



## Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 07:12 AM JST

PDB ID : 7VH6 / pdb\_00007vh6  
EMDB ID : EMD-31988  
Title : Cryo-EM structure of the hexameric plasma membrane H<sup>+</sup>-ATPase in the active state (pH 6.0, BeF<sub>3</sub><sup>-</sup>, conformation 1, C1 symmetry)  
Authors : Zhao, P.; Zhao, C.; Chen, D.; Yun, C.; Li, H.; Bai, L.  
Deposited on : 2021-09-21  
Resolution : 3.80 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

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

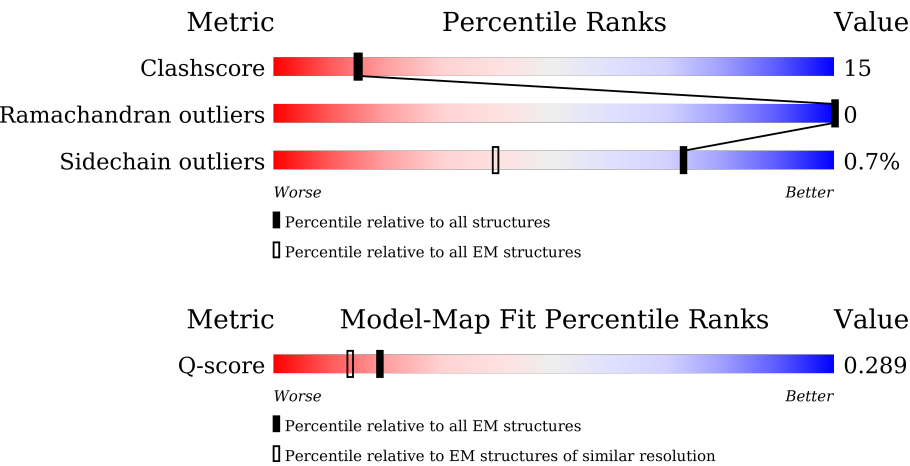
EMDB validation analysis : 0.0.1.dev133  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.50

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 3.80 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) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 10198 ( 3.30 - 4.30 )                                    |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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 EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain                                                                          |
|-----|-------|--------|-------------------------------------------------------------------------------------------|
| 1   | A     | 918    | <div><div>10%</div><div><div></div><div>60%</div><div>23%</div><div>16%</div></div></div> |
| 1   | B     | 918    | <div><div>16%</div><div><div></div><div>60%</div><div>23%</div><div>16%</div></div></div> |
| 1   | C     | 918    | <div><div>29%</div><div><div></div><div>60%</div><div>24%</div><div>16%</div></div></div> |
| 1   | D     | 918    | <div><div>44%</div><div><div></div><div>60%</div><div>23%</div><div>16%</div></div></div> |

Continued on next page...

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | E     | 918    |                  |
| 1   | F     | 918    |                  |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 2   | BEF  | A     | 1001 | -         | -        | X       | -                |
| 2   | BEF  | B     | 1001 | -         | -        | X       | -                |
| 2   | BEF  | C     | 1001 | -         | -        | X       | -                |
| 2   | BEF  | D     | 1001 | -         | -        | X       | -                |
| 2   | BEF  | E     | 1001 | -         | -        | X       | -                |
| 2   | BEF  | F     | 1001 | -         | -        | X       | -                |

## 2 Entry composition [i](#)

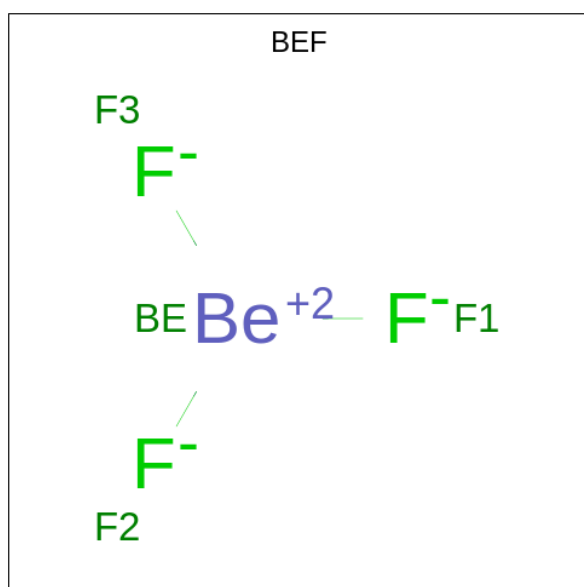
There are 3 unique types of molecules in this entry. The entry contains 38202 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Plasma membrane ATPase 1.

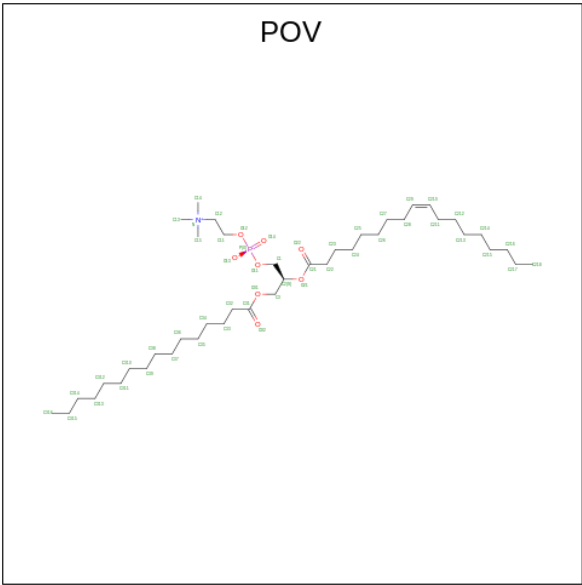
| Mol | Chain | Residues | Atoms |      |     |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|----|---------|-------|
| 1   | A     | 768      | Total | C    | N   | O    | S  | 0       | 0     |
|     |       |          | 5869  | 3802 | 967 | 1073 | 27 |         |       |
| 1   | B     | 768      | Total | C    | N   | O    | S  | 0       | 0     |
|     |       |          | 5869  | 3802 | 967 | 1073 | 27 |         |       |
| 1   | C     | 768      | Total | C    | N   | O    | S  | 0       | 0     |
|     |       |          | 5869  | 3802 | 967 | 1073 | 27 |         |       |
| 1   | D     | 768      | Total | C    | N   | O    | S  | 0       | 0     |
|     |       |          | 5869  | 3802 | 967 | 1073 | 27 |         |       |
| 1   | E     | 768      | Total | C    | N   | O    | S  | 0       | 0     |
|     |       |          | 5869  | 3802 | 967 | 1073 | 27 |         |       |
| 1   | F     | 768      | Total | C    | N   | O    | S  | 0       | 0     |
|     |       |          | 5869  | 3802 | 967 | 1073 | 27 |         |       |

- Molecule 2 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 2   | A     | 1        | Total | Be | F | 0       |
|     |       |          | 4     | 1  | 3 |         |
| 2   | B     | 1        | Total | Be | F | 0       |
|     |       |          | 4     | 1  | 3 |         |
| 2   | C     | 1        | Total | Be | F | 0       |
|     |       |          | 4     | 1  | 3 |         |
| 2   | D     | 1        | Total | Be | F | 0       |
|     |       |          | 4     | 1  | 3 |         |
| 2   | E     | 1        | Total | Be | F | 0       |
|     |       |          | 4     | 1  | 3 |         |
| 2   | F     | 1        | Total | Be | F | 0       |
|     |       |          | 4     | 1  | 3 |         |

- Molecule 3 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (CCD ID: POV) (formula: C<sub>42</sub>H<sub>82</sub>NO<sub>8</sub>P) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 3   | A     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 52    | 42 | 1 | 8 | 1 |         |
| 3   | A     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 52    | 42 | 1 | 8 | 1 |         |
| 3   | A     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 52    | 42 | 1 | 8 | 1 |         |
| 3   | A     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 52    | 42 | 1 | 8 | 1 |         |
| 3   | A     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 52    | 42 | 1 | 8 | 1 |         |

Continued on next page...

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 3   | A     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 52    | 42 | 1 | 8 | 1 |         |
| 3   | A     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 52    | 42 | 1 | 8 | 1 |         |
| 3   | A     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 52    | 42 | 1 | 8 | 1 |         |
| 3   | A     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 52    | 42 | 1 | 8 | 1 |         |
| 3   | A     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 52    | 42 | 1 | 8 | 1 |         |
| 3   | B     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 52    | 42 | 1 | 8 | 1 |         |
| 3   | B     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 52    | 42 | 1 | 8 | 1 |         |
| 3   | B     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 52    | 42 | 1 | 8 | 1 |         |
| 3   | B     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 52    | 42 | 1 | 8 | 1 |         |
| 3   | B     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 52    | 42 | 1 | 8 | 1 |         |
| 3   | B     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 52    | 42 | 1 | 8 | 1 |         |
| 3   | B     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 52    | 42 | 1 | 8 | 1 |         |
| 3   | B     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 52    | 42 | 1 | 8 | 1 |         |
| 3   | C     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 52    | 42 | 1 | 8 | 1 |         |
| 3   | C     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 52    | 42 | 1 | 8 | 1 |         |
| 3   | C     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 52    | 42 | 1 | 8 | 1 |         |
| 3   | C     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 52    | 42 | 1 | 8 | 1 |         |
| 3   | C     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 52    | 42 | 1 | 8 | 1 |         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 3   | C     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 52    | 42 | 1 | 8 | 1 |         |
| 3   | C     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 52    | 42 | 1 | 8 | 1 |         |
| 3   | C     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 52    | 42 | 1 | 8 | 1 |         |
| 3   | D     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 52    | 42 | 1 | 8 | 1 |         |
| 3   | D     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 52    | 42 | 1 | 8 | 1 |         |
| 3   | D     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 52    | 42 | 1 | 8 | 1 |         |
| 3   | D     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 52    | 42 | 1 | 8 | 1 |         |
| 3   | D     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 52    | 42 | 1 | 8 | 1 |         |
| 3   | D     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 52    | 42 | 1 | 8 | 1 |         |
| 3   | D     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 52    | 42 | 1 | 8 | 1 |         |
| 3   | D     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 52    | 42 | 1 | 8 | 1 |         |
| 3   | D     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 52    | 42 | 1 | 8 | 1 |         |
| 3   | E     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 52    | 42 | 1 | 8 | 1 |         |
| 3   | E     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 52    | 42 | 1 | 8 | 1 |         |
| 3   | E     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 52    | 42 | 1 | 8 | 1 |         |
| 3   | E     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 52    | 42 | 1 | 8 | 1 |         |
| 3   | E     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 52    | 42 | 1 | 8 | 1 |         |
| 3   | E     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 52    | 42 | 1 | 8 | 1 |         |
| 3   | E     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 52    | 42 | 1 | 8 | 1 |         |

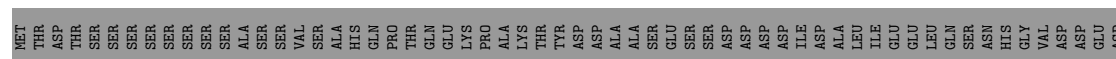
*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 3   | E     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 52    | 42 | 1 | 8 | 1 |         |
| 3   | F     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 52    | 42 | 1 | 8 | 1 |         |
| 3   | F     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 52    | 42 | 1 | 8 | 1 |         |
| 3   | F     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 52    | 42 | 1 | 8 | 1 |         |
| 3   | F     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 52    | 42 | 1 | 8 | 1 |         |
| 3   | F     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 52    | 42 | 1 | 8 | 1 |         |
| 3   | F     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 52    | 42 | 1 | 8 | 1 |         |
| 3   | F     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 52    | 42 | 1 | 8 | 1 |         |



Chain B: 











## 4 Experimental information

| Property                             | Value                     | Source    |
|--------------------------------------|---------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE           | Depositor |
| Imposed symmetry                     | POINT, Not provided       |           |
| Number of particles used             | 63661                     | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF         | Depositor |
| CTF correction method                | NONE                      | Depositor |
| Microscope                           | FEI TITAN KRIOS           | Depositor |
| Voltage (kV)                         | 300                       | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 1.6                       | Depositor |
| Minimum defocus (nm)                 | Not provided              |           |
| Maximum defocus (nm)                 | Not provided              |           |
| Magnification                        | Not provided              |           |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k) | Depositor |
| Maximum map value                    | 0.060                     | Depositor |
| Minimum map value                    | -0.035                    | Depositor |
| Average map value                    | 0.000                     | Depositor |
| Map value standard deviation         | 0.002                     | Depositor |
| Recommended contour level            | 0.012                     | Depositor |
| Map size ( $\text{\AA}$ )            | 312.0, 312.0, 312.0       | wwPDB     |
| Map dimensions                       | 300, 300, 300             | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0          | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.04, 1.04, 1.04          | Depositor |

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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     | 0.28         | 1/5989 (0.0%)  | 0.55        | 4/8141 (0.0%)   |
| 1   | B     | 0.28         | 1/5989 (0.0%)  | 0.55        | 4/8141 (0.0%)   |
| 1   | C     | 0.28         | 1/5989 (0.0%)  | 0.55        | 4/8141 (0.0%)   |
| 1   | D     | 0.28         | 1/5989 (0.0%)  | 0.55        | 4/8141 (0.0%)   |
| 1   | E     | 0.28         | 1/5989 (0.0%)  | 0.55        | 4/8141 (0.0%)   |
| 1   | F     | 0.28         | 1/5989 (0.0%)  | 0.55        | 4/8141 (0.0%)   |
| All | All   | 0.28         | 6/35934 (0.0%) | 0.55        | 24/48846 (0.0%) |

All (6) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 1   | B     | 198 | PRO  | CG-CD | -10.91 | 1.13        | 1.50     |
| 1   | F     | 198 | PRO  | CG-CD | -10.91 | 1.13        | 1.50     |
| 1   | D     | 198 | PRO  | CG-CD | -10.90 | 1.13        | 1.50     |
| 1   | E     | 198 | PRO  | CG-CD | -10.89 | 1.13        | 1.50     |
| 1   | A     | 198 | PRO  | CG-CD | -10.89 | 1.13        | 1.50     |
| 1   | C     | 198 | PRO  | CG-CD | -10.86 | 1.13        | 1.50     |

All (24) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1   | C     | 198 | PRO  | N-CD-CG | -12.83 | 83.96       | 103.20   |
| 1   | A     | 198 | PRO  | N-CD-CG | -12.82 | 83.97       | 103.20   |
| 1   | F     | 198 | PRO  | N-CD-CG | -12.81 | 83.98       | 103.20   |
| 1   | E     | 198 | PRO  | N-CD-CG | -12.81 | 83.99       | 103.20   |
| 1   | B     | 198 | PRO  | N-CD-CG | -12.80 | 84.00       | 103.20   |
| 1   | D     | 198 | PRO  | N-CD-CG | -12.78 | 84.04       | 103.20   |
| 1   | D     | 198 | PRO  | CA-N-CD | -8.64  | 99.90       | 112.00   |
| 1   | A     | 198 | PRO  | CA-N-CD | -8.64  | 99.91       | 112.00   |
| 1   | B     | 198 | PRO  | CA-N-CD | -8.64  | 99.91       | 112.00   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | E     | 198 | PRO  | CA-N-CD  | -8.63 | 99.92       | 112.00   |
| 1   | F     | 198 | PRO  | CA-N-CD  | -8.62 | 99.93       | 112.00   |
| 1   | C     | 198 | PRO  | CA-N-CD  | -8.59 | 99.98       | 112.00   |
| 1   | F     | 211 | PRO  | CA-N-CD  | -7.62 | 101.33      | 112.00   |
| 1   | A     | 211 | PRO  | CA-N-CD  | -7.62 | 101.34      | 112.00   |
| 1   | C     | 211 | PRO  | CA-N-CD  | -7.62 | 101.34      | 112.00   |
| 1   | B     | 211 | PRO  | CA-N-CD  | -7.61 | 101.34      | 112.00   |
| 1   | D     | 211 | PRO  | CA-N-CD  | -7.61 | 101.35      | 112.00   |
| 1   | E     | 211 | PRO  | CA-N-CD  | -7.60 | 101.36      | 112.00   |
| 1   | B     | 198 | PRO  | CA-CB-CG | -7.36 | 90.52       | 104.50   |
| 1   | A     | 198 | PRO  | CA-CB-CG | -7.35 | 90.54       | 104.50   |
| 1   | D     | 198 | PRO  | CA-CB-CG | -7.34 | 90.54       | 104.50   |
| 1   | C     | 198 | PRO  | CA-CB-CG | -7.34 | 90.56       | 104.50   |
| 1   | F     | 198 | PRO  | CA-CB-CG | -7.34 | 90.56       | 104.50   |
| 1   | E     | 198 | PRO  | CA-CB-CG | -7.33 | 90.58       | 104.50   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in 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     | 5869  | 0        | 5973     | 185     | 0            |
| 1   | B     | 5869  | 0        | 5973     | 184     | 0            |
| 1   | C     | 5869  | 0        | 5973     | 200     | 0            |
| 1   | D     | 5869  | 0        | 5973     | 194     | 0            |
| 1   | E     | 5869  | 0        | 5973     | 176     | 0            |
| 1   | F     | 5869  | 0        | 5973     | 191     | 0            |
| 2   | A     | 4     | 0        | 0        | 3       | 0            |
| 2   | B     | 4     | 0        | 0        | 3       | 0            |
| 2   | C     | 4     | 0        | 0        | 3       | 0            |
| 2   | D     | 4     | 0        | 0        | 3       | 0            |
| 2   | E     | 4     | 0        | 0        | 3       | 0            |
| 2   | F     | 4     | 0        | 0        | 3       | 0            |
| 3   | A     | 572   | 0        | 900      | 67      | 0            |
| 3   | B     | 468   | 0        | 736      | 48      | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3   | C     | 468   | 0        | 734      | 58      | 0            |
| 3   | D     | 520   | 0        | 818      | 55      | 0            |
| 3   | E     | 468   | 0        | 736      | 45      | 0            |
| 3   | F     | 468   | 0        | 736      | 45      | 0            |
| All | All   | 38202 | 0        | 40498    | 1173    | 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 15.

All (1173) 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) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:400:SER:O    | 1:C:404:LEU:HG    | 1.23                     | 1.32              |
| 1:F:400:SER:O    | 1:F:404:LEU:HG    | 1.21                     | 1.30              |
| 1:D:400:SER:O    | 1:D:404:LEU:HG    | 1.23                     | 1.29              |
| 1:B:400:SER:O    | 1:B:404:LEU:HG    | 1.24                     | 1.28              |
| 1:F:315:ARG:NE   | 3:F:1002:POV:O13  | 1.67                     | 1.28              |
| 1:A:400:SER:O    | 1:A:404:LEU:HG    | 1.23                     | 1.27              |
| 1:E:400:SER:O    | 1:E:404:LEU:HG    | 1.23                     | 1.26              |
| 1:B:315:ARG:NE   | 3:B:1004:POV:O13  | 1.68                     | 1.25              |
| 1:A:315:ARG:NE   | 3:A:1003:POV:O13  | 1.70                     | 1.22              |
| 1:E:316:THR:CG2  | 1:F:783:GLY:H     | 1.52                     | 1.20              |
| 1:C:316:THR:CG2  | 1:D:783:GLY:H     | 1.58                     | 1.16              |
| 1:E:315:ARG:NE   | 3:E:1003:POV:O13  | 1.80                     | 1.14              |
| 1:A:316:THR:CG2  | 1:B:783:GLY:H     | 1.60                     | 1.13              |
| 1:D:768:ILE:HD12 | 3:D:1004:POV:H21J | 1.16                     | 1.10              |
| 1:C:768:ILE:HD12 | 3:C:1004:POV:H21J | 1.28                     | 1.09              |
| 1:A:781:LYS:O    | 1:F:316:THR:HG21  | 1.51                     | 1.09              |
| 1:A:783:GLY:H    | 1:F:316:THR:CG2   | 1.66                     | 1.07              |
| 1:E:316:THR:HG21 | 1:F:781:LYS:O     | 1.55                     | 1.05              |
| 1:B:316:THR:HG21 | 1:C:781:LYS:O     | 1.57                     | 1.03              |
| 1:D:316:THR:HG21 | 1:E:781:LYS:O     | 1.60                     | 1.02              |
| 1:D:316:THR:CG2  | 1:E:783:GLY:H     | 1.74                     | 1.00              |
| 1:B:316:THR:CG2  | 1:C:783:GLY:H     | 1.74                     | 1.00              |
| 1:D:400:SER:HB3  | 1:D:403:ASP:HB3   | 1.44                     | 0.98              |
| 1:F:400:SER:HB3  | 1:F:403:ASP:HB3   | 1.46                     | 0.98              |
| 1:C:400:SER:HB3  | 1:C:403:ASP:HB3   | 1.43                     | 0.96              |
| 1:E:316:THR:CG2  | 1:F:783:GLY:N     | 2.30                     | 0.95              |
| 1:E:768:ILE:HD13 | 3:E:1004:POV:H31D | 1.50                     | 0.93              |
| 1:A:400:SER:HB3  | 1:A:403:ASP:HB3   | 1.46                     | 0.93              |
| 1:A:316:THR:HG21 | 1:B:781:LYS:O     | 1.67                     | 0.92              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:E:768:ILE:CD1  | 3:E:1004:POV:H31D | 2.00                     | 0.92              |
| 1:C:316:THR:HG21 | 1:D:781:LYS:O     | 1.68                     | 0.92              |
| 1:C:306:LEU:CD1  | 1:D:868:VAL:CG2   | 2.48                     | 0.92              |
| 1:D:315:ARG:HB3  | 3:D:1002:POV:H14B | 1.50                     | 0.90              |
| 1:E:400:SER:HB3  | 1:E:403:ASP:HB3   | 1.53                     | 0.90              |
| 1:C:315:ARG:NH1  | 3:C:1003:POV:O13  | 2.05                     | 0.90              |
| 1:E:314:TYR:O    | 1:F:779:LEU:HD22  | 1.72                     | 0.89              |
| 1:C:316:THR:CG2  | 1:D:783:GLY:N     | 2.35                     | 0.89              |
| 1:E:313:PHE:O    | 1:F:783:GLY:O     | 1.91                     | 0.89              |
| 1:A:316:THR:HG22 | 1:B:783:GLY:H     | 1.35                     | 0.89              |
| 1:D:315:ARG:NH1  | 3:D:1003:POV:O13  | 2.05                     | 0.88              |
| 1:A:314:TYR:O    | 1:B:779:LEU:HD22  | 1.75                     | 0.87              |
| 1:A:779:LEU:HD22 | 1:F:314:TYR:O     | 1.73                     | 0.87              |
| 1:B:768:ILE:CD1  | 3:B:1005:POV:H31D | 2.05                     | 0.86              |
| 1:C:712:ILE:HG13 | 3:C:1003:POV:H32A | 1.55                     | 0.86              |
| 1:F:400:SER:CB   | 1:F:403:ASP:HB3   | 2.04                     | 0.86              |
| 1:B:768:ILE:HD13 | 3:B:1005:POV:H31D | 1.58                     | 0.86              |
| 1:F:768:ILE:HD13 | 3:F:1003:POV:H31D | 1.57                     | 0.86              |
| 1:C:315:ARG:HB3  | 3:C:1002:POV:H14B | 1.56                     | 0.86              |
| 1:A:783:GLY:H    | 1:F:316:THR:HG22  | 1.41                     | 0.85              |
| 1:C:306:LEU:HD11 | 1:D:868:VAL:HG23  | 1.58                     | 0.85              |
| 1:E:316:THR:HG22 | 1:F:783:GLY:N     | 1.92                     | 0.85              |
| 1:C:768:ILE:CD1  | 3:C:1004:POV:H31D | 2.06                     | 0.85              |
| 1:E:400:SER:CB   | 1:E:403:ASP:HB3   | 2.07                     | 0.84              |
| 1:A:768:ILE:CD1  | 3:A:1004:POV:H31D | 2.08                     | 0.84              |
| 1:A:316:THR:CG2  | 1:B:783:GLY:N     | 2.41                     | 0.83              |
| 1:A:314:TYR:O    | 1:B:779:LEU:CD2   | 2.27                     | 0.83              |
| 1:A:783:GLY:O    | 1:F:313:PHE:O     | 1.97                     | 0.83              |
| 1:B:400:SER:HB3  | 1:B:403:ASP:HB3   | 1.58                     | 0.83              |
| 1:C:400:SER:CB   | 1:C:403:ASP:HB3   | 2.08                     | 0.82              |
| 1:A:316:THR:HG22 | 1:B:783:GLY:N     | 1.92                     | 0.82              |
| 1:A:400:SER:CB   | 1:A:403:ASP:HB3   | 2.08                     | 0.82              |
| 1:E:306:LEU:CD1  | 1:F:868:VAL:CG2   | 2.57                     | 0.82              |
| 1:C:314:TYR:O    | 1:D:779:LEU:HD22  | 1.77                     | 0.82              |
| 1:F:768:ILE:CD1  | 3:F:1003:POV:H31D | 2.09                     | 0.82              |
| 1:E:316:THR:HG23 | 1:F:783:GLY:H     | 1.44                     | 0.82              |
| 1:A:768:ILE:HD13 | 3:A:1004:POV:H31D | 1.62                     | 0.82              |
| 1:A:781:LYS:C    | 1:F:316:THR:HG21  | 2.04                     | 0.81              |
| 1:D:400:SER:CB   | 1:D:403:ASP:HB3   | 2.09                     | 0.81              |
| 1:A:772:ILE:HD13 | 3:A:1010:POV:H31C | 1.63                     | 0.81              |
| 1:B:400:SER:CB   | 1:B:403:ASP:HB3   | 2.10                     | 0.81              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:B:1003:POV:H31C | 1:C:772:ILE:HD13  | 1.63                     | 0.80              |
| 1:C:316:THR:HG22  | 1:D:783:GLY:N     | 1.97                     | 0.80              |
| 3:D:1005:POV:H34A | 3:D:1005:POV:H27  | 1.61                     | 0.80              |
| 1:A:779:LEU:CD2   | 1:F:314:TYR:O     | 2.30                     | 0.80              |
| 1:C:313:PHE:O     | 1:D:783:GLY:O     | 1.99                     | 0.80              |
| 1:F:400:SER:O     | 1:F:404:LEU:CG    | 2.18                     | 0.80              |
| 3:F:1004:POV:H34A | 3:F:1004:POV:H27  | 1.64                     | 0.78              |
| 1:E:708:LEU:HD21  | 3:E:1003:POV:H312 | 1.64                     | 0.78              |
| 1:A:783:GLY:N     | 1:F:316:THR:CG2   | 2.47                     | 0.78              |
| 1:D:307:LEU:HD12  | 3:D:1002:POV:H36A | 1.65                     | 0.78              |
| 1:A:783:GLY:N     | 1:F:316:THR:HG22  | 1.99                     | 0.77              |
| 1:C:307:LEU:HD12  | 3:C:1002:POV:H36A | 1.65                     | 0.77              |
| 1:B:313:PHE:O     | 1:C:783:GLY:O     | 2.01                     | 0.77              |
| 1:E:319:ILE:HD13  | 1:F:857:ARG:HG2   | 1.67                     | 0.77              |
| 1:D:430:LEU:O     | 1:D:435:LYS:HE2   | 1.85                     | 0.77              |
| 1:E:306:LEU:HD11  | 1:F:868:VAL:HG23  | 1.66                     | 0.77              |
| 1:D:768:ILE:HD12  | 3:D:1004:POV:C218 | 2.08                     | 0.76              |
| 3:B:1006:POV:H27  | 3:B:1006:POV:H34A | 1.66                     | 0.76              |
| 1:F:708:LEU:HD21  | 3:F:1002:POV:H312 | 1.67                     | 0.76              |
| 1:A:319:ILE:HD13  | 1:B:857:ARG:HG2   | 1.67                     | 0.75              |
| 3:C:1005:POV:H27  | 3:C:1005:POV:H34A | 1.66                     | 0.75              |
| 1:C:768:ILE:HD11  | 3:C:1004:POV:H31D | 1.66                     | 0.75              |
| 1:D:316:THR:HG22  | 1:E:783:GLY:H     | 1.50                     | 0.75              |
| 3:E:1005:POV:H27  | 3:E:1005:POV:H34A | 1.66                     | 0.75              |
| 3:A:1005:POV:H27  | 3:A:1005:POV:H34A | 1.69                     | 0.74              |
| 3:A:1002:POV:H31C | 1:B:772:ILE:HD13  | 1.69                     | 0.74              |
| 1:C:307:LEU:CD1   | 3:C:1002:POV:H36A | 2.18                     | 0.74              |
| 1:B:314:TYR:O     | 1:C:779:LEU:HD22  | 1.86                     | 0.74              |
| 1:D:314:TYR:O     | 1:E:779:LEU:HD22  | 1.88                     | 0.74              |
| 1:C:306:LEU:HD11  | 1:D:868:VAL:CG2   | 2.15                     | 0.73              |
| 1:E:314:TYR:O     | 1:F:779:LEU:CD2   | 2.36                     | 0.73              |
| 1:E:306:LEU:HD11  | 1:F:868:VAL:CG2   | 2.18                     | 0.73              |
| 1:E:316:THR:HG21  | 1:F:781:LYS:C     | 2.14                     | 0.73              |
| 1:D:768:ILE:CD1   | 3:D:1004:POV:H31D | 2.18                     | 0.73              |
| 1:F:550:LEU:HD23  | 1:F:678:LEU:HD22  | 1.70                     | 0.73              |
| 1:C:550:LEU:HD23  | 1:C:678:LEU:HD22  | 1.70                     | 0.73              |
| 1:C:306:LEU:CD1   | 1:D:868:VAL:HG21  | 2.19                     | 0.73              |
| 1:A:550:LEU:HD23  | 1:A:678:LEU:HD22  | 1.70                     | 0.72              |
| 1:D:550:LEU:HD23  | 1:D:678:LEU:HD22  | 1.70                     | 0.72              |
| 3:E:1002:POV:H31C | 1:F:772:ILE:HD13  | 1.71                     | 0.72              |
| 1:A:316:THR:HG21  | 1:B:781:LYS:C     | 2.13                     | 0.72              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:E:400:SER:O     | 1:E:404:LEU:CG    | 2.19                     | 0.72              |
| 1:B:316:THR:HG22  | 1:C:783:GLY:H     | 1.51                     | 0.72              |
| 1:A:700:LEU:HD11  | 1:A:760:ILE:HD13  | 1.70                     | 0.72              |
| 1:D:313:PHE:O     | 1:E:783:GLY:O     | 2.08                     | 0.72              |
| 1:B:430:LEU:O     | 1:B:435:LYS:HE2   | 1.89                     | 0.72              |
| 1:E:700:LEU:HD11  | 1:E:760:ILE:HD13  | 1.70                     | 0.72              |
| 1:D:768:ILE:CD1   | 3:D:1004:POV:H21J | 2.08                     | 0.72              |
| 1:C:700:LEU:HD11  | 1:C:760:ILE:HD13  | 1.70                     | 0.72              |
| 1:B:700:LEU:HD11  | 1:B:760:ILE:HD13  | 1.70                     | 0.71              |
| 1:E:550:LEU:HD23  | 1:E:678:LEU:HD22  | 1.70                     | 0.71              |
| 1:F:700:LEU:HD11  | 1:F:760:ILE:HD13  | 1.70                     | 0.71              |
| 1:B:550:LEU:HD23  | 1:B:678:LEU:HD22  | 1.70                     | 0.71              |
| 1:D:700:LEU:HD11  | 1:D:760:ILE:HD13  | 1.70                     | 0.71              |
| 1:B:316:THR:HG21  | 1:C:781:LYS:C     | 2.15                     | 0.71              |
| 1:C:314:TYR:O     | 1:D:779:LEU:CD2   | 2.39                     | 0.71              |
| 1:A:857:ARG:HG2   | 1:F:319:ILE:HD13  | 1.71                     | 0.71              |
| 1:C:314:TYR:CD1   | 1:D:776:THR:HG22  | 2.26                     | 0.70              |
| 1:C:430:LEU:HB2   | 1:C:435:LYS:HB3   | 1.73                     | 0.70              |
| 1:B:319:ILE:HD13  | 1:C:857:ARG:HG2   | 1.73                     | 0.70              |
| 1:C:306:LEU:HD13  | 1:D:868:VAL:HG21  | 1.73                     | 0.70              |
| 1:F:430:LEU:HB2   | 1:F:435:LYS:HB3   | 1.73                     | 0.70              |
| 3:D:1005:POV:H27A | 3:D:1006:POV:H27A | 1.74                     | 0.70              |
| 1:E:314:TYR:CD1   | 1:F:776:THR:HG22  | 2.27                     | 0.70              |
| 1:C:400:SER:O     | 1:C:404:LEU:CG    | 2.20                     | 0.69              |
| 1:D:316:THR:HG21  | 1:E:781:LYS:C     | 2.16                     | 0.69              |
| 1:C:319:ILE:HD13  | 1:D:857:ARG:HG2   | 1.75                     | 0.69              |
| 1:B:316:THR:HG22  | 1:C:783:GLY:N     | 2.08                     | 0.69              |
| 1:D:307:LEU:CD1   | 3:D:1002:POV:H36A | 2.22                     | 0.69              |
| 1:C:768:ILE:CD1   | 3:C:1004:POV:C313 | 2.71                     | 0.69              |
| 1:D:316:THR:CG2   | 1:E:783:GLY:N     | 2.54                     | 0.69              |
| 1:D:316:THR:HG22  | 1:E:783:GLY:N     | 2.08                     | 0.69              |
| 1:B:398:GLY:HA3   | 1:B:404:LEU:HD11  | 1.75                     | 0.69              |
| 1:D:314:TYR:O     | 1:E:779:LEU:CD2   | 2.40                     | 0.69              |
| 1:B:314:TYR:O     | 1:C:779:LEU:CD2   | 2.41                     | 0.68              |
| 1:C:398:GLY:HA3   | 1:C:404:LEU:HD11  | 1.75                     | 0.68              |
| 1:D:398:GLY:HA3   | 1:D:404:LEU:HD11  | 1.75                     | 0.68              |
| 1:D:315:ARG:HD3   | 3:D:1002:POV:H13A | 1.75                     | 0.68              |
| 1:E:430:LEU:HB2   | 1:E:435:LYS:HB3   | 1.74                     | 0.68              |
| 1:B:316:THR:CG2   | 1:C:783:GLY:N     | 2.54                     | 0.68              |
| 1:F:398:GLY:HA3   | 1:F:404:LEU:HD11  | 1.74                     | 0.68              |
| 1:B:306:LEU:CD1   | 1:C:868:VAL:CG2   | 2.72                     | 0.68              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:E:398:GLY:HA3   | 1:E:404:LEU:HD11  | 1.75                     | 0.68              |
| 1:D:319:ILE:HD13  | 1:E:857:ARG:HG2   | 1.74                     | 0.68              |
| 1:A:398:GLY:HA3   | 1:A:404:LEU:HD11  | 1.75                     | 0.68              |
| 3:A:1005:POV:H27A | 3:A:1006:POV:H27A | 1.75                     | 0.67              |
| 1:A:306:LEU:CD1   | 1:B:868:VAL:CG2   | 2.71                     | 0.67              |
| 3:C:1005:POV:H27A | 3:C:1006:POV:H27A | 1.75                     | 0.67              |
| 1:D:701:HIS:ND1   | 1:D:766:LEU:HB3   | 2.10                     | 0.67              |
| 1:E:712:ILE:HG13  | 3:E:1003:POV:H34  | 1.77                     | 0.67              |
| 1:C:768:ILE:HD11  | 3:C:1004:POV:C313 | 2.24                     | 0.67              |
| 1:C:701:HIS:ND1   | 1:C:766:LEU:HB3   | 2.10                     | 0.67              |
| 3:C:1004:POV:H38  | 3:C:1005:POV:H311 | 1.76                     | 0.67              |
| 1:A:701:HIS:ND1   | 1:A:766:LEU:HB3   | 2.10                     | 0.67              |
| 1:B:430:LEU:HB2   | 1:B:435:LYS:HB3   | 1.76                     | 0.67              |
| 1:E:701:HIS:ND1   | 1:E:766:LEU:HB3   | 2.10                     | 0.67              |
| 1:F:701:HIS:ND1   | 1:F:766:LEU:HB3   | 2.10                     | 0.67              |
| 1:B:701:HIS:ND1   | 1:B:766:LEU:HB3   | 2.10                     | 0.66              |
| 1:E:634:ASP:OD1   | 2:E:1001:BEF:F3   | 2.03                     | 0.66              |
| 1:E:306:LEU:CD1   | 1:F:868:VAL:HG21  | 2.25                     | 0.66              |
| 1:E:318:GLY:HA2   | 1:F:786:GLN:NE2   | 2.11                     | 0.66              |
| 1:A:314:TYR:CE2   | 3:A:1002:POV:H27A | 2.31                     | 0.66              |
| 1:A:400:SER:O     | 1:A:404:LEU:CG    | 2.20                     | 0.66              |
| 3:F:1004:POV:H27A | 3:F:1005:POV:H27A | 1.77                     | 0.66              |
| 3:B:1006:POV:H27A | 3:B:1007:POV:H27A | 1.77                     | 0.65              |
| 1:B:314:TYR:CE2   | 3:B:1003:POV:H27A | 2.31                     | 0.65              |
| 1:B:712:ILE:HG13  | 3:B:1004:POV:H34  | 1.78                     | 0.65              |
| 1:D:400:SER:O     | 1:D:404:LEU:CG    | 2.20                     | 0.65              |
| 1:C:751:ASN:ND2   | 1:C:883:ASP:OD1   | 2.30                     | 0.64              |
| 1:A:751:ASN:ND2   | 1:A:883:ASP:OD1   | 2.30                     | 0.64              |
| 1:E:773:THR:HG21  | 1:E:798:GLN:HG3   | 1.79                     | 0.64              |
| 1:C:316:THR:HG23  | 1:D:783:GLY:H     | 1.55                     | 0.64              |
| 1:F:751:ASN:ND2   | 1:F:883:ASP:OD1   | 2.30                     | 0.64              |
| 1:B:773:THR:HG21  | 1:B:798:GLN:HG3   | 1.79                     | 0.64              |
| 1:D:773:THR:HG21  | 1:D:798:GLN:HG3   | 1.79                     | 0.64              |
| 1:A:313:PHE:O     | 1:B:783:GLY:O     | 2.15                     | 0.64              |
| 1:A:773:THR:HG21  | 1:A:798:GLN:HG3   | 1.79                     | 0.64              |
| 1:D:768:ILE:HD11  | 3:D:1004:POV:H31D | 1.78                     | 0.64              |
| 1:D:751:ASN:ND2   | 1:D:883:ASP:OD1   | 2.30                     | 0.64              |
| 1:C:404:LEU:HD22  | 1:C:527:LEU:HB3   | 1.80                     | 0.64              |
| 1:A:306:LEU:HD11  | 1:B:868:VAL:CG2   | 2.28                     | 0.64              |
| 1:B:751:ASN:ND2   | 1:B:883:ASP:OD1   | 2.30                     | 0.64              |
| 1:E:751:ASN:ND2   | 1:E:883:ASP:OD1   | 2.30                     | 0.64              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:F:404:LEU:HD22 | 1:F:527:LEU:HB3   | 1.80                     | 0.64              |
| 3:F:1003:POV:H38 | 3:F:1004:POV:H311 | 1.80                     | 0.64              |
| 1:D:360:VAL:HG12 | 1:D:664:ILE:HG12  | 1.81                     | 0.63              |
| 1:B:404:LEU:HD22 | 1:B:527:LEU:HB3   | 1.80                     | 0.63              |
| 1:A:360:VAL:HG12 | 1:A:664:ILE:HG12  | 1.81                     | 0.63              |
| 1:E:360:VAL:HG12 | 1:E:664:ILE:HG12  | 1.81                     | 0.63              |
| 1:E:404:LEU:HD22 | 1:E:527:LEU:HB3   | 1.80                     | 0.63              |
| 1:F:773:THR:HG21 | 1:F:798:GLN:HG3   | 1.79                     | 0.63              |
| 1:D:430:LEU:HB2  | 1:D:435:LYS:HB3   | 1.81                     | 0.63              |
| 3:B:1005:POV:H24 | 3:B:1006:POV:H23  | 1.79                     | 0.63              |
| 1:C:773:THR:HG21 | 1:C:798:GLN:HG3   | 1.79                     | 0.62              |
| 1:A:306:LEU:HD11 | 1:B:868:VAL:HG23  | 1.81                     | 0.62              |
| 1:D:404:LEU:HD22 | 1:D:527:LEU:HB3   | 1.81                     | 0.62              |
| 1:A:404:LEU:HD22 | 1:A:527:LEU:HB3   | 1.80                     | 0.62              |
| 1:C:316:THR:HG21 | 1:D:781:LYS:C     | 2.24                     | 0.62              |
| 1:C:768:ILE:HD13 | 3:C:1004:POV:H312 | 1.80                     | 0.62              |
| 1:B:360:VAL:HG12 | 1:B:664:ILE:HG12  | 1.81                     | 0.62              |
| 1:B:768:ILE:HD11 | 3:B:1005:POV:H31D | 1.82                     | 0.62              |
| 1:A:868:VAL:CG2  | 1:F:306:LEU:CD1   | 2.77                     | 0.62              |
| 1:C:360:VAL:HG12 | 1:C:664:ILE:HG12  | 1.81                     | 0.62              |
| 1:D:306:LEU:CD1  | 1:E:868:VAL:CG2   | 2.78                     | 0.62              |
| 1:E:429:SER:O    | 1:E:431:LYS:NZ    | 2.33                     | 0.62              |
| 1:A:776:THR:HG22 | 1:F:314:TYR:CD1   | 2.35                     | 0.61              |
| 3:A:1004:POV:H38 | 3:A:1005:POV:H311 | 1.82                     | 0.61              |
| 1:F:360:VAL:HG12 | 1:F:664:ILE:HG12  | 1.80                     | 0.61              |
| 1:D:429:SER:O    | 1:D:431:LYS:NZ    | 2.33                     | 0.61              |
| 1:E:314:TYR:CE2  | 3:E:1002:POV:H27A | 2.36                     | 0.61              |
| 1:A:429:SER:O    | 1:A:431:LYS:NZ    | 2.33                     | 0.61              |
| 1:B:429:SER:O    | 1:B:431:LYS:NZ    | 2.33                     | 0.61              |
| 1:C:316:THR:HG21 | 1:D:783:GLY:H     | 1.63                     | 0.61              |
| 1:C:429:SER:O    | 1:C:431:LYS:NZ    | 2.33                     | 0.61              |
| 1:E:182:VAL:HG12 | 1:E:202:LEU:HG    | 1.83                     | 0.61              |
| 1:B:182:VAL:HG12 | 1:B:202:LEU:HG    | 1.83                     | 0.60              |
| 1:B:306:LEU:HD11 | 1:C:868:VAL:HG23  | 1.83                     | 0.60              |
| 1:F:389:SER:HB3  | 1:F:535:PRO:HG3   | 1.84                     | 0.60              |
| 1:F:429:SER:O    | 1:F:431:LYS:NZ    | 2.33                     | 0.60              |
| 1:A:389:SER:HB3  | 1:A:535:PRO:HG3   | 1.84                     | 0.60              |
| 1:D:389:SER:HB3  | 1:D:535:PRO:HG3   | 1.83                     | 0.60              |
| 1:E:309:TRP:CH2  | 1:F:860:ILE:HG21  | 2.36                     | 0.60              |
| 1:C:389:SER:HB3  | 1:C:535:PRO:HG3   | 1.84                     | 0.60              |
| 1:A:378:ASP:O    | 1:A:382:THR:OG1   | 2.20                     | 0.60              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:636:VAL:HG12 | 1:C:657:ALA:HB3   | 1.83                     | 0.60              |
| 1:D:636:VAL:HG12 | 1:D:657:ALA:HB3   | 1.83                     | 0.60              |
| 1:F:636:VAL:HG12 | 1:F:657:ALA:HB3   | 1.84                     | 0.60              |
| 1:A:636:VAL:HG12 | 1:A:657:ALA:HB3   | 1.84                     | 0.60              |
| 3:B:1005:POV:H38 | 3:B:1006:POV:H311 | 1.83                     | 0.60              |
| 1:F:378:ASP:O    | 1:F:382:THR:OG1   | 2.20                     | 0.60              |
| 1:B:385:LYS:O    | 1:B:386:ASN:ND2   | 2.35                     | 0.60              |
| 1:B:389:SER:HB3  | 1:B:535:PRO:HG3   | 1.84                     | 0.60              |
| 1:D:182:VAL:HG12 | 1:D:202:LEU:HG    | 1.83                     | 0.60              |
| 1:D:712:ILE:HG13 | 3:D:1003:POV:H32A | 1.83                     | 0.60              |
| 1:A:182:VAL:HG12 | 1:A:202:LEU:HG    | 1.83                     | 0.60              |
| 1:D:684:ILE:HG22 | 1:D:688:MET:HE2   | 1.83                     | 0.60              |
| 1:E:389:SER:HB3  | 1:E:535:PRO:HG3   | 1.84                     | 0.60              |
| 1:F:182:VAL:HG12 | 1:F:202:LEU:HG    | 1.83                     | 0.60              |
| 1:B:797:LEU:HD22 | 1:B:840:THR:HG21  | 1.84                     | 0.59              |
| 1:C:182:VAL:HG12 | 1:C:202:LEU:HG    | 1.83                     | 0.59              |
| 1:A:684:ILE:HG22 | 1:A:688:MET:HE2   | 1.83                     | 0.59              |
| 1:C:315:ARG:HD3  | 3:C:1002:POV:H13A | 1.83                     | 0.59              |
| 1:C:615:LYS:HD3  | 1:C:638:ASP:HB3   | 1.84                     | 0.59              |
| 1:C:768:ILE:HD13 | 3:C:1004:POV:H31D | 1.81                     | 0.59              |
| 1:D:378:ASP:O    | 1:D:382:THR:OG1   | 2.20                     | 0.59              |
| 1:F:684:ILE:HG22 | 1:F:688:MET:HE2   | 1.83                     | 0.59              |
| 1:A:694:TYR:CZ   | 1:A:698:LEU:HD11  | 2.37                     | 0.59              |
| 1:C:297:LEU:HD21 | 1:C:696:ILE:HG23  | 1.85                     | 0.59              |
| 1:C:378:ASP:O    | 1:C:382:THR:OG1   | 2.20                     | 0.59              |
| 1:C:410:LEU:HA   | 1:C:414:ARG:HH12  | 1.68                     | 0.59              |
| 1:C:684:ILE:HG22 | 1:C:688:MET:HE2   | 1.83                     | 0.59              |
| 1:D:694:TYR:CZ   | 1:D:698:LEU:HD11  | 2.37                     | 0.59              |
| 1:A:768:ILE:HD11 | 3:A:1004:POV:H31D | 1.84                     | 0.59              |
| 1:B:694:TYR:CZ   | 1:B:698:LEU:HD11  | 2.37                     | 0.59              |
| 1:D:410:LEU:HA   | 1:D:414:ARG:HH12  | 1.68                     | 0.59              |
| 1:F:297:LEU:HD21 | 1:F:696:ILE:HG23  | 1.85                     | 0.59              |
| 1:E:797:LEU:HD22 | 1:E:840:THR:HG21  | 1.85                     | 0.59              |
| 1:F:410:LEU:HA   | 1:F:414:ARG:HH12  | 1.68                     | 0.59              |
| 1:A:382:THR:O    | 1:A:537:ARG:NH2   | 2.36                     | 0.59              |
| 1:A:410:LEU:HA   | 1:A:414:ARG:HH12  | 1.68                     | 0.59              |
| 1:B:297:LEU:HD21 | 1:B:696:ILE:HG23  | 1.85                     | 0.59              |
| 1:E:297:LEU:HD21 | 1:E:696:ILE:HG23  | 1.85                     | 0.59              |
| 1:F:615:LYS:HD3  | 1:F:638:ASP:HB3   | 1.84                     | 0.59              |
| 1:B:684:ILE:HG22 | 1:B:688:MET:HE2   | 1.83                     | 0.59              |
| 3:D:1004:POV:H38 | 3:D:1005:POV:H311 | 1.85                     | 0.59              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:F:797:LEU:HD22 | 1:F:840:THR:HG21  | 1.85                     | 0.59              |
| 1:A:772:ILE:CD1  | 3:A:1010:POV:H31C | 2.31                     | 0.59              |
| 1:B:410:LEU:HA   | 1:B:414:ARG:HH12  | 1.68                     | 0.59              |
| 1:C:385:LYS:O    | 1:C:386:ASN:ND2   | 2.35                     | 0.59              |
| 1:C:797:LEU:HD22 | 1:C:840:THR:HG21  | 1.85                     | 0.59              |
| 1:E:636:VAL:HG12 | 1:E:657:ALA:HB3   | 1.84                     | 0.59              |
| 1:A:783:GLY:H    | 1:F:316:THR:HG23  | 1.62                     | 0.59              |
| 1:B:378:ASP:O    | 1:B:382:THR:OG1   | 2.20                     | 0.59              |
| 1:C:315:ARG:CZ   | 3:C:1003:POV:O13  | 2.50                     | 0.59              |
| 1:D:615:LYS:HD3  | 1:D:638:ASP:HB3   | 1.84                     | 0.59              |
| 1:E:410:LEU:HA   | 1:E:414:ARG:HH12  | 1.68                     | 0.59              |
| 1:E:684:ILE:HG22 | 1:E:688:MET:HE2   | 1.83                     | 0.59              |
| 1:E:694:TYR:CZ   | 1:E:698:LEU:HD11  | 2.38                     | 0.59              |
| 1:F:694:TYR:CZ   | 1:F:698:LEU:HD11  | 2.38                     | 0.59              |
| 1:A:712:ILE:HG13 | 3:A:1003:POV:H34  | 1.83                     | 0.59              |
| 1:A:615:LYS:HD3  | 1:A:638:ASP:HB3   | 1.84                     | 0.58              |
| 1:B:400:SER:O    | 1:B:404:LEU:CG    | 2.21                     | 0.58              |
| 1:E:615:LYS:HD3  | 1:E:638:ASP:HB3   | 1.84                     | 0.58              |
| 1:F:385:LYS:O    | 1:F:386:ASN:ND2   | 2.35                     | 0.58              |
| 1:A:797:LEU:HD22 | 1:A:840:THR:HG21  | 1.85                     | 0.58              |
| 1:D:382:THR:O    | 1:D:537:ARG:NH2   | 2.36                     | 0.58              |
| 1:B:636:VAL:HG12 | 1:B:657:ALA:HB3   | 1.84                     | 0.58              |
| 1:D:315:ARG:NE   | 3:D:1003:POV:O13  | 2.36                     | 0.58              |
| 1:B:708:LEU:HD21 | 3:B:1004:POV:H312 | 1.84                     | 0.58              |
| 1:D:306:LEU:HD11 | 1:E:868:VAL:CG2   | 2.34                     | 0.58              |
| 1:D:768:ILE:CD1  | 3:D:1004:POV:C313 | 2.82                     | 0.58              |
| 1:D:773:THR:O    | 1:D:776:THR:OG1   | 2.22                     | 0.58              |
| 1:F:773:THR:O    | 1:F:776:THR:OG1   | 2.21                     | 0.58              |
| 1:C:694:TYR:CZ   | 1:C:698:LEU:HD11  | 2.37                     | 0.58              |
| 1:D:797:LEU:HD22 | 1:D:840:THR:HG21  | 1.85                     | 0.58              |
| 1:E:382:THR:O    | 1:E:537:ARG:NH2   | 2.36                     | 0.58              |
| 1:A:297:LEU:HD21 | 1:A:696:ILE:HG23  | 1.85                     | 0.58              |
| 1:B:382:THR:O    | 1:B:537:ARG:NH2   | 2.36                     | 0.58              |
| 1:D:297:LEU:HD21 | 1:D:696:ILE:HG23  | 1.85                     | 0.58              |
| 1:D:307:LEU:CD1  | 3:D:1002:POV:C36  | 2.81                     | 0.58              |
| 1:E:768:ILE:HD11 | 3:E:1004:POV:H31D | 1.81                     | 0.58              |
| 1:A:772:ILE:HD13 | 3:A:1010:POV:C312 | 2.33                     | 0.58              |
| 1:B:306:LEU:HD11 | 1:C:868:VAL:CG2   | 2.33                     | 0.58              |
| 1:F:430:LEU:O    | 1:F:435:LYS:HE2   | 2.04                     | 0.58              |
| 1:C:773:THR:O    | 1:C:776:THR:OG1   | 2.22                     | 0.58              |
| 1:D:315:ARG:CZ   | 3:D:1003:POV:O13  | 2.51                     | 0.58              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:768:ILE:HD11  | 3:D:1004:POV:C313 | 2.34                     | 0.58              |
| 1:A:773:THR:O     | 1:A:776:THR:OG1   | 2.22                     | 0.58              |
| 1:B:615:LYS:HD3   | 1:B:638:ASP:HB3   | 1.84                     | 0.58              |
| 1:E:306:LEU:HD13  | 1:F:868:VAL:HG21  | 1.84                     | 0.58              |
| 1:E:378:ASP:O     | 1:E:382:THR:OG1   | 2.20                     | 0.58              |
| 1:E:773:THR:O     | 1:E:776:THR:OG1   | 2.21                     | 0.58              |
| 1:E:313:PHE:O     | 1:F:783:GLY:C     | 2.47                     | 0.57              |
| 3:E:1010:POV:H32  | 3:E:1010:POV:H22A | 1.86                     | 0.57              |
| 1:A:708:LEU:HD21  | 3:A:1003:POV:H312 | 1.86                     | 0.57              |
| 1:C:306:LEU:CD1   | 1:D:868:VAL:HG23  | 2.21                     | 0.57              |
| 1:E:396:VAL:HG21  | 1:E:528:GLY:HA3   | 1.86                     | 0.57              |
| 1:C:315:ARG:NE    | 3:C:1003:POV:O13  | 2.36                     | 0.57              |
| 1:B:396:VAL:HG21  | 1:B:528:GLY:HA3   | 1.86                     | 0.57              |
| 1:C:396:VAL:HG21  | 1:C:528:GLY:HA3   | 1.86                     | 0.57              |
| 3:B:1003:POV:C312 | 1:C:772:ILE:HD13  | 2.34                     | 0.57              |
| 1:F:382:THR:O     | 1:F:537:ARG:NH2   | 2.36                     | 0.57              |
| 1:C:768:ILE:CD1   | 3:C:1004:POV:H21J | 2.19                     | 0.57              |
| 3:E:1004:POV:H38  | 3:E:1005:POV:H311 | 1.85                     | 0.57              |
| 3:A:1011:POV:H32  | 3:A:1011:POV:H22A | 1.87                     | 0.57              |
| 1:B:773:THR:O     | 1:B:776:THR:OG1   | 2.22                     | 0.57              |
| 1:C:382:THR:O     | 1:C:537:ARG:NH2   | 2.36                     | 0.57              |
| 1:F:396:VAL:HG21  | 1:F:528:GLY:HA3   | 1.86                     | 0.57              |
| 1:C:309:TRP:CH2   | 1:D:860:ILE:HG21  | 2.39                     | 0.56              |
| 3:E:1005:POV:H27A | 3:E:1006:POV:H27A | 1.87                     | 0.56              |
| 1:F:805:TRP:NE1   | 1:F:833:ASP:OD2   | 2.38                     | 0.56              |
| 3:A:1004:POV:H1   | 3:A:1004:POV:H14B | 1.87                     | 0.56              |
| 1:B:224:GLN:HB2   | 1:B:253:ARG:HB2   | 1.87                     | 0.56              |
| 1:C:768:ILE:HD12  | 3:C:1004:POV:C218 | 2.19                     | 0.56              |
| 3:C:1002:POV:H13  | 3:C:1003:POV:H15A | 1.87                     | 0.56              |
| 1:E:434:PRO:O     | 1:E:438:ASP:HB2   | 2.05                     | 0.56              |
| 1:B:434:PRO:O     | 1:B:438:ASP:HB2   | 2.05                     | 0.56              |
| 1:C:224:GLN:HB2   | 1:C:253:ARG:HB2   | 1.87                     | 0.56              |
| 1:C:567:GLU:OE1   | 1:C:570:ARG:NH1   | 2.39                     | 0.56              |
| 1:C:805:TRP:NE1   | 1:C:833:ASP:OD2   | 2.38                     | 0.56              |
| 1:E:224:GLN:HB2   | 1:E:253:ARG:HB2   | 1.87                     | 0.56              |
| 3:E:1002:POV:H314 | 1:F:772:ILE:CD1   | 2.35                     | 0.56              |
| 3:E:1006:POV:H32  | 3:E:1008:POV:H32A | 1.87                     | 0.56              |
| 1:F:567:GLU:OE1   | 1:F:570:ARG:NH1   | 2.39                     | 0.56              |
| 1:D:306:LEU:HD11  | 1:E:868:VAL:HG23  | 1.87                     | 0.56              |
| 1:F:224:GLN:HB2   | 1:F:253:ARG:HB2   | 1.87                     | 0.56              |
| 1:A:805:TRP:NE1   | 1:A:833:ASP:OD2   | 2.38                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:567:GLU:OE1   | 1:B:570:ARG:NH1   | 2.39                     | 0.56              |
| 1:D:567:GLU:OE1   | 1:D:570:ARG:NH1   | 2.39                     | 0.56              |
| 3:D:1002:POV:H13  | 3:D:1003:POV:H15A | 1.85                     | 0.56              |
| 1:C:307:LEU:CD1   | 3:C:1002:POV:C36  | 2.84                     | 0.56              |
| 1:D:396:VAL:HG21  | 1:D:528:GLY:HA3   | 1.86                     | 0.56              |
| 1:D:434:PRO:O     | 1:D:438:ASP:HB2   | 2.05                     | 0.56              |
| 1:A:567:GLU:OE1   | 1:A:570:ARG:NH1   | 2.39                     | 0.56              |
| 1:C:519:ARG:NH1   | 1:C:521:GLU:OE2   | 2.39                     | 0.56              |
| 1:F:434:PRO:O     | 1:F:438:ASP:HB2   | 2.05                     | 0.56              |
| 1:A:868:VAL:HG23  | 1:F:306:LEU:HD11  | 1.88                     | 0.56              |
| 1:E:567:GLU:OE1   | 1:E:570:ARG:NH1   | 2.39                     | 0.56              |
| 1:F:519:ARG:NH1   | 1:F:521:GLU:OE2   | 2.39                     | 0.56              |
| 1:D:224:GLN:HB2   | 1:D:253:ARG:HB2   | 1.87                     | 0.55              |
| 1:E:805:TRP:NE1   | 1:E:833:ASP:OD2   | 2.38                     | 0.55              |
| 3:E:1002:POV:H31C | 1:F:772:ILE:CD1   | 2.36                     | 0.55              |
| 1:F:610:VAL:HG11  | 1:F:615:LYS:HG3   | 1.89                     | 0.55              |
| 1:A:224:GLN:HB2   | 1:A:253:ARG:HB2   | 1.87                     | 0.55              |
| 1:A:519:ARG:NH1   | 1:A:521:GLU:OE2   | 2.39                     | 0.55              |
| 3:A:1002:POV:H212 | 3:A:1002:POV:H39A | 1.88                     | 0.55              |
| 1:B:438:ASP:OD1   | 1:B:438:ASP:O     | 2.25                     | 0.55              |
| 1:B:519:ARG:NH1   | 1:B:521:GLU:OE2   | 2.39                     | 0.55              |
| 3:B:1002:POV:H32  | 3:B:1002:POV:H22A | 1.88                     | 0.55              |
| 1:C:434:PRO:O     | 1:C:438:ASP:HB2   | 2.06                     | 0.55              |
| 1:D:805:TRP:NE1   | 1:D:833:ASP:OD2   | 2.38                     | 0.55              |
| 1:F:380:THR:OG1   | 2:F:1001:BEF:F3   | 2.15                     | 0.55              |
| 1:F:701:HIS:HD2   | 1:F:702:LEU:HG    | 1.72                     | 0.55              |
| 3:B:1007:POV:H32  | 3:B:1009:POV:H32A | 1.89                     | 0.55              |
| 1:F:419:LEU:O     | 1:F:424:LYS:NZ    | 2.39                     | 0.55              |
| 1:A:396:VAL:HG21  | 1:A:528:GLY:HA3   | 1.86                     | 0.55              |
| 1:C:610:VAL:HG11  | 1:C:615:LYS:HG3   | 1.88                     | 0.55              |
| 1:E:519:ARG:NH1   | 1:E:521:GLU:OE2   | 2.39                     | 0.55              |
| 1:A:434:PRO:O     | 1:A:438:ASP:HB2   | 2.06                     | 0.55              |
| 1:D:519:ARG:NH1   | 1:D:521:GLU:OE2   | 2.39                     | 0.55              |
| 3:D:1004:POV:H24  | 3:D:1005:POV:H23  | 1.88                     | 0.55              |
| 1:F:712:ILE:HG13  | 3:F:1002:POV:H34  | 1.86                     | 0.55              |
| 1:C:701:HIS:HD2   | 1:C:702:LEU:HG    | 1.72                     | 0.55              |
| 1:C:768:ILE:HD13  | 3:C:1004:POV:C313 | 2.34                     | 0.55              |
| 1:E:438:ASP:OD1   | 1:E:438:ASP:O     | 2.25                     | 0.55              |
| 1:A:438:ASP:OD1   | 1:A:438:ASP:O     | 2.25                     | 0.55              |
| 1:B:314:TYR:CD1   | 1:C:776:THR:HG22  | 2.42                     | 0.55              |
| 1:B:380:THR:OG1   | 2:B:1001:BEF:F3   | 2.15                     | 0.55              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:380:THR:OG1   | 2:D:1001:BEF:F3   | 2.15                     | 0.55              |
| 1:A:610:VAL:HG11  | 1:A:615:LYS:HG3   | 1.88                     | 0.55              |
| 1:B:805:TRP:NE1   | 1:B:833:ASP:OD2   | 2.38                     | 0.55              |
| 1:D:309:TRP:NE1   | 1:D:326:THR:OG1   | 2.40                     | 0.55              |
| 1:D:438:ASP:OD1   | 1:D:438:ASP:O     | 2.24                     | 0.55              |
| 1:E:610:VAL:HG11  | 1:E:615:LYS:HG3   | 1.89                     | 0.55              |
| 3:A:1010:POV:H39A | 3:A:1010:POV:H212 | 1.87                     | 0.55              |
| 1:C:380:THR:OG1   | 2:C:1001:BEF:F3   | 2.15                     | 0.55              |
| 1:A:586:LEU:O     | 1:A:617:ARG:NH2   | 2.40                     | 0.55              |
| 1:C:419:LEU:O     | 1:C:424:LYS:NZ    | 2.39                     | 0.55              |
| 1:D:514:GLY:HA2   | 1:D:529:VAL:HA    | 1.89                     | 0.55              |
| 1:B:701:HIS:HD2   | 1:B:702:LEU:HG    | 1.72                     | 0.54              |
| 1:C:586:LEU:O     | 1:C:617:ARG:NH2   | 2.40                     | 0.54              |
| 1:D:610:VAL:HG11  | 1:D:615:LYS:HG3   | 1.89                     | 0.54              |
| 1:A:306:LEU:CD1   | 1:B:868:VAL:HG21  | 2.37                     | 0.54              |
| 1:A:514:GLY:HA2   | 1:A:529:VAL:HA    | 1.89                     | 0.54              |
| 1:B:400:SER:OG    | 1:B:403:ASP:HB3   | 2.07                     | 0.54              |
| 1:B:610:VAL:HG11  | 1:B:615:LYS:HG3   | 1.88                     | 0.54              |
| 1:D:419:LEU:O     | 1:D:424:LYS:NZ    | 2.39                     | 0.54              |
| 3:D:1007:POV:H3   | 3:E:1010:POV:H15B | 1.89                     | 0.54              |
| 1:D:768:ILE:HD13  | 3:D:1004:POV:H31D | 1.90                     | 0.54              |
| 1:F:309:TRP:NE1   | 1:F:326:THR:OG1   | 2.40                     | 0.54              |
| 1:F:586:LEU:O     | 1:F:617:ARG:NH2   | 2.40                     | 0.54              |
| 1:A:701:HIS:HD2   | 1:A:702:LEU:HG    | 1.72                     | 0.54              |
| 1:B:318:GLY:HA2   | 1:C:786:GLN:NE2   | 2.22                     | 0.54              |
| 1:C:438:ASP:O     | 1:C:438:ASP:OD1   | 2.24                     | 0.54              |
| 1:D:586:LEU:O     | 1:D:617:ARG:NH2   | 2.40                     | 0.54              |
| 1:F:438:ASP:OD1   | 1:F:438:ASP:O     | 2.24                     | 0.54              |
| 1:A:786:GLN:NE2   | 1:F:318:GLY:HA2   | 2.23                     | 0.54              |
| 1:B:634:ASP:OD1   | 2:B:1001:BEF:F3   | 2.16                     | 0.54              |
| 1:A:380:THR:OG1   | 2:A:1001:BEF:F3   | 2.15                     | 0.54              |
| 1:A:414:ARG:NH1   | 1:A:439:ALA:O     | 2.41                     | 0.54              |
| 1:B:306:LEU:CD1   | 1:C:868:VAL:HG21  | 2.37                     | 0.54              |
| 3:F:1005:POV:H32  | 3:F:1007:POV:H32A | 1.88                     | 0.54              |
| 1:E:419:LEU:O     | 1:E:424:LYS:NZ    | 2.39                     | 0.54              |
| 1:B:586:LEU:O     | 1:B:617:ARG:NH2   | 2.40                     | 0.54              |
| 1:D:179:THR:HA    | 1:D:192:PRO:HA    | 1.90                     | 0.54              |
| 1:A:179:THR:HA    | 1:A:192:PRO:HA    | 1.90                     | 0.54              |
| 1:B:514:GLY:HA2   | 1:B:529:VAL:HA    | 1.89                     | 0.54              |
| 1:A:781:LYS:O     | 1:F:316:THR:CG2   | 2.42                     | 0.54              |
| 3:A:1006:POV:H32  | 3:A:1008:POV:H32A | 1.89                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:701:HIS:HD2   | 1:D:702:LEU:HG    | 1.72                     | 0.54              |
| 1:E:586:LEU:O     | 1:E:617:ARG:NH2   | 2.40                     | 0.54              |
| 1:A:419:LEU:O     | 1:A:424:LYS:NZ    | 2.39                     | 0.53              |
| 1:D:384:THR:HA    | 1:D:536:PRO:HA    | 1.90                     | 0.53              |
| 1:D:634:ASP:OD1   | 2:D:1001:BEF:F3   | 2.16                     | 0.53              |
| 1:E:701:HIS:HD2   | 1:E:702:LEU:HG    | 1.72                     | 0.53              |
| 1:A:430:LEU:HB2   | 1:A:435:LYS:HB3   | 1.90                     | 0.53              |
| 1:A:768:ILE:HG21  | 3:A:1010:POV:H217 | 1.90                     | 0.53              |
| 1:C:309:TRP:NE1   | 1:C:326:THR:OG1   | 2.40                     | 0.53              |
| 3:D:1002:POV:H13B | 3:D:1003:POV:H13B | 1.89                     | 0.53              |
| 1:A:384:THR:HA    | 1:A:536:PRO:HA    | 1.90                     | 0.53              |
| 1:C:514:GLY:HA2   | 1:C:529:VAL:HA    | 1.89                     | 0.53              |
| 3:C:1002:POV:H13B | 3:C:1003:POV:H13B | 1.91                     | 0.53              |
| 1:D:414:ARG:NH1   | 1:D:439:ALA:O     | 2.41                     | 0.53              |
| 1:F:414:ARG:NH1   | 1:F:439:ALA:O     | 2.41                     | 0.53              |
| 1:A:783:GLY:C     | 1:F:313:PHE:O     | 2.52                     | 0.53              |
| 1:B:414:ARG:NH1   | 1:B:439:ALA:O     | 2.41                     | 0.53              |
| 1:C:414:ARG:NH1   | 1:C:439:ALA:O     | 2.41                     | 0.53              |
| 3:C:1010:POV:H22A | 3:C:1010:POV:H32  | 1.90                     | 0.53              |
| 1:F:514:GLY:HA2   | 1:F:529:VAL:HA    | 1.89                     | 0.53              |
| 1:B:309:TRP:NE1   | 1:B:326:THR:OG1   | 2.40                     | 0.53              |
| 1:C:634:ASP:OD1   | 2:C:1001:BEF:F3   | 2.16                     | 0.53              |
| 1:E:414:ARG:NH1   | 1:E:439:ALA:O     | 2.41                     | 0.53              |
| 1:B:798:GLN:HE21  | 1:B:861:TRP:HE1   | 1.57                     | 0.53              |
| 3:E:1002:POV:H210 | 3:F:1003:POV:H216 | 1.90                     | 0.53              |
| 1:F:634:ASP:OD1   | 2:F:1001:BEF:F3   | 2.16                     | 0.53              |
| 1:B:419:LEU:O     | 1:B:424:LYS:NZ    | 2.39                     | 0.53              |
| 1:C:798:GLN:HE21  | 1:C:861:TRP:HE1   | 1.57                     | 0.53              |
| 1:E:309:TRP:NE1   | 1:E:326:THR:OG1   | 2.40                     | 0.53              |
| 1:E:514:GLY:HA2   | 1:E:529:VAL:HA    | 1.89                     | 0.53              |
| 1:E:798:GLN:HE21  | 1:E:861:TRP:HE1   | 1.57                     | 0.53              |
| 1:F:798:GLN:HE21  | 1:F:861:TRP:HE1   | 1.57                     | 0.53              |
| 1:B:384:THR:HA    | 1:B:536:PRO:HA    | 1.90                     | 0.53              |
| 3:F:1004:POV:H21C | 3:F:1005:POV:H21B | 1.90                     | 0.53              |
| 1:A:634:ASP:OD1   | 2:A:1001:BEF:F3   | 2.16                     | 0.53              |
| 1:C:384:THR:HA    | 1:C:536:PRO:HA    | 1.90                     | 0.53              |
| 1:E:400:SER:OG    | 1:E:403:ASP:HB3   | 2.08                     | 0.53              |
| 1:F:708:LEU:CD2   | 3:F:1002:POV:H312 | 2.38                     | 0.53              |
| 1:F:656:ASP:OD1   | 1:F:659:ARG:NH1   | 2.42                     | 0.53              |
| 3:A:1002:POV:H31C | 1:B:772:ILE:CD1   | 2.38                     | 0.52              |
| 3:A:1010:POV:H27A | 1:F:314:TYR:CE2   | 2.43                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:A:1011:POV:H15B | 3:F:1006:POV:H3   | 1.91                     | 0.52              |
| 1:B:674:ILE:O     | 1:B:678:LEU:N     | 2.36                     | 0.52              |
| 3:B:1003:POV:H314 | 1:C:772:ILE:CD1   | 2.39                     | 0.52              |
| 1:C:656:ASP:OD1   | 1:C:659:ARG:NH1   | 2.42                     | 0.52              |
| 1:F:179:THR:HA    | 1:F:192:PRO:HA    | 1.90                     | 0.52              |
| 3:B:1010:POV:H37A | 3:C:1009:POV:H27A | 1.90                     | 0.52              |
| 1:F:581:ALA:HB2   | 1:F:610:VAL:HG22  | 1.91                     | 0.52              |
| 3:B:1008:POV:H3   | 3:C:1010:POV:H15B | 1.90                     | 0.52              |
| 1:C:366:ILE:O     | 1:C:681:SER:OG    | 2.23                     | 0.52              |
| 1:C:581:ALA:HB2   | 1:C:610:VAL:HG22  | 1.91                     | 0.52              |
| 1:F:384:THR:HA    | 1:F:536:PRO:HA    | 1.90                     | 0.52              |
| 1:A:581:ALA:HB2   | 1:A:610:VAL:HG22  | 1.91                     | 0.52              |
| 1:A:772:ILE:CD1   | 3:A:1010:POV:H314 | 2.39                     | 0.52              |
| 1:B:179:THR:HA    | 1:B:192:PRO:HA    | 1.90                     | 0.52              |
| 1:E:384:THR:HA    | 1:E:536:PRO:HA    | 1.90                     | 0.52              |
| 3:E:1002:POV:C312 | 1:F:772:ILE:HD13  | 2.37                     | 0.52              |
| 1:A:656:ASP:OD1   | 1:A:659:ARG:NH1   | 2.43                     | 0.52              |
| 1:B:315:ARG:CZ    | 3:B:1004:POV:O13  | 2.50                     | 0.52              |
| 1:D:656:ASP:OD1   | 1:D:659:ARG:NH1   | 2.43                     | 0.52              |
| 1:E:656:ASP:OD1   | 1:E:659:ARG:NH1   | 2.42                     | 0.52              |
| 1:B:656:ASP:OD1   | 1:B:659:ARG:NH1   | 2.43                     | 0.52              |
| 1:C:198:PRO:HA    | 1:C:260:VAL:HG23  | 1.92                     | 0.52              |
| 1:E:179:THR:HA    | 1:E:192:PRO:HA    | 1.90                     | 0.52              |
| 1:E:198:PRO:HA    | 1:E:260:VAL:HG23  | 1.92                     | 0.52              |
| 1:B:198:PRO:HA    | 1:B:260:VAL:HG23  | 1.92                     | 0.52              |
| 3:B:1004:POV:H29  | 3:B:1007:POV:H310 | 1.92                     | 0.52              |
| 1:F:204:LEU:HD12  | 1:F:208:THR:HG21  | 1.92                     | 0.52              |
| 1:C:179:THR:HA    | 1:C:192:PRO:HA    | 1.90                     | 0.52              |
| 1:D:366:ILE:O     | 1:D:681:SER:OG    | 2.23                     | 0.52              |
| 1:D:674:ILE:O     | 1:D:678:LEU:N     | 2.36                     | 0.52              |
| 1:E:414:ARG:HE    | 1:E:440:LEU:HD13  | 1.75                     | 0.52              |
| 1:B:414:ARG:HE    | 1:B:440:LEU:HD13  | 1.75                     | 0.52              |
| 3:B:1006:POV:H21C | 3:B:1007:POV:H21B | 1.91                     | 0.52              |
| 1:D:204:LEU:HD12  | 1:D:208:THR:HG21  | 1.92                     | 0.52              |
| 1:D:318:GLY:HA2   | 1:E:786:GLN:NE2   | 2.25                     | 0.52              |
| 1:B:312:CYS:HB3   | 1:B:322:ILE:HG12  | 1.92                     | 0.52              |
| 1:C:414:ARG:HE    | 1:C:440:LEU:HD13  | 1.75                     | 0.52              |
| 1:E:408:ALA:HB1   | 1:E:474:LYS:HD3   | 1.92                     | 0.52              |
| 1:A:366:ILE:O     | 1:A:681:SER:OG    | 2.23                     | 0.51              |
| 1:D:414:ARG:HE    | 1:D:440:LEU:HD13  | 1.75                     | 0.51              |
| 1:F:198:PRO:HA    | 1:F:260:VAL:HG23  | 1.92                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:204:LEU:HD12  | 1:A:208:THR:HG21  | 1.92                     | 0.51              |
| 1:B:408:ALA:HB1   | 1:B:474:LYS:HD3   | 1.92                     | 0.51              |
| 1:B:581:ALA:HB2   | 1:B:610:VAL:HG22  | 1.91                     | 0.51              |
| 1:C:204:LEU:HD12  | 1:C:208:THR:HG21  | 1.92                     | 0.51              |
| 1:E:312:CYS:HB3   | 1:E:322:ILE:HG12  | 1.92                     | 0.51              |
| 1:A:408:ALA:HB1   | 1:A:474:LYS:HD3   | 1.92                     | 0.51              |
| 1:C:459:THR:HB    | 1:C:473:VAL:HG23  | 1.93                     | 0.51              |
| 1:C:768:ILE:HD13  | 3:C:1004:POV:C312 | 2.40                     | 0.51              |
| 1:D:312:CYS:HB3   | 1:D:322:ILE:HG12  | 1.92                     | 0.51              |
| 1:D:408:ALA:HB1   | 1:D:474:LYS:HD3   | 1.92                     | 0.51              |
| 1:D:581:ALA:HB2   | 1:D:610:VAL:HG22  | 1.91                     | 0.51              |
| 1:E:204:LEU:HD12  | 1:E:208:THR:HG21  | 1.92                     | 0.51              |
| 3:E:1002:POV:H39A | 3:E:1002:POV:H212 | 1.92                     | 0.51              |
| 1:F:414:ARG:HE    | 1:F:440:LEU:HD13  | 1.75                     | 0.51              |
| 1:F:459:THR:HB    | 1:F:473:VAL:HG23  | 1.93                     | 0.51              |
| 1:A:459:THR:HB    | 1:A:473:VAL:HG23  | 1.93                     | 0.51              |
| 3:A:1007:POV:H3   | 3:B:1002:POV:H15B | 1.93                     | 0.51              |
| 1:D:459:THR:HB    | 1:D:473:VAL:HG23  | 1.93                     | 0.51              |
| 1:E:128:MET:HE3   | 1:E:336:VAL:HA    | 1.93                     | 0.51              |
| 1:E:459:THR:HB    | 1:E:473:VAL:HG23  | 1.93                     | 0.51              |
| 3:E:1002:POV:H217 | 1:F:768:ILE:HG21  | 1.92                     | 0.51              |
| 1:A:312:CYS:HB3   | 1:A:322:ILE:HG12  | 1.92                     | 0.51              |
| 3:B:1005:POV:H1   | 3:B:1005:POV:H14B | 1.92                     | 0.51              |
| 1:A:309:TRP:NE1   | 1:A:326:THR:OG1   | 2.40                     | 0.51              |
| 1:A:367:GLU:HB3   | 1:A:688:MET:HE1   | 1.92                     | 0.51              |
| 1:A:798:GLN:HE21  | 1:A:861:TRP:HE1   | 1.57                     | 0.51              |
| 1:B:128:MET:HE3   | 1:B:336:VAL:HA    | 1.93                     | 0.51              |
| 1:C:674:ILE:O     | 1:C:678:LEU:N     | 2.37                     | 0.51              |
| 1:A:414:ARG:HE    | 1:A:440:LEU:HD13  | 1.75                     | 0.51              |
| 1:B:367:GLU:HB3   | 1:B:688:MET:HE1   | 1.92                     | 0.51              |
| 1:F:674:ILE:O     | 1:F:678:LEU:N     | 2.36                     | 0.51              |
| 1:F:518:LYS:HD3   | 1:F:524:TRP:CE2   | 2.46                     | 0.51              |
| 1:A:314:TYR:OH    | 3:A:1002:POV:H29  | 2.11                     | 0.51              |
| 1:A:518:LYS:HD3   | 1:A:524:TRP:CE2   | 2.46                     | 0.51              |
| 1:B:459:THR:HB    | 1:B:473:VAL:HG23  | 1.93                     | 0.51              |
| 1:C:367:GLU:HB3   | 1:C:688:MET:HE1   | 1.92                     | 0.51              |
| 1:D:198:PRO:HA    | 1:D:260:VAL:HG23  | 1.92                     | 0.51              |
| 1:D:798:GLN:HE21  | 1:D:861:TRP:HE1   | 1.57                     | 0.51              |
| 1:E:217:VAL:HG12  | 1:E:218:THR:HG23  | 1.93                     | 0.51              |
| 1:E:581:ALA:HB2   | 1:E:610:VAL:HG22  | 1.91                     | 0.51              |
| 1:A:128:MET:HE3   | 1:A:336:VAL:HA    | 1.93                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:380:THR:OG1   | 1:A:381:GLY:N     | 2.44                     | 0.51              |
| 1:B:217:VAL:HG12  | 1:B:218:THR:HG23  | 1.93                     | 0.51              |
| 1:C:217:VAL:HG12  | 1:C:218:THR:HG23  | 1.93                     | 0.51              |
| 1:D:380:THR:OG1   | 1:D:381:GLY:N     | 2.44                     | 0.51              |
| 1:F:312:CYS:HB3   | 1:F:322:ILE:HG12  | 1.92                     | 0.51              |
| 1:A:198:PRO:HA    | 1:A:260:VAL:HG23  | 1.92                     | 0.50              |
| 1:E:307:LEU:HD23  | 3:E:1003:POV:H31E | 1.92                     | 0.50              |
| 3:F:1003:POV:H24  | 3:F:1004:POV:H23  | 1.93                     | 0.50              |
| 1:D:128:MET:HE3   | 1:D:336:VAL:HA    | 1.93                     | 0.50              |
| 1:D:518:LYS:HD3   | 1:D:524:TRP:CE2   | 2.46                     | 0.50              |
| 1:F:367:GLU:HB3   | 1:F:688:MET:HE1   | 1.92                     | 0.50              |
| 1:F:380:THR:OG1   | 1:F:381:GLY:N     | 2.44                     | 0.50              |
| 3:A:1010:POV:H13B | 3:F:1002:POV:H13B | 1.94                     | 0.50              |
| 1:B:204:LEU:HD12  | 1:B:208:THR:HG21  | 1.92                     | 0.50              |
| 1:C:380:THR:OG1   | 1:C:381:GLY:N     | 2.44                     | 0.50              |
| 1:C:518:LYS:HD3   | 1:C:524:TRP:CE2   | 2.46                     | 0.50              |
| 3:C:1006:POV:H37A | 3:D:1011:POV:H27A | 1.93                     | 0.50              |
| 3:C:1007:POV:H1   | 3:D:1011:POV:H15B | 1.94                     | 0.50              |
| 1:E:518:LYS:HD3   | 1:E:524:TRP:CE2   | 2.46                     | 0.50              |
| 1:F:408:ALA:HB1   | 1:F:474:LYS:HD3   | 1.92                     | 0.50              |
| 1:C:408:ALA:HB1   | 1:C:474:LYS:HD3   | 1.92                     | 0.50              |
| 1:E:367:GLU:HB3   | 1:E:688:MET:HE1   | 1.92                     | 0.50              |
| 1:E:380:THR:OG1   | 1:E:381:GLY:N     | 2.44                     | 0.50              |
| 1:F:217:VAL:HG12  | 1:F:218:THR:HG23  | 1.93                     | 0.50              |
| 1:B:518:LYS:HD3   | 1:B:524:TRP:CE2   | 2.46                     | 0.50              |
| 1:D:367:GLU:HB3   | 1:D:688:MET:HE1   | 1.93                     | 0.50              |
| 3:D:1011:POV:H32  | 3:D:1011:POV:H22A | 1.94                     | 0.50              |
| 1:F:550:LEU:O     | 1:F:682:ARG:NH2   | 2.41                     | 0.50              |
| 3:A:1007:POV:H25  | 3:A:1007:POV:H32  | 1.93                     | 0.50              |
| 1:C:312:CYS:HB3   | 1:C:322:ILE:HG12  | 1.92                     | 0.50              |
| 1:C:318:GLY:HA2   | 1:D:786:GLN:NE2   | 2.26                     | 0.50              |
| 1:F:379:LYS:HA    | 1:F:383:LEU:HD12  | 1.94                     | 0.50              |
| 1:A:769:GLY:HA2   | 3:A:1010:POV:H31H | 1.94                     | 0.50              |
| 1:C:128:MET:HE3   | 1:C:336:VAL:HA    | 1.93                     | 0.50              |
| 1:C:379:LYS:HA    | 1:C:383:LEU:HD12  | 1.94                     | 0.50              |
| 3:C:1002:POV:H39A | 3:C:1002:POV:H212 | 1.94                     | 0.50              |
| 1:A:150:LEU:HD23  | 1:A:336:VAL:HG12  | 1.94                     | 0.49              |
| 1:A:786:GLN:HE22  | 1:F:319:ILE:H     | 1.59                     | 0.49              |
| 1:B:380:THR:O     | 1:B:384:THR:OG1   | 2.29                     | 0.49              |
| 1:C:150:LEU:HD23  | 1:C:336:VAL:HG12  | 1.94                     | 0.49              |
| 3:D:1009:POV:H31F | 3:D:1010:POV:H21G | 1.94                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:315:ARG:CZ    | 3:A:1003:POV:O13  | 2.54                     | 0.49              |
| 1:D:306:LEU:CD1   | 1:E:868:VAL:HG21  | 2.42                     | 0.49              |
| 1:A:217:VAL:HG12  | 1:A:218:THR:HG23  | 1.93                     | 0.49              |
| 3:A:1004:POV:H24  | 3:A:1005:POV:H23  | 1.93                     | 0.49              |
| 3:C:1009:POV:H35  | 3:D:1008:POV:H27  | 1.94                     | 0.49              |
| 1:E:379:LYS:HA    | 1:E:383:LEU:HD12  | 1.94                     | 0.49              |
| 1:E:846:SER:OG    | 1:E:847:GLU:N     | 2.45                     | 0.49              |
| 1:F:128:MET:HE3   | 1:F:336:VAL:HA    | 1.93                     | 0.49              |
| 3:F:1006:POV:H25  | 3:F:1006:POV:H32  | 1.94                     | 0.49              |
| 1:B:380:THR:OG1   | 1:B:381:GLY:N     | 2.44                     | 0.49              |
| 3:C:1007:POV:H3   | 3:D:1011:POV:H15B | 1.95                     | 0.49              |
| 1:D:217:VAL:HG12  | 1:D:218:THR:HG23  | 1.93                     | 0.49              |
| 1:A:674:ILE:O     | 1:A:678:LEU:N     | 2.36                     | 0.49              |
| 1:A:783:GLY:HA2   | 1:F:313:PHE:O     | 2.13                     | 0.49              |
| 1:B:150:LEU:HD23  | 1:B:336:VAL:HG12  | 1.94                     | 0.49              |
| 1:B:379:LYS:HA    | 1:B:383:LEU:HD12  | 1.94                     | 0.49              |
| 1:B:846:SER:OG    | 1:B:847:GLU:N     | 2.45                     | 0.49              |
| 1:D:150:LEU:HD23  | 1:D:336:VAL:HG12  | 1.94                     | 0.49              |
| 1:A:551:GLY:HA3   | 1:A:747:PRO:HD3   | 1.95                     | 0.49              |
| 1:B:551:GLY:HA3   | 1:B:747:PRO:HD3   | 1.95                     | 0.49              |
| 1:F:846:SER:OG    | 1:F:847:GLU:N     | 2.45                     | 0.49              |
| 1:D:551:GLY:HA3   | 1:D:747:PRO:HD3   | 1.95                     | 0.49              |
| 1:E:872:PHE:HB3   | 1:E:876:MET:HE2   | 1.95                     | 0.49              |
| 1:E:708:LEU:CD2   | 3:E:1003:POV:H312 | 2.38                     | 0.49              |
| 1:E:551:GLY:HA3   | 1:E:747:PRO:HD3   | 1.95                     | 0.49              |
| 3:A:1002:POV:H314 | 1:B:772:ILE:CD1   | 2.43                     | 0.49              |
| 1:B:872:PHE:HB3   | 1:B:876:MET:HE2   | 1.95                     | 0.49              |
| 1:C:846:SER:OG    | 1:C:847:GLU:N     | 2.45                     | 0.49              |
| 1:D:846:SER:OG    | 1:D:847:GLU:N     | 2.45                     | 0.49              |
| 1:E:150:LEU:HD23  | 1:E:336:VAL:HG12  | 1.94                     | 0.49              |
| 3:E:1007:POV:H1   | 3:F:1010:POV:H15B | 1.95                     | 0.49              |
| 3:E:1007:POV:H3   | 3:F:1010:POV:H15B | 1.95                     | 0.49              |
| 1:F:150:LEU:HD23  | 1:F:336:VAL:HG12  | 1.94                     | 0.49              |
| 3:A:1003:POV:H29  | 3:A:1006:POV:H310 | 1.94                     | 0.48              |
| 3:A:1012:POV:H31F | 3:B:1010:POV:H21G | 1.95                     | 0.48              |
| 3:A:1012:POV:H33A | 3:D:1009:POV:H23A | 1.94                     | 0.48              |
| 1:C:332:ILE:HG21  | 1:C:702:LEU:HB2   | 1.95                     | 0.48              |
| 1:B:391:HIS:HB3   | 1:B:394:TYR:HD2   | 1.78                     | 0.48              |
| 1:C:430:LEU:O     | 1:C:435:LYS:HE2   | 2.13                     | 0.48              |
| 1:A:846:SER:OG    | 1:A:847:GLU:N     | 2.45                     | 0.48              |
| 1:C:550:LEU:O     | 1:C:682:ARG:NH2   | 2.41                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:872:PHE:HB3   | 1:A:876:MET:HE2   | 1.95                     | 0.48              |
| 1:E:306:LEU:CD1   | 1:F:868:VAL:HG23  | 2.35                     | 0.48              |
| 1:F:872:PHE:HB3   | 1:F:876:MET:HE2   | 1.95                     | 0.48              |
| 1:A:379:LYS:HA    | 1:A:383:LEU:HD12  | 1.94                     | 0.48              |
| 3:D:1007:POV:H1   | 3:E:1010:POV:H15B | 1.94                     | 0.48              |
| 1:F:332:ILE:HG21  | 1:F:702:LEU:HB2   | 1.95                     | 0.48              |
| 3:F:1004:POV:H29  | 3:F:1004:POV:H26  | 1.53                     | 0.48              |
| 1:C:551:GLY:HA3   | 1:C:747:PRO:HD3   | 1.95                     | 0.48              |
| 1:C:872:PHE:HB3   | 1:C:876:MET:HE2   | 1.95                     | 0.48              |
| 1:E:391:HIS:HB3   | 1:E:394:TYR:HD2   | 1.78                     | 0.48              |
| 1:B:309:TRP:CH2   | 1:C:860:ILE:HG21  | 2.49                     | 0.48              |
| 1:C:637:ASN:OD1   | 1:C:638:ASP:N     | 2.47                     | 0.48              |
| 1:D:379:LYS:HA    | 1:D:383:LEU:HD12  | 1.94                     | 0.48              |
| 1:D:391:HIS:HB3   | 1:D:394:TYR:HD2   | 1.78                     | 0.48              |
| 1:E:380:THR:O     | 1:E:384:THR:OG1   | 2.29                     | 0.48              |
| 1:E:550:LEU:O     | 1:E:682:ARG:NH2   | 2.41                     | 0.48              |
| 1:F:637:ASN:OD1   | 1:F:638:ASP:N     | 2.47                     | 0.48              |
| 3:B:1003:POV:H217 | 1:C:768:ILE:HG21  | 1.95                     | 0.48              |
| 1:D:872:PHE:HB3   | 1:D:876:MET:HE2   | 1.95                     | 0.48              |
| 1:A:307:LEU:HD23  | 3:A:1003:POV:H31E | 1.95                     | 0.48              |
| 3:A:1007:POV:H1   | 3:B:1002:POV:H15B | 1.96                     | 0.48              |
| 1:C:391:HIS:HB3   | 1:C:394:TYR:HD2   | 1.78                     | 0.48              |
| 3:F:1008:POV:H31F | 3:F:1009:POV:H21G | 1.96                     | 0.48              |
| 1:C:280:ALA:HB2   | 1:C:643:LYS:HD2   | 1.96                     | 0.48              |
| 3:D:1005:POV:H26  | 3:D:1005:POV:H29  | 1.57                     | 0.48              |
| 1:F:280:ALA:HB2   | 1:F:643:LYS:HD2   | 1.96                     | 0.48              |
| 1:F:391:HIS:HB3   | 1:F:394:TYR:HD2   | 1.78                     | 0.48              |
| 1:F:551:GLY:HA3   | 1:F:747:PRO:HD3   | 1.95                     | 0.48              |
| 3:A:1002:POV:C312 | 1:B:772:ILE:HD13  | 2.41                     | 0.47              |
| 1:B:280:ALA:HB2   | 1:B:643:LYS:HD2   | 1.96                     | 0.47              |
| 1:C:380:THR:O     | 1:C:384:THR:OG1   | 2.29                     | 0.47              |
| 1:E:307:LEU:CD2   | 3:E:1003:POV:H31E | 2.44                     | 0.47              |
| 1:E:332:ILE:HG21  | 1:E:702:LEU:HB2   | 1.95                     | 0.47              |
| 3:A:1008:POV:H212 | 3:F:1009:POV:H39A | 1.96                     | 0.47              |
| 1:A:550:LEU:O     | 1:A:682:ARG:NH2   | 2.41                     | 0.47              |
| 1:A:868:VAL:CG2   | 1:F:306:LEU:HD11  | 2.44                     | 0.47              |
| 1:B:332:ILE:HG21  | 1:B:702:LEU:HB2   | 1.95                     | 0.47              |
| 1:B:378:ASP:OD2   | 2:B:1001:BEF:F2   | 2.22                     | 0.47              |
| 3:B:1003:POV:H39A | 3:B:1003:POV:H212 | 1.96                     | 0.47              |
| 1:A:391:HIS:HB3   | 1:A:394:TYR:HD2   | 1.78                     | 0.47              |
| 3:A:1010:POV:H13A | 3:A:1010:POV:H11A | 1.52                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:E:280:ALA:HB2   | 1:E:643:LYS:HD2   | 1.96                     | 0.47              |
| 1:E:481:LEU:HD21  | 1:E:495:HIS:HA    | 1.97                     | 0.47              |
| 1:A:637:ASN:OD1   | 1:A:638:ASP:N     | 2.47                     | 0.47              |
| 1:B:307:LEU:HD23  | 3:B:1004:POV:H31E | 1.96                     | 0.47              |
| 1:B:481:LEU:HD21  | 1:B:495:HIS:HA    | 1.97                     | 0.47              |
| 3:C:1003:POV:H29  | 3:C:1006:POV:H310 | 1.96                     | 0.47              |
| 1:D:378:ASP:OD2   | 2:D:1001:BEF:F2   | 2.22                     | 0.47              |
| 1:A:280:ALA:HB2   | 1:A:643:LYS:HD2   | 1.96                     | 0.47              |
| 3:B:1008:POV:H1   | 3:C:1010:POV:H15B | 1.96                     | 0.47              |
| 3:C:1006:POV:H32  | 3:C:1008:POV:H32A | 1.97                     | 0.47              |
| 1:D:314:TYR:CD1   | 1:E:776:THR:HG22  | 2.50                     | 0.47              |
| 1:D:332:ILE:HG21  | 1:D:702:LEU:HB2   | 1.95                     | 0.47              |
| 1:F:380:THR:O     | 1:F:384:THR:OG1   | 2.29                     | 0.47              |
| 1:C:313:PHE:O     | 1:D:783:GLY:C     | 2.56                     | 0.47              |
| 1:C:378:ASP:OD2   | 2:C:1001:BEF:F2   | 2.22                     | 0.47              |
| 1:D:280:ALA:HB2   | 1:D:643:LYS:HD2   | 1.96                     | 0.47              |
| 1:A:332:ILE:HG21  | 1:A:702:LEU:HB2   | 1.95                     | 0.47              |
| 1:C:809:ILE:HD12  | 1:C:809:ILE:H     | 1.80                     | 0.47              |
| 1:D:365:ALA:HB1   | 1:D:647:THR:HG23  | 1.97                     | 0.47              |
| 1:A:378:ASP:OD2   | 2:A:1001:BEF:F2   | 2.22                     | 0.47              |
| 1:C:481:LEU:HD21  | 1:C:495:HIS:HA    | 1.97                     | 0.47              |
| 3:C:1006:POV:H210 | 3:C:1008:POV:H39  | 1.96                     | 0.47              |
| 1:A:868:VAL:HG21  | 1:F:306:LEU:CD1   | 2.44                     | 0.46              |
| 3:A:1002:POV:H13  | 3:A:1003:POV:H15A | 1.97                     | 0.46              |
| 1:A:380:THR:O     | 1:A:384:THR:OG1   | 2.29                     | 0.46              |
| 3:A:1011:POV:H15B | 3:F:1006:POV:H1   | 1.98                     | 0.46              |
| 1:B:550:LEU:O     | 1:B:682:ARG:NH2   | 2.41                     | 0.46              |
| 3:D:1004:POV:H34  | 3:D:1004:POV:H210 | 1.97                     | 0.46              |
| 1:F:378:ASP:OD2   | 2:F:1001:BEF:F2   | 2.22                     | 0.46              |
| 1:F:481:LEU:HD21  | 1:F:495:HIS:HA    | 1.97                     | 0.46              |
| 3:F:1002:POV:H29  | 3:F:1005:POV:H310 | 1.97                     | 0.46              |
| 1:A:701:HIS:CD2   | 1:A:702:LEU:HG    | 2.50                     | 0.46              |
| 1:C:701:HIS:CD2   | 1:C:702:LEU:HG    | 2.50                     | 0.46              |
| 1:E:701:HIS:CD2   | 1:E:702:LEU:HG    | 2.50                     | 0.46              |
| 1:F:809:ILE:H     | 1:F:809:ILE:HD12  | 1.80                     | 0.46              |
| 3:B:1007:POV:H11  | 3:B:1007:POV:H15A | 1.62                     | 0.46              |
| 3:C:1008:POV:H14A | 3:C:1008:POV:H11  | 1.62                     | 0.46              |
| 1:D:637:ASN:OD1   | 1:D:638:ASP:N     | 2.47                     | 0.46              |
| 3:D:1010:POV:H3   | 3:D:1010:POV:O13  | 2.16                     | 0.46              |
| 1:F:365:ALA:HB1   | 1:F:647:THR:HG23  | 1.97                     | 0.46              |
| 1:F:701:HIS:CD2   | 1:F:702:LEU:HG    | 2.50                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:365:ALA:HB1   | 1:A:647:THR:HG23  | 1.97                     | 0.46              |
| 3:B:1003:POV:H31C | 1:C:772:ILE:CD1   | 2.39                     | 0.46              |
| 1:D:768:ILE:HD13  | 3:D:1004:POV:C313 | 2.45                     | 0.46              |
| 3:F:1005:POV:H11  | 3:F:1005:POV:H15A | 1.59                     | 0.46              |
| 1:D:701:HIS:CD2   | 1:D:702:LEU:HG    | 2.50                     | 0.46              |
| 1:D:809:ILE:H     | 1:D:809:ILE:HD12  | 1.81                     | 0.46              |
| 1:A:213:ASP:OD1   | 1:A:267:THR:N     | 2.49                     | 0.46              |
| 1:A:860:ILE:HG21  | 1:F:309:TRP:CH2   | 2.51                     | 0.46              |
| 1:D:316:THR:HG23  | 1:E:783:GLY:H     | 1.73                     | 0.46              |
| 3:F:1009:POV:H3   | 3:F:1009:POV:O13  | 2.16                     | 0.46              |
| 1:B:365:ALA:HB1   | 1:B:647:THR:HG23  | 1.97                     | 0.46              |
| 1:B:650:ALA:HB3   | 1:B:665:VAL:HA    | 1.98                     | 0.46              |
| 1:D:650:ALA:HB3   | 1:D:665:VAL:HA    | 1.98                     | 0.46              |
| 1:E:458:VAL:HG23  | 1:E:474:LYS:HB2   | 1.98                     | 0.46              |
| 3:E:1006:POV:H15A | 3:E:1006:POV:H11  | 1.59                     | 0.46              |
| 1:F:458:VAL:HG23  | 1:F:474:LYS:HB2   | 1.98                     | 0.46              |
| 1:C:458:VAL:HG23  | 1:C:474:LYS:HB2   | 1.98                     | 0.46              |
| 1:E:365:ALA:HB1   | 1:E:647:THR:HG23  | 1.97                     | 0.46              |
| 1:E:674:ILE:O     | 1:E:678:LEU:N     | 2.36                     | 0.46              |
| 3:F:1008:POV:H28  | 3:F:1008:POV:H211 | 1.73                     | 0.46              |
| 1:A:458:VAL:HG23  | 1:A:474:LYS:HB2   | 1.98                     | 0.46              |
| 1:B:348:VAL:HB    | 1:B:737:ALA:HB1   | 1.98                     | 0.46              |
| 1:B:458:VAL:HG23  | 1:B:474:LYS:HB2   | 1.98                     | 0.46              |
| 3:B:1010:POV:O13  | 3:B:1010:POV:H3   | 2.15                     | 0.46              |
| 3:D:1002:POV:H13A | 3:D:1002:POV:H11A | 1.50                     | 0.46              |
| 3:D:1006:POV:H11  | 3:D:1006:POV:H15A | 1.60                     | 0.46              |
| 1:E:348:VAL:HB    | 1:E:737:ALA:HB1   | 1.98                     | 0.46              |
| 1:F:213:ASP:OD1   | 1:F:267:THR:N     | 2.49                     | 0.46              |
| 1:A:481:LEU:HD21  | 1:A:495:HIS:HA    | 1.97                     | 0.45              |
| 1:A:650:ALA:HB3   | 1:A:665:VAL:HA    | 1.98                     | 0.45              |
| 1:B:313:PHE:O     | 1:C:783:GLY:C     | 2.60                     | 0.45              |
| 1:C:365:ALA:HB1   | 1:C:647:THR:HG23  | 1.97                     | 0.45              |
| 1:C:385:LYS:NZ    | 1:C:536:PRO:O     | 2.50                     | 0.45              |
| 1:A:430:LEU:HB2   | 1:A:435:LYS:CB    | 2.47                     | 0.45              |
| 1:B:385:LYS:NZ    | 1:B:536:PRO:O     | 2.49                     | 0.45              |
| 1:D:213:ASP:OD1   | 1:D:267:THR:N     | 2.49                     | 0.45              |
| 1:E:650:ALA:HB3   | 1:E:665:VAL:HA    | 1.98                     | 0.45              |
| 3:A:1005:POV:H29  | 3:A:1005:POV:H26  | 1.61                     | 0.45              |
| 1:B:213:ASP:OD1   | 1:B:267:THR:N     | 2.49                     | 0.45              |
| 1:B:701:HIS:CD2   | 1:B:702:LEU:HG    | 2.50                     | 0.45              |
| 1:D:458:VAL:HG23  | 1:D:474:LYS:HB2   | 1.98                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:A:1012:POV:H37  | 3:C:1009:POV:H27  | 1.99                     | 0.45              |
| 1:C:310:THR:HG23  | 1:D:772:ILE:CG2   | 2.46                     | 0.45              |
| 3:D:1009:POV:H28  | 3:D:1009:POV:H211 | 1.79                     | 0.45              |
| 1:F:385:LYS:NZ    | 1:F:536:PRO:O     | 2.49                     | 0.45              |
| 3:A:1002:POV:H21E | 3:A:1007:POV:H31H | 1.98                     | 0.45              |
| 1:C:213:ASP:OD1   | 1:C:267:THR:N     | 2.49                     | 0.45              |
| 1:C:517:ARG:O     | 1:C:525:GLU:N     | 2.36                     | 0.45              |
| 1:D:481:LEU:HD21  | 1:D:495:HIS:HA    | 1.97                     | 0.45              |
| 1:E:637:ASN:OD1   | 1:E:638:ASP:N     | 2.47                     | 0.45              |
| 1:E:809:ILE:HD12  | 1:E:809:ILE:H     | 1.80                     | 0.45              |
| 1:A:809:ILE:HD12  | 1:A:809:ILE:H     | 1.81                     | 0.45              |
| 3:A:1010:POV:H13  | 3:F:1002:POV:H15A | 1.98                     | 0.45              |
| 1:E:385:LYS:NZ    | 1:E:536:PRO:O     | 2.49                     | 0.45              |
| 1:A:385:LYS:NZ    | 1:A:536:PRO:O     | 2.49                     | 0.45              |
| 3:C:1007:POV:H29  | 3:C:1007:POV:H26A | 1.79                     | 0.45              |
| 1:E:213:ASP:OD1   | 1:E:267:THR:N     | 2.49                     | 0.45              |
| 3:F:1010:POV:H32  | 3:F:1010:POV:H22A | 1.98                     | 0.45              |
| 1:B:809:ILE:HD12  | 1:B:809:ILE:H     | 1.80                     | 0.45              |
| 3:C:1009:POV:H211 | 3:C:1009:POV:H28  | 1.76                     | 0.45              |
| 1:F:315:ARG:CZ    | 3:F:1002:POV:O13  | 2.54                     | 0.45              |
| 3:B:1002:POV:H312 | 3:B:1002:POV:H214 | 1.99                     | 0.45              |
| 1:C:562:VAL:HG22  | 1:C:608:ALA:HB3   | 1.99                     | 0.45              |
| 1:D:385:LYS:NZ    | 1:D:536:PRO:O     | 2.50                     | 0.45              |
| 1:D:411:ALA:HB3   | 1:D:474:LYS:HG3   | 1.99                     | 0.45              |
| 1:D:550:LEU:O     | 1:D:682:ARG:NH2   | 2.41                     | 0.45              |
| 1:F:464:SER:HB2   | 1:F:468:GLU:HB2   | 1.99                     | 0.45              |
| 3:F:1005:POV:H21J | 3:F:1010:POV:H31F | 1.98                     | 0.45              |
| 1:B:316:THR:HG23  | 1:C:783:GLY:H     | 1.70                     | 0.45              |
| 1:B:637:ASN:OD1   | 1:B:638:ASP:N     | 2.47                     | 0.45              |
| 1:D:464:SER:HB2   | 1:D:468:GLU:HB2   | 1.99                     | 0.45              |
| 1:D:555:LYS:NZ    | 1:D:604:ALA:O     | 2.41                     | 0.45              |
| 1:F:650:ALA:HB3   | 1:F:665:VAL:HA    | 1.98                     | 0.45              |
| 1:A:464:SER:HB2   | 1:A:468:GLU:HB2   | 1.99                     | 0.44              |
| 1:A:776:THR:HG22  | 1:F:314:TYR:CE1   | 2.52                     | 0.44              |
| 1:C:316:THR:HG22  | 1:D:783:GLY:CA    | 2.47                     | 0.44              |
| 1:C:464:SER:HB2   | 1:C:468:GLU:HB2   | 1.99                     | 0.44              |
| 3:C:1002:POV:H21D | 1:D:768:ILE:HG21  | 1.99                     | 0.44              |
| 3:C:1005:POV:H21C | 3:C:1006:POV:H21B | 2.00                     | 0.44              |
| 3:C:1006:POV:H15A | 3:C:1006:POV:H11  | 1.59                     | 0.44              |
| 3:D:1007:POV:H25  | 3:D:1007:POV:H32  | 1.97                     | 0.44              |
| 1:E:562:VAL:HG22  | 1:E:608:ALA:HB3   | 2.00                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:E:1002:POV:H314 | 1:F:772:ILE:HD11  | 1.99                     | 0.44              |
| 1:B:306:LEU:HD13  | 1:C:868:VAL:HG21  | 1.98                     | 0.44              |
| 1:B:562:VAL:HG22  | 1:B:608:ALA:HB3   | 1.99                     | 0.44              |
| 1:D:380:THR:O     | 1:D:384:THR:OG1   | 2.29                     | 0.44              |
| 3:E:1009:POV:H3   | 3:E:1009:POV:O13  | 2.18                     | 0.44              |
| 1:A:411:ALA:HB3   | 1:A:474:LYS:HG3   | 1.99                     | 0.44              |
| 1:A:702:LEU:HD21  | 1:A:799:ILE:HD13  | 1.99                     | 0.44              |
| 1:C:650:ALA:HB3   | 1:C:665:VAL:HA    | 1.98                     | 0.44              |
| 1:D:768:ILE:HD13  | 3:D:1004:POV:H312 | 1.99                     | 0.44              |
| 1:F:562:VAL:HG22  | 1:F:608:ALA:HB3   | 1.99                     | 0.44              |
| 3:F:1002:POV:H21E | 3:F:1002:POV:H39  | 2.00                     | 0.44              |
| 1:A:314:TYR:CD1   | 1:B:776:THR:HG22  | 2.53                     | 0.44              |
| 1:A:510:PHE:HE1   | 1:A:567:GLU:HG2   | 1.83                     | 0.44              |
| 1:C:400:SER:HA    | 1:C:401:PRO:HD2   | 1.91                     | 0.44              |
| 1:D:348:VAL:HB    | 1:D:737:ALA:HB1   | 1.99                     | 0.44              |
| 1:D:702:LEU:HD21  | 1:D:799:ILE:HD13  | 1.99                     | 0.44              |
| 1:E:412:ALA:O     | 1:E:414:ARG:NH2   | 2.51                     | 0.44              |
| 1:F:346:MET:SD    | 1:F:363:LEU:HB3   | 2.58                     | 0.44              |
| 1:A:346:MET:SD    | 1:A:363:LEU:HB3   | 2.58                     | 0.44              |
| 1:B:412:ALA:O     | 1:B:414:ARG:NH2   | 2.51                     | 0.44              |
| 1:C:346:MET:SD    | 1:C:363:LEU:HB3   | 2.58                     | 0.44              |
| 1:F:348:VAL:HB    | 1:F:737:ALA:HB1   | 1.98                     | 0.44              |
| 3:A:1009:POV:H3   | 3:A:1009:POV:O13  | 2.16                     | 0.44              |
| 1:B:464:SER:HB2   | 1:B:468:GLU:HB2   | 1.98                     | 0.44              |
| 1:B:510:PHE:HE1   | 1:B:567:GLU:HG2   | 1.83                     | 0.44              |
| 1:C:704:ILE:HG12  | 3:C:1003:POV:H31D | 1.99                     | 0.44              |
| 1:D:346:MET:SD    | 1:D:363:LEU:HB3   | 2.58                     | 0.44              |
| 3:E:1002:POV:H13B | 3:E:1003:POV:H13B | 2.00                     | 0.44              |
| 1:A:412:ALA:O     | 1:A:414:ARG:NH2   | 2.51                     | 0.44              |
| 3:A:1002:POV:H31H | 1:B:769:GLY:HA2   | 1.99                     | 0.44              |
| 3:B:1009:POV:H11  | 3:B:1009:POV:H14A | 1.60                     | 0.44              |
| 3:C:1008:POV:H28  | 3:C:1008:POV:H211 | 1.79                     | 0.44              |
| 3:C:1010:POV:H15A | 3:C:1010:POV:H11  | 1.75                     | 0.44              |
| 1:D:375:LEU:HB3   | 1:D:554:VAL:HG12  | 2.00                     | 0.44              |
| 1:D:510:PHE:HE1   | 1:D:567:GLU:HG2   | 1.83                     | 0.44              |
| 1:E:510:PHE:HE1   | 1:E:567:GLU:HG2   | 1.83                     | 0.44              |
| 1:F:411:ALA:HB3   | 1:F:474:LYS:HG3   | 1.99                     | 0.44              |
| 1:A:348:VAL:HB    | 1:A:737:ALA:HB1   | 1.98                     | 0.44              |
| 3:A:1002:POV:H13B | 3:A:1003:POV:H13B | 2.00                     | 0.44              |
| 1:B:702:LEU:HD21  | 1:B:799:ILE:HD13  | 1.99                     | 0.44              |
| 3:B:1006:POV:H26  | 3:B:1006:POV:H29  | 1.54                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:348:VAL:HB    | 1:C:737:ALA:HB1   | 1.98                     | 0.44              |
| 1:C:411:ALA:HB3   | 1:C:474:LYS:HG3   | 1.99                     | 0.44              |
| 3:F:1007:POV:H14A | 3:F:1007:POV:H11  | 1.60                     | 0.44              |
| 1:A:717:LEU:HB3   | 1:A:722:ILE:HD11  | 2.00                     | 0.43              |
| 3:B:1008:POV:H37  | 3:C:1005:POV:H210 | 2.00                     | 0.43              |
| 1:D:717:LEU:HB3   | 1:D:722:ILE:HD11  | 2.00                     | 0.43              |
| 1:E:346:MET:SD    | 1:E:363:LEU:HB3   | 2.58                     | 0.43              |
| 1:E:464:SER:HB2   | 1:E:468:GLU:HB2   | 1.99                     | 0.43              |
| 1:E:702:LEU:HD21  | 1:E:799:ILE:HD13  | 1.99                     | 0.43              |
| 1:A:375:LEU:HB3   | 1:A:554:VAL:HG12  | 2.00                     | 0.43              |
| 1:B:123:PRO:HA    | 1:B:126:PHE:HD2   | 1.83                     | 0.43              |
| 1:D:412:ALA:O     | 1:D:414:ARG:NH2   | 2.51                     | 0.43              |
| 1:A:123:PRO:HG2   | 1:A:294:GLY:HA3   | 2.01                     | 0.43              |
| 1:A:562:VAL:HG22  | 1:A:608:ALA:HB3   | 1.99                     | 0.43              |
| 1:B:123:PRO:HG2   | 1:B:294:GLY:HA3   | 2.01                     | 0.43              |
| 1:D:562:VAL:HG22  | 1:D:608:ALA:HB3   | 1.99                     | 0.43              |
| 1:E:123:PRO:HA    | 1:E:126:PHE:HD2   | 1.84                     | 0.43              |
| 1:E:717:LEU:HB3   | 1:E:722:ILE:HD11  | 2.00                     | 0.43              |
| 1:F:768:ILE:HD11  | 3:F:1003:POV:H31D | 1.96                     | 0.43              |
| 1:A:123:PRO:HA    | 1:A:126:PHE:HD2   | 1.83                     | 0.43              |
| 3:B:1006:POV:H21E | 3:B:1007:POV:H21D | 2.00                     | 0.43              |
| 1:C:412:ALA:O     | 1:C:414:ARG:NH2   | 2.51                     | 0.43              |
| 1:D:123:PRO:HA    | 1:D:126:PHE:HD2   | 1.83                     | 0.43              |
| 1:F:517:ARG:O     | 1:F:525:GLU:N     | 2.36                     | 0.43              |
| 1:F:717:LEU:HB3   | 1:F:722:ILE:HD11  | 2.00                     | 0.43              |
| 1:A:306:LEU:HD13  | 1:B:868:VAL:HG21  | 1.99                     | 0.43              |
| 1:F:702:LEU:HD21  | 1:F:799:ILE:HD13  | 1.99                     | 0.43              |
| 1:B:346:MET:SD    | 1:B:363:LEU:HB3   | 2.58                     | 0.43              |
| 1:B:488:HIS:ND1   | 1:B:489:PRO:O     | 2.52                     | 0.43              |
| 1:C:309:TRP:CZ3   | 1:D:860:ILE:CG2   | 3.02                     | 0.43              |
| 1:C:717:LEU:HB3   | 1:C:722:ILE:HD11  | 2.00                     | 0.43              |
| 3:C:1009:POV:H3   | 3:C:1009:POV:O13  | 2.18                     | 0.43              |
| 1:D:407:THR:HG23  | 1:D:472:CYS:SG    | 2.59                     | 0.43              |
| 1:E:634:ASP:OD1   | 2:E:1001:BEF:F1   | 2.26                     | 0.43              |
| 1:F:510:PHE:HE1   | 1:F:567:GLU:HG2   | 1.83                     | 0.43              |
| 3:A:1006:POV:H15A | 3:A:1006:POV:H11  | 1.60                     | 0.43              |
| 3:B:1003:POV:H13A | 3:B:1003:POV:H11A | 1.55                     | 0.43              |
| 1:C:616:TYR:CE2   | 1:C:644:LYS:HD2   | 2.54                     | 0.43              |
| 1:C:702:LEU:HD21  | 1:C:799:ILE:HD13  | 1.99                     | 0.43              |
| 1:D:123:PRO:HG2   | 1:D:294:GLY:HA3   | 2.01                     | 0.43              |
| 1:E:123:PRO:HG2   | 1:E:294:GLY:HA3   | 2.01                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:E:309:TRP:CZ3   | 1:F:860:ILE:CG2   | 3.01                     | 0.43              |
| 3:E:1005:POV:H21C | 3:E:1006:POV:H21B | 2.00                     | 0.43              |
| 1:A:488:HIS:ND1   | 1:A:489:PRO:O     | 2.52                     | 0.43              |
| 1:A:616:TYR:CE2   | 1:A:644:LYS:HD2   | 2.54                     | 0.43              |
| 1:D:518:LYS:HB3   | 1:D:524:TRP:HA    | 2.01                     | 0.43              |
| 3:D:1007:POV:H35  | 3:E:1005:POV:H210 | 1.99                     | 0.43              |
| 1:E:316:THR:HG22  | 1:F:783:GLY:CA    | 2.49                     | 0.43              |
| 1:E:411:ALA:HB3   | 1:E:474:LYS:HG3   | 1.99                     | 0.43              |
| 1:E:445:VAL:HG22  | 1:E:462:VAL:HG12  | 2.01                     | 0.43              |
| 1:E:488:HIS:ND1   | 1:E:489:PRO:O     | 2.52                     | 0.43              |
| 3:E:1008:POV:H211 | 3:E:1008:POV:H28  | 1.81                     | 0.43              |
| 1:F:412:ALA:O     | 1:F:414:ARG:NH2   | 2.51                     | 0.43              |
| 1:A:318:GLY:HA2   | 1:B:786:GLN:NE2   | 2.34                     | 0.43              |
| 3:A:1008:POV:H11  | 3:A:1008:POV:H14A | 1.61                     | 0.43              |
| 1:B:411:ALA:HB3   | 1:B:474:LYS:HG3   | 1.99                     | 0.43              |
| 1:C:375:LEU:HB3   | 1:C:554:VAL:HG12  | 2.00                     | 0.43              |
| 1:D:517:ARG:O     | 1:D:525:GLU:N     | 2.36                     | 0.43              |
| 1:D:704:ILE:HG12  | 3:D:1003:POV:H31D | 2.00                     | 0.43              |
| 1:F:616:TYR:CE2   | 1:F:644:LYS:HD2   | 2.54                     | 0.43              |
| 1:F:625:ARG:HD3   | 1:F:627:TYR:CE2   | 2.54                     | 0.43              |
| 1:A:625:ARG:HD3   | 1:A:627:TYR:CE2   | 2.54                     | 0.43              |
| 3:A:1006:POV:H37A | 3:B:1002:POV:H27A | 2.01                     | 0.43              |
| 1:B:616:TYR:CE2   | 1:B:644:LYS:HD2   | 2.54                     | 0.43              |
| 1:D:488:HIS:ND1   | 1:D:489:PRO:O     | 2.52                     | 0.43              |
| 1:E:616:TYR:CE2   | 1:E:644:LYS:HD2   | 2.54                     | 0.43              |
| 1:E:625:ARG:HD3   | 1:E:627:TYR:CE2   | 2.54                     | 0.43              |
| 1:F:123:PRO:HA    | 1:F:126:PHE:HD2   | 1.83                     | 0.43              |
| 1:F:407:THR:HG23  | 1:F:472:CYS:SG    | 2.59                     | 0.43              |
| 1:A:518:LYS:HB3   | 1:A:524:TRP:HA    | 2.01                     | 0.42              |
| 1:B:407:THR:HG23  | 1:B:472:CYS:SG    | 2.59                     | 0.42              |
| 1:B:717:LEU:HB3   | 1:B:722:ILE:HD11  | 2.00                     | 0.42              |
| 1:C:123:PRO:HG2   | 1:C:294:GLY:HA3   | 2.01                     | 0.42              |
| 1:C:510:PHE:HE1   | 1:C:567:GLU:HG2   | 1.83                     | 0.42              |
| 1:C:687:ARG:NH1   | 1:C:739:ASP:O     | 2.52                     | 0.42              |
| 1:E:498:TYR:O     | 1:E:502:VAL:N     | 2.43                     | 0.42              |
| 1:F:400:SER:OG    | 1:F:403:ASP:HB3   | 2.17                     | 0.42              |
| 1:A:407:THR:HG23  | 1:A:472:CYS:SG    | 2.59                     | 0.42              |
| 1:A:868:VAL:HG21  | 1:F:306:LEU:HD13  | 2.01                     | 0.42              |
| 1:B:625:ARG:HD3   | 1:B:627:TYR:CE2   | 2.54                     | 0.42              |
| 1:C:625:ARG:HD3   | 1:C:627:TYR:CE2   | 2.54                     | 0.42              |
| 1:D:430:LEU:HB2   | 1:D:435:LYS:CB    | 2.47                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:616:TYR:CE2   | 1:D:644:LYS:HD2   | 2.54                     | 0.42              |
| 3:D:1002:POV:H39A | 3:D:1002:POV:H212 | 2.00                     | 0.42              |
| 1:E:366:ILE:O     | 1:E:681:SER:OG    | 2.23                     | 0.42              |
| 3:E:1010:POV:H312 | 3:E:1010:POV:H214 | 2.00                     | 0.42              |
| 1:F:375:LEU:HB3   | 1:F:554:VAL:HG12  | 2.00                     | 0.42              |
| 1:B:375:LEU:HB3   | 1:B:554:VAL:HG12  | 2.00                     | 0.42              |
| 1:B:752:LEU:HG    | 1:B:756:TRP:CD1   | 2.55                     | 0.42              |
| 1:D:625:ARG:HD3   | 1:D:627:TYR:CE2   | 2.54                     | 0.42              |
| 1:F:123:PRO:HG2   | 1:F:294:GLY:HA3   | 2.01                     | 0.42              |
| 3:F:1006:POV:H26A | 3:F:1006:POV:H29  | 1.79                     | 0.42              |
| 3:A:1012:POV:H14A | 3:A:1012:POV:O14  | 2.19                     | 0.42              |
| 3:A:1012:POV:H28  | 3:A:1012:POV:H211 | 1.76                     | 0.42              |
| 1:B:518:LYS:HB3   | 1:B:524:TRP:HA    | 2.01                     | 0.42              |
| 1:C:445:VAL:HG22  | 1:C:462:VAL:HG12  | 2.01                     | 0.42              |
| 3:D:1005:POV:H21C | 3:D:1006:POV:H21B | 2.01                     | 0.42              |
| 3:D:1006:POV:H32  | 3:D:1008:POV:H32A | 2.00                     | 0.42              |
| 1:B:386:ASN:C     | 1:B:386:ASN:HD22  | 2.27                     | 0.42              |
| 1:C:407:THR:HG23  | 1:C:472:CYS:SG    | 2.59                     | 0.42              |
| 1:C:488:HIS:ND1   | 1:C:489:PRO:O     | 2.52                     | 0.42              |
| 1:D:445:VAL:HG22  | 1:D:462:VAL:HG12  | 2.00                     | 0.42              |
| 1:D:471:VAL:HB    | 1:D:518:LYS:HG3   | 2.02                     | 0.42              |
| 1:E:375:LEU:HB3   | 1:E:554:VAL:HG12  | 2.00                     | 0.42              |
| 1:E:407:THR:HG23  | 1:E:472:CYS:SG    | 2.59                     | 0.42              |
| 1:E:619:VAL:O     | 1:E:623:GLN:HG2   | 2.20                     | 0.42              |
| 3:E:1009:POV:H32  | 3:E:1009:POV:H24A | 2.00                     | 0.42              |
| 1:F:619:VAL:O     | 1:F:623:GLN:HG2   | 2.20                     | 0.42              |
| 1:F:687:ARG:NH1   | 1:F:739:ASP:O     | 2.52                     | 0.42              |
| 1:A:471:VAL:HB    | 1:A:518:LYS:HG3   | 2.02                     | 0.42              |
| 1:A:498:TYR:O     | 1:A:502:VAL:N     | 2.43                     | 0.42              |
| 1:A:772:ILE:HD11  | 3:A:1010:POV:H314 | 2.02                     | 0.42              |
| 1:B:445:VAL:HG22  | 1:B:462:VAL:HG12  | 2.01                     | 0.42              |
| 1:C:314:TYR:CE1   | 1:D:776:THR:HG22  | 2.53                     | 0.42              |
| 1:D:723:VAL:O     | 1:D:727:ILE:HG13  | 2.20                     | 0.42              |
| 3:D:1003:POV:H21E | 3:D:1003:POV:H39  | 2.01                     | 0.42              |
| 1:E:309:TRP:CH2   | 1:F:860:ILE:CG2   | 3.02                     | 0.42              |
| 1:E:314:TYR:CE1   | 1:F:776:THR:HG22  | 2.52                     | 0.42              |
| 1:E:471:VAL:HB    | 1:E:518:LYS:HG3   | 2.02                     | 0.42              |
| 1:E:752:LEU:HG    | 1:E:756:TRP:CD1   | 2.55                     | 0.42              |
| 3:E:1005:POV:H29  | 3:E:1005:POV:H26  | 1.56                     | 0.42              |
| 1:A:723:VAL:O     | 1:A:727:ILE:HG13  | 2.20                     | 0.42              |
| 1:A:752:LEU:HG    | 1:A:756:TRP:CD1   | 2.55                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:777:MET:HE3   | 1:A:791:MET:HA    | 2.02                     | 0.42              |
| 3:A:1006:POV:H28  | 3:A:1006:POV:H211 | 1.84                     | 0.42              |
| 1:B:723:VAL:O     | 1:B:727:ILE:HG13  | 2.20                     | 0.42              |
| 3:B:1010:POV:H211 | 3:B:1010:POV:H28  | 1.75                     | 0.42              |
| 1:C:123:PRO:HA    | 1:C:126:PHE:HD2   | 1.84                     | 0.42              |
| 1:C:752:LEU:HG    | 1:C:756:TRP:CD1   | 2.55                     | 0.42              |
| 3:C:1004:POV:H210 | 3:C:1004:POV:H34  | 2.01                     | 0.42              |
| 3:C:1004:POV:H2   | 3:C:1004:POV:H25  | 2.02                     | 0.42              |
| 1:D:315:ARG:HB3   | 3:D:1002:POV:C14  | 2.36                     | 0.42              |
| 1:E:518:LYS:HB3   | 1:E:524:TRP:HA    | 2.01                     | 0.42              |
| 1:E:723:VAL:O     | 1:E:727:ILE:HG13  | 2.20                     | 0.42              |
| 1:E:736:ILE:HD13  | 1:E:736:ILE:HA    | 1.90                     | 0.42              |
| 3:E:1009:POV:H39A | 3:F:1007:POV:H212 | 2.01                     | 0.42              |
| 1:F:723:VAL:O     | 1:F:727:ILE:HG13  | 2.20                     | 0.42              |
| 1:F:752:LEU:HG    | 1:F:756:TRP:CD1   | 2.55                     | 0.42              |
| 1:A:307:LEU:CD2   | 3:A:1003:POV:H31E | 2.50                     | 0.42              |
| 3:A:1011:POV:H28  | 3:A:1011:POV:H21A | 1.75                     | 0.42              |
| 1:B:471:VAL:HB    | 1:B:518:LYS:HG3   | 2.02                     | 0.42              |
| 3:B:1010:POV:H37  | 3:C:1008:POV:H27  | 2.00                     | 0.42              |
| 1:C:518:LYS:HB3   | 1:C:524:TRP:HA    | 2.01                     | 0.42              |
| 1:C:723:VAL:O     | 1:C:727:ILE:HG13  | 2.20                     | 0.42              |
| 1:D:619:VAL:O     | 1:D:623:GLN:HG2   | 2.20                     | 0.42              |
| 1:D:687:ARG:NH1   | 1:D:739:ASP:O     | 2.52                     | 0.42              |
| 1:D:752:LEU:HG    | 1:D:756:TRP:CD1   | 2.55                     | 0.42              |
| 1:D:777:MET:HE3   | 1:D:791:MET:HA    | 2.02                     | 0.42              |
| 1:E:310:THR:HG23  | 1:F:772:ILE:CG2   | 2.50                     | 0.42              |
| 3:E:1005:POV:H11A | 3:E:1005:POV:H15B | 1.88                     | 0.42              |
| 1:F:386:ASN:C     | 1:F:386:ASN:HD22  | 2.27                     | 0.42              |
| 1:F:445:VAL:HG22  | 1:F:462:VAL:HG12  | 2.01                     | 0.42              |
| 1:F:518:LYS:HB3   | 1:F:524:TRP:HA    | 2.01                     | 0.42              |
| 3:F:1007:POV:H37A | 3:F:1009:POV:H28A | 2.01                     | 0.42              |
| 3:A:1011:POV:H27A | 3:F:1005:POV:H37A | 2.00                     | 0.42              |
| 1:B:307:LEU:CD2   | 3:B:1004:POV:H31E | 2.50                     | 0.42              |
| 1:B:314:TYR:CE1   | 1:C:776:THR:HG22  | 2.55                     | 0.42              |
| 3:B:1006:POV:H11A | 3:B:1006:POV:H15B | 1.88                     | 0.42              |
| 1:C:267:THR:O     | 1:C:271:ARG:N     | 2.44                     | 0.42              |
| 1:C:471:VAL:HB    | 1:C:518:LYS:HG3   | 2.02                     | 0.42              |
| 1:C:505:LEU:HG    | 1:C:510:PHE:HB2   | 2.01                     | 0.42              |
| 1:E:476:ALA:HB3   | 1:E:479:PHE:HD2   | 1.85                     | 0.42              |
| 1:F:267:THR:O     | 1:F:271:ARG:N     | 2.44                     | 0.42              |
| 3:F:1003:POV:H210 | 3:F:1003:POV:H34  | 2.01                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:445:VAL:HG22  | 1:A:462:VAL:HG12  | 2.01                     | 0.42              |
| 1:A:619:VAL:O     | 1:A:623:GLN:HG2   | 2.20                     | 0.42              |
| 3:A:1004:POV:H34  | 3:A:1004:POV:H210 | 2.02                     | 0.42              |
| 1:B:542:GLN:O     | 1:B:545:SER:N     | 2.53                     | 0.42              |
| 1:B:619:VAL:O     | 1:B:623:GLN:HG2   | 2.20                     | 0.42              |
| 3:B:1002:POV:H11  | 3:B:1002:POV:H15A | 1.73                     | 0.42              |
| 1:C:777:MET:HE3   | 1:C:791:MET:HA    | 2.02                     | 0.42              |
| 1:D:505:LEU:HG    | 1:D:510:PHE:HB2   | 2.01                     | 0.42              |
| 1:E:505:LEU:HG    | 1:E:510:PHE:HB2   | 2.01                     | 0.42              |
| 1:E:542:GLN:O     | 1:E:545:SER:N     | 2.53                     | 0.42              |
| 1:F:488:HIS:ND1   | 1:F:489:PRO:O     | 2.52                     | 0.42              |
| 1:F:734:LEU:HD23  | 1:F:734:LEU:HA    | 1.90                     | 0.42              |
| 1:A:555:LYS:NZ    | 1:A:604:ALA:O     | 2.41                     | 0.41              |
| 3:B:1004:POV:H11A | 3:B:1004:POV:H14B | 1.82                     | 0.41              |
| 1:C:619:VAL:O     | 1:C:623:GLN:HG2   | 2.20                     | 0.41              |
| 3:C:1002:POV:H31F | 1:D:868:VAL:HG11  | 2.02                     | 0.41              |
| 1:D:617:ARG:O     | 1:D:621:ILE:HG12  | 2.20                     | 0.41              |
| 1:F:797:LEU:O     | 1:F:801:LEU:HD23  | 2.20                     | 0.41              |
| 1:A:617:ARG:O     | 1:A:621:ILE:HG12  | 2.20                     | 0.41              |
| 3:A:1008:POV:H27  | 3:F:1009:POV:H35  | 2.02                     | 0.41              |
| 3:A:1010:POV:H31G | 3:A:1010:POV:H31D | 1.81                     | 0.41              |
| 1:B:366:ILE:O     | 1:B:681:SER:OG    | 2.23                     | 0.41              |
| 1:B:505:LEU:HG    | 1:B:510:PHE:HB2   | 2.01                     | 0.41              |
| 1:B:734:LEU:HD23  | 1:B:734:LEU:HA    | 1.89                     | 0.41              |
| 1:B:797:LEU:O     | 1:B:801:LEU:HD23  | 2.20                     | 0.41              |
| 1:C:797:LEU:O     | 1:C:801:LEU:HD23  | 2.20                     | 0.41              |
| 3:E:1003:POV:H21E | 3:E:1003:POV:H39  | 2.02                     | 0.41              |
| 1:F:471:VAL:HB    | 1:F:518:LYS:HG3   | 2.02                     | 0.41              |
| 3:F:1008:POV:H15B | 3:F:1008:POV:H11  | 1.78                     | 0.41              |
| 1:A:542:GLN:O     | 1:A:545:SER:N     | 2.53                     | 0.41              |
| 3:A:1007:POV:H13B | 3:A:1007:POV:H11A | 1.73                     | 0.41              |
| 1:B:476:ALA:HB3   | 1:B:479:PHE:HD2   | 1.85                     | 0.41              |
| 3:C:1006:POV:H37  | 3:C:1007:POV:H28  | 2.02                     | 0.41              |
| 3:E:1002:POV:H13A | 3:E:1002:POV:H11A | 1.55                     | 0.41              |
| 1:F:505:LEU:HG    | 1:F:510:PHE:HB2   | 2.01                     | 0.41              |
| 1:F:777:MET:HE3   | 1:F:791:MET:HA    | 2.02                     | 0.41              |
| 1:A:316:THR:HG23  | 1:B:783:GLY:H     | 1.68                     | 0.41              |
| 1:A:505:LEU:HG    | 1:A:510:PHE:HB2   | 2.01                     | 0.41              |
| 1:C:152:MET:O     | 1:C:156:GLY:N     | 2.51                     | 0.41              |
| 1:D:704:ILE:HG21  | 3:D:1004:POV:H314 | 2.02                     | 0.41              |
| 3:D:1010:POV:H28  | 3:D:1010:POV:H211 | 1.75                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:E:617:ARG:O     | 1:E:621:ILE:HG12  | 2.20                     | 0.41              |
| 1:E:797:LEU:O     | 1:E:801:LEU:HD23  | 2.20                     | 0.41              |
| 1:A:128:MET:O     | 1:A:132:ALA:N     | 2.48                     | 0.41              |
| 1:A:316:THR:HG22  | 1:B:783:GLY:CA    | 2.49                     | 0.41              |
| 3:A:1002:POV:H13A | 3:A:1002:POV:H11A | 1.53                     | 0.41              |
| 3:A:1002:POV:H31G | 3:A:1002:POV:H31D | 1.80                     | 0.41              |
| 1:B:516:ALA:HA    | 1:B:527:LEU:H     | 1.86                     | 0.41              |
| 1:B:777:MET:HE3   | 1:B:791:MET:HA    | 2.02                     | 0.41              |
| 1:C:386:ASN:C     | 1:C:386:ASN:HD22  | 2.27                     | 0.41              |
| 1:C:476:ALA:HB3   | 1:C:479:PHE:HD2   | 1.85                     | 0.41              |
| 1:D:542:GLN:O     | 1:D:545:SER:N     | 2.53                     | 0.41              |
| 1:E:516:ALA:HA    | 1:E:527:LEU:H     | 1.86                     | 0.41              |
| 1:E:777:MET:HE3   | 1:E:791:MET:HA    | 2.02                     | 0.41              |
| 1:F:379:LYS:NZ    | 1:F:564:ILE:HG23  | 2.36                     | 0.41              |
| 1:A:361:GLN:NE2   | 1:A:659:ARG:O     | 2.52                     | 0.41              |
| 1:A:544:VAL:HG13  | 1:A:554:VAL:HG21  | 2.03                     | 0.41              |
| 1:C:297:LEU:HD23  | 1:C:297:LEU:HA    | 1.91                     | 0.41              |
| 1:C:544:VAL:HG13  | 1:C:554:VAL:HG21  | 2.03                     | 0.41              |
| 1:C:685:PHE:HA    | 1:C:688:MET:HE3   | 2.03                     | 0.41              |
| 1:E:544:VAL:HG13  | 1:E:554:VAL:HG21  | 2.03                     | 0.41              |
| 1:F:297:LEU:HD23  | 1:F:297:LEU:HA    | 1.92                     | 0.41              |
| 1:F:617:ARG:O     | 1:F:621:ILE:HG12  | 2.20                     | 0.41              |
| 3:F:1009:POV:H11  | 3:F:1009:POV:H14A | 1.82                     | 0.41              |
| 1:A:687:ARG:NH1   | 1:A:739:ASP:O     | 2.52                     | 0.41              |
| 1:C:734:LEU:HD23  | 1:C:734:LEU:HA    | 1.90                     | 0.41              |
| 3:E:1007:POV:H29  | 3:E:1007:POV:H26A | 1.85                     | 0.41              |
| 1:F:685:PHE:HA    | 1:F:688:MET:HE3   | 2.03                     | 0.41              |
| 3:A:1010:POV:H21A | 3:A:1010:POV:H28A | 1.85                     | 0.41              |
| 1:B:379:LYS:NZ    | 1:B:564:ILE:HG23  | 2.36                     | 0.41              |
| 1:C:379:LYS:NZ    | 1:C:564:ILE:HG23  | 2.36                     | 0.41              |
| 1:C:516:ALA:HA    | 1:C:527:LEU:H     | 1.86                     | 0.41              |
| 3:D:1005:POV:H15B | 3:D:1005:POV:H11A | 1.83                     | 0.41              |
| 1:F:307:LEU:HD23  | 3:F:1002:POV:H31E | 2.03                     | 0.41              |
| 1:F:476:ALA:HB3   | 1:F:479:PHE:HD2   | 1.85                     | 0.41              |
| 3:F:1004:POV:H21E | 3:F:1005:POV:H21D | 2.03                     | 0.41              |
| 1:A:286:PHE:HZ    | 1:A:342:VAL:HG11  | 1.86                     | 0.41              |
| 3:A:1011:POV:H312 | 3:A:1011:POV:H214 | 2.03                     | 0.41              |
| 1:B:267:THR:O     | 1:B:271:ARG:N     | 2.44                     | 0.41              |
| 1:B:310:THR:OG1   | 3:B:1003:POV:H312 | 2.21                     | 0.41              |
| 1:B:325:TYR:HB3   | 1:B:710:ILE:HD13  | 2.03                     | 0.41              |
| 1:B:544:VAL:HG13  | 1:B:554:VAL:HG21  | 2.03                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:617:ARG:O     | 1:B:621:ILE:HG12  | 2.20                     | 0.41              |
| 1:C:617:ARG:O     | 1:C:621:ILE:HG12  | 2.20                     | 0.41              |
| 3:C:1005:POV:H28A | 3:C:1005:POV:H211 | 1.81                     | 0.41              |
| 1:D:307:LEU:HD13  | 3:D:1002:POV:C36  | 2.51                     | 0.41              |
| 1:D:567:GLU:HA    | 1:D:570:ARG:NH1   | 2.35                     | 0.41              |
| 1:E:379:LYS:NZ    | 1:E:564:ILE:HG23  | 2.36                     | 0.41              |
| 1:E:685:PHE:HA    | 1:E:688:MET:HE3   | 2.03                     | 0.41              |
| 1:E:687:ARG:NH1   | 1:E:739:ASP:O     | 2.52                     | 0.41              |
| 1:F:430:LEU:HB2   | 1:F:435:LYS:CB    | 2.47                     | 0.41              |
| 1:F:516:ALA:HA    | 1:F:527:LEU:H     | 1.86                     | 0.41              |
| 1:F:544:VAL:HG13  | 1:F:554:VAL:HG21  | 2.03                     | 0.41              |
| 1:F:804:ASN:HB3   | 1:F:829:VAL:HG13  | 2.03                     | 0.41              |
| 1:A:325:TYR:HB3   | 1:A:710:ILE:HD13  | 2.03                     | 0.41              |
| 1:A:797:LEU:O     | 1:A:801:LEU:HD23  | 2.20                     | 0.41              |
| 1:B:287:THR:HA    | 1:B:290:LEU:HB3   | 2.03                     | 0.41              |
| 1:B:685:PHE:HA    | 1:B:688:MET:HE3   | 2.03                     | 0.41              |
| 1:C:804:ASN:HB3   | 1:C:829:VAL:HG13  | 2.03                     | 0.41              |
| 1:D:516:ALA:HA    | 1:D:527:LEU:H     | 1.86                     | 0.41              |
| 1:D:685:PHE:HA    | 1:D:688:MET:HE3   | 2.03                     | 0.41              |
| 1:D:797:LEU:O     | 1:D:801:LEU:HD23  | 2.20                     | 0.41              |
| 1:F:542:GLN:O     | 1:F:545:SER:N     | 2.53                     | 0.41              |
| 1:A:476:ALA:HB3   | 1:A:479:PHE:HD2   | 1.85                     | 0.40              |
| 1:A:685:PHE:HA    | 1:A:688:MET:HE3   | 2.03                     | 0.40              |
| 1:C:555:LYS:NZ    | 1:C:604:ALA:O     | 2.41                     | 0.40              |
| 1:D:544:VAL:HG13  | 1:D:554:VAL:HG21  | 2.03                     | 0.40              |
| 1:D:648:GLY:H     | 1:D:663:ASP:HB2   | 1.86                     | 0.40              |
| 1:F:287:THR:HA    | 1:F:290:LEU:HB3   | 2.03                     | 0.40              |
| 1:F:567:GLU:HA    | 1:F:570:ARG:NH1   | 2.35                     | 0.40              |
| 1:A:379:LYS:NZ    | 1:A:564:ILE:HG23  | 2.36                     | 0.40              |
| 1:A:407:THR:HG21  | 1:A:527:LEU:HD12  | 2.03                     | 0.40              |
| 1:A:516:ALA:HA    | 1:A:527:LEU:H     | 1.86                     | 0.40              |
| 1:B:400:SER:OG    | 1:B:403:ASP:CB    | 2.69                     | 0.40              |
| 3:B:1003:POV:H13B | 3:B:1004:POV:H13B | 2.03                     | 0.40              |
| 1:C:286:PHE:HZ    | 1:C:342:VAL:HG11  | 1.86                     | 0.40              |
| 1:C:287:THR:HA    | 1:C:290:LEU:HB3   | 2.03                     | 0.40              |
| 1:C:325:TYR:HB3   | 1:C:710:ILE:HD13  | 2.03                     | 0.40              |
| 1:C:542:GLN:O     | 1:C:545:SER:N     | 2.53                     | 0.40              |
| 3:C:1002:POV:H13A | 3:C:1002:POV:H11A | 1.51                     | 0.40              |
| 3:C:1005:POV:H15B | 3:C:1005:POV:H11A | 1.85                     | 0.40              |
| 1:D:286:PHE:HZ    | 1:D:342:VAL:HG11  | 1.86                     | 0.40              |
| 1:D:325:TYR:HB3   | 1:D:710:ILE:HD13  | 2.03                     | 0.40              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:1007:POV:H23  | 3:E:1010:POV:H22  | 2.02                     | 0.40              |
| 1:E:325:TYR:HB3   | 1:E:710:ILE:HD13  | 2.03                     | 0.40              |
| 1:B:687:ARG:NH1   | 1:B:739:ASP:O     | 2.52                     | 0.40              |
| 1:B:752:LEU:HD12  | 1:B:752:LEU:HA    | 1.93                     | 0.40              |
| 3:B:1010:POV:H11  | 3:B:1010:POV:H14A | 1.87                     | 0.40              |
| 1:D:476:ALA:HB3   | 1:D:479:PHE:HD2   | 1.85                     | 0.40              |
| 1:D:721:LEU:HD23  | 1:D:796:PHE:HB2   | 2.04                     | 0.40              |
| 1:D:808:PHE:HE1   | 1:D:829:VAL:HG11  | 1.87                     | 0.40              |
| 3:D:1005:POV:H28A | 3:D:1005:POV:H211 | 1.84                     | 0.40              |
| 3:D:1010:POV:H39A | 3:E:1008:POV:H212 | 2.02                     | 0.40              |
| 1:E:778:PHE:O     | 3:E:1004:POV:H14A | 2.21                     | 0.40              |
| 1:F:286:PHE:HZ    | 1:F:342:VAL:HG11  | 1.86                     | 0.40              |
| 1:A:794:ILE:HG23  | 1:A:858:VAL:HG21  | 2.04                     | 0.40              |
| 1:B:736:ILE:HD11  | 1:B:807:ILE:HG12  | 2.03                     | 0.40              |
| 1:B:808:PHE:HE1   | 1:B:829:VAL:HG11  | 1.87                     | 0.40              |
| 1:C:239:LYS:NZ    | 1:C:245:THR:HA    | 2.37                     | 0.40              |
| 3:C:1002:POV:H28A | 3:C:1002:POV:H21A | 1.82                     | 0.40              |
| 1:D:587:GLY:C     | 1:D:617:ARG:HH22  | 2.30                     | 0.40              |
| 1:E:232:GLY:HA3   | 1:E:380:THR:HG21  | 2.03                     | 0.40              |
| 1:E:239:LYS:NZ    | 1:E:245:THR:HA    | 2.37                     | 0.40              |
| 1:E:287:THR:HA    | 1:E:290:LEU:HB3   | 2.03                     | 0.40              |
| 1:E:567:GLU:HA    | 1:E:570:ARG:NH1   | 2.35                     | 0.40              |
| 1:E:587:GLY:C     | 1:E:617:ARG:HH22  | 2.30                     | 0.40              |
| 1:F:484:VAL:HG23  | 1:F:524:TRP:HD1   | 1.86                     | 0.40              |
| 3:F:1004:POV:H3A  | 3:F:1005:POV:H2   | 2.03                     | 0.40              |
| 3:F:1010:POV:H15A | 3:F:1010:POV:H11  | 1.75                     | 0.40              |
| 1:A:517:ARG:O     | 1:A:525:GLU:N     | 2.36                     | 0.40              |
| 1:A:648:GLY:H     | 1:A:663:ASP:HB2   | 1.86                     | 0.40              |
| 1:B:567:GLU:HA    | 1:B:570:ARG:NH1   | 2.35                     | 0.40              |
| 1:B:721:LEU:HD23  | 1:B:796:PHE:HB2   | 2.04                     | 0.40              |
| 1:B:804:ASN:HB3   | 1:B:829:VAL:HG13  | 2.03                     | 0.40              |
| 1:D:287:THR:HA    | 1:D:290:LEU:HB3   | 2.03                     | 0.40              |
| 1:D:309:TRP:CH2   | 1:E:860:ILE:HG21  | 2.56                     | 0.40              |
| 1:D:379:LYS:NZ    | 1:D:564:ILE:HG23  | 2.36                     | 0.40              |
| 1:D:407:THR:HG21  | 1:D:527:LEU:HD12  | 2.03                     | 0.40              |
| 1:E:378:ASP:OD2   | 2:E:1001:BEF:F2   | 2.29                     | 0.40              |
| 3:E:1007:POV:H28  | 3:E:1007:POV:H211 | 1.94                     | 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 PDB entries followed by that with respect to all EM entries.

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

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1   | A     | 760/918 (83%)   | 734 (97%)  | 26 (3%)  | 0        | 100         | 100 |
| 1   | B     | 760/918 (83%)   | 734 (97%)  | 26 (3%)  | 0        | 100         | 100 |
| 1   | C     | 760/918 (83%)   | 734 (97%)  | 26 (3%)  | 0        | 100         | 100 |
| 1   | D     | 760/918 (83%)   | 734 (97%)  | 26 (3%)  | 0        | 100         | 100 |
| 1   | E     | 760/918 (83%)   | 734 (97%)  | 26 (3%)  | 0        | 100         | 100 |
| 1   | F     | 760/918 (83%)   | 734 (97%)  | 26 (3%)  | 0        | 100         | 100 |
| All | All   | 4560/5508 (83%) | 4404 (97%) | 156 (3%) | 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 PDB entries followed by that with respect to all EM entries.

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

| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1   | A     | 622/752 (83%)   | 618 (99%)  | 4 (1%)   | 78          | 79 |
| 1   | B     | 622/752 (83%)   | 617 (99%)  | 5 (1%)   | 73          | 76 |
| 1   | C     | 622/752 (83%)   | 616 (99%)  | 6 (1%)   | 68          | 74 |
| 1   | D     | 622/752 (83%)   | 618 (99%)  | 4 (1%)   | 78          | 79 |
| 1   | E     | 622/752 (83%)   | 618 (99%)  | 4 (1%)   | 78          | 79 |
| 1   | F     | 622/752 (83%)   | 618 (99%)  | 4 (1%)   | 78          | 79 |
| All | All   | 3732/4512 (83%) | 3705 (99%) | 27 (1%)  | 73          | 77 |

All (27) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 399 | VAL  |
| 1   | A     | 400 | SER  |
| 1   | A     | 432 | GLN  |
| 1   | A     | 433 | TYR  |
| 1   | B     | 386 | ASN  |
| 1   | B     | 400 | SER  |
| 1   | B     | 432 | GLN  |
| 1   | B     | 433 | TYR  |
| 1   | B     | 435 | LYS  |
| 1   | C     | 386 | ASN  |
| 1   | C     | 399 | VAL  |
| 1   | C     | 400 | SER  |
| 1   | C     | 432 | GLN  |
| 1   | C     | 433 | TYR  |
| 1   | C     | 435 | LYS  |
| 1   | D     | 399 | VAL  |
| 1   | D     | 400 | SER  |
| 1   | D     | 433 | TYR  |
| 1   | D     | 435 | LYS  |
| 1   | E     | 400 | SER  |
| 1   | E     | 432 | GLN  |
| 1   | E     | 433 | TYR  |
| 1   | E     | 435 | LYS  |
| 1   | F     | 386 | ASN  |
| 1   | F     | 400 | SER  |
| 1   | F     | 433 | TYR  |
| 1   | F     | 435 | LYS  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 154 | ASN  |
| 1   | A     | 391 | HIS  |
| 1   | A     | 500 | ASN  |
| 1   | A     | 623 | GLN  |
| 1   | A     | 701 | HIS  |
| 1   | A     | 787 | ASN  |
| 1   | A     | 792 | ASN  |
| 1   | B     | 154 | ASN  |
| 1   | B     | 386 | ASN  |
| 1   | B     | 391 | HIS  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 623 | GLN  |
| 1   | B     | 701 | HIS  |
| 1   | B     | 787 | ASN  |
| 1   | C     | 154 | ASN  |
| 1   | C     | 386 | ASN  |
| 1   | C     | 391 | HIS  |
| 1   | C     | 613 | GLN  |
| 1   | C     | 623 | GLN  |
| 1   | C     | 701 | HIS  |
| 1   | C     | 787 | ASN  |
| 1   | C     | 792 | ASN  |
| 1   | D     | 154 | ASN  |
| 1   | D     | 391 | HIS  |
| 1   | D     | 500 | ASN  |
| 1   | D     | 623 | GLN  |
| 1   | D     | 701 | HIS  |
| 1   | D     | 787 | ASN  |
| 1   | D     | 792 | ASN  |
| 1   | E     | 154 | ASN  |
| 1   | E     | 391 | HIS  |
| 1   | E     | 613 | GLN  |
| 1   | E     | 623 | GLN  |
| 1   | E     | 701 | HIS  |
| 1   | E     | 787 | ASN  |
| 1   | F     | 154 | ASN  |
| 1   | F     | 386 | ASN  |
| 1   | F     | 391 | HIS  |
| 1   | F     | 613 | GLN  |
| 1   | F     | 623 | GLN  |
| 1   | F     | 701 | HIS  |
| 1   | F     | 787 | ASN  |
| 1   | F     | 792 | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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](#)

63 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   | POV  | C     | 1007 | 3    | 51,51,51     | 1.22 | 5 (9%)   | 57,59,59    | 1.26 | 3 (5%)   |
| 3   | POV  | F     | 1004 | -    | 51,51,51     | 1.19 | 5 (9%)   | 57,59,59    | 1.18 | 3 (5%)   |
| 2   | BEF  | B     | 1001 | -    | 0,3,3        | -    | -        | -           | -    | -        |
| 3   | POV  | F     | 1009 | -    | 51,51,51     | 1.18 | 4 (7%)   | 57,59,59    | 1.15 | 3 (5%)   |
| 3   | POV  | E     | 1005 | -    | 51,51,51     | 1.18 | 4 (7%)   | 57,59,59    | 1.17 | 4 (7%)   |
| 3   | POV  | A     | 1004 | -    | 51,51,51     | 1.19 | 5 (9%)   | 57,59,59    | 1.10 | 2 (3%)   |
| 3   | POV  | A     | 1012 | -    | 51,51,51     | 1.19 | 4 (7%)   | 57,59,59    | 1.18 | 2 (3%)   |
| 2   | BEF  | F     | 1001 | -    | 0,3,3        | -    | -        | -           | -    | -        |
| 3   | POV  | C     | 1006 | -    | 51,51,51     | 1.18 | 4 (7%)   | 57,59,59    | 1.22 | 3 (5%)   |
| 3   | POV  | B     | 1002 | 3    | 51,51,51     | 1.21 | 5 (9%)   | 57,59,59    | 1.15 | 2 (3%)   |
| 3   | POV  | E     | 1010 | 3    | 51,51,51     | 1.20 | 5 (9%)   | 57,59,59    | 1.15 | 2 (3%)   |
| 3   | POV  | D     | 1008 | -    | 51,51,51     | 1.19 | 4 (7%)   | 57,59,59    | 1.16 | 2 (3%)   |
| 3   | POV  | E     | 1003 | -    | 51,51,51     | 1.22 | 6 (11%)  | 57,59,59    | 1.15 | 3 (5%)   |
| 3   | POV  | E     | 1002 | -    | 51,51,51     | 1.20 | 4 (7%)   | 57,59,59    | 1.13 | 2 (3%)   |
| 3   | POV  | B     | 1010 | -    | 51,51,51     | 1.18 | 4 (7%)   | 57,59,59    | 1.18 | 3 (5%)   |
| 3   | POV  | F     | 1005 | -    | 51,51,51     | 1.19 | 4 (7%)   | 57,59,59    | 1.19 | 2 (3%)   |
| 3   | POV  | B     | 1009 | -    | 51,51,51     | 1.19 | 4 (7%)   | 57,59,59    | 1.15 | 3 (5%)   |
| 3   | POV  | B     | 1007 | -    | 51,51,51     | 1.19 | 4 (7%)   | 57,59,59    | 1.18 | 2 (3%)   |
| 3   | POV  | D     | 1007 | 3    | 51,51,51     | 1.22 | 5 (9%)   | 57,59,59    | 1.24 | 3 (5%)   |
| 3   | POV  | B     | 1004 | -    | 51,51,51     | 1.20 | 4 (7%)   | 57,59,59    | 1.20 | 3 (5%)   |
| 3   | POV  | A     | 1009 | -    | 51,51,51     | 1.18 | 4 (7%)   | 57,59,59    | 1.18 | 3 (5%)   |
| 3   | POV  | C     | 1002 | -    | 51,51,51     | 1.20 | 4 (7%)   | 57,59,59    | 1.10 | 2 (3%)   |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | POV  | A     | 1007 | 3    | 51,51,51     | 1.22 | 5 (9%)   | 57,59,59    | 1.23 | 3 (5%)   |
| 3   | POV  | D     | 1004 | -    | 51,51,51     | 1.18 | 5 (9%)   | 57,59,59    | 1.16 | 2 (3%)   |
| 3   | POV  | F     | 1002 | -    | 51,51,51     | 1.20 | 4 (7%)   | 57,59,59    | 1.17 | 2 (3%)   |
| 3   | POV  | F     | 1003 | -    | 51,51,51     | 1.19 | 4 (7%)   | 57,59,59    | 1.11 | 2 (3%)   |
| 3   | POV  | F     | 1010 | 3    | 51,51,51     | 1.21 | 6 (11%)  | 57,59,59    | 1.15 | 2 (3%)   |
| 3   | POV  | E     | 1008 | -    | 51,51,51     | 1.19 | 4 (7%)   | 57,59,59    | 1.14 | 2 (3%)   |
| 3   | POV  | B     | 1006 | -    | 51,51,51     | 1.19 | 5 (9%)   | 57,59,59    | 1.17 | 3 (5%)   |
| 3   | POV  | A     | 1008 | -    | 51,51,51     | 1.19 | 4 (7%)   | 57,59,59    | 1.13 | 2 (3%)   |
| 2   | BEF  | D     | 1001 | -    | 0,3,3        | -    | -        | -           | -    | -        |
| 3   | POV  | D     | 1006 | -    | 51,51,51     | 1.19 | 4 (7%)   | 57,59,59    | 1.21 | 2 (3%)   |
| 3   | POV  | C     | 1009 | -    | 51,51,51     | 1.18 | 4 (7%)   | 57,59,59    | 1.19 | 3 (5%)   |
| 3   | POV  | A     | 1010 | -    | 51,51,51     | 1.20 | 4 (7%)   | 57,59,59    | 1.16 | 3 (5%)   |
| 3   | POV  | B     | 1005 | -    | 51,51,51     | 1.19 | 5 (9%)   | 57,59,59    | 1.12 | 2 (3%)   |
| 3   | POV  | D     | 1005 | -    | 51,51,51     | 1.18 | 4 (7%)   | 57,59,59    | 1.18 | 3 (5%)   |
| 3   | POV  | C     | 1003 | -    | 51,51,51     | 1.23 | 5 (9%)   | 57,59,59    | 1.17 | 3 (5%)   |
| 3   | POV  | A     | 1005 | -    | 51,51,51     | 1.19 | 4 (7%)   | 57,59,59    | 1.17 | 3 (5%)   |
| 3   | POV  | D     | 1002 | -    | 51,51,51     | 1.20 | 4 (7%)   | 57,59,59    | 1.10 | 2 (3%)   |
| 3   | POV  | C     | 1004 | 1    | 51,51,51     | 1.19 | 4 (7%)   | 57,59,59    | 1.12 | 2 (3%)   |
| 3   | POV  | C     | 1005 | -    | 51,51,51     | 1.18 | 4 (7%)   | 57,59,59    | 1.18 | 3 (5%)   |
| 3   | POV  | C     | 1008 | -    | 51,51,51     | 1.19 | 4 (7%)   | 57,59,59    | 1.17 | 3 (5%)   |
| 3   | POV  | F     | 1008 | -    | 51,51,51     | 1.19 | 4 (7%)   | 57,59,59    | 1.22 | 3 (5%)   |
| 2   | BEF  | E     | 1001 | -    | 0,3,3        | -    | -        | -           | -    | -        |
| 3   | POV  | A     | 1006 | -    | 51,51,51     | 1.19 | 4 (7%)   | 57,59,59    | 1.18 | 2 (3%)   |
| 3   | POV  | D     | 1009 | -    | 51,51,51     | 1.18 | 4 (7%)   | 57,59,59    | 1.21 | 3 (5%)   |
| 3   | POV  | F     | 1006 | 3    | 51,51,51     | 1.23 | 6 (11%)  | 57,59,59    | 1.25 | 3 (5%)   |
| 3   | POV  | D     | 1003 | -    | 51,51,51     | 1.24 | 6 (11%)  | 57,59,59    | 1.16 | 3 (5%)   |
| 3   | POV  | D     | 1010 | -    | 51,51,51     | 1.18 | 4 (7%)   | 57,59,59    | 1.17 | 3 (5%)   |
| 3   | POV  | E     | 1004 | -    | 51,51,51     | 1.21 | 5 (9%)   | 57,59,59    | 1.07 | 2 (3%)   |
| 3   | POV  | A     | 1002 | -    | 51,51,51     | 1.20 | 4 (7%)   | 57,59,59    | 1.14 | 2 (3%)   |
| 3   | POV  | B     | 1003 | -    | 51,51,51     | 1.19 | 4 (7%)   | 57,59,59    | 1.17 | 2 (3%)   |
| 3   | POV  | E     | 1006 | -    | 51,51,51     | 1.19 | 4 (7%)   | 57,59,59    | 1.17 | 3 (5%)   |
| 2   | BEF  | A     | 1001 | -    | 0,3,3        | -    | -        | -           | -    | -        |
| 3   | POV  | D     | 1011 | 3    | 51,51,51     | 1.19 | 4 (7%)   | 57,59,59    | 1.16 | 2 (3%)   |
| 2   | BEF  | C     | 1001 | -    | 0,3,3        | -    | -        | -           | -    | -        |
| 3   | POV  | B     | 1008 | 3    | 51,51,51     | 1.21 | 5 (9%)   | 57,59,59    | 1.25 | 3 (5%)   |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | POV  | E     | 1009 | -    | 51,51,51     | 1.19 | 4 (7%)   | 57,59,59    | 1.17 | 3 (5%)   |
| 3   | POV  | E     | 1007 | 3    | 51,51,51     | 1.22 | 5 (9%)   | 57,59,59    | 1.25 | 3 (5%)   |
| 3   | POV  | F     | 1007 | -    | 51,51,51     | 1.20 | 4 (7%)   | 57,59,59    | 1.15 | 3 (5%)   |
| 3   | POV  | A     | 1003 | -    | 51,51,51     | 1.21 | 4 (7%)   | 57,59,59    | 1.20 | 2 (3%)   |
| 3   | POV  | C     | 1010 | 3    | 51,51,51     | 1.19 | 5 (9%)   | 57,59,59    | 1.19 | 2 (3%)   |
| 3   | POV  | A     | 1011 | 3    | 51,51,51     | 1.21 | 5 (9%)   | 57,59,59    | 1.14 | 2 (3%)   |

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

| Mol | Type | Chain | Res  | Link | Chirals | Torsions    | Rings |
|-----|------|-------|------|------|---------|-------------|-------|
| 3   | POV  | C     | 1007 | 3    | -       | 24/55/55/55 | -     |
| 3   | POV  | F     | 1004 | -    | -       | 27/55/55/55 | -     |
| 3   | POV  | F     | 1009 | -    | -       | 22/55/55/55 | -     |
| 3   | POV  | E     | 1005 | -    | -       | 27/55/55/55 | -     |
| 3   | POV  | A     | 1004 | -    | -       | 24/55/55/55 | -     |
| 3   | POV  | A     | 1012 | -    | -       | 21/55/55/55 | -     |
| 3   | POV  | C     | 1006 | -    | -       | 30/55/55/55 | -     |
| 3   | POV  | B     | 1002 | 3    | -       | 26/55/55/55 | -     |
| 3   | POV  | E     | 1010 | 3    | -       | 24/55/55/55 | -     |
| 3   | POV  | D     | 1008 | -    | -       | 28/55/55/55 | -     |
| 3   | POV  | E     | 1003 | -    | -       | 27/55/55/55 | -     |
| 3   | POV  | E     | 1002 | -    | -       | 25/55/55/55 | -     |
| 3   | POV  | B     | 1010 | -    | -       | 23/55/55/55 | -     |
| 3   | POV  | F     | 1005 | -    | -       | 27/55/55/55 | -     |
| 3   | POV  | B     | 1009 | -    | -       | 28/55/55/55 | -     |
| 3   | POV  | B     | 1007 | -    | -       | 28/55/55/55 | -     |
| 3   | POV  | D     | 1007 | 3    | -       | 24/55/55/55 | -     |
| 3   | POV  | B     | 1004 | -    | -       | 24/55/55/55 | -     |
| 3   | POV  | A     | 1009 | -    | -       | 25/55/55/55 | -     |
| 3   | POV  | C     | 1002 | -    | -       | 27/55/55/55 | -     |
| 3   | POV  | A     | 1007 | 3    | -       | 23/55/55/55 | -     |
| 3   | POV  | D     | 1004 | -    | -       | 24/55/55/55 | -     |
| 3   | POV  | F     | 1002 | -    | -       | 26/55/55/55 | -     |

Continued on next page...

*Continued from previous page...*

| Mol | Type | Chain | Res  | Link | Chirals | Torsions    | Rings |
|-----|------|-------|------|------|---------|-------------|-------|
| 3   | POV  | F     | 1003 | -    | -       | 24/55/55/55 | -     |
| 3   | POV  | F     | 1010 | 3    | -       | 24/55/55/55 | -     |
| 3   | POV  | E     | 1008 | -    | -       | 26/55/55/55 | -     |
| 3   | POV  | B     | 1006 | -    | -       | 27/55/55/55 | -     |
| 3   | POV  | A     | 1008 | -    | -       | 29/55/55/55 | -     |
| 3   | POV  | D     | 1006 | -    | -       | 29/55/55/55 | -     |
| 3   | POV  | C     | 1009 | -    | -       | 23/55/55/55 | -     |
| 3   | POV  | A     | 1010 | -    | -       | 26/55/55/55 | -     |
| 3   | POV  | B     | 1005 | -    | -       | 25/55/55/55 | -     |
| 3   | POV  | D     | 1005 | -    | -       | 26/55/55/55 | -     |
| 3   | POV  | C     | 1003 | -    | -       | 26/55/55/55 | -     |
| 3   | POV  | A     | 1005 | -    | -       | 26/55/55/55 | -     |
| 3   | POV  | D     | 1002 | -    | -       | 26/55/55/55 | -     |
| 3   | POV  | C     | 1004 | 1    | -       | 23/55/55/55 | -     |
| 3   | POV  | C     | 1005 | -    | -       | 27/55/55/55 | -     |
| 3   | POV  | C     | 1008 | -    | -       | 25/55/55/55 | -     |
| 3   | POV  | F     | 1008 | -    | -       | 20/55/55/55 | -     |
| 3   | POV  | A     | 1006 | -    | -       | 28/55/55/55 | -     |
| 3   | POV  | D     | 1009 | -    | -       | 20/55/55/55 | -     |
| 3   | POV  | F     | 1006 | 3    | -       | 22/55/55/55 | -     |
| 3   | POV  | D     | 1003 | -    | -       | 26/55/55/55 | -     |
| 3   | POV  | D     | 1010 | -    | -       | 22/55/55/55 | -     |
| 3   | POV  | E     | 1004 | -    | -       | 27/55/55/55 | -     |
| 3   | POV  | A     | 1002 | -    | -       | 26/55/55/55 | -     |
| 3   | POV  | B     | 1003 | -    | -       | 30/55/55/55 | -     |
| 3   | POV  | E     | 1006 | -    | -       | 29/55/55/55 | -     |
| 3   | POV  | D     | 1011 | 3    | -       | 22/55/55/55 | -     |
| 3   | POV  | B     | 1008 | 3    | -       | 23/55/55/55 | -     |
| 3   | POV  | E     | 1009 | -    | -       | 23/55/55/55 | -     |
| 3   | POV  | E     | 1007 | 3    | -       | 21/55/55/55 | -     |
| 3   | POV  | F     | 1007 | -    | -       | 32/55/55/55 | -     |
| 3   | POV  | A     | 1003 | -    | -       | 24/55/55/55 | -     |
| 3   | POV  | C     | 1010 | 3    | -       | 22/55/55/55 | -     |
| 3   | POV  | A     | 1011 | 3    | -       | 21/55/55/55 | -     |

All (252) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 3   | F     | 1004 | POV  | O31-C31 | 3.83 | 1.44        | 1.33     |
| 3   | D     | 1003 | POV  | O31-C31 | 3.81 | 1.44        | 1.33     |
| 3   | D     | 1002 | POV  | O31-C31 | 3.79 | 1.44        | 1.33     |
| 3   | C     | 1003 | POV  | O31-C31 | 3.78 | 1.44        | 1.33     |
| 3   | A     | 1005 | POV  | O31-C31 | 3.78 | 1.44        | 1.33     |
| 3   | A     | 1008 | POV  | O31-C31 | 3.78 | 1.44        | 1.33     |
| 3   | E     | 1003 | POV  | O31-C31 | 3.78 | 1.44        | 1.33     |
| 3   | C     | 1002 | POV  | O31-C31 | 3.77 | 1.44        | 1.33     |
| 3   | E     | 1005 | POV  | O31-C31 | 3.76 | 1.44        | 1.33     |
| 3   | C     | 1005 | POV  | O31-C31 | 3.76 | 1.44        | 1.33     |
| 3   | B     | 1002 | POV  | O31-C31 | 3.76 | 1.44        | 1.33     |
| 3   | B     | 1006 | POV  | O31-C31 | 3.75 | 1.44        | 1.33     |
| 3   | A     | 1002 | POV  | O31-C31 | 3.75 | 1.44        | 1.33     |
| 3   | E     | 1008 | POV  | O31-C31 | 3.75 | 1.44        | 1.33     |
| 3   | A     | 1011 | POV  | O31-C31 | 3.74 | 1.44        | 1.33     |
| 3   | E     | 1006 | POV  | O31-C31 | 3.73 | 1.44        | 1.33     |
| 3   | B     | 1007 | POV  | O31-C31 | 3.73 | 1.44        | 1.33     |
| 3   | F     | 1006 | POV  | O31-C31 | 3.73 | 1.44        | 1.33     |
| 3   | E     | 1007 | POV  | O31-C31 | 3.72 | 1.44        | 1.33     |
| 3   | F     | 1002 | POV  | O31-C31 | 3.72 | 1.44        | 1.33     |
| 3   | F     | 1007 | POV  | O31-C31 | 3.72 | 1.44        | 1.33     |
| 3   | B     | 1004 | POV  | O31-C31 | 3.72 | 1.44        | 1.33     |
| 3   | D     | 1005 | POV  | O31-C31 | 3.72 | 1.44        | 1.33     |
| 3   | F     | 1005 | POV  | O31-C31 | 3.72 | 1.44        | 1.33     |
| 3   | A     | 1012 | POV  | O31-C31 | 3.71 | 1.44        | 1.33     |
| 3   | E     | 1010 | POV  | O31-C31 | 3.71 | 1.44        | 1.33     |
| 3   | F     | 1009 | POV  | O31-C31 | 3.71 | 1.44        | 1.33     |
| 3   | D     | 1007 | POV  | O31-C31 | 3.70 | 1.44        | 1.33     |
| 3   | B     | 1009 | POV  | O31-C31 | 3.70 | 1.44        | 1.33     |
| 3   | F     | 1010 | POV  | O31-C31 | 3.70 | 1.44        | 1.33     |
| 3   | E     | 1002 | POV  | O31-C31 | 3.70 | 1.44        | 1.33     |
| 3   | A     | 1010 | POV  | O31-C31 | 3.70 | 1.44        | 1.33     |
| 3   | A     | 1006 | POV  | O31-C31 | 3.70 | 1.44        | 1.33     |
| 3   | D     | 1006 | POV  | O31-C31 | 3.70 | 1.44        | 1.33     |
| 3   | D     | 1008 | POV  | O31-C31 | 3.69 | 1.44        | 1.33     |
| 3   | B     | 1008 | POV  | O31-C31 | 3.69 | 1.44        | 1.33     |
| 3   | E     | 1009 | POV  | O31-C31 | 3.69 | 1.44        | 1.33     |
| 3   | B     | 1003 | POV  | O31-C31 | 3.68 | 1.44        | 1.33     |
| 3   | A     | 1003 | POV  | O31-C31 | 3.68 | 1.44        | 1.33     |
| 3   | C     | 1006 | POV  | O31-C31 | 3.68 | 1.44        | 1.33     |
| 3   | D     | 1011 | POV  | O31-C31 | 3.68 | 1.44        | 1.33     |
| 3   | F     | 1008 | POV  | O31-C31 | 3.68 | 1.44        | 1.33     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 3   | C     | 1008 | POV  | O31-C31 | 3.67 | 1.44        | 1.33     |
| 3   | A     | 1009 | POV  | O31-C31 | 3.67 | 1.44        | 1.33     |
| 3   | A     | 1007 | POV  | O31-C31 | 3.66 | 1.44        | 1.33     |
| 3   | B     | 1010 | POV  | O31-C31 | 3.65 | 1.44        | 1.33     |
| 3   | C     | 1007 | POV  | O31-C31 | 3.65 | 1.44        | 1.33     |
| 3   | C     | 1010 | POV  | O31-C31 | 3.65 | 1.44        | 1.33     |
| 3   | E     | 1004 | POV  | O31-C31 | 3.65 | 1.44        | 1.33     |
| 3   | D     | 1009 | POV  | O31-C31 | 3.63 | 1.43        | 1.33     |
| 3   | C     | 1009 | POV  | O31-C31 | 3.62 | 1.43        | 1.33     |
| 3   | D     | 1010 | POV  | O31-C31 | 3.62 | 1.43        | 1.33     |
| 3   | F     | 1003 | POV  | O31-C31 | 3.61 | 1.43        | 1.33     |
| 3   | D     | 1004 | POV  | O31-C31 | 3.59 | 1.43        | 1.33     |
| 3   | C     | 1004 | POV  | O31-C31 | 3.59 | 1.43        | 1.33     |
| 3   | B     | 1005 | POV  | O31-C31 | 3.57 | 1.43        | 1.33     |
| 3   | A     | 1004 | POV  | O31-C31 | 3.51 | 1.43        | 1.33     |
| 3   | F     | 1006 | POV  | O21-C21 | 3.07 | 1.43        | 1.34     |
| 3   | E     | 1007 | POV  | O21-C21 | 3.05 | 1.42        | 1.34     |
| 3   | D     | 1007 | POV  | O21-C21 | 3.03 | 1.42        | 1.34     |
| 3   | A     | 1007 | POV  | O21-C21 | 3.02 | 1.42        | 1.34     |
| 3   | B     | 1008 | POV  | O21-C21 | 3.00 | 1.42        | 1.34     |
| 3   | C     | 1007 | POV  | O21-C21 | 2.99 | 1.42        | 1.34     |
| 3   | E     | 1009 | POV  | O21-C21 | 2.95 | 1.42        | 1.34     |
| 3   | B     | 1010 | POV  | O21-C21 | 2.91 | 1.42        | 1.34     |
| 3   | C     | 1009 | POV  | O21-C21 | 2.91 | 1.42        | 1.34     |
| 3   | F     | 1010 | POV  | O21-C21 | 2.90 | 1.42        | 1.34     |
| 3   | E     | 1003 | POV  | O21-C21 | 2.90 | 1.42        | 1.34     |
| 3   | C     | 1010 | POV  | O21-C21 | 2.89 | 1.42        | 1.34     |
| 3   | B     | 1002 | POV  | O21-C21 | 2.89 | 1.42        | 1.34     |
| 3   | D     | 1010 | POV  | O21-C21 | 2.87 | 1.42        | 1.34     |
| 3   | F     | 1004 | POV  | O21-C21 | 2.87 | 1.42        | 1.34     |
| 3   | F     | 1009 | POV  | O21-C21 | 2.86 | 1.42        | 1.34     |
| 3   | A     | 1005 | POV  | O21-C21 | 2.86 | 1.42        | 1.34     |
| 3   | A     | 1009 | POV  | O21-C21 | 2.85 | 1.42        | 1.34     |
| 3   | E     | 1010 | POV  | O21-C21 | 2.85 | 1.42        | 1.34     |
| 3   | A     | 1011 | POV  | O21-C21 | 2.84 | 1.42        | 1.34     |
| 3   | D     | 1003 | POV  | O21-C21 | 2.84 | 1.42        | 1.34     |
| 3   | C     | 1005 | POV  | O21-C21 | 2.83 | 1.42        | 1.34     |
| 3   | D     | 1005 | POV  | O21-C21 | 2.83 | 1.42        | 1.34     |
| 3   | E     | 1005 | POV  | O21-C21 | 2.83 | 1.42        | 1.34     |
| 3   | F     | 1008 | POV  | O21-C21 | 2.82 | 1.42        | 1.34     |
| 3   | D     | 1006 | POV  | O21-C21 | 2.82 | 1.42        | 1.34     |
| 3   | D     | 1011 | POV  | O21-C21 | 2.82 | 1.42        | 1.34     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 3   | A     | 1010 | POV  | O21-C21 | 2.82 | 1.42        | 1.34     |
| 3   | D     | 1005 | POV  | P-O12   | 2.81 | 1.70        | 1.59     |
| 3   | E     | 1004 | POV  | O21-C21 | 2.81 | 1.42        | 1.34     |
| 3   | B     | 1004 | POV  | O21-C21 | 2.81 | 1.42        | 1.34     |
| 3   | C     | 1006 | POV  | O21-C21 | 2.81 | 1.42        | 1.34     |
| 3   | F     | 1002 | POV  | O21-C21 | 2.81 | 1.42        | 1.34     |
| 3   | D     | 1009 | POV  | O21-C21 | 2.80 | 1.42        | 1.34     |
| 3   | A     | 1012 | POV  | O21-C21 | 2.79 | 1.42        | 1.34     |
| 3   | D     | 1002 | POV  | O21-C21 | 2.79 | 1.42        | 1.34     |
| 3   | B     | 1006 | POV  | O21-C21 | 2.79 | 1.42        | 1.34     |
| 3   | B     | 1007 | POV  | O21-C21 | 2.78 | 1.42        | 1.34     |
| 3   | B     | 1006 | POV  | P-O12   | 2.78 | 1.70        | 1.59     |
| 3   | A     | 1002 | POV  | O21-C21 | 2.78 | 1.42        | 1.34     |
| 3   | F     | 1005 | POV  | O21-C21 | 2.78 | 1.42        | 1.34     |
| 3   | C     | 1004 | POV  | O21-C21 | 2.77 | 1.42        | 1.34     |
| 3   | F     | 1004 | POV  | P-O12   | 2.77 | 1.70        | 1.59     |
| 3   | E     | 1008 | POV  | P-O12   | 2.77 | 1.70        | 1.59     |
| 3   | C     | 1003 | POV  | O21-C21 | 2.76 | 1.42        | 1.34     |
| 3   | A     | 1006 | POV  | O21-C21 | 2.76 | 1.42        | 1.34     |
| 3   | C     | 1005 | POV  | P-O12   | 2.76 | 1.70        | 1.59     |
| 3   | A     | 1005 | POV  | P-O12   | 2.75 | 1.70        | 1.59     |
| 3   | F     | 1003 | POV  | O21-C21 | 2.75 | 1.42        | 1.34     |
| 3   | C     | 1008 | POV  | P-O12   | 2.75 | 1.70        | 1.59     |
| 3   | C     | 1002 | POV  | O21-C21 | 2.75 | 1.42        | 1.34     |
| 3   | A     | 1004 | POV  | O21-C21 | 2.74 | 1.42        | 1.34     |
| 3   | B     | 1005 | POV  | O21-C21 | 2.74 | 1.42        | 1.34     |
| 3   | E     | 1006 | POV  | O21-C21 | 2.74 | 1.42        | 1.34     |
| 3   | A     | 1003 | POV  | O21-C21 | 2.73 | 1.42        | 1.34     |
| 3   | B     | 1009 | POV  | P-O12   | 2.73 | 1.70        | 1.59     |
| 3   | D     | 1008 | POV  | P-O12   | 2.73 | 1.70        | 1.59     |
| 3   | F     | 1007 | POV  | P-O12   | 2.73 | 1.70        | 1.59     |
| 3   | A     | 1008 | POV  | P-O12   | 2.73 | 1.70        | 1.59     |
| 3   | E     | 1005 | POV  | P-O12   | 2.73 | 1.70        | 1.59     |
| 3   | A     | 1003 | POV  | P-O12   | 2.72 | 1.70        | 1.59     |
| 3   | E     | 1002 | POV  | O21-C21 | 2.71 | 1.42        | 1.34     |
| 3   | B     | 1003 | POV  | O21-C21 | 2.70 | 1.41        | 1.34     |
| 3   | C     | 1003 | POV  | P-O12   | 2.69 | 1.70        | 1.59     |
| 3   | D     | 1004 | POV  | O21-C21 | 2.68 | 1.41        | 1.34     |
| 3   | C     | 1004 | POV  | P-O12   | 2.68 | 1.70        | 1.59     |
| 3   | C     | 1008 | POV  | O21-C21 | 2.68 | 1.41        | 1.34     |
| 3   | D     | 1003 | POV  | P-O12   | 2.67 | 1.70        | 1.59     |
| 3   | E     | 1004 | POV  | P-O12   | 2.67 | 1.70        | 1.59     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 3   | D     | 1004 | POV  | P-O12   | 2.66 | 1.70        | 1.59     |
| 3   | D     | 1008 | POV  | O21-C21 | 2.66 | 1.41        | 1.34     |
| 3   | B     | 1005 | POV  | P-O12   | 2.66 | 1.70        | 1.59     |
| 3   | E     | 1008 | POV  | O21-C21 | 2.65 | 1.41        | 1.34     |
| 3   | E     | 1003 | POV  | P-O12   | 2.64 | 1.70        | 1.59     |
| 3   | F     | 1002 | POV  | P-O12   | 2.64 | 1.70        | 1.59     |
| 3   | F     | 1007 | POV  | O21-C21 | 2.64 | 1.41        | 1.34     |
| 3   | B     | 1004 | POV  | P-O12   | 2.63 | 1.70        | 1.59     |
| 3   | A     | 1008 | POV  | O21-C21 | 2.63 | 1.41        | 1.34     |
| 3   | B     | 1009 | POV  | O21-C21 | 2.62 | 1.41        | 1.34     |
| 3   | A     | 1004 | POV  | P-O12   | 2.61 | 1.69        | 1.59     |
| 3   | F     | 1003 | POV  | P-O12   | 2.60 | 1.69        | 1.59     |
| 3   | A     | 1011 | POV  | P-O12   | 2.59 | 1.69        | 1.59     |
| 3   | A     | 1007 | POV  | P-O12   | 2.58 | 1.69        | 1.59     |
| 3   | E     | 1007 | POV  | P-O12   | 2.58 | 1.69        | 1.59     |
| 3   | B     | 1002 | POV  | P-O12   | 2.57 | 1.69        | 1.59     |
| 3   | B     | 1008 | POV  | P-O12   | 2.57 | 1.69        | 1.59     |
| 3   | F     | 1010 | POV  | P-O12   | 2.57 | 1.69        | 1.59     |
| 3   | F     | 1006 | POV  | P-O12   | 2.57 | 1.69        | 1.59     |
| 3   | D     | 1007 | POV  | P-O12   | 2.55 | 1.69        | 1.59     |
| 3   | C     | 1007 | POV  | P-O12   | 2.55 | 1.69        | 1.59     |
| 3   | C     | 1010 | POV  | P-O12   | 2.55 | 1.69        | 1.59     |
| 3   | D     | 1003 | POV  | C12-C11 | 2.55 | 1.59        | 1.51     |
| 3   | C     | 1003 | POV  | C12-C11 | 2.54 | 1.59        | 1.51     |
| 3   | E     | 1009 | POV  | P-O12   | 2.53 | 1.69        | 1.59     |
| 3   | A     | 1009 | POV  | P-O12   | 2.53 | 1.69        | 1.59     |
| 3   | A     | 1012 | POV  | P-O12   | 2.52 | 1.69        | 1.59     |
| 3   | E     | 1010 | POV  | P-O12   | 2.52 | 1.69        | 1.59     |
| 3   | B     | 1005 | POV  | C12-C11 | 2.51 | 1.59        | 1.51     |
| 3   | B     | 1007 | POV  | P-O12   | 2.51 | 1.69        | 1.59     |
| 3   | F     | 1008 | POV  | P-O12   | 2.50 | 1.69        | 1.59     |
| 3   | D     | 1011 | POV  | P-O12   | 2.50 | 1.69        | 1.59     |
| 3   | D     | 1009 | POV  | P-O12   | 2.50 | 1.69        | 1.59     |
| 3   | E     | 1004 | POV  | C12-C11 | 2.49 | 1.59        | 1.51     |
| 3   | C     | 1009 | POV  | P-O12   | 2.49 | 1.69        | 1.59     |
| 3   | A     | 1006 | POV  | P-O12   | 2.49 | 1.69        | 1.59     |
| 3   | E     | 1006 | POV  | P-O12   | 2.48 | 1.69        | 1.59     |
| 3   | B     | 1010 | POV  | P-O12   | 2.48 | 1.69        | 1.59     |
| 3   | D     | 1004 | POV  | C12-C11 | 2.48 | 1.59        | 1.51     |
| 3   | D     | 1006 | POV  | P-O12   | 2.47 | 1.69        | 1.59     |
| 3   | D     | 1010 | POV  | P-O12   | 2.47 | 1.69        | 1.59     |
| 3   | C     | 1004 | POV  | C12-C11 | 2.47 | 1.59        | 1.51     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 3   | F     | 1005 | POV  | P-O12   | 2.46 | 1.69        | 1.59     |
| 3   | C     | 1006 | POV  | P-O12   | 2.46 | 1.69        | 1.59     |
| 3   | C     | 1002 | POV  | P-O12   | 2.46 | 1.69        | 1.59     |
| 3   | F     | 1009 | POV  | P-O12   | 2.45 | 1.69        | 1.59     |
| 3   | A     | 1004 | POV  | C12-C11 | 2.44 | 1.59        | 1.51     |
| 3   | D     | 1002 | POV  | P-O12   | 2.44 | 1.69        | 1.59     |
| 3   | E     | 1002 | POV  | P-O12   | 2.42 | 1.69        | 1.59     |
| 3   | B     | 1003 | POV  | P-O12   | 2.42 | 1.69        | 1.59     |
| 3   | F     | 1003 | POV  | C12-C11 | 2.41 | 1.58        | 1.51     |
| 3   | A     | 1002 | POV  | P-O12   | 2.40 | 1.69        | 1.59     |
| 3   | A     | 1010 | POV  | P-O12   | 2.40 | 1.69        | 1.59     |
| 3   | F     | 1010 | POV  | C12-C11 | 2.37 | 1.58        | 1.51     |
| 3   | A     | 1003 | POV  | C12-C11 | 2.36 | 1.58        | 1.51     |
| 3   | B     | 1002 | POV  | C12-C11 | 2.36 | 1.58        | 1.51     |
| 3   | A     | 1011 | POV  | C12-C11 | 2.35 | 1.58        | 1.51     |
| 3   | C     | 1007 | POV  | C12-C11 | 2.34 | 1.58        | 1.51     |
| 3   | D     | 1002 | POV  | C12-C11 | 2.33 | 1.58        | 1.51     |
| 3   | C     | 1010 | POV  | C12-C11 | 2.33 | 1.58        | 1.51     |
| 3   | F     | 1006 | POV  | C12-C11 | 2.32 | 1.58        | 1.51     |
| 3   | E     | 1007 | POV  | C12-C11 | 2.31 | 1.58        | 1.51     |
| 3   | A     | 1007 | POV  | C12-C11 | 2.31 | 1.58        | 1.51     |
| 3   | B     | 1007 | POV  | C12-C11 | 2.31 | 1.58        | 1.51     |
| 3   | C     | 1006 | POV  | C12-C11 | 2.31 | 1.58        | 1.51     |
| 3   | B     | 1009 | POV  | C12-C11 | 2.30 | 1.58        | 1.51     |
| 3   | D     | 1007 | POV  | C12-C11 | 2.30 | 1.58        | 1.51     |
| 3   | D     | 1006 | POV  | C12-C11 | 2.30 | 1.58        | 1.51     |
| 3   | E     | 1006 | POV  | C12-C11 | 2.30 | 1.58        | 1.51     |
| 3   | A     | 1006 | POV  | C12-C11 | 2.30 | 1.58        | 1.51     |
| 3   | F     | 1007 | POV  | C12-C11 | 2.30 | 1.58        | 1.51     |
| 3   | E     | 1008 | POV  | C12-C11 | 2.29 | 1.58        | 1.51     |
| 3   | A     | 1005 | POV  | C12-C11 | 2.29 | 1.58        | 1.51     |
| 3   | E     | 1010 | POV  | C12-C11 | 2.29 | 1.58        | 1.51     |
| 3   | F     | 1004 | POV  | C12-C11 | 2.29 | 1.58        | 1.51     |
| 3   | C     | 1008 | POV  | C12-C11 | 2.29 | 1.58        | 1.51     |
| 3   | F     | 1008 | POV  | C12-C11 | 2.29 | 1.58        | 1.51     |
| 3   | F     | 1002 | POV  | C12-C11 | 2.29 | 1.58        | 1.51     |
| 3   | B     | 1008 | POV  | C12-C11 | 2.29 | 1.58        | 1.51     |
| 3   | F     | 1005 | POV  | C12-C11 | 2.29 | 1.58        | 1.51     |
| 3   | B     | 1004 | POV  | C12-C11 | 2.29 | 1.58        | 1.51     |
| 3   | A     | 1008 | POV  | C12-C11 | 2.28 | 1.58        | 1.51     |
| 3   | A     | 1012 | POV  | C12-C11 | 2.28 | 1.58        | 1.51     |
| 3   | D     | 1009 | POV  | C12-C11 | 2.28 | 1.58        | 1.51     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 3   | B     | 1006 | POV  | C12-C11 | 2.28 | 1.58        | 1.51     |
| 3   | C     | 1002 | POV  | C12-C11 | 2.28 | 1.58        | 1.51     |
| 3   | D     | 1008 | POV  | C12-C11 | 2.27 | 1.58        | 1.51     |
| 3   | E     | 1002 | POV  | C12-C11 | 2.27 | 1.58        | 1.51     |
| 3   | A     | 1010 | POV  | C12-C11 | 2.27 | 1.58        | 1.51     |
| 3   | D     | 1011 | POV  | C12-C11 | 2.26 | 1.58        | 1.51     |
| 3   | A     | 1002 | POV  | C12-C11 | 2.26 | 1.58        | 1.51     |
| 3   | C     | 1005 | POV  | C12-C11 | 2.26 | 1.58        | 1.51     |
| 3   | D     | 1005 | POV  | C12-C11 | 2.25 | 1.58        | 1.51     |
| 3   | E     | 1005 | POV  | C12-C11 | 2.24 | 1.58        | 1.51     |
| 3   | B     | 1003 | POV  | C12-C11 | 2.24 | 1.58        | 1.51     |
| 3   | E     | 1009 | POV  | C12-C11 | 2.22 | 1.58        | 1.51     |
| 3   | C     | 1009 | POV  | C12-C11 | 2.22 | 1.58        | 1.51     |
| 3   | E     | 1003 | POV  | C12-C11 | 2.22 | 1.58        | 1.51     |
| 3   | A     | 1009 | POV  | C12-C11 | 2.21 | 1.58        | 1.51     |
| 3   | D     | 1010 | POV  | C12-C11 | 2.17 | 1.58        | 1.51     |
| 3   | B     | 1010 | POV  | C12-C11 | 2.16 | 1.58        | 1.51     |
| 3   | F     | 1009 | POV  | C12-C11 | 2.13 | 1.58        | 1.51     |
| 3   | F     | 1006 | POV  | C22-C21 | 2.12 | 1.56        | 1.50     |
| 3   | B     | 1008 | POV  | C22-C21 | 2.09 | 1.56        | 1.50     |
| 3   | A     | 1007 | POV  | C22-C21 | 2.08 | 1.56        | 1.50     |
| 3   | E     | 1007 | POV  | C22-C21 | 2.08 | 1.56        | 1.50     |
| 3   | E     | 1004 | POV  | P-O11   | 2.06 | 1.67        | 1.59     |
| 3   | B     | 1002 | POV  | C22-C21 | 2.06 | 1.56        | 1.50     |
| 3   | C     | 1003 | POV  | P-O11   | 2.05 | 1.67        | 1.59     |
| 3   | D     | 1003 | POV  | P-O11   | 2.05 | 1.67        | 1.59     |
| 3   | F     | 1004 | POV  | C22-C21 | 2.05 | 1.56        | 1.50     |
| 3   | E     | 1003 | POV  | C22-C21 | 2.04 | 1.56        | 1.50     |
| 3   | A     | 1011 | POV  | C22-C21 | 2.04 | 1.56        | 1.50     |
| 3   | F     | 1010 | POV  | C22-C21 | 2.03 | 1.56        | 1.50     |
| 3   | C     | 1010 | POV  | C22-C21 | 2.03 | 1.56        | 1.50     |
| 3   | E     | 1010 | POV  | C22-C21 | 2.03 | 1.56        | 1.50     |
| 3   | C     | 1007 | POV  | C22-C21 | 2.03 | 1.56        | 1.50     |
| 3   | D     | 1007 | POV  | C22-C21 | 2.03 | 1.56        | 1.50     |
| 3   | E     | 1003 | POV  | P-O11   | 2.02 | 1.67        | 1.59     |
| 3   | B     | 1005 | POV  | P-O11   | 2.02 | 1.67        | 1.59     |
| 3   | F     | 1006 | POV  | P-O11   | 2.01 | 1.67        | 1.59     |
| 3   | B     | 1006 | POV  | C22-C21 | 2.01 | 1.56        | 1.50     |
| 3   | D     | 1004 | POV  | P-O11   | 2.01 | 1.67        | 1.59     |
| 3   | D     | 1003 | POV  | C22-C21 | 2.01 | 1.56        | 1.50     |
| 3   | A     | 1004 | POV  | P-O11   | 2.01 | 1.67        | 1.59     |
| 3   | F     | 1010 | POV  | P-O11   | 2.00 | 1.67        | 1.59     |

All (145) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 3   | F     | 1006 | POV  | O21-C21-C22 | 5.07 | 122.43      | 111.50   |
| 3   | E     | 1007 | POV  | O21-C21-C22 | 4.87 | 122.00      | 111.50   |
| 3   | A     | 1007 | POV  | O21-C21-C22 | 4.80 | 121.85      | 111.50   |
| 3   | D     | 1007 | POV  | O21-C21-C22 | 4.78 | 121.81      | 111.50   |
| 3   | C     | 1007 | POV  | O21-C21-C22 | 4.73 | 121.69      | 111.50   |
| 3   | B     | 1008 | POV  | O21-C21-C22 | 4.70 | 121.64      | 111.50   |
| 3   | D     | 1006 | POV  | O21-C21-C22 | 4.40 | 120.99      | 111.50   |
| 3   | C     | 1006 | POV  | O21-C21-C22 | 4.37 | 120.91      | 111.50   |
| 3   | D     | 1004 | POV  | O21-C21-C22 | 4.33 | 120.84      | 111.50   |
| 3   | F     | 1005 | POV  | O21-C21-C22 | 4.29 | 120.75      | 111.50   |
| 3   | B     | 1005 | POV  | O21-C21-C22 | 4.28 | 120.72      | 111.50   |
| 3   | B     | 1007 | POV  | O21-C21-C22 | 4.23 | 120.61      | 111.50   |
| 3   | A     | 1006 | POV  | O21-C21-C22 | 4.21 | 120.58      | 111.50   |
| 3   | B     | 1002 | POV  | O21-C21-C22 | 4.21 | 120.57      | 111.50   |
| 3   | C     | 1010 | POV  | O21-C21-C22 | 4.21 | 120.56      | 111.50   |
| 3   | F     | 1010 | POV  | O21-C21-C22 | 4.20 | 120.55      | 111.50   |
| 3   | E     | 1006 | POV  | O21-C21-C22 | 4.17 | 120.48      | 111.50   |
| 3   | E     | 1003 | POV  | O21-C21-C22 | 4.13 | 120.41      | 111.50   |
| 3   | E     | 1010 | POV  | O21-C21-C22 | 4.13 | 120.41      | 111.50   |
| 3   | A     | 1004 | POV  | O21-C21-C22 | 4.09 | 120.31      | 111.50   |
| 3   | A     | 1011 | POV  | O21-C21-C22 | 4.07 | 120.27      | 111.50   |
| 3   | E     | 1004 | POV  | O21-C21-C22 | 4.06 | 120.26      | 111.50   |
| 3   | F     | 1003 | POV  | O21-C21-C22 | 4.05 | 120.22      | 111.50   |
| 3   | A     | 1003 | POV  | O21-C21-C22 | 4.04 | 120.21      | 111.50   |
| 3   | E     | 1009 | POV  | O21-C21-C22 | 4.03 | 120.19      | 111.50   |
| 3   | D     | 1011 | POV  | O21-C21-C22 | 3.96 | 120.03      | 111.50   |
| 3   | C     | 1009 | POV  | O21-C21-C22 | 3.94 | 119.99      | 111.50   |
| 3   | D     | 1003 | POV  | O21-C21-C22 | 3.93 | 119.96      | 111.50   |
| 3   | A     | 1012 | POV  | O21-C21-C22 | 3.92 | 119.96      | 111.50   |
| 3   | D     | 1009 | POV  | O21-C21-C22 | 3.89 | 119.89      | 111.50   |
| 3   | B     | 1006 | POV  | O21-C21-C22 | 3.89 | 119.87      | 111.50   |
| 3   | A     | 1002 | POV  | O21-C21-C22 | 3.88 | 119.86      | 111.50   |
| 3   | F     | 1008 | POV  | O21-C21-C22 | 3.87 | 119.85      | 111.50   |
| 3   | C     | 1003 | POV  | O21-C21-C22 | 3.86 | 119.83      | 111.50   |
| 3   | C     | 1004 | POV  | O21-C21-C22 | 3.85 | 119.80      | 111.50   |
| 3   | D     | 1010 | POV  | O21-C21-C22 | 3.85 | 119.80      | 111.50   |
| 3   | B     | 1003 | POV  | O21-C21-C22 | 3.85 | 119.79      | 111.50   |
| 3   | F     | 1004 | POV  | O21-C21-C22 | 3.85 | 119.79      | 111.50   |
| 3   | C     | 1005 | POV  | O21-C21-C22 | 3.83 | 119.75      | 111.50   |
| 3   | B     | 1004 | POV  | O21-C21-C22 | 3.82 | 119.73      | 111.50   |
| 3   | B     | 1010 | POV  | O21-C21-C22 | 3.80 | 119.70      | 111.50   |
| 3   | F     | 1002 | POV  | O21-C21-C22 | 3.77 | 119.63      | 111.50   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3   | E     | 1002 | POV  | O21-C21-C22 | 3.76  | 119.61      | 111.50   |
| 3   | A     | 1005 | POV  | O21-C21-C22 | 3.72  | 119.52      | 111.50   |
| 3   | F     | 1009 | POV  | O21-C21-C22 | 3.72  | 119.51      | 111.50   |
| 3   | A     | 1009 | POV  | O21-C21-C22 | 3.71  | 119.50      | 111.50   |
| 3   | C     | 1008 | POV  | O21-C21-C22 | 3.71  | 119.49      | 111.50   |
| 3   | D     | 1005 | POV  | O21-C21-C22 | 3.68  | 119.42      | 111.50   |
| 3   | F     | 1007 | POV  | O21-C21-C22 | 3.67  | 119.42      | 111.50   |
| 3   | B     | 1009 | POV  | O21-C21-C22 | 3.65  | 119.37      | 111.50   |
| 3   | D     | 1002 | POV  | O21-C21-C22 | 3.62  | 119.30      | 111.50   |
| 3   | D     | 1008 | POV  | O21-C21-C22 | 3.60  | 119.26      | 111.50   |
| 3   | E     | 1008 | POV  | O21-C21-C22 | 3.60  | 119.25      | 111.50   |
| 3   | C     | 1002 | POV  | O21-C21-C22 | 3.59  | 119.25      | 111.50   |
| 3   | A     | 1008 | POV  | O21-C21-C22 | 3.56  | 119.17      | 111.50   |
| 3   | A     | 1010 | POV  | O21-C21-C22 | 3.53  | 119.11      | 111.50   |
| 3   | E     | 1005 | POV  | O21-C21-C22 | 3.46  | 118.96      | 111.50   |
| 3   | A     | 1010 | POV  | O31-C31-C32 | 3.31  | 122.29      | 111.91   |
| 3   | D     | 1003 | POV  | O31-C31-C32 | 3.23  | 122.06      | 111.91   |
| 3   | A     | 1003 | POV  | O31-C31-C32 | 3.19  | 121.91      | 111.91   |
| 3   | B     | 1004 | POV  | O31-C31-C32 | 3.10  | 121.64      | 111.91   |
| 3   | C     | 1003 | POV  | O31-C31-C32 | 3.09  | 121.59      | 111.91   |
| 3   | B     | 1003 | POV  | O31-C31-C32 | 2.96  | 121.19      | 111.91   |
| 3   | A     | 1002 | POV  | O31-C31-C32 | 2.94  | 121.12      | 111.91   |
| 3   | F     | 1002 | POV  | O31-C31-C32 | 2.93  | 121.09      | 111.91   |
| 3   | B     | 1008 | POV  | C3-C2-C1    | -2.91 | 104.91      | 111.79   |
| 3   | D     | 1007 | POV  | O31-C31-C32 | 2.91  | 121.03      | 111.91   |
| 3   | E     | 1002 | POV  | O31-C31-C32 | 2.89  | 120.99      | 111.91   |
| 3   | C     | 1007 | POV  | O31-C31-C32 | 2.88  | 120.95      | 111.91   |
| 3   | A     | 1007 | POV  | C3-C2-C1    | -2.87 | 104.99      | 111.79   |
| 3   | C     | 1007 | POV  | C3-C2-C1    | -2.87 | 105.01      | 111.79   |
| 3   | E     | 1003 | POV  | O31-C31-C32 | 2.84  | 120.82      | 111.91   |
| 3   | B     | 1008 | POV  | O31-C31-C32 | 2.82  | 120.76      | 111.91   |
| 3   | E     | 1007 | POV  | C3-C2-C1    | -2.80 | 105.16      | 111.79   |
| 3   | C     | 1002 | POV  | O31-C31-C32 | 2.79  | 120.66      | 111.91   |
| 3   | F     | 1006 | POV  | C3-C2-C1    | -2.78 | 105.21      | 111.79   |
| 3   | D     | 1002 | POV  | O31-C31-C32 | 2.76  | 120.57      | 111.91   |
| 3   | A     | 1007 | POV  | O31-C31-C32 | 2.73  | 120.48      | 111.91   |
| 3   | F     | 1006 | POV  | O31-C31-C32 | 2.73  | 120.46      | 111.91   |
| 3   | E     | 1007 | POV  | O31-C31-C32 | 2.72  | 120.44      | 111.91   |
| 3   | F     | 1007 | POV  | O31-C31-C32 | 2.70  | 120.37      | 111.91   |
| 3   | F     | 1010 | POV  | O31-C31-C32 | 2.68  | 120.31      | 111.91   |
| 3   | C     | 1008 | POV  | O31-C31-C32 | 2.67  | 120.29      | 111.91   |
| 3   | B     | 1002 | POV  | O31-C31-C32 | 2.66  | 120.26      | 111.91   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3   | E     | 1008 | POV  | O31-C31-C32 | 2.65  | 120.22      | 111.91   |
| 3   | D     | 1011 | POV  | O31-C31-C32 | 2.63  | 120.15      | 111.91   |
| 3   | E     | 1010 | POV  | O31-C31-C32 | 2.59  | 120.05      | 111.91   |
| 3   | A     | 1011 | POV  | O31-C31-C32 | 2.59  | 120.05      | 111.91   |
| 3   | B     | 1009 | POV  | O31-C31-C32 | 2.58  | 120.01      | 111.91   |
| 3   | D     | 1007 | POV  | C3-C2-C1    | -2.57 | 105.71      | 111.79   |
| 3   | D     | 1008 | POV  | O31-C31-C32 | 2.54  | 119.89      | 111.91   |
| 3   | C     | 1010 | POV  | O31-C31-C32 | 2.54  | 119.87      | 111.91   |
| 3   | A     | 1008 | POV  | O31-C31-C32 | 2.53  | 119.86      | 111.91   |
| 3   | C     | 1009 | POV  | O31-C31-C32 | 2.53  | 119.84      | 111.91   |
| 3   | A     | 1009 | POV  | O31-C31-C32 | 2.51  | 119.79      | 111.91   |
| 3   | E     | 1009 | POV  | O31-C31-C32 | 2.50  | 119.75      | 111.91   |
| 3   | B     | 1010 | POV  | O31-C31-C32 | 2.48  | 119.70      | 111.91   |
| 3   | F     | 1009 | POV  | O31-C31-C32 | 2.47  | 119.66      | 111.91   |
| 3   | F     | 1004 | POV  | O31-C31-C32 | 2.47  | 119.65      | 111.91   |
| 3   | D     | 1010 | POV  | O31-C31-C32 | 2.47  | 119.65      | 111.91   |
| 3   | D     | 1009 | POV  | O31-C31-C32 | 2.46  | 119.64      | 111.91   |
| 3   | F     | 1008 | POV  | O31-C31-C32 | 2.43  | 119.52      | 111.91   |
| 3   | F     | 1003 | POV  | O31-C31-C32 | 2.42  | 119.50      | 111.91   |
| 3   | C     | 1005 | POV  | C11-C12-N   | -2.39 | 107.81      | 115.78   |
| 3   | A     | 1012 | POV  | O31-C31-C32 | 2.38  | 119.38      | 111.91   |
| 3   | D     | 1005 | POV  | C11-C12-N   | -2.37 | 107.86      | 115.78   |
| 3   | C     | 1006 | POV  | O31-C31-C32 | 2.36  | 119.32      | 111.91   |
| 3   | E     | 1006 | POV  | O31-C31-C32 | 2.35  | 119.29      | 111.91   |
| 3   | A     | 1006 | POV  | O31-C31-C32 | 2.35  | 119.29      | 111.91   |
| 3   | B     | 1007 | POV  | O31-C31-C32 | 2.34  | 119.25      | 111.91   |
| 3   | E     | 1005 | POV  | C11-C12-N   | -2.33 | 108.01      | 115.78   |
| 3   | F     | 1007 | POV  | C2-O21-C21  | -2.33 | 112.06      | 117.79   |
| 3   | D     | 1006 | POV  | O31-C31-C32 | 2.32  | 119.18      | 111.91   |
| 3   | A     | 1004 | POV  | O31-C31-C32 | 2.31  | 119.17      | 111.91   |
| 3   | F     | 1005 | POV  | O31-C31-C32 | 2.31  | 119.16      | 111.91   |
| 3   | B     | 1006 | POV  | O31-C31-C32 | 2.30  | 119.14      | 111.91   |
| 3   | C     | 1004 | POV  | O31-C31-C32 | 2.30  | 119.12      | 111.91   |
| 3   | D     | 1004 | POV  | O31-C31-C32 | 2.29  | 119.11      | 111.91   |
| 3   | A     | 1005 | POV  | C11-C12-N   | -2.29 | 108.13      | 115.78   |
| 3   | B     | 1006 | POV  | C11-C12-N   | -2.28 | 108.18      | 115.78   |
| 3   | C     | 1005 | POV  | O31-C31-C32 | 2.27  | 119.04      | 111.91   |
| 3   | C     | 1009 | POV  | C3-C2-C1    | -2.25 | 106.46      | 111.79   |
| 3   | A     | 1005 | POV  | O31-C31-C32 | 2.21  | 118.84      | 111.91   |
| 3   | B     | 1005 | POV  | O31-C31-C32 | 2.21  | 118.83      | 111.91   |
| 3   | E     | 1004 | POV  | O31-C31-C32 | 2.20  | 118.83      | 111.91   |
| 3   | F     | 1004 | POV  | C11-C12-N   | -2.20 | 108.44      | 115.78   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 3   | D     | 1010 | POV  | C3-C2-C1    | -2.19 | 106.60      | 111.79   |
| 3   | D     | 1005 | POV  | O31-C31-C32 | 2.19  | 118.77      | 111.91   |
| 3   | B     | 1010 | POV  | C3-C2-C1    | -2.17 | 106.66      | 111.79   |
| 3   | D     | 1009 | POV  | C3-C2-C1    | -2.13 | 106.75      | 111.79   |
| 3   | B     | 1004 | POV  | C24-C23-C22 | -2.13 | 105.53      | 113.19   |
| 3   | E     | 1009 | POV  | C3-C2-C1    | -2.12 | 106.76      | 111.79   |
| 3   | B     | 1009 | POV  | C2-O21-C21  | -2.10 | 112.61      | 117.79   |
| 3   | F     | 1008 | POV  | C3-C2-C1    | -2.09 | 106.84      | 111.79   |
| 3   | D     | 1003 | POV  | C24-C23-C22 | -2.08 | 105.70      | 113.19   |
| 3   | E     | 1003 | POV  | C24-C23-C22 | -2.08 | 105.71      | 113.19   |
| 3   | E     | 1005 | POV  | O31-C31-C32 | 2.07  | 118.40      | 111.91   |
| 3   | A     | 1009 | POV  | C3-C2-C1    | -2.06 | 106.92      | 111.79   |
| 3   | C     | 1003 | POV  | C24-C23-C22 | -2.06 | 105.80      | 113.19   |
| 3   | C     | 1006 | POV  | C3-C2-C1    | -2.05 | 106.95      | 111.79   |
| 3   | F     | 1009 | POV  | C3-C2-C1    | -2.03 | 106.97      | 111.79   |
| 3   | C     | 1008 | POV  | C2-O21-C21  | -2.01 | 112.84      | 117.79   |
| 3   | E     | 1005 | POV  | C2-O21-C21  | -2.01 | 112.84      | 117.79   |
| 3   | A     | 1010 | POV  | O31-C31-O32 | -2.01 | 118.52      | 123.59   |
| 3   | E     | 1006 | POV  | C2-O21-C21  | -2.00 | 112.86      | 117.79   |

There are no chirality outliers.

All (1434) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms          |
|-----|-------|------|------|----------------|
| 3   | A     | 1002 | POV  | C1-O11-P-O14   |
| 3   | A     | 1003 | POV  | C12-C11-O12-P  |
| 3   | A     | 1004 | POV  | C1-O11-P-O13   |
| 3   | A     | 1005 | POV  | C22-C21-O21-C2 |
| 3   | A     | 1006 | POV  | C1-O11-P-O14   |
| 3   | A     | 1006 | POV  | C11-O12-P-O13  |
| 3   | A     | 1006 | POV  | C11-O12-P-O14  |
| 3   | A     | 1006 | POV  | O12-C11-C12-N  |
| 3   | A     | 1007 | POV  | C11-O12-P-O11  |
| 3   | A     | 1007 | POV  | C11-O12-P-O13  |
| 3   | A     | 1007 | POV  | C11-O12-P-O14  |
| 3   | A     | 1007 | POV  | O12-C11-C12-N  |
| 3   | A     | 1007 | POV  | C22-C21-O21-C2 |
| 3   | A     | 1007 | POV  | O22-C21-O21-C2 |
| 3   | A     | 1008 | POV  | C1-O11-P-O12   |
| 3   | A     | 1008 | POV  | C1-O11-P-O13   |
| 3   | A     | 1008 | POV  | C1-O11-P-O14   |
| 3   | A     | 1008 | POV  | O12-C11-C12-N  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms          |
|-----|-------|------|------|----------------|
| 3   | A     | 1008 | POV  | C12-C11-O12-P  |
| 3   | A     | 1008 | POV  | C22-C21-O21-C2 |
| 3   | A     | 1010 | POV  | C1-O11-P-O14   |
| 3   | A     | 1011 | POV  | C1-O11-P-O14   |
| 3   | A     | 1011 | POV  | C11-O12-P-O14  |
| 3   | A     | 1011 | POV  | C22-C21-O21-C2 |
| 3   | A     | 1011 | POV  | O22-C21-O21-C2 |
| 3   | A     | 1012 | POV  | O12-C11-C12-N  |
| 3   | B     | 1002 | POV  | C11-O12-P-O11  |
| 3   | B     | 1002 | POV  | C11-O12-P-O14  |
| 3   | B     | 1002 | POV  | C22-C21-O21-C2 |
| 3   | B     | 1002 | POV  | O22-C21-O21-C2 |
| 3   | B     | 1003 | POV  | C1-O11-P-O14   |
| 3   | B     | 1004 | POV  | C11-O12-P-O13  |
| 3   | B     | 1004 | POV  | C12-C11-O12-P  |
| 3   | B     | 1005 | POV  | C1-O11-P-O13   |
| 3   | B     | 1006 | POV  | C22-C21-O21-C2 |
| 3   | B     | 1007 | POV  | C1-O11-P-O14   |
| 3   | B     | 1007 | POV  | C11-O12-P-O13  |
| 3   | B     | 1007 | POV  | C11-O12-P-O14  |
| 3   | B     | 1007 | POV  | O12-C11-C12-N  |
| 3   | B     | 1008 | POV  | C11-O12-P-O13  |
| 3   | B     | 1008 | POV  | C11-O12-P-O14  |
| 3   | B     | 1008 | POV  | O12-C11-C12-N  |
| 3   | B     | 1008 | POV  | C22-C21-O21-C2 |
| 3   | B     | 1008 | POV  | O22-C21-O21-C2 |
| 3   | B     | 1009 | POV  | C1-O11-P-O12   |
| 3   | B     | 1009 | POV  | C1-O11-P-O13   |
| 3   | B     | 1009 | POV  | C1-O11-P-O14   |
| 3   | B     | 1009 | POV  | O12-C11-C12-N  |
| 3   | B     | 1009 | POV  | C12-C11-O12-P  |
| 3   | B     | 1009 | POV  | C22-C21-O21-C2 |
| 3   | C     | 1002 | POV  | C1-O11-P-O14   |
| 3   | C     | 1003 | POV  | C1-O11-P-O12   |
| 3   | C     | 1003 | POV  | C1-O11-P-O13   |
| 3   | C     | 1003 | POV  | C1-O11-P-O14   |
| 3   | C     | 1003 | POV  | O12-C11-C12-N  |
| 3   | C     | 1003 | POV  | C12-C11-O12-P  |
| 3   | C     | 1004 | POV  | C1-O11-P-O13   |
| 3   | C     | 1004 | POV  | C22-C21-O21-C2 |
| 3   | C     | 1005 | POV  | C22-C21-O21-C2 |
| 3   | C     | 1006 | POV  | C1-O11-P-O14   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms          |
|-----|-------|------|------|----------------|
| 3   | C     | 1006 | POV  | C11-O12-P-O13  |
| 3   | C     | 1006 | POV  | C11-O12-P-O14  |
| 3   | C     | 1006 | POV  | O12-C11-C12-N  |
| 3   | C     | 1007 | POV  | C11-O12-P-O13  |
| 3   | C     | 1007 | POV  | C11-O12-P-O14  |
| 3   | C     | 1007 | POV  | O12-C11-C12-N  |
| 3   | C     | 1007 | POV  | C22-C21-O21-C2 |
| 3   | C     | 1007 | POV  | O22-C21-O21-C2 |
| 3   | C     | 1008 | POV  | C1-O11-P-O13   |
| 3   | C     | 1008 | POV  | C1-O11-P-O14   |
| 3   | C     | 1008 | POV  | O12-C11-C12-N  |
| 3   | C     | 1008 | POV  | C12-C11-O12-P  |
| 3   | C     | 1008 | POV  | C22-C21-O21-C2 |
| 3   | C     | 1010 | POV  | C1-O11-P-O14   |
| 3   | C     | 1010 | POV  | C22-C21-O21-C2 |
| 3   | C     | 1010 | POV  | O22-C21-O21-C2 |
| 3   | D     | 1002 | POV  | C1-O11-P-O14   |
| 3   | D     | 1003 | POV  | C1-O11-P-O12   |
| 3   | D     | 1003 | POV  | C1-O11-P-O13   |
| 3   | D     | 1003 | POV  | C1-O11-P-O14   |
| 3   | D     | 1003 | POV  | O12-C11-C12-N  |
| 3   | D     | 1003 | POV  | C12-C11-O12-P  |
| 3   | D     | 1004 | POV  | C1-O11-P-O13   |
| 3   | D     | 1004 | POV  | C22-C21-O21-C2 |
| 3   | D     | 1005 | POV  | C22-C21-O21-C2 |
| 3   | D     | 1006 | POV  | C1-O11-P-O14   |
| 3   | D     | 1006 | POV  | C11-O12-P-O13  |
| 3   | D     | 1006 | POV  | C11-O12-P-O14  |
| 3   | D     | 1006 | POV  | O12-C11-C12-N  |
| 3   | D     | 1007 | POV  | C11-O12-P-O13  |
| 3   | D     | 1007 | POV  | C11-O12-P-O14  |
| 3   | D     | 1007 | POV  | O12-C11-C12-N  |
| 3   | D     | 1007 | POV  | C22-C21-O21-C2 |
| 3   | D     | 1007 | POV  | O22-C21-O21-C2 |
| 3   | D     | 1008 | POV  | C1-O11-P-O13   |
| 3   | D     | 1008 | POV  | C1-O11-P-O14   |
| 3   | D     | 1008 | POV  | O12-C11-C12-N  |
| 3   | D     | 1008 | POV  | C12-C11-O12-P  |
| 3   | D     | 1008 | POV  | C22-C21-O21-C2 |
| 3   | D     | 1009 | POV  | O12-C11-C12-N  |
| 3   | D     | 1011 | POV  | C11-O12-P-O14  |
| 3   | D     | 1011 | POV  | C22-C21-O21-C2 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms          |
|-----|-------|------|------|----------------|
| 3   | D     | 1011 | POV  | O22-C21-O21-C2 |
| 3   | E     | 1002 | POV  | C1-O11-P-O14   |
| 3   | E     | 1003 | POV  | C1-O11-P-O14   |
| 3   | E     | 1003 | POV  | C11-O12-P-O13  |
| 3   | E     | 1003 | POV  | C11-O12-P-O14  |
| 3   | E     | 1004 | POV  | C1-O11-P-O13   |
| 3   | E     | 1004 | POV  | C1-O11-P-O14   |
| 3   | E     | 1004 | POV  | C22-C21-O21-C2 |
| 3   | E     | 1005 | POV  | C22-C21-O21-C2 |
| 3   | E     | 1006 | POV  | C1-O11-P-O14   |
| 3   | E     | 1006 | POV  | C11-O12-P-O13  |
| 3   | E     | 1006 | POV  | C11-O12-P-O14  |
| 3   | E     | 1006 | POV  | O12-C11-C12-N  |
| 3   | E     | 1007 | POV  | C11-O12-P-O11  |
| 3   | E     | 1007 | POV  | C11-O12-P-O13  |
| 3   | E     | 1007 | POV  | C11-O12-P-O14  |
| 3   | E     | 1007 | POV  | O12-C11-C12-N  |
| 3   | E     | 1007 | POV  | C22-C21-O21-C2 |
| 3   | E     | 1007 | POV  | O22-C21-O21-C2 |
| 3   | E     | 1008 | POV  | C1-O11-P-O12   |
| 3   | E     | 1008 | POV  | C1-O11-P-O13   |
| 3   | E     | 1008 | POV  | C1-O11-P-O14   |
| 3   | E     | 1008 | POV  | O12-C11-C12-N  |
| 3   | E     | 1008 | POV  | C12-C11-O12-P  |
| 3   | E     | 1008 | POV  | C22-C21-O21-C2 |
| 3   | E     | 1010 | POV  | C11-O12-P-O14  |
| 3   | E     | 1010 | POV  | C22-C21-O21-C2 |
| 3   | E     | 1010 | POV  | O22-C21-O21-C2 |
| 3   | F     | 1002 | POV  | C11-O12-P-O13  |
| 3   | F     | 1002 | POV  | C11-O12-P-O14  |
| 3   | F     | 1002 | POV  | C12-C11-O12-P  |
| 3   | F     | 1003 | POV  | C1-O11-P-O13   |
| 3   | F     | 1003 | POV  | C1-O11-P-O14   |
| 3   | F     | 1003 | POV  | C22-C21-O21-C2 |
| 3   | F     | 1004 | POV  | C22-C21-O21-C2 |
| 3   | F     | 1005 | POV  | C1-O11-P-O14   |
| 3   | F     | 1005 | POV  | C11-O12-P-O13  |
| 3   | F     | 1005 | POV  | C11-O12-P-O14  |
| 3   | F     | 1005 | POV  | O12-C11-C12-N  |
| 3   | F     | 1006 | POV  | C11-O12-P-O13  |
| 3   | F     | 1006 | POV  | C11-O12-P-O14  |
| 3   | F     | 1006 | POV  | O12-C11-C12-N  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms          |
|-----|-------|------|------|----------------|
| 3   | F     | 1006 | POV  | C22-C21-O21-C2 |
| 3   | F     | 1006 | POV  | O22-C21-O21-C2 |
| 3   | F     | 1007 | POV  | C1-O11-P-O12   |
| 3   | F     | 1007 | POV  | C1-O11-P-O13   |
| 3   | F     | 1007 | POV  | C1-O11-P-O14   |
| 3   | F     | 1007 | POV  | O12-C11-C12-N  |
| 3   | F     | 1007 | POV  | C12-C11-O12-P  |
| 3   | F     | 1007 | POV  | C22-C21-O21-C2 |
| 3   | F     | 1008 | POV  | O12-C11-C12-N  |
| 3   | F     | 1010 | POV  | C11-O12-P-O14  |
| 3   | F     | 1010 | POV  | C22-C21-O21-C2 |
| 3   | F     | 1010 | POV  | O22-C21-O21-C2 |
| 3   | A     | 1011 | POV  | O32-C31-O31-C3 |
| 3   | B     | 1002 | POV  | O32-C31-O31-C3 |
| 3   | C     | 1010 | POV  | O32-C31-O31-C3 |
| 3   | E     | 1010 | POV  | O32-C31-O31-C3 |
| 3   | F     | 1010 | POV  | O32-C31-O31-C3 |
| 3   | A     | 1004 | POV  | O22-C21-O21-C2 |
| 3   | A     | 1005 | POV  | O22-C21-O21-C2 |
| 3   | A     | 1008 | POV  | O22-C21-O21-C2 |
| 3   | B     | 1005 | POV  | O22-C21-O21-C2 |
| 3   | B     | 1006 | POV  | O22-C21-O21-C2 |
| 3   | B     | 1009 | POV  | O22-C21-O21-C2 |
| 3   | C     | 1004 | POV  | O22-C21-O21-C2 |
| 3   | C     | 1008 | POV  | O22-C21-O21-C2 |
| 3   | D     | 1004 | POV  | O22-C21-O21-C2 |
| 3   | D     | 1005 | POV  | O22-C21-O21-C2 |
| 3   | D     | 1008 | POV  | O22-C21-O21-C2 |
| 3   | E     | 1004 | POV  | O22-C21-O21-C2 |
| 3   | E     | 1005 | POV  | O22-C21-O21-C2 |
| 3   | E     | 1008 | POV  | O22-C21-O21-C2 |
| 3   | F     | 1003 | POV  | O22-C21-O21-C2 |
| 3   | F     | 1007 | POV  | O22-C21-O21-C2 |
| 3   | A     | 1007 | POV  | C32-C31-O31-C3 |
| 3   | D     | 1007 | POV  | C32-C31-O31-C3 |
| 3   | F     | 1006 | POV  | C32-C31-O31-C3 |
| 3   | A     | 1004 | POV  | C22-C21-O21-C2 |
| 3   | B     | 1005 | POV  | C22-C21-O21-C2 |
| 3   | D     | 1011 | POV  | O32-C31-O31-C3 |
| 3   | A     | 1011 | POV  | C32-C31-O31-C3 |
| 3   | B     | 1002 | POV  | C32-C31-O31-C3 |
| 3   | B     | 1008 | POV  | C32-C31-O31-C3 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 3   | C     | 1007 | POV  | C32-C31-O31-C3  |
| 3   | C     | 1010 | POV  | C32-C31-O31-C3  |
| 3   | D     | 1011 | POV  | C32-C31-O31-C3  |
| 3   | E     | 1007 | POV  | C32-C31-O31-C3  |
| 3   | E     | 1010 | POV  | C32-C31-O31-C3  |
| 3   | F     | 1010 | POV  | C32-C31-O31-C3  |
| 3   | C     | 1005 | POV  | O22-C21-O21-C2  |
| 3   | F     | 1004 | POV  | O22-C21-O21-C2  |
| 3   | F     | 1006 | POV  | O32-C31-O31-C3  |
| 3   | A     | 1007 | POV  | O32-C31-O31-C3  |
| 3   | D     | 1007 | POV  | O32-C31-O31-C3  |
| 3   | E     | 1007 | POV  | O32-C31-O31-C3  |
| 3   | E     | 1006 | POV  | C22-C21-O21-C2  |
| 3   | B     | 1008 | POV  | O32-C31-O31-C3  |
| 3   | C     | 1007 | POV  | O32-C31-O31-C3  |
| 3   | C     | 1008 | POV  | C32-C31-O31-C3  |
| 3   | A     | 1002 | POV  | C22-C21-O21-C2  |
| 3   | B     | 1003 | POV  | C22-C21-O21-C2  |
| 3   | C     | 1002 | POV  | C22-C21-O21-C2  |
| 3   | E     | 1006 | POV  | O22-C21-O21-C2  |
| 3   | D     | 1004 | POV  | C11-C12-N-C13   |
| 3   | D     | 1004 | POV  | C11-C12-N-C14   |
| 3   | A     | 1008 | POV  | C32-C31-O31-C3  |
| 3   | A     | 1009 | POV  | C32-C31-O31-C3  |
| 3   | B     | 1009 | POV  | C32-C31-O31-C3  |
| 3   | B     | 1010 | POV  | C32-C31-O31-C3  |
| 3   | C     | 1009 | POV  | C32-C31-O31-C3  |
| 3   | D     | 1008 | POV  | C32-C31-O31-C3  |
| 3   | D     | 1010 | POV  | C32-C31-O31-C3  |
| 3   | E     | 1009 | POV  | C32-C31-O31-C3  |
| 3   | F     | 1009 | POV  | C32-C31-O31-C3  |
| 3   | B     | 1002 | POV  | C31-C32-C33-C34 |
| 3   | A     | 1006 | POV  | C22-C21-O21-C2  |
| 3   | A     | 1010 | POV  | C22-C21-O21-C2  |
| 3   | B     | 1007 | POV  | C22-C21-O21-C2  |
| 3   | D     | 1002 | POV  | C22-C21-O21-C2  |
| 3   | E     | 1002 | POV  | C22-C21-O21-C2  |
| 3   | A     | 1010 | POV  | C21-C22-C23-C24 |
| 3   | C     | 1010 | POV  | C21-C22-C23-C24 |
| 3   | C     | 1010 | POV  | C31-C32-C33-C34 |
| 3   | D     | 1006 | POV  | C31-C32-C33-C34 |
| 3   | D     | 1009 | POV  | C31-C32-C33-C34 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 3   | E     | 1009 | POV  | C21-C22-C23-C24 |
| 3   | E     | 1010 | POV  | C31-C32-C33-C34 |
| 3   | A     | 1009 | POV  | O32-C31-O31-C3  |
| 3   | E     | 1008 | POV  | C32-C31-O31-C3  |
| 3   | A     | 1002 | POV  | C21-C22-C23-C24 |
| 3   | A     | 1006 | POV  | C31-C32-C33-C34 |
| 3   | A     | 1007 | POV  | C21-C22-C23-C24 |
| 3   | A     | 1012 | POV  | C31-C32-C33-C34 |
| 3   | B     | 1006 | POV  | C31-C32-C33-C34 |
| 3   | B     | 1007 | POV  | C31-C32-C33-C34 |
| 3   | C     | 1002 | POV  | C21-C22-C23-C24 |
| 3   | C     | 1006 | POV  | C31-C32-C33-C34 |
| 3   | C     | 1009 | POV  | C21-C22-C23-C24 |
| 3   | D     | 1010 | POV  | C21-C22-C23-C24 |
| 3   | D     | 1011 | POV  | C21-C22-C23-C24 |
| 3   | F     | 1004 | POV  | C31-C32-C33-C34 |
| 3   | C     | 1009 | POV  | O32-C31-O31-C3  |
| 3   | F     | 1009 | POV  | O32-C31-O31-C3  |
| 3   | A     | 1005 | POV  | C31-C32-C33-C34 |
| 3   | A     | 1009 | POV  | C21-C22-C23-C24 |
| 3   | A     | 1011 | POV  | C31-C32-C33-C34 |
| 3   | A     | 1012 | POV  | C21-C22-C23-C24 |
| 3   | B     | 1005 | POV  | C21-C22-C23-C24 |
| 3   | B     | 1008 | POV  | C21-C22-C23-C24 |
| 3   | B     | 1010 | POV  | C21-C22-C23-C24 |
| 3   | C     | 1005 | POV  | C31-C32-C33-C34 |
| 3   | C     | 1007 | POV  | C21-C22-C23-C24 |
| 3   | D     | 1005 | POV  | C31-C32-C33-C34 |
| 3   | D     | 1006 | POV  | C21-C22-C23-C24 |
| 3   | D     | 1007 | POV  | C21-C22-C23-C24 |
| 3   | D     | 1009 | POV  | C21-C22-C23-C24 |
| 3   | D     | 1011 | POV  | C31-C32-C33-C34 |
| 3   | E     | 1002 | POV  | C21-C22-C23-C24 |
| 3   | E     | 1004 | POV  | C21-C22-C23-C24 |
| 3   | E     | 1005 | POV  | C31-C32-C33-C34 |
| 3   | E     | 1006 | POV  | C31-C32-C33-C34 |
| 3   | E     | 1007 | POV  | C21-C22-C23-C24 |
| 3   | F     | 1005 | POV  | C31-C32-C33-C34 |
| 3   | F     | 1006 | POV  | C21-C22-C23-C24 |
| 3   | F     | 1008 | POV  | C31-C32-C33-C34 |
| 3   | F     | 1009 | POV  | C21-C22-C23-C24 |
| 3   | F     | 1010 | POV  | C31-C32-C33-C34 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 3   | A     | 1002 | POV  | O22-C21-O21-C2  |
| 3   | C     | 1004 | POV  | C21-C22-C23-C24 |
| 3   | D     | 1002 | POV  | C21-C22-C23-C24 |
| 3   | D     | 1004 | POV  | C21-C22-C23-C24 |
| 3   | F     | 1003 | POV  | C21-C22-C23-C24 |
| 3   | F     | 1008 | POV  | C21-C22-C23-C24 |
| 3   | C     | 1006 | POV  | C22-C21-O21-C2  |
| 3   | F     | 1005 | POV  | C22-C21-O21-C2  |
| 3   | A     | 1008 | POV  | O32-C31-O31-C3  |
| 3   | B     | 1010 | POV  | O32-C31-O31-C3  |
| 3   | D     | 1008 | POV  | O32-C31-O31-C3  |
| 3   | E     | 1009 | POV  | O32-C31-O31-C3  |
| 3   | A     | 1004 | POV  | C21-C22-C23-C24 |
| 3   | B     | 1003 | POV  | C21-C22-C23-C24 |
| 3   | D     | 1010 | POV  | O32-C31-O31-C3  |
| 3   | B     | 1002 | POV  | C21-C22-C23-C24 |
| 3   | E     | 1010 | POV  | C21-C22-C23-C24 |
| 3   | A     | 1010 | POV  | O22-C21-O21-C2  |
| 3   | B     | 1003 | POV  | O22-C21-O21-C2  |
| 3   | C     | 1002 | POV  | O22-C21-O21-C2  |
| 3   | F     | 1007 | POV  | C32-C31-O31-C3  |
| 3   | F     | 1008 | POV  | C32-C31-O31-C3  |
| 3   | B     | 1009 | POV  | O32-C31-O31-C3  |
| 3   | C     | 1008 | POV  | O32-C31-O31-C3  |
| 3   | E     | 1008 | POV  | O32-C31-O31-C3  |
| 3   | B     | 1010 | POV  | C22-C21-O21-C2  |
| 3   | D     | 1006 | POV  | C22-C21-O21-C2  |
| 3   | F     | 1009 | POV  | C22-C21-O21-C2  |
| 3   | A     | 1003 | POV  | C1-O11-P-O12    |
| 3   | A     | 1004 | POV  | C1-O11-P-O12    |
| 3   | A     | 1005 | POV  | C11-O12-P-O11   |
| 3   | A     | 1006 | POV  | C11-O12-P-O11   |
| 3   | A     | 1011 | POV  | C1-O11-P-O12    |
| 3   | A     | 1011 | POV  | C11-O12-P-O11   |
| 3   | A     | 1012 | POV  | C11-O12-P-O11   |
| 3   | B     | 1002 | POV  | C1-O11-P-O12    |
| 3   | B     | 1004 | POV  | C1-O11-P-O12    |
| 3   | B     | 1004 | POV  | C11-O12-P-O11   |
| 3   | B     | 1005 | POV  | C1-O11-P-O12    |
| 3   | B     | 1006 | POV  | C11-O12-P-O11   |
| 3   | B     | 1007 | POV  | C11-O12-P-O11   |
| 3   | B     | 1008 | POV  | C11-O12-P-O11   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 3   | C     | 1004 | POV  | C1-O11-P-O12    |
| 3   | C     | 1005 | POV  | C11-O12-P-O11   |
| 3   | C     | 1006 | POV  | C11-O12-P-O11   |
| 3   | C     | 1007 | POV  | C11-O12-P-O11   |
| 3   | C     | 1008 | POV  | C1-O11-P-O12    |
| 3   | C     | 1010 | POV  | C11-O12-P-O11   |
| 3   | D     | 1002 | POV  | C1-O11-P-O12    |
| 3   | D     | 1004 | POV  | C1-O11-P-O12    |
| 3   | D     | 1005 | POV  | C11-O12-P-O11   |
| 3   | D     | 1006 | POV  | C11-O12-P-O11   |
| 3   | D     | 1007 | POV  | C11-O12-P-O11   |
| 3   | D     | 1008 | POV  | C1-O11-P-O12    |
| 3   | D     | 1009 | POV  | C11-O12-P-O11   |
| 3   | D     | 1011 | POV  | C1-O11-P-O12    |
| 3   | D     | 1011 | POV  | C11-O12-P-O11   |
| 3   | E     | 1003 | POV  | C1-O11-P-O12    |
| 3   | E     | 1003 | POV  | C11-O12-P-O11   |
| 3   | E     | 1004 | POV  | C1-O11-P-O12    |
| 3   | E     | 1005 | POV  | C11-O12-P-O11   |
| 3   | E     | 1006 | POV  | C11-O12-P-O11   |
| 3   | E     | 1010 | POV  | C1-O11-P-O12    |
| 3   | E     | 1010 | POV  | C11-O12-P-O11   |
| 3   | F     | 1002 | POV  | C1-O11-P-O12    |
| 3   | F     | 1002 | POV  | C11-O12-P-O11   |
| 3   | F     | 1003 | POV  | C1-O11-P-O12    |
| 3   | F     | 1004 | POV  | C11-O12-P-O11   |
| 3   | F     | 1005 | POV  | C11-O12-P-O11   |
| 3   | F     | 1006 | POV  | C11-O12-P-O11   |
| 3   | F     | 1008 | POV  | C11-O12-P-O11   |
| 3   | F     | 1010 | POV  | C1-O11-P-O12    |
| 3   | F     | 1010 | POV  | C11-O12-P-O11   |
| 3   | A     | 1006 | POV  | C32-C31-O31-C3  |
| 3   | C     | 1006 | POV  | C32-C31-O31-C3  |
| 3   | D     | 1009 | POV  | C32-C31-O31-C3  |
| 3   | F     | 1005 | POV  | C21-C22-C23-C24 |
| 3   | A     | 1006 | POV  | O22-C21-O21-C2  |
| 3   | A     | 1009 | POV  | O22-C21-O21-C2  |
| 3   | B     | 1007 | POV  | O22-C21-O21-C2  |
| 3   | B     | 1010 | POV  | O22-C21-O21-C2  |
| 3   | C     | 1006 | POV  | O22-C21-O21-C2  |
| 3   | D     | 1002 | POV  | O22-C21-O21-C2  |
| 3   | D     | 1006 | POV  | O22-C21-O21-C2  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms               |
|-----|-------|------|------|---------------------|
| 3   | E     | 1002 | POV  | O22-C21-O21-C2      |
| 3   | F     | 1005 | POV  | O22-C21-O21-C2      |
| 3   | F     | 1009 | POV  | O22-C21-O21-C2      |
| 3   | A     | 1012 | POV  | C32-C31-O31-C3      |
| 3   | C     | 1005 | POV  | C33-C34-C35-C36     |
| 3   | A     | 1009 | POV  | C22-C21-O21-C2      |
| 3   | D     | 1010 | POV  | C22-C21-O21-C2      |
| 3   | E     | 1009 | POV  | C22-C21-O21-C2      |
| 3   | A     | 1010 | POV  | C39-C310-C311-C312  |
| 3   | B     | 1006 | POV  | C33-C34-C35-C36     |
| 3   | B     | 1010 | POV  | C22-C23-C24-C25     |
| 3   | D     | 1003 | POV  | C310-C311-C312-C313 |
| 3   | D     | 1009 | POV  | C310-C311-C312-C313 |
| 3   | E     | 1002 | POV  | C24-C25-C26-C27     |
| 3   | E     | 1008 | POV  | C24-C25-C26-C27     |
| 3   | E     | 1010 | POV  | C212-C213-C214-C215 |
| 3   | F     | 1002 | POV  | C312-C313-C314-C315 |
| 3   | F     | 1004 | POV  | C33-C34-C35-C36     |
| 3   | F     | 1010 | POV  | C212-C213-C214-C215 |
| 3   | A     | 1002 | POV  | C39-C310-C311-C312  |
| 3   | A     | 1003 | POV  | C310-C311-C312-C313 |
| 3   | A     | 1011 | POV  | C212-C213-C214-C215 |
| 3   | A     | 1012 | POV  | C310-C311-C312-C313 |
| 3   | B     | 1006 | POV  | C22-C23-C24-C25     |
| 3   | C     | 1002 | POV  | C24-C25-C26-C27     |
| 3   | D     | 1002 | POV  | C24-C25-C26-C27     |
| 3   | E     | 1002 | POV  | C39-C310-C311-C312  |
| 3   | F     | 1002 | POV  | C311-C310-C39-C38   |
| 3   | D     | 1010 | POV  | O22-C21-O21-C2      |
| 3   | E     | 1009 | POV  | O22-C21-O21-C2      |
| 3   | A     | 1003 | POV  | C31-C32-C33-C34     |
| 3   | A     | 1008 | POV  | C24-C25-C26-C27     |
| 3   | A     | 1010 | POV  | C24-C25-C26-C27     |
| 3   | B     | 1003 | POV  | C24-C25-C26-C27     |
| 3   | C     | 1003 | POV  | C39-C310-C311-C312  |
| 3   | C     | 1010 | POV  | C212-C213-C214-C215 |
| 3   | D     | 1003 | POV  | C311-C310-C39-C38   |
| 3   | D     | 1005 | POV  | C22-C23-C24-C25     |
| 3   | E     | 1005 | POV  | C33-C34-C35-C36     |
| 3   | A     | 1003 | POV  | C32-C33-C34-C35     |
| 3   | A     | 1005 | POV  | C22-C23-C24-C25     |
| 3   | A     | 1005 | POV  | C33-C34-C35-C36     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms               |
|-----|-------|------|------|---------------------|
| 3   | B     | 1003 | POV  | C39-C310-C311-C312  |
| 3   | D     | 1005 | POV  | C33-C34-C35-C36     |
| 3   | D     | 1006 | POV  | C32-C33-C34-C35     |
| 3   | D     | 1011 | POV  | C212-C213-C214-C215 |
| 3   | F     | 1009 | POV  | C22-C23-C24-C25     |
| 3   | A     | 1003 | POV  | C39-C310-C311-C312  |
| 3   | A     | 1009 | POV  | C22-C23-C24-C25     |
| 3   | B     | 1004 | POV  | C39-C310-C311-C312  |
| 3   | C     | 1002 | POV  | C39-C310-C311-C312  |
| 3   | C     | 1003 | POV  | C311-C310-C39-C38   |
| 3   | E     | 1003 | POV  | C39-C310-C311-C312  |
| 3   | F     | 1002 | POV  | C39-C310-C311-C312  |
| 3   | A     | 1011 | POV  | C21-C22-C23-C24     |
| 3   | D     | 1003 | POV  | C31-C32-C33-C34     |
| 3   | F     | 1010 | POV  | C21-C22-C23-C24     |
| 3   | A     | 1010 | POV  | C212-C213-C214-C215 |
| 3   | B     | 1002 | POV  | C212-C213-C214-C215 |
| 3   | D     | 1002 | POV  | C39-C310-C311-C312  |
| 3   | D     | 1010 | POV  | C22-C23-C24-C25     |
| 3   | E     | 1009 | POV  | C22-C23-C24-C25     |
| 3   | F     | 1008 | POV  | C22-C23-C24-C25     |
| 3   | F     | 1007 | POV  | O32-C31-O31-C3      |
| 3   | F     | 1008 | POV  | O32-C31-O31-C3      |
| 3   | B     | 1004 | POV  | C310-C311-C312-C313 |
| 3   | C     | 1003 | POV  | C310-C311-C312-C313 |
| 3   | E     | 1002 | POV  | C212-C213-C214-C215 |
| 3   | E     | 1003 | POV  | C310-C311-C312-C313 |
| 3   | E     | 1010 | POV  | C22-C23-C24-C25     |
| 3   | F     | 1004 | POV  | C22-C23-C24-C25     |
| 3   | A     | 1002 | POV  | C24-C25-C26-C27     |
| 3   | A     | 1006 | POV  | C22-C23-C24-C25     |
| 3   | A     | 1008 | POV  | C211-C212-C213-C214 |
| 3   | A     | 1012 | POV  | C311-C312-C313-C314 |
| 3   | B     | 1003 | POV  | C212-C213-C214-C215 |
| 3   | C     | 1005 | POV  | C22-C23-C24-C25     |
| 3   | C     | 1006 | POV  | C32-C33-C34-C35     |
| 3   | C     | 1008 | POV  | C212-C213-C214-C215 |
| 3   | D     | 1002 | POV  | C212-C213-C214-C215 |
| 3   | D     | 1003 | POV  | C32-C33-C34-C35     |
| 3   | D     | 1009 | POV  | C311-C312-C313-C314 |
| 3   | E     | 1006 | POV  | C32-C33-C34-C35     |
| 3   | F     | 1005 | POV  | C22-C23-C24-C25     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms               |
|-----|-------|------|------|---------------------|
| 3   | F     | 1005 | POV  | C32-C33-C34-C35     |
| 3   | F     | 1007 | POV  | C212-C213-C214-C215 |
| 3   | C     | 1002 | POV  | C212-C213-C214-C215 |
| 3   | D     | 1003 | POV  | C39-C310-C311-C312  |
| 3   | E     | 1003 | POV  | C311-C310-C39-C38   |
| 3   | F     | 1010 | POV  | C22-C23-C24-C25     |
| 3   | C     | 1009 | POV  | O22-C21-O21-C2      |
| 3   | C     | 1009 | POV  | C22-C21-O21-C2      |
| 3   | A     | 1012 | POV  | C22-C23-C24-C25     |
| 3   | B     | 1005 | POV  | C23-C24-C25-C26     |
| 3   | B     | 1007 | POV  | C32-C33-C34-C35     |
| 3   | C     | 1008 | POV  | C211-C212-C213-C214 |
| 3   | C     | 1009 | POV  | C22-C23-C24-C25     |
| 3   | D     | 1008 | POV  | C24-C25-C26-C27     |
| 3   | D     | 1009 | POV  | C22-C23-C24-C25     |
| 3   | C     | 1003 | POV  | C26-C27-C28-C29     |
| 3   | D     | 1002 | POV  | C210-C211-C212-C213 |
| 3   | E     | 1007 | POV  | C210-C211-C212-C213 |
| 3   | A     | 1003 | POV  | C311-C310-C39-C38   |
| 3   | A     | 1006 | POV  | C32-C33-C34-C35     |
| 3   | B     | 1002 | POV  | C22-C23-C24-C25     |
| 3   | B     | 1004 | POV  | C32-C33-C34-C35     |
| 3   | B     | 1009 | POV  | C212-C213-C214-C215 |
| 3   | B     | 1009 | POV  | C36-C37-C38-C39     |
| 3   | C     | 1008 | POV  | C36-C37-C38-C39     |
| 3   | C     | 1010 | POV  | C22-C23-C24-C25     |
| 3   | D     | 1008 | POV  | C211-C212-C213-C214 |
| 3   | E     | 1003 | POV  | C24-C25-C26-C27     |
| 3   | E     | 1003 | POV  | C32-C33-C34-C35     |
| 3   | E     | 1004 | POV  | C23-C24-C25-C26     |
| 3   | E     | 1008 | POV  | C212-C213-C214-C215 |
| 3   | F     | 1002 | POV  | C24-C25-C26-C27     |
| 3   | F     | 1003 | POV  | C23-C24-C25-C26     |
| 3   | F     | 1008 | POV  | C310-C311-C312-C313 |
| 3   | F     | 1008 | POV  | C311-C312-C313-C314 |
| 3   | D     | 1004 | POV  | C11-C12-N-C15       |
| 3   | B     | 1003 | POV  | C311-C310-C39-C38   |
| 3   | D     | 1002 | POV  | C311-C310-C39-C38   |
| 3   | D     | 1008 | POV  | C212-C213-C214-C215 |
| 3   | A     | 1002 | POV  | C212-C213-C214-C215 |
| 3   | B     | 1004 | POV  | C311-C310-C39-C38   |
| 3   | B     | 1009 | POV  | C211-C212-C213-C214 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms               |
|-----|-------|------|------|---------------------|
| 3   | C     | 1003 | POV  | C312-C313-C314-C315 |
| 3   | C     | 1007 | POV  | C312-C313-C314-C315 |
| 3   | C     | 1008 | POV  | C24-C25-C26-C27     |
| 3   | E     | 1008 | POV  | C211-C212-C213-C214 |
| 3   | E     | 1008 | POV  | C36-C37-C38-C39     |
| 3   | F     | 1007 | POV  | C211-C212-C213-C214 |
| 3   | A     | 1006 | POV  | C21-C22-C23-C24     |
| 3   | C     | 1006 | POV  | O32-C31-O31-C3      |
| 3   | A     | 1008 | POV  | C36-C37-C38-C39     |
| 3   | B     | 1007 | POV  | C22-C23-C24-C25     |
| 3   | C     | 1002 | POV  | C311-C310-C39-C38   |
| 3   | C     | 1003 | POV  | C32-C33-C34-C35     |
| 3   | D     | 1008 | POV  | C36-C37-C38-C39     |
| 3   | E     | 1003 | POV  | C312-C313-C314-C315 |
| 3   | F     | 1007 | POV  | C36-C37-C38-C39     |
| 3   | F     | 1005 | POV  | C32-C31-O31-C3      |
| 3   | B     | 1009 | POV  | C24-C25-C26-C27     |
| 3   | D     | 1004 | POV  | C23-C24-C25-C26     |
| 3   | F     | 1006 | POV  | C312-C313-C314-C315 |
| 3   | A     | 1011 | POV  | C22-C23-C24-C25     |
| 3   | C     | 1008 | POV  | C37-C38-C39-C310    |
| 3   | E     | 1006 | POV  | C24-C25-C26-C27     |
| 3   | A     | 1006 | POV  | O32-C31-O31-C3      |
| 3   | D     | 1009 | POV  | O32-C31-O31-C3      |
| 3   | F     | 1002 | POV  | C32-C33-C34-C35     |
| 3   | F     | 1007 | POV  | C24-C25-C26-C27     |
| 3   | A     | 1002 | POV  | C311-C310-C39-C38   |
| 3   | C     | 1004 | POV  | C23-C24-C25-C26     |
| 3   | C     | 1006 | POV  | C24-C25-C26-C27     |
| 3   | C     | 1006 | POV  | C21-C22-C23-C24     |
| 3   | B     | 1007 | POV  | C24-C25-C26-C27     |
| 3   | B     | 1007 | POV  | C32-C31-O31-C3      |
| 3   | D     | 1006 | POV  | C32-C31-O31-C3      |
| 3   | C     | 1009 | POV  | C211-C212-C213-C214 |
| 3   | B     | 1009 | POV  | C37-C38-C39-C310    |
| 3   | D     | 1006 | POV  | C22-C23-C24-C25     |
| 3   | D     | 1011 | POV  | C22-C23-C24-C25     |
| 3   | F     | 1009 | POV  | C310-C311-C312-C313 |
| 3   | A     | 1002 | POV  | C210-C211-C212-C213 |
| 3   | A     | 1005 | POV  | C210-C211-C212-C213 |
| 3   | B     | 1008 | POV  | C210-C211-C212-C213 |
| 3   | C     | 1002 | POV  | C210-C211-C212-C213 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms               |
|-----|-------|------|------|---------------------|
| 3   | C     | 1007 | POV  | C210-C211-C212-C213 |
| 3   | D     | 1007 | POV  | C210-C211-C212-C213 |
| 3   | E     | 1005 | POV  | C210-C211-C212-C213 |
| 3   | F     | 1006 | POV  | C210-C211-C212-C213 |
| 3   | D     | 1010 | POV  | C211-C212-C213-C214 |
| 3   | C     | 1003 | POV  | C311-C312-C313-C314 |
| 3   | C     | 1009 | POV  | C310-C311-C312-C313 |
| 3   | A     | 1012 | POV  | O32-C31-O31-C3      |
| 3   | A     | 1008 | POV  | C212-C213-C214-C215 |
| 3   | A     | 1009 | POV  | C310-C311-C312-C313 |
| 3   | B     | 1004 | POV  | C312-C313-C314-C315 |
| 3   | E     | 1009 | POV  | C212-C213-C214-C215 |
| 3   | F     | 1007 | POV  | C37-C38-C39-C310    |
| 3   | A     | 1010 | POV  | C311-C310-C39-C38   |
| 3   | C     | 1005 | POV  | C311-C312-C313-C314 |
| 3   | F     | 1003 | POV  | C311-C312-C313-C314 |
| 3   | F     | 1008 | POV  | C32-C33-C34-C35     |
| 3   | A     | 1003 | POV  | C24-C25-C26-C27     |
| 3   | B     | 1010 | POV  | C211-C212-C213-C214 |
| 3   | D     | 1005 | POV  | C311-C312-C313-C314 |
| 3   | D     | 1007 | POV  | C312-C313-C314-C315 |
| 3   | D     | 1009 | POV  | C32-C33-C34-C35     |
| 3   | E     | 1004 | POV  | C11-C12-N-C14       |
| 3   | B     | 1007 | POV  | C21-C22-C23-C24     |
| 3   | A     | 1008 | POV  | C37-C38-C39-C310    |
| 3   | E     | 1004 | POV  | C311-C312-C313-C314 |
| 3   | E     | 1008 | POV  | C37-C38-C39-C310    |
| 3   | E     | 1006 | POV  | C32-C31-O31-C3      |
| 3   | A     | 1012 | POV  | C22-C21-O21-C2      |
| 3   | F     | 1002 | POV  | C310-C311-C312-C313 |
| 3   | B     | 1004 | POV  | C31-C32-C33-C34     |
| 3   | A     | 1005 | POV  | C24-C25-C26-C27     |
| 3   | B     | 1004 | POV  | C24-C25-C26-C27     |
| 3   | E     | 1002 | POV  | C311-C310-C39-C38   |
| 3   | E     | 1006 | POV  | C22-C23-C24-C25     |
| 3   | E     | 1009 | POV  | C211-C212-C213-C214 |
| 3   | E     | 1010 | POV  | C33-C34-C35-C36     |
| 3   | D     | 1003 | POV  | C311-C312-C313-C314 |
| 3   | E     | 1005 | POV  | C311-C312-C313-C314 |
| 3   | E     | 1005 | POV  | C24-C25-C26-C27     |
| 3   | B     | 1007 | POV  | O32-C31-O31-C3      |
| 3   | D     | 1006 | POV  | O32-C31-O31-C3      |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms               |
|-----|-------|------|------|---------------------|
| 3   | F     | 1005 | POV  | O32-C31-O31-C3      |
| 3   | A     | 1003 | POV  | C26-C27-C28-C29     |
| 3   | A     | 1007 | POV  | C210-C211-C212-C213 |
| 3   | A     | 1011 | POV  | C26-C27-C28-C29     |
| 3   | B     | 1002 | POV  | C26-C27-C28-C29     |
| 3   | B     | 1003 | POV  | C210-C211-C212-C213 |
| 3   | B     | 1004 | POV  | C26-C27-C28-C29     |
| 3   | C     | 1010 | POV  | C26-C27-C28-C29     |
| 3   | D     | 1003 | POV  | C26-C27-C28-C29     |
| 3   | D     | 1005 | POV  | C210-C211-C212-C213 |
| 3   | D     | 1011 | POV  | C26-C27-C28-C29     |
| 3   | E     | 1002 | POV  | C210-C211-C212-C213 |
| 3   | F     | 1002 | POV  | C26-C27-C28-C29     |
| 3   | F     | 1008 | POV  | O22-C21-O21-C2      |
| 3   | C     | 1003 | POV  | C31-C32-C33-C34     |
| 3   | E     | 1003 | POV  | C31-C32-C33-C34     |
| 3   | A     | 1007 | POV  | C312-C313-C314-C315 |
| 3   | A     | 1012 | POV  | C32-C33-C34-C35     |
| 3   | A     | 1003 | POV  | C312-C313-C314-C315 |
| 3   | A     | 1012 | POV  | C39-C310-C311-C312  |
| 3   | D     | 1003 | POV  | C24-C25-C26-C27     |
| 3   | A     | 1004 | POV  | C311-C312-C313-C314 |
| 3   | A     | 1011 | POV  | C33-C34-C35-C36     |
| 3   | B     | 1002 | POV  | C33-C34-C35-C36     |
| 3   | B     | 1006 | POV  | C311-C312-C313-C314 |
| 3   | B     | 1010 | POV  | C212-C213-C214-C215 |
| 3   | E     | 1007 | POV  | C312-C313-C314-C315 |
| 3   | F     | 1007 | POV  | C22-C23-C24-C25     |
| 3   | B     | 1003 | POV  | C25-C26-C27-C28     |
| 3   | C     | 1008 | POV  | C35-C36-C37-C38     |
| 3   | D     | 1010 | POV  | C310-C311-C312-C313 |
| 3   | E     | 1002 | POV  | C25-C26-C27-C28     |
| 3   | D     | 1003 | POV  | C312-C313-C314-C315 |
| 3   | D     | 1004 | POV  | C311-C312-C313-C314 |
| 3   | D     | 1005 | POV  | C24-C25-C26-C27     |
| 3   | D     | 1006 | POV  | C24-C25-C26-C27     |
| 3   | D     | 1008 | POV  | C37-C38-C39-C310    |
| 3   | E     | 1009 | POV  | C311-C312-C313-C314 |
| 3   | F     | 1010 | POV  | C33-C34-C35-C36     |
| 3   | D     | 1009 | POV  | C22-C21-O21-C2      |
| 3   | F     | 1008 | POV  | C22-C21-O21-C2      |
| 3   | A     | 1004 | POV  | C23-C24-C25-C26     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms               |
|-----|-------|------|------|---------------------|
| 3   | B     | 1009 | POV  | C35-C36-C37-C38     |
| 3   | A     | 1008 | POV  | C22-C23-C24-C25     |
| 3   | A     | 1009 | POV  | C211-C212-C213-C214 |
| 3   | A     | 1012 | POV  | O22-C21-O21-C2      |
| 3   | A     | 1009 | POV  | C212-C213-C214-C215 |
| 3   | F     | 1009 | POV  | C212-C213-C214-C215 |
| 3   | D     | 1011 | POV  | C33-C34-C35-C36     |
| 3   | A     | 1010 | POV  | C210-C211-C212-C213 |
| 3   | E     | 1003 | POV  | C26-C27-C28-C29     |
| 3   | E     | 1010 | POV  | C26-C27-C28-C29     |
| 3   | F     | 1010 | POV  | C26-C27-C28-C29     |
| 3   | B     | 1005 | POV  | C311-C312-C313-C314 |
| 3   | A     | 1006 | POV  | C24-C25-C26-C27     |
| 3   | A     | 1008 | POV  | C35-C36-C37-C38     |
| 3   | D     | 1008 | POV  | C35-C36-C37-C38     |
| 3   | F     | 1009 | POV  | C211-C212-C213-C214 |
| 3   | F     | 1007 | POV  | C35-C36-C37-C38     |
| 3   | E     | 1006 | POV  | O32-C31-O31-C3      |
| 3   | B     | 1004 | POV  | C36-C37-C38-C39     |
| 3   | C     | 1008 | POV  | C22-C23-C24-C25     |
| 3   | C     | 1009 | POV  | C212-C213-C214-C215 |
| 3   | D     | 1003 | POV  | C36-C37-C38-C39     |
| 3   | D     | 1006 | POV  | C214-C215-C216-C217 |
| 3   | E     | 1009 | POV  | C310-C311-C312-C313 |
| 3   | A     | 1010 | POV  | C1-O11-P-O12        |
| 3   | B     | 1003 | POV  | C1-O11-P-O12        |
| 3   | C     | 1002 | POV  | C1-O11-P-O12        |
| 3   | E     | 1002 | POV  | C1-O11-P-O12        |
| 3   | C     | 1002 | POV  | C310-C311-C312-C313 |
| 3   | D     | 1002 | POV  | C310-C311-C312-C313 |
| 3   | D     | 1010 | POV  | C39-C310-C311-C312  |
| 3   | B     | 1003 | POV  | C313-C314-C315-C316 |
| 3   | D     | 1008 | POV  | C22-C23-C24-C25     |
| 3   | F     | 1005 | POV  | C24-C25-C26-C27     |
| 3   | F     | 1009 | POV  | C311-C312-C313-C314 |
| 3   | A     | 1002 | POV  | C25-C26-C27-C28     |
| 3   | B     | 1004 | POV  | C214-C215-C216-C217 |
| 3   | B     | 1009 | POV  | C22-C23-C24-C25     |
| 3   | C     | 1010 | POV  | C214-C215-C216-C217 |
| 3   | B     | 1006 | POV  | C24-C25-C26-C27     |
| 3   | C     | 1005 | POV  | C24-C25-C26-C27     |
| 3   | D     | 1009 | POV  | C39-C310-C311-C312  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms               |
|-----|-------|------|------|---------------------|
| 3   | E     | 1006 | POV  | C214-C215-C216-C217 |
| 3   | F     | 1004 | POV  | C24-C25-C26-C27     |
| 3   | F     | 1009 | POV  | C39-C310-C311-C312  |
| 3   | C     | 1005 | POV  | C210-C211-C212-C213 |
| 3   | A     | 1005 | POV  | C311-C312-C313-C314 |
| 3   | B     | 1005 | POV  | C37-C38-C39-C310    |
| 3   | C     | 1009 | POV  | C39-C310-C311-C312  |
| 3   | E     | 1004 | POV  | C22-C23-C24-C25     |
| 3   | C     | 1002 | POV  | C25-C26-C27-C28     |
| 3   | C     | 1006 | POV  | C22-C23-C24-C25     |
| 3   | C     | 1003 | POV  | C214-C215-C216-C217 |
| 3   | C     | 1010 | POV  | C33-C34-C35-C36     |
| 3   | F     | 1002 | POV  | C31-C32-C33-C34     |
| 3   | A     | 1003 | POV  | C36-C37-C38-C39     |
| 3   | C     | 1003 | POV  | C36-C37-C38-C39     |
| 3   | A     | 1005 | POV  | C1-C2-C3-O31        |
| 3   | A     | 1008 | POV  | C1-C2-C3-O31        |
| 3   | A     | 1010 | POV  | C1-C2-C3-O31        |
| 3   | B     | 1006 | POV  | C1-C2-C3-O31        |
| 3   | B     | 1009 | POV  | C1-C2-C3-O31        |
| 3   | C     | 1004 | POV  | C311-C312-C313-C314 |
| 3   | C     | 1005 | POV  | C1-C2-C3-O31        |
| 3   | C     | 1008 | POV  | C1-C2-C3-O31        |
| 3   | D     | 1005 | POV  | C1-C2-C3-O31        |
| 3   | D     | 1008 | POV  | C1-C2-C3-O31        |
| 3   | F     | 1007 | POV  | C1-C2-C3-O31        |
| 3   | A     | 1007 | POV  | C313-C314-C315-C316 |
| 3   | A     | 1009 | POV  | C311-C312-C313-C314 |
| 3   | B     | 1006 | POV  | C23-C24-C25-C26     |
| 3   | B     | 1008 | POV  | C313-C314-C315-C316 |
| 3   | A     | 1006 | POV  | C39-C310-C311-C312  |
| 3   | B     | 1004 | POV  | C311-C312-C313-C314 |
| 3   | E     | 1006 | POV  | C21-C22-C23-C24     |
| 3   | A     | 1003 | POV  | C214-C215-C216-C217 |
| 3   | A     | 1004 | POV  | C24-C25-C26-C27     |
| 3   | A     | 1004 | POV  | C37-C38-C39-C310    |
| 3   | B     | 1008 | POV  | C312-C313-C314-C315 |
| 3   | F     | 1008 | POV  | C39-C310-C311-C312  |
| 3   | B     | 1006 | POV  | C210-C211-C212-C213 |
| 3   | D     | 1003 | POV  | C210-C211-C212-C213 |
| 3   | F     | 1004 | POV  | C210-C211-C212-C213 |
| 3   | C     | 1003 | POV  | C24-C25-C26-C27     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms               |
|-----|-------|------|------|---------------------|
| 3   | C     | 1006 | POV  | C214-C215-C216-C217 |
| 3   | D     | 1004 | POV  | C22-C23-C24-C25     |
| 3   | D     | 1010 | POV  | C212-C213-C214-C215 |
| 3   | D     | 1007 | POV  | C313-C314-C315-C316 |
| 3   | E     | 1010 | POV  | C214-C215-C216-C217 |
| 3   | B     | 1010 | POV  | C39-C310-C311-C312  |
| 3   | E     | 1002 | POV  | C313-C314-C315-C316 |
| 3   | A     | 1002 | POV  | C31-C32-C33-C34     |
| 3   | C     | 1006 | POV  | C39-C310-C311-C312  |
| 3   | C     | 1004 | POV  | C37-C38-C39-C310    |
| 3   | E     | 1008 | POV  | C35-C36-C37-C38     |
| 3   | F     | 1005 | POV  | C214-C215-C216-C217 |
| 3   | D     | 1009 | POV  | O22-C21-O21-C2      |
| 3   | B     | 1010 | POV  | C310-C311-C312-C313 |
| 3   | A     | 1010 | POV  | C25-C26-C27-C28     |
| 3   | C     | 1007 | POV  | C313-C314-C315-C316 |
| 3   | E     | 1003 | POV  | C311-C312-C313-C314 |
| 3   | F     | 1004 | POV  | C23-C24-C25-C26     |
| 3   | A     | 1009 | POV  | C39-C310-C311-C312  |
| 3   | A     | 1005 | POV  | O11-C1-C2-O21       |
| 3   | E     | 1004 | POV  | O11-C1-C2-O21       |
| 3   | F     | 1003 | POV  | O11-C1-C2-O21       |
| 3   | F     | 1004 | POV  | O11-C1-C2-O21       |
| 3   | D     | 1002 | POV  | C36-C37-C38-C39     |
| 3   | E     | 1007 | POV  | C313-C314-C315-C316 |
| 3   | D     | 1003 | POV  | C214-C215-C216-C217 |
| 3   | A     | 1006 | POV  | C210-C211-C212-C213 |
| 3   | D     | 1006 | POV  | C210-C211-C212-C213 |
| 3   | B     | 1002 | POV  | C214-C215-C216-C217 |
| 3   | F     | 1006 | POV  | C313-C314-C315-C316 |
| 3   | A     | 1008 | POV  | O21-C2-C3-O31       |
| 3   | F     | 1005 | POV  | C39-C310-C311-C312  |
| 3   | F     | 1002 | POV  | C36-C37-C38-C39     |
| 3   | A     | 1003 | POV  | C311-C312-C313-C314 |
| 3   | D     | 1005 | POV  | C23-C24-C25-C26     |
| 3   | E     | 1002 | POV  | C32-C33-C34-C35     |
| 3   | E     | 1004 | POV  | C37-C38-C39-C310    |
| 3   | E     | 1008 | POV  | C34-C35-C36-C37     |
| 3   | E     | 1003 | POV  | C214-C215-C216-C217 |
| 3   | F     | 1002 | POV  | C214-C215-C216-C217 |
| 3   | A     | 1010 | POV  | C310-C311-C312-C313 |
| 3   | B     | 1003 | POV  | C310-C311-C312-C313 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms               |
|-----|-------|------|------|---------------------|
| 3   | F     | 1008 | POV  | C312-C313-C314-C315 |
| 3   | D     | 1010 | POV  | C311-C312-C313-C314 |
| 3   | F     | 1002 | POV  | C210-C211-C212-C213 |
| 3   | B     | 1006 | POV  | C32-C33-C34-C35     |
| 3   | E     | 1004 | POV  | C11-C12-N-C15       |
| 3   | B     | 1009 | POV  | C34-C35-C36-C37     |
| 3   | C     | 1009 | POV  | C311-C312-C313-C314 |
| 3   | D     | 1008 | POV  | C34-C35-C36-C37     |
| 3   | E     | 1002 | POV  | C310-C311-C312-C313 |
| 3   | E     | 1003 | POV  | C36-C37-C38-C39     |
| 3   | D     | 1002 | POV  | C25-C26-C27-C28     |
| 3   | C     | 1002 | POV  | C313-C314-C315-C316 |
| 3   | C     | 1005 | POV  | C23-C24-C25-C26     |
| 3   | E     | 1008 | POV  | C311-C310-C39-C38   |
| 3   | A     | 1005 | POV  | C32-C31-O31-C3      |
| 3   | B     | 1006 | POV  | C32-C31-O31-C3      |
| 3   | E     | 1002 | POV  | C32-C31-O31-C3      |
| 3   | B     | 1003 | POV  | C31-C32-C33-C34     |
| 3   | A     | 1002 | POV  | C313-C314-C315-C316 |
| 3   | A     | 1011 | POV  | C214-C215-C216-C217 |
| 3   | F     | 1007 | POV  | C34-C35-C36-C37     |
| 3   | A     | 1002 | POV  | C310-C311-C312-C313 |
| 3   | E     | 1002 | POV  | C35-C36-C37-C38     |
| 3   | F     | 1004 | POV  | C311-C312-C313-C314 |
| 3   | A     | 1005 | POV  | C23-C24-C25-C26     |
| 3   | F     | 1007 | POV  | C32-C33-C34-C35     |
| 3   | A     | 1002 | POV  | C32-C33-C34-C35     |
| 3   | E     | 1005 | POV  | C32-C33-C34-C35     |
| 3   | F     | 1010 | POV  | C214-C215-C216-C217 |
| 3   | C     | 1002 | POV  | C1-C2-C3-O31        |
| 3   | E     | 1005 | POV  | C1-C2-C3-O31        |
| 3   | E     | 1008 | POV  | C1-C2-C3-O31        |
| 3   | F     | 1004 | POV  | C1-C2-C3-O31        |
| 3   | B     | 1010 | POV  | C311-C312-C313-C314 |
| 3   | A     | 1002 | POV  | C213-C214-C215-C216 |
| 3   | A     | 1006 | POV  | C211-C212-C213-C214 |
| 3   | D     | 1006 | POV  | C39-C310-C311-C312  |
| 3   | A     | 1010 | POV  | C313-C314-C315-C316 |
| 3   | B     | 1009 | POV  | C32-C33-C34-C35     |
| 3   | F     | 1004 | POV  | C32-C33-C34-C35     |
| 3   | F     | 1007 | POV  | C311-C310-C39-C38   |
| 3   | D     | 1004 | POV  | C37-C38-C39-C310    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms               |
|-----|-------|------|------|---------------------|
| 3   | C     | 1010 | POV  | C1-O11-P-O12        |
| 3   | D     | 1002 | POV  | C31-C32-C33-C34     |
| 3   | A     | 1006 | POV  | C311-C310-C39-C38   |
| 3   | A     | 1002 | POV  | O11-C1-C2-O21       |
| 3   | A     | 1010 | POV  | O11-C1-C2-O21       |
| 3   | A     | 1011 | POV  | O11-C1-C2-O21       |
| 3   | B     | 1003 | POV  | O11-C1-C2-O21       |
| 3   | C     | 1002 | POV  | O11-C1-C2-O21       |
| 3   | C     | 1005 | POV  | O11-C1-C2-O21       |
| 3   | D     | 1005 | POV  | O11-C1-C2-O21       |
| 3   | D     | 1011 | POV  | O11-C1-C2-O21       |
| 3   | E     | 1010 | POV  | O11-C1-C2-O21       |
| 3   | C     | 1004 | POV  | C32-C31-O31-C3      |
| 3   | F     | 1003 | POV  | C32-C31-O31-C3      |
| 3   | A     | 1004 | POV  | C22-C23-C24-C25     |
| 3   | A     | 1006 | POV  | C214-C215-C216-C217 |
| 3   | B     | 1009 | POV  | C312-C313-C314-C315 |
| 3   | E     | 1008 | POV  | C32-C33-C34-C35     |
| 3   | F     | 1005 | POV  | C211-C212-C213-C214 |
| 3   | E     | 1006 | POV  | C39-C310-C311-C312  |
| 3   | D     | 1008 | POV  | O21-C2-C3-O31       |
| 3   | E     | 1008 | POV  | O21-C2-C3-O31       |
| 3   | A     | 1008 | POV  | C34-C35-C36-C37     |
| 3   | E     | 1002 | POV  | C213-C214-C215-C216 |
| 3   | E     | 1008 | POV  | C312-C313-C314-C315 |
| 3   | B     | 1010 | POV  | C311-C310-C39-C38   |
| 3   | D     | 1009 | POV  | C312-C313-C314-C315 |
| 3   | E     | 1006 | POV  | C211-C212-C213-C214 |
| 3   | A     | 1005 | POV  | C212-C213-C214-C215 |
| 3   | D     | 1005 | POV  | C212-C213-C214-C215 |
| 3   | F     | 1005 | POV  | C311-C310-C39-C38   |
| 3   | A     | 1009 | POV  | C31-C32-C33-C34     |
| 3   | C     | 1002 | POV  | C213-C214-C215-C216 |
| 3   | B     | 1003 | POV  | C213-C214-C215-C216 |
| 3   | E     | 1005 | POV  | C23-C24-C25-C26     |
| 3   | A     | 1012 | POV  | C211-C212-C213-C214 |
| 3   | E     | 1008 | POV  | C22-C23-C24-C25     |
| 3   | F     | 1003 | POV  | C37-C38-C39-C310    |
| 3   | F     | 1008 | POV  | C211-C212-C213-C214 |
| 3   | A     | 1007 | POV  | C212-C213-C214-C215 |
| 3   | C     | 1006 | POV  | C211-C212-C213-C214 |
| 3   | E     | 1009 | POV  | C39-C310-C311-C312  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms               |
|-----|-------|------|------|---------------------|
| 3   | C     | 1003 | POV  | C215-C216-C217-C218 |
| 3   | E     | 1004 | POV  | C35-C36-C37-C38     |
| 3   | A     | 1005 | POV  | C312-C313-C314-C315 |
| 3   | A     | 1006 | POV  | C310-C311-C312-C313 |
| 3   | C     | 1002 | POV  | C36-C37-C38-C39     |
| 3   | E     | 1003 | POV  | C215-C216-C217-C218 |
| 3   | F     | 1002 | POV  | C215-C216-C217-C218 |
| 3   | A     | 1003 | POV  | C215-C216-C217-C218 |
| 3   | B     | 1007 | POV  | C39-C310-C311-C312  |
| 3   | D     | 1003 | POV  | C35-C36-C37-C38     |
| 3   | E     | 1004 | POV  | C310-C311-C312-C313 |
| 3   | A     | 1005 | POV  | C32-C33-C34-C35     |
| 3   | F     | 1009 | POV  | C23-C24-C25-C26     |
| 3   | A     | 1011 | POV  | O11-C1-C2-C3        |
| 3   | E     | 1004 | POV  | O11-C1-C2-C3        |
| 3   | F     | 1003 | POV  | O11-C1-C2-C3        |
| 3   | D     | 1005 | POV  | C311-C310-C39-C38   |
| 3   | D     | 1010 | POV  | C32-C33-C34-C35     |
| 3   | B     | 1007 | POV  | C210-C211-C212-C213 |
| 3   | C     | 1004 | POV  | C210-C211-C212-C213 |
| 3   | A     | 1008 | POV  | C311-C310-C39-C38   |
| 3   | A     | 1010 | POV  | C213-C214-C215-C216 |
| 3   | B     | 1003 | POV  | C32-C33-C34-C35     |
| 3   | B     | 1003 | POV  | C36-C37-C38-C39     |
| 3   | F     | 1002 | POV  | C313-C314-C315-C316 |
| 3   | C     | 1005 | POV  | C212-C213-C214-C215 |
| 3   | D     | 1002 | POV  | C213-C214-C215-C216 |
| 3   | F     | 1004 | POV  | C212-C213-C214-C215 |
| 3   | C     | 1005 | POV  | C32-C31-O31-C3      |
| 3   | C     | 1009 | POV  | C23-C24-C25-C26     |
| 3   | F     | 1002 | POV  | C35-C36-C37-C38     |
| 3   | A     | 1004 | POV  | C32-C33-C34-C35     |
| 3   | E     | 1009 | POV  | C312-C313-C314-C315 |
| 3   | A     | 1008 | POV  | C32-C33-C34-C35     |
| 3   | B     | 1004 | POV  | C215-C216-C217-C218 |
| 3   | E     | 1004 | POV  | C32-C31-O31-C3      |
| 3   | E     | 1005 | POV  | C32-C31-O31-C3      |
| 3   | D     | 1005 | POV  | C312-C313-C314-C315 |
| 3   | A     | 1003 | POV  | C210-C211-C212-C213 |
| 3   | E     | 1003 | POV  | C210-C211-C212-C213 |
| 3   | A     | 1003 | POV  | C2-C1-O11-P         |
| 3   | D     | 1002 | POV  | C1-C2-C3-O31        |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms               |
|-----|-------|------|------|---------------------|
| 3   | B     | 1002 | POV  | O11-C1-C2-O21       |
| 3   | B     | 1006 | POV  | O11-C1-C2-O21       |
| 3   | C     | 1004 | POV  | O11-C1-C2-O21       |
| 3   | C     | 1010 | POV  | O11-C1-C2-O21       |
| 3   | D     | 1002 | POV  | O11-C1-C2-O21       |
| 3   | E     | 1002 | POV  | O11-C1-C2-O21       |
| 3   | E     | 1005 | POV  | O11-C1-C2-O21       |
| 3   | F     | 1009 | POV  | O11-C1-C2-O21       |
| 3   | F     | 1010 | POV  | O11-C1-C2-O21       |
| 3   | B     | 1007 | POV  | C214-C215-C216-C217 |
| 3   | D     | 1006 | POV  | C34-C35-C36-C37     |
| 3   | C     | 1004 | POV  | O32-C31-O31-C3      |
| 3   | A     | 1002 | POV  | C36-C37-C38-C39     |
| 3   | C     | 1006 | POV  | C310-C311-C312-C313 |
| 3   | D     | 1009 | POV  | C23-C24-C25-C26     |
| 3   | A     | 1005 | POV  | O32-C31-O31-C3      |
| 3   | B     | 1006 | POV  | O32-C31-O31-C3      |
| 3   | C     | 1006 | POV  | C311-C310-C39-C38   |
| 3   | A     | 1005 | POV  | O21-C2-C3-O31       |
| 3   | A     | 1010 | POV  | O21-C2-C3-O31       |
| 3   | A     | 1011 | POV  | O21-C2-C3-O31       |
| 3   | B     | 1007 | POV  | O21-C2-C3-O31       |
| 3   | B     | 1009 | POV  | O21-C2-C3-O31       |
| 3   | C     | 1008 | POV  | O21-C2-C3-O31       |
| 3   | D     | 1005 | POV  | O21-C2-C3-O31       |
| 3   | E     | 1006 | POV  | O21-C2-C3-O31       |
| 3   | F     | 1007 | POV  | O21-C2-C3-O31       |
| 3   | C     | 1004 | POV  | C22-C23-C24-C25     |
| 3   | B     | 1010 | POV  | C23-C24-C25-C26     |
| 3   | F     | 1005 | POV  | C210-C211-C212-C213 |
| 3   | A     | 1002 | POV  | C35-C36-C37-C38     |
| 3   | C     | 1004 | POV  | C311-C310-C39-C38   |
| 3   | D     | 1003 | POV  | C215-C216-C217-C218 |
| 3   | D     | 1004 | POV  | C39-C310-C311-C312  |
| 3   | E     | 1002 | POV  | O32-C31-O31-C3      |
| 3   | F     | 1003 | POV  | O32-C31-O31-C3      |
| 3   | A     | 1007 | POV  | C35-C36-C37-C38     |
| 3   | B     | 1006 | POV  | C311-C310-C39-C38   |
| 3   | D     | 1009 | POV  | C211-C212-C213-C214 |
| 3   | E     | 1005 | POV  | C22-C23-C24-C25     |
| 3   | E     | 1005 | POV  | O32-C31-O31-C3      |
| 3   | B     | 1009 | POV  | C311-C310-C39-C38   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms               |
|-----|-------|------|------|---------------------|
| 3   | D     | 1011 | POV  | C214-C215-C216-C217 |
| 3   | A     | 1006 | POV  | C213-C214-C215-C216 |
| 3   | B     | 1003 | POV  | C35-C36-C37-C38     |
| 3   | C     | 1005 | POV  | O32-C31-O31-C3      |
| 3   | E     | 1009 | POV  | C31-C32-C33-C34     |
| 3   | B     | 1003 | POV  | C214-C215-C216-C217 |
| 3   | C     | 1004 | POV  | C24-C25-C26-C27     |
| 3   | D     | 1005 | POV  | C32-C31-O31-C3      |
| 3   | C     | 1003 | POV  | C35-C36-C37-C38     |
| 3   | F     | 1004 | POV  | C26-C27-C28-C29     |
| 3   | A     | 1002 | POV  | C1-O11-P-O12        |
| 3   | A     | 1003 | POV  | C11-O12-P-O11       |
| 3   | A     | 1006 | POV  | C1-O11-P-O12        |
| 3   | B     | 1007 | POV  | C1-O11-P-O12        |
| 3   | C     | 1006 | POV  | C1-O11-P-O12        |
| 3   | D     | 1006 | POV  | C1-O11-P-O12        |
| 3   | E     | 1006 | POV  | C1-O11-P-O12        |
| 3   | F     | 1005 | POV  | C1-O11-P-O12        |
| 3   | C     | 1003 | POV  | C2-C1-O11-P         |
| 3   | B     | 1006 | POV  | C37-C38-C39-C310    |
| 3   | E     | 1002 | POV  | C36-C37-C38-C39     |
| 3   | A     | 1002 | POV  | C1-O11-P-O13        |
| 3   | A     | 1002 | POV  | C11-O12-P-O13       |
| 3   | A     | 1003 | POV  | C1-O11-P-O13        |
| 3   | A     | 1003 | POV  | C1-O11-P-O14        |
| 3   | A     | 1004 | POV  | C1-O11-P-O14        |
| 3   | A     | 1005 | POV  | C11-O12-P-O13       |
| 3   | A     | 1005 | POV  | C11-O12-P-O14       |
| 3   | A     | 1010 | POV  | C1-O11-P-O13        |
| 3   | A     | 1010 | POV  | C11-O12-P-O13       |
| 3   | A     | 1012 | POV  | C11-O12-P-O13       |
| 3   | B     | 1002 | POV  | C1-O11-P-O13        |
| 3   | B     | 1002 | POV  | C1-O11-P-O14        |
| 3   | B     | 1003 | POV  | C1-O11-P-O13        |
| 3   | B     | 1003 | POV  | C11-O12-P-O13       |
| 3   | B     | 1004 | POV  | C1-O11-P-O13        |
| 3   | B     | 1004 | POV  | C1-O11-P-O14        |
| 3   | B     | 1005 | POV  | C1-O11-P-O14        |
| 3   | B     | 1006 | POV  | C11-O12-P-O13       |
| 3   | B     | 1006 | POV  | C11-O12-P-O14       |
| 3   | C     | 1002 | POV  | C1-O11-P-O13        |
| 3   | C     | 1002 | POV  | C11-O12-P-O13       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms               |
|-----|-------|------|------|---------------------|
| 3   | C     | 1004 | POV  | C1-O11-P-O14        |
| 3   | C     | 1005 | POV  | C11-O12-P-O13       |
| 3   | C     | 1005 | POV  | C11-O12-P-O14       |
| 3   | C     | 1010 | POV  | C11-O12-P-O14       |
| 3   | D     | 1002 | POV  | C1-O11-P-O13        |
| 3   | D     | 1002 | POV  | C11-O12-P-O13       |
| 3   | D     | 1004 | POV  | C1-O11-P-O14        |
| 3   | D     | 1004 | POV  | C11-O12-P-O14       |
| 3   | D     | 1005 | POV  | C11-O12-P-O13       |
| 3   | D     | 1005 | POV  | C11-O12-P-O14       |
| 3   | D     | 1009 | POV  | C11-O12-P-O13       |
| 3   | D     | 1011 | POV  | C1-O11-P-O13        |
| 3   | D     | 1011 | POV  | C1-O11-P-O14        |
| 3   | E     | 1002 | POV  | C1-O11-P-O13        |
| 3   | E     | 1002 | POV  | C11-O12-P-O13       |
| 3   | E     | 1005 | POV  | C11-O12-P-O13       |
| 3   | E     | 1005 | POV  | C11-O12-P-O14       |
| 3   | E     | 1010 | POV  | C1-O11-P-O13        |
| 3   | E     | 1010 | POV  | C1-O11-P-O14        |
| 3   | F     | 1002 | POV  | C1-O11-P-O13        |
| 3   | F     | 1002 | POV  | C1-O11-P-O14        |
| 3   | F     | 1004 | POV  | C11-O12-P-O13       |
| 3   | F     | 1004 | POV  | C11-O12-P-O14       |
| 3   | F     | 1008 | POV  | C11-O12-P-O13       |
| 3   | F     | 1010 | POV  | C1-O11-P-O13        |
| 3   | F     | 1010 | POV  | C1-O11-P-O14        |
| 3   | D     | 1006 | POV  | C211-C212-C213-C214 |
| 3   | F     | 1003 | POV  | C35-C36-C37-C38     |
| 3   | B     | 1005 | POV  | C32-C31-O31-C3      |
| 3   | A     | 1005 | POV  | O11-C1-C2-C3        |
| 3   | B     | 1002 | POV  | O11-C1-C2-C3        |
| 3   | B     | 1006 | POV  | O11-C1-C2-C3        |
| 3   | C     | 1010 | POV  | O11-C1-C2-C3        |
| 3   | D     | 1005 | POV  | O11-C1-C2-C3        |
| 3   | D     | 1011 | POV  | O11-C1-C2-C3        |
| 3   | E     | 1005 | POV  | O11-C1-C2-C3        |
| 3   | E     | 1010 | POV  | O11-C1-C2-C3        |
| 3   | F     | 1004 | POV  | O11-C1-C2-C3        |
| 3   | F     | 1010 | POV  | O11-C1-C2-C3        |
| 3   | A     | 1005 | POV  | C311-C310-C39-C38   |
| 3   | C     | 1007 | POV  | C33-C34-C35-C36     |
| 3   | C     | 1008 | POV  | C34-C35-C36-C37     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms               |
|-----|-------|------|------|---------------------|
| 3   | D     | 1004 | POV  | C310-C311-C312-C313 |
| 3   | F     | 1003 | POV  | C22-C23-C24-C25     |
| 3   | C     | 1003 | POV  | C313-C314-C315-C316 |
| 3   | D     | 1008 | POV  | C32-C33-C34-C35     |
| 3   | E     | 1005 | POV  | C212-C213-C214-C215 |
| 3   | A     | 1007 | POV  | C12-C11-O12-P       |
| 3   | B     | 1008 | POV  | C12-C11-O12-P       |
| 3   | C     | 1007 | POV  | C12-C11-O12-P       |
| 3   | D     | 1007 | POV  | C12-C11-O12-P       |
| 3   | E     | 1003 | POV  | C12-C11-O12-P       |
| 3   | E     | 1007 | POV  | C12-C11-O12-P       |
| 3   | F     | 1006 | POV  | C12-C11-O12-P       |
| 3   | D     | 1006 | POV  | C311-C310-C39-C38   |
| 3   | E     | 1002 | POV  | C31-C32-C33-C34     |
| 3   | E     | 1003 | POV  | C35-C36-C37-C38     |
| 3   | E     | 1005 | POV  | C311-C310-C39-C38   |
| 3   | D     | 1004 | POV  | C32-C31-O31-C3      |
| 3   | D     | 1008 | POV  | C311-C310-C39-C38   |
| 3   | D     | 1011 | POV  | C310-C311-C312-C313 |
| 3   | A     | 1012 | POV  | C312-C313-C314-C315 |
| 3   | C     | 1009 | POV  | C25-C26-C27-C28     |
| 3   | E     | 1009 | POV  | C23-C24-C25-C26     |
| 3   | D     | 1005 | POV  | O32-C31-O31-C3      |
| 3   | E     | 1004 | POV  | O32-C31-O31-C3      |
| 3   | B     | 1010 | POV  | C25-C26-C27-C28     |
| 3   | A     | 1007 | POV  | C11-C12-N-C13       |
| 3   | B     | 1005 | POV  | C11-C12-N-C14       |
| 3   | F     | 1006 | POV  | C11-C12-N-C13       |
| 3   | E     | 1006 | POV  | C310-C311-C312-C313 |
| 3   | F     | 1003 | POV  | C212-C213-C214-C215 |
| 3   | E     | 1005 | POV  | O21-C21-C22-C23     |
| 3   | A     | 1003 | POV  | O12-C11-C12-N       |
| 3   | A     | 1005 | POV  | O12-C11-C12-N       |
| 3   | A     | 1009 | POV  | O12-C11-C12-N       |
| 3   | A     | 1011 | POV  | O12-C11-C12-N       |
| 3   | B     | 1002 | POV  | O12-C11-C12-N       |
| 3   | B     | 1004 | POV  | O12-C11-C12-N       |
| 3   | B     | 1006 | POV  | O12-C11-C12-N       |
| 3   | C     | 1005 | POV  | O12-C11-C12-N       |
| 3   | C     | 1010 | POV  | O12-C11-C12-N       |
| 3   | D     | 1005 | POV  | O12-C11-C12-N       |
| 3   | D     | 1011 | POV  | O12-C11-C12-N       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms               |
|-----|-------|------|------|---------------------|
| 3   | E     | 1003 | POV  | O12-C11-C12-N       |
| 3   | E     | 1005 | POV  | O12-C11-C12-N       |
| 3   | E     | 1007 | POV  | C36-C37-C38-C39     |
| 3   | E     | 1010 | POV  | O12-C11-C12-N       |
| 3   | F     | 1002 | POV  | O12-C11-C12-N       |
| 3   | F     | 1004 | POV  | O12-C11-C12-N       |
| 3   | F     | 1010 | POV  | O12-C11-C12-N       |
| 3   | B     | 1006 | POV  | O21-C2-C3-O31       |
| 3   | C     | 1002 | POV  | O21-C2-C3-O31       |
| 3   | C     | 1005 | POV  | O21-C2-C3-O31       |
| 3   | D     | 1011 | POV  | O21-C2-C3-O31       |
| 3   | E     | 1005 | POV  | O21-C2-C3-O31       |
| 3   | E     | 1010 | POV  | O21-C2-C3-O31       |
| 3   | F     | 1004 | POV  | O21-C2-C3-O31       |
| 3   | D     | 1010 | POV  | C311-C310-C39-C38   |
| 3   | A     | 1012 | POV  | C23-C24-C25-C26     |
| 3   | B     | 1004 | POV  | C35-C36-C37-C38     |
| 3   | D     | 1002 | POV  | C313-C314-C315-C316 |
| 3   | D     | 1003 | POV  | C2-C1-O11-P         |
| 3   | E     | 1010 | POV  | C310-C311-C312-C313 |
| 3   | E     | 1009 | POV  | C25-C26-C27-C28     |
| 3   | F     | 1008 | POV  | C23-C24-C25-C26     |
| 3   | B     | 1005 | POV  | O32-C31-O31-C3      |
| 3   | D     | 1004 | POV  | O32-C31-O31-C3      |
| 3   | F     | 1007 | POV  | C312-C313-C314-C315 |
| 3   | A     | 1006 | POV  | C23-C24-C25-C26     |
| 3   | F     | 1003 | POV  | C310-C311-C312-C313 |
| 3   | B     | 1010 | POV  | C31-C32-C33-C34     |
| 3   | B     | 1005 | POV  | C11-C12-N-C15       |
| 3   | B     | 1008 | POV  | C11-C12-N-C13       |
| 3   | C     | 1006 | POV  | C11-C12-N-C15       |
| 3   | C     | 1007 | POV  | C11-C12-N-C13       |
| 3   | D     | 1005 | POV  | C32-C33-C34-C35     |
| 3   | E     | 1004 | POV  | C211-C212-C213-C214 |
| 3   | A     | 1002 | POV  | C214-C215-C216-C217 |
| 3   | E     | 1006 | POV  | C311-C310-C39-C38   |
| 3   | E     | 1010 | POV  | C25-C26-C27-C28     |
| 3   | F     | 1004 | POV  | C312-C313-C314-C315 |
| 3   | B     | 1006 | POV  | C212-C213-C214-C215 |
| 3   | D     | 1007 | POV  | C36-C37-C38-C39     |
| 3   | F     | 1009 | POV  | C25-C26-C27-C28     |
| 3   | B     | 1004 | POV  | C213-C214-C215-C216 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms               |
|-----|-------|------|------|---------------------|
| 3   | D     | 1010 | POV  | C25-C26-C27-C28     |
| 3   | A     | 1004 | POV  | C211-C212-C213-C214 |
| 3   | F     | 1003 | POV  | C39-C310-C311-C312  |
| 3   | C     | 1002 | POV  | C214-C215-C216-C217 |
| 3   | E     | 1005 | POV  | C312-C313-C314-C315 |
| 3   | E     | 1006 | POV  | C34-C35-C36-C37     |
| 3   | D     | 1006 | POV  | C213-C214-C215-C216 |
| 3   | C     | 1004 | POV  | O11-C1-C2-C3        |
| 3   | C     | 1005 | POV  | O11-C1-C2-C3        |
| 3   | E     | 1002 | POV  | C214-C215-C216-C217 |
| 3   | D     | 1006 | POV  | C310-C311-C312-C313 |
| 3   | F     | 1006 | POV  | C35-C36-C37-C38     |
| 3   | A     | 1005 | POV  | C37-C38-C39-C310    |
| 3   | C     | 1005 | POV  | C34-C35-C36-C37     |
| 3   | B     | 1004 | POV  | C2-C1-O11-P         |
| 3   | E     | 1003 | POV  | C2-C1-O11-P         |
| 3   | F     | 1002 | POV  | C2-C1-O11-P         |
| 3   | F     | 1009 | POV  | C2-C1-O11-P         |
| 3   | C     | 1008 | POV  | C312-C313-C314-C315 |
| 3   | E     | 1004 | POV  | C212-C213-C214-C215 |
| 3   | E     | 1004 | POV  | C11-C12-N-C13       |
| 3   | A     | 1007 | POV  | C22-C23-C24-C25     |
| 3   | B     | 1005 | POV  | C24-C25-C26-C27     |
| 3   | E     | 1010 | POV  | C24-C25-C26-C27     |
| 3   | B     | 1002 | POV  | C36-C37-C38-C39     |
| 3   | A     | 1002 | POV  | C11-O12-P-O11       |
| 3   | A     | 1007 | POV  | C1-O11-P-O12        |
| 3   | A     | 1008 | POV  | C11-O12-P-O11       |
| 3   | A     | 1009 | POV  | C11-O12-P-O11       |
| 3   | B     | 1003 | POV  | C11-O12-P-O11       |
| 3   | B     | 1008 | POV  | C1-O11-P-O12        |
| 3   | B     | 1009 | POV  | C11-O12-P-O11       |
| 3   | B     | 1010 | POV  | C11-O12-P-O11       |
| 3   | C     | 1002 | POV  | C11-O12-P-O11       |
| 3   | C     | 1003 | POV  | C11-O12-P-O11       |
| 3   | C     | 1007 | POV  | C1-O11-P-O12        |
| 3   | C     | 1008 | POV  | C11-O12-P-O11       |
| 3   | C     | 1009 | POV  | C11-O12-P-O11       |
| 3   | D     | 1002 | POV  | C11-O12-P-O11       |
| 3   | D     | 1003 | POV  | C11-O12-P-O11       |
| 3   | D     | 1007 | POV  | C1-O11-P-O12        |
| 3   | D     | 1008 | POV  | C11-O12-P-O11       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms               |
|-----|-------|------|------|---------------------|
| 3   | D     | 1010 | POV  | C11-O12-P-O11       |
| 3   | E     | 1007 | POV  | C1-O11-P-O12        |
| 3   | E     | 1008 | POV  | C11-O12-P-O11       |
| 3   | E     | 1009 | POV  | C11-O12-P-O11       |
| 3   | F     | 1006 | POV  | C1-O11-P-O12        |
| 3   | F     | 1007 | POV  | C11-O12-P-O11       |
| 3   | F     | 1009 | POV  | C11-O12-P-O11       |
| 3   | F     | 1003 | POV  | C24-C25-C26-C27     |
| 3   | A     | 1009 | POV  | C311-C310-C39-C38   |
| 3   | C     | 1009 | POV  | C214-C215-C216-C217 |
| 3   | E     | 1010 | POV  | C1-C2-C3-O31        |
| 3   | C     | 1002 | POV  | C35-C36-C37-C38     |
| 3   | E     | 1006 | POV  | C23-C24-C25-C26     |
| 3   | D     | 1004 | POV  | C35-C36-C37-C38     |
| 3   | F     | 1010 | POV  | C24-C25-C26-C27     |
| 3   | D     | 1007 | POV  | C11-C12-N-C13       |
| 3   | E     | 1007 | POV  | C11-C12-N-C13       |
| 3   | B     | 1005 | POV  | C210-C211-C212-C213 |
| 3   | A     | 1010 | POV  | C36-C37-C38-C39     |
| 3   | A     | 1004 | POV  | C32-C31-O31-C3      |
| 3   | F     | 1009 | POV  | C311-C310-C39-C38   |
| 3   | C     | 1005 | POV  | C32-C33-C34-C35     |
| 3   | E     | 1004 | POV  | C32-C33-C34-C35     |
| 3   | A     | 1003 | POV  | C35-C36-C37-C38     |
| 3   | A     | 1004 | POV  | C311-C310-C39-C38   |
| 3   | B     | 1010 | POV  | C32-C33-C34-C35     |
| 3   | E     | 1005 | POV  | C37-C38-C39-C310    |
| 3   | A     | 1012 | POV  | C2-C1-O11-P         |
| 3   | D     | 1009 | POV  | C2-C1-O11-P         |
| 3   | F     | 1008 | POV  | C2-C1-O11-P         |
| 3   | A     | 1010 | POV  | C35-C36-C37-C38     |
| 3   | B     | 1005 | POV  | C211-C212-C213-C214 |
| 3   | C     | 1002 | POV  | C31-C32-C33-C34     |
| 3   | C     | 1008 | POV  | C32-C33-C34-C35     |
| 3   | C     | 1006 | POV  | C210-C211-C212-C213 |
| 3   | D     | 1006 | POV  | C26-C27-C28-C29     |
| 3   | E     | 1006 | POV  | C210-C211-C212-C213 |
| 3   | A     | 1004 | POV  | O32-C31-O31-C3      |
| 3   | B     | 1007 | POV  | C211-C212-C213-C214 |
| 3   | F     | 1005 | POV  | C310-C311-C312-C313 |
| 3   | F     | 1004 | POV  | C32-C31-O31-C3      |
| 3   | A     | 1002 | POV  | O11-C1-C2-C3        |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms               |
|-----|-------|------|------|---------------------|
| 3   | A     | 1003 | POV  | C213-C214-C215-C216 |
| 3   | A     | 1009 | POV  | C23-C24-C25-C26     |
| 3   | B     | 1006 | POV  | C310-C311-C312-C313 |
| 3   | A     | 1009 | POV  | O11-C1-C2-O21       |
| 3   | B     | 1005 | POV  | C32-C33-C34-C35     |
| 3   | D     | 1003 | POV  | C37-C38-C39-C310    |
| 3   | D     | 1002 | POV  | C35-C36-C37-C38     |
| 3   | B     | 1002 | POV  | O21-C2-C3-O31       |
| 3   | C     | 1010 | POV  | O21-C2-C3-O31       |
| 3   | D     | 1002 | POV  | O21-C2-C3-O31       |
| 3   | C     | 1006 | POV  | C213-C214-C215-C216 |
| 3   | C     | 1005 | POV  | C311-C310-C39-C38   |
| 3   | B     | 1010 | POV  | C2-C1-O11-P         |
| 3   | D     | 1010 | POV  | C2-C1-O11-P         |
| 3   | C     | 1005 | POV  | O21-C21-C22-C23     |
| 3   | B     | 1005 | POV  | C310-C311-C312-C313 |
| 3   | C     | 1007 | POV  | C36-C37-C38-C39     |
| 3   | B     | 1006 | POV  | C26-C27-C28-C29     |
| 3   | D     | 1004 | POV  | C210-C211-C212-C213 |
| 3   | B     | 1007 | POV  | C23-C24-C25-C26     |
| 3   | F     | 1009 | POV  | C312-C313-C314-C315 |
| 3   | A     | 1003 | POV  | C33-C34-C35-C36     |
| 3   | A     | 1004 | POV  | C35-C36-C37-C38     |
| 3   | A     | 1009 | POV  | C32-C33-C34-C35     |
| 3   | B     | 1003 | POV  | C22-C23-C24-C25     |
| 3   | C     | 1004 | POV  | C32-C33-C34-C35     |
| 3   | D     | 1010 | POV  | C23-C24-C25-C26     |
| 3   | E     | 1003 | POV  | C313-C314-C315-C316 |
| 3   | B     | 1005 | POV  | C22-C23-C24-C25     |
| 3   | B     | 1007 | POV  | C310-C311-C312-C313 |
| 3   | F     | 1004 | POV  | C311-C310-C39-C38   |
| 3   | F     | 1004 | POV  | O32-C31-O31-C3      |
| 3   | A     | 1009 | POV  | C25-C26-C27-C28     |
| 3   | A     | 1012 | POV  | C210-C211-C212-C213 |
| 3   | A     | 1012 | POV  | C26-C27-C28-C29     |
| 3   | D     | 1009 | POV  | C210-C211-C212-C213 |
| 3   | D     | 1009 | POV  | C26-C27-C28-C29     |
| 3   | E     | 1009 | POV  | C26-C27-C28-C29     |
| 3   | A     | 1007 | POV  | C11-C12-N-C14       |
| 3   | A     | 1007 | POV  | C11-C12-N-C15       |
| 3   | B     | 1005 | POV  | C11-C12-N-C13       |
| 3   | F     | 1006 | POV  | C11-C12-N-C15       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms               |
|-----|-------|------|------|---------------------|
| 3   | C     | 1009 | POV  | C312-C313-C314-C315 |
| 3   | E     | 1008 | POV  | C21-C22-C23-C24     |
| 3   | C     | 1004 | POV  | C35-C36-C37-C38     |
| 3   | A     | 1007 | POV  | C33-C34-C35-C36     |
| 3   | C     | 1007 | POV  | C35-C36-C37-C38     |
| 3   | C     | 1009 | POV  | C31-C32-C33-C34     |
| 3   | D     | 1008 | POV  | C312-C313-C314-C315 |
| 3   | C     | 1009 | POV  | C32-C33-C34-C35     |
| 3   | A     | 1009 | POV  | C26-C27-C28-C29     |
| 3   | B     | 1010 | POV  | C26-C27-C28-C29     |
| 3   | B     | 1006 | POV  | C312-C313-C314-C315 |
| 3   | A     | 1008 | POV  | C21-C22-C23-C24     |
| 3   | D     | 1002 | POV  | C214-C215-C216-C217 |
| 3   | D     | 1007 | POV  | C212-C213-C214-C215 |
| 3   | B     | 1010 | POV  | C312-C313-C314-C315 |
| 3   | B     | 1008 | POV  | C33-C34-C35-C36     |
| 3   | D     | 1007 | POV  | C33-C34-C35-C36     |
| 3   | A     | 1012 | POV  | O21-C2-C3-O31       |
| 3   | D     | 1003 | POV  | O21-C2-C3-O31       |
| 3   | D     | 1006 | POV  | O21-C2-C3-O31       |
| 3   | F     | 1005 | POV  | O21-C2-C3-O31       |
| 3   | F     | 1005 | POV  | C213-C214-C215-C216 |
| 3   | B     | 1004 | POV  | C210-C211-C212-C213 |
| 3   | C     | 1003 | POV  | C210-C211-C212-C213 |
| 3   | C     | 1006 | POV  | C26-C27-C28-C29     |
| 3   | A     | 1008 | POV  | C31-C32-C33-C34     |
| 3   | B     | 1006 | POV  | C34-C35-C36-C37     |
| 3   | F     | 1002 | POV  | C213-C214-C215-C216 |
| 3   | F     | 1006 | POV  | C33-C34-C35-C36     |
| 3   | B     | 1005 | POV  | C35-C36-C37-C38     |
| 3   | A     | 1004 | POV  | C39-C310-C311-C312  |
| 3   | E     | 1004 | POV  | C312-C313-C314-C315 |
| 3   | D     | 1003 | POV  | C313-C314-C315-C316 |
| 3   | F     | 1003 | POV  | C313-C314-C315-C316 |
| 3   | A     | 1009 | POV  | C2-C1-O11-P         |
| 3   | B     | 1008 | POV  | C35-C36-C37-C38     |
| 3   | C     | 1007 | POV  | C212-C213-C214-C215 |
| 3   | E     | 1006 | POV  | C213-C214-C215-C216 |
| 3   | D     | 1003 | POV  | C213-C214-C215-C216 |
| 3   | A     | 1008 | POV  | C312-C313-C314-C315 |
| 3   | E     | 1004 | POV  | C24-C25-C26-C27     |
| 3   | A     | 1006 | POV  | C34-C35-C36-C37     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms               |
|-----|-------|------|------|---------------------|
| 3   | B     | 1005 | POV  | C27-C28-C29-C210    |
| 3   | D     | 1004 | POV  | C27-C28-C29-C210    |
| 3   | E     | 1004 | POV  | C27-C28-C29-C210    |
| 3   | B     | 1010 | POV  | O11-C1-C2-O21       |
| 3   | C     | 1009 | POV  | O11-C1-C2-O21       |
| 3   | D     | 1010 | POV  | O11-C1-C2-O21       |
| 3   | E     | 1005 | POV  | C310-C311-C312-C313 |
| 3   | F     | 1006 | POV  | C22-C23-C24-C25     |
| 3   | D     | 1003 | POV  | O21-C21-C22-C23     |
| 3   | C     | 1007 | POV  | C22-C23-C24-C25     |
| 3   | F     | 1007 | POV  | C11-C12-N-C14       |
| 3   | D     | 1004 | POV  | C311-C310-C39-C38   |
| 3   | A     | 1009 | POV  | O11-C1-C2-C3        |
| 3   | B     | 1003 | POV  | O11-C1-C2-C3        |
| 3   | B     | 1010 | POV  | O11-C1-C2-C3        |
| 3   | C     | 1009 | POV  | O11-C1-C2-C3        |
| 3   | D     | 1010 | POV  | O11-C1-C2-C3        |
| 3   | E     | 1002 | POV  | O11-C1-C2-C3        |
| 3   | F     | 1009 | POV  | O11-C1-C2-C3        |
| 3   | F     | 1004 | POV  | O21-C21-C22-C23     |
| 3   | A     | 1011 | POV  | C310-C311-C312-C313 |
| 3   | C     | 1003 | POV  | C213-C214-C215-C216 |
| 3   | C     | 1002 | POV  | O32-C31-O31-C3      |
| 3   | F     | 1007 | POV  | C31-C32-C33-C34     |
| 3   | F     | 1002 | POV  | C311-C312-C313-C314 |
| 3   | E     | 1009 | POV  | C2-C1-O11-P         |
| 3   | A     | 1006 | POV  | C26-C27-C28-C29     |
| 3   | F     | 1008 | POV  | C26-C27-C28-C29     |
| 3   | C     | 1006 | POV  | O21-C2-C3-O31       |
| 3   | F     | 1010 | POV  | O21-C2-C3-O31       |
| 3   | B     | 1004 | POV  | O21-C21-C22-C23     |
| 3   | E     | 1008 | POV  | O21-C21-C22-C23     |
| 3   | C     | 1002 | POV  | C32-C31-O31-C3      |
| 3   | F     | 1003 | POV  | C27-C28-C29-C210    |
| 3   | A     | 1008 | POV  | C313-C314-C315-C316 |
| 3   | B     | 1002 | POV  | C24-C25-C26-C27     |
| 3   | C     | 1008 | POV  | C311-C310-C39-C38   |
| 3   | D     | 1002 | POV  | C37-C38-C39-C310    |
| 3   | E     | 1004 | POV  | C39-C310-C311-C312  |
| 3   | F     | 1010 | POV  | C25-C26-C27-C28     |
| 3   | D     | 1005 | POV  | C37-C38-C39-C310    |
| 3   | B     | 1008 | POV  | C11-C12-N-C15       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms               |
|-----|-------|------|------|---------------------|
| 3   | C     | 1006 | POV  | C11-C12-N-C14       |
| 3   | E     | 1006 | POV  | C11-C12-N-C15       |
| 3   | F     | 1006 | POV  | C11-C12-N-C14       |
| 3   | C     | 1008 | POV  | O21-C21-C22-C23     |
| 3   | E     | 1009 | POV  | C32-C33-C34-C35     |
| 3   | A     | 1004 | POV  | C210-C211-C212-C213 |
| 3   | A     | 1009 | POV  | C210-C211-C212-C213 |
| 3   | B     | 1007 | POV  | C26-C27-C28-C29     |
| 3   | B     | 1009 | POV  | C210-C211-C212-C213 |
| 3   | C     | 1010 | POV  | C310-C311-C312-C313 |
| 3   | A     | 1007 | POV  | C27-C28-C29-C210    |
| 3   | E     | 1007 | POV  | C27-C28-C29-C210    |
| 3   | F     | 1005 | POV  | C34-C35-C36-C37     |
| 3   | A     | 1005 | POV  | C34-C35-C36-C37     |
| 3   | A     | 1008 | POV  | O21-C21-C22-C23     |
| 3   | B     | 1009 | POV  | O21-C21-C22-C23     |
| 3   | E     | 1003 | POV  | O21-C21-C22-C23     |
| 3   | B     | 1007 | POV  | C311-C310-C39-C38   |
| 3   | B     | 1003 | POV  | C32-C31-O31-C3      |
| 3   | E     | 1003 | POV  | C33-C34-C35-C36     |
| 3   | D     | 1008 | POV  | O21-C21-C22-C23     |
| 3   | B     | 1002 | POV  | C310-C311-C312-C313 |
| 3   | A     | 1004 | POV  | C27-C28-C29-C210    |
| 3   | B     | 1008 | POV  | C27-C28-C29-C210    |
| 3   | C     | 1004 | POV  | C27-C28-C29-C210    |
| 3   | D     | 1010 | POV  | C26-C27-C28-C29     |
| 3   | A     | 1010 | POV  | C214-C215-C216-C217 |
| 3   | A     | 1011 | POV  | C1-C2-C3-O31        |
| 3   | B     | 1002 | POV  | C1-C2-C3-O31        |
| 3   | C     | 1009 | POV  | C2-C1-O11-P         |
| 3   | C     | 1010 | POV  | C1-C2-C3-O31        |
| 3   | D     | 1011 | POV  | C1-C2-C3-O31        |
| 3   | F     | 1010 | POV  | C1-C2-C3-O31        |
| 3   | E     | 1009 | POV  | O11-C1-C2-O21       |
| 3   | F     | 1007 | POV  | O21-C21-C22-C23     |
| 3   | C     | 1006 | POV  | C11-C12-N-C13       |
| 3   | C     | 1007 | POV  | C11-C12-N-C15       |
| 3   | D     | 1006 | POV  | C11-C12-N-C15       |
| 3   | D     | 1008 | POV  | C11-C12-N-C14       |
| 3   | E     | 1007 | POV  | C11-C12-N-C15       |
| 3   | F     | 1005 | POV  | C11-C12-N-C15       |
| 3   | B     | 1003 | POV  | O32-C31-O31-C3      |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms               |
|-----|-------|------|------|---------------------|
| 3   | B     | 1008 | POV  | C22-C23-C24-C25     |
| 3   | C     | 1003 | POV  | O21-C21-C22-C23     |
| 3   | B     | 1009 | POV  | C27-C28-C29-C210    |
| 3   | C     | 1007 | POV  | C27-C28-C29-C210    |
| 3   | F     | 1004 | POV  | C27-C28-C29-C210    |
| 3   | D     | 1007 | POV  | C22-C23-C24-C25     |
| 3   | A     | 1005 | POV  | C26-C27-C28-C29     |
| 3   | E     | 1009 | POV  | C210-C211-C212-C213 |
| 3   | F     | 1008 | POV  | C210-C211-C212-C213 |
| 3   | A     | 1010 | POV  | O11-C1-C2-C3        |
| 3   | C     | 1002 | POV  | O11-C1-C2-C3        |
| 3   | E     | 1009 | POV  | O11-C1-C2-C3        |
| 3   | F     | 1005 | POV  | C23-C24-C25-C26     |
| 3   | C     | 1006 | POV  | C311-C312-C313-C314 |
| 3   | A     | 1006 | POV  | O21-C2-C3-O31       |
| 3   | A     | 1002 | POV  | C29-C210-C211-C212  |
| 3   | A     | 1010 | POV  | C29-C210-C211-C212  |
| 3   | C     | 1004 | POV  | C29-C210-C211-C212  |
| 3   | F     | 1010 | POV  | C36-C37-C38-C39     |
| 3   | B     | 1007 | POV  | C34-C35-C36-C37     |
| 3   | A     | 1006 | POV  | C11-C12-N-C15       |
| 3   | C     | 1007 | POV  | C11-C12-N-C14       |
| 3   | D     | 1007 | POV  | C11-C12-N-C15       |
| 3   | C     | 1005 | POV  | C310-C311-C312-C313 |
| 3   | D     | 1007 | POV  | C35-C36-C37-C38     |
| 3   | D     | 1007 | POV  | C27-C28-C29-C210    |
| 3   | D     | 1008 | POV  | C27-C28-C29-C210    |
| 3   | F     | 1006 | POV  | C27-C28-C29-C210    |
| 3   | B     | 1005 | POV  | C311-C310-C39-C38   |
| 3   | F     | 1009 | POV  | C214-C215-C216-C217 |
| 3   | A     | 1010 | POV  | C32-C33-C34-C35     |
| 3   | F     | 1003 | POV  | C211-C212-C213-C214 |
| 3   | B     | 1009 | POV  | O22-C21-C22-C23     |
| 3   | E     | 1003 | POV  | C213-C214-C215-C216 |
| 3   | D     | 1004 | POV  | C29-C210-C211-C212  |
| 3   | D     | 1005 | POV  | C26-C27-C28-C29     |
| 3   | D     | 1008 | POV  | O22-C21-C22-C23     |
| 3   | F     | 1007 | POV  | O22-C21-C22-C23     |
| 3   | A     | 1004 | POV  | O11-C1-C2-O21       |
| 3   | D     | 1010 | POV  | C312-C313-C314-C315 |
| 3   | C     | 1005 | POV  | C312-C313-C314-C315 |
| 3   | A     | 1008 | POV  | O22-C21-C22-C23     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms               |
|-----|-------|------|------|---------------------|
| 3   | E     | 1008 | POV  | O22-C21-C22-C23     |
| 3   | F     | 1009 | POV  | C32-C33-C34-C35     |
| 3   | C     | 1008 | POV  | O22-C21-C22-C23     |
| 3   | A     | 1009 | POV  | C214-C215-C216-C217 |
| 3   | A     | 1004 | POV  | C11-C12-N-C14       |
| 3   | A     | 1004 | POV  | C11-O12-P-O14       |
| 3   | A     | 1007 | POV  | C1-O11-P-O14        |
| 3   | A     | 1009 | POV  | C11-O12-P-O14       |
| 3   | B     | 1003 | POV  | C11-O12-P-O14       |
| 3   | B     | 1005 | POV  | C11-O12-P-O14       |
| 3   | B     | 1007 | POV  | C11-C12-N-C15       |
| 3   | B     | 1008 | POV  | C11-C12-N-C14       |
| 3   | B     | 1008 | POV  | C1-O11-P-O14        |
| 3   | B     | 1009 | POV  | C11-C12-N-C14       |
| 3   | B     | 1010 | POV  | C11-O12-P-O14       |
| 3   | C     | 1004 | POV  | C11-O12-P-O14       |
| 3   | C     | 1007 | POV  | C1-O11-P-O14        |
| 3   | C     | 1009 | POV  | C11-O12-P-O14       |
| 3   | D     | 1007 | POV  | C11-C12-N-C14       |
| 3   | D     | 1007 | POV  | C1-O11-P-O14        |
| 3   | D     | 1010 | POV  | C11-O12-P-O14       |
| 3   | E     | 1003 | POV  | C1-O11-P-O13        |
| 3   | E     | 1004 | POV  | C11-O12-P-O14       |
| 3   | E     | 1007 | POV  | C1-O11-P-O14        |
| 3   | E     | 1009 | POV  | C11-O12-P-O14       |
| 3   | F     | 1006 | POV  | C1-O11-P-O14        |
| 3   | F     | 1007 | POV  | C11-O12-P-O14       |
| 3   | F     | 1009 | POV  | C11-O12-P-O14       |
| 3   | D     | 1002 | POV  | O11-C1-C2-C3        |
| 3   | D     | 1004 | POV  | C24-C25-C26-C27     |
| 3   | C     | 1005 | POV  | C26-C27-C28-C29     |
| 3   | B     | 1003 | POV  | C29-C210-C211-C212  |
| 3   | D     | 1006 | POV  | C27-C28-C29-C210    |
| 3   | B     | 1002 | POV  | C34-C35-C36-C37     |
| 3   | F     | 1004 | POV  | C313-C314-C315-C316 |
| 3   | A     | 1002 | POV  | C37-C38-C39-C310    |
| 3   | C     | 1003 | POV  | C211-C212-C213-C214 |
| 3   | D     | 1008 | POV  | C11-C12-N-C15       |
| 3   | E     | 1007 | POV  | C11-C12-N-C14       |
| 3   | F     | 1003 | POV  | C11-C12-N-C14       |
| 3   | F     | 1007 | POV  | C11-C12-N-C13       |
| 3   | F     | 1007 | POV  | C11-C12-N-C15       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms               |
|-----|-------|------|------|---------------------|
| 3   | A     | 1008 | POV  | C27-C28-C29-C210    |
| 3   | D     | 1005 | POV  | C27-C28-C29-C210    |
| 3   | F     | 1005 | POV  | O31-C31-C32-C33     |
| 3   | C     | 1003 | POV  | C37-C38-C39-C310    |
| 3   | A     | 1010 | POV  | C37-C38-C39-C310    |
| 3   | B     | 1003 | POV  | C37-C38-C39-C310    |
| 3   | B     | 1007 | POV  | C213-C214-C215-C216 |
| 3   | C     | 1010 | POV  | C24-C25-C26-C27     |
| 3   | B     | 1007 | POV  | O31-C31-C32-C33     |
| 3   | D     | 1006 | POV  | O31-C31-C32-C33     |
| 3   | E     | 1006 | POV  | O31-C31-C32-C33     |
| 3   | B     | 1005 | POV  | O11-C1-C2-O21       |
| 3   | C     | 1009 | POV  | O21-C21-C22-C23     |
| 3   | E     | 1005 | POV  | C27-C28-C29-C210    |
| 3   | F     | 1007 | POV  | C27-C28-C29-C210    |
| 3   | C     | 1004 | POV  | C39-C310-C311-C312  |
| 3   | B     | 1002 | POV  | C39-C310-C311-C312  |
| 3   | F     | 1002 | POV  | O21-C21-C22-C23     |
| 3   | F     | 1007 | POV  | C210-C211-C212-C213 |
| 3   | D     | 1006 | POV  | O32-C31-C32-C33     |
| 3   | E     | 1007 | POV  | C35-C36-C37-C38     |
| 3   | A     | 1003 | POV  | O21-C21-C22-C23     |
| 3   | A     | 1006 | POV  | O31-C31-C32-C33     |
| 3   | C     | 1006 | POV  | O31-C31-C32-C33     |
| 3   | E     | 1006 | POV  | C11-C12-N-C13       |
| 3   | F     | 1003 | POV  | C11-C12-N-C13       |
| 3   | C     | 1006 | POV  | C27-C28-C29-C210    |
| 3   | A     | 1004 | POV  | C310-C311-C312-C313 |
| 3   | B     | 1008 | POV  | C212-C213-C214-C215 |
| 3   | E     | 1006 | POV  | O32-C31-C32-C33     |

There are no ring outliers.

63 monomers are involved in 305 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 3   | C     | 1007 | POV  | 4       | 0            |
| 3   | F     | 1004 | POV  | 8       | 0            |
| 2   | B     | 1001 | BEF  | 3       | 0            |
| 3   | F     | 1009 | POV  | 6       | 0            |
| 3   | E     | 1005 | POV  | 7       | 0            |
| 3   | A     | 1004 | POV  | 7       | 0            |
| 3   | A     | 1012 | POV  | 5       | 0            |

*Continued on next page...*

*Continued from previous page...*

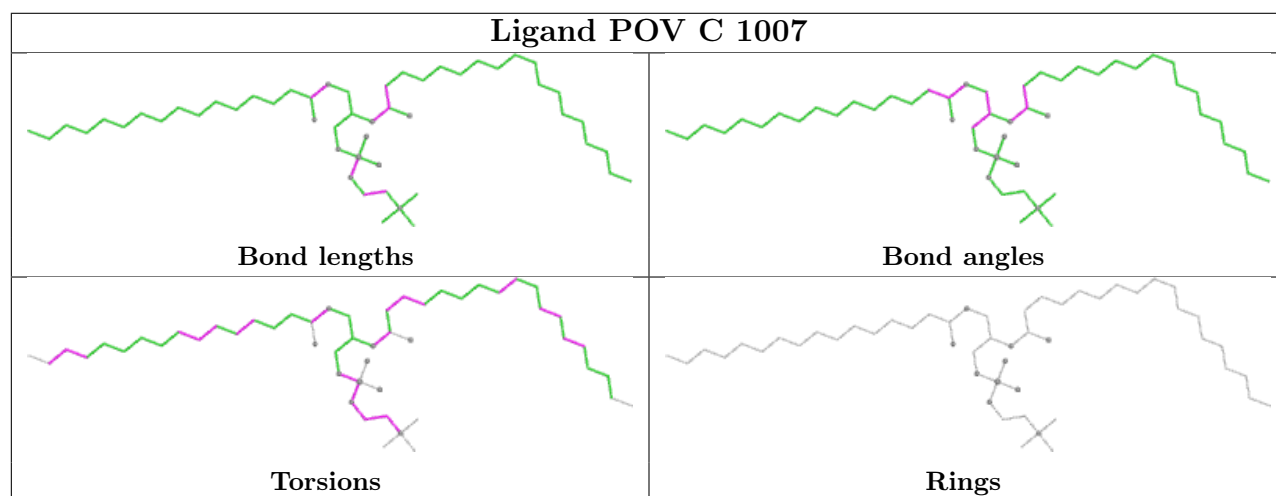
| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 2   | F     | 1001 | BEF  | 3       | 0            |
| 3   | C     | 1006 | POV  | 8       | 0            |
| 3   | B     | 1002 | POV  | 6       | 0            |
| 3   | E     | 1010 | POV  | 5       | 0            |
| 3   | D     | 1008 | POV  | 2       | 0            |
| 3   | E     | 1003 | POV  | 8       | 0            |
| 3   | E     | 1002 | POV  | 11      | 0            |
| 3   | B     | 1010 | POV  | 6       | 0            |
| 3   | F     | 1005 | POV  | 9       | 0            |
| 3   | B     | 1009 | POV  | 2       | 0            |
| 3   | B     | 1007 | POV  | 6       | 0            |
| 3   | D     | 1007 | POV  | 5       | 0            |
| 3   | B     | 1004 | POV  | 9       | 0            |
| 3   | A     | 1009 | POV  | 1       | 0            |
| 3   | C     | 1002 | POV  | 12      | 0            |
| 3   | A     | 1007 | POV  | 5       | 0            |
| 3   | D     | 1004 | POV  | 14      | 0            |
| 3   | F     | 1002 | POV  | 10      | 0            |
| 3   | F     | 1003 | POV  | 7       | 0            |
| 3   | F     | 1010 | POV  | 5       | 0            |
| 3   | E     | 1008 | POV  | 3       | 0            |
| 3   | B     | 1006 | POV  | 8       | 0            |
| 3   | A     | 1008 | POV  | 4       | 0            |
| 2   | D     | 1001 | BEF  | 3       | 0            |
| 3   | D     | 1006 | POV  | 4       | 0            |
| 3   | C     | 1009 | POV  | 5       | 0            |
| 3   | A     | 1010 | POV  | 14      | 0            |
| 3   | B     | 1005 | POV  | 6       | 0            |
| 3   | D     | 1005 | POV  | 8       | 0            |
| 3   | C     | 1003 | POV  | 8       | 0            |
| 3   | A     | 1005 | POV  | 5       | 0            |
| 3   | D     | 1002 | POV  | 11      | 0            |
| 3   | C     | 1004 | POV  | 14      | 0            |
| 3   | C     | 1005 | POV  | 7       | 0            |
| 3   | C     | 1008 | POV  | 5       | 0            |
| 3   | F     | 1008 | POV  | 3       | 0            |
| 2   | E     | 1001 | BEF  | 3       | 0            |
| 3   | A     | 1006 | POV  | 6       | 0            |
| 3   | D     | 1009 | POV  | 3       | 0            |
| 3   | F     | 1006 | POV  | 4       | 0            |
| 3   | D     | 1003 | POV  | 8       | 0            |
| 3   | D     | 1010 | POV  | 4       | 0            |

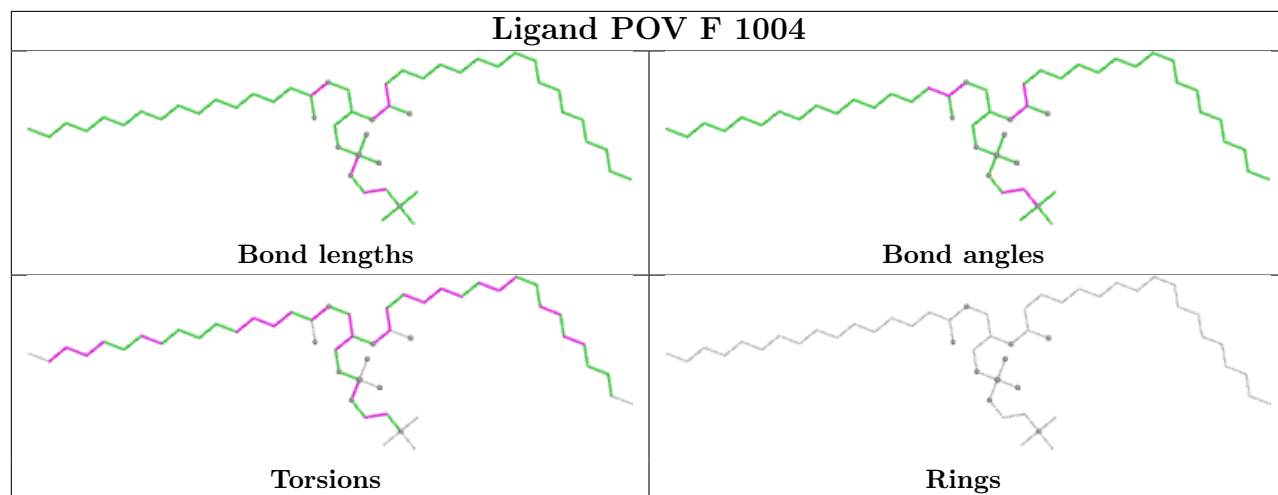
*Continued on next page...*

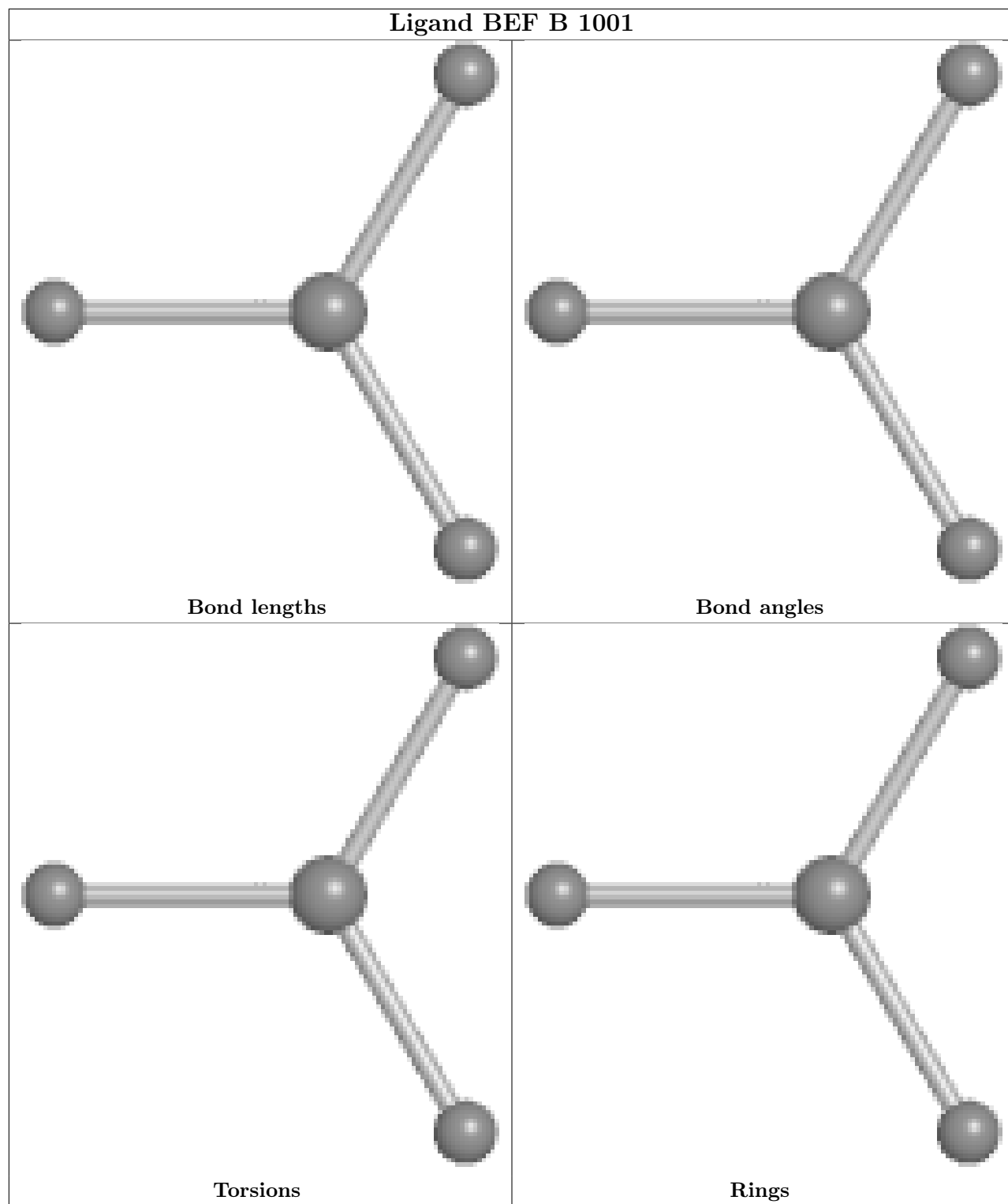
Continued from previous page...

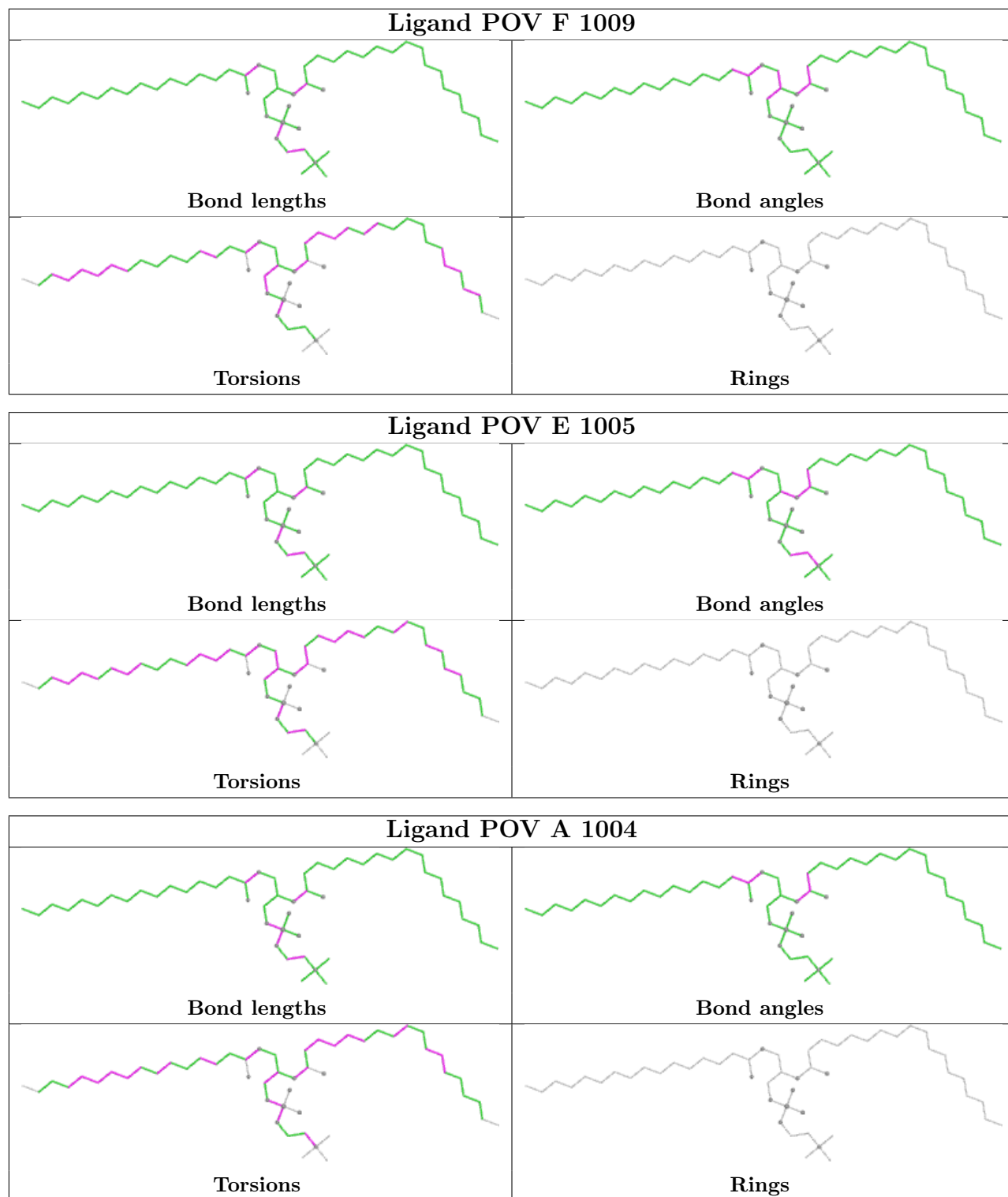
| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 3   | E     | 1004 | POV  | 5       | 0            |
| 3   | A     | 1002 | POV  | 13      | 0            |
| 3   | B     | 1003 | POV  | 10      | 0            |
| 3   | E     | 1006 | POV  | 4       | 0            |
| 2   | A     | 1001 | BEF  | 3       | 0            |
| 3   | D     | 1011 | POV  | 4       | 0            |
| 2   | C     | 1001 | BEF  | 3       | 0            |
| 3   | B     | 1008 | POV  | 3       | 0            |
| 3   | E     | 1009 | POV  | 3       | 0            |
| 3   | E     | 1007 | POV  | 4       | 0            |
| 3   | F     | 1007 | POV  | 4       | 0            |
| 3   | A     | 1003 | POV  | 9       | 0            |
| 3   | C     | 1010 | POV  | 4       | 0            |
| 3   | A     | 1011 | POV  | 6       | 0            |

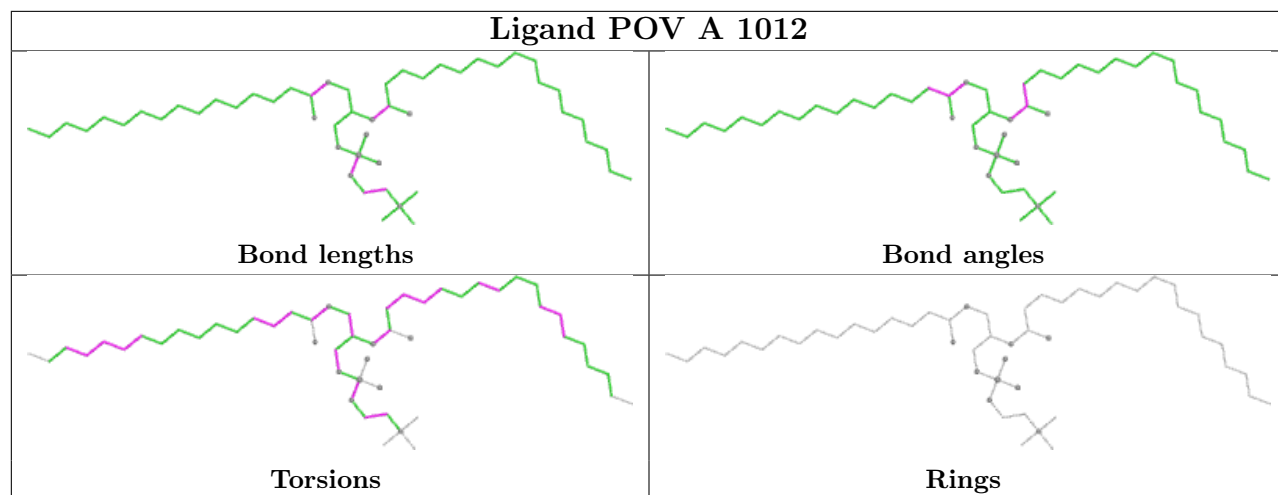
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

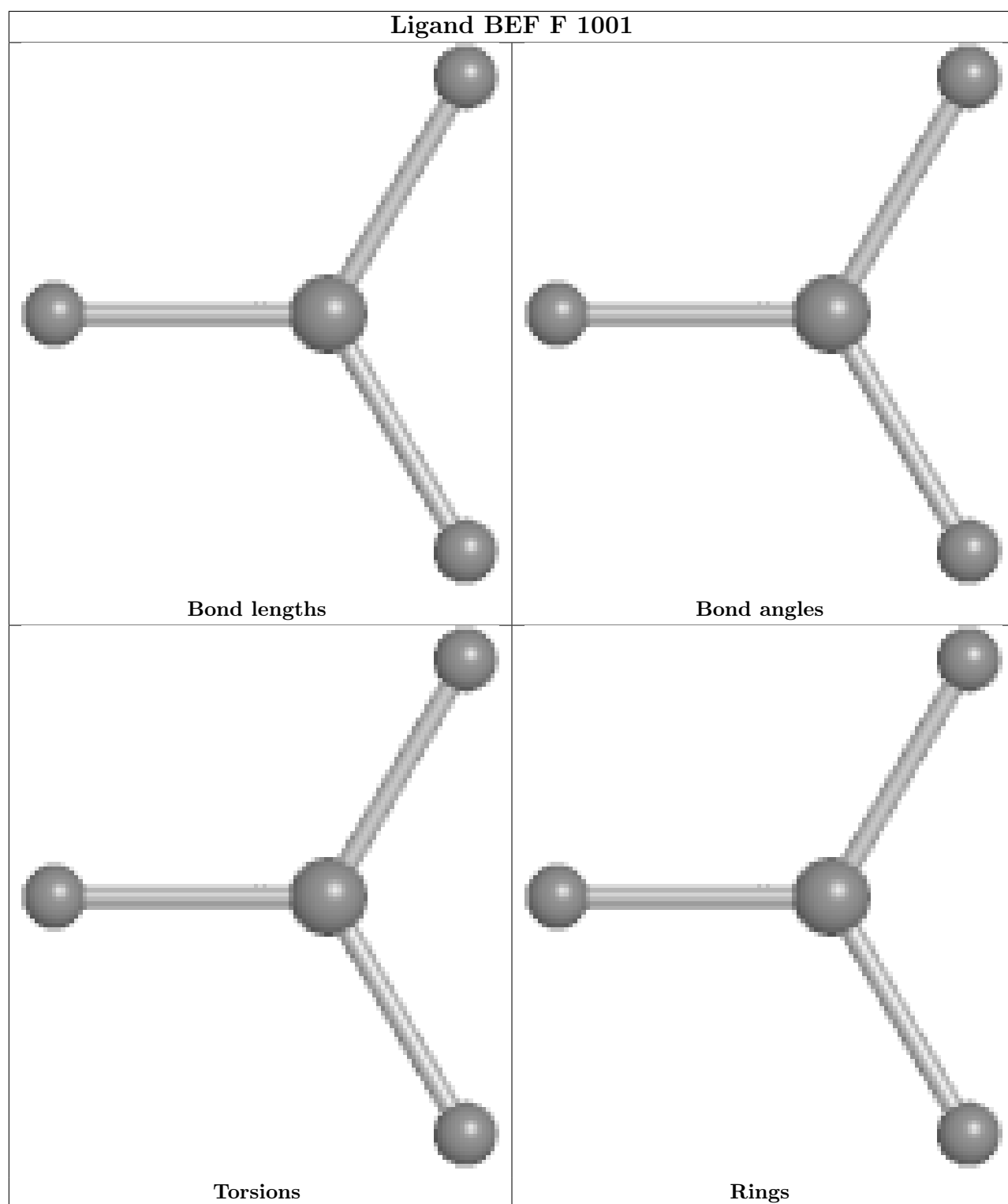


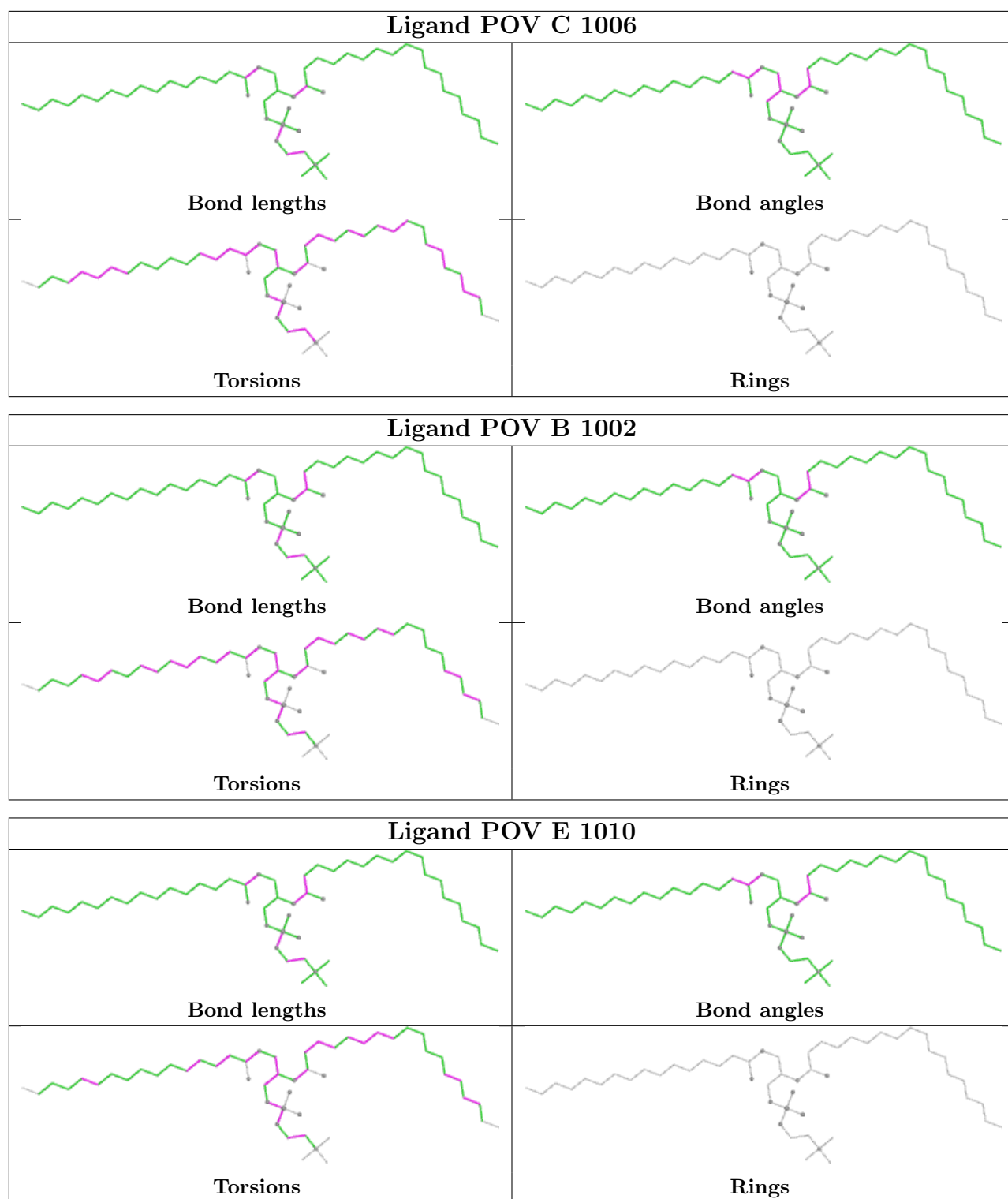


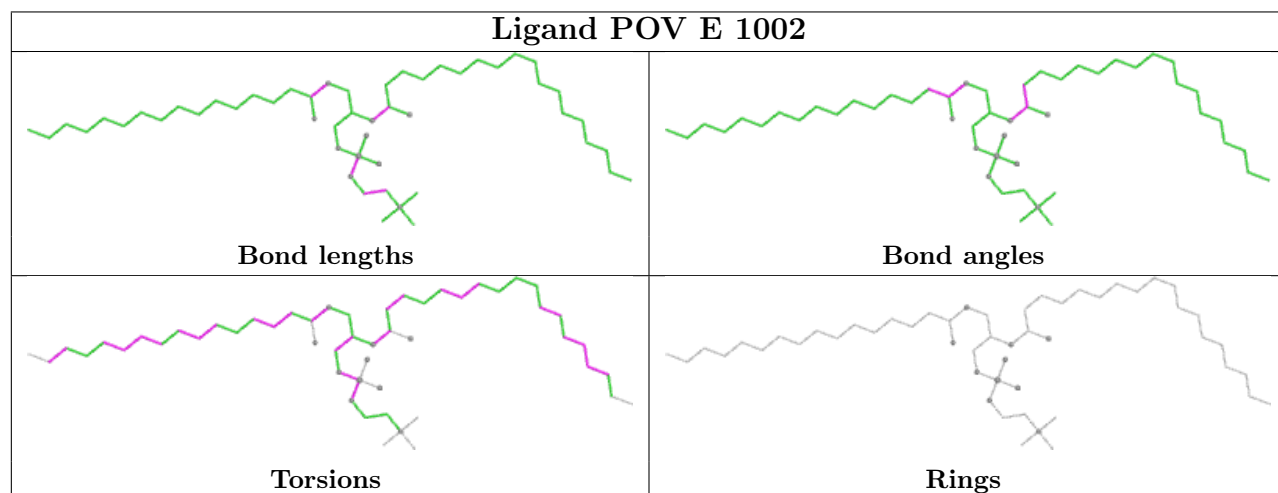
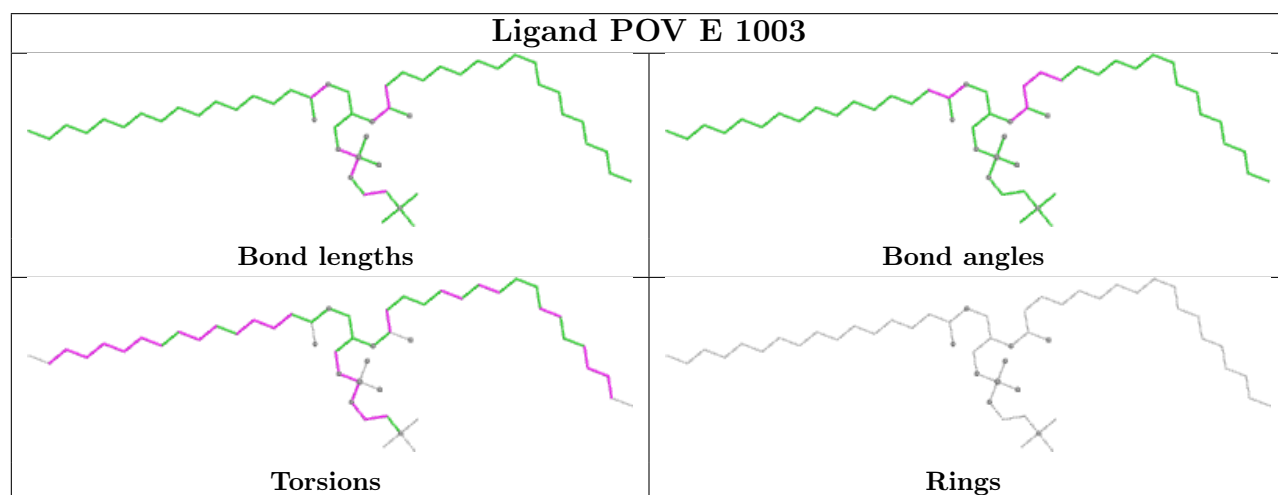
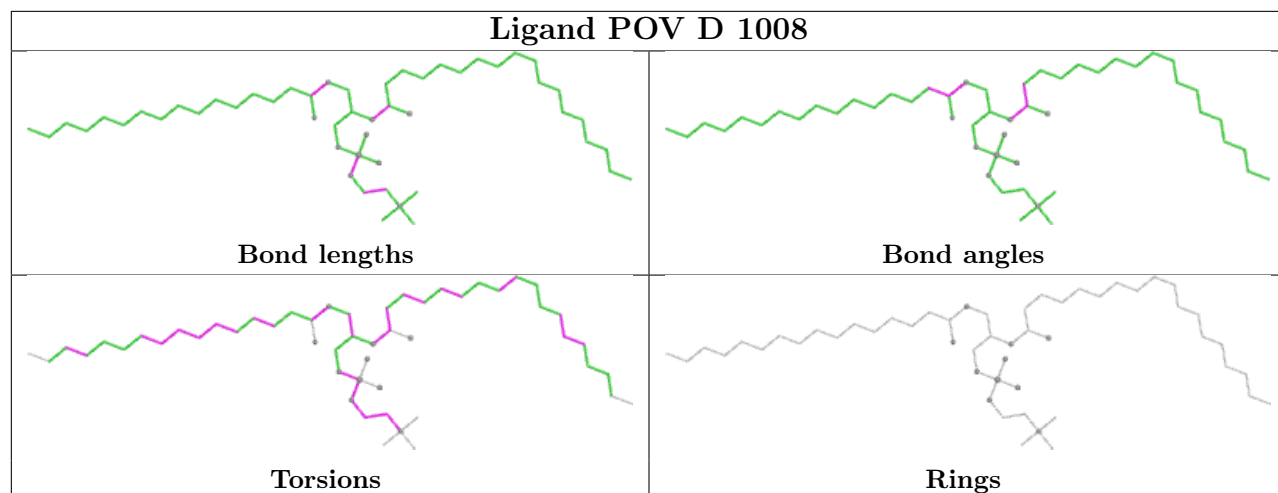


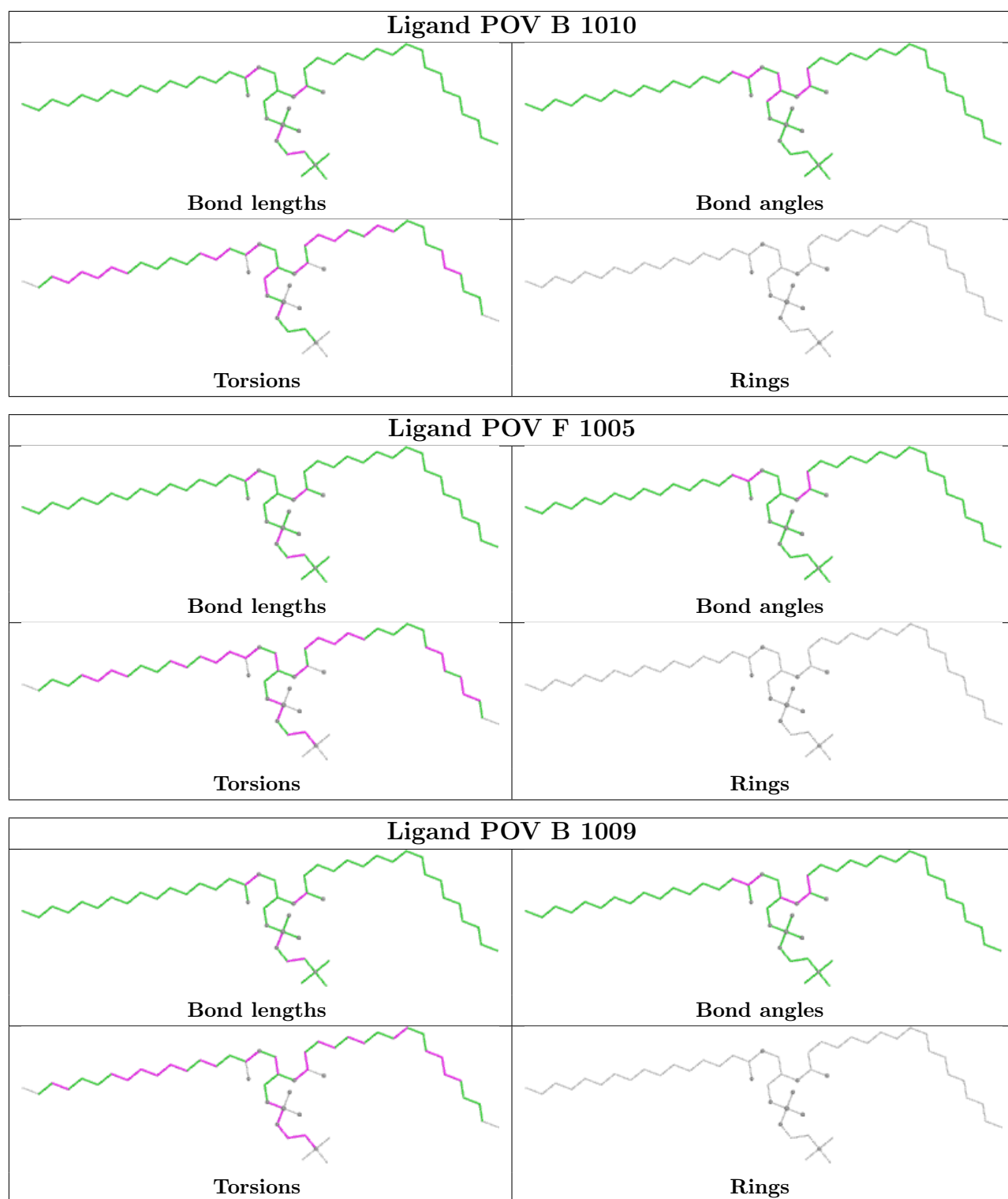


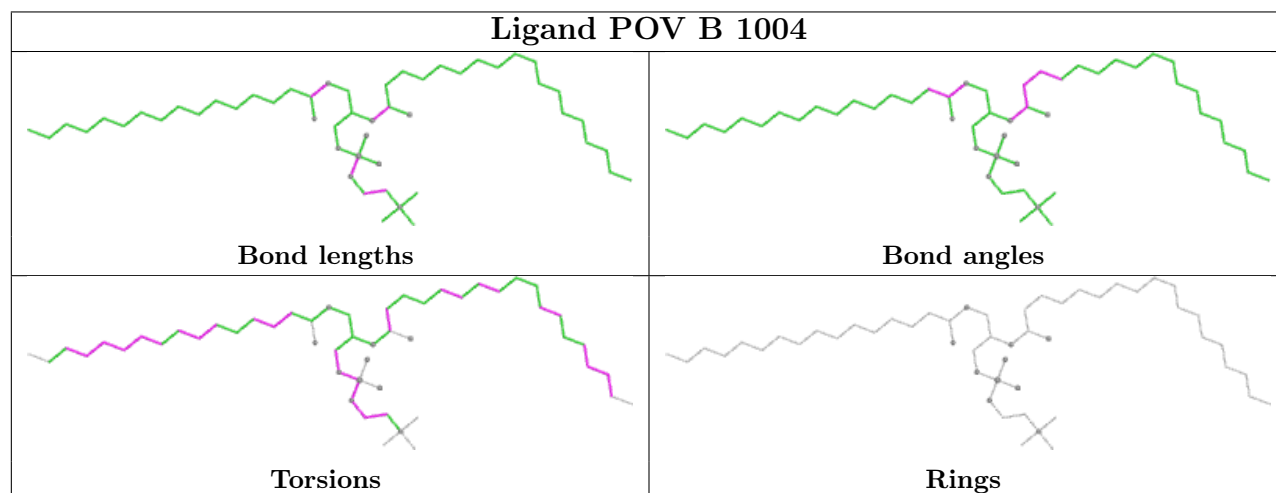
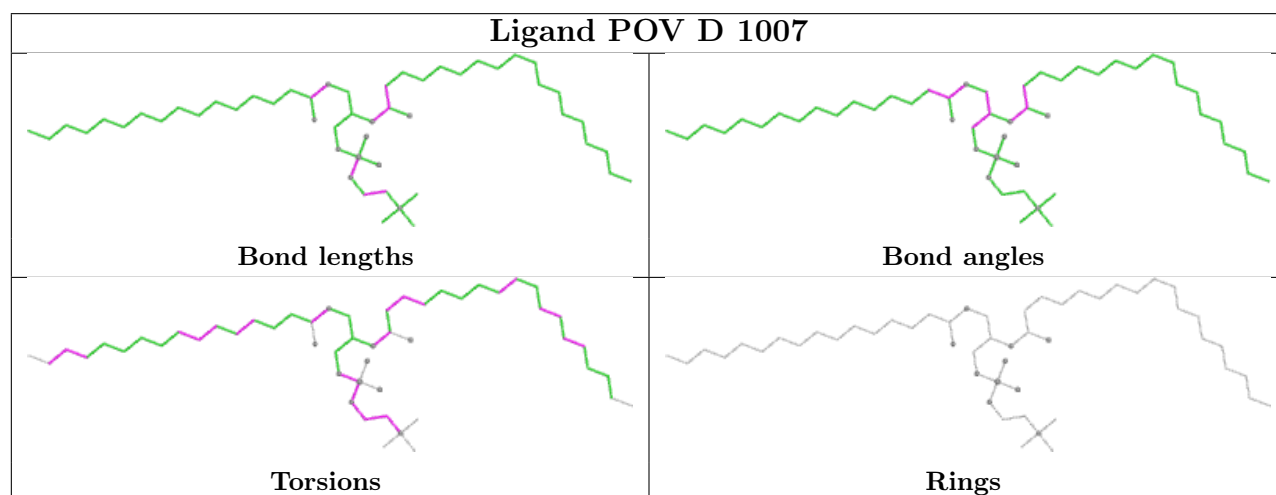
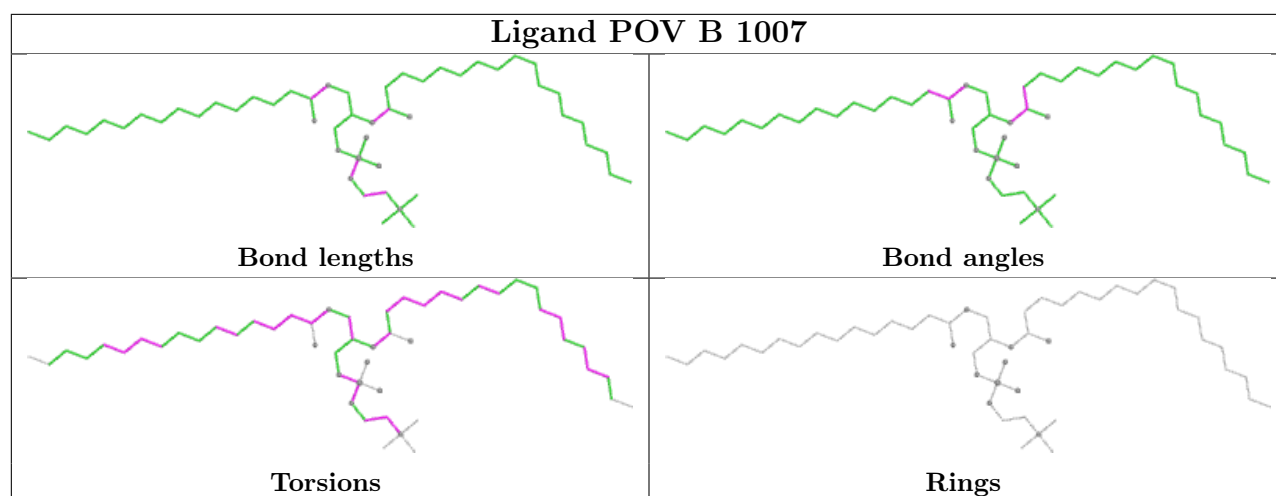


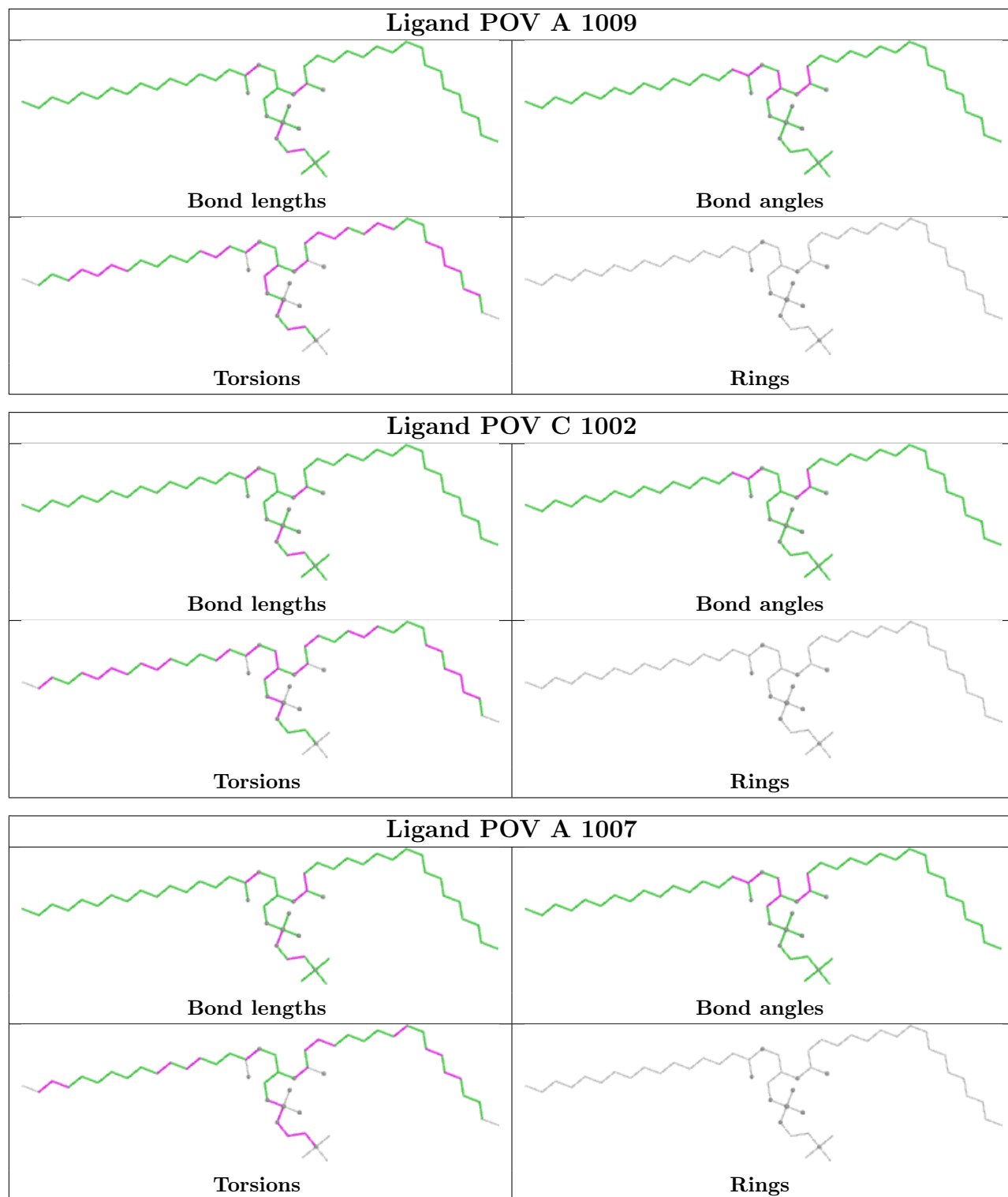


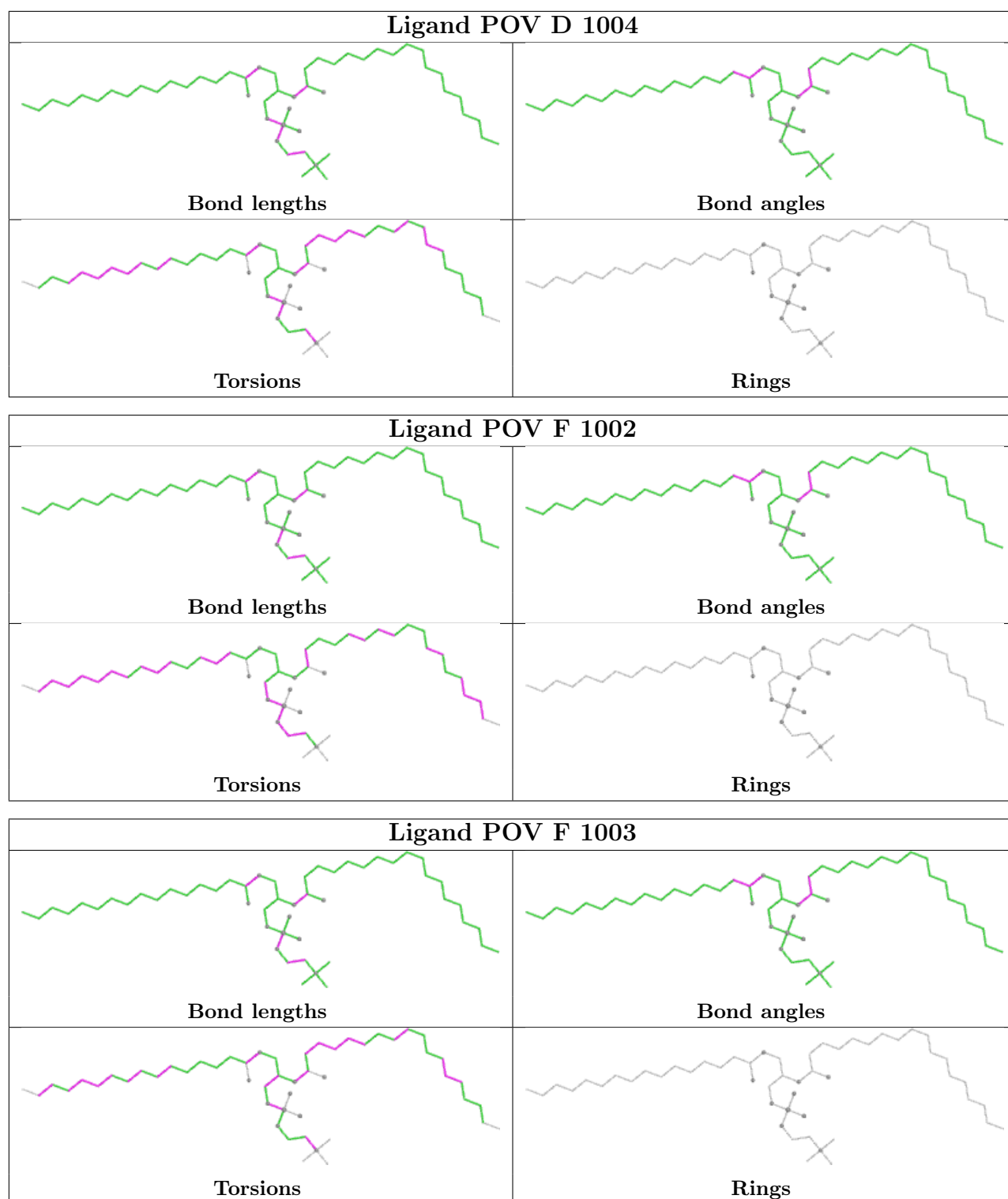


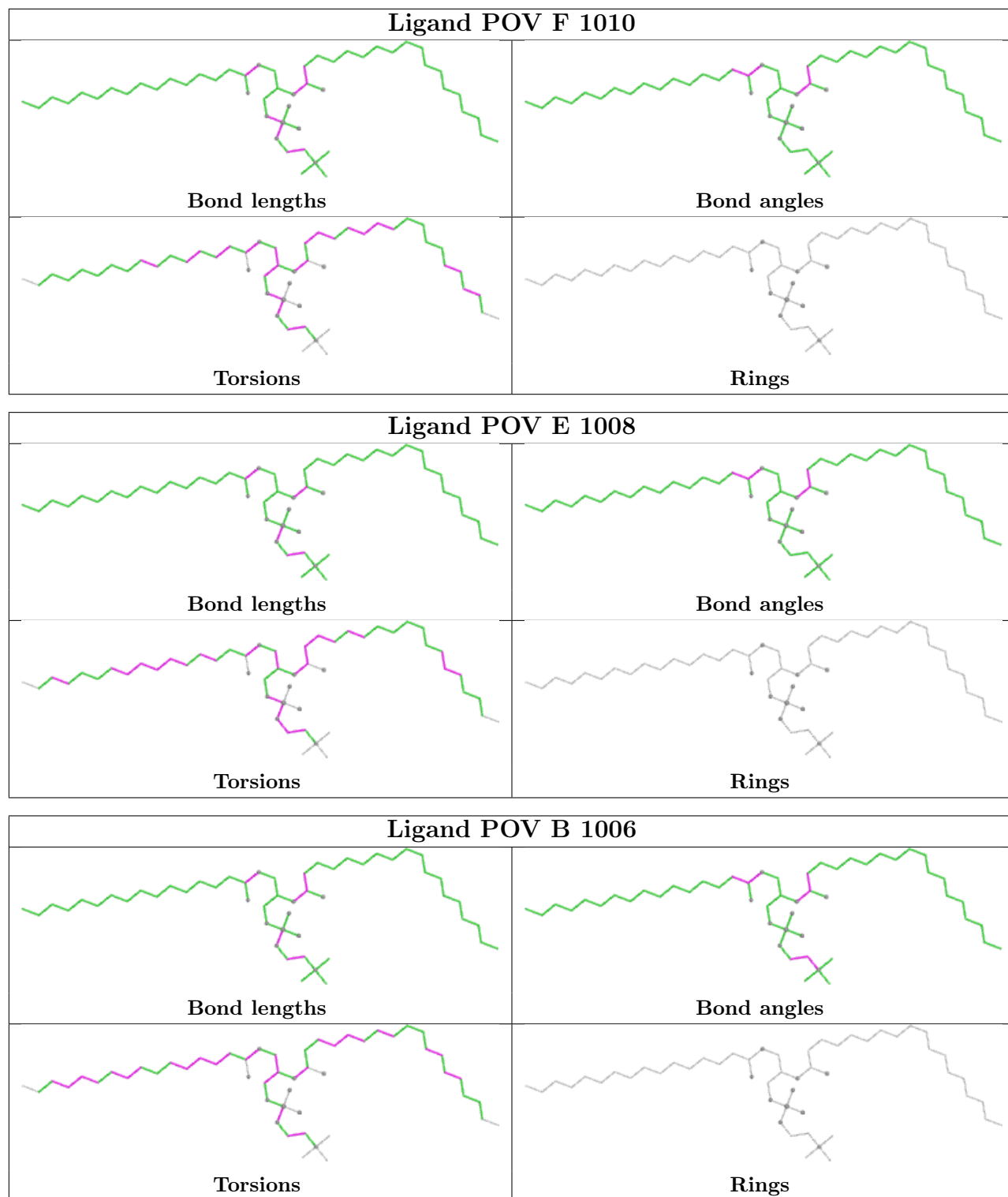


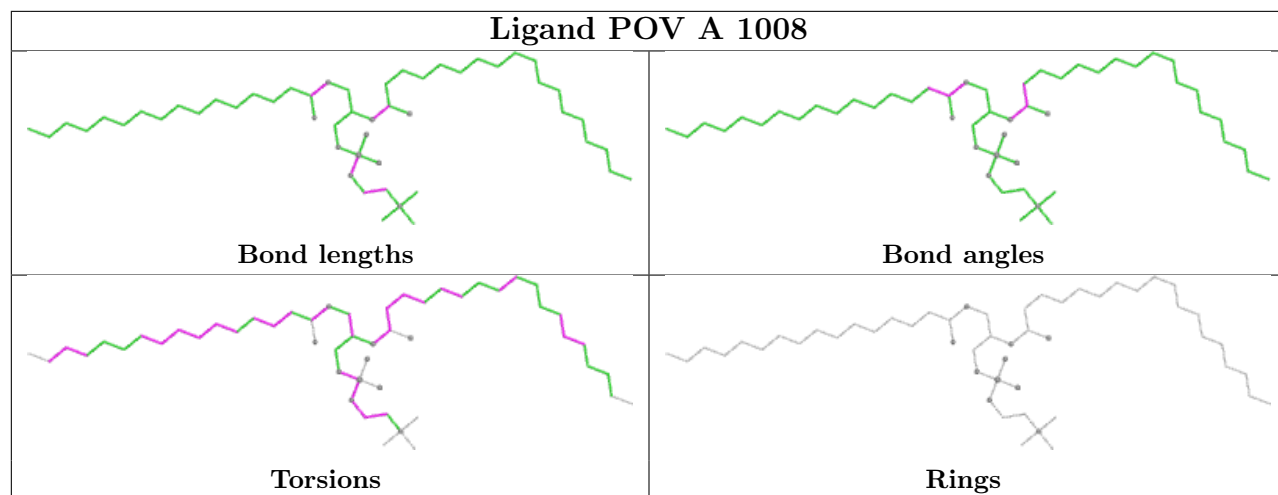


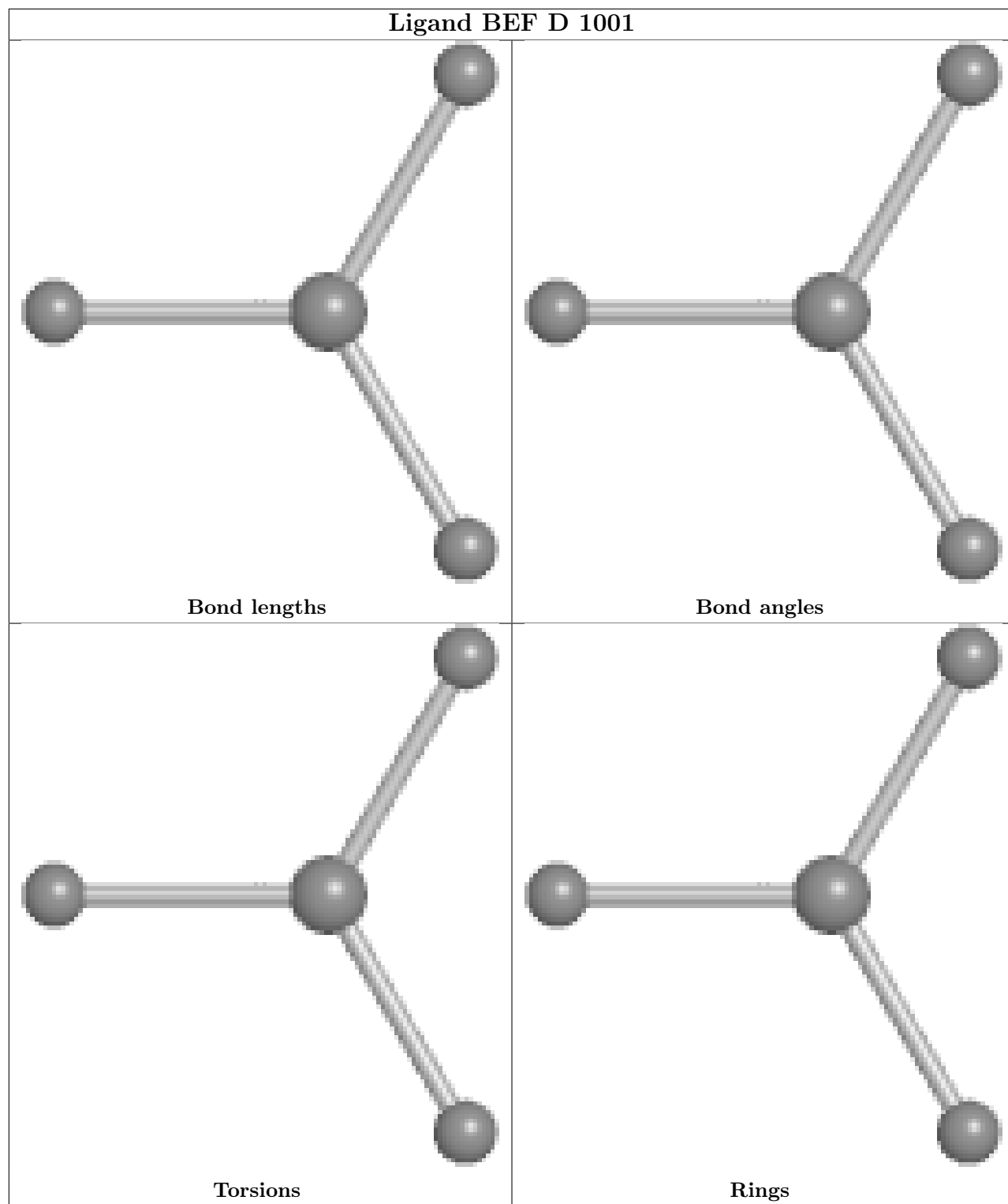


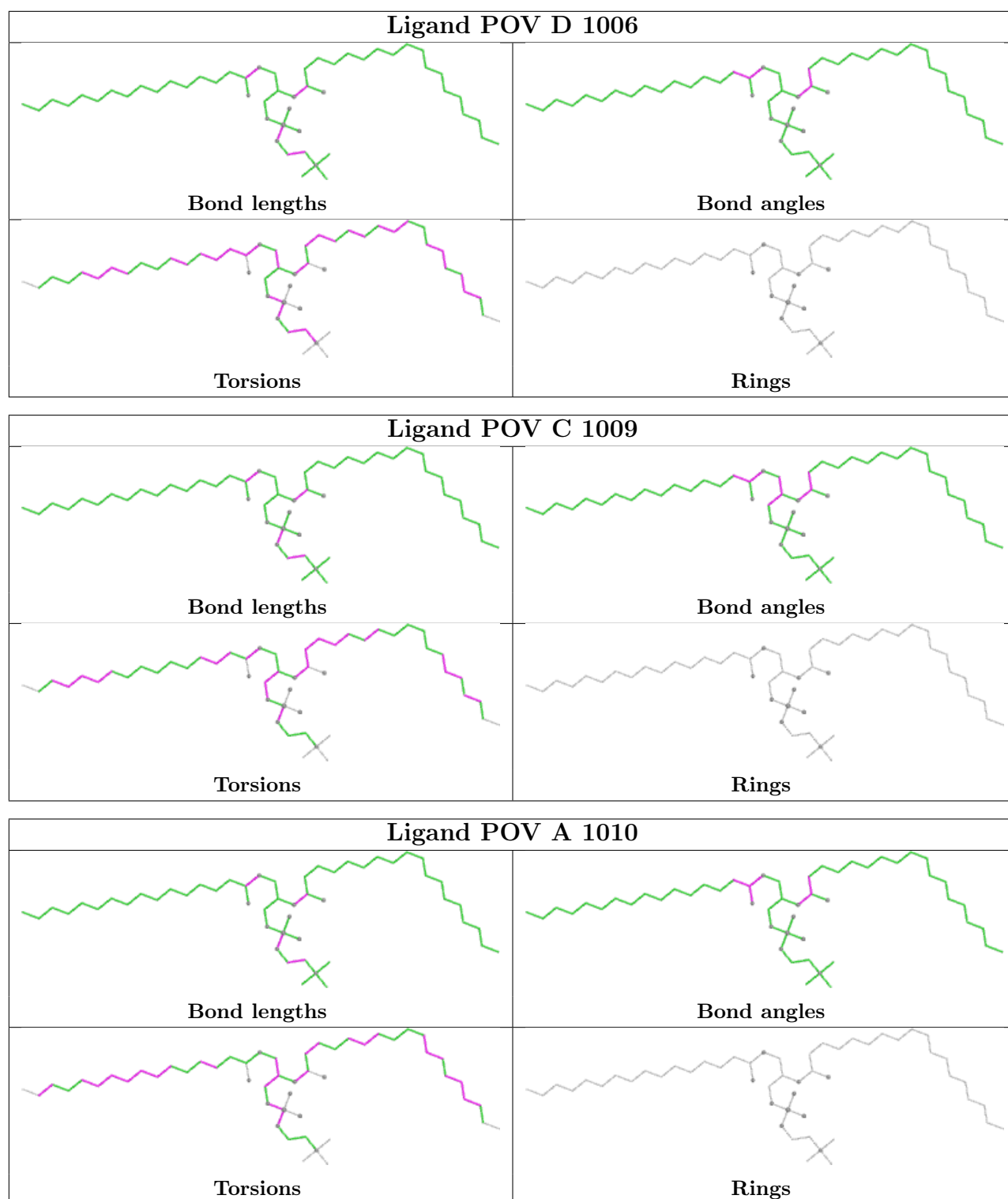


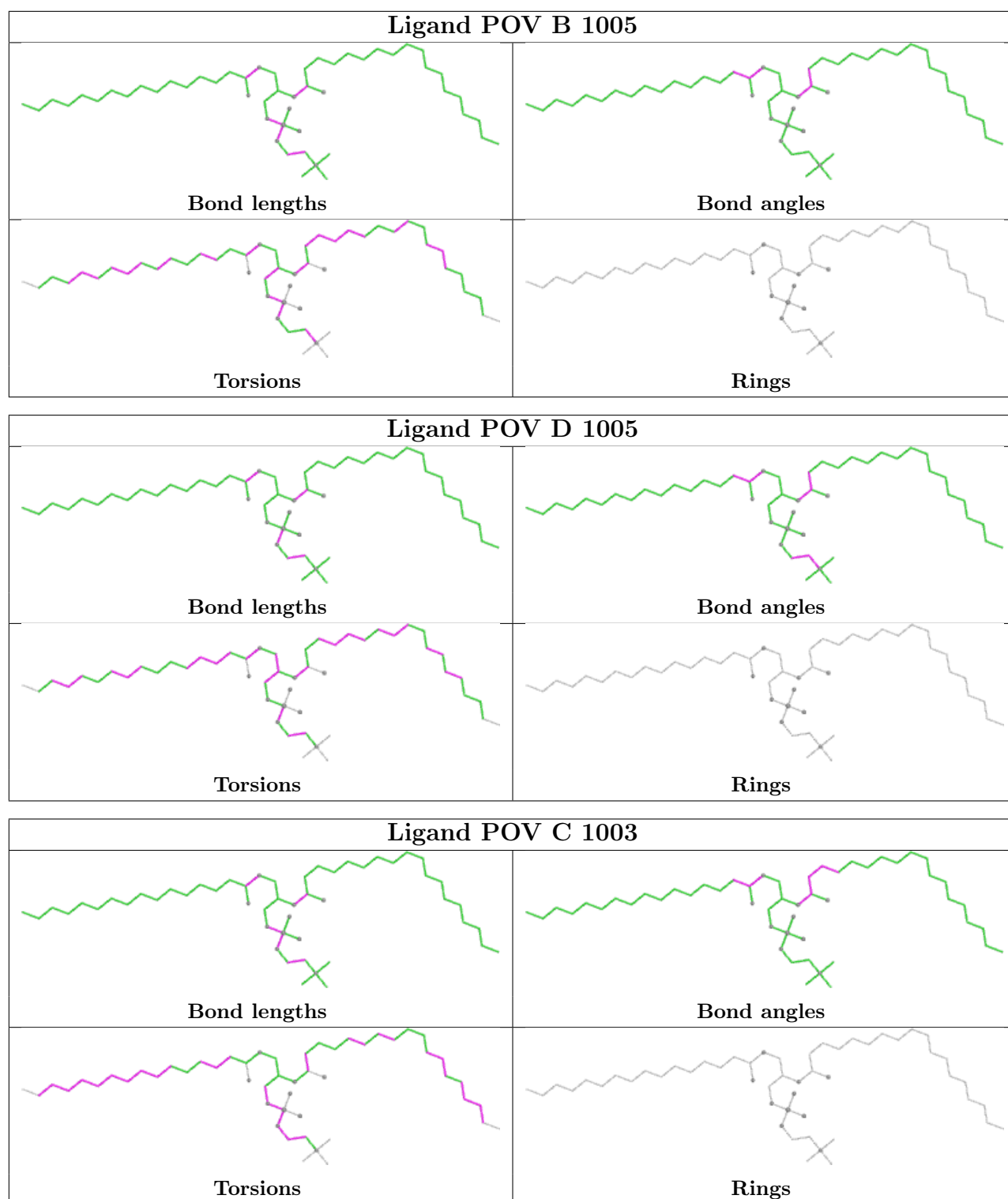


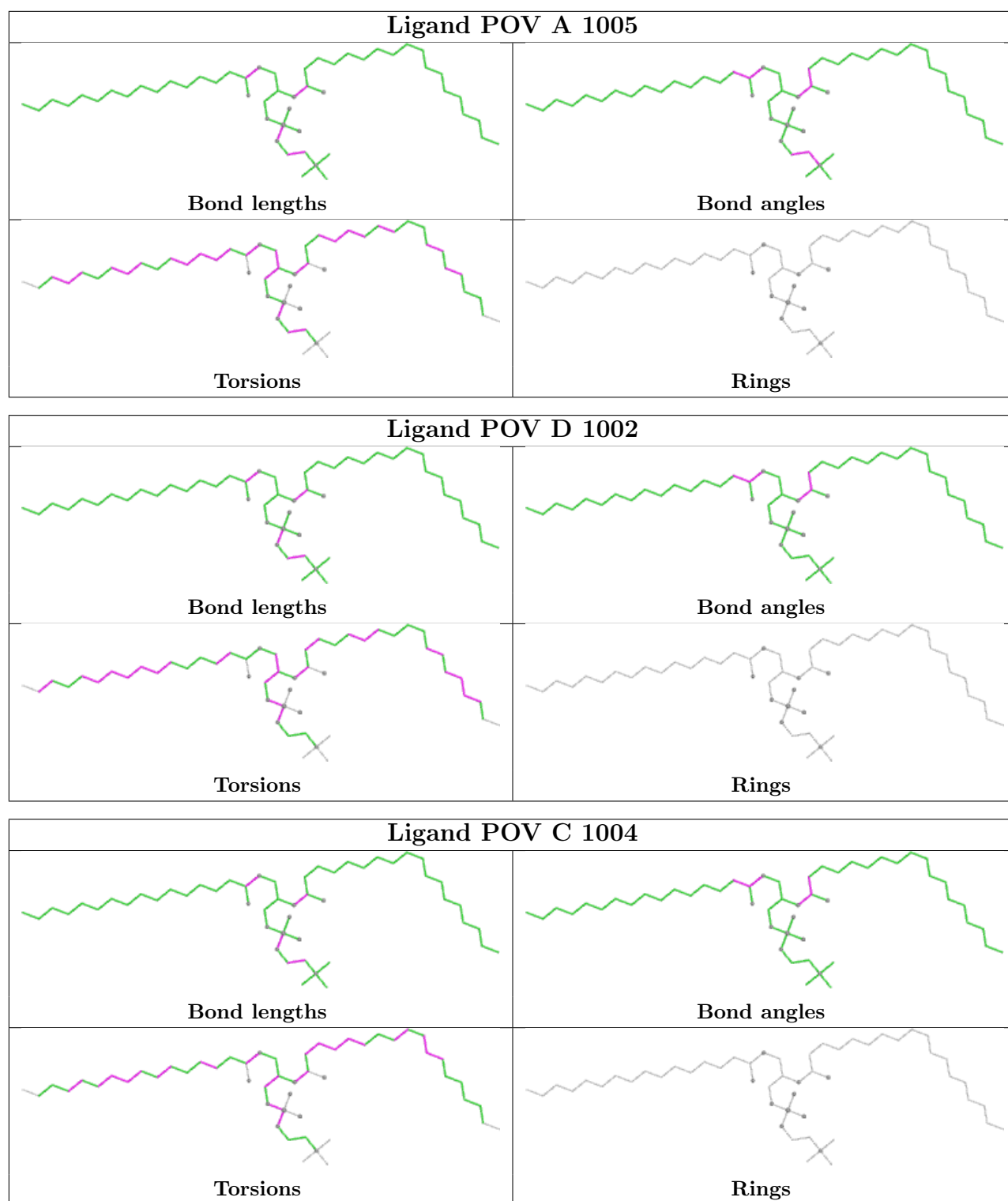


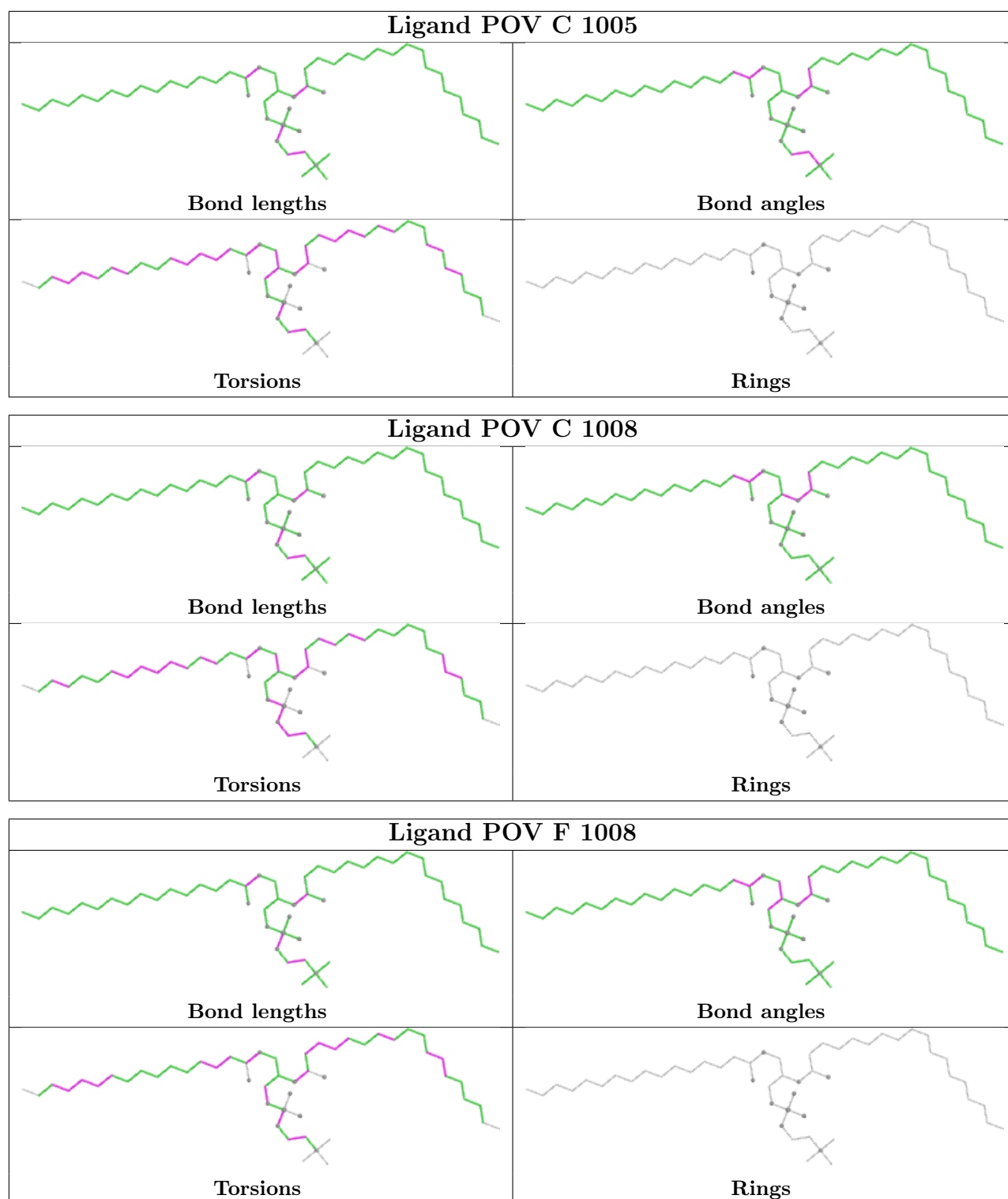


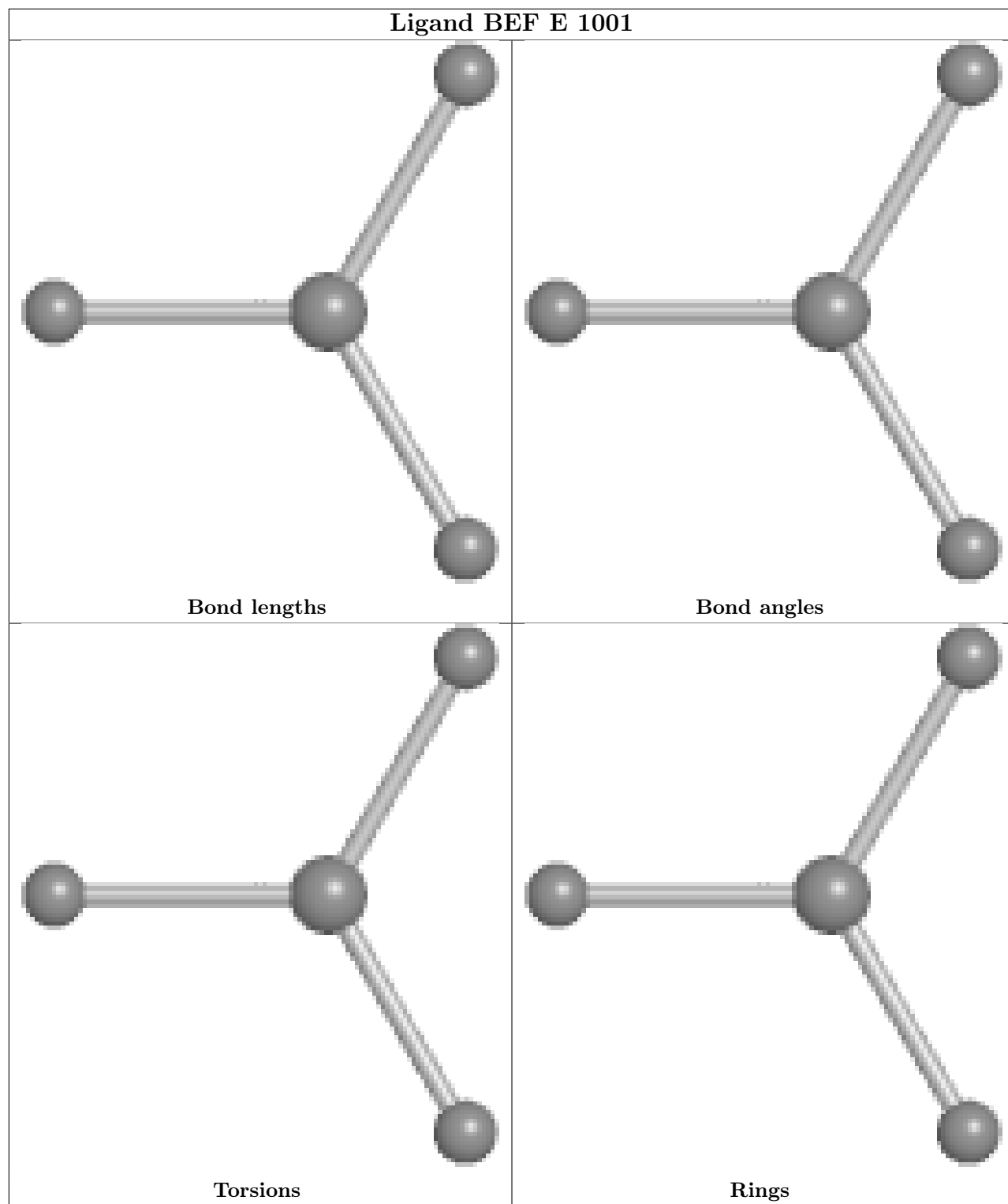


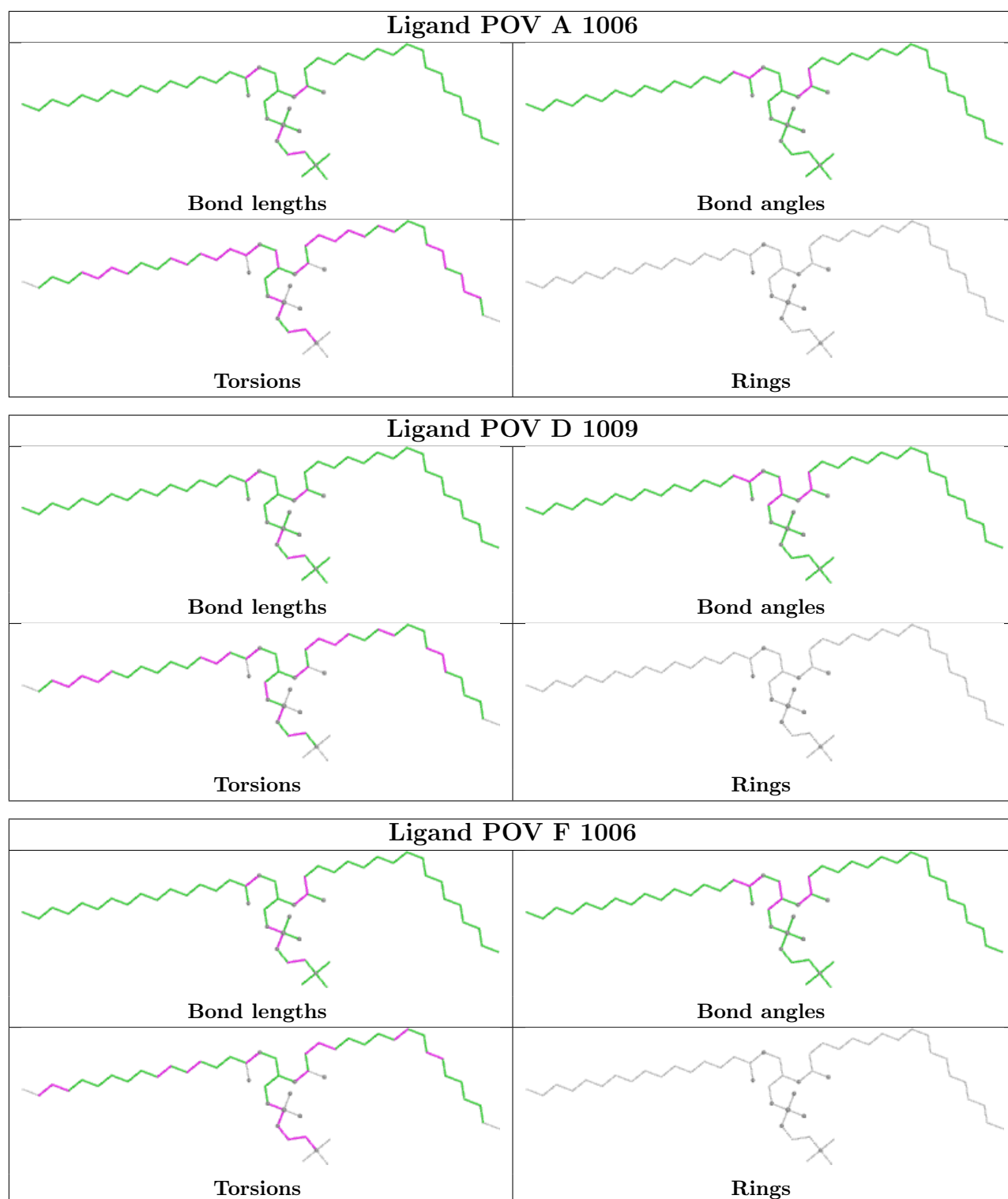


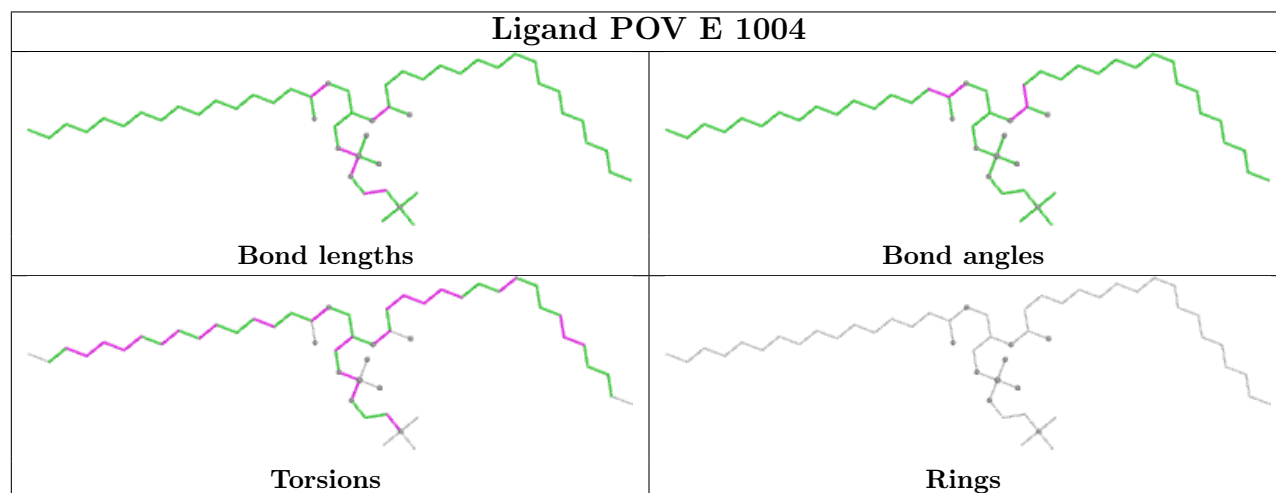
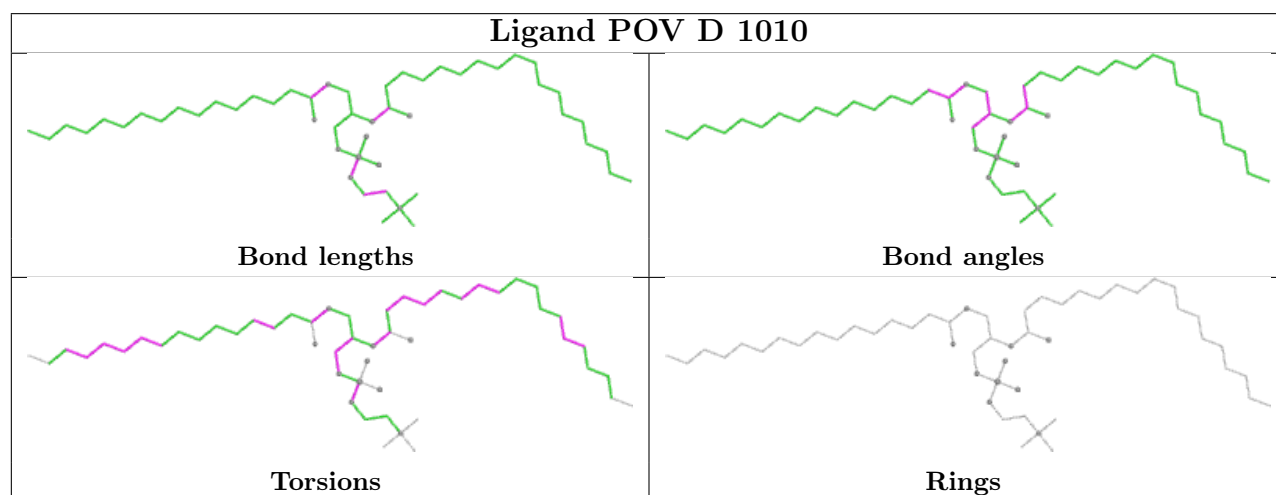
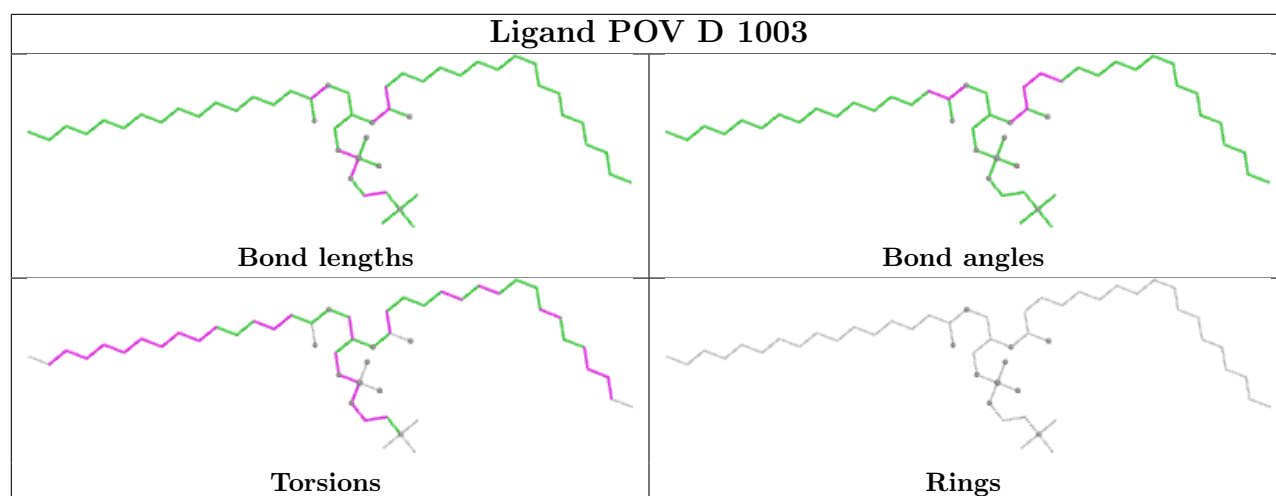


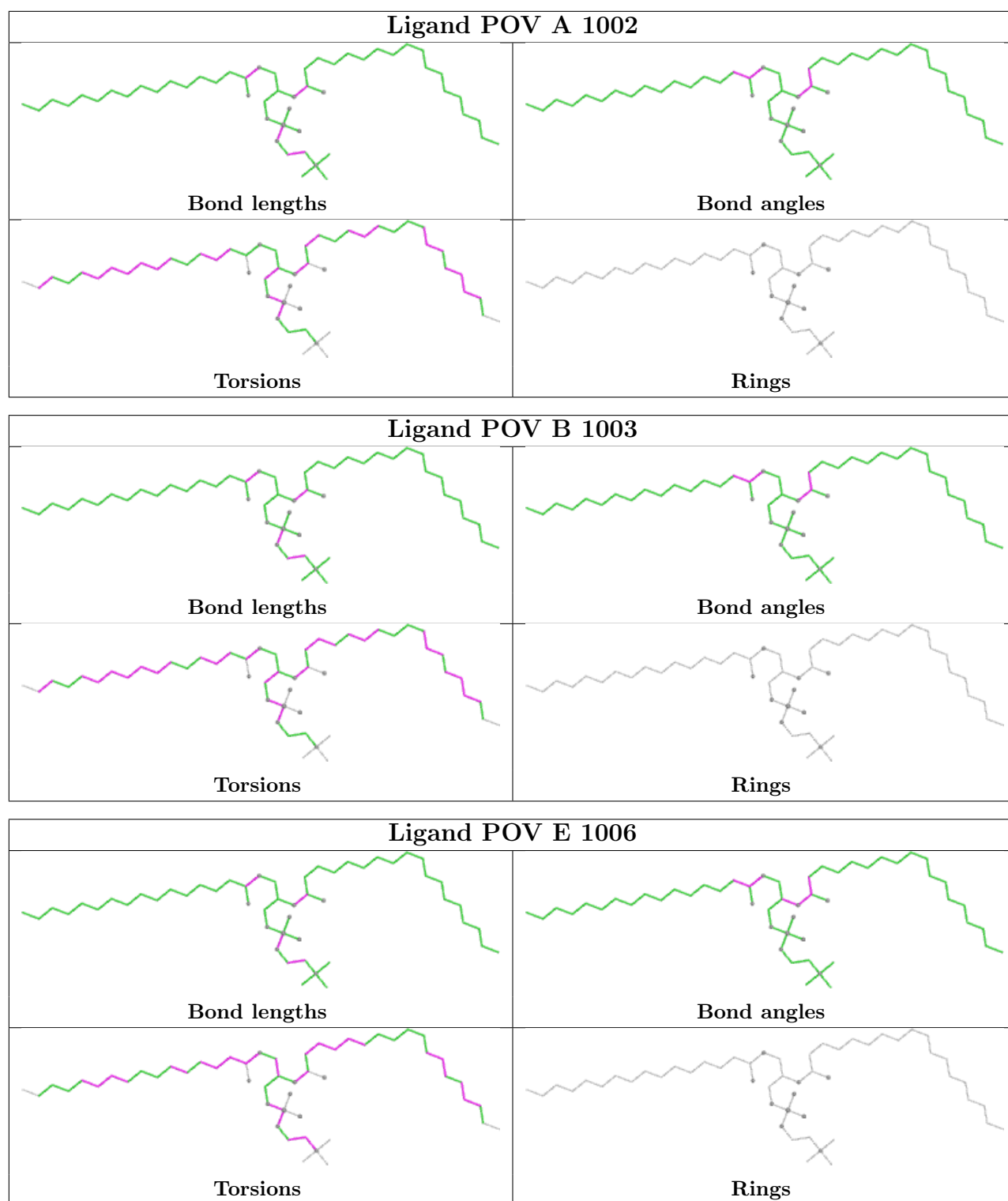


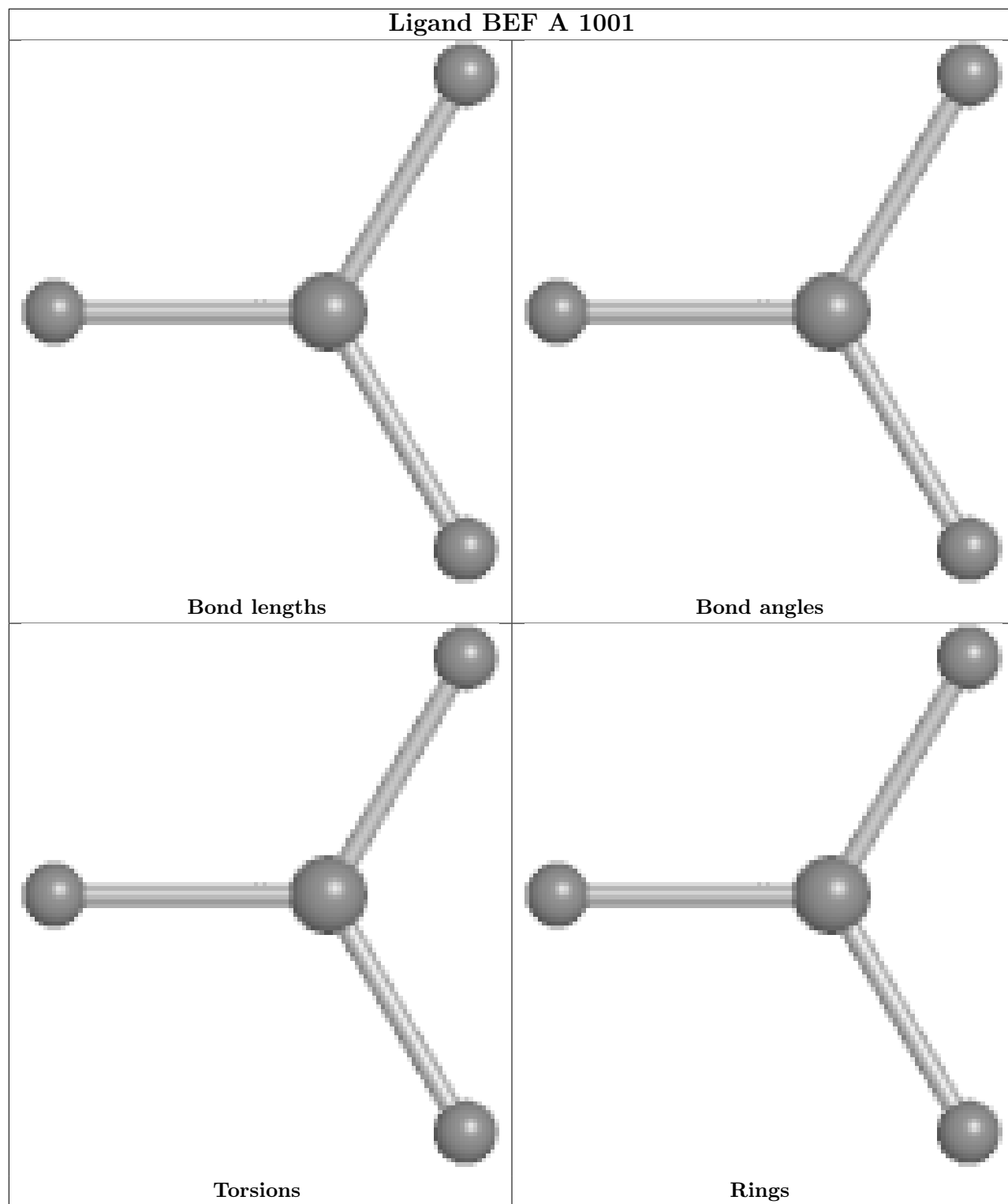


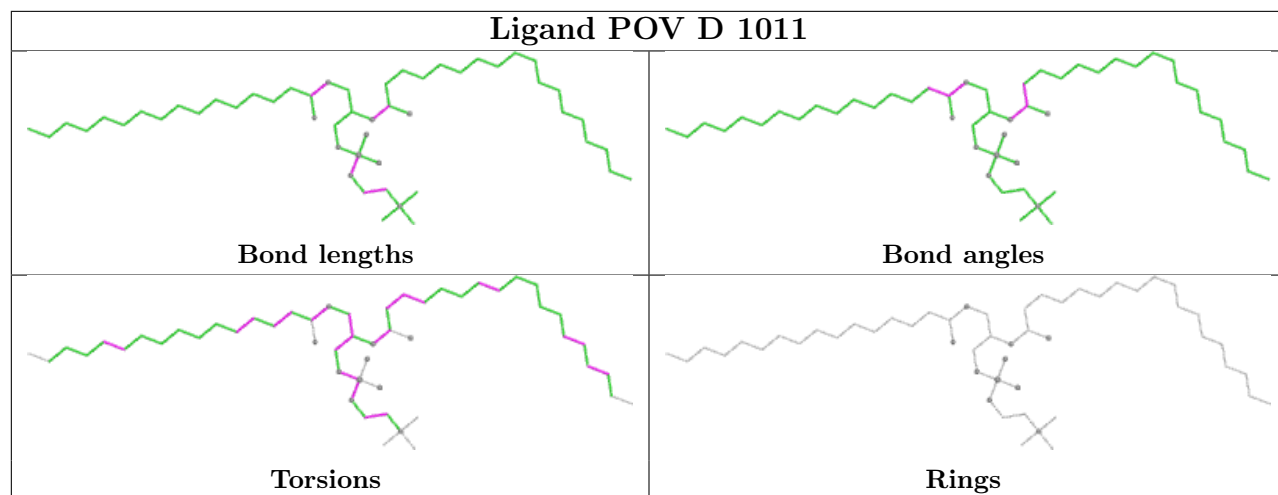


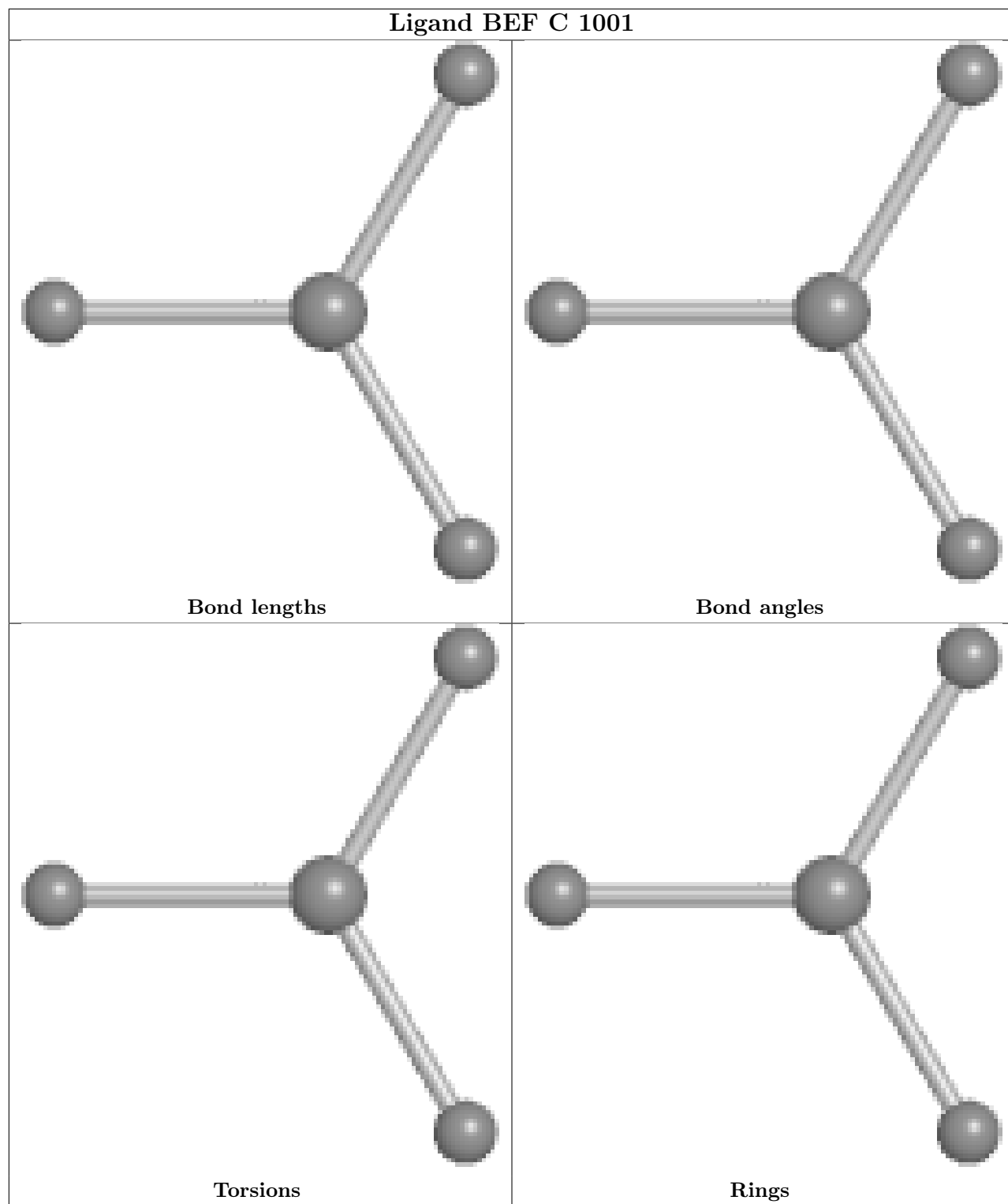


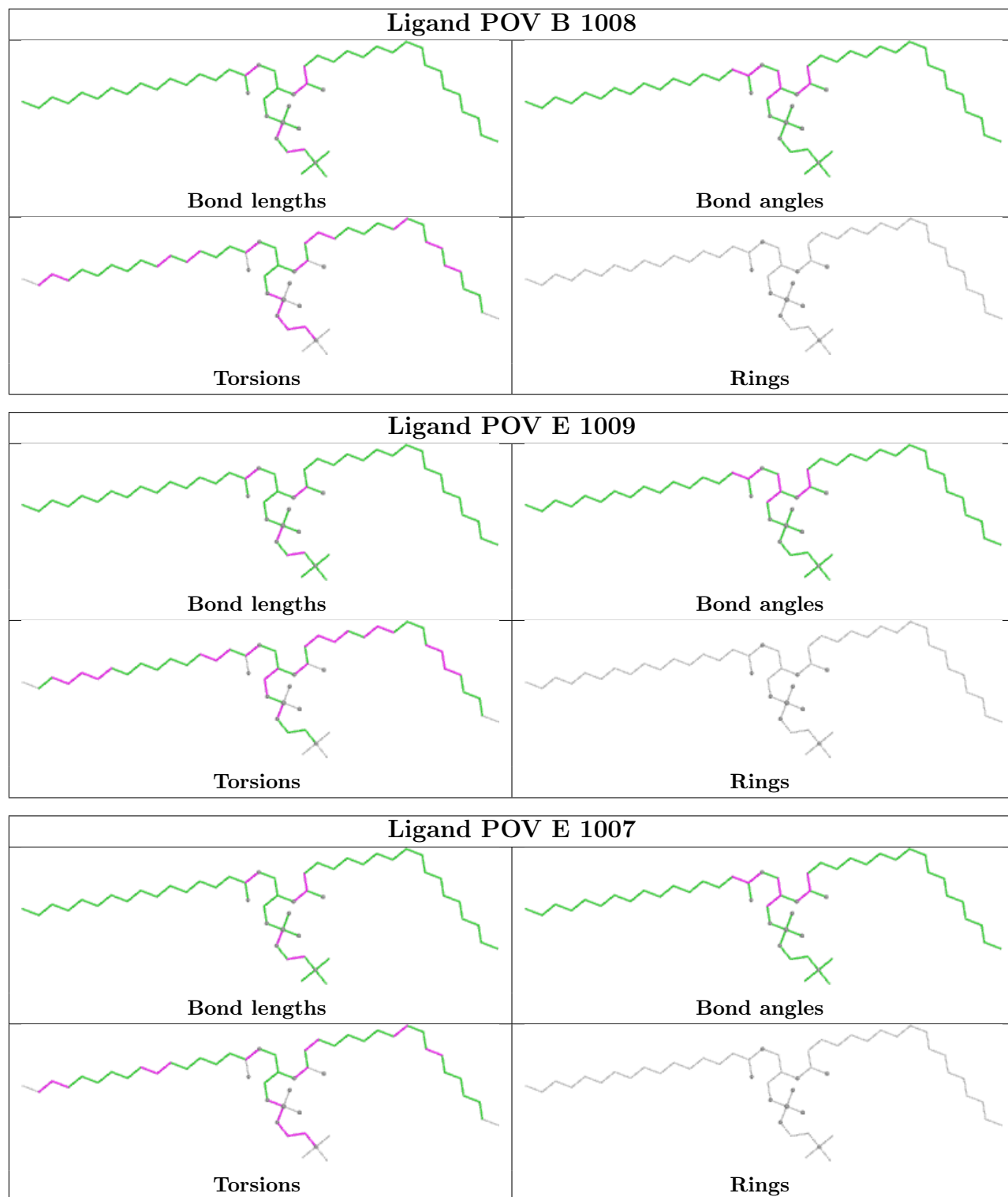


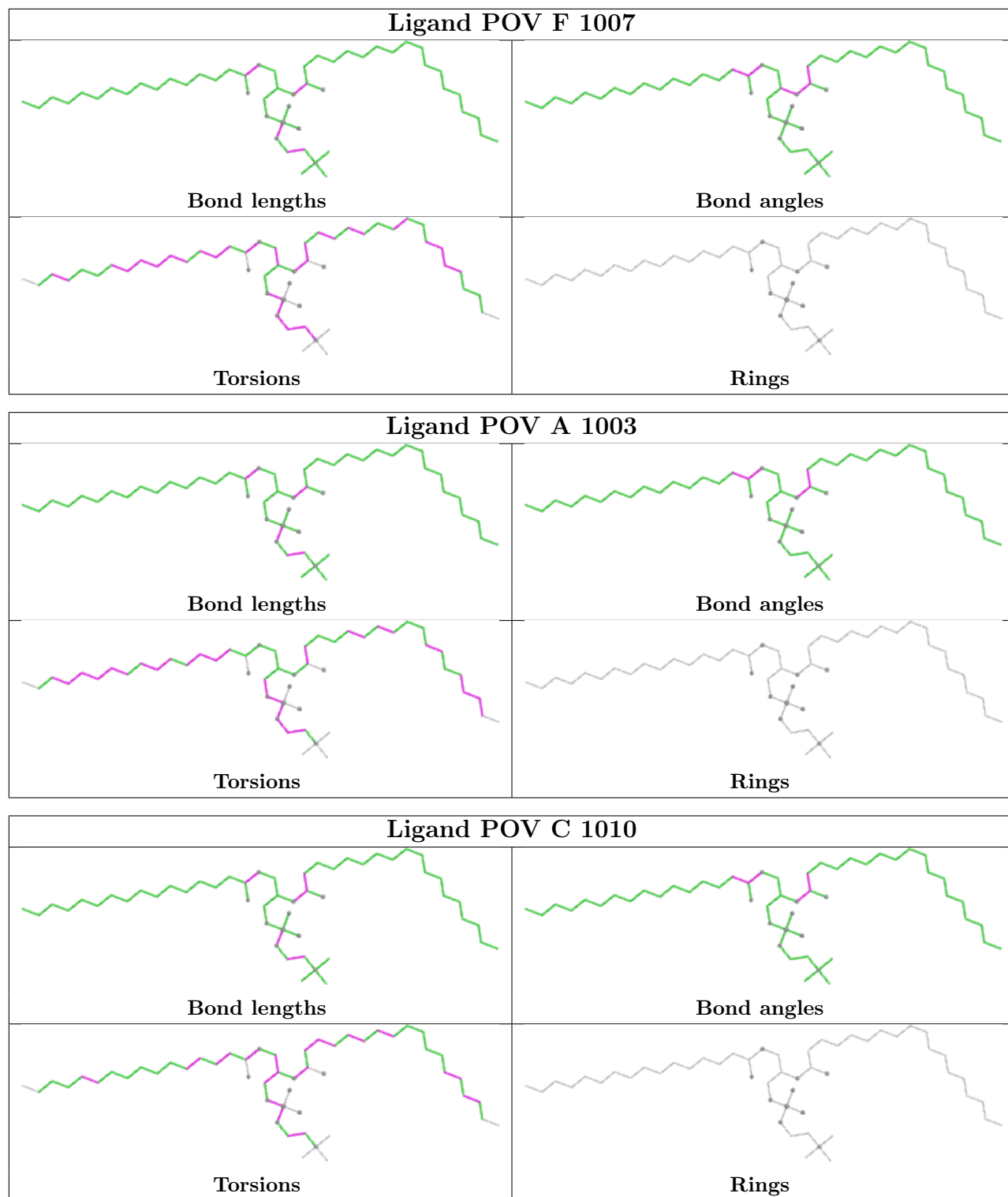


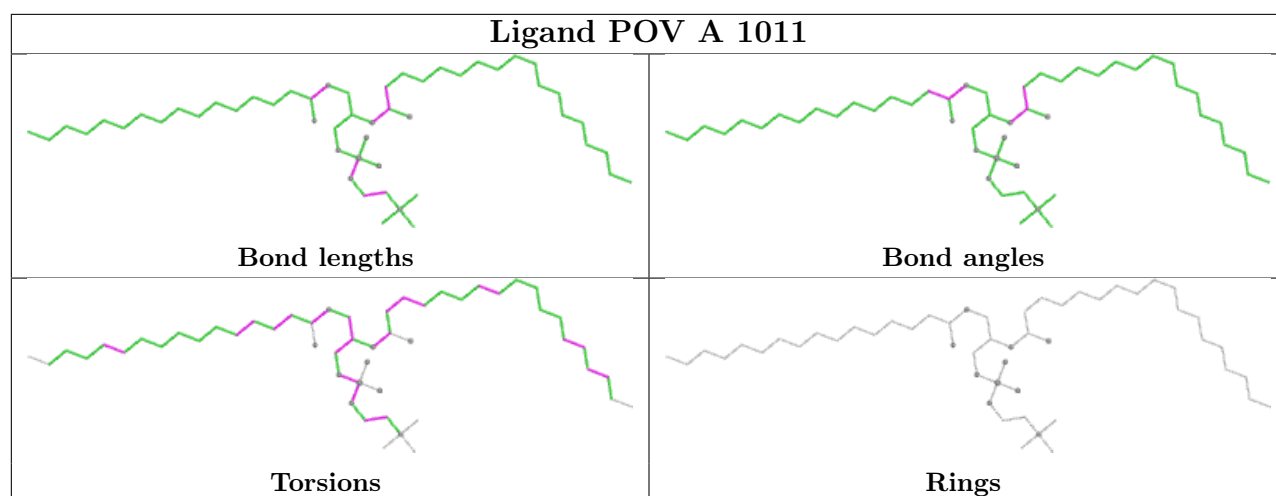












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

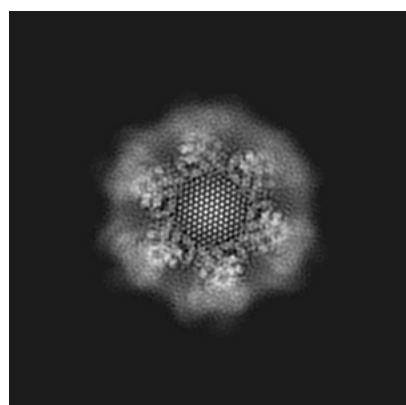
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31988. These allow visual inspection of the internal detail of the map and identification of artifacts.

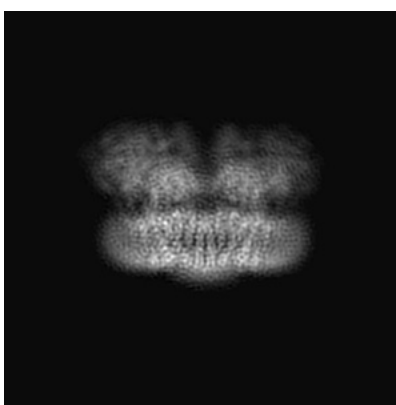
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

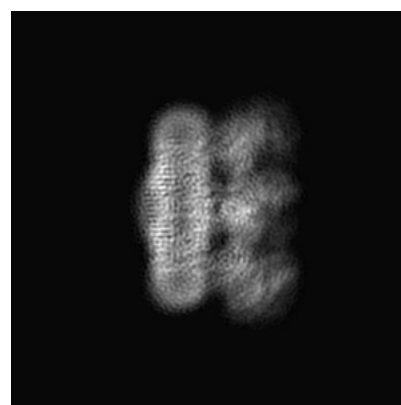
#### 6.1.1 Primary map



X



Y

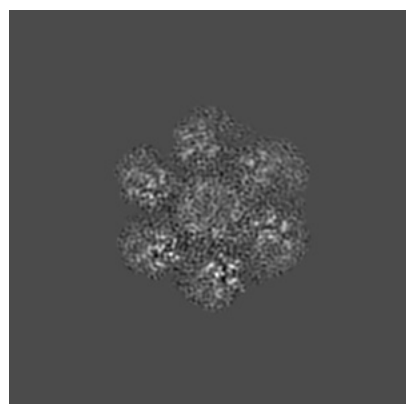


Z

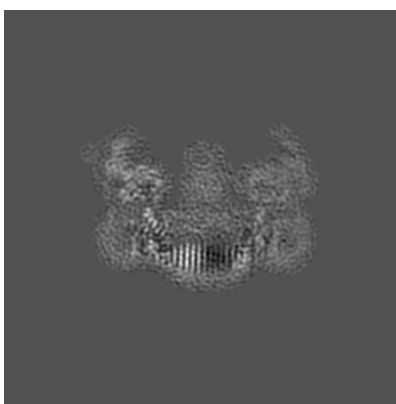
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

#### 6.2.1 Primary map



X Index: 150



Y Index: 150

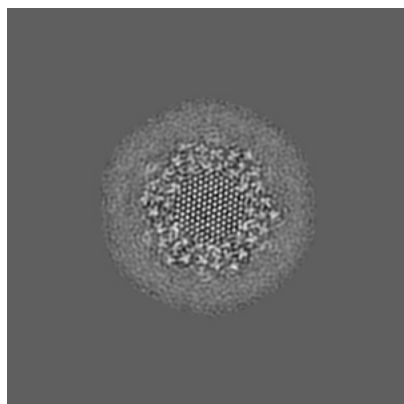


Z Index: 150

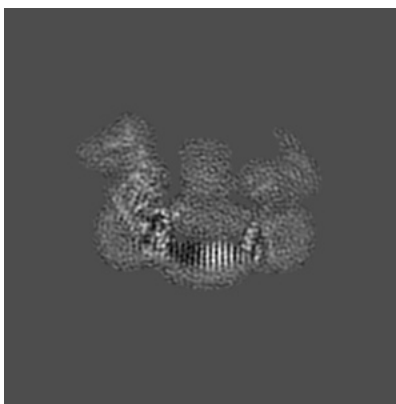
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

### 6.3.1 Primary map



X Index: 116



Y Index: 156

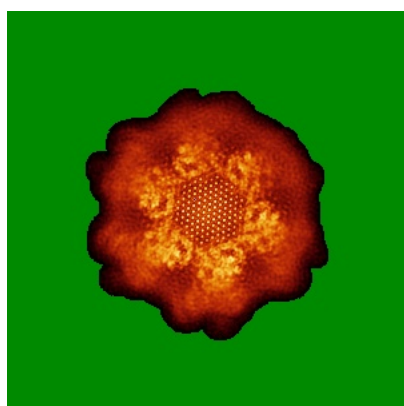


Z Index: 121

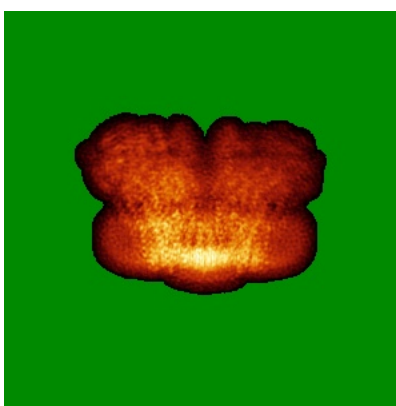
The images above show the largest variance slices of the map in three orthogonal directions.

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

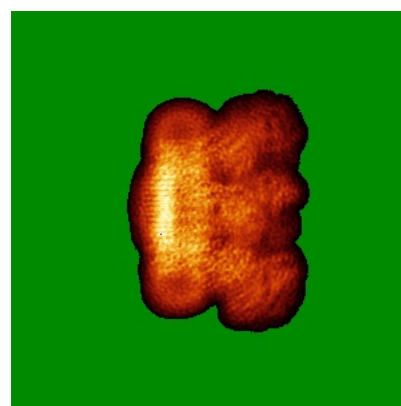
### 6.4.1 Primary map



X



Y

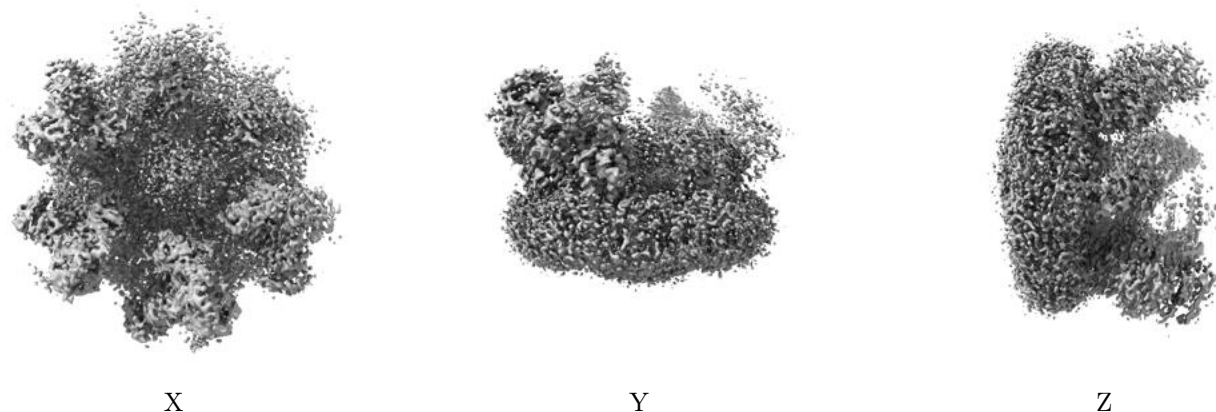


Z

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

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.012. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

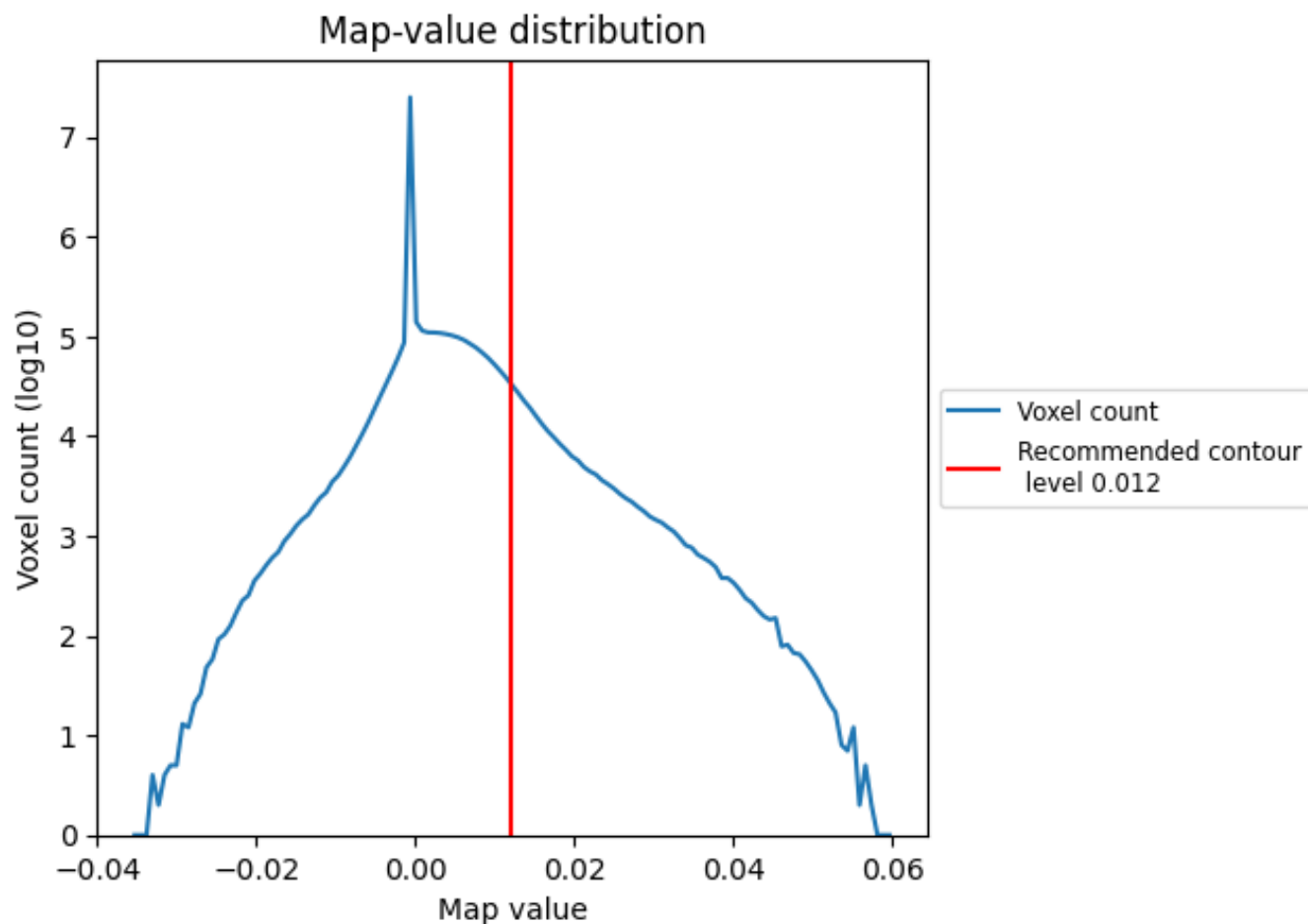
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

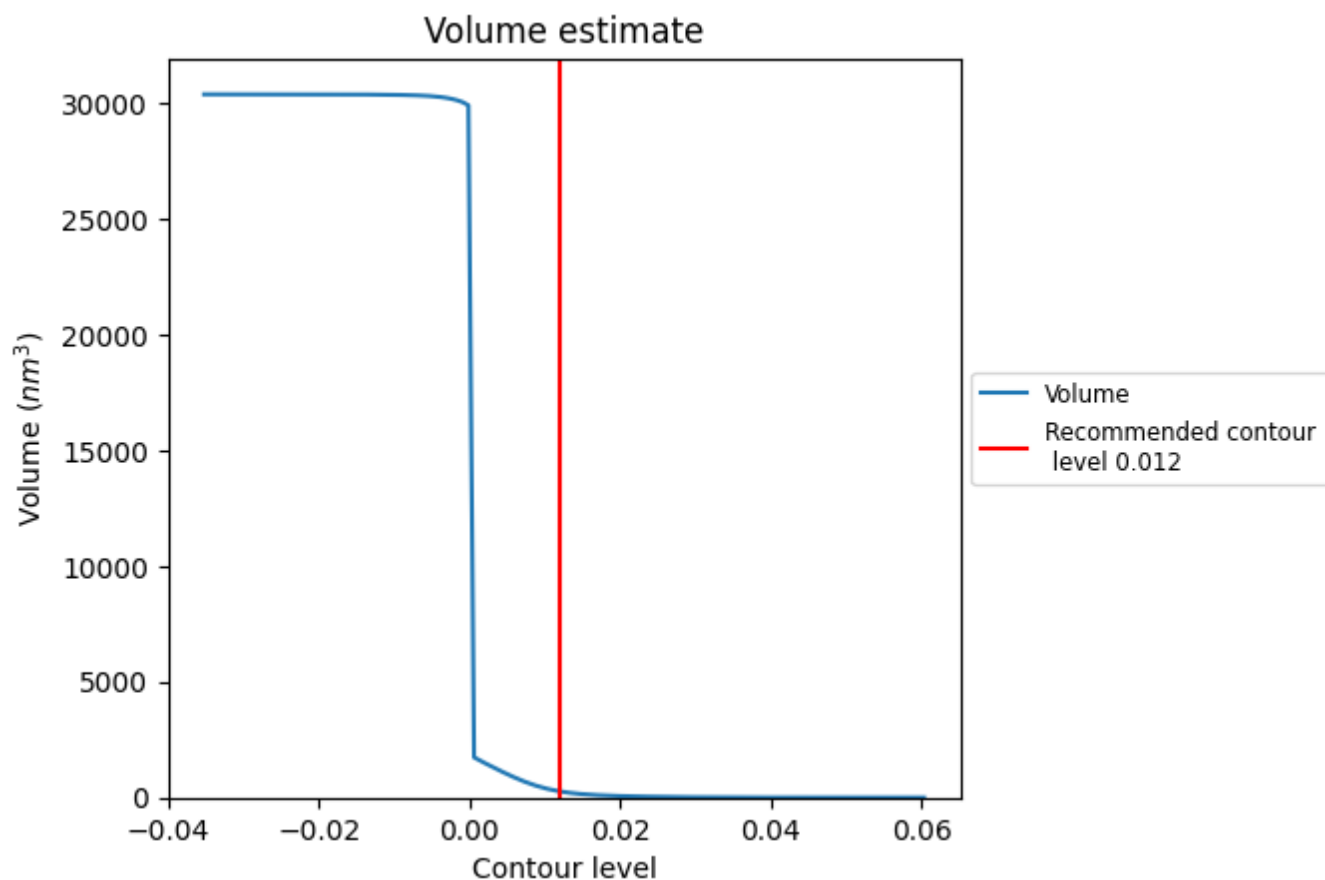
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

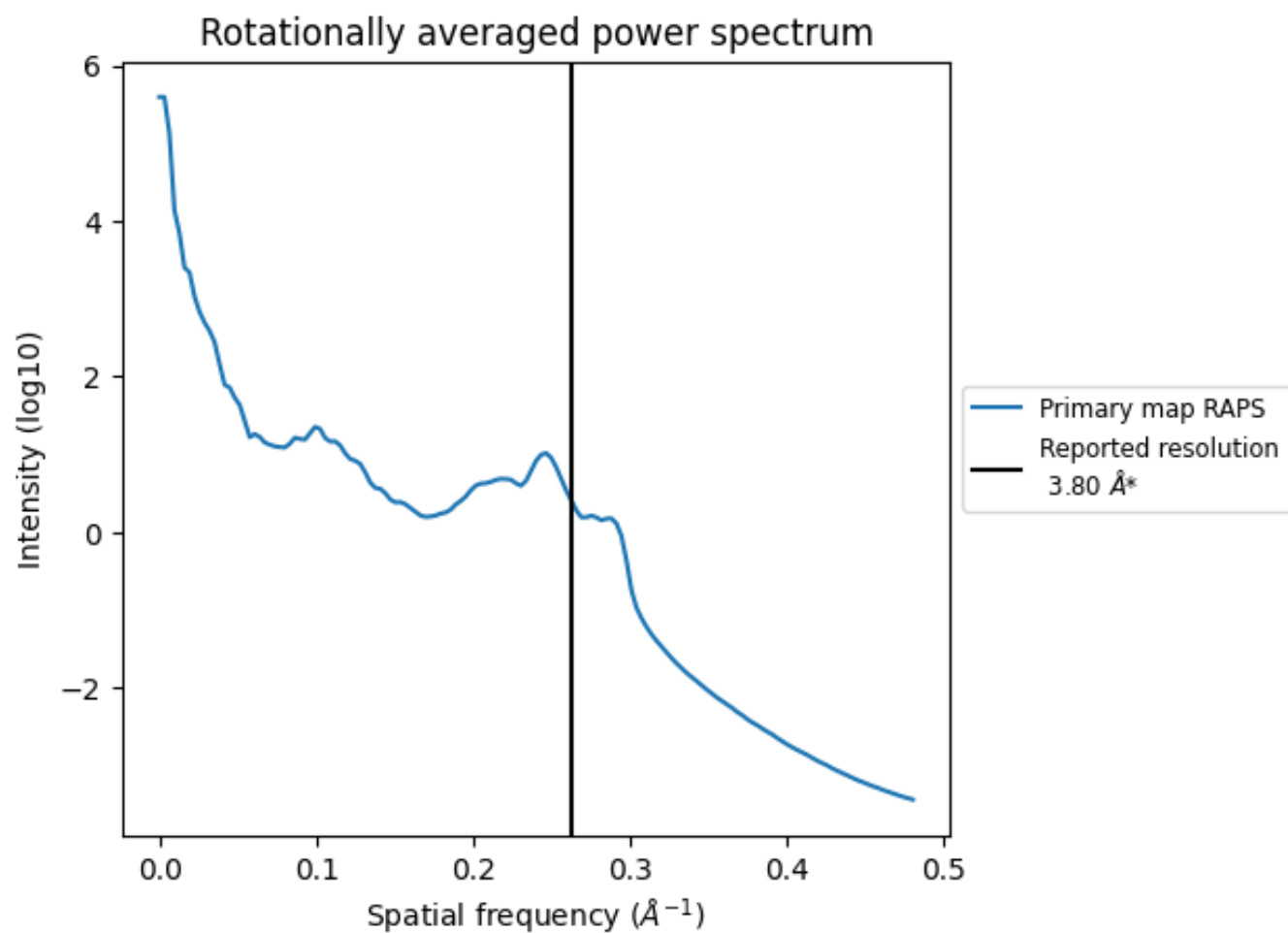
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 267 nm<sup>3</sup>; this corresponds to an approximate mass of 241 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ



\*Reported resolution corresponds to spatial frequency of 0.263 Å<sup>-1</sup>

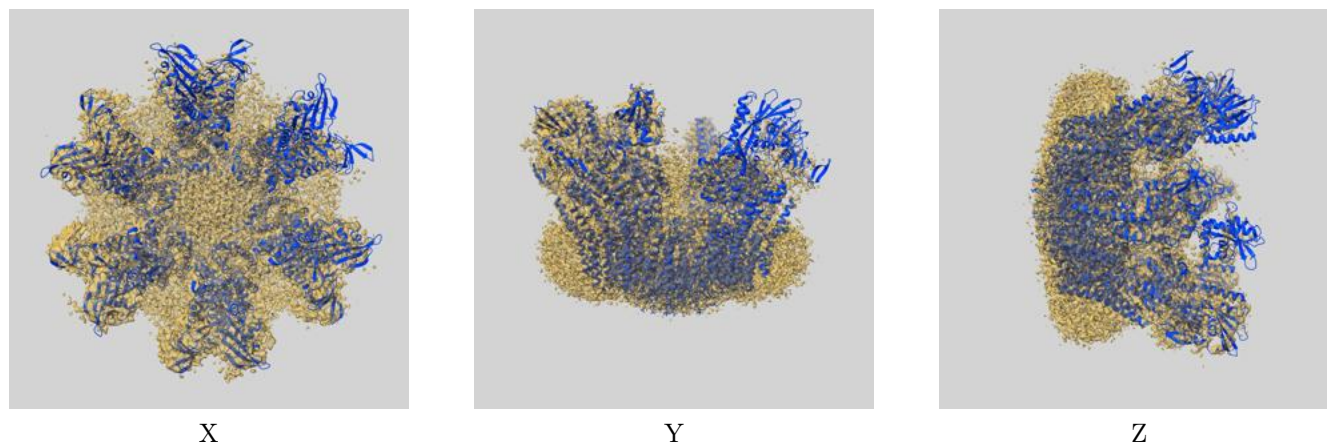
## 8 Fourier-Shell correlation ⓘ

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

## 9 Map-model fit [i](#)

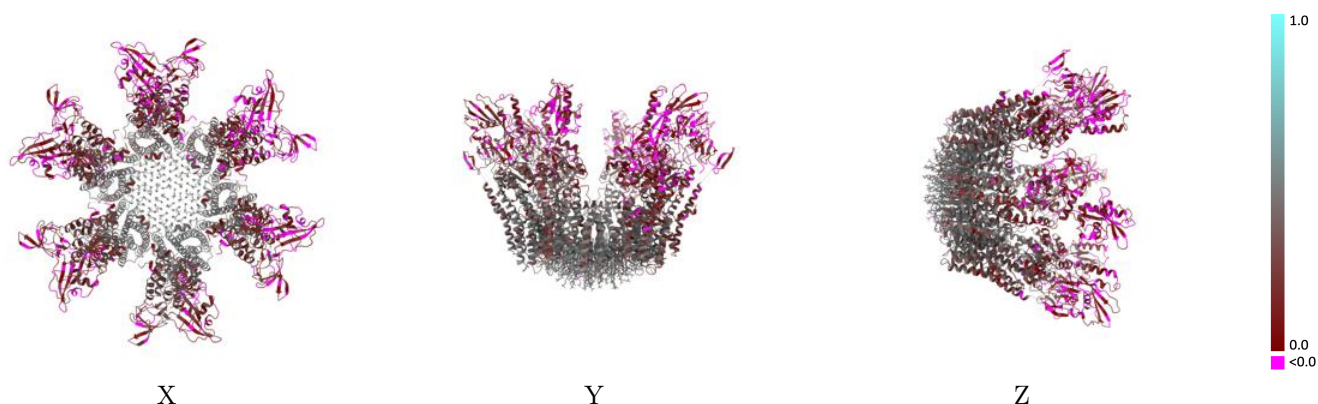
This section contains information regarding the fit between EMDB map EMD-31988 and PDB model 7VH6. Per-residue inclusion information can be found in section [3](#) on page [9](#).

### 9.1 Map-model overlay [i](#)



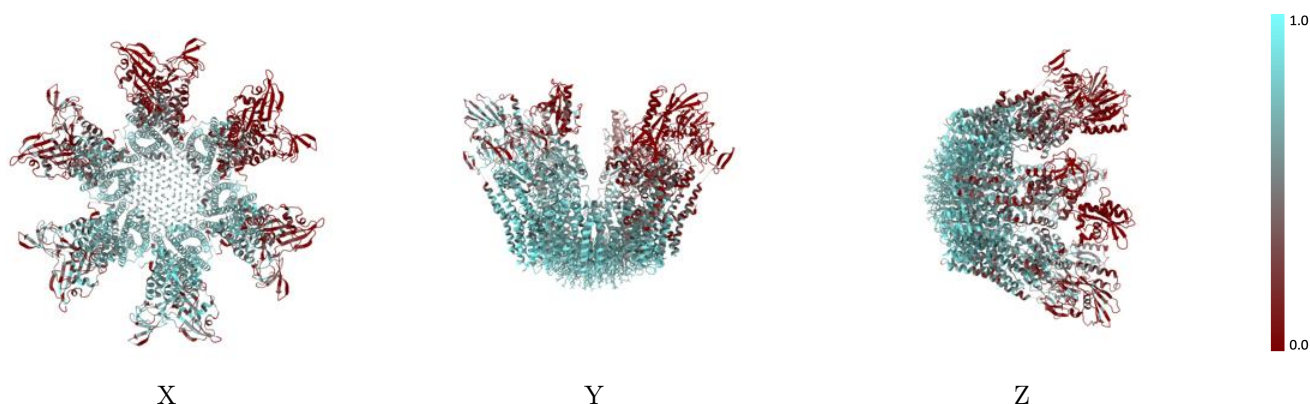
The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



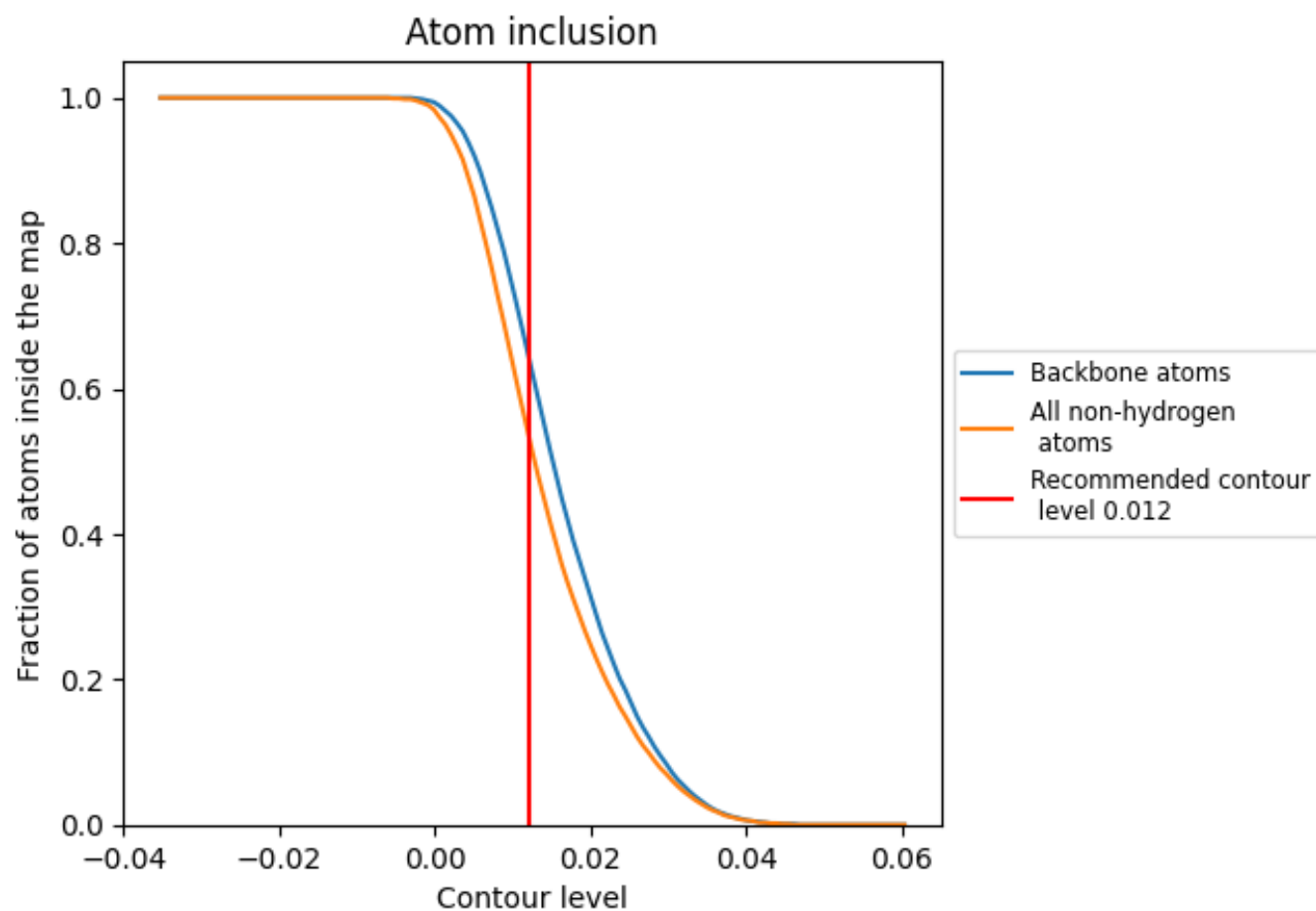
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.012).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 65% of all backbone atoms, 54% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.012) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion     | Q-score            |
|-------|--------------------|--------------------|
| All   | <div></div> 0.5380 | <div></div> 0.2890 |
| A     | <div></div> 0.6940 | <div></div> 0.3680 |
| B     | <div></div> 0.6390 | <div></div> 0.3170 |
| C     | <div></div> 0.5320 | <div></div> 0.2870 |
| D     | <div></div> 0.4090 | <div></div> 0.2460 |
| E     | <div></div> 0.3860 | <div></div> 0.2290 |
| F     | <div></div> 0.5650 | <div></div> 0.2870 |

