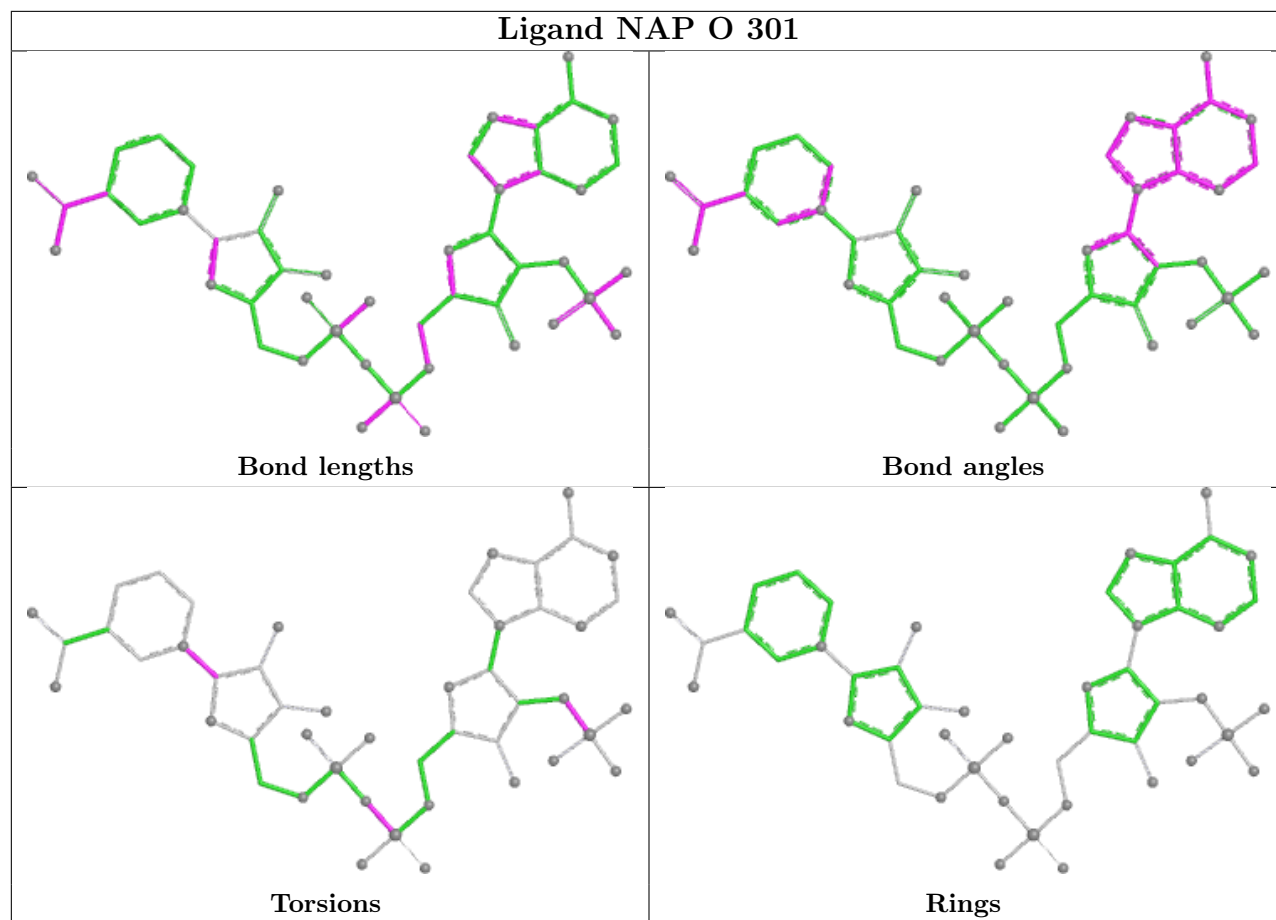
## Ligand H4M F 302

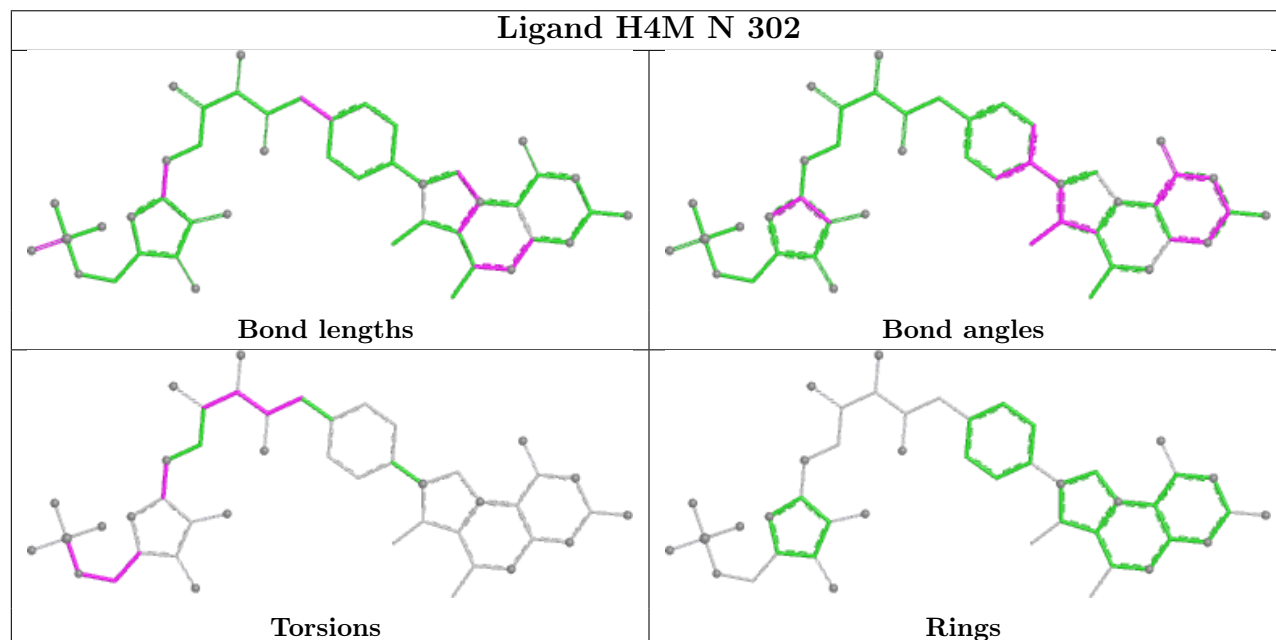
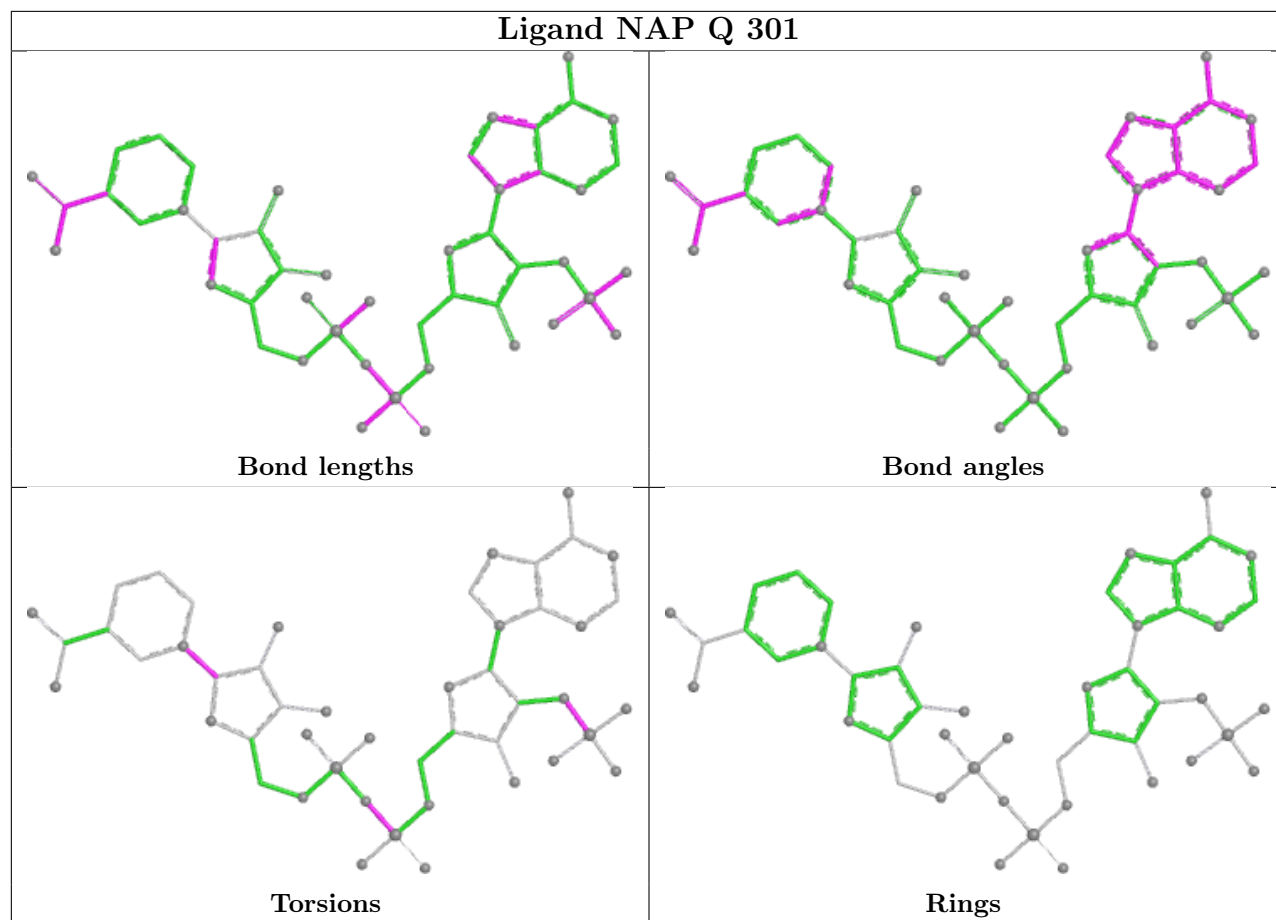


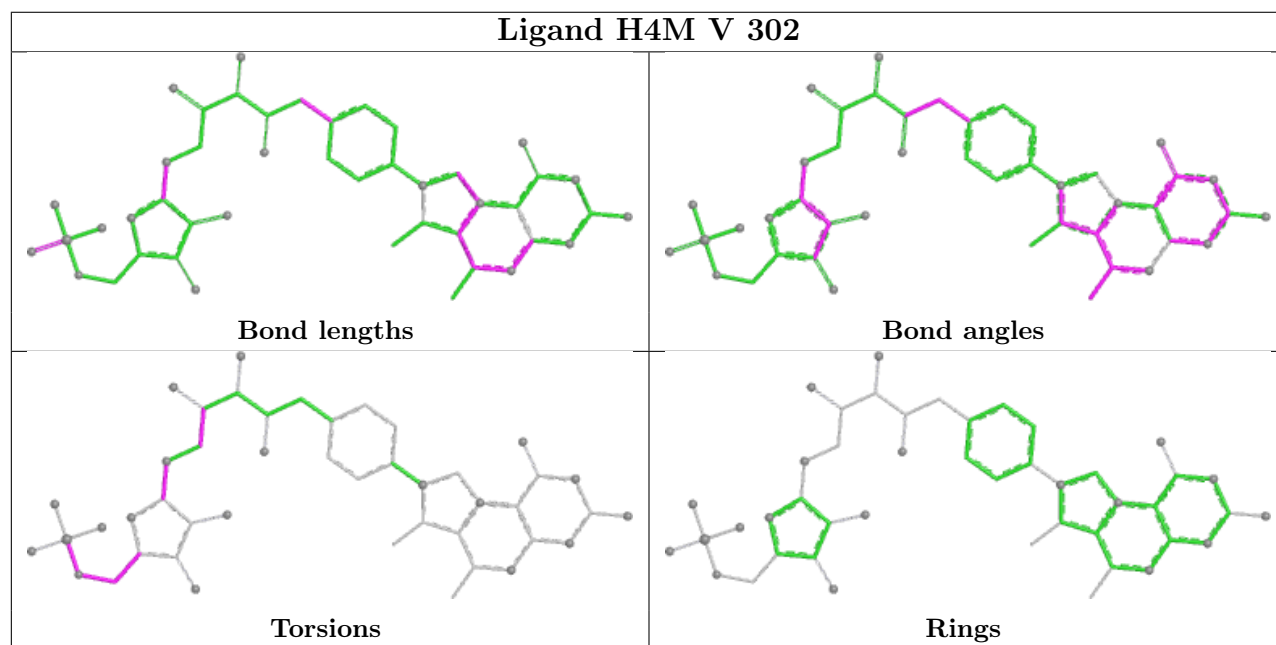
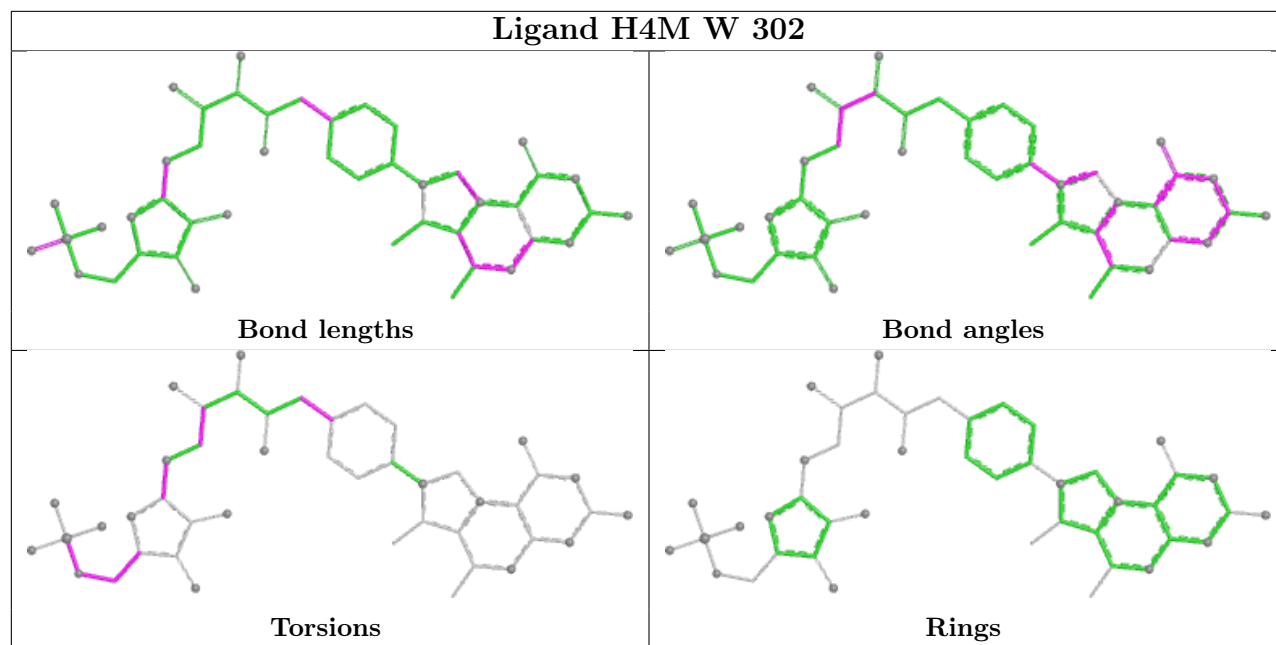




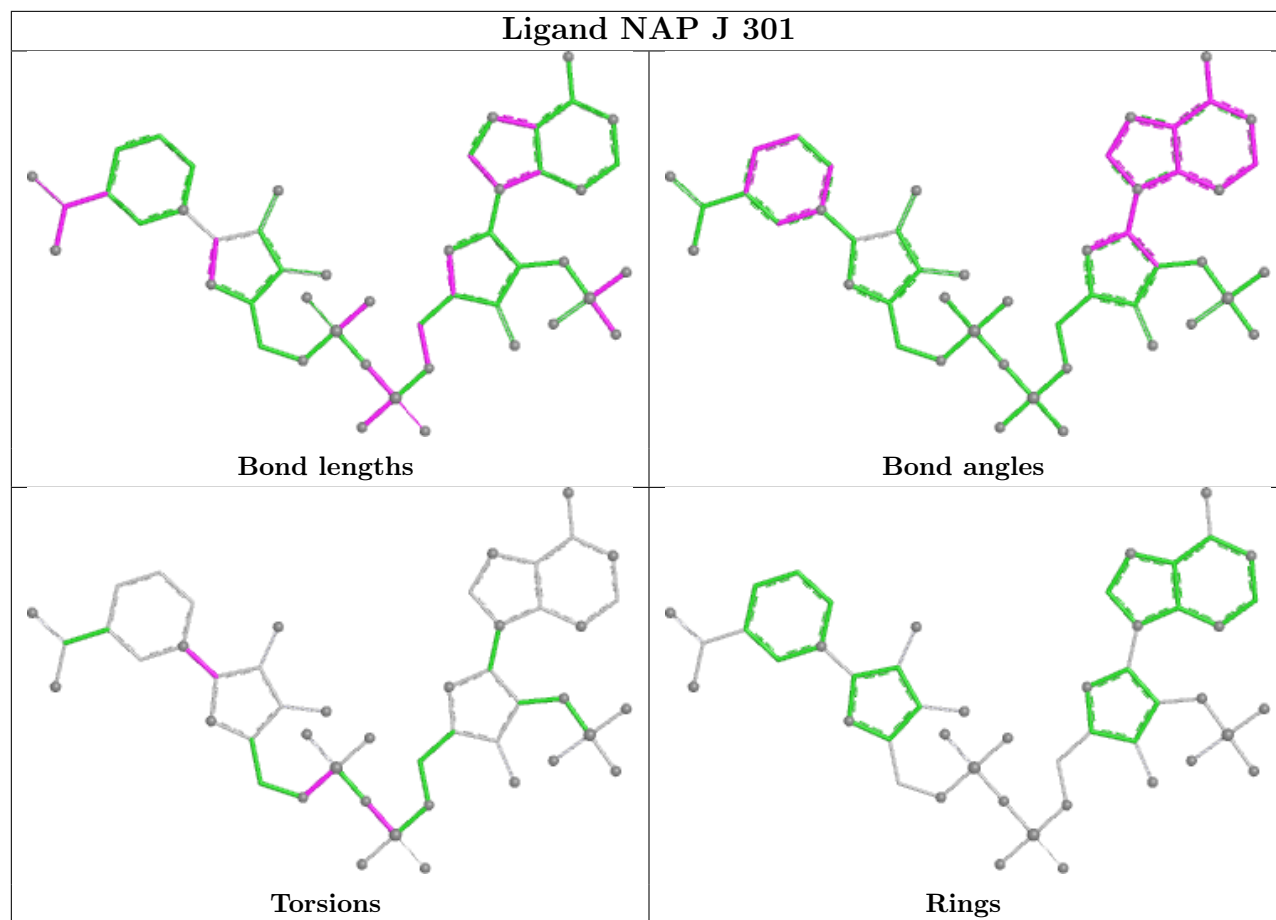


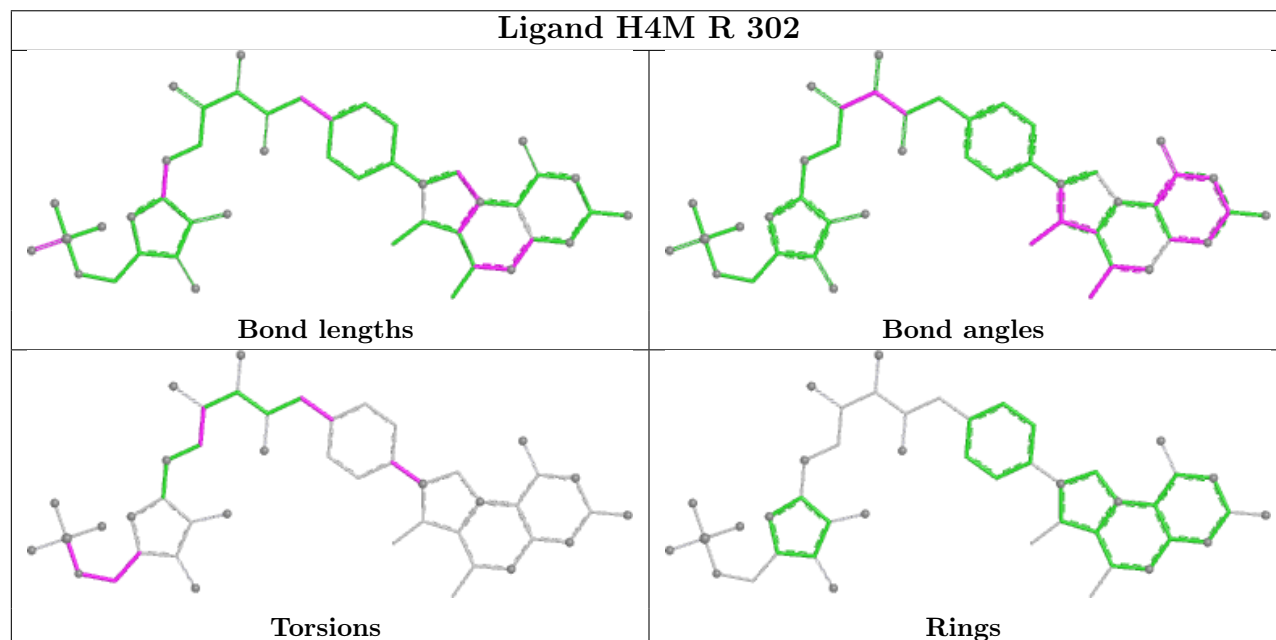
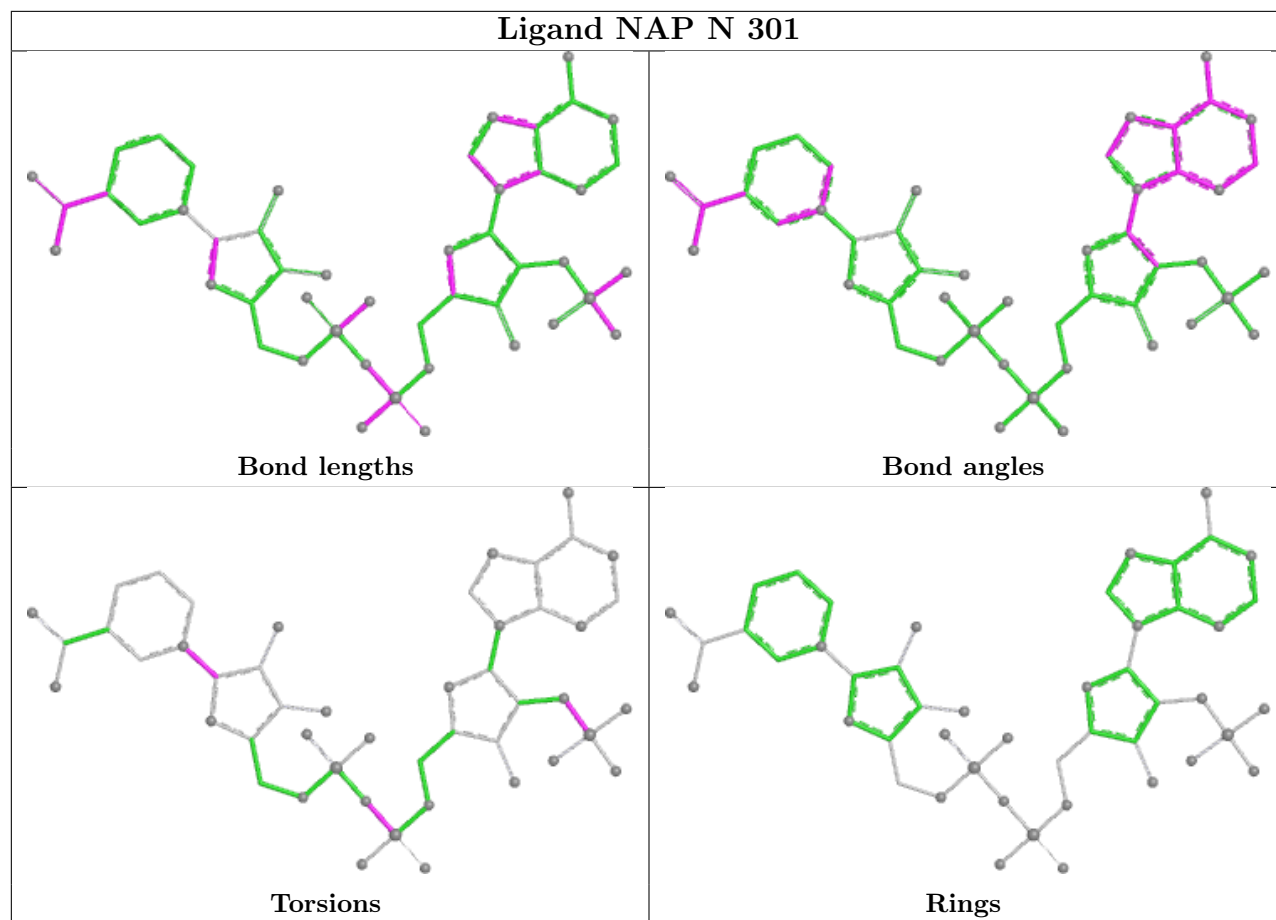


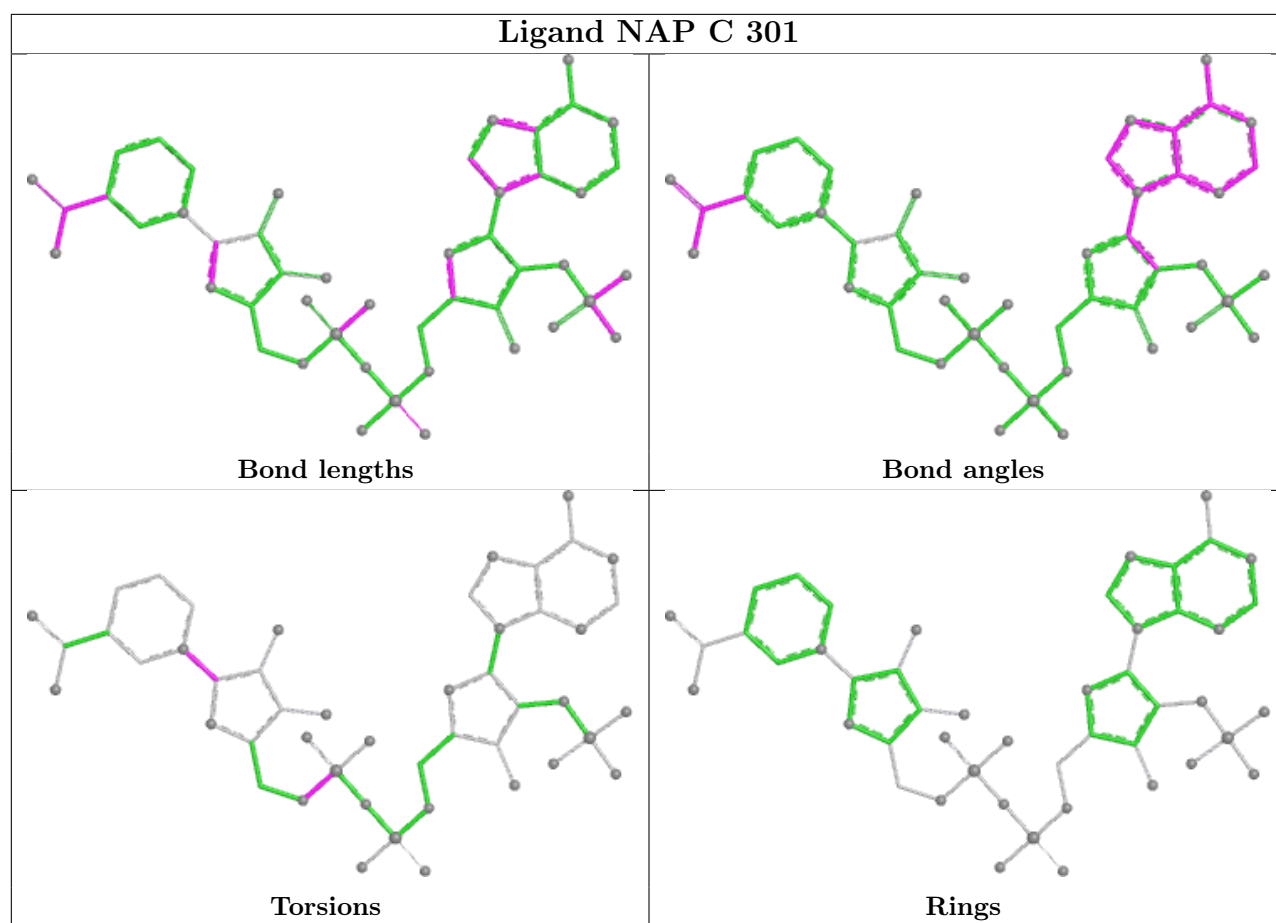




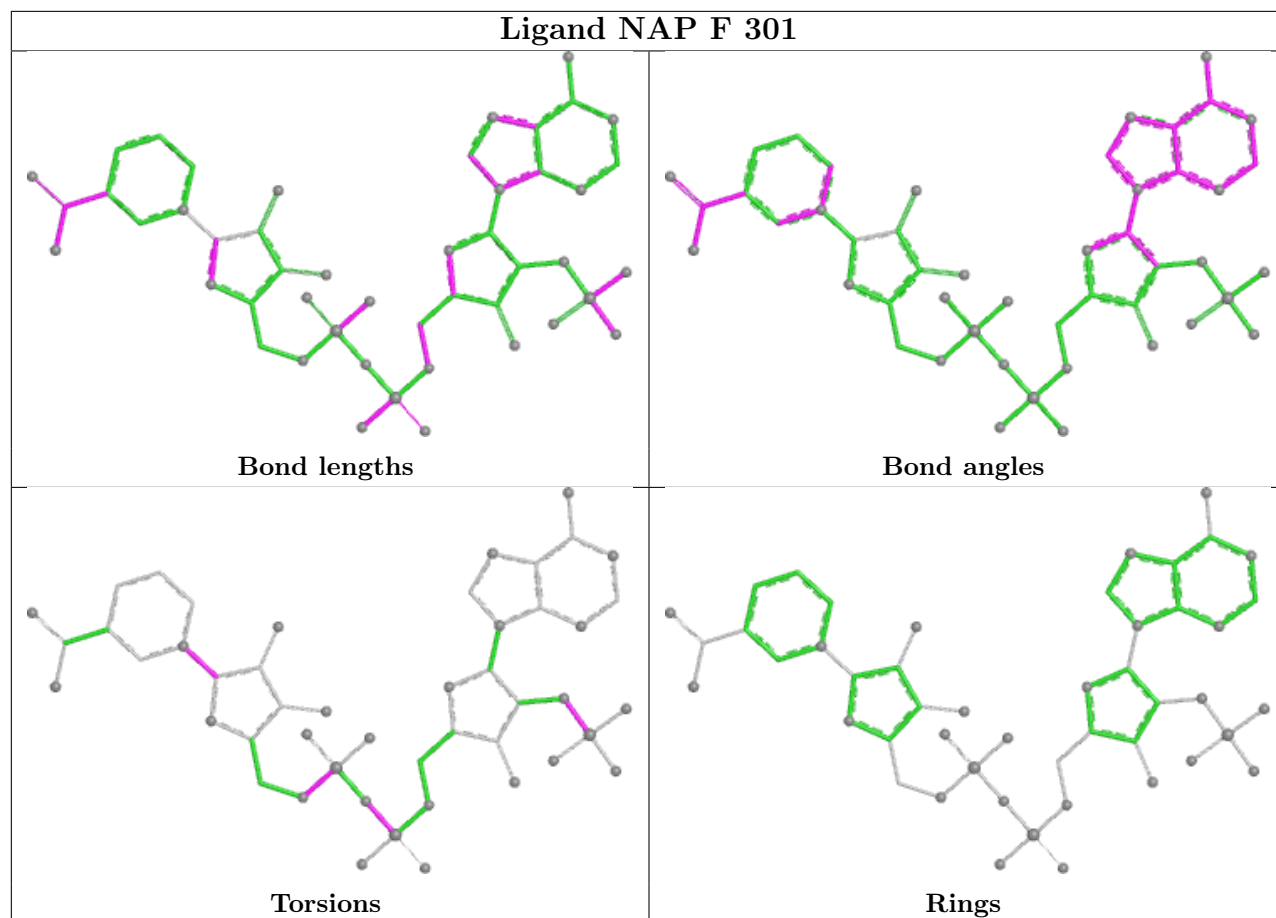
## Ligand NAP J 301



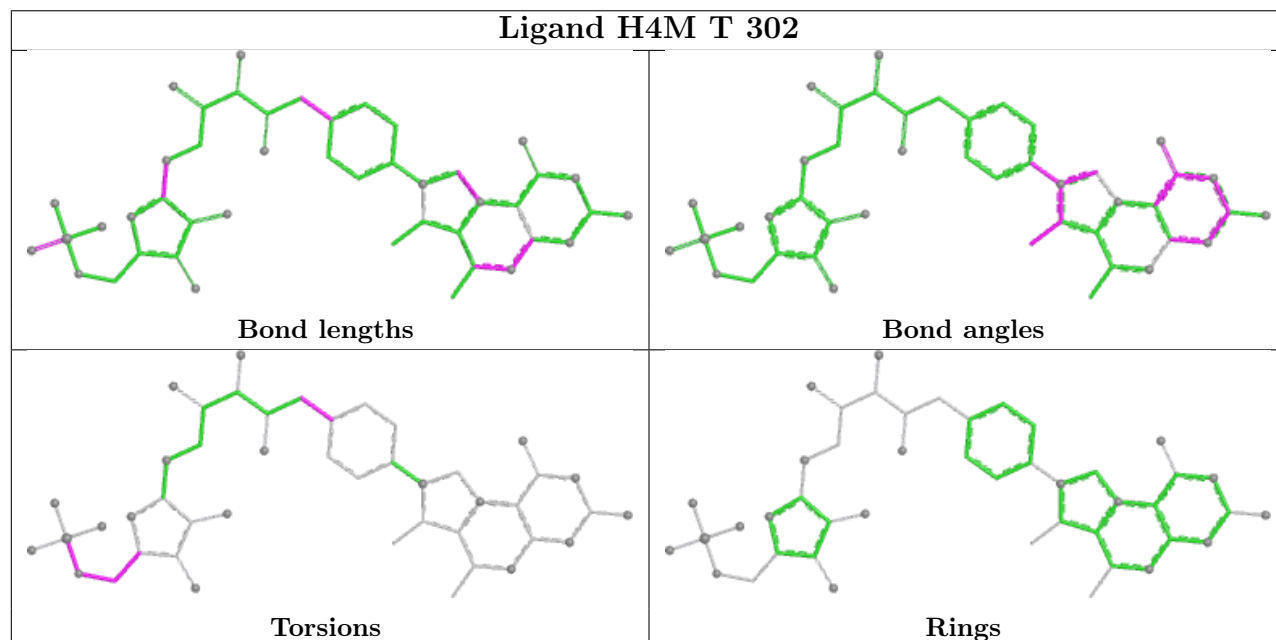


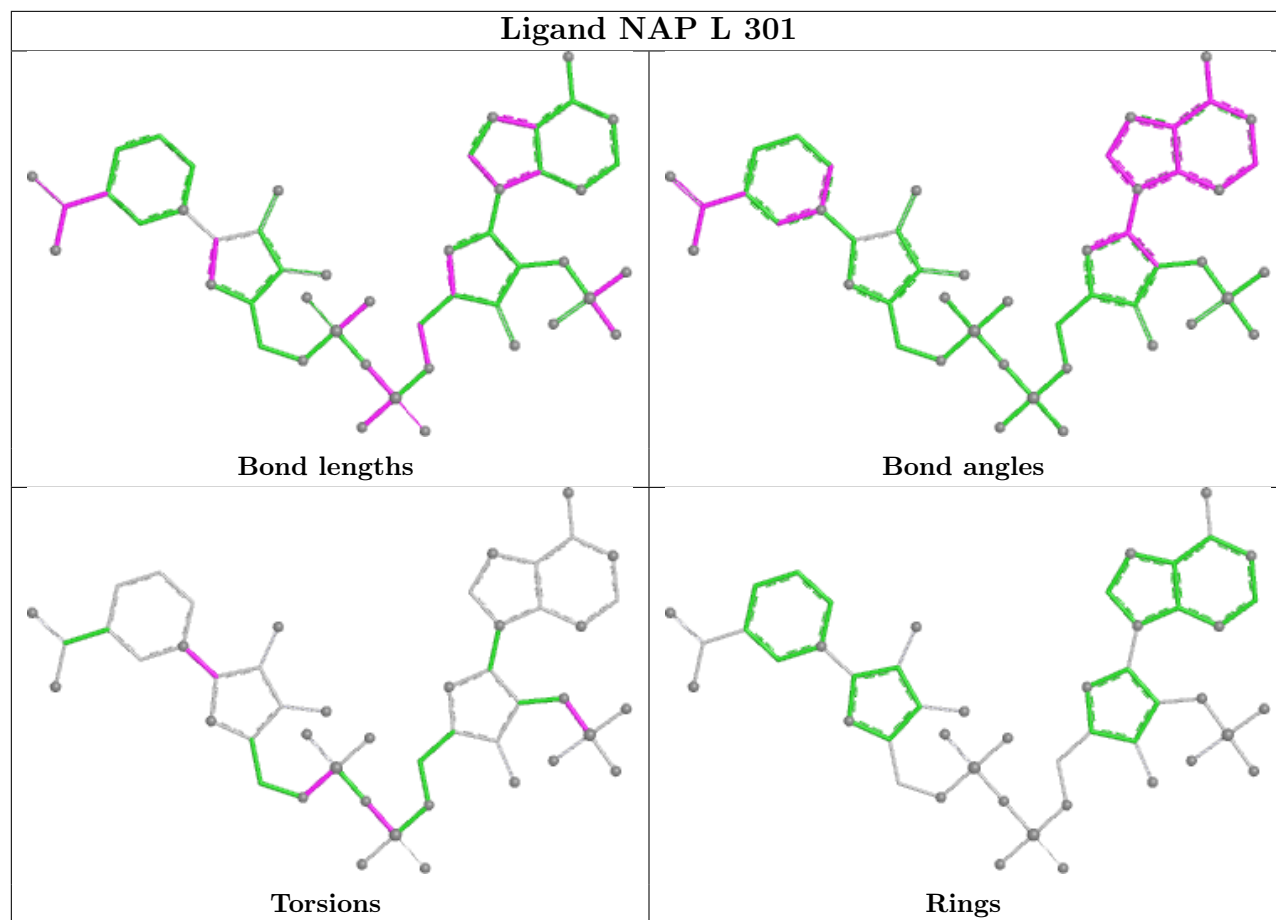


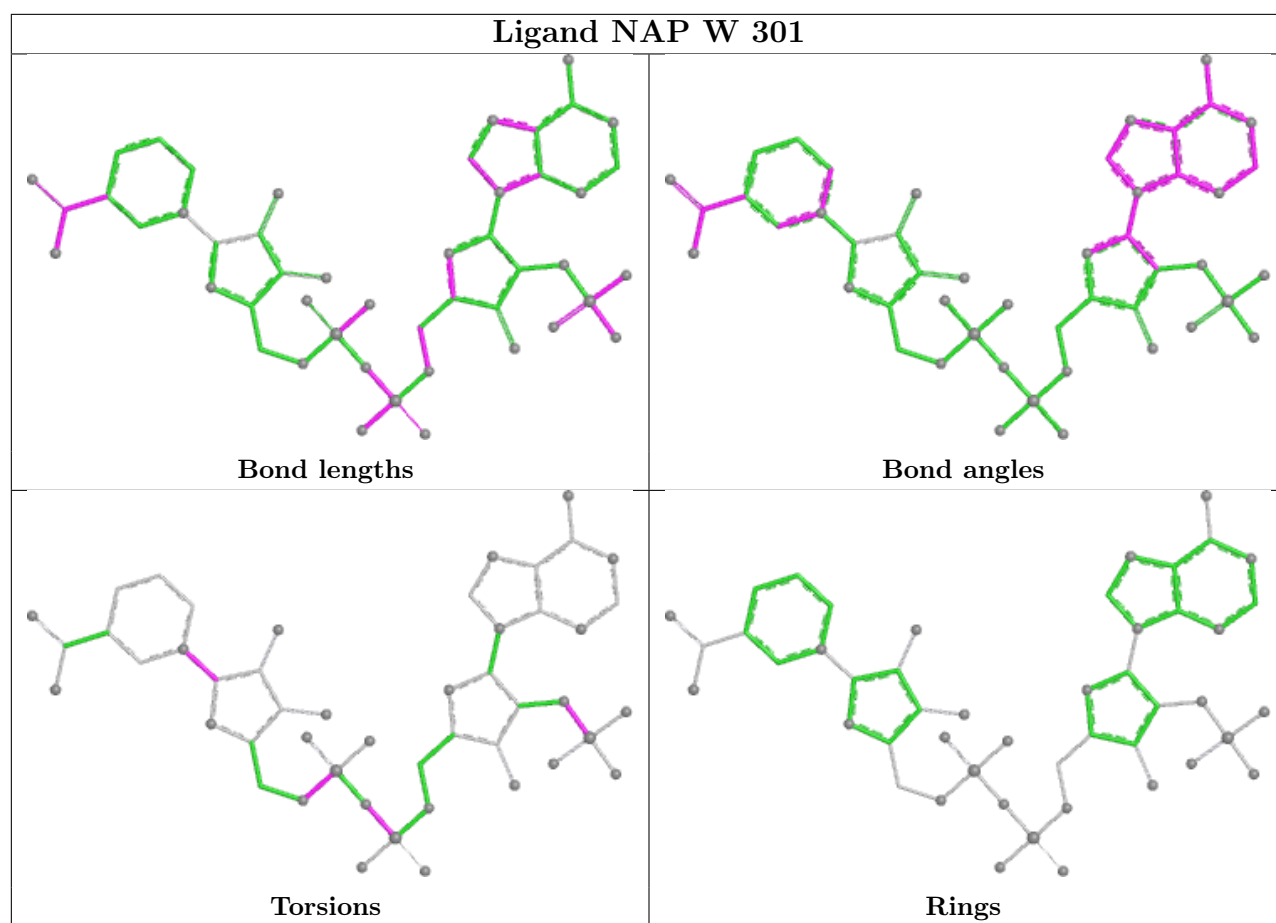
## Ligand NAP F 301

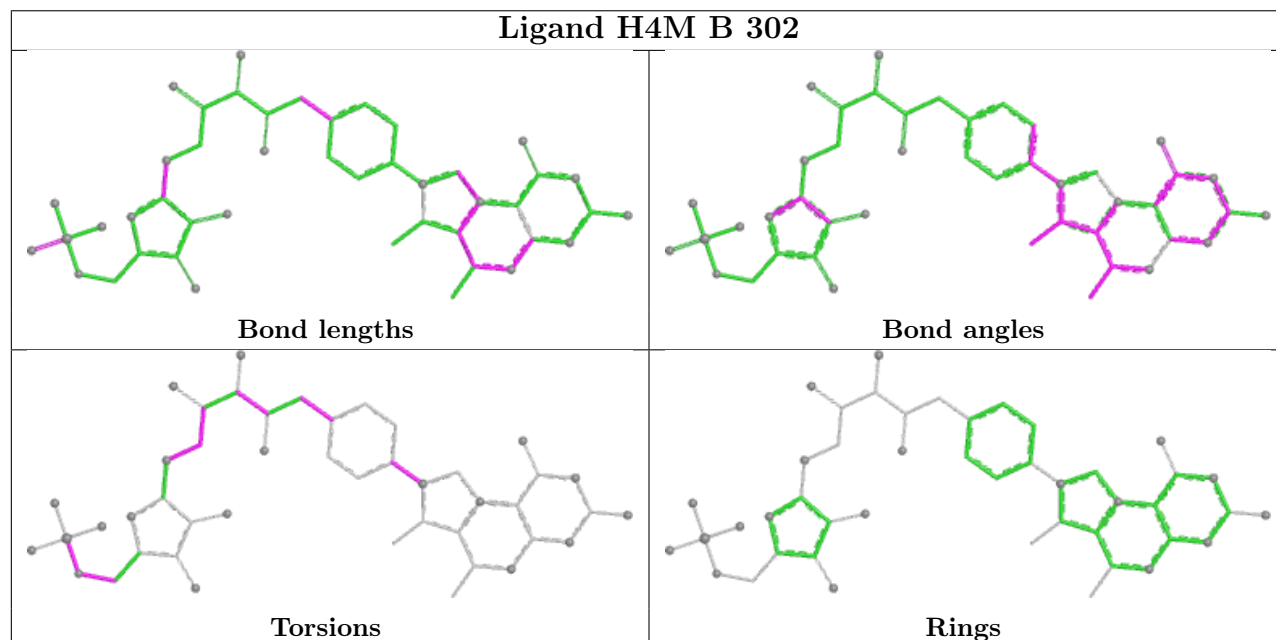
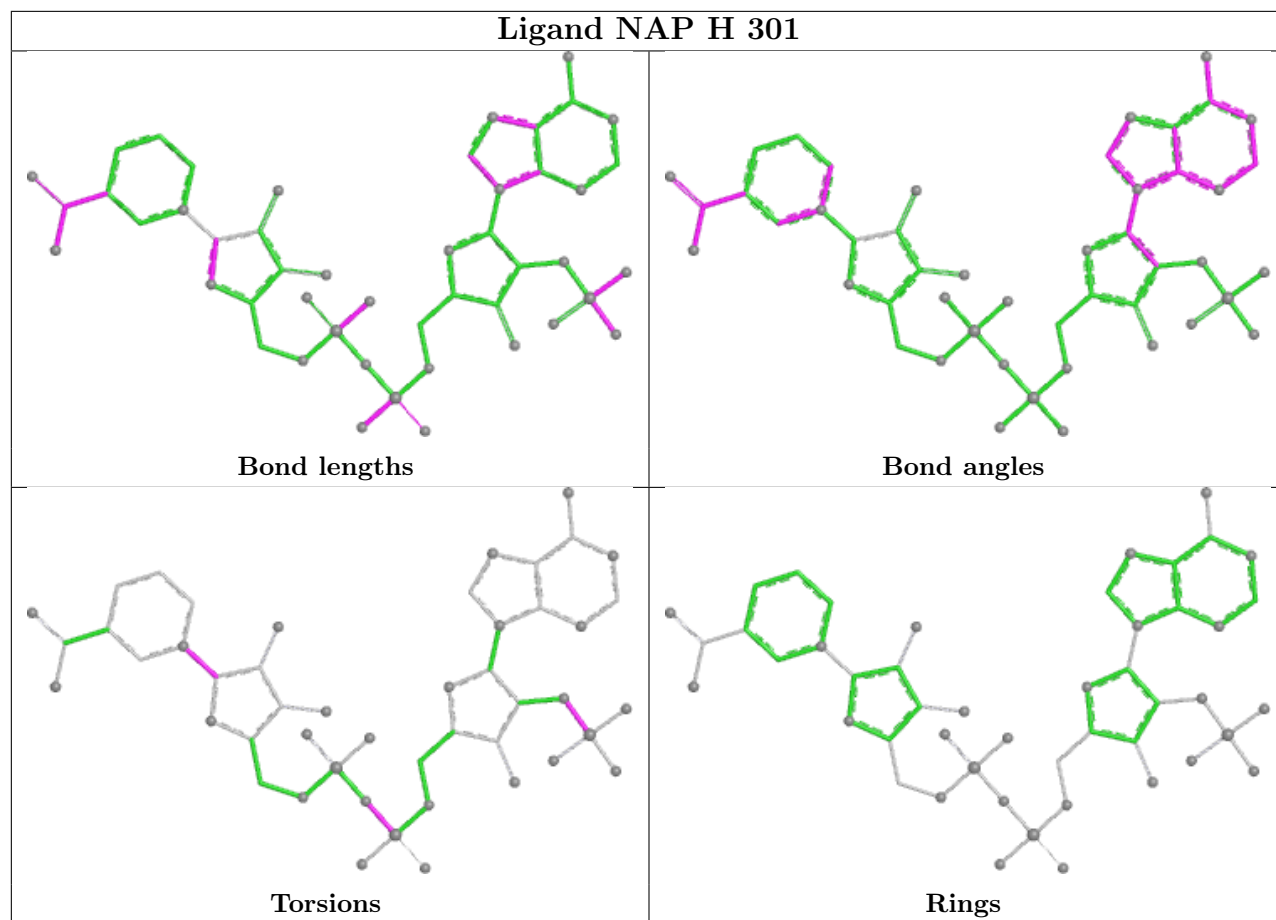


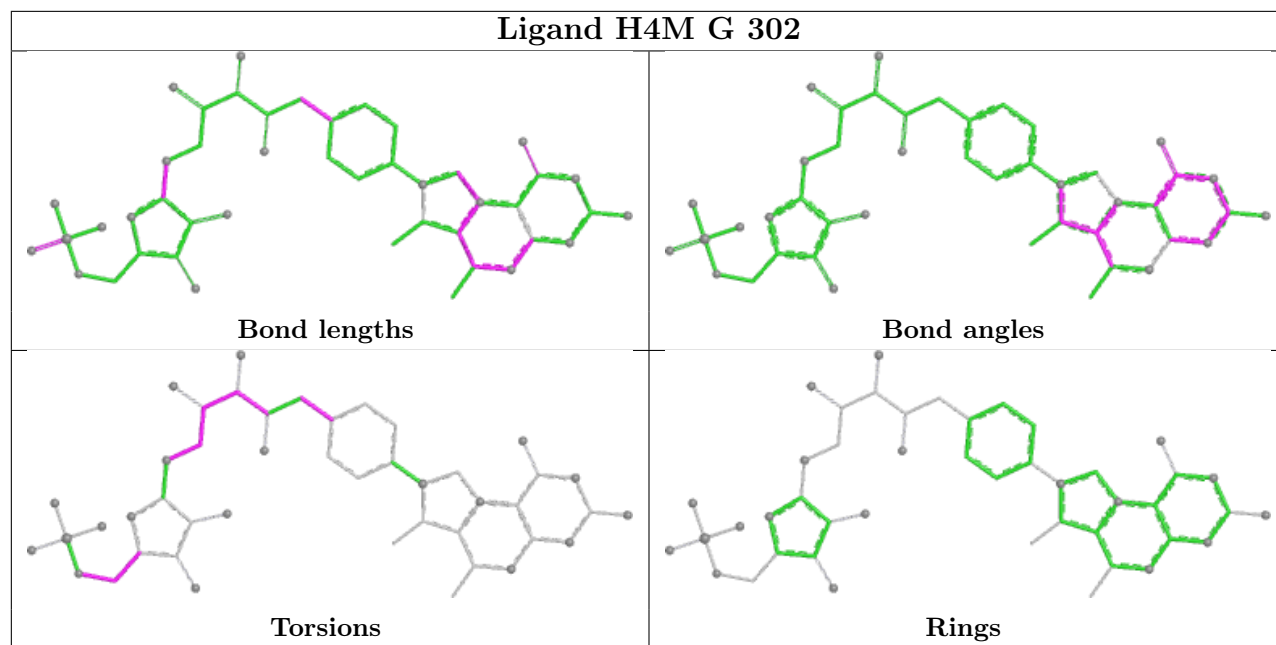
## Ligand H4M T 302











## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed      | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9  |
|-----|-------|---------------|--------|---------------|-----------------------|--------|
| 1   | A     | 287/288 (99%) | -0.14  | 0 100 100     | 16, 22, 35, 50        | 0      |
| 1   | B     | 287/288 (99%) | -0.11  | 3 (1%) 79 82  | 16, 22, 35, 56        | 0      |
| 1   | C     | 287/288 (99%) | 0.04   | 1 (0%) 90 91  | 15, 27, 45, 56        | 1 (0%) |
| 1   | D     | 287/288 (99%) | 0.08   | 1 (0%) 90 91  | 16, 26, 41, 57        | 1 (0%) |
| 1   | E     | 287/288 (99%) | -0.16  | 0 100 100     | 12, 22, 35, 49        | 1 (0%) |
| 1   | F     | 287/288 (99%) | -0.05  | 2 (0%) 84 87  | 16, 23, 36, 48        | 0      |
| 1   | G     | 287/288 (99%) | -0.23  | 1 (0%) 90 91  | 16, 22, 37, 46        | 0      |
| 1   | H     | 287/288 (99%) | -0.25  | 3 (1%) 79 82  | 11, 20, 33, 46        | 4 (1%) |
| 1   | I     | 287/288 (99%) | -0.04  | 2 (0%) 84 87  | 14, 25, 44, 55        | 1 (0%) |
| 1   | J     | 287/288 (99%) | -0.11  | 2 (0%) 84 87  | 18, 24, 37, 44        | 0      |
| 1   | K     | 287/288 (99%) | -0.07  | 0 100 100     | 15, 23, 37, 53        | 1 (0%) |
| 1   | L     | 287/288 (99%) | 0.16   | 0 100 100     | 20, 28, 48, 69        | 3 (1%) |
| 1   | M     | 287/288 (99%) | -0.26  | 2 (0%) 84 87  | 15, 20, 33, 52        | 0      |
| 1   | N     | 287/288 (99%) | -0.14  | 1 (0%) 90 91  | 12, 22, 36, 48        | 3 (1%) |
| 1   | O     | 287/288 (99%) | 0.07   | 2 (0%) 84 87  | 10, 27, 46, 60        | 1 (0%) |
| 1   | P     | 287/288 (99%) | 0.31   | 4 (1%) 73 77  | 18, 29, 45, 59        | 1 (0%) |
| 1   | Q     | 287/288 (99%) | -0.03  | 4 (1%) 73 77  | 16, 23, 38, 56        | 0      |
| 1   | R     | 287/288 (99%) | 0.50   | 5 (1%) 69 72  | 18, 34, 49, 64        | 3 (1%) |
| 1   | S     | 287/288 (99%) | 0.84   | 22 (7%) 19 21 | 24, 39, 54, 67        | 1 (0%) |
| 1   | T     | 287/288 (99%) | 0.14   | 0 100 100     | 20, 27, 39, 55        | 0      |
| 1   | U     | 287/288 (99%) | 0.80   | 15 (5%) 33 35 | 23, 39, 53, 65        | 1 (0%) |
| 1   | V     | 287/288 (99%) | 2.05   | 140 (48%) 0 0 | 24, 56, 82, 94        | 2 (0%) |
| 1   | W     | 287/288 (99%) | 0.25   | 4 (1%) 73 77  | 17, 28, 41, 59        | 2 (0%) |
| 1   | X     | 287/288 (99%) | 1.26   | 55 (19%) 3 3  | 28, 46, 70, 100       | 0      |

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| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2  |    |    | OWAB(Å <sup>2</sup> ) | Q<0.9   |
|-----|-------|-----------------|--------|----------|----|----|-----------------------|---------|
| All | All   | 6888/6912 (99%) | 0.21   | 269 (3%) | 43 | 47 | 10, 26, 52, 100       | 26 (0%) |

All (269) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | X     | 85  | PHE  | 7.9  |
| 1   | V     | 184 | ALA  | 6.2  |
| 1   | V     | 209 | TRP  | 5.7  |
| 1   | V     | 241 | TYR  | 5.7  |
| 1   | V     | 193 | VAL  | 5.7  |
| 1   | V     | 181 | ALA  | 5.5  |
| 1   | V     | 207 | ALA  | 5.4  |
| 1   | V     | 203 | LEU  | 5.0  |
| 1   | V     | 192 | PHE  | 5.0  |
| 1   | V     | 215 | ILE  | 5.0  |
| 1   | V     | 229 | ILE  | 5.0  |
| 1   | V     | 232 | ILE  | 4.9  |
| 1   | V     | 189 | GLY  | 4.9  |
| 1   | V     | 231 | GLY  | 4.9  |
| 1   | V     | 190 | ALA  | 4.9  |
| 1   | V     | 210 | GLN  | 4.6  |
| 1   | V     | 219 | ALA  | 4.6  |
| 1   | V     | 110 | VAL  | 4.6  |
| 1   | V     | 124 | VAL  | 4.6  |
| 1   | X     | 118 | VAL  | 4.5  |
| 1   | V     | 113 | ALA  | 4.5  |
| 1   | V     | 243 | GLY  | 4.4  |
| 1   | V     | 145 | ALA  | 4.4  |
| 1   | V     | 201 | LEU  | 4.3  |
| 1   | V     | 218 | VAL  | 4.3  |
| 1   | V     | 252 | ILE  | 4.3  |
| 1   | V     | 204 | LEU  | 4.3  |
| 1   | V     | 147 | VAL  | 4.3  |
| 1   | X     | 255 | LEU  | 4.2  |
| 1   | X     | 115 | GLY  | 4.2  |
| 1   | V     | 126 | LEU  | 4.1  |
| 1   | V     | 230 | GLY  | 4.1  |
| 1   | V     | 108 | ALA  | 4.1  |
| 1   | V     | 186 | ALA  | 4.1  |
| 1   | V     | 227 | LEU  | 4.0  |
| 1   | V     | 208 | ALA  | 4.0  |
| 1   | V     | 140 | LEU  | 4.0  |

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| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 1   | V     | 283    | LEU  | 3.9  |
| 1   | V     | 106    | GLY  | 3.9  |
| 1   | V     | 144    | GLY  | 3.9  |
| 1   | V     | 238    | GLY  | 3.9  |
| 1   | V     | 233    | ASP  | 3.9  |
| 1   | V     | 217    | ILE  | 3.9  |
| 1   | V     | 205    | PRO  | 3.8  |
| 1   | V     | 188    | LYS  | 3.8  |
| 1   | V     | 111    | VAL  | 3.8  |
| 1   | V     | 214    | SER  | 3.8  |
| 1   | V     | 172    | VAL  | 3.7  |
| 1   | V     | 177    | THR  | 3.7  |
| 1   | V     | 123    | ALA  | 3.7  |
| 1   | V     | 178    | ALA  | 3.7  |
| 1   | V     | 250    | LEU  | 3.7  |
| 1   | V     | 246    | ALA  | 3.7  |
| 1   | V     | 182[A] | SER  | 3.6  |
| 1   | V     | 247    | PHE  | 3.6  |
| 1   | V     | 125    | VAL  | 3.6  |
| 1   | V     | 109    | LEU  | 3.6  |
| 1   | V     | 187    | VAL  | 3.6  |
| 1   | V     | 175    | ALA  | 3.6  |
| 1   | V     | 185    | GLU  | 3.5  |
| 1   | V     | 221    | TYR  | 3.5  |
| 1   | X     | 88     | PHE  | 3.5  |
| 1   | V     | 149    | LEU  | 3.5  |
| 1   | X     | 113    | ALA  | 3.5  |
| 1   | F     | 242    | GLY  | 3.4  |
| 1   | P     | 85     | PHE  | 3.4  |
| 1   | V     | 154    | LEU  | 3.4  |
| 1   | V     | 199    | ILE  | 3.4  |
| 1   | X     | 120    | GLY  | 3.4  |
| 1   | V     | 248    | GLY  | 3.4  |
| 1   | V     | 180    | ASP  | 3.4  |
| 1   | X     | 170    | VAL  | 3.3  |
| 1   | V     | 150    | CYS  | 3.3  |
| 1   | V     | 242    | GLY  | 3.3  |
| 1   | V     | 173    | THR  | 3.3  |
| 1   | V     | 107    | VAL  | 3.3  |
| 1   | V     | 122    | LYS  | 3.3  |
| 1   | V     | 195    | THR  | 3.3  |
| 1   | V     | 213    | SER  | 3.3  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | V     | 141 | ALA  | 3.3  |
| 1   | V     | 157 | ALA  | 3.3  |
| 1   | V     | 174 | ALA  | 3.3  |
| 1   | V     | 137 | ALA  | 3.2  |
| 1   | V     | 146 | GLU  | 3.2  |
| 1   | V     | 151 | GLY  | 3.2  |
| 1   | V     | 130 | GLY  | 3.2  |
| 1   | V     | 253 | GLY  | 3.2  |
| 1   | X     | 144 | GLY  | 3.2  |
| 1   | V     | 257 | LEU  | 3.1  |
| 1   | V     | 105 | ALA  | 3.1  |
| 1   | V     | 114 | ALA  | 3.1  |
| 1   | U     | 201 | LEU  | 3.1  |
| 1   | X     | 201 | LEU  | 3.1  |
| 1   | I     | 2   | SER  | 3.1  |
| 1   | V     | 120 | GLY  | 3.1  |
| 1   | V     | 159 | ALA  | 3.1  |
| 1   | V     | 148 | VAL  | 3.1  |
| 1   | V     | 194 | PHE  | 3.1  |
| 1   | X     | 56  | LYS  | 3.1  |
| 1   | V     | 170 | VAL  | 3.0  |
| 1   | V     | 142 | GLY  | 3.0  |
| 1   | X     | 189 | GLY  | 3.0  |
| 1   | V     | 211 | ASN  | 3.0  |
| 1   | V     | 161 | ALA  | 3.0  |
| 1   | V     | 235 | THR  | 3.0  |
| 1   | X     | 173 | THR  | 3.0  |
| 1   | X     | 169 | LYS  | 3.0  |
| 1   | X     | 246 | ALA  | 3.0  |
| 1   | V     | 128 | GLY  | 3.0  |
| 1   | X     | 142 | GLY  | 3.0  |
| 1   | V     | 127 | ALA  | 2.9  |
| 1   | V     | 281 | TYR  | 2.9  |
| 1   | V     | 244 | LYS  | 2.9  |
| 1   | V     | 239 | LYS  | 2.9  |
| 1   | V     | 116 | GLY  | 2.9  |
| 1   | X     | 86  | GLY  | 2.9  |
| 1   | V     | 160 | ALA  | 2.9  |
| 1   | R     | 282 | LYS  | 2.9  |
| 1   | Q     | 180 | ASP  | 2.9  |
| 1   | X     | 110 | VAL  | 2.9  |
| 1   | I     | 201 | LEU  | 2.9  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | V     | 249 | ALA  | 2.8  |
| 1   | X     | 232 | ILE  | 2.8  |
| 1   | X     | 242 | GLY  | 2.8  |
| 1   | S     | 124 | VAL  | 2.8  |
| 1   | V     | 255 | LEU  | 2.8  |
| 1   | Q     | 181 | ALA  | 2.8  |
| 1   | V     | 136 | SER  | 2.8  |
| 1   | V     | 115 | GLY  | 2.8  |
| 1   | V     | 220 | ASP  | 2.8  |
| 1   | V     | 234 | ALA  | 2.8  |
| 1   | S     | 288 | ALA  | 2.7  |
| 1   | P     | 178 | ALA  | 2.7  |
| 1   | V     | 139 | LEU  | 2.7  |
| 1   | X     | 214 | SER  | 2.7  |
| 1   | V     | 118 | VAL  | 2.7  |
| 1   | S     | 178 | ALA  | 2.7  |
| 1   | X     | 111 | VAL  | 2.7  |
| 1   | X     | 2   | SER  | 2.7  |
| 1   | V     | 228 | GLY  | 2.6  |
| 1   | V     | 254 | GLY  | 2.6  |
| 1   | V     | 206 | GLN  | 2.6  |
| 1   | M     | 256 | LYS  | 2.6  |
| 1   | V     | 56  | LYS  | 2.6  |
| 1   | V     | 176 | GLU  | 2.6  |
| 1   | U     | 199 | ILE  | 2.6  |
| 1   | X     | 199 | ILE  | 2.6  |
| 1   | V     | 117 | SER  | 2.6  |
| 1   | X     | 58  | LYS  | 2.6  |
| 1   | V     | 212 | GLU  | 2.6  |
| 1   | R     | 243 | GLY  | 2.6  |
| 1   | V     | 155 | ASP  | 2.6  |
| 1   | X     | 243 | GLY  | 2.6  |
| 1   | V     | 216 | GLU  | 2.5  |
| 1   | V     | 236 | ASP  | 2.5  |
| 1   | V     | 196 | ALA  | 2.5  |
| 1   | X     | 217 | ILE  | 2.5  |
| 1   | V     | 152 | ARG  | 2.5  |
| 1   | X     | 257 | LEU  | 2.5  |
| 1   | V     | 133 | GLY  | 2.5  |
| 1   | X     | 254 | GLY  | 2.5  |
| 1   | V     | 191 | HIS  | 2.5  |
| 1   | B     | 199 | ILE  | 2.5  |

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| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 1   | H     | 199    | ILE  | 2.5  |
| 1   | P     | 243    | GLY  | 2.5  |
| 1   | V     | 168    | PHE  | 2.5  |
| 1   | X     | 116    | GLY  | 2.4  |
| 1   | X     | 251    | GLY  | 2.4  |
| 1   | O     | 155    | ASP  | 2.4  |
| 1   | X     | 168    | PHE  | 2.4  |
| 1   | X     | 57     | GLU  | 2.4  |
| 1   | S     | 172    | VAL  | 2.4  |
| 1   | S     | 218    | VAL  | 2.4  |
| 1   | S     | 207    | ALA  | 2.4  |
| 1   | S     | 219    | ALA  | 2.4  |
| 1   | V     | 288    | ALA  | 2.4  |
| 1   | V     | 258    | LYS  | 2.4  |
| 1   | U     | 242    | GLY  | 2.4  |
| 1   | U     | 171    | ASN  | 2.4  |
| 1   | V     | 226    | PRO  | 2.4  |
| 1   | X     | 129    | THR  | 2.4  |
| 1   | H     | 85     | PHE  | 2.4  |
| 1   | W     | 85     | PHE  | 2.4  |
| 1   | X     | 84     | PHE  | 2.4  |
| 1   | S     | 209    | TRP  | 2.4  |
| 1   | S     | 208    | ALA  | 2.4  |
| 1   | V     | 158    | GLN  | 2.4  |
| 1   | V     | 153    | LYS  | 2.4  |
| 1   | X     | 140    | LEU  | 2.4  |
| 1   | X     | 282    | LYS  | 2.4  |
| 1   | X     | 60     | SER  | 2.3  |
| 1   | Q     | 185    | GLU  | 2.3  |
| 1   | Q     | 184    | ALA  | 2.3  |
| 1   | X     | 288    | ALA  | 2.3  |
| 1   | S     | 187    | VAL  | 2.3  |
| 1   | V     | 171    | ASN  | 2.3  |
| 1   | U     | 120    | GLY  | 2.3  |
| 1   | V     | 259    | LEU  | 2.3  |
| 1   | X     | 50     | ILE  | 2.3  |
| 1   | X     | 250    | LEU  | 2.3  |
| 1   | J     | 256    | LYS  | 2.3  |
| 1   | R     | 169    | LYS  | 2.3  |
| 1   | U     | 268    | PHE  | 2.3  |
| 1   | D     | 171[A] | ASN  | 2.3  |
| 1   | X     | 171    | ASN  | 2.3  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | S     | 173 | THR  | 2.3  |
| 1   | N     | 116 | GLY  | 2.3  |
| 1   | S     | 243 | GLY  | 2.3  |
| 1   | V     | 245 | ARG  | 2.3  |
| 1   | U     | 56  | LYS  | 2.3  |
| 1   | R     | 199 | ILE  | 2.3  |
| 1   | X     | 283 | LEU  | 2.3  |
| 1   | W     | 2   | SER  | 2.3  |
| 1   | X     | 223 | ALA  | 2.2  |
| 1   | V     | 222 | ASN  | 2.2  |
| 1   | X     | 87  | PRO  | 2.2  |
| 1   | U     | 118 | VAL  | 2.2  |
| 1   | O     | 201 | LEU  | 2.2  |
| 1   | S     | 215 | ILE  | 2.2  |
| 1   | X     | 281 | TYR  | 2.2  |
| 1   | W     | 180 | ASP  | 2.2  |
| 1   | S     | 146 | GLU  | 2.2  |
| 1   | M     | 82  | LYS  | 2.2  |
| 1   | V     | 102 | THR  | 2.2  |
| 1   | S     | 168 | PHE  | 2.2  |
| 1   | X     | 147 | VAL  | 2.2  |
| 1   | W     | 185 | GLU  | 2.2  |
| 1   | S     | 241 | TYR  | 2.2  |
| 1   | V     | 104 | ALA  | 2.2  |
| 1   | X     | 108 | ALA  | 2.2  |
| 1   | V     | 119 | LYS  | 2.2  |
| 1   | S     | 115 | GLY  | 2.2  |
| 1   | H     | 206 | GLN  | 2.2  |
| 1   | B     | 85  | PHE  | 2.2  |
| 1   | C     | 180 | ASP  | 2.2  |
| 1   | U     | 58  | LYS  | 2.2  |
| 1   | U     | 119 | LYS  | 2.2  |
| 1   | X     | 109 | LEU  | 2.1  |
| 1   | V     | 183 | ARG  | 2.1  |
| 1   | S     | 192 | PHE  | 2.1  |
| 1   | V     | 164 | VAL  | 2.1  |
| 1   | X     | 55  | GLY  | 2.1  |
| 1   | S     | 127 | ALA  | 2.1  |
| 1   | V     | 103 | ALA  | 2.1  |
| 1   | V     | 198 | ALA  | 2.1  |
| 1   | J     | 287 | MET  | 2.1  |
| 1   | P     | 241 | TYR  | 2.1  |

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| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 1   | B     | 56     | LYS  | 2.1  |
| 1   | R     | 115    | GLY  | 2.1  |
| 1   | S     | 193    | VAL  | 2.1  |
| 1   | S     | 223    | ALA  | 2.1  |
| 1   | U     | 92     | CYS  | 2.1  |
| 1   | U     | 239    | LYS  | 2.1  |
| 1   | X     | 165    | ASN  | 2.1  |
| 1   | V     | 129    | THR  | 2.0  |
| 1   | U     | 265    | ALA  | 2.0  |
| 1   | U     | 154    | LEU  | 2.0  |
| 1   | X     | 154    | LEU  | 2.0  |
| 1   | V     | 280    | ILE  | 2.0  |
| 1   | X     | 241    | TYR  | 2.0  |
| 1   | V     | 200    | GLY  | 2.0  |
| 1   | X     | 238    | GLY  | 2.0  |
| 1   | F     | 169    | LYS  | 2.0  |
| 1   | V     | 121    | LYS  | 2.0  |
| 1   | X     | 39     | PRO  | 2.0  |
| 1   | V     | 279[A] | GLU  | 2.0  |
| 1   | G     | 85     | PHE  | 2.0  |
| 1   | S     | 154    | LEU  | 2.0  |
| 1   | U     | 267    | LEU  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 3   | H4M  | F     | 302 | 45/54 | 0.67 | 0.23 | 20,39,43,47                | 45    |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 3   | H4M  | U     | 302 | 45/54 | 0.70 | 0.25 | 49,56,58,59                 | 45    |
| 3   | H4M  | L     | 302 | 45/54 | 0.72 | 0.25 | 33,42,48,49                 | 45    |
| 3   | H4M  | C     | 302 | 45/54 | 0.72 | 0.18 | 22,33,46,48                 | 45    |
| 3   | H4M  | R     | 302 | 45/54 | 0.73 | 0.21 | 30,45,60,61                 | 45    |
| 3   | H4M  | V     | 302 | 45/54 | 0.74 | 0.18 | 39,44,56,58                 | 45    |
| 3   | H4M  | O     | 302 | 45/54 | 0.76 | 0.23 | 28,42,47,49                 | 45    |
| 3   | H4M  | S     | 302 | 45/54 | 0.77 | 0.20 | 39,45,57,57                 | 45    |
| 3   | H4M  | I     | 302 | 45/54 | 0.77 | 0.19 | 23,38,45,47                 | 45    |
| 3   | H4M  | N     | 302 | 45/54 | 0.77 | 0.28 | 46,58,60,61                 | 45    |
| 3   | H4M  | X     | 302 | 45/54 | 0.77 | 0.20 | 27,61,80,81                 | 45    |
| 3   | H4M  | W     | 302 | 45/54 | 0.78 | 0.18 | 28,37,50,51                 | 45    |
| 3   | H4M  | Q     | 302 | 45/54 | 0.80 | 0.20 | 41,47,60,62                 | 45    |
| 3   | H4M  | D     | 301 | 45/54 | 0.81 | 0.17 | 30,41,74,74                 | 0     |
| 3   | H4M  | K     | 302 | 45/54 | 0.81 | 0.18 | 20,35,41,44                 | 45    |
| 2   | NAP  | W     | 301 | 48/48 | 0.83 | 0.39 | 72,82,92,95                 | 0     |
| 3   | H4M  | P     | 302 | 45/54 | 0.84 | 0.15 | 21,33,55,57                 | 45    |
| 3   | H4M  | H     | 302 | 45/54 | 0.85 | 0.16 | 18,26,39,43                 | 45    |
| 3   | H4M  | B     | 302 | 45/54 | 0.85 | 0.17 | 16,24,36,37                 | 45    |
| 2   | NAP  | V     | 301 | 48/48 | 0.86 | 0.14 | 43,47,51,52                 | 0     |
| 3   | H4M  | T     | 302 | 45/54 | 0.87 | 0.18 | 43,47,53,54                 | 45    |
| 3   | H4M  | J     | 302 | 45/54 | 0.88 | 0.13 | 20,32,56,58                 | 0     |
| 3   | H4M  | G     | 302 | 45/54 | 0.88 | 0.14 | 23,34,60,63                 | 0     |
| 3   | H4M  | M     | 302 | 45/54 | 0.89 | 0.14 | 21,32,67,69                 | 0     |
| 3   | H4M  | E     | 302 | 45/54 | 0.90 | 0.15 | 30,42,46,47                 | 45    |
| 3   | H4M  | A     | 302 | 45/54 | 0.91 | 0.11 | 17,26,54,57                 | 0     |
| 2   | NAP  | S     | 301 | 48/48 | 0.91 | 0.13 | 40,48,53,57                 | 0     |
| 2   | NAP  | E     | 301 | 48/48 | 0.92 | 0.15 | 30,38,46,49                 | 0     |
| 2   | NAP  | U     | 301 | 48/48 | 0.92 | 0.13 | 42,54,60,60                 | 0     |
| 2   | NAP  | L     | 301 | 48/48 | 0.94 | 0.11 | 39,42,50,53                 | 0     |
| 2   | NAP  | O     | 301 | 48/48 | 0.94 | 0.11 | 33,42,53,55                 | 0     |
| 4   | SO4  | H     | 303 | 5/5   | 0.94 | 0.11 | 36,45,47,56                 | 0     |
| 4   | SO4  | P     | 303 | 5/5   | 0.94 | 0.10 | 40,43,47,53                 | 0     |
| 4   | SO4  | V     | 303 | 5/5   | 0.94 | 0.11 | 45,46,56,60                 | 0     |
| 2   | NAP  | T     | 301 | 48/48 | 0.95 | 0.11 | 28,38,46,46                 | 0     |
| 2   | NAP  | X     | 301 | 48/48 | 0.95 | 0.08 | 25,34,49,63                 | 0     |
| 4   | SO4  | A     | 303 | 5/5   | 0.95 | 0.10 | 35,43,45,51                 | 0     |
| 2   | NAP  | G     | 301 | 48/48 | 0.96 | 0.08 | 20,27,35,38                 | 0     |
| 4   | SO4  | D     | 303 | 5/5   | 0.96 | 0.08 | 34,38,40,46                 | 0     |
| 2   | NAP  | Q     | 301 | 48/48 | 0.96 | 0.10 | 23,29,37,45                 | 0     |
| 4   | SO4  | J     | 303 | 5/5   | 0.96 | 0.10 | 38,46,55,55                 | 0     |
| 4   | SO4  | M     | 303 | 5/5   | 0.96 | 0.10 | 33,35,46,50                 | 0     |
| 2   | NAP  | J     | 301 | 48/48 | 0.96 | 0.10 | 22,33,39,41                 | 0     |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 4   | SO4  | S     | 303 | 5/5   | 0.96 | 0.10 | 42,43,57,57                 | 0     |
| 2   | NAP  | A     | 301 | 48/48 | 0.96 | 0.09 | 20,31,36,38                 | 0     |
| 2   | NAP  | N     | 301 | 48/48 | 0.97 | 0.08 | 24,27,36,41                 | 0     |
| 2   | NAP  | R     | 301 | 48/48 | 0.97 | 0.06 | 24,31,36,41                 | 0     |
| 2   | NAP  | F     | 301 | 48/48 | 0.97 | 0.07 | 20,27,33,36                 | 0     |
| 2   | NAP  | P     | 301 | 48/48 | 0.97 | 0.07 | 25,28,35,36                 | 0     |
| 2   | NAP  | H     | 301 | 48/48 | 0.98 | 0.05 | 16,19,25,32                 | 0     |
| 2   | NAP  | I     | 301 | 48/48 | 0.98 | 0.06 | 21,26,33,36                 | 0     |
| 2   | NAP  | B     | 301 | 48/48 | 0.98 | 0.05 | 18,23,28,37                 | 0     |
| 2   | NAP  | K     | 301 | 48/48 | 0.98 | 0.05 | 18,23,31,38                 | 0     |
| 2   | NAP  | C     | 301 | 48/48 | 0.98 | 0.06 | 23,29,33,39                 | 0     |
| 2   | NAP  | M     | 301 | 48/48 | 0.98 | 0.05 | 15,19,25,26                 | 0     |
| 2   | NAP  | D     | 302 | 48/48 | 0.98 | 0.05 | 18,24,29,33                 | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.