



## Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 02:54 PM UTC

PDB ID : 8FOB / pdb\_00008fob  
EMDB ID : EMD-29344  
Title : Cryo-EM structure of human TRPV6 in the open state  
Authors : Neuberger, A.; Yelshanskaya, M.V.; Nadezhdin, K.D.; Sobolevsky, A.I.  
Deposited on : 2022-12-30  
Resolution : 2.71 Å (reported)  
Based on initial model : 7MIJ

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.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
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 EMD 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) : 2.49

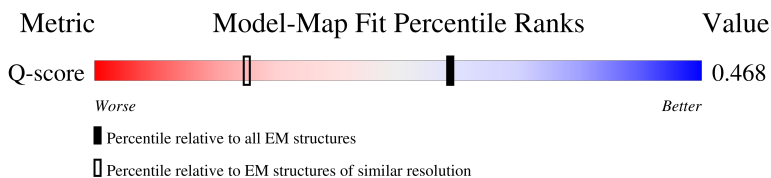
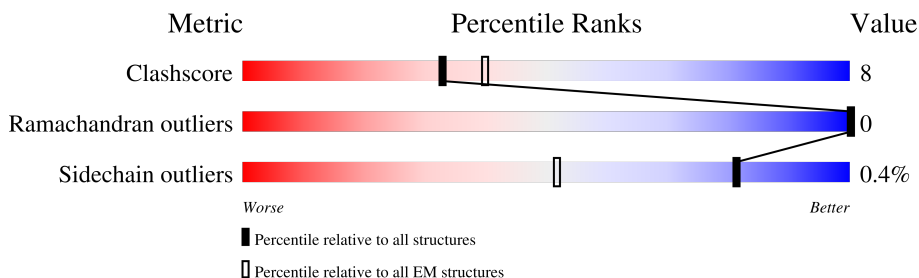
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.71 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                       | 10297 ( 2.21 - 3.21 )                                    |

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     | 725    | <div> <div>15%</div> <div>70%</div> <div>11%</div> <div>18%</div> </div> |
| 1   | B     | 725    | <div> <div>15%</div> <div>70%</div> <div>12%</div> <div>18%</div> </div> |
| 1   | C     | 725    | <div> <div>15%</div> <div>70%</div> <div>12%</div> <div>18%</div> </div> |
| 1   | D     | 725    | <div> <div>15%</div> <div>69%</div> <div>13%</div> <div>18%</div> </div> |

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   | Y01  | A     | 801 | X         | -        | -       | -                |
| 2   | Y01  | A     | 802 | X         | -        | -       | -                |
| 2   | Y01  | A     | 810 | X         | -        | -       | -                |
| 2   | Y01  | B     | 801 | X         | -        | -       | -                |
| 2   | Y01  | B     | 803 | X         | -        | -       | -                |
| 2   | Y01  | B     | 804 | X         | -        | -       | -                |
| 2   | Y01  | C     | 801 | X         | -        | -       | -                |
| 2   | Y01  | C     | 803 | X         | -        | -       | -                |
| 2   | Y01  | C     | 804 | X         | -        | -       | -                |
| 2   | Y01  | C     | 805 | X         | -        | -       | -                |
| 2   | Y01  | D     | 804 | X         | -        | -       | -                |
| 2   | Y01  | D     | 805 | X         | -        | -       | -                |

2 Entry composition ⓘ

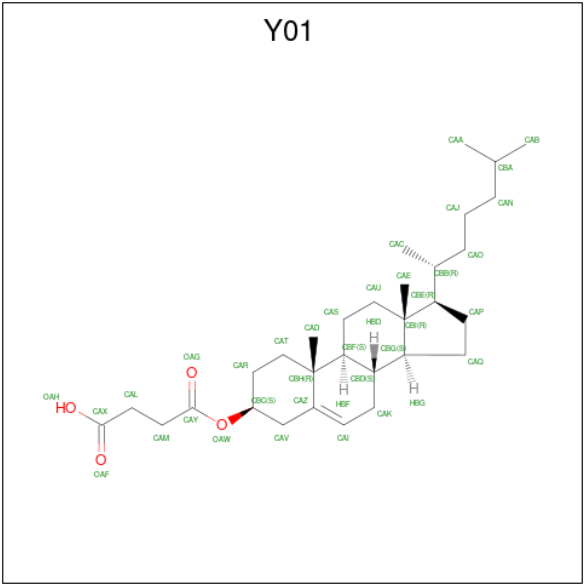
There are 6 unique types of molecules in this entry. The entry contains 20390 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Transient receptor potential cation channel subfamily V member 6.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1   | A     | 594      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4766  | 3078 | 806 | 843 | 39 |         |       |
| 1   | B     | 594      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4766  | 3078 | 806 | 843 | 39 |         |       |
| 1   | C     | 594      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4766  | 3078 | 806 | 843 | 39 |         |       |
| 1   | D     | 594      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4766  | 3078 | 806 | 843 | 39 |         |       |

- Molecule 2 is CHOLESTEROL HEMISUCCINATE (CCD ID: Y01) (formula: C<sub>31</sub>H<sub>50</sub>O<sub>4</sub>).



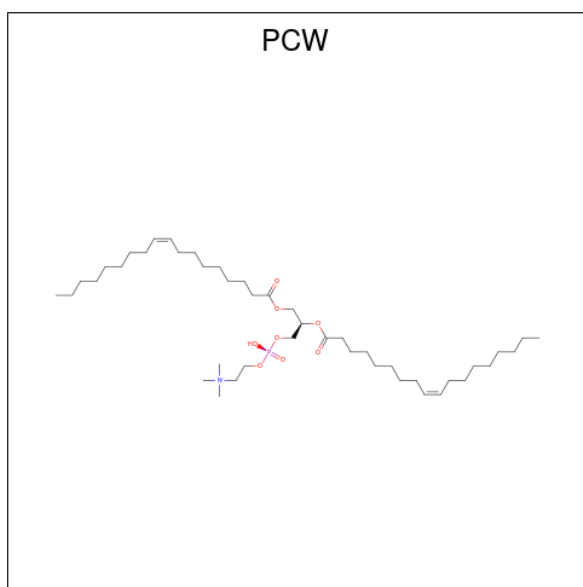
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 2   | A     | 1        | Total | C  | O | 0       |
|     |       |          | 35    | 31 | 4 |         |
| 2   | A     | 1        | Total | C  | O | 0       |
|     |       |          | 35    | 31 | 4 |         |

Continued on next page...

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 2   | A     | 1        | Total | C  | O | 0       |
|     |       |          | 35    | 31 | 4 |         |
| 2   | B     | 1        | Total | C  | O | 0       |
|     |       |          | 35    | 31 | 4 |         |
| 2   | B     | 1        | Total | C  | O | 0       |
|     |       |          | 35    | 31 | 4 |         |
| 2   | B     | 1        | Total | C  | O | 0       |
|     |       |          | 35    | 31 | 4 |         |
| 2   | C     | 1        | Total | C  | O | 0       |
|     |       |          | 35    | 31 | 4 |         |
| 2   | C     | 1        | Total | C  | O | 0       |
|     |       |          | 35    | 31 | 4 |         |
| 2   | C     | 1        | Total | C  | O | 0       |
|     |       |          | 35    | 31 | 4 |         |
| 2   | C     | 1        | Total | C  | O | 0       |
|     |       |          | 35    | 31 | 4 |         |
| 2   | D     | 1        | Total | C  | O | 0       |
|     |       |          | 35    | 31 | 4 |         |
| 2   | D     | 1        | Total | C  | O | 0       |
|     |       |          | 35    | 31 | 4 |         |

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



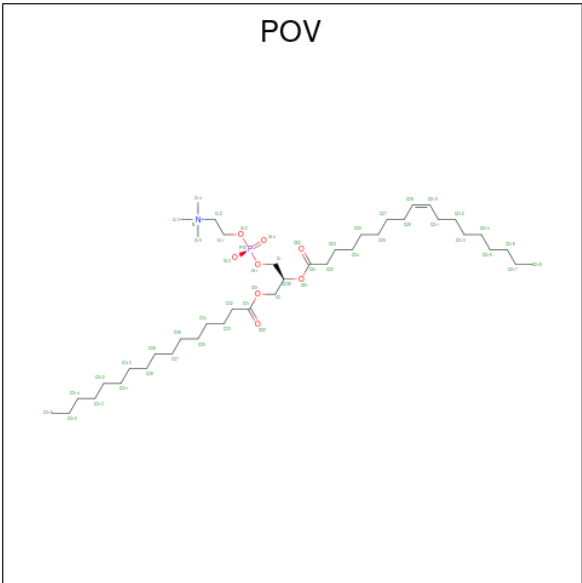
| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 3   | A     | 1        | Total | C  | 0       |
|     |       |          | 13    | 13 |         |

*Continued on next page...*

Continued from previous page...

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 3   | B     | 1        | Total | C  | 0       |
|     |       |          | 13    | 13 |         |
| 3   | C     | 1        | Total | C  | 0       |
|     |       |          | 13    | 13 |         |
| 3   | D     | 1        | Total | C  | 0       |
|     |       |          | 13    | 13 |         |

- Molecule 4 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylamm onio)ethyl phosphate (CCD ID: POV) (formula: C<sub>42</sub>H<sub>82</sub>NO<sub>8</sub>P).



| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 4   | A     | 1        | Total | C  |   |   |   | 0       |
|     |       |          | 13    | 13 |   |   |   |         |
| 4   | A     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 52    | 42 | 1 | 8 | 1 |         |
| 4   | A     | 1        | Total | C  |   |   |   | 0       |
|     |       |          | 14    | 14 |   |   |   |         |
| 4   | A     | 1        | Total | C  | O |   |   | 0       |
|     |       |          | 18    | 16 | 2 |   |   |         |
| 4   | A     | 1        | Total | C  |   |   |   | 0       |
|     |       |          | 20    | 20 |   |   |   |         |
| 4   | A     | 1        | Total | C  | O |   |   | 0       |
|     |       |          | 31    | 28 | 3 |   |   |         |
| 4   | A     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 52    | 42 | 1 | 8 | 1 |         |
| 4   | B     | 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 |
|-----|-------|----------|------------------------------|---------|
| 4   | B     | 1        | Total C<br>13 13             | 0       |
| 4   | B     | 1        | Total C N O P<br>52 42 1 8 1 | 0       |
| 4   | B     | 1        | Total C<br>14 14             | 0       |
| 4   | B     | 1        | Total C O<br>18 16 2         | 0       |
| 4   | B     | 1        | Total C<br>20 20             | 0       |
| 4   | B     | 1        | Total C O<br>31 28 3         | 0       |
| 4   | C     | 1        | Total C N O P<br>52 42 1 8 1 | 0       |
| 4   | C     | 1        | Total C<br>13 13             | 0       |
| 4   | C     | 1        | Total C N O P<br>52 42 1 8 1 | 0       |
| 4   | C     | 1        | Total C<br>14 14             | 0       |
| 4   | C     | 1        | Total C O<br>18 16 2         | 0       |
| 4   | C     | 1        | Total C<br>20 20             | 0       |
| 4   | C     | 1        | Total C O<br>31 28 3         | 0       |
| 4   | D     | 1        | Total C<br>20 20             | 0       |
| 4   | D     | 1        | Total C O<br>31 28 3         | 0       |
| 4   | D     | 1        | Total C N O P<br>52 42 1 8 1 | 0       |
| 4   | D     | 1        | Total C<br>13 13             | 0       |
| 4   | D     | 1        | Total C N O P<br>52 42 1 8 1 | 0       |
| 4   | D     | 1        | Total C<br>14 14             | 0       |
| 4   | D     | 1        | Total C O<br>18 16 2         | 0       |

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 5   | A     | 2        | Total | Ca | 0       |
|     |       |          | 2     | 2  |         |

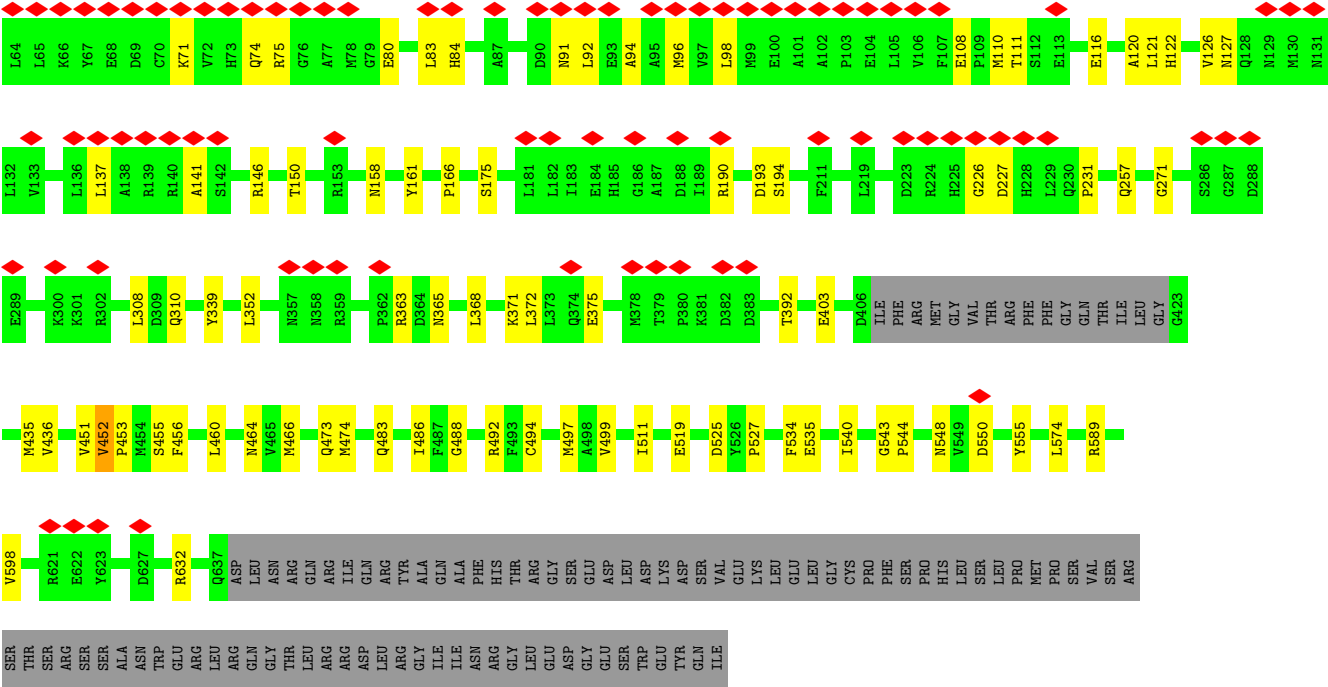
- Molecule 6 is water.

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 6   | A     | 13       | Total | O  | 0       |
|     |       |          | 13    | 13 |         |
| 6   | B     | 13       | Total | O  | 0       |
|     |       |          | 13    | 13 |         |
| 6   | C     | 13       | Total | O  | 0       |
|     |       |          | 13    | 13 |         |
| 6   | D     | 13       | Total | O  | 0       |
|     |       |          | 13    | 13 |         |









## 4 Experimental information

| Property                             | Value                  | Source    |
|--------------------------------------|------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE        | Depositor |
| Imposed symmetry                     | POINT, Not provided    |           |
| Number of particles used             | 76442                  | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF      | Depositor |
| CTF correction method                | NONE                   | Depositor |
| Microscope                           | TFS KRIOS              | Depositor |
| Voltage (kV)                         | 300                    | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 60                     | Depositor |
| Minimum defocus (nm)                 | 800                    | Depositor |
| Maximum defocus (nm)                 | 2000                   | Depositor |
| Magnification                        | Not provided           |           |
| Image detector                       | GATAN K3 (6k x 4k)     | Depositor |
| Maximum map value                    | 3.364                  | Depositor |
| Minimum map value                    | -2.390                 | Depositor |
| Average map value                    | 0.031                  | Depositor |
| Map value standard deviation         | 0.128                  | Depositor |
| Recommended contour level            | 0.51                   | Depositor |
| Map size ( $\text{\AA}$ )            | 215.04, 215.04, 215.04 | wwPDB     |
| Map dimensions                       | 256, 256, 256          | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0       | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 0.84, 0.84, 0.84       | Depositor |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, POV, Y01, PCW

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     | 0.31         | 0/4875      | 0.74        | 4/6616 (0.1%)   |
| 1   | B     | 0.31         | 0/4875      | 0.74        | 4/6616 (0.1%)   |
| 1   | C     | 0.31         | 0/4875      | 0.74        | 4/6616 (0.1%)   |
| 1   | D     | 0.31         | 0/4875      | 0.74        | 4/6616 (0.1%)   |
| All | All   | 0.31         | 0/19500     | 0.74        | 16/26464 (0.1%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 1                   |
| 1   | B     | 0                   | 1                   |
| 1   | C     | 0                   | 1                   |
| 1   | D     | 0                   | 1                   |
| All | All   | 0                   | 4                   |

There are no bond length outliers.

All (16) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1   | D     | 175 | SER  | CA-C-N | 5.58 | 129.18      | 120.82   |
| 1   | D     | 175 | SER  | C-N-CA | 5.58 | 129.18      | 120.82   |
| 1   | A     | 175 | SER  | CA-C-N | 5.57 | 129.17      | 120.82   |
| 1   | A     | 175 | SER  | C-N-CA | 5.57 | 129.17      | 120.82   |
| 1   | B     | 175 | SER  | CA-C-N | 5.55 | 129.14      | 120.82   |
| 1   | B     | 175 | SER  | C-N-CA | 5.55 | 129.14      | 120.82   |
| 1   | C     | 175 | SER  | CA-C-N | 5.54 | 129.13      | 120.82   |
| 1   | C     | 175 | SER  | C-N-CA | 5.54 | 129.13      | 120.82   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1   | C     | 403 | GLU  | CA-C-N | 5.35 | 123.61      | 120.24   |
| 1   | C     | 403 | GLU  | C-N-CA | 5.35 | 123.61      | 120.24   |
| 1   | B     | 403 | GLU  | CA-C-N | 5.32 | 123.59      | 120.24   |
| 1   | B     | 403 | GLU  | C-N-CA | 5.32 | 123.59      | 120.24   |
| 1   | A     | 403 | GLU  | CA-C-N | 5.32 | 123.59      | 120.24   |
| 1   | A     | 403 | GLU  | C-N-CA | 5.32 | 123.59      | 120.24   |
| 1   | D     | 403 | GLU  | CA-C-N | 5.27 | 123.56      | 120.24   |
| 1   | D     | 403 | GLU  | C-N-CA | 5.27 | 123.56      | 120.24   |

There are no chirality outliers.

All (4) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | A     | 519 | GLU  | Peptide |
| 1   | B     | 519 | GLU  | Peptide |
| 1   | C     | 519 | GLU  | Peptide |
| 1   | D     | 519 | GLU  | Peptide |

## 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     | 4766  | 0        | 4818     | 52      | 0            |
| 1   | B     | 4766  | 0        | 4818     | 53      | 0            |
| 1   | C     | 4766  | 0        | 4818     | 54      | 0            |
| 1   | D     | 4766  | 0        | 4818     | 58      | 0            |
| 2   | A     | 105   | 0        | 135      | 35      | 0            |
| 2   | B     | 105   | 0        | 135      | 38      | 0            |
| 2   | C     | 140   | 0        | 180      | 49      | 0            |
| 2   | D     | 70    | 0        | 90       | 21      | 0            |
| 3   | A     | 13    | 0        | 20       | 0       | 0            |
| 3   | B     | 13    | 0        | 20       | 0       | 0            |
| 3   | C     | 13    | 0        | 20       | 0       | 0            |
| 3   | D     | 13    | 0        | 20       | 0       | 0            |
| 4   | A     | 200   | 0        | 316      | 12      | 0            |
| 4   | B     | 200   | 0        | 316      | 8       | 0            |
| 4   | C     | 200   | 0        | 316      | 10      | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4   | D     | 200   | 0        | 316      | 8       | 0            |
| 5   | A     | 2     | 0        | 0        | 0       | 0            |
| 6   | A     | 13    | 0        | 0        | 0       | 0            |
| 6   | B     | 13    | 0        | 0        | 0       | 0            |
| 6   | C     | 13    | 0        | 0        | 0       | 0            |
| 6   | D     | 13    | 0        | 0        | 0       | 0            |
| All | All   | 20390 | 0        | 21156    | 348     | 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 8.

All (348) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 2:C:804:Y01:CBH | 2:C:804:Y01:CAT | 1.78                     | 1.61              |
| 2:A:801:Y01:CBH | 2:A:801:Y01:CAT | 1.80                     | 1.60              |
| 2:A:810:Y01:CBH | 2:A:810:Y01:CAT | 1.79                     | 1.60              |
| 2:C:805:Y01:CAT | 2:C:805:Y01:CBH | 1.79                     | 1.60              |
| 2:B:804:Y01:CBH | 2:B:804:Y01:CAT | 1.78                     | 1.59              |
| 2:B:803:Y01:CBH | 2:B:803:Y01:CAT | 1.80                     | 1.58              |
| 2:D:805:Y01:CBH | 2:D:805:Y01:CAT | 1.78                     | 1.58              |
| 2:A:802:Y01:CBH | 2:A:802:Y01:CAT | 1.78                     | 1.58              |
| 2:C:803:Y01:CBH | 2:C:803:Y01:CAT | 1.80                     | 1.57              |
| 2:C:801:Y01:CBH | 2:C:801:Y01:CAT | 1.79                     | 1.57              |
| 2:B:801:Y01:CBH | 2:B:801:Y01:CAT | 1.79                     | 1.54              |
| 2:D:804:Y01:CBH | 2:D:804:Y01:CAT | 1.80                     | 1.54              |
| 2:B:801:Y01:CAZ | 2:B:801:Y01:CAV | 1.90                     | 1.48              |
| 2:B:804:Y01:CAZ | 2:B:804:Y01:CAV | 1.91                     | 1.48              |
| 2:C:803:Y01:CAZ | 2:C:803:Y01:CAV | 1.91                     | 1.48              |
| 2:B:803:Y01:CAZ | 2:B:803:Y01:CAV | 1.91                     | 1.48              |
| 2:D:805:Y01:CAV | 2:D:805:Y01:CAZ | 1.91                     | 1.48              |
| 2:C:805:Y01:CAZ | 2:C:805:Y01:CAV | 1.91                     | 1.48              |
| 2:C:801:Y01:CAZ | 2:C:801:Y01:CAV | 1.91                     | 1.47              |
| 2:C:804:Y01:CAV | 2:C:804:Y01:CAZ | 1.91                     | 1.47              |
| 2:A:802:Y01:CAZ | 2:A:802:Y01:CAV | 1.91                     | 1.47              |
| 2:A:801:Y01:CAV | 2:A:801:Y01:CAZ | 1.91                     | 1.47              |
| 2:A:810:Y01:CAZ | 2:A:810:Y01:CAV | 1.90                     | 1.46              |
| 2:D:804:Y01:CAZ | 2:D:804:Y01:CAV | 1.91                     | 1.44              |
| 2:D:805:Y01:CAT | 2:D:805:Y01:CAZ | 2.43                     | 0.97              |
| 2:C:804:Y01:CAT | 2:C:804:Y01:CAZ | 2.43                     | 0.96              |
| 2:A:802:Y01:CAT | 2:A:802:Y01:CAZ | 2.43                     | 0.95              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:804:Y01:CAT  | 2:B:804:Y01:CAZ  | 2.44                     | 0.94              |
| 2:D:804:Y01:CAT  | 2:D:804:Y01:CAZ  | 2.50                     | 0.90              |
| 2:A:810:Y01:CAT  | 2:A:810:Y01:CAZ  | 2.49                     | 0.90              |
| 2:A:801:Y01:CAT  | 2:A:801:Y01:CAZ  | 2.49                     | 0.90              |
| 2:B:803:Y01:CAT  | 2:B:803:Y01:CAZ  | 2.49                     | 0.89              |
| 2:C:805:Y01:CAT  | 2:C:805:Y01:CAZ  | 2.49                     | 0.89              |
| 2:C:801:Y01:CAT  | 2:C:801:Y01:CAZ  | 2.50                     | 0.89              |
| 2:B:801:Y01:CAT  | 2:B:801:Y01:CAZ  | 2.49                     | 0.88              |
| 2:C:803:Y01:CAT  | 2:C:803:Y01:CAZ  | 2.49                     | 0.87              |
| 2:C:804:Y01:CAT  | 2:C:804:Y01:CBF  | 2.61                     | 0.79              |
| 2:D:805:Y01:CAT  | 2:D:805:Y01:CBF  | 2.61                     | 0.77              |
| 2:A:802:Y01:CAT  | 2:A:802:Y01:CBF  | 2.61                     | 0.77              |
| 2:B:803:Y01:CAT  | 2:B:803:Y01:CBF  | 2.64                     | 0.76              |
| 2:B:804:Y01:CAT  | 2:B:804:Y01:CBF  | 2.61                     | 0.75              |
| 2:C:803:Y01:CAT  | 2:C:803:Y01:CBF  | 2.65                     | 0.74              |
| 2:A:801:Y01:CAT  | 2:A:801:Y01:CBF  | 2.65                     | 0.74              |
| 2:D:804:Y01:CAT  | 2:D:804:Y01:CBF  | 2.66                     | 0.74              |
| 2:C:805:Y01:CAT  | 2:C:805:Y01:CBF  | 2.66                     | 0.73              |
| 2:A:810:Y01:CAT  | 2:A:810:Y01:CBF  | 2.65                     | 0.73              |
| 2:B:801:Y01:CAT  | 2:B:801:Y01:CBF  | 2.65                     | 0.72              |
| 2:C:801:Y01:CAT  | 2:C:801:Y01:CBF  | 2.64                     | 0.72              |
| 2:C:805:Y01:CAT  | 2:C:805:Y01:CAD  | 2.72                     | 0.65              |
| 2:A:801:Y01:CAT  | 2:A:801:Y01:CAD  | 2.74                     | 0.65              |
| 2:A:810:Y01:CAV  | 2:A:810:Y01:CAI  | 2.74                     | 0.64              |
| 2:B:801:Y01:CAT  | 2:B:801:Y01:CAD  | 2.74                     | 0.64              |
| 2:D:805:Y01:CAT  | 2:D:805:Y01:CAD  | 2.74                     | 0.64              |
| 2:B:803:Y01:CAV  | 2:B:803:Y01:CAI  | 2.74                     | 0.64              |
| 2:C:804:Y01:CBH  | 2:C:804:Y01:CAV  | 2.67                     | 0.63              |
| 1:C:486:ILE:HD12 | 2:C:804:Y01:HAD3 | 1.80                     | 0.63              |
| 2:B:804:Y01:CAT  | 2:B:804:Y01:CAD  | 2.74                     | 0.62              |
| 1:A:486:ILE:HD12 | 2:A:802:Y01:HAD3 | 1.81                     | 0.62              |
| 2:A:801:Y01:CAV  | 2:A:801:Y01:CAI  | 2.75                     | 0.62              |
| 2:C:803:Y01:CAT  | 2:C:803:Y01:CAD  | 2.74                     | 0.62              |
| 2:D:804:Y01:CAV  | 2:D:804:Y01:CAI  | 2.74                     | 0.62              |
| 2:C:803:Y01:CAV  | 2:C:803:Y01:CAI  | 2.75                     | 0.62              |
| 2:A:802:Y01:CAT  | 2:A:802:Y01:CAD  | 2.74                     | 0.62              |
| 1:B:71:LYS:HB3   | 1:B:74:GLN:HB2   | 1.83                     | 0.61              |
| 1:A:71:LYS:HB3   | 1:A:74:GLN:HB2   | 1.82                     | 0.61              |
| 2:C:804:Y01:CAT  | 2:C:804:Y01:CAD  | 2.74                     | 0.61              |
| 2:A:802:Y01:CBH  | 2:A:802:Y01:CAV  | 2.67                     | 0.61              |
| 1:B:486:ILE:HD12 | 2:B:804:Y01:HAD3 | 1.82                     | 0.61              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:804:Y01:CAT  | 2:D:804:Y01:CAD  | 2.74                     | 0.61              |
| 1:C:71:LYS:HB3   | 1:C:74:GLN:HB2   | 1.83                     | 0.61              |
| 2:C:801:Y01:CAT  | 2:C:801:Y01:CAD  | 2.74                     | 0.61              |
| 2:B:801:Y01:CAV  | 2:B:801:Y01:CAI  | 2.76                     | 0.60              |
| 1:D:71:LYS:HB3   | 1:D:74:GLN:HB2   | 1.83                     | 0.60              |
| 2:A:810:Y01:HAO2 | 1:D:494:CYS:HB2  | 1.84                     | 0.59              |
| 1:D:486:ILE:HD12 | 2:D:805:Y01:HAD3 | 1.84                     | 0.59              |
| 1:A:492:ARG:HD2  | 1:D:474:MET:HB3  | 1.84                     | 0.59              |
| 2:A:810:Y01:CAT  | 2:A:810:Y01:CAD  | 2.75                     | 0.59              |
| 2:C:805:Y01:CAV  | 2:C:805:Y01:CAI  | 2.76                     | 0.59              |
| 2:A:801:Y01:CAT  | 2:A:801:Y01:CAS  | 2.81                     | 0.59              |
| 1:B:227:ASP:HA   | 1:B:231:PRO:HB3  | 1.85                     | 0.59              |
| 1:D:227:ASP:HA   | 1:D:231:PRO:HB3  | 1.85                     | 0.58              |
| 2:D:804:Y01:CAT  | 2:D:804:Y01:CAS  | 2.81                     | 0.58              |
| 2:B:803:Y01:CAT  | 2:B:803:Y01:CAS  | 2.81                     | 0.58              |
| 2:C:801:Y01:CAV  | 2:C:801:Y01:CAI  | 2.77                     | 0.58              |
| 1:C:452:VAL:HG13 | 1:C:453:PRO:HD3  | 1.86                     | 0.58              |
| 2:C:803:Y01:CAT  | 2:C:803:Y01:CAS  | 2.81                     | 0.58              |
| 1:A:227:ASP:HA   | 1:A:231:PRO:HB3  | 1.85                     | 0.58              |
| 2:D:805:Y01:CBH  | 2:D:805:Y01:CAV  | 2.67                     | 0.58              |
| 1:B:452:VAL:HG13 | 1:B:453:PRO:HD3  | 1.86                     | 0.58              |
| 1:A:452:VAL:HG13 | 1:A:453:PRO:HD3  | 1.86                     | 0.58              |
| 1:D:452:VAL:HG13 | 1:D:453:PRO:HD3  | 1.86                     | 0.58              |
| 1:B:53:ALA:O     | 1:B:91:ASN:ND2   | 2.38                     | 0.57              |
| 1:C:53:ALA:O     | 1:C:91:ASN:ND2   | 2.38                     | 0.57              |
| 1:C:227:ASP:HA   | 1:C:231:PRO:HB3  | 1.85                     | 0.57              |
| 1:D:53:ALA:O     | 1:D:91:ASN:ND2   | 2.38                     | 0.57              |
| 1:C:363:ARG:HB3  | 1:D:550:ASP:H    | 1.69                     | 0.57              |
| 2:A:802:Y01:CAV  | 2:A:802:Y01:CAI  | 2.79                     | 0.56              |
| 1:A:53:ALA:O     | 1:A:91:ASN:ND2   | 2.38                     | 0.56              |
| 2:B:803:Y01:CAT  | 2:B:803:Y01:CAD  | 2.74                     | 0.56              |
| 1:A:525:ASP:HB3  | 1:A:527:PRO:HD2  | 1.88                     | 0.56              |
| 1:B:494:CYS:HB2  | 2:C:801:Y01:HAO2 | 1.87                     | 0.55              |
| 1:B:525:ASP:HB3  | 1:B:527:PRO:HD2  | 1.88                     | 0.55              |
| 1:B:42:LYS:NZ    | 1:B:46:GLU:OE2   | 2.38                     | 0.55              |
| 1:A:42:LYS:NZ    | 1:A:46:GLU:OE2   | 2.38                     | 0.55              |
| 1:B:41:GLN:OE1   | 1:B:54:LYS:NZ    | 2.40                     | 0.55              |
| 2:B:804:Y01:CAV  | 2:B:804:Y01:CAI  | 2.79                     | 0.55              |
| 1:D:42:LYS:NZ    | 1:D:46:GLU:OE2   | 2.38                     | 0.55              |
| 1:C:525:ASP:HB3  | 1:C:527:PRO:HD2  | 1.88                     | 0.55              |
| 1:A:494:CYS:HB2  | 2:B:801:Y01:HAO2 | 1.89                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:41:GLN:OE1   | 1:C:54:LYS:NZ    | 2.40                     | 0.54              |
| 1:C:42:LYS:NZ    | 1:C:46:GLU:OE2   | 2.38                     | 0.54              |
| 2:B:804:Y01:CBH  | 2:B:804:Y01:CAV  | 2.67                     | 0.54              |
| 1:D:525:ASP:HB3  | 1:D:527:PRO:HD2  | 1.87                     | 0.54              |
| 1:A:41:GLN:OE1   | 1:A:54:LYS:NZ    | 2.40                     | 0.54              |
| 1:D:41:GLN:OE1   | 1:D:54:LYS:NZ    | 2.40                     | 0.54              |
| 1:A:632:ARG:NH2  | 1:B:34:ASP:OD1   | 2.41                     | 0.53              |
| 1:C:494:CYS:HB2  | 2:C:805:Y01:HAO2 | 1.90                     | 0.53              |
| 1:D:111:THR:HA   | 1:D:116:GLU:HA   | 1.91                     | 0.53              |
| 1:A:111:THR:HA   | 1:A:116:GLU:HA   | 1.91                     | 0.53              |
| 1:C:111:THR:HA   | 1:C:116:GLU:HA   | 1.91                     | 0.53              |
| 1:B:460:LEU:O    | 1:B:464:ASN:ND2  | 2.42                     | 0.52              |
| 1:A:460:LEU:O    | 1:A:464:ASN:ND2  | 2.42                     | 0.52              |
| 1:C:460:LEU:O    | 1:C:464:ASN:ND2  | 2.42                     | 0.52              |
| 2:C:804:Y01:CAV  | 2:C:804:Y01:CAI  | 2.79                     | 0.52              |
| 1:B:111:THR:HA   | 1:B:116:GLU:HA   | 1.91                     | 0.52              |
| 1:B:137:LEU:HD23 | 1:B:141:ALA:HB3  | 1.92                     | 0.52              |
| 1:A:190:ARG:NH2  | 1:A:226:GLY:O    | 2.43                     | 0.52              |
| 1:A:363:ARG:HB3  | 1:B:550:ASP:H    | 1.75                     | 0.52              |
| 1:D:190:ARG:NH2  | 1:D:226:GLY:O    | 2.43                     | 0.52              |
| 1:D:460:LEU:O    | 1:D:464:ASN:ND2  | 2.42                     | 0.52              |
| 1:D:45:TRP:HA    | 1:D:51:LEU:HD12  | 1.92                     | 0.51              |
| 1:B:190:ARG:NH2  | 1:B:226:GLY:O    | 2.43                     | 0.51              |
| 1:C:137:LEU:HD23 | 1:C:141:ALA:HB3  | 1.92                     | 0.51              |
| 1:C:190:ARG:NH2  | 1:C:226:GLY:O    | 2.43                     | 0.51              |
| 1:B:352:LEU:O    | 1:B:371:LYS:NZ   | 2.43                     | 0.51              |
| 1:A:137:LEU:HD23 | 1:A:141:ALA:HB3  | 1.92                     | 0.51              |
| 1:A:352:LEU:O    | 1:A:371:LYS:NZ   | 2.43                     | 0.51              |
| 1:C:632:ARG:NH2  | 1:D:34:ASP:OD1   | 2.43                     | 0.51              |
| 1:C:352:LEU:O    | 1:C:371:LYS:NZ   | 2.43                     | 0.51              |
| 1:B:45:TRP:HA    | 1:B:51:LEU:HD12  | 1.92                     | 0.51              |
| 1:D:352:LEU:O    | 1:D:371:LYS:NZ   | 2.43                     | 0.51              |
| 1:A:45:TRP:HA    | 1:A:51:LEU:HD12  | 1.92                     | 0.51              |
| 1:C:45:TRP:HA    | 1:C:51:LEU:HD12  | 1.92                     | 0.50              |
| 1:B:368:LEU:HD12 | 1:C:514:THR:HA   | 1.93                     | 0.50              |
| 2:C:801:Y01:CBH  | 2:C:801:Y01:CAV  | 2.69                     | 0.50              |
| 1:A:75:ARG:NH2   | 1:A:108:GLU:OE1  | 2.45                     | 0.50              |
| 1:D:137:LEU:HD23 | 1:D:141:ALA:HB3  | 1.92                     | 0.50              |
| 1:B:339:TYR:OH   | 1:B:392:THR:O    | 2.27                     | 0.50              |
| 2:B:804:Y01:CAT  | 2:B:804:Y01:CAS  | 2.89                     | 0.50              |
| 1:B:632:ARG:NH2  | 1:C:34:ASP:OD1   | 2.44                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:550:ASP:H    | 1:D:363:ARG:HB3  | 1.77                     | 0.49              |
| 2:D:805:Y01:CAT  | 2:D:805:Y01:CAS  | 2.91                     | 0.49              |
| 1:D:75:ARG:NH2   | 1:D:108:GLU:OE1  | 2.45                     | 0.49              |
| 1:C:75:ARG:NH2   | 1:C:108:GLU:OE1  | 2.45                     | 0.49              |
| 1:D:535:GLU:HG2  | 1:D:540:ILE:HD11 | 1.95                     | 0.49              |
| 2:D:805:Y01:CAV  | 2:D:805:Y01:CAI  | 2.79                     | 0.49              |
| 1:A:92:LEU:HG    | 1:A:96:MET:HE2   | 1.95                     | 0.49              |
| 1:B:75:ARG:NH2   | 1:B:108:GLU:OE1  | 2.45                     | 0.49              |
| 2:C:804:Y01:CAT  | 2:C:804:Y01:CAS  | 2.90                     | 0.49              |
| 1:D:466:MET:HA   | 4:D:801:POV:H21H | 1.95                     | 0.48              |
| 4:A:807:POV:H21A | 4:A:807:POV:H21D | 1.67                     | 0.48              |
| 1:C:92:LEU:HG    | 1:C:96:MET:HE2   | 1.95                     | 0.48              |
| 2:C:801:Y01:CAT  | 2:C:801:Y01:CAS  | 2.91                     | 0.48              |
| 1:A:535:GLU:HG2  | 1:A:540:ILE:HD11 | 1.95                     | 0.48              |
| 2:A:802:Y01:CAT  | 2:A:802:Y01:CAS  | 2.92                     | 0.48              |
| 1:C:489:ASP:OD2  | 1:C:581:THR:OG1  | 2.26                     | 0.48              |
| 2:A:810:Y01:CAT  | 2:A:810:Y01:CAS  | 2.92                     | 0.48              |
| 1:C:535:GLU:HG2  | 1:C:540:ILE:HD11 | 1.95                     | 0.48              |
| 1:B:474:MET:HB3  | 1:C:492:ARG:HD2  | 1.94                     | 0.48              |
| 2:B:801:Y01:CAT  | 2:B:801:Y01:CAS  | 2.91                     | 0.48              |
| 2:C:804:Y01:HBB  | 2:C:804:Y01:HAE2 | 1.72                     | 0.48              |
| 1:B:92:LEU:HG    | 1:B:96:MET:HE2   | 1.95                     | 0.48              |
| 1:A:339:TYR:OH   | 1:A:392:THR:O    | 2.27                     | 0.48              |
| 1:A:161:TYR:OH   | 1:A:193:ASP:OD2  | 2.29                     | 0.47              |
| 1:B:511:ILE:HG21 | 1:B:555:TYR:HB2  | 1.96                     | 0.47              |
| 1:B:535:GLU:HG2  | 1:B:540:ILE:HD11 | 1.95                     | 0.47              |
| 1:C:534:PHE:HE1  | 2:C:805:Y01:HBA  | 1.78                     | 0.47              |
| 1:D:511:ILE:HG21 | 1:D:555:TYR:HB2  | 1.96                     | 0.47              |
| 2:A:810:Y01:HBA  | 1:D:534:PHE:HE1  | 1.79                     | 0.47              |
| 2:B:804:Y01:HAE2 | 2:B:804:Y01:HBB  | 1.73                     | 0.47              |
| 1:C:161:TYR:OH   | 1:C:193:ASP:OD2  | 2.29                     | 0.47              |
| 1:B:489:ASP:OD2  | 1:B:581:THR:OG1  | 2.26                     | 0.47              |
| 1:D:92:LEU:HG    | 1:D:96:MET:HE2   | 1.95                     | 0.47              |
| 1:D:146:ARG:NH2  | 1:D:194:SER:OG   | 2.48                     | 0.47              |
| 1:C:146:ARG:NH2  | 1:C:194:SER:OG   | 2.48                     | 0.47              |
| 1:A:511:ILE:HG21 | 1:A:555:TYR:HB2  | 1.96                     | 0.47              |
| 1:C:121:LEU:HG   | 1:C:141:ALA:HB1  | 1.97                     | 0.47              |
| 1:A:121:LEU:HG   | 1:A:141:ALA:HB1  | 1.97                     | 0.47              |
| 1:A:488:GLY:O    | 1:A:492:ARG:NE   | 2.42                     | 0.47              |
| 1:B:146:ARG:NH2  | 1:B:194:SER:OG   | 2.48                     | 0.47              |
| 2:B:803:Y01:CAT  | 2:B:803:Y01:HAS1 | 2.44                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:511:ILE:HG21 | 1:C:555:TYR:HB2  | 1.96                     | 0.47              |
| 1:A:534:PHE:HE1  | 2:B:801:Y01:HBA  | 1.80                     | 0.46              |
| 1:B:363:ARG:HB3  | 1:C:550:ASP:H    | 1.79                     | 0.46              |
| 1:C:339:TYR:OH   | 1:C:392:THR:O    | 2.27                     | 0.46              |
| 1:A:34:ASP:OD1   | 1:D:632:ARG:NH2  | 2.49                     | 0.46              |
| 1:A:146:ARG:NH2  | 1:A:194:SER:OG   | 2.48                     | 0.46              |
| 2:A:801:Y01:CAT  | 2:A:801:Y01:HAS1 | 2.46                     | 0.46              |
| 1:B:83:LEU:HD23  | 1:B:98:LEU:HD22  | 1.97                     | 0.46              |
| 4:B:807:POV:H37A | 4:B:807:POV:H31A | 1.56                     | 0.46              |
| 1:C:474:MET:HB3  | 1:D:492:ARG:HD2  | 1.96                     | 0.46              |
| 1:D:43:ARG:NH1   | 1:D:46:GLU:OE2   | 2.49                     | 0.46              |
| 1:B:43:ARG:NH1   | 1:B:46:GLU:OE2   | 2.49                     | 0.46              |
| 1:D:436:VAL:HG13 | 4:D:810:POV:H21C | 1.97                     | 0.46              |
| 1:B:121:LEU:HG   | 1:B:141:ALA:HB1  | 1.97                     | 0.46              |
| 2:C:805:Y01:CAZ  | 2:C:805:Y01:CBC  | 2.84                     | 0.46              |
| 1:D:435:MET:HE1  | 4:D:807:POV:H31C | 1.98                     | 0.46              |
| 1:A:83:LEU:HD23  | 1:A:98:LEU:HD22  | 1.98                     | 0.46              |
| 1:C:466:MET:HA   | 4:C:811:POV:H21H | 1.97                     | 0.46              |
| 1:B:161:TYR:OH   | 1:B:193:ASP:OD2  | 2.29                     | 0.46              |
| 4:B:811:POV:H210 | 4:C:808:POV:H32A | 1.98                     | 0.46              |
| 1:C:84:HIS:HD2   | 1:C:120:ALA:HB2  | 1.81                     | 0.46              |
| 1:D:121:LEU:HG   | 1:D:141:ALA:HB1  | 1.97                     | 0.46              |
| 1:D:122:HIS:CD2  | 1:D:166:PRO:HG3  | 2.51                     | 0.46              |
| 1:A:84:HIS:HD2   | 1:A:120:ALA:HB2  | 1.81                     | 0.46              |
| 1:A:368:LEU:HD12 | 1:B:514:THR:HA   | 1.98                     | 0.46              |
| 1:B:122:HIS:CD2  | 1:B:166:PRO:HG3  | 2.51                     | 0.46              |
| 1:B:534:PHE:HE1  | 2:C:801:Y01:HBA  | 1.81                     | 0.46              |
| 1:C:43:ARG:NH1   | 1:C:46:GLU:OE2   | 2.49                     | 0.46              |
| 1:C:83:LEU:HD23  | 1:C:98:LEU:HD22  | 1.97                     | 0.46              |
| 1:C:122:HIS:CD2  | 1:C:166:PRO:HG3  | 2.51                     | 0.46              |
| 4:A:808:POV:H213 | 4:A:808:POV:H210 | 1.75                     | 0.45              |
| 1:D:84:HIS:HD2   | 1:D:120:ALA:HB2  | 1.81                     | 0.45              |
| 4:D:810:POV:H21A | 4:D:810:POV:H21D | 1.66                     | 0.45              |
| 1:B:435:MET:HE1  | 4:B:806:POV:H31C | 1.98                     | 0.45              |
| 2:C:805:Y01:CAT  | 2:C:805:Y01:CAS  | 2.94                     | 0.45              |
| 1:A:43:ARG:NH1   | 1:A:46:GLU:OE2   | 2.49                     | 0.45              |
| 1:B:84:HIS:HD2   | 1:B:120:ALA:HB2  | 1.81                     | 0.45              |
| 2:B:803:Y01:CBH  | 2:B:803:Y01:CAV  | 2.71                     | 0.45              |
| 1:B:497:MET:HE1  | 1:B:574:LEU:HD22 | 1.99                     | 0.45              |
| 1:C:363:ARG:NH1  | 1:D:548:ASN:O    | 2.50                     | 0.45              |
| 1:A:371:LYS:HG2  | 1:A:375:GLU:HG3  | 1.99                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:802:Y01:CBH  | 2:A:802:Y01:CAR  | 2.85                     | 0.45              |
| 1:C:451:VAL:O    | 1:C:455:SER:N    | 2.49                     | 0.45              |
| 1:C:497:MET:HE1  | 1:C:574:LEU:HD22 | 1.99                     | 0.45              |
| 1:A:514:THR:HA   | 1:D:368:LEU:HD12 | 1.99                     | 0.45              |
| 1:D:371:LYS:HG2  | 1:D:375:GLU:HG3  | 1.99                     | 0.45              |
| 1:C:308:LEU:HD11 | 1:C:598:VAL:HG21 | 1.99                     | 0.45              |
| 1:D:83:LEU:HD23  | 1:D:98:LEU:HD22  | 1.97                     | 0.45              |
| 2:A:802:Y01:HBB  | 2:A:802:Y01:HAE2 | 1.71                     | 0.45              |
| 1:D:451:VAL:O    | 1:D:455:SER:N    | 2.49                     | 0.45              |
| 1:A:257:GLN:NE2  | 1:A:310:GLN:OE1  | 2.49                     | 0.45              |
| 2:C:805:Y01:HAP2 | 2:C:805:Y01:HAO1 | 1.83                     | 0.45              |
| 1:A:308:LEU:HD11 | 1:A:598:VAL:HG21 | 1.98                     | 0.44              |
| 4:A:809:POV:H310 | 4:A:809:POV:H37  | 1.54                     | 0.44              |
| 2:B:801:Y01:HAP2 | 2:B:801:Y01:HAO1 | 1.84                     | 0.44              |
| 4:B:811:POV:H37  | 4:B:811:POV:H310 | 1.58                     | 0.44              |
| 1:D:308:LEU:HD11 | 1:D:598:VAL:HG21 | 1.98                     | 0.44              |
| 4:C:811:POV:H210 | 4:C:811:POV:H213 | 1.72                     | 0.44              |
| 4:A:811:POV:H26A | 1:D:456:PHE:HZ   | 1.82                     | 0.44              |
| 1:B:371:LYS:HG2  | 1:B:375:GLU:HG3  | 1.99                     | 0.44              |
| 1:A:474:MET:HB3  | 1:B:492:ARG:HD2  | 2.00                     | 0.44              |
| 1:B:308:LEU:HD11 | 1:B:598:VAL:HG21 | 1.98                     | 0.44              |
| 1:C:488:GLY:O    | 1:C:492:ARG:NE   | 2.42                     | 0.44              |
| 4:C:802:POV:H39  | 4:C:802:POV:H31C | 1.87                     | 0.44              |
| 1:D:543:GLY:HA2  | 1:D:544:PRO:HD3  | 1.85                     | 0.44              |
| 1:A:122:HIS:CD2  | 1:A:166:PRO:HG3  | 2.51                     | 0.44              |
| 1:B:466:MET:HA   | 4:B:810:POV:H21H | 1.99                     | 0.44              |
| 1:D:91:ASN:HB3   | 1:D:94:ALA:HB3   | 1.99                     | 0.44              |
| 2:A:802:Y01:HAO2 | 2:A:802:Y01:HAP1 | 1.62                     | 0.44              |
| 2:B:801:Y01:HBB  | 2:B:801:Y01:HAN2 | 1.70                     | 0.44              |
| 1:C:371:LYS:HG2  | 1:C:375:GLU:HG3  | 1.99                     | 0.44              |
| 1:D:161:TYR:OH   | 1:D:193:ASP:OD2  | 2.29                     | 0.44              |
| 1:D:352:LEU:HD23 | 1:D:368:LEU:HD13 | 2.00                     | 0.44              |
| 2:A:801:Y01:HAE2 | 2:A:801:Y01:HBB  | 1.75                     | 0.44              |
| 1:D:497:MET:HE1  | 1:D:574:LEU:HD22 | 1.99                     | 0.44              |
| 2:D:805:Y01:CBH  | 2:D:805:Y01:CAR  | 2.83                     | 0.44              |
| 1:A:436:VAL:HG13 | 4:A:807:POV:H21C | 2.00                     | 0.44              |
| 2:A:801:Y01:CAS  | 2:A:801:Y01:HAT2 | 2.47                     | 0.44              |
| 4:C:808:POV:H37A | 4:C:808:POV:H31A | 1.55                     | 0.43              |
| 1:D:339:TYR:OH   | 1:D:392:THR:O    | 2.27                     | 0.43              |
| 4:A:805:POV:H32A | 4:D:802:POV:H210 | 1.99                     | 0.43              |
| 2:B:803:Y01:CAS  | 2:B:803:Y01:HAT2 | 2.48                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:803:Y01:CAT  | 2:C:803:Y01:HAS1 | 2.47                     | 0.43              |
| 2:C:804:Y01:CBH  | 2:C:804:Y01:CAR  | 2.85                     | 0.43              |
| 1:A:497:MET:HE1  | 1:A:574:LEU:HD22 | 1.99                     | 0.43              |
| 2:B:801:Y01:CAZ  | 2:B:801:Y01:CBC  | 2.84                     | 0.43              |
| 1:C:91:ASN:HB3   | 1:C:94:ALA:HB3   | 1.99                     | 0.43              |
| 1:C:425:PHE:HB2  | 2:C:803:Y01:HAL2 | 2.00                     | 0.43              |
| 2:C:804:Y01:HAP1 | 2:C:804:Y01:HAO2 | 1.51                     | 0.43              |
| 1:C:352:LEU:HD23 | 1:C:368:LEU:HD13 | 2.00                     | 0.43              |
| 1:C:473:GLN:O    | 1:C:589:ARG:NH2  | 2.52                     | 0.43              |
| 4:C:808:POV:H211 | 4:C:808:POV:H28  | 1.91                     | 0.43              |
| 1:A:352:LEU:HD23 | 1:A:368:LEU:HD13 | 2.00                     | 0.43              |
| 2:B:804:Y01:CAS  | 2:B:804:Y01:HAT2 | 2.49                     | 0.43              |
| 1:B:91:ASN:HB3   | 1:B:94:ALA:HB3   | 1.99                     | 0.43              |
| 1:B:473:GLN:O    | 1:B:589:ARG:NH2  | 2.52                     | 0.43              |
| 4:D:802:POV:H310 | 4:D:802:POV:H37  | 1.62                     | 0.43              |
| 1:B:257:GLN:NE2  | 1:B:310:GLN:OE1  | 2.50                     | 0.43              |
| 2:B:804:Y01:HAP1 | 2:B:804:Y01:HAO2 | 1.53                     | 0.43              |
| 1:C:257:GLN:NE2  | 1:C:310:GLN:OE1  | 2.50                     | 0.43              |
| 1:C:271:GLY:H    | 1:D:127:ASN:ND2  | 2.17                     | 0.43              |
| 2:C:801:Y01:HBB  | 2:C:801:Y01:HAN2 | 1.74                     | 0.42              |
| 2:C:803:Y01:CAS  | 2:C:803:Y01:HAT2 | 2.49                     | 0.42              |
| 2:D:804:Y01:CAT  | 2:D:804:Y01:HAS1 | 2.49                     | 0.42              |
| 1:B:150:THR:O    | 1:B:158:ASN:ND2  | 2.53                     | 0.42              |
| 1:A:425:PHE:HB2  | 2:A:801:Y01:HAL2 | 2.02                     | 0.42              |
| 2:A:810:Y01:CAZ  | 2:A:810:Y01:CBC  | 2.84                     | 0.42              |
| 2:D:805:Y01:HAE2 | 2:D:805:Y01:HBB  | 1.72                     | 0.42              |
| 2:B:801:Y01:HBB  | 2:B:801:Y01:HAE2 | 1.81                     | 0.42              |
| 1:D:150:THR:O    | 1:D:158:ASN:ND2  | 2.53                     | 0.42              |
| 1:D:473:GLN:O    | 1:D:589:ARG:NH2  | 2.52                     | 0.42              |
| 1:A:91:ASN:HB3   | 1:A:94:ALA:HB3   | 1.99                     | 0.42              |
| 1:B:352:LEU:HD23 | 1:B:368:LEU:HD13 | 2.00                     | 0.42              |
| 2:C:805:Y01:CBH  | 2:C:805:Y01:CAV  | 2.69                     | 0.42              |
| 4:D:801:POV:H210 | 4:D:801:POV:H213 | 1.69                     | 0.42              |
| 1:A:271:GLY:H    | 1:B:127:ASN:ND2  | 2.18                     | 0.42              |
| 2:B:804:Y01:CBH  | 2:B:804:Y01:CAR  | 2.84                     | 0.42              |
| 1:C:436:VAL:HG13 | 4:C:810:POV:H21C | 2.02                     | 0.42              |
| 1:B:488:GLY:O    | 1:B:492:ARG:NE   | 2.42                     | 0.42              |
| 1:A:466:MET:HA   | 4:A:808:POV:H21H | 2.00                     | 0.42              |
| 2:C:801:Y01:HAP2 | 2:C:801:Y01:HAO1 | 1.81                     | 0.42              |
| 1:D:483:GLN:HB2  | 2:D:805:Y01:HBC  | 2.00                     | 0.42              |
| 1:D:488:GLY:O    | 1:D:492:ARG:NE   | 2.42                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:473:GLN:O    | 1:A:589:ARG:NH2  | 2.52                     | 0.41              |
| 1:C:271:GLY:HA3  | 1:D:126:VAL:HG12 | 2.01                     | 0.41              |
| 1:B:65:LEU:HD13  | 1:B:65:LEU:HA    | 1.94                     | 0.41              |
| 4:C:812:POV:H310 | 4:C:812:POV:H37  | 1.60                     | 0.41              |
| 4:A:805:POV:H37A | 4:A:805:POV:H31A | 1.56                     | 0.41              |
| 4:A:809:POV:H210 | 4:B:807:POV:H32A | 2.02                     | 0.41              |
| 1:C:435:MET:HE1  | 4:C:807:POV:H31C | 2.01                     | 0.41              |
| 1:A:150:THR:O    | 1:A:158:ASN:ND2  | 2.53                     | 0.41              |
| 2:C:805:Y01:HAE2 | 2:C:805:Y01:HBB  | 1.80                     | 0.41              |
| 1:A:543:GLY:HA2  | 1:A:544:PRO:HD3  | 1.85                     | 0.41              |
| 1:D:80:GLU:HG2   | 1:D:110:MET:HE2  | 2.03                     | 0.41              |
| 2:C:805:Y01:CBH  | 2:C:805:Y01:CAR  | 2.88                     | 0.41              |
| 2:D:804:Y01:HAE2 | 2:D:804:Y01:HBB  | 1.77                     | 0.41              |
| 4:D:808:POV:H37A | 4:D:808:POV:H31A | 1.58                     | 0.41              |
| 2:A:802:Y01:HAC2 | 2:A:802:Y01:HAJ2 | 1.94                     | 0.41              |
| 2:B:801:Y01:CBH  | 2:B:801:Y01:CAV  | 2.69                     | 0.41              |
| 2:B:803:Y01:HBB  | 2:B:803:Y01:HAE2 | 1.78                     | 0.41              |
| 4:B:809:POV:H21D | 4:B:809:POV:H21A | 1.67                     | 0.41              |
| 4:A:805:POV:H31H | 4:A:805:POV:H31D | 1.92                     | 0.41              |
| 4:B:810:POV:H210 | 4:B:810:POV:H213 | 1.73                     | 0.41              |
| 1:C:150:THR:O    | 1:C:158:ASN:ND2  | 2.53                     | 0.41              |
| 4:C:810:POV:H21D | 4:C:810:POV:H21A | 1.71                     | 0.41              |
| 1:D:257:GLN:NE2  | 1:D:310:GLN:OE1  | 2.50                     | 0.41              |
| 4:A:806:POV:H21B | 4:A:806:POV:H215 | 1.91                     | 0.41              |
| 1:B:371:LYS:HG2  | 1:B:372:LEU:H    | 1.86                     | 0.41              |
| 1:A:126:VAL:HG12 | 1:D:271:GLY:HA3  | 2.03                     | 0.40              |
| 1:A:371:LYS:HG2  | 1:A:372:LEU:H    | 1.86                     | 0.40              |
| 2:C:801:Y01:HAB1 | 2:C:801:Y01:HAJ1 | 1.94                     | 0.40              |
| 1:B:486:ILE:HA   | 1:B:490:LEU:HD12 | 2.03                     | 0.40              |
| 2:A:802:Y01:HAA1 | 2:A:802:Y01:HAJ1 | 1.92                     | 0.40              |
| 1:B:80:GLU:HG2   | 1:B:110:MET:HE2  | 2.03                     | 0.40              |
| 4:A:811:POV:H31C | 4:A:811:POV:H39  | 1.87                     | 0.40              |
| 1:C:466:MET:HG3  | 1:D:499:VAL:HG11 | 2.03                     | 0.40              |
| 1:D:371:LYS:HG2  | 1:D:372:LEU:H    | 1.86                     | 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     | 590/725 (81%)   | 541 (92%)  | 49 (8%)  | 0        | 100         | 100 |
| 1   | B     | 590/725 (81%)   | 540 (92%)  | 50 (8%)  | 0        | 100         | 100 |
| 1   | C     | 590/725 (81%)   | 541 (92%)  | 49 (8%)  | 0        | 100         | 100 |
| 1   | D     | 590/725 (81%)   | 541 (92%)  | 49 (8%)  | 0        | 100         | 100 |
| All | All   | 2360/2900 (81%) | 2163 (92%) | 197 (8%) | 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     | 516/633 (82%)   | 514 (100%)  | 2 (0%)   | 84          | 92 |
| 1   | B     | 516/633 (82%)   | 514 (100%)  | 2 (0%)   | 84          | 92 |
| 1   | C     | 516/633 (82%)   | 514 (100%)  | 2 (0%)   | 84          | 92 |
| 1   | D     | 516/633 (82%)   | 514 (100%)  | 2 (0%)   | 84          | 92 |
| All | All   | 2064/2532 (82%) | 2056 (100%) | 8 (0%)   | 81          | 92 |

All (8) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 365 | ASN  |
| 1   | A     | 452 | VAL  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 365 | ASN  |
| 1   | B     | 452 | VAL  |
| 1   | C     | 365 | ASN  |
| 1   | C     | 452 | VAL  |
| 1   | D     | 365 | ASN  |
| 1   | D     | 452 | VAL  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 31  | GLN  |
| 1   | A     | 37  | ASN  |
| 1   | A     | 122 | HIS  |
| 1   | A     | 127 | ASN  |
| 1   | A     | 131 | ASN  |
| 1   | A     | 197 | ASN  |
| 1   | A     | 206 | GLN  |
| 1   | A     | 258 | HIS  |
| 1   | A     | 464 | ASN  |
| 1   | A     | 637 | GLN  |
| 1   | B     | 31  | GLN  |
| 1   | B     | 37  | ASN  |
| 1   | B     | 122 | HIS  |
| 1   | B     | 127 | ASN  |
| 1   | B     | 131 | ASN  |
| 1   | B     | 197 | ASN  |
| 1   | B     | 206 | GLN  |
| 1   | B     | 258 | HIS  |
| 1   | B     | 464 | ASN  |
| 1   | B     | 637 | GLN  |
| 1   | C     | 37  | ASN  |
| 1   | C     | 122 | HIS  |
| 1   | C     | 127 | ASN  |
| 1   | C     | 131 | ASN  |
| 1   | C     | 197 | ASN  |
| 1   | C     | 206 | GLN  |
| 1   | C     | 258 | HIS  |
| 1   | C     | 464 | ASN  |
| 1   | C     | 637 | GLN  |
| 1   | D     | 31  | GLN  |
| 1   | D     | 37  | ASN  |
| 1   | D     | 122 | HIS  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 127 | ASN  |
| 1   | D     | 131 | ASN  |
| 1   | D     | 174 | ASN  |
| 1   | D     | 197 | ASN  |
| 1   | D     | 206 | GLN  |
| 1   | D     | 258 | HIS  |
| 1   | D     | 464 | ASN  |
| 1   | D     | 637 | GLN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 46 ligands modelled in this entry, 2 are monoatomic - leaving 44 for Mogul analysis.

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 | $\# Z  > 2$ |
| 4   | POV  | D     | 808 | -    | 51,51,51     | 1.07 | 2 (3%)      | 57,59,59    | 0.97 | 4 (7%)      |
| 4   | POV  | C     | 808 | -    | 51,51,51     | 1.07 | 2 (3%)      | 57,59,59    | 1.00 | 3 (5%)      |
| 4   | POV  | D     | 803 | -    | 51,51,51     | 1.11 | 5 (9%)      | 57,59,59    | 0.91 | 3 (5%)      |
| 2   | Y01  | B     | 801 | -    | 38,38,38     | 7.76 | 21 (55%)    | 57,57,57    | 3.48 | 26 (45%)    |
| 3   | PCW  | B     | 805 | -    | 12,12,53     | 0.80 | 0           | 11,11,61    | 0.49 | 0           |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 2   | Y01  | A     | 801 | -    | 38,38,38     | 7.79 | 20 (52%) | 57,57,57    | 3.13 | 26 (45%) |
| 2   | Y01  | C     | 804 | -    | 38,38,38     | 7.73 | 22 (57%) | 57,57,57    | 3.46 | 24 (42%) |
| 2   | Y01  | A     | 802 | -    | 38,38,38     | 7.74 | 22 (57%) | 57,57,57    | 3.38 | 25 (43%) |
| 4   | POV  | C     | 802 | -    | 51,51,51     | 1.11 | 5 (9%)   | 57,59,59    | 0.90 | 3 (5%)   |
| 4   | POV  | D     | 802 | -    | 29,29,51     | 0.92 | 1 (3%)   | 28,28,59    | 0.73 | 1 (3%)   |
| 4   | POV  | D     | 807 | -    | 12,12,51     | 0.65 | 0        | 11,11,59    | 0.43 | 0        |
| 4   | POV  | A     | 808 | -    | 18,18,51     | 0.73 | 0        | 16,16,59    | 0.40 | 0        |
| 4   | POV  | A     | 806 | -    | 13,13,51     | 0.73 | 0        | 12,12,59    | 0.36 | 0        |
| 2   | Y01  | A     | 810 | -    | 38,38,38     | 7.75 | 21 (55%) | 57,57,57    | 3.52 | 24 (42%) |
| 4   | POV  | D     | 809 | -    | 13,13,51     | 0.72 | 0        | 12,12,59    | 0.36 | 0        |
| 2   | Y01  | C     | 803 | -    | 38,38,38     | 7.79 | 20 (52%) | 57,57,57    | 3.12 | 26 (45%) |
| 4   | POV  | B     | 806 | -    | 12,12,51     | 0.67 | 0        | 11,11,59    | 0.39 | 0        |
| 2   | Y01  | C     | 801 | -    | 38,38,38     | 7.77 | 21 (55%) | 57,57,57    | 3.48 | 26 (45%) |
| 4   | POV  | A     | 805 | -    | 51,51,51     | 1.07 | 2 (3%)   | 57,59,59    | 0.97 | 4 (7%)   |
| 2   | Y01  | C     | 805 | -    | 38,38,38     | 7.77 | 21 (55%) | 57,57,57    | 3.57 | 26 (45%) |
| 4   | POV  | B     | 802 | -    | 51,51,51     | 1.10 | 3 (5%)   | 57,59,59    | 0.90 | 3 (5%)   |
| 2   | Y01  | B     | 803 | -    | 38,38,38     | 7.80 | 20 (52%) | 57,57,57    | 3.13 | 26 (45%) |
| 4   | POV  | A     | 811 | -    | 51,51,51     | 1.11 | 5 (9%)   | 57,59,59    | 0.90 | 3 (5%)   |
| 4   | POV  | B     | 807 | -    | 51,51,51     | 1.07 | 2 (3%)   | 57,59,59    | 0.99 | 3 (5%)   |
| 4   | POV  | C     | 807 | -    | 12,12,51     | 0.66 | 0        | 11,11,59    | 0.42 | 0        |
| 4   | POV  | C     | 812 | -    | 29,29,51     | 0.93 | 1 (3%)   | 28,28,59    | 0.73 | 1 (3%)   |
| 3   | PCW  | A     | 803 | -    | 12,12,53     | 0.81 | 0        | 11,11,61    | 0.50 | 0        |
| 4   | POV  | C     | 809 | -    | 13,13,51     | 0.73 | 0        | 12,12,59    | 0.36 | 0        |
| 2   | Y01  | D     | 805 | -    | 38,38,38     | 7.72 | 21 (55%) | 57,57,57    | 3.48 | 24 (42%) |
| 4   | POV  | B     | 810 | -    | 18,18,51     | 0.73 | 0        | 16,16,59    | 0.40 | 0        |
| 4   | POV  | D     | 801 | -    | 18,18,51     | 0.72 | 0        | 16,16,59    | 0.41 | 0        |
| 3   | PCW  | D     | 806 | -    | 12,12,53     | 0.81 | 0        | 11,11,61    | 0.49 | 0        |
| 4   | POV  | B     | 811 | -    | 29,29,51     | 0.93 | 1 (3%)   | 28,28,59    | 0.72 | 1 (3%)   |
| 2   | Y01  | D     | 804 | -    | 38,38,38     | 7.81 | 20 (52%) | 57,57,57    | 3.15 | 27 (47%) |
| 4   | POV  | C     | 810 | -    | 17,17,51     | 1.51 | 2 (11%)  | 17,17,59    | 0.89 | 0        |
| 4   | POV  | B     | 808 | -    | 13,13,51     | 0.73 | 0        | 12,12,59    | 0.35 | 0        |
| 4   | POV  | B     | 809 | -    | 17,17,51     | 1.51 | 2 (11%)  | 17,17,59    | 0.90 | 0        |
| 2   | Y01  | B     | 804 | -    | 38,38,38     | 7.74 | 22 (57%) | 57,57,57    | 3.48 | 24 (42%) |
| 4   | POV  | A     | 809 | -    | 29,29,51     | 0.93 | 1 (3%)   | 28,28,59    | 0.72 | 1 (3%)   |
| 4   | POV  | D     | 810 | -    | 17,17,51     | 1.51 | 2 (11%)  | 17,17,59    | 0.89 | 0        |
| 4   | POV  | A     | 807 | -    | 17,17,51     | 1.50 | 2 (11%)  | 17,17,59    | 0.90 | 0        |
| 4   | POV  | C     | 811 | -    | 18,18,51     | 0.72 | 0        | 16,16,59    | 0.41 | 0        |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | PCW  | C     | 806 | -    | 12,12,53     | 0.81 | 0        | 11,11,61    | 0.50 | 0        |
| 4   | POV  | A     | 804 | -    | 12,12,51     | 0.65 | 0        | 11,11,59    | 0.44 | 0        |

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

| Mol | Type | Chain | Res | Link | Chirals   | Torsions    | Rings   |
|-----|------|-------|-----|------|-----------|-------------|---------|
| 4   | POV  | D     | 808 | -    | -         | 28/55/55/55 | -       |
| 4   | POV  | C     | 808 | -    | -         | 26/55/55/55 | -       |
| 4   | POV  | D     | 803 | -    | -         | 24/55/55/55 | -       |
| 2   | Y01  | B     | 801 | -    | 4/4/12/13 | 16/19/77/77 | 0/4/4/4 |
| 3   | PCW  | B     | 805 | -    | -         | 4/10/10/57  | -       |
| 2   | Y01  | A     | 801 | -    | 4/4/12/13 | 12/19/77/77 | 0/4/4/4 |
| 2   | Y01  | C     | 804 | -    | 4/4/12/13 | 12/19/77/77 | 0/4/4/4 |
| 2   | Y01  | A     | 802 | -    | 4/4/12/13 | 12/19/77/77 | 0/4/4/4 |
| 4   | POV  | C     | 802 | -    | -         | 23/55/55/55 | -       |
| 4   | POV  | D     | 802 | -    | -         | 12/26/26/55 | -       |
| 4   | POV  | D     | 807 | -    | -         | 5/10/10/55  | -       |
| 4   | POV  | A     | 808 | -    | -         | 10/14/14/55 | -       |
| 4   | POV  | A     | 806 | -    | -         | 5/11/11/55  | -       |
| 2   | Y01  | A     | 810 | -    | 4/4/12/13 | 14/19/77/77 | 0/4/4/4 |
| 4   | POV  | D     | 809 | -    | -         | 5/11/11/55  | -       |
| 2   | Y01  | C     | 803 | -    | 4/4/12/13 | 12/19/77/77 | 0/4/4/4 |
| 4   | POV  | B     | 806 | -    | -         | 5/10/10/55  | -       |
| 2   | Y01  | C     | 801 | -    | 4/4/12/13 | 14/19/77/77 | 0/4/4/4 |
| 4   | POV  | A     | 805 | -    | -         | 29/55/55/55 | -       |
| 2   | Y01  | C     | 805 | -    | 4/4/12/13 | 14/19/77/77 | 0/4/4/4 |
| 4   | POV  | B     | 802 | -    | -         | 22/55/55/55 | -       |
| 2   | Y01  | B     | 803 | -    | 4/4/12/13 | 12/19/77/77 | 0/4/4/4 |
| 4   | POV  | A     | 811 | -    | -         | 24/55/55/55 | -       |
| 4   | POV  | B     | 807 | -    | -         | 28/55/55/55 | -       |
| 4   | POV  | C     | 807 | -    | -         | 5/10/10/55  | -       |
| 4   | POV  | C     | 812 | -    | -         | 12/26/26/55 | -       |
| 3   | PCW  | A     | 803 | -    | -         | 3/10/10/57  | -       |

Continued on next page...

*Continued from previous page...*

| Mol | Type | Chain | Res | Link | Chirals   | Torsions    | Rings   |
|-----|------|-------|-----|------|-----------|-------------|---------|
| 4   | POV  | C     | 809 | -    | -         | 5/11/11/55  | -       |
| 2   | Y01  | D     | 805 | -    | 4/4/12/13 | 12/19/77/77 | 0/4/4/4 |
| 4   | POV  | B     | 810 | -    | -         | 10/14/14/55 | -       |
| 4   | POV  | D     | 801 | -    | -         | 10/14/14/55 | -       |
| 3   | PCW  | D     | 806 | -    | -         | 4/10/10/57  | -       |
| 4   | POV  | B     | 811 | -    | -         | 13/26/26/55 | -       |
| 2   | Y01  | D     | 804 | -    | 4/4/12/13 | 14/19/77/77 | 0/4/4/4 |
| 4   | POV  | C     | 810 | -    | -         | 7/15/15/55  | -       |
| 4   | POV  | B     | 808 | -    | -         | 6/11/11/55  | -       |
| 4   | POV  | B     | 809 | -    | -         | 7/15/15/55  | -       |
| 2   | Y01  | B     | 804 | -    | 4/4/12/13 | 12/19/77/77 | 0/4/4/4 |
| 4   | POV  | A     | 809 | -    | -         | 12/26/26/55 | -       |
| 4   | POV  | D     | 810 | -    | -         | 7/15/15/55  | -       |
| 4   | POV  | A     | 807 | -    | -         | 7/15/15/55  | -       |
| 4   | POV  | C     | 811 | -    | -         | 10/14/14/55 | -       |
| 3   | PCW  | C     | 806 | -    | -         | 3/10/10/57  | -       |
| 4   | POV  | A     | 804 | -    | -         | 5/10/10/55  | -       |

All (289) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 2   | D     | 804 | Y01  | CAK-CBD | -22.52 | 1.16        | 1.53     |
| 2   | C     | 805 | Y01  | CAK-CBD | -22.45 | 1.16        | 1.53     |
| 2   | C     | 801 | Y01  | CAK-CBD | -22.41 | 1.16        | 1.53     |
| 2   | A     | 801 | Y01  | CAK-CBD | -22.41 | 1.16        | 1.53     |
| 2   | C     | 803 | Y01  | CAK-CBD | -22.40 | 1.16        | 1.53     |
| 2   | B     | 803 | Y01  | CAK-CBD | -22.40 | 1.16        | 1.53     |
| 2   | B     | 801 | Y01  | CAK-CBD | -22.37 | 1.17        | 1.53     |
| 2   | A     | 810 | Y01  | CAK-CBD | -22.30 | 1.17        | 1.53     |
| 2   | A     | 802 | Y01  | CAK-CBD | -21.89 | 1.17        | 1.53     |
| 2   | B     | 804 | Y01  | CAK-CBD | -21.82 | 1.17        | 1.53     |
| 2   | D     | 805 | Y01  | CAK-CBD | -21.81 | 1.17        | 1.53     |
| 2   | C     | 804 | Y01  | CAK-CBD | -21.81 | 1.17        | 1.53     |
| 2   | D     | 804 | Y01  | CBD-CBG | -20.96 | 1.14        | 1.53     |
| 2   | B     | 803 | Y01  | CBD-CBG | -20.87 | 1.14        | 1.53     |
| 2   | C     | 803 | Y01  | CBD-CBG | -20.83 | 1.14        | 1.53     |
| 2   | A     | 801 | Y01  | CBD-CBG | -20.81 | 1.14        | 1.53     |
| 2   | C     | 805 | Y01  | CBD-CBG | -20.54 | 1.15        | 1.53     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 2   | C     | 801 | Y01  | CBD-CBG | -20.53 | 1.15        | 1.53     |
| 2   | B     | 801 | Y01  | CBD-CBG | -20.50 | 1.15        | 1.53     |
| 2   | A     | 810 | Y01  | CBD-CBG | -20.37 | 1.15        | 1.53     |
| 2   | A     | 802 | Y01  | CBD-CBG | -20.35 | 1.15        | 1.53     |
| 2   | B     | 804 | Y01  | CBD-CBG | -20.17 | 1.15        | 1.53     |
| 2   | C     | 804 | Y01  | CBD-CBG | -20.11 | 1.15        | 1.53     |
| 2   | D     | 805 | Y01  | CBD-CBG | -20.09 | 1.15        | 1.53     |
| 2   | B     | 804 | Y01  | CAV-CAZ | 19.98  | 1.91        | 1.51     |
| 2   | D     | 805 | Y01  | CAV-CAZ | 19.97  | 1.91        | 1.51     |
| 2   | C     | 804 | Y01  | CAV-CAZ | 19.90  | 1.91        | 1.51     |
| 2   | A     | 801 | Y01  | CAV-CAZ | 19.87  | 1.91        | 1.51     |
| 2   | B     | 803 | Y01  | CAV-CAZ | 19.86  | 1.91        | 1.51     |
| 2   | C     | 803 | Y01  | CAV-CAZ | 19.83  | 1.91        | 1.51     |
| 2   | A     | 802 | Y01  | CAV-CAZ | 19.81  | 1.91        | 1.51     |
| 2   | D     | 804 | Y01  | CAV-CAZ | 19.69  | 1.91        | 1.51     |
| 2   | C     | 801 | Y01  | CAV-CAZ | 19.63  | 1.91        | 1.51     |
| 2   | C     | 805 | Y01  | CAV-CAZ | 19.62  | 1.91        | 1.51     |
| 2   | B     | 801 | Y01  | CAV-CAZ | 19.56  | 1.90        | 1.51     |
| 2   | A     | 810 | Y01  | CAV-CAZ | 19.44  | 1.90        | 1.51     |
| 2   | C     | 804 | Y01  | CBH-CAZ | -16.49 | 1.21        | 1.52     |
| 2   | B     | 804 | Y01  | CBH-CAZ | -16.47 | 1.21        | 1.52     |
| 2   | A     | 802 | Y01  | CBH-CAZ | -16.38 | 1.21        | 1.52     |
| 2   | D     | 805 | Y01  | CBH-CAZ | -16.38 | 1.21        | 1.52     |
| 2   | A     | 810 | Y01  | CBH-CAZ | -15.69 | 1.23        | 1.52     |
| 2   | B     | 801 | Y01  | CBH-CAZ | -15.62 | 1.23        | 1.52     |
| 2   | C     | 801 | Y01  | CBH-CAZ | -15.62 | 1.23        | 1.52     |
| 2   | C     | 805 | Y01  | CBH-CAZ | -15.59 | 1.23        | 1.52     |
| 2   | B     | 803 | Y01  | CBH-CAZ | -15.57 | 1.23        | 1.52     |
| 2   | D     | 804 | Y01  | CBH-CAZ | -15.55 | 1.23        | 1.52     |
| 2   | A     | 801 | Y01  | CBH-CAZ | -15.52 | 1.23        | 1.52     |
| 2   | C     | 803 | Y01  | CBH-CAZ | -15.49 | 1.23        | 1.52     |
| 2   | D     | 804 | Y01  | CAT-CBH | 14.32  | 1.80        | 1.54     |
| 2   | C     | 803 | Y01  | CAT-CBH | 14.22  | 1.80        | 1.54     |
| 2   | B     | 803 | Y01  | CAT-CBH | 14.16  | 1.80        | 1.54     |
| 2   | A     | 801 | Y01  | CAT-CBH | 14.15  | 1.80        | 1.54     |
| 2   | A     | 810 | Y01  | CAT-CBH | 13.99  | 1.79        | 1.54     |
| 2   | B     | 801 | Y01  | CAT-CBH | 13.96  | 1.79        | 1.54     |
| 2   | C     | 801 | Y01  | CAT-CBH | 13.88  | 1.79        | 1.54     |
| 2   | C     | 805 | Y01  | CAT-CBH | 13.86  | 1.79        | 1.54     |
| 2   | D     | 804 | Y01  | CAU-CBI | -13.48 | 1.30        | 1.54     |
| 2   | A     | 801 | Y01  | CAU-CBI | -13.37 | 1.30        | 1.54     |
| 2   | B     | 803 | Y01  | CAU-CBI | -13.36 | 1.30        | 1.54     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 2   | C     | 803 | Y01  | CAU-CBI | -13.34 | 1.30        | 1.54     |
| 2   | B     | 804 | Y01  | CAT-CBH | 13.27  | 1.78        | 1.54     |
| 2   | B     | 804 | Y01  | CAU-CBI | -13.25 | 1.31        | 1.54     |
| 2   | C     | 804 | Y01  | CAU-CBI | -13.25 | 1.31        | 1.54     |
| 2   | A     | 802 | Y01  | CAU-CBI | -13.23 | 1.31        | 1.54     |
| 2   | C     | 804 | Y01  | CAT-CBH | 13.23  | 1.78        | 1.54     |
| 2   | D     | 805 | Y01  | CAU-CBI | -13.21 | 1.31        | 1.54     |
| 2   | A     | 802 | Y01  | CAT-CBH | 13.09  | 1.78        | 1.54     |
| 2   | D     | 805 | Y01  | CAT-CBH | 13.07  | 1.78        | 1.54     |
| 2   | B     | 801 | Y01  | CAU-CBI | -12.96 | 1.31        | 1.54     |
| 2   | C     | 801 | Y01  | CAU-CBI | -12.96 | 1.31        | 1.54     |
| 2   | C     | 805 | Y01  | CAU-CBI | -12.93 | 1.31        | 1.54     |
| 2   | A     | 810 | Y01  | CAU-CBI | -12.91 | 1.31        | 1.54     |
| 2   | B     | 801 | Y01  | CBI-CBE | 8.67   | 1.70        | 1.55     |
| 2   | C     | 801 | Y01  | CBI-CBE | 8.64   | 1.70        | 1.55     |
| 2   | A     | 810 | Y01  | CBI-CBE | 8.58   | 1.70        | 1.55     |
| 2   | C     | 805 | Y01  | CBI-CBE | 8.54   | 1.70        | 1.55     |
| 2   | C     | 804 | Y01  | CBI-CBE | 8.25   | 1.70        | 1.55     |
| 2   | D     | 805 | Y01  | CBI-CBE | 8.25   | 1.70        | 1.55     |
| 2   | A     | 802 | Y01  | CBI-CBE | 8.24   | 1.70        | 1.55     |
| 2   | B     | 804 | Y01  | CBI-CBE | 8.23   | 1.70        | 1.55     |
| 2   | C     | 803 | Y01  | CBI-CBE | 8.22   | 1.70        | 1.55     |
| 2   | A     | 801 | Y01  | CBI-CBE | 8.21   | 1.70        | 1.55     |
| 2   | D     | 804 | Y01  | CBI-CBE | 8.19   | 1.70        | 1.55     |
| 2   | B     | 803 | Y01  | CBI-CBE | 8.15   | 1.70        | 1.55     |
| 2   | C     | 804 | Y01  | CAQ-CAP | 7.28   | 1.73        | 1.54     |
| 2   | B     | 804 | Y01  | CAQ-CAP | 7.27   | 1.73        | 1.54     |
| 2   | A     | 810 | Y01  | CBI-CBG | 7.27   | 1.68        | 1.55     |
| 2   | D     | 805 | Y01  | CAQ-CAP | 7.24   | 1.73        | 1.54     |
| 2   | C     | 801 | Y01  | CBI-CBG | 7.20   | 1.68        | 1.55     |
| 2   | B     | 801 | Y01  | CBI-CBG | 7.18   | 1.68        | 1.55     |
| 2   | A     | 802 | Y01  | CAQ-CAP | 7.13   | 1.73        | 1.54     |
| 2   | C     | 805 | Y01  | CBI-CBG | 7.08   | 1.68        | 1.55     |
| 2   | D     | 804 | Y01  | CAQ-CAP | 6.93   | 1.72        | 1.54     |
| 2   | C     | 803 | Y01  | CAQ-CAP | 6.89   | 1.72        | 1.54     |
| 2   | A     | 801 | Y01  | CAQ-CAP | 6.88   | 1.72        | 1.54     |
| 2   | B     | 803 | Y01  | CAQ-CAP | 6.86   | 1.72        | 1.54     |
| 2   | A     | 802 | Y01  | CBI-CBG | 6.86   | 1.67        | 1.55     |
| 2   | D     | 805 | Y01  | CBI-CBG | 6.76   | 1.67        | 1.55     |
| 2   | C     | 805 | Y01  | CAQ-CAP | 6.75   | 1.72        | 1.54     |
| 2   | B     | 804 | Y01  | CBI-CBG | 6.72   | 1.67        | 1.55     |
| 2   | C     | 804 | Y01  | CBI-CBG | 6.72   | 1.67        | 1.55     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | B     | 801 | Y01  | CAQ-CAP | 6.71  | 1.72        | 1.54     |
| 2   | C     | 801 | Y01  | CAQ-CAP | 6.71  | 1.72        | 1.54     |
| 2   | A     | 810 | Y01  | CAQ-CAP | 6.67  | 1.72        | 1.54     |
| 2   | A     | 801 | Y01  | CBI-CBG | 6.62  | 1.67        | 1.55     |
| 2   | B     | 803 | Y01  | CBI-CBG | 6.58  | 1.67        | 1.55     |
| 2   | C     | 803 | Y01  | CBI-CBG | 6.57  | 1.67        | 1.55     |
| 2   | D     | 804 | Y01  | CBI-CBG | 6.47  | 1.66        | 1.55     |
| 2   | A     | 801 | Y01  | CAQ-CBG | 5.49  | 1.65        | 1.54     |
| 2   | B     | 803 | Y01  | CAQ-CBG | 5.49  | 1.65        | 1.54     |
| 2   | D     | 805 | Y01  | CAQ-CBG | 5.48  | 1.65        | 1.54     |
| 2   | C     | 803 | Y01  | CAQ-CBG | 5.47  | 1.65        | 1.54     |
| 2   | C     | 804 | Y01  | CAQ-CBG | 5.46  | 1.65        | 1.54     |
| 2   | A     | 802 | Y01  | CAQ-CBG | 5.43  | 1.65        | 1.54     |
| 2   | D     | 804 | Y01  | CAQ-CBG | 5.41  | 1.65        | 1.54     |
| 2   | B     | 804 | Y01  | CAQ-CBG | 5.40  | 1.65        | 1.54     |
| 2   | B     | 803 | Y01  | CAU-CAS | -5.33 | 1.42        | 1.53     |
| 2   | C     | 803 | Y01  | CAU-CAS | -5.31 | 1.42        | 1.53     |
| 2   | A     | 810 | Y01  | CAQ-CBG | 5.30  | 1.65        | 1.54     |
| 2   | A     | 801 | Y01  | CAU-CAS | -5.29 | 1.42        | 1.53     |
| 2   | D     | 804 | Y01  | CAU-CAS | -5.26 | 1.42        | 1.53     |
| 2   | B     | 801 | Y01  | CAQ-CBG | 5.23  | 1.65        | 1.54     |
| 2   | C     | 805 | Y01  | CAQ-CBG | 5.21  | 1.65        | 1.54     |
| 2   | C     | 801 | Y01  | CAQ-CBG | 5.18  | 1.65        | 1.54     |
| 2   | A     | 802 | Y01  | CAI-CAZ | 5.04  | 1.43        | 1.33     |
| 2   | C     | 805 | Y01  | CAI-CAZ | 5.03  | 1.43        | 1.33     |
| 2   | C     | 801 | Y01  | CAI-CAZ | 5.03  | 1.43        | 1.33     |
| 2   | C     | 804 | Y01  | CAI-CAZ | 5.02  | 1.43        | 1.33     |
| 2   | B     | 804 | Y01  | CAI-CAZ | 5.02  | 1.43        | 1.33     |
| 2   | B     | 803 | Y01  | CAI-CAZ | 5.01  | 1.43        | 1.33     |
| 2   | A     | 801 | Y01  | CAI-CAZ | 5.00  | 1.43        | 1.33     |
| 2   | D     | 805 | Y01  | CAI-CAZ | 4.96  | 1.43        | 1.33     |
| 2   | C     | 803 | Y01  | CAI-CAZ | 4.95  | 1.43        | 1.33     |
| 2   | C     | 804 | Y01  | CAU-CAS | -4.93 | 1.43        | 1.53     |
| 2   | B     | 801 | Y01  | CAI-CAZ | 4.92  | 1.43        | 1.33     |
| 2   | A     | 802 | Y01  | CAU-CAS | -4.91 | 1.43        | 1.53     |
| 2   | B     | 804 | Y01  | CAU-CAS | -4.89 | 1.43        | 1.53     |
| 2   | D     | 804 | Y01  | CAI-CAZ | 4.87  | 1.43        | 1.33     |
| 2   | D     | 805 | Y01  | CAU-CAS | -4.85 | 1.43        | 1.53     |
| 2   | A     | 810 | Y01  | CAI-CAZ | 4.82  | 1.42        | 1.33     |
| 2   | C     | 805 | Y01  | CAU-CAS | -4.80 | 1.43        | 1.53     |
| 2   | B     | 801 | Y01  | CAU-CAS | -4.72 | 1.44        | 1.53     |
| 2   | A     | 810 | Y01  | CAU-CAS | -4.70 | 1.44        | 1.53     |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2   | C     | 801 | Y01  | CAU-CAS  | -4.68 | 1.44        | 1.53     |
| 2   | B     | 803 | Y01  | CBB-CBE  | -4.67 | 1.46        | 1.54     |
| 2   | C     | 803 | Y01  | CBB-CBE  | -4.57 | 1.46        | 1.54     |
| 2   | A     | 801 | Y01  | CBB-CBE  | -4.55 | 1.46        | 1.54     |
| 2   | D     | 804 | Y01  | CBB-CBE  | -4.50 | 1.46        | 1.54     |
| 2   | C     | 805 | Y01  | OAW-CAY  | 4.40  | 1.46        | 1.34     |
| 2   | C     | 804 | Y01  | CBB-CBE  | -4.38 | 1.46        | 1.54     |
| 2   | A     | 810 | Y01  | OAW-CAY  | 4.38  | 1.46        | 1.34     |
| 2   | C     | 805 | Y01  | CAT-CAR  | 4.38  | 1.62        | 1.53     |
| 2   | B     | 804 | Y01  | CBH-CBF  | -4.38 | 1.49        | 1.56     |
| 2   | B     | 804 | Y01  | CBB-CBE  | -4.38 | 1.46        | 1.54     |
| 2   | A     | 802 | Y01  | CBB-CBE  | -4.37 | 1.46        | 1.54     |
| 2   | B     | 801 | Y01  | OAW-CAY  | 4.36  | 1.46        | 1.34     |
| 2   | D     | 805 | Y01  | CBB-CBE  | -4.34 | 1.47        | 1.54     |
| 2   | A     | 810 | Y01  | CAT-CAR  | 4.34  | 1.62        | 1.53     |
| 2   | C     | 804 | Y01  | CBH-CBF  | -4.32 | 1.49        | 1.56     |
| 2   | C     | 801 | Y01  | OAW-CAY  | 4.32  | 1.46        | 1.34     |
| 2   | C     | 805 | Y01  | CBH-CBF  | -4.32 | 1.49        | 1.56     |
| 2   | B     | 801 | Y01  | CAT-CAR  | 4.28  | 1.61        | 1.53     |
| 2   | C     | 801 | Y01  | CBB-CBE  | -4.27 | 1.47        | 1.54     |
| 2   | D     | 805 | Y01  | CBH-CBF  | -4.27 | 1.49        | 1.56     |
| 2   | A     | 802 | Y01  | CBH-CBF  | -4.24 | 1.49        | 1.56     |
| 2   | C     | 801 | Y01  | CBH-CBF  | -4.23 | 1.49        | 1.56     |
| 4   | B     | 809 | POV  | C29-C210 | 4.23  | 1.55        | 1.31     |
| 2   | B     | 801 | Y01  | CBB-CBE  | -4.22 | 1.47        | 1.54     |
| 4   | C     | 810 | POV  | C29-C210 | 4.21  | 1.55        | 1.31     |
| 2   | A     | 810 | Y01  | CBH-CBF  | -4.20 | 1.49        | 1.56     |
| 4   | D     | 810 | POV  | C29-C210 | 4.20  | 1.55        | 1.31     |
| 4   | A     | 807 | POV  | C29-C210 | 4.20  | 1.55        | 1.31     |
| 2   | C     | 801 | Y01  | CAT-CAR  | 4.19  | 1.61        | 1.53     |
| 2   | A     | 810 | Y01  | CBB-CBE  | -4.18 | 1.47        | 1.54     |
| 2   | C     | 805 | Y01  | CBB-CBE  | -4.15 | 1.47        | 1.54     |
| 2   | B     | 801 | Y01  | CBH-CBF  | -4.12 | 1.49        | 1.56     |
| 2   | C     | 803 | Y01  | OAW-CAY  | 4.05  | 1.45        | 1.34     |
| 2   | D     | 804 | Y01  | OAW-CAY  | 4.04  | 1.45        | 1.34     |
| 2   | D     | 804 | Y01  | CAT-CAR  | 4.02  | 1.61        | 1.53     |
| 2   | B     | 803 | Y01  | OAW-CAY  | 3.95  | 1.45        | 1.34     |
| 2   | A     | 801 | Y01  | OAW-CAY  | 3.94  | 1.45        | 1.34     |
| 2   | D     | 805 | Y01  | OAW-CAY  | 3.91  | 1.45        | 1.34     |
| 2   | C     | 804 | Y01  | OAW-CAY  | 3.86  | 1.45        | 1.34     |
| 2   | B     | 804 | Y01  | OAW-CAY  | 3.84  | 1.45        | 1.34     |
| 2   | D     | 805 | Y01  | CBD-CBF  | -3.83 | 1.46        | 1.53     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | A     | 802 | Y01  | OAW-CAY | 3.83  | 1.45        | 1.34     |
| 2   | C     | 803 | Y01  | CAT-CAR | 3.83  | 1.61        | 1.53     |
| 2   | B     | 803 | Y01  | CAT-CAR | 3.81  | 1.61        | 1.53     |
| 2   | A     | 801 | Y01  | CAT-CAR | 3.81  | 1.61        | 1.53     |
| 2   | C     | 804 | Y01  | CBD-CBF | -3.79 | 1.46        | 1.53     |
| 2   | A     | 802 | Y01  | CBD-CBF | -3.79 | 1.46        | 1.53     |
| 2   | B     | 804 | Y01  | CBD-CBF | -3.78 | 1.46        | 1.53     |
| 2   | A     | 810 | Y01  | CBD-CBF | -3.77 | 1.46        | 1.53     |
| 2   | C     | 801 | Y01  | CBD-CBF | -3.77 | 1.46        | 1.53     |
| 2   | B     | 801 | Y01  | CBD-CBF | -3.76 | 1.46        | 1.53     |
| 2   | C     | 805 | Y01  | CBD-CBF | -3.74 | 1.46        | 1.53     |
| 2   | C     | 804 | Y01  | CAT-CAR | 3.66  | 1.60        | 1.53     |
| 2   | A     | 802 | Y01  | CAT-CAR | 3.65  | 1.60        | 1.53     |
| 2   | B     | 804 | Y01  | CAT-CAR | 3.65  | 1.60        | 1.53     |
| 2   | D     | 805 | Y01  | CAT-CAR | 3.53  | 1.60        | 1.53     |
| 2   | B     | 803 | Y01  | CBD-CBF | -3.47 | 1.47        | 1.53     |
| 2   | A     | 801 | Y01  | CBD-CBF | -3.44 | 1.47        | 1.53     |
| 2   | C     | 803 | Y01  | CBD-CBF | -3.42 | 1.47        | 1.53     |
| 2   | D     | 804 | Y01  | CAV-CBC | -3.31 | 1.44        | 1.52     |
| 4   | B     | 807 | POV  | O21-C21 | 3.30  | 1.43        | 1.34     |
| 2   | D     | 804 | Y01  | CBD-CBF | -3.28 | 1.47        | 1.53     |
| 4   | A     | 805 | POV  | O21-C21 | 3.27  | 1.43        | 1.34     |
| 4   | D     | 808 | POV  | O21-C21 | 3.26  | 1.43        | 1.34     |
| 4   | C     | 808 | POV  | O21-C21 | 3.23  | 1.43        | 1.34     |
| 4   | D     | 810 | POV  | O21-C21 | 3.21  | 1.41        | 1.30     |
| 4   | C     | 810 | POV  | O21-C21 | 3.20  | 1.41        | 1.30     |
| 4   | B     | 809 | POV  | O21-C21 | 3.19  | 1.41        | 1.30     |
| 4   | A     | 807 | POV  | O21-C21 | 3.18  | 1.41        | 1.30     |
| 2   | C     | 803 | Y01  | CAV-CBC | -3.13 | 1.45        | 1.52     |
| 2   | B     | 803 | Y01  | CAV-CBC | -3.08 | 1.45        | 1.52     |
| 2   | A     | 801 | Y01  | CAV-CBC | -3.04 | 1.45        | 1.52     |
| 4   | D     | 803 | POV  | O21-C21 | 3.03  | 1.42        | 1.34     |
| 4   | B     | 802 | POV  | O21-C21 | 2.98  | 1.42        | 1.34     |
| 4   | C     | 802 | POV  | O21-C21 | 2.97  | 1.42        | 1.34     |
| 4   | A     | 811 | POV  | O21-C21 | 2.97  | 1.42        | 1.34     |
| 2   | B     | 803 | Y01  | CBH-CBF | -2.88 | 1.51        | 1.56     |
| 2   | A     | 801 | Y01  | CBH-CBF | -2.85 | 1.51        | 1.56     |
| 2   | A     | 810 | Y01  | CAV-CBC | -2.81 | 1.45        | 1.52     |
| 2   | B     | 801 | Y01  | CAV-CBC | -2.75 | 1.46        | 1.52     |
| 2   | C     | 803 | Y01  | CBH-CBF | -2.75 | 1.51        | 1.56     |
| 4   | D     | 803 | POV  | O31-C31 | 2.73  | 1.41        | 1.33     |
| 2   | C     | 805 | Y01  | CAV-CBC | -2.71 | 1.46        | 1.52     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4   | A     | 811 | POV  | O31-C31 | 2.71  | 1.41        | 1.33     |
| 4   | C     | 812 | POV  | O31-C31 | 2.71  | 1.41        | 1.33     |
| 4   | C     | 802 | POV  | O31-C31 | 2.70  | 1.41        | 1.33     |
| 4   | B     | 811 | POV  | O31-C31 | 2.70  | 1.41        | 1.33     |
| 2   | A     | 802 | Y01  | CAV-CBC | -2.69 | 1.46        | 1.52     |
| 4   | A     | 809 | POV  | O31-C31 | 2.69  | 1.41        | 1.33     |
| 2   | A     | 802 | Y01  | CAO-CBB | 2.69  | 1.61        | 1.54     |
| 4   | B     | 802 | POV  | O31-C31 | 2.68  | 1.41        | 1.33     |
| 2   | C     | 801 | Y01  | CAV-CBC | -2.68 | 1.46        | 1.52     |
| 4   | D     | 802 | POV  | O31-C31 | 2.67  | 1.41        | 1.33     |
| 2   | C     | 804 | Y01  | CAO-CBB | 2.65  | 1.60        | 1.54     |
| 2   | D     | 805 | Y01  | CAO-CBB | 2.63  | 1.60        | 1.54     |
| 2   | B     | 804 | Y01  | CAO-CBB | 2.62  | 1.60        | 1.54     |
| 2   | C     | 804 | Y01  | CAV-CBC | -2.62 | 1.46        | 1.52     |
| 2   | D     | 805 | Y01  | CAV-CBC | -2.59 | 1.46        | 1.52     |
| 4   | C     | 808 | POV  | O31-C31 | 2.58  | 1.40        | 1.33     |
| 4   | B     | 807 | POV  | O31-C31 | 2.57  | 1.40        | 1.33     |
| 4   | D     | 808 | POV  | O31-C31 | 2.57  | 1.40        | 1.33     |
| 2   | D     | 804 | Y01  | CBH-CBF | -2.55 | 1.52        | 1.56     |
| 2   | B     | 804 | Y01  | CAV-CBC | -2.54 | 1.46        | 1.52     |
| 4   | A     | 805 | POV  | O31-C31 | 2.51  | 1.40        | 1.33     |
| 4   | A     | 811 | POV  | O21-C2  | -2.47 | 1.40        | 1.46     |
| 4   | B     | 802 | POV  | O21-C2  | -2.45 | 1.40        | 1.46     |
| 4   | C     | 802 | POV  | O21-C2  | -2.41 | 1.40        | 1.46     |
| 2   | D     | 804 | Y01  | CAO-CBB | 2.41  | 1.60        | 1.54     |
| 4   | D     | 803 | POV  | O21-C2  | -2.38 | 1.41        | 1.46     |
| 2   | A     | 802 | Y01  | CAK-CAI | 2.36  | 1.55        | 1.50     |
| 2   | B     | 803 | Y01  | CAO-CBB | 2.35  | 1.60        | 1.54     |
| 2   | D     | 805 | Y01  | CAK-CAI | 2.35  | 1.55        | 1.50     |
| 2   | B     | 804 | Y01  | CAK-CAI | 2.35  | 1.55        | 1.50     |
| 2   | B     | 801 | Y01  | CAM-CAY | 2.33  | 1.57        | 1.50     |
| 2   | C     | 803 | Y01  | CAO-CBB | 2.33  | 1.60        | 1.54     |
| 2   | A     | 801 | Y01  | CAO-CBB | 2.33  | 1.60        | 1.54     |
| 2   | C     | 804 | Y01  | CAK-CAI | 2.33  | 1.54        | 1.50     |
| 2   | A     | 810 | Y01  | CAM-CAY | 2.31  | 1.57        | 1.50     |
| 2   | C     | 805 | Y01  | CAM-CAY | 2.31  | 1.57        | 1.50     |
| 2   | C     | 805 | Y01  | CAS-CBF | -2.30 | 1.50        | 1.53     |
| 2   | C     | 801 | Y01  | CAM-CAY | 2.26  | 1.57        | 1.50     |
| 2   | D     | 805 | Y01  | CAR-CBC | -2.22 | 1.45        | 1.51     |
| 2   | A     | 802 | Y01  | CAR-CBC | -2.21 | 1.45        | 1.51     |
| 2   | A     | 810 | Y01  | CAO-CBB | 2.20  | 1.59        | 1.54     |
| 2   | B     | 801 | Y01  | CAO-CBB | 2.19  | 1.59        | 1.54     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | B     | 801 | Y01  | CAS-CBF | -2.19 | 1.50        | 1.53     |
| 2   | D     | 804 | Y01  | CAR-CBC | -2.18 | 1.45        | 1.51     |
| 2   | A     | 810 | Y01  | CAS-CBF | -2.18 | 1.50        | 1.53     |
| 2   | C     | 804 | Y01  | CAR-CBC | -2.15 | 1.45        | 1.51     |
| 2   | C     | 805 | Y01  | CAO-CBB | 2.15  | 1.59        | 1.54     |
| 2   | C     | 801 | Y01  | CAO-CBB | 2.13  | 1.59        | 1.54     |
| 2   | B     | 804 | Y01  | CAR-CBC | -2.13 | 1.45        | 1.51     |
| 2   | A     | 802 | Y01  | CAS-CBF | -2.11 | 1.50        | 1.53     |
| 2   | C     | 804 | Y01  | CAS-CBF | -2.10 | 1.50        | 1.53     |
| 2   | B     | 803 | Y01  | CAR-CBC | -2.09 | 1.45        | 1.51     |
| 2   | C     | 801 | Y01  | CAS-CBF | -2.08 | 1.50        | 1.53     |
| 4   | D     | 803 | POV  | P-O12   | 2.08  | 1.67        | 1.59     |
| 2   | A     | 801 | Y01  | CAR-CBC | -2.07 | 1.45        | 1.51     |
| 2   | C     | 803 | Y01  | CAR-CBC | -2.06 | 1.45        | 1.51     |
| 4   | A     | 811 | POV  | P-O12   | 2.04  | 1.67        | 1.59     |
| 4   | C     | 802 | POV  | P-O11   | 2.04  | 1.67        | 1.59     |
| 4   | A     | 811 | POV  | P-O11   | 2.04  | 1.67        | 1.59     |
| 4   | D     | 803 | POV  | P-O11   | 2.03  | 1.67        | 1.59     |
| 2   | B     | 804 | Y01  | CAS-CBF | -2.03 | 1.50        | 1.53     |
| 4   | C     | 802 | POV  | P-O12   | 2.03  | 1.67        | 1.59     |

All (334) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 2   | C     | 805 | Y01  | CAD-CBH-CBF | -13.77 | 96.20       | 111.66   |
| 2   | A     | 810 | Y01  | CAD-CBH-CBF | -13.47 | 96.54       | 111.66   |
| 2   | C     | 801 | Y01  | CAD-CBH-CBF | -13.25 | 96.78       | 111.66   |
| 2   | B     | 801 | Y01  | CAD-CBH-CBF | -13.16 | 96.90       | 111.66   |
| 2   | B     | 804 | Y01  | CAD-CBH-CBF | -10.24 | 100.17      | 111.66   |
| 2   | C     | 804 | Y01  | CAD-CBH-CBF | -9.76  | 100.71      | 111.66   |
| 2   | D     | 805 | Y01  | CAD-CBH-CBF | -9.75  | 100.72      | 111.66   |
| 2   | A     | 802 | Y01  | CAD-CBH-CBF | -9.58  | 100.91      | 111.66   |
| 2   | B     | 803 | Y01  | CAD-CBH-CBF | -8.39  | 102.24      | 111.66   |
| 2   | A     | 801 | Y01  | CAD-CBH-CBF | -8.19  | 102.46      | 111.66   |
| 2   | C     | 803 | Y01  | CAD-CBH-CBF | -8.06  | 102.62      | 111.66   |
| 2   | B     | 803 | Y01  | CAV-CAZ-CAI | -8.03  | 109.68      | 120.57   |
| 2   | D     | 804 | Y01  | CAV-CAZ-CAI | -8.00  | 109.72      | 120.57   |
| 2   | C     | 803 | Y01  | CAV-CAZ-CAI | -7.83  | 109.96      | 120.57   |
| 2   | C     | 804 | Y01  | CAU-CBI-CBE | -7.82  | 105.09      | 116.60   |
| 2   | B     | 804 | Y01  | CAU-CBI-CBE | -7.81  | 105.10      | 116.60   |
| 2   | D     | 805 | Y01  | CAU-CBI-CBE | -7.81  | 105.10      | 116.60   |
| 2   | A     | 801 | Y01  | CAV-CAZ-CAI | -7.77  | 110.04      | 120.57   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | D     | 804 | Y01  | CAD-CBH-CBF | -7.57 | 103.16      | 111.66   |
| 2   | A     | 810 | Y01  | CAV-CAZ-CAI | -7.57 | 110.31      | 120.57   |
| 2   | C     | 804 | Y01  | CBG-CBI-CBE | 7.45  | 108.65      | 100.10   |
| 2   | D     | 805 | Y01  | CBG-CBI-CBE | 7.37  | 108.56      | 100.10   |
| 2   | C     | 805 | Y01  | CBG-CBI-CBE | 7.30  | 108.48      | 100.10   |
| 2   | A     | 802 | Y01  | CAU-CBI-CBE | -7.30 | 105.85      | 116.60   |
| 2   | B     | 804 | Y01  | CBG-CBI-CBE | 7.27  | 108.45      | 100.10   |
| 2   | C     | 805 | Y01  | CAV-CAZ-CAI | -7.22 | 110.78      | 120.57   |
| 2   | A     | 802 | Y01  | CBG-CBI-CBE | 7.18  | 108.33      | 100.10   |
| 2   | B     | 801 | Y01  | CAV-CAZ-CAI | -7.14 | 110.89      | 120.57   |
| 2   | C     | 801 | Y01  | CBG-CBI-CBE | 7.02  | 108.16      | 100.10   |
| 2   | A     | 810 | Y01  | CBG-CBI-CBE | 7.01  | 108.14      | 100.10   |
| 2   | B     | 801 | Y01  | CBG-CBI-CBE | 7.00  | 108.13      | 100.10   |
| 2   | B     | 801 | Y01  | CAK-CAI-CAZ | -6.91 | 113.35      | 125.02   |
| 2   | A     | 810 | Y01  | CAK-CAI-CAZ | -6.89 | 113.38      | 125.02   |
| 2   | C     | 801 | Y01  | CAK-CAI-CAZ | -6.88 | 113.40      | 125.02   |
| 2   | C     | 805 | Y01  | CAK-CAI-CAZ | -6.87 | 113.42      | 125.02   |
| 2   | A     | 801 | Y01  | CBF-CBH-CAZ | 6.84  | 119.67      | 109.65   |
| 2   | C     | 801 | Y01  | CAV-CAZ-CAI | -6.83 | 111.31      | 120.57   |
| 2   | C     | 803 | Y01  | CBF-CBH-CAZ | 6.80  | 119.61      | 109.65   |
| 2   | D     | 805 | Y01  | CAT-CAR-CBC | 6.78  | 121.39      | 110.33   |
| 2   | B     | 803 | Y01  | CBF-CBH-CAZ | 6.72  | 119.49      | 109.65   |
| 2   | D     | 804 | Y01  | CBF-CBH-CAZ | 6.71  | 119.48      | 109.65   |
| 2   | A     | 802 | Y01  | CAK-CAI-CAZ | -6.65 | 113.79      | 125.02   |
| 2   | A     | 802 | Y01  | CAT-CAR-CBC | 6.59  | 121.08      | 110.33   |
| 2   | C     | 804 | Y01  | CAT-CAR-CBC | 6.51  | 120.95      | 110.33   |
| 2   | B     | 804 | Y01  | CBF-CBH-CAZ | 6.36  | 118.97      | 109.65   |
| 2   | D     | 804 | Y01  | CAK-CAI-CAZ | -6.36 | 114.28      | 125.02   |
| 2   | D     | 804 | Y01  | CAU-CBI-CBE | -6.31 | 107.31      | 116.60   |
| 2   | D     | 805 | Y01  | CBF-CBH-CAZ | 6.30  | 118.87      | 109.65   |
| 2   | B     | 803 | Y01  | CAK-CAI-CAZ | -6.28 | 114.42      | 125.02   |
| 2   | C     | 801 | Y01  | CBF-CBH-CAZ | 6.26  | 118.81      | 109.65   |
| 2   | D     | 805 | Y01  | CBD-CAK-CAI | 6.26  | 121.44      | 112.76   |
| 2   | C     | 804 | Y01  | CAK-CAI-CAZ | -6.25 | 114.46      | 125.02   |
| 2   | C     | 804 | Y01  | CBF-CBH-CAZ | 6.23  | 118.77      | 109.65   |
| 2   | A     | 801 | Y01  | CAK-CAI-CAZ | -6.21 | 114.53      | 125.02   |
| 2   | B     | 801 | Y01  | CBF-CBH-CAZ | 6.19  | 118.72      | 109.65   |
| 2   | B     | 804 | Y01  | CBD-CAK-CAI | 6.18  | 121.33      | 112.76   |
| 2   | C     | 803 | Y01  | CAK-CAI-CAZ | -6.18 | 114.59      | 125.02   |
| 2   | B     | 804 | Y01  | CAK-CAI-CAZ | -6.17 | 114.60      | 125.02   |
| 2   | D     | 805 | Y01  | CAK-CAI-CAZ | -6.16 | 114.62      | 125.02   |
| 2   | A     | 810 | Y01  | CBF-CBH-CAZ | 6.15  | 118.65      | 109.65   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | D     | 804 | Y01  | CBG-CBI-CBE | 6.11  | 107.11      | 100.10   |
| 2   | B     | 804 | Y01  | CAT-CAR-CBC | 6.09  | 120.26      | 110.33   |
| 2   | C     | 805 | Y01  | CBF-CBH-CAZ | 6.09  | 118.56      | 109.65   |
| 2   | A     | 802 | Y01  | CAV-CAZ-CAI | -6.07 | 112.34      | 120.57   |
| 2   | A     | 802 | Y01  | CBF-CBH-CAZ | 6.06  | 118.53      | 109.65   |
| 2   | C     | 804 | Y01  | CBD-CAK-CAI | 6.05  | 121.14      | 112.76   |
| 2   | C     | 805 | Y01  | CAS-CAU-CBI | 5.99  | 122.85      | 112.74   |
| 2   | C     | 804 | Y01  | CAV-CAZ-CAI | -5.90 | 112.57      | 120.57   |
| 2   | D     | 805 | Y01  | CAV-CAZ-CAI | -5.87 | 112.61      | 120.57   |
| 2   | B     | 801 | Y01  | CAS-CAU-CBI | 5.87  | 122.64      | 112.74   |
| 2   | C     | 801 | Y01  | CAS-CAU-CBI | 5.86  | 122.63      | 112.74   |
| 2   | A     | 810 | Y01  | CAS-CAU-CBI | 5.84  | 122.59      | 112.74   |
| 2   | B     | 804 | Y01  | CAV-CAZ-CAI | -5.79 | 112.72      | 120.57   |
| 2   | A     | 801 | Y01  | CBG-CBI-CBE | 5.76  | 106.70      | 100.10   |
| 2   | C     | 803 | Y01  | CBG-CBI-CBE | 5.69  | 106.63      | 100.10   |
| 2   | B     | 801 | Y01  | OAW-CAY-CAM | 5.68  | 123.77      | 111.48   |
| 2   | A     | 810 | Y01  | OAW-CAY-CAM | 5.66  | 123.74      | 111.48   |
| 2   | C     | 805 | Y01  | OAW-CAY-CAM | 5.65  | 123.70      | 111.48   |
| 2   | A     | 801 | Y01  | CAU-CBI-CBE | -5.64 | 108.29      | 116.60   |
| 2   | C     | 803 | Y01  | CAU-CBI-CBE | -5.61 | 108.34      | 116.60   |
| 2   | C     | 801 | Y01  | OAW-CAY-CAM | 5.54  | 123.46      | 111.48   |
| 2   | A     | 810 | Y01  | CBD-CAK-CAI | 5.39  | 120.23      | 112.76   |
| 2   | B     | 803 | Y01  | CAS-CAU-CBI | 5.37  | 121.81      | 112.74   |
| 2   | C     | 803 | Y01  | OAW-CAY-CAM | 5.36  | 123.08      | 111.48   |
| 2   | C     | 803 | Y01  | CAS-CAU-CBI | 5.36  | 121.78      | 112.74   |
| 2   | A     | 801 | Y01  | CAS-CAU-CBI | 5.35  | 121.77      | 112.74   |
| 2   | B     | 803 | Y01  | CBG-CBI-CBE | 5.35  | 106.24      | 100.10   |
| 2   | D     | 804 | Y01  | CAU-CBI-CBG | 5.35  | 115.25      | 107.25   |
| 2   | A     | 802 | Y01  | CBD-CAK-CAI | 5.33  | 120.14      | 112.76   |
| 2   | D     | 804 | Y01  | CAS-CAU-CBI | 5.33  | 121.73      | 112.74   |
| 2   | B     | 803 | Y01  | CAU-CBI-CBE | -5.32 | 108.77      | 116.60   |
| 2   | A     | 801 | Y01  | OAW-CAY-CAM | 5.31  | 122.97      | 111.48   |
| 2   | A     | 802 | Y01  | CAS-CAU-CBI | 5.30  | 121.69      | 112.74   |
| 2   | B     | 803 | Y01  | CAU-CBI-CBG | 5.30  | 115.17      | 107.25   |
| 2   | D     | 805 | Y01  | CAK-CBD-CBF | 5.28  | 115.82      | 109.72   |
| 2   | C     | 803 | Y01  | CAU-CBI-CBG | 5.27  | 115.14      | 107.25   |
| 2   | A     | 801 | Y01  | CAU-CBI-CBG | 5.23  | 115.07      | 107.25   |
| 2   | B     | 804 | Y01  | CAK-CBD-CBF | 5.22  | 115.75      | 109.72   |
| 2   | C     | 803 | Y01  | CAT-CAR-CBC | 5.22  | 118.84      | 110.33   |
| 2   | C     | 804 | Y01  | CAS-CAU-CBI | 5.21  | 121.53      | 112.74   |
| 2   | B     | 804 | Y01  | CAS-CAU-CBI | 5.21  | 121.53      | 112.74   |
| 2   | D     | 804 | Y01  | OAW-CAY-CAM | 5.20  | 122.72      | 111.48   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | B     | 804 | Y01  | CBC-CAV-CAZ | 5.19  | 119.11      | 111.45   |
| 2   | B     | 803 | Y01  | CAT-CAR-CBC | 5.17  | 118.76      | 110.33   |
| 2   | D     | 805 | Y01  | CAS-CAU-CBI | 5.17  | 121.46      | 112.74   |
| 2   | A     | 801 | Y01  | CAT-CAR-CBC | 5.17  | 118.76      | 110.33   |
| 2   | D     | 805 | Y01  | CBC-CAV-CAZ | 5.16  | 119.08      | 111.45   |
| 2   | D     | 804 | Y01  | CAT-CAR-CBC | 5.13  | 118.70      | 110.33   |
| 2   | B     | 803 | Y01  | OAW-CAY-CAM | 5.11  | 122.53      | 111.48   |
| 2   | C     | 804 | Y01  | CAK-CBD-CBF | 5.03  | 115.54      | 109.72   |
| 2   | C     | 805 | Y01  | CBD-CAK-CAI | 5.03  | 119.73      | 112.76   |
| 2   | C     | 801 | Y01  | CBI-CBG-CBD | 4.96  | 121.46      | 114.41   |
| 2   | B     | 801 | Y01  | CBI-CBG-CBD | 4.94  | 121.43      | 114.41   |
| 2   | C     | 805 | Y01  | CBI-CBG-CBD | 4.93  | 121.41      | 114.41   |
| 2   | B     | 804 | Y01  | CAU-CBI-CBG | 4.92  | 114.60      | 107.25   |
| 2   | C     | 804 | Y01  | CBC-CAV-CAZ | 4.91  | 118.71      | 111.45   |
| 2   | C     | 804 | Y01  | CAU-CBI-CBG | 4.90  | 114.58      | 107.25   |
| 2   | D     | 805 | Y01  | CAU-CBI-CBG | 4.83  | 114.47      | 107.25   |
| 2   | A     | 802 | Y01  | CBC-CAV-CAZ | 4.82  | 118.57      | 111.45   |
| 2   | A     | 810 | Y01  | CBI-CBG-CBD | 4.82  | 121.25      | 114.41   |
| 2   | A     | 810 | Y01  | CAU-CBI-CBE | -4.79 | 109.55      | 116.60   |
| 2   | B     | 801 | Y01  | CBD-CAK-CAI | 4.77  | 119.38      | 112.76   |
| 2   | C     | 801 | Y01  | CBD-CAK-CAI | 4.76  | 119.36      | 112.76   |
| 2   | C     | 805 | Y01  | CAT-CAR-CBC | 4.71  | 118.02      | 110.33   |
| 2   | A     | 802 | Y01  | CBI-CBG-CBD | 4.67  | 121.04      | 114.41   |
| 2   | C     | 801 | Y01  | CAS-CBF-CBH | 4.60  | 118.75      | 113.08   |
| 2   | A     | 802 | Y01  | CAU-CBI-CBG | 4.59  | 114.11      | 107.25   |
| 2   | B     | 804 | Y01  | CBH-CBF-CBD | 4.52  | 119.32      | 112.71   |
| 2   | A     | 802 | Y01  | OAW-CAY-CAM | 4.52  | 121.25      | 111.48   |
| 2   | C     | 805 | Y01  | CAU-CBI-CBE | -4.50 | 109.97      | 116.60   |
| 2   | B     | 801 | Y01  | CAT-CAR-CBC | 4.49  | 117.65      | 110.33   |
| 2   | D     | 805 | Y01  | OAW-CAY-CAM | 4.49  | 121.19      | 111.48   |
| 2   | C     | 801 | Y01  | CAT-CAR-CBC | 4.48  | 117.65      | 110.33   |
| 2   | C     | 804 | Y01  | OAW-CAY-CAM | 4.45  | 121.12      | 111.48   |
| 2   | D     | 805 | Y01  | CBH-CBF-CBD | 4.45  | 119.21      | 112.71   |
| 2   | C     | 805 | Y01  | CAS-CBF-CBH | 4.42  | 118.53      | 113.08   |
| 2   | A     | 810 | Y01  | CBH-CBF-CBD | 4.40  | 119.15      | 112.71   |
| 2   | B     | 804 | Y01  | OAW-CAY-CAM | 4.39  | 120.99      | 111.48   |
| 2   | B     | 801 | Y01  | CAU-CBI-CBE | -4.39 | 110.14      | 116.60   |
| 2   | B     | 801 | Y01  | CAS-CBF-CBH | 4.39  | 118.49      | 113.08   |
| 2   | C     | 801 | Y01  | CAE-CBI-CBE | -4.38 | 103.73      | 111.68   |
| 2   | C     | 805 | Y01  | CBH-CBF-CBD | 4.35  | 119.07      | 112.71   |
| 2   | C     | 801 | Y01  | CBH-CBF-CBD | 4.34  | 119.06      | 112.71   |
| 2   | C     | 801 | Y01  | CAU-CBI-CBE | -4.33 | 110.23      | 116.60   |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | B     | 803 | Y01  | CBI-CBG-CBD | 4.33  | 120.56      | 114.41   |
| 2   | C     | 804 | Y01  | CBH-CBF-CBD | 4.32  | 119.03      | 112.71   |
| 2   | B     | 801 | Y01  | CAE-CBI-CBE | -4.31 | 103.85      | 111.68   |
| 2   | A     | 810 | Y01  | CAS-CBF-CBH | 4.30  | 118.38      | 113.08   |
| 2   | A     | 810 | Y01  | CAT-CAR-CBC | 4.30  | 117.34      | 110.33   |
| 2   | C     | 805 | Y01  | CAE-CBI-CBE | -4.30 | 103.89      | 111.68   |
| 2   | A     | 801 | Y01  | CBI-CBG-CBD | 4.28  | 120.49      | 114.41   |
| 2   | A     | 802 | Y01  | CAK-CBD-CBF | 4.26  | 114.65      | 109.72   |
| 2   | B     | 801 | Y01  | CBH-CBF-CBD | 4.21  | 118.87      | 112.71   |
| 2   | C     | 803 | Y01  | CBI-CBG-CBD | 4.21  | 120.39      | 114.41   |
| 2   | D     | 804 | Y01  | CBI-CBG-CBD | 4.18  | 120.35      | 114.41   |
| 2   | A     | 810 | Y01  | CAK-CBD-CBF | 4.12  | 114.48      | 109.72   |
| 2   | C     | 801 | Y01  | CAK-CBD-CBF | 4.12  | 114.48      | 109.72   |
| 2   | D     | 804 | Y01  | CBF-CBD-CBG | 4.05  | 114.38      | 109.09   |
| 2   | C     | 805 | Y01  | CAK-CBD-CBF | 4.00  | 114.34      | 109.72   |
| 2   | A     | 802 | Y01  | CBH-CBF-CBD | 3.98  | 118.53      | 112.71   |
| 2   | C     | 804 | Y01  | CBI-CBG-CBD | 3.96  | 120.03      | 114.41   |
| 2   | B     | 801 | Y01  | CAK-CBD-CBF | 3.95  | 114.28      | 109.72   |
| 2   | A     | 810 | Y01  | CAE-CBI-CBE | -3.95 | 104.52      | 111.68   |
| 4   | C     | 808 | POV  | O21-C21-C22 | 3.91  | 119.94      | 111.48   |
| 2   | D     | 805 | Y01  | CBI-CBE-CBB | -3.85 | 113.55      | 119.50   |
| 2   | B     | 803 | Y01  | CAC-CBB-CAO | -3.84 | 104.39      | 110.34   |
| 2   | C     | 804 | Y01  | CBI-CBE-CBB | -3.83 | 113.58      | 119.50   |
| 2   | B     | 804 | Y01  | CBI-CBE-CBB | -3.82 | 113.60      | 119.50   |
| 2   | A     | 810 | Y01  | CAC-CBB-CAO | -3.81 | 104.44      | 110.34   |
| 2   | B     | 801 | Y01  | CAC-CBB-CAO | -3.79 | 104.47      | 110.34   |
| 2   | D     | 805 | Y01  | CBI-CBG-CBD | 3.77  | 119.77      | 114.41   |
| 2   | D     | 804 | Y01  | CBC-CAV-CAZ | 3.77  | 117.01      | 111.45   |
| 2   | B     | 803 | Y01  | CBC-CAV-CAZ | 3.76  | 117.00      | 111.45   |
| 2   | A     | 801 | Y01  | CBC-CAV-CAZ | 3.76  | 117.00      | 111.45   |
| 4   | B     | 807 | POV  | O21-C21-C22 | 3.75  | 119.60      | 111.48   |
| 2   | C     | 805 | Y01  | CAU-CBI-CBG | 3.75  | 112.86      | 107.25   |
| 2   | B     | 804 | Y01  | CBI-CBG-CBD | 3.75  | 119.73      | 114.41   |
| 2   | C     | 805 | Y01  | CAC-CBB-CAO | -3.73 | 104.57      | 110.34   |
| 2   | C     | 803 | Y01  | CAC-CBB-CAO | -3.72 | 104.58      | 110.34   |
| 2   | C     | 801 | Y01  | CAC-CBB-CAO | -3.71 | 104.60      | 110.34   |
| 2   | B     | 804 | Y01  | CAC-CBB-CBE | -3.71 | 107.32      | 112.88   |
| 2   | A     | 801 | Y01  | CAC-CBB-CAO | -3.69 | 104.63      | 110.34   |
| 2   | C     | 803 | Y01  | CBC-CAV-CAZ | 3.66  | 116.86      | 111.45   |
| 2   | B     | 803 | Y01  | CBD-CAK-CAI | 3.66  | 117.83      | 112.76   |
| 4   | A     | 805 | POV  | O21-C21-C22 | 3.60  | 119.27      | 111.48   |
| 2   | A     | 810 | Y01  | CAU-CBI-CBG | 3.58  | 112.60      | 107.25   |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | C     | 804 | Y01  | CAC-CBB-CBE | -3.58 | 107.51      | 112.88   |
| 4   | C     | 802 | POV  | O21-C21-C22 | 3.57  | 119.21      | 111.48   |
| 4   | D     | 803 | POV  | O21-C21-C22 | 3.56  | 119.19      | 111.48   |
| 4   | A     | 811 | POV  | O21-C21-C22 | 3.56  | 119.17      | 111.48   |
| 2   | A     | 802 | Y01  | CBI-CBE-CBB | -3.54 | 114.03      | 119.50   |
| 2   | B     | 801 | Y01  | CAU-CBI-CBG | 3.51  | 112.50      | 107.25   |
| 2   | C     | 803 | Y01  | CBF-CBD-CBG | 3.50  | 113.66      | 109.09   |
| 2   | A     | 801 | Y01  | CBF-CBD-CBG | 3.49  | 113.65      | 109.09   |
| 4   | B     | 802 | POV  | O21-C21-C22 | 3.48  | 119.02      | 111.48   |
| 4   | D     | 808 | POV  | O21-C21-C22 | 3.47  | 118.99      | 111.48   |
| 2   | C     | 801 | Y01  | CAU-CBI-CBG | 3.47  | 112.44      | 107.25   |
| 2   | A     | 801 | Y01  | CBD-CAK-CAI | 3.47  | 117.57      | 112.76   |
| 2   | D     | 805 | Y01  | CAC-CBB-CBE | -3.47 | 107.68      | 112.88   |
| 2   | C     | 803 | Y01  | CBD-CAK-CAI | 3.47  | 117.57      | 112.76   |
| 2   | B     | 803 | Y01  | CBF-CBD-CBG | 3.45  | 113.59      | 109.09   |
| 2   | B     | 804 | Y01  | CAP-CBE-CBI | 3.44  | 107.88      | 103.84   |
| 2   | D     | 804 | Y01  | CAS-CBF-CBH | 3.33  | 117.20      | 113.08   |
| 2   | D     | 805 | Y01  | CAP-CBE-CBI | 3.30  | 107.72      | 103.84   |
| 2   | A     | 802 | Y01  | CAR-CBC-CAV | 3.27  | 115.53      | 110.97   |
| 2   | C     | 804 | Y01  | CAP-CBE-CBI | 3.26  | 107.68      | 103.84   |
| 2   | A     | 802 | Y01  | CAC-CBB-CBE | -3.26 | 107.99      | 112.88   |
| 2   | D     | 805 | Y01  | CAS-CBF-CBH | 3.24  | 117.07      | 113.08   |
| 2   | A     | 802 | Y01  | CAO-CBB-CBE | 3.23  | 117.02      | 110.33   |
| 2   | C     | 804 | Y01  | CAO-CBB-CBE | 3.18  | 116.92      | 110.33   |
| 2   | B     | 804 | Y01  | CAR-CBC-CAV | 3.18  | 115.39      | 110.97   |
| 2   | C     | 805 | Y01  | CAD-CBH-CAZ | 3.17  | 113.22      | 108.38   |
| 2   | D     | 804 | Y01  | CAC-CBB-CAO | -3.16 | 105.44      | 110.34   |
| 2   | D     | 805 | Y01  | CAR-CBC-CAV | 3.12  | 115.31      | 110.97   |
| 2   | B     | 804 | Y01  | CAO-CBB-CBE | 3.11  | 116.79      | 110.33   |
| 2   | D     | 805 | Y01  | CAO-CBB-CBE | 3.10  | 116.77      | 110.33   |
| 2   | A     | 802 | Y01  | CAS-CBF-CBH | 3.10  | 116.90      | 113.08   |
| 2   | B     | 804 | Y01  | CAS-CBF-CBH | 3.09  | 116.89      | 113.08   |
| 2   | C     | 804 | Y01  | CAR-CBC-CAV | 3.08  | 115.25      | 110.97   |
| 2   | D     | 805 | Y01  | CBH-CAZ-CAI | -3.01 | 118.54      | 122.93   |
| 2   | C     | 804 | Y01  | CBH-CAZ-CAI | -2.95 | 118.61      | 122.93   |
| 2   | A     | 801 | Y01  | CAK-CBD-CBF | 2.91  | 113.09      | 109.72   |
| 2   | C     | 804 | Y01  | CAS-CBF-CBH | 2.91  | 116.67      | 113.08   |
| 2   | C     | 803 | Y01  | CAS-CBF-CBH | 2.88  | 116.63      | 113.08   |
| 2   | B     | 803 | Y01  | CAE-CBI-CBE | -2.87 | 106.48      | 111.68   |
| 2   | C     | 803 | Y01  | CAK-CBD-CBF | 2.87  | 113.03      | 109.72   |
| 2   | B     | 804 | Y01  | CBH-CAZ-CAI | -2.87 | 118.74      | 122.93   |
| 2   | D     | 804 | Y01  | CAC-CBB-CBE | -2.85 | 108.60      | 112.88   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | C     | 804 | Y01  | CAD-CBH-CAZ | 2.85  | 112.74      | 108.38   |
| 2   | D     | 804 | Y01  | CBI-CBE-CBB | -2.84 | 115.11      | 119.50   |
| 2   | A     | 802 | Y01  | CAD-CBH-CAZ | 2.82  | 112.68      | 108.38   |
| 2   | C     | 803 | Y01  | CAE-CBI-CBE | -2.81 | 106.57      | 111.68   |
| 2   | A     | 801 | Y01  | CBI-CBE-CBB | -2.81 | 115.15      | 119.50   |
| 2   | A     | 802 | Y01  | CBH-CAZ-CAI | -2.81 | 118.82      | 122.93   |
| 2   | B     | 803 | Y01  | CAC-CBB-CBE | -2.80 | 108.68      | 112.88   |
| 2   | A     | 801 | Y01  | CAE-CBI-CBE | -2.80 | 106.60      | 111.68   |
| 2   | C     | 803 | Y01  | CBI-CBE-CBB | -2.80 | 115.18      | 119.50   |
| 2   | A     | 810 | Y01  | OAW-CAY-OAG | -2.78 | 117.21      | 123.70   |
| 4   | C     | 808 | POV  | O31-C31-C32 | 2.78  | 120.31      | 111.83   |
| 2   | A     | 801 | Y01  | CAS-CBF-CBH | 2.77  | 116.50      | 113.08   |
| 4   | B     | 807 | POV  | O31-C31-C32 | 2.77  | 120.27      | 111.83   |
| 2   | B     | 804 | Y01  | CAD-CBH-CAZ | 2.76  | 112.61      | 108.38   |
| 4   | D     | 808 | POV  | O31-C31-C32 | 2.74  | 120.20      | 111.83   |
| 2   | D     | 804 | Y01  | CAK-CBD-CBF | 2.74  | 112.89      | 109.72   |
| 2   | D     | 805 | Y01  | CAD-CBH-CAZ | 2.74  | 112.57      | 108.38   |
| 2   | B     | 803 | Y01  | CAK-CBD-CBF | 2.74  | 112.89      | 109.72   |
| 2   | B     | 803 | Y01  | CBI-CBE-CBB | -2.72 | 115.29      | 119.50   |
| 2   | A     | 801 | Y01  | CAC-CBB-CBE | -2.72 | 108.81      | 112.88   |
| 2   | B     | 801 | Y01  | OAW-CAY-OAG | -2.72 | 117.36      | 123.70   |
| 2   | C     | 805 | Y01  | OAW-CAY-OAG | -2.71 | 117.38      | 123.70   |
| 2   | C     | 805 | Y01  | OAW-CBC-CAV | 2.70  | 113.60      | 108.04   |
| 2   | C     | 803 | Y01  | CBH-CBF-CBD | 2.68  | 116.64      | 112.71   |
| 4   | A     | 805 | POV  | O31-C31-C32 | 2.68  | 120.02      | 111.83   |
| 2   | D     | 804 | Y01  | CBD-CAK-CAI | 2.68  | 116.47      | 112.76   |
| 2   | A     | 801 | Y01  | CBH-CBF-CBD | 2.68  | 116.63      | 112.71   |
| 4   | D     | 802 | POV  | O31-C31-C32 | 2.67  | 119.99      | 111.83   |
| 2   | D     | 804 | Y01  | OAW-CBC-CAV | -2.67 | 102.53      | 108.04   |
| 4   | C     | 812 | POV  | O31-C31-C32 | 2.67  | 119.97      | 111.83   |
| 2   | C     | 801 | Y01  | OAW-CBC-CAV | 2.66  | 113.52      | 108.04   |
| 4   | B     | 811 | POV  | O31-C31-C32 | 2.65  | 119.92      | 111.83   |
| 2   | A     | 810 | Y01  | CAD-CBH-CAZ | 2.63  | 112.40      | 108.38   |
| 4   | B     | 802 | POV  | O31-C31-C32 | 2.62  | 119.82      | 111.83   |
| 2   | D     | 804 | Y01  | CAO-CBB-CBE | 2.62  | 115.76      | 110.33   |
| 4   | A     | 811 | POV  | O31-C31-C32 | 2.61  | 119.81      | 111.83   |
| 2   | C     | 801 | Y01  | OAW-CAY-OAG | -2.61 | 117.59      | 123.70   |
| 2   | C     | 803 | Y01  | CAC-CBB-CBE | -2.61 | 108.97      | 112.88   |
| 2   | A     | 810 | Y01  | OAW-CBC-CAR | 2.61  | 114.53      | 108.37   |
| 2   | C     | 801 | Y01  | CAD-CBH-CAZ | 2.60  | 112.36      | 108.38   |
| 2   | C     | 801 | Y01  | CAQ-CBG-CBD | -2.60 | 114.95      | 119.10   |
| 4   | A     | 809 | POV  | O31-C31-C32 | 2.60  | 119.76      | 111.83   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | B     | 801 | Y01  | CAD-CBH-CAZ | 2.60  | 112.35      | 108.38   |
| 2   | A     | 801 | Y01  | CAO-CBB-CBE | 2.57  | 115.66      | 110.33   |
| 2   | B     | 803 | Y01  | CAS-CBF-CBH | 2.56  | 116.24      | 113.08   |
| 4   | C     | 802 | POV  | O31-C31-C32 | 2.56  | 119.64      | 111.83   |
| 2   | B     | 803 | Y01  | CBH-CBF-CBD | 2.56  | 116.45      | 112.71   |
| 2   | A     | 801 | Y01  | OAW-CAY-OAG | -2.55 | 117.74      | 123.70   |
| 2   | D     | 804 | Y01  | OAW-CBC-CAR | 2.55  | 114.40      | 108.37   |
| 4   | D     | 803 | POV  | O31-C31-C32 | 2.53  | 119.56      | 111.83   |
| 2   | C     | 805 | Y01  | OAW-CBC-CAR | 2.53  | 114.36      | 108.37   |
| 2   | C     | 803 | Y01  | OAW-CBC-CAR | 2.52  | 114.32      | 108.37   |
| 2   | B     | 801 | Y01  | OAW-CBC-CAV | 2.51  | 113.21      | 108.04   |
| 2   | C     | 805 | Y01  | CAQ-CBG-CBD | -2.51 | 115.10      | 119.10   |
| 2   | A     | 802 | Y01  | CAE-CBI-CBE | -2.49 | 107.16      | 111.68   |
| 2   | C     | 803 | Y01  | CAO-CBB-CBE | 2.49  | 115.49      | 110.33   |
| 2   | B     | 803 | Y01  | CAO-CBB-CBE | 2.49  | 115.48      | 110.33   |
| 2   | D     | 804 | Y01  | CBH-CBF-CBD | 2.48  | 116.34      | 112.71   |
| 2   | B     | 801 | Y01  | CAQ-CBG-CBD | -2.47 | 115.16      | 119.10   |
| 2   | A     | 810 | Y01  | OAW-CBC-CAV | 2.45  | 113.08      | 108.04   |
| 2   | D     | 804 | Y01  | CAE-CBI-CBE | -2.45 | 107.24      | 111.68   |
| 2   | B     | 801 | Y01  | CBC-CAV-CAZ | 2.45  | 115.06      | 111.45   |
| 2   | A     | 802 | Y01  | CAT-CBH-CBF | -2.43 | 105.53      | 108.74   |
| 4   | B     | 807 | POV  | C14-N-C12   | 2.42  | 119.54      | 109.91   |
| 2   | B     | 801 | Y01  | OAW-CBC-CAR | 2.40  | 114.04      | 108.37   |
| 2   | C     | 805 | Y01  | CBC-CAV-CAZ | 2.39  | 114.98      | 111.45   |
| 4   | D     | 808 | POV  | C14-N-C12   | 2.38  | 119.37      | 109.91   |
| 2   | C     | 801 | Y01  | CBF-CBD-CBG | 2.38  | 112.20      | 109.09   |
| 2   | B     | 801 | Y01  | CBF-CBD-CBG | 2.37  | 112.19      | 109.09   |
| 2   | C     | 805 | Y01  | CBF-CBD-CBG | 2.37  | 112.18      | 109.09   |
| 2   | C     | 804 | Y01  | CAT-CBH-CBF | -2.35 | 105.63      | 108.74   |
| 2   | C     | 801 | Y01  | CBC-CAV-CAZ | 2.33  | 114.89      | 111.45   |
| 2   | B     | 803 | Y01  | OAW-CBC-CAR | 2.33  | 113.87      | 108.37   |
| 2   | C     | 803 | Y01  | OAW-CAY-OAG | -2.32 | 118.29      | 123.70   |
| 2   | B     | 803 | Y01  | CAT-CBH-CBF | -2.31 | 105.67      | 108.74   |
| 4   | A     | 811 | POV  | C14-N-C12   | 2.31  | 119.11      | 109.91   |
| 2   | B     | 803 | Y01  | OAW-CAY-OAG | -2.30 | 118.32      | 123.70   |
| 2   | A     | 801 | Y01  | OAW-CBC-CAR | 2.29  | 113.79      | 108.37   |
| 4   | C     | 802 | POV  | C14-N-C12   | 2.29  | 119.02      | 109.91   |
| 4   | B     | 802 | POV  | C14-N-C12   | 2.29  | 119.01      | 109.91   |
| 4   | A     | 805 | POV  | C14-N-C12   | 2.28  | 118.96      | 109.91   |
| 4   | C     | 808 | POV  | C14-N-C12   | 2.27  | 118.95      | 109.91   |
| 2   | D     | 805 | Y01  | CAT-CBH-CBF | -2.27 | 105.73      | 108.74   |
| 2   | A     | 810 | Y01  | CBC-CAV-CAZ | 2.26  | 114.78      | 111.45   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | C     | 801 | Y01  | OAW-CBC-CAR | 2.22  | 113.61      | 108.37   |
| 4   | D     | 803 | POV  | C14-N-C12   | 2.22  | 118.72      | 109.91   |
| 2   | C     | 805 | Y01  | CBH-CAZ-CAI | -2.18 | 119.75      | 122.93   |
| 2   | B     | 804 | Y01  | CAT-CBH-CBF | -2.17 | 105.86      | 108.74   |
| 2   | D     | 804 | Y01  | OAW-CAY-OAG | -2.16 | 118.64      | 123.70   |
| 2   | B     | 803 | Y01  | OAH-CAX-CAL | 2.16  | 120.81      | 114.00   |
| 4   | D     | 808 | POV  | C2-O21-C21  | 2.13  | 122.90      | 117.80   |
| 4   | A     | 805 | POV  | C2-O21-C21  | 2.10  | 122.81      | 117.80   |
| 2   | A     | 810 | Y01  | CAQ-CBG-CBD | -2.09 | 115.76      | 119.10   |
| 2   | C     | 801 | Y01  | CBH-CAZ-CAI | -2.09 | 119.88      | 122.93   |
| 2   | A     | 802 | Y01  | CBF-CBD-CBG | 2.09  | 111.81      | 109.09   |
| 2   | B     | 801 | Y01  | CBH-CAZ-CAI | -2.06 | 119.93      | 122.93   |
| 2   | A     | 801 | Y01  | OAH-CAX-CAL | 2.05  | 120.49      | 114.00   |
| 2   | C     | 805 | Y01  | OAH-CAX-CAL | 2.05  | 120.49      | 114.00   |
| 2   | A     | 801 | Y01  | CAT-CBH-CBF | -2.05 | 106.02      | 108.74   |
| 2   | C     | 803 | Y01  | OAH-CAX-CAL | 2.05  | 120.48      | 114.00   |
| 2   | D     | 804 | Y01  | CAQ-CBG-CBD | -2.04 | 115.85      | 119.10   |
| 2   | B     | 801 | Y01  | OAH-CAX-CAL | 2.03  | 120.42      | 114.00   |
| 2   | D     | 804 | Y01  | OAH-CAX-CAL | 2.03  | 120.40      | 114.00   |
| 2   | C     | 801 | Y01  | OAH-CAX-CAL | 2.02  | 120.38      | 114.00   |
| 2   | C     | 803 | Y01  | CAT-CBH-CBF | -2.01 | 106.08      | 108.74   |
| 2   | A     | 810 | Y01  | CBH-CAZ-CAI | -2.01 | 120.00      | 122.93   |

All (48) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 2   | A     | 801 | Y01  | CBC  |
| 2   | A     | 801 | Y01  | CBG  |
| 2   | A     | 801 | Y01  | CBF  |
| 2   | A     | 801 | Y01  | CBD  |
| 2   | A     | 802 | Y01  | CBC  |
| 2   | A     | 802 | Y01  | CBG  |
| 2   | A     | 802 | Y01  | CBF  |
| 2   | A     | 802 | Y01  | CBD  |
| 2   | A     | 810 | Y01  | CBC  |
| 2   | A     | 810 | Y01  | CBG  |
| 2   | A     | 810 | Y01  | CBF  |
| 2   | A     | 810 | Y01  | CBD  |
| 2   | B     | 801 | Y01  | CBC  |
| 2   | B     | 801 | Y01  | CBG  |
| 2   | B     | 801 | Y01  | CBF  |
| 2   | B     | 801 | Y01  | CBD  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 2   | B     | 803 | Y01  | CBC  |
| 2   | B     | 803 | Y01  | CBG  |
| 2   | B     | 803 | Y01  | CBF  |
| 2   | B     | 803 | Y01  | CBD  |
| 2   | B     | 804 | Y01  | CBC  |
| 2   | B     | 804 | Y01  | CBG  |
| 2   | B     | 804 | Y01  | CBF  |
| 2   | B     | 804 | Y01  | CBD  |
| 2   | C     | 801 | Y01  | CBC  |
| 2   | C     | 801 | Y01  | CBG  |
| 2   | C     | 801 | Y01  | CBF  |
| 2   | C     | 801 | Y01  | CBD  |
| 2   | C     | 803 | Y01  | CBC  |
| 2   | C     | 803 | Y01  | CBG  |
| 2   | C     | 803 | Y01  | CBF  |
| 2   | C     | 803 | Y01  | CBD  |
| 2   | C     | 804 | Y01  | CBC  |
| 2   | C     | 804 | Y01  | CBG  |
| 2   | C     | 804 | Y01  | CBF  |
| 2   | C     | 804 | Y01  | CBD  |
| 2   | C     | 805 | Y01  | CBC  |
| 2   | C     | 805 | Y01  | CBG  |
| 2   | C     | 805 | Y01  | CBF  |
| 2   | C     | 805 | Y01  | CBD  |
| 2   | D     | 804 | Y01  | CBC  |
| 2   | D     | 804 | Y01  | CBG  |
| 2   | D     | 804 | Y01  | CBF  |
| 2   | D     | 804 | Y01  | CBD  |
| 2   | D     | 805 | Y01  | CBC  |
| 2   | D     | 805 | Y01  | CBG  |
| 2   | D     | 805 | Y01  | CBF  |
| 2   | D     | 805 | Y01  | CBD  |

All (532) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | A     | 801 | Y01  | CAC-CBB-CBE-CBI |
| 2   | A     | 801 | Y01  | CAM-CAY-OAW-CBC |
| 2   | A     | 801 | Y01  | CAX-CAL-CAM-CAY |
| 2   | A     | 802 | Y01  | CAO-CBB-CBE-CAP |
| 2   | A     | 802 | Y01  | CAO-CBB-CBE-CBI |
| 2   | A     | 802 | Y01  | CAC-CBB-CBE-CBI |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | A     | 802 | Y01  | CAM-CAY-OAW-CBC |
| 2   | A     | 810 | Y01  | CAV-CBC-OAW-CAY |
| 2   | A     | 810 | Y01  | CAM-CAY-OAW-CBC |
| 2   | B     | 801 | Y01  | CAV-CBC-OAW-CAY |
| 2   | B     | 801 | Y01  | CAM-CAY-OAW-CBC |
| 2   | B     | 803 | Y01  | CAC-CBB-CBE-CBI |
| 2   | B     | 803 | Y01  | CAM-CAY-OAW-CBC |
| 2   | B     | 803 | Y01  | CAX-CAL-CAM-CAY |
| 2   | B     | 804 | Y01  | CAC-CBB-CBE-CAP |
| 2   | B     | 804 | Y01  | CAC-CBB-CBE-CBI |
| 2   | B     | 804 | Y01  | CAM-CAY-OAW-CBC |
| 2   | C     | 801 | Y01  | CAV-CBC-OAW-CAY |
| 2   | C     | 801 | Y01  | CAM-CAY-OAW-CBC |
| 2   | C     | 803 | Y01  | CAC-CBB-CBE-CBI |
| 2   | C     | 803 | Y01  | CAM-CAY-OAW-CBC |
| 2   | C     | 804 | Y01  | CAO-CBB-CBE-CBI |
| 2   | C     | 804 | Y01  | CAC-CBB-CBE-CAP |
| 2   | C     | 804 | Y01  | CAC-CBB-CBE-CBI |
| 2   | C     | 804 | Y01  | CAM-CAY-OAW-CBC |
| 2   | C     | 805 | Y01  | CAV-CBC-OAW-CAY |
| 2   | C     | 805 | Y01  | CAM-CAY-OAW-CBC |
| 2   | D     | 804 | Y01  | CAC-CBB-CBE-CBI |
| 2   | D     | 804 | Y01  | CAM-CAY-OAW-CBC |
| 2   | D     | 805 | Y01  | CAC-CBB-CBE-CAP |
| 2   | D     | 805 | Y01  | CAC-CBB-CBE-CBI |
| 2   | D     | 805 | Y01  | CAM-CAY-OAW-CBC |
| 4   | A     | 805 | POV  | C1-O11-P-O12    |
| 4   | A     | 805 | POV  | C1-O11-P-O13    |
| 4   | A     | 805 | POV  | C11-O12-P-O11   |
| 4   | A     | 805 | POV  | O12-C11-C12-N   |
| 4   | A     | 811 | POV  | C11-O12-P-O13   |
| 4   | B     | 802 | POV  | C11-O12-P-O11   |
| 4   | B     | 802 | POV  | C11-O12-P-O13   |
| 4   | B     | 807 | POV  | C1-O11-P-O12    |
| 4   | B     | 807 | POV  | C1-O11-P-O13    |
| 4   | B     | 807 | POV  | C11-O12-P-O11   |
| 4   | B     | 807 | POV  | C11-O12-P-O13   |
| 4   | B     | 807 | POV  | O12-C11-C12-N   |
| 4   | C     | 802 | POV  | C11-O12-P-O13   |
| 4   | C     | 808 | POV  | C1-O11-P-O12    |
| 4   | C     | 808 | POV  | C11-O12-P-O11   |
| 4   | C     | 808 | POV  | O12-C11-C12-N   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms               |
|-----|-------|-----|------|---------------------|
| 4   | D     | 803 | POV  | C11-O12-P-O13       |
| 4   | D     | 808 | POV  | C1-O11-P-O12        |
| 4   | D     | 808 | POV  | C1-O11-P-O13        |
| 4   | D     | 808 | POV  | C11-O12-P-O11       |
| 4   | D     | 808 | POV  | C11-O12-P-O13       |
| 4   | D     | 808 | POV  | O12-C11-C12-N       |
| 2   | A     | 810 | Y01  | CAN-CAJ-CAO-CBB     |
| 2   | B     | 801 | Y01  | CAN-CAJ-CAO-CBB     |
| 2   | C     | 801 | Y01  | CAN-CAJ-CAO-CBB     |
| 2   | A     | 802 | Y01  | CAC-CBB-CBE-CAP     |
| 2   | D     | 804 | Y01  | CAC-CBB-CBE-CAP     |
| 2   | B     | 804 | Y01  | CAO-CBB-CBE-CBI     |
| 2   | D     | 805 | Y01  | CAO-CBB-CBE-CBI     |
| 2   | C     | 805 | Y01  | CAN-CAJ-CAO-CBB     |
| 2   | A     | 801 | Y01  | OAG-CAY-OAW-CBC     |
| 2   | A     | 802 | Y01  | OAG-CAY-OAW-CBC     |
| 2   | A     | 810 | Y01  | OAG-CAY-OAW-CBC     |
| 2   | B     | 801 | Y01  | OAG-CAY-OAW-CBC     |
| 2   | B     | 803 | Y01  | OAG-CAY-OAW-CBC     |
| 2   | B     | 804 | Y01  | OAG-CAY-OAW-CBC     |
| 2   | C     | 801 | Y01  | OAG-CAY-OAW-CBC     |
| 2   | C     | 803 | Y01  | OAG-CAY-OAW-CBC     |
| 2   | C     | 804 | Y01  | OAG-CAY-OAW-CBC     |
| 2   | C     | 805 | Y01  | OAG-CAY-OAW-CBC     |
| 2   | D     | 804 | Y01  | OAG-CAY-OAW-CBC     |
| 2   | D     | 805 | Y01  | OAG-CAY-OAW-CBC     |
| 2   | A     | 802 | Y01  | CAJ-CAO-CBB-CAC     |
| 2   | B     | 804 | Y01  | CAJ-CAO-CBB-CAC     |
| 2   | C     | 804 | Y01  | CAJ-CAO-CBB-CAC     |
| 2   | D     | 805 | Y01  | CAJ-CAO-CBB-CAC     |
| 2   | A     | 801 | Y01  | CAC-CBB-CBE-CAP     |
| 2   | B     | 803 | Y01  | CAC-CBB-CBE-CAP     |
| 2   | C     | 803 | Y01  | CAC-CBB-CBE-CAP     |
| 2   | B     | 804 | Y01  | CAO-CBB-CBE-CAP     |
| 2   | C     | 804 | Y01  | CAO-CBB-CBE-CAP     |
| 2   | D     | 805 | Y01  | CAO-CBB-CBE-CAP     |
| 2   | A     | 801 | Y01  | CAO-CBB-CBE-CBI     |
| 2   | B     | 803 | Y01  | CAO-CBB-CBE-CBI     |
| 2   | C     | 803 | Y01  | CAO-CBB-CBE-CBI     |
| 2   | D     | 804 | Y01  | CAO-CBB-CBE-CBI     |
| 2   | D     | 804 | Y01  | CAO-CBB-CBE-CAP     |
| 4   | A     | 807 | POV  | C211-C212-C213-C214 |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms               |
|-----|-------|-----|------|---------------------|
| 2   | B     | 803 | Y01  | CAJ-CAO-CBB-CAC     |
| 2   | A     | 810 | Y01  | CAC-CBB-CBE-CBI     |
| 2   | A     | 801 | Y01  | CAO-CBB-CBE-CAP     |
| 2   | C     | 803 | Y01  | CAO-CBB-CBE-CAP     |
| 4   | C     | 810 | POV  | C211-C212-C213-C214 |
| 2   | A     | 810 | Y01  | CAJ-CAO-CBB-CAC     |
| 2   | B     | 801 | Y01  | CAJ-CAO-CBB-CAC     |
| 2   | C     | 801 | Y01  | CAJ-CAO-CBB-CAC     |
| 2   | C     | 805 | Y01  | CAJ-CAO-CBB-CAC     |
| 2   | A     | 810 | Y01  | CAJ-CAO-CBB-CBE     |
| 2   | B     | 801 | Y01  | CAJ-CAO-CBB-CBE     |
| 2   | B     | 803 | Y01  | CAJ-CAO-CBB-CBE     |
| 2   | C     | 801 | Y01  | CAJ-CAO-CBB-CBE     |
| 2   | C     | 805 | Y01  | CAJ-CAO-CBB-CBE     |
| 4   | C     | 808 | POV  | C37-C38-C39-C310    |
| 4   | D     | 810 | POV  | C211-C212-C213-C214 |
| 4   | A     | 809 | POV  | C32-C33-C34-C35     |
| 4   | A     | 809 | POV  | C37-C38-C39-C310    |
| 4   | B     | 806 | POV  | C32-C33-C34-C35     |
| 4   | C     | 812 | POV  | C32-C33-C34-C35     |
| 2   | C     | 803 | Y01  | CAX-CAL-CAM-CAY     |
| 4   | B     | 811 | POV  | C37-C38-C39-C310    |
| 2   | C     | 803 | Y01  | CAJ-CAO-CBB-CAC     |
| 4   | A     | 805 | POV  | C37-C38-C39-C310    |
| 4   | A     | 811 | POV  | C21-C22-C23-C24     |
| 4   | C     | 802 | POV  | C21-C22-C23-C24     |
| 4   | D     | 803 | POV  | C21-C22-C23-C24     |
| 2   | B     | 803 | Y01  | CAO-CBB-CBE-CAP     |
| 2   | B     | 804 | Y01  | CAJ-CAO-CBB-CBE     |
| 2   | C     | 804 | Y01  | CAJ-CAO-CBB-CBE     |
| 2   | D     | 805 | Y01  | CAJ-CAO-CBB-CBE     |
| 4   | B     | 807 | POV  | C37-C38-C39-C310    |
| 4   | D     | 808 | POV  | C37-C38-C39-C310    |
| 2   | A     | 801 | Y01  | CAJ-CAO-CBB-CAC     |
| 2   | D     | 804 | Y01  | CAJ-CAO-CBB-CAC     |
| 4   | D     | 802 | POV  | C37-C38-C39-C310    |
| 4   | B     | 802 | POV  | C21-C22-C23-C24     |
| 4   | C     | 812 | POV  | C37-C38-C39-C310    |
| 2   | A     | 802 | Y01  | CAJ-CAO-CBB-CBE     |
| 2   | C     | 803 | Y01  | CAJ-CAO-CBB-CBE     |
| 4   | B     | 811 | POV  | C32-C33-C34-C35     |
| 2   | B     | 801 | Y01  | CAC-CBB-CBE-CBI     |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms               |
|-----|-------|-----|------|---------------------|
| 2   | C     | 801 | Y01  | CAC-CBB-CBE-CBI     |
| 4   | A     | 807 | POV  | C211-C210-C29-C28   |
| 4   | C     | 810 | POV  | C211-C210-C29-C28   |
| 4   | D     | 810 | POV  | C211-C210-C29-C28   |
| 4   | A     | 811 | POV  | O22-C21-O21-C2      |
| 4   | A     | 809 | POV  | C32-C31-O31-C3      |
| 2   | A     | 802 | Y01  | CAN-CAJ-CAO-CBB     |
| 2   | D     | 805 | Y01  | CAN-CAJ-CAO-CBB     |
| 2   | A     | 801 | Y01  | CAJ-CAO-CBB-CBE     |
| 2   | D     | 804 | Y01  | CAJ-CAO-CBB-CBE     |
| 2   | B     | 804 | Y01  | CAN-CAJ-CAO-CBB     |
| 2   | C     | 801 | Y01  | CAO-CAJ-CAN-CBA     |
| 2   | C     | 805 | Y01  | CAO-CAJ-CAN-CBA     |
| 4   | C     | 812 | POV  | C32-C31-O31-C3      |
| 2   | D     | 804 | Y01  | CAX-CAL-CAM-CAY     |
| 2   | C     | 804 | Y01  | CAN-CAJ-CAO-CBB     |
| 4   | A     | 811 | POV  | C22-C21-O21-C2      |
| 4   | B     | 802 | POV  | C22-C21-O21-C2      |
| 4   | C     | 802 | POV  | C22-C21-O21-C2      |
| 4   | B     | 802 | POV  | O22-C21-O21-C2      |
| 4   | C     | 802 | POV  | O22-C21-O21-C2      |
| 2   | C     | 805 | Y01  | CAC-CBB-CBE-CBI     |
| 4   | B     | 809 | POV  | C211-C210-C29-C28   |
| 2   | B     | 801 | Y01  | CAJ-CAN-CBA-CAA     |
| 2   | C     | 801 | Y01  | CAJ-CAN-CBA-CAA     |
| 2   | C     | 805 | Y01  | CAJ-CAN-CBA-CAA     |
| 4   | C     | 807 | POV  | C32-C33-C34-C35     |
| 4   | D     | 802 | POV  | C32-C31-O31-C3      |
| 4   | C     | 807 | POV  | C34-C35-C36-C37     |
| 4   | D     | 808 | POV  | C310-C311-C312-C313 |
| 4   | A     | 805 | POV  | C311-C310-C39-C38   |
| 4   | B     | 807 | POV  | C311-C310-C39-C38   |
| 4   | D     | 802 | POV  | C34-C35-C36-C37     |
| 4   | D     | 807 | POV  | C34-C35-C36-C37     |
| 4   | C     | 808 | POV  | C25-C26-C27-C28     |
| 4   | D     | 808 | POV  | C311-C310-C39-C38   |
| 4   | B     | 811 | POV  | C34-C35-C36-C37     |
| 4   | D     | 808 | POV  | C25-C26-C27-C28     |
| 4   | A     | 805 | POV  | C24-C25-C26-C27     |
| 4   | A     | 808 | POV  | C34-C35-C36-C37     |
| 4   | C     | 811 | POV  | C34-C35-C36-C37     |
| 4   | D     | 801 | POV  | C34-C35-C36-C37     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms               |
|-----|-------|-----|------|---------------------|
| 2   | A     | 810 | Y01  | CAJ-CAN-CBA-CAA     |
| 3   | D     | 806 | PCW  | C16-C17-C18-C19     |
| 2   | A     | 810 | Y01  | CAO-CBB-CBE-CBI     |
| 4   | A     | 805 | POV  | C310-C311-C312-C313 |
| 4   | B     | 807 | POV  | C25-C26-C27-C28     |
| 4   | B     | 810 | POV  | C34-C35-C36-C37     |
| 2   | B     | 801 | Y01  | CAO-CAJ-CAN-CBA     |
| 4   | D     | 803 | POV  | C22-C21-O21-C2      |
| 4   | A     | 805 | POV  | C25-C26-C27-C28     |
| 4   | A     | 808 | POV  | C36-C37-C38-C39     |
| 4   | C     | 811 | POV  | C36-C37-C38-C39     |
| 4   | C     | 808 | POV  | C310-C311-C312-C313 |
| 4   | C     | 812 | POV  | C34-C35-C36-C37     |
| 4   | D     | 801 | POV  | C36-C37-C38-C39     |
| 4   | D     | 808 | POV  | C24-C25-C26-C27     |
| 4   | C     | 808 | POV  | C24-C25-C26-C27     |
| 4   | B     | 807 | POV  | C310-C311-C312-C313 |
| 2   | C     | 804 | Y01  | CAJ-CAN-CBA-CAB     |
| 4   | A     | 809 | POV  | O32-C31-O31-C3      |
| 4   | C     | 812 | POV  | O32-C31-O31-C3      |
| 4   | C     | 802 | POV  | C310-C311-C312-C313 |
| 4   | A     | 811 | POV  | C310-C311-C312-C313 |
| 4   | B     | 810 | POV  | C36-C37-C38-C39     |
| 4   | D     | 803 | POV  | C310-C311-C312-C313 |
| 4   | B     | 810 | POV  | C213-C214-C215-C216 |
| 4   | A     | 806 | POV  | C214-C215-C216-C217 |
| 4   | A     | 809 | POV  | C311-C310-C39-C38   |
| 4   | B     | 802 | POV  | C310-C311-C312-C313 |
| 4   | B     | 807 | POV  | C24-C25-C26-C27     |
| 4   | C     | 808 | POV  | C311-C310-C39-C38   |
| 4   | C     | 810 | POV  | C23-C24-C25-C26     |
| 4   | D     | 810 | POV  | C23-C24-C25-C26     |
| 4   | A     | 811 | POV  | C33-C34-C35-C36     |
| 4   | B     | 806 | POV  | C34-C35-C36-C37     |
| 4   | B     | 808 | POV  | C214-C215-C216-C217 |
| 4   | C     | 809 | POV  | C214-C215-C216-C217 |
| 4   | D     | 809 | POV  | C214-C215-C216-C217 |
| 4   | A     | 809 | POV  | C34-C35-C36-C37     |
| 4   | B     | 802 | POV  | C33-C34-C35-C36     |
| 4   | B     | 809 | POV  | C23-C24-C25-C26     |
| 2   | A     | 802 | Y01  | CAJ-CAN-CBA-CAB     |
| 4   | D     | 808 | POV  | C22-C21-O21-C2      |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms               |
|-----|-------|-----|------|---------------------|
| 4   | D     | 803 | POV  | C32-C31-O31-C3      |
| 4   | C     | 802 | POV  | C33-C34-C35-C36     |
| 4   | A     | 807 | POV  | C23-C24-C25-C26     |
| 4   | D     | 802 | POV  | O32-C31-O31-C3      |
| 4   | A     | 804 | POV  | C34-C35-C36-C37     |
| 4   | D     | 803 | POV  | C33-C34-C35-C36     |
| 4   | D     | 803 | POV  | O22-C21-O21-C2      |
| 4   | B     | 807 | POV  | C32-C31-O31-C3      |
| 4   | C     | 808 | POV  | C32-C31-O31-C3      |
| 4   | B     | 811 | POV  | C311-C310-C39-C38   |
| 4   | D     | 801 | POV  | C213-C214-C215-C216 |
| 4   | C     | 812 | POV  | C311-C310-C39-C38   |
| 4   | C     | 811 | POV  | C213-C214-C215-C216 |
| 2   | A     | 810 | Y01  | CAC-CBB-CBE-CAP     |
| 4   | A     | 805 | POV  | C22-C21-O21-C2      |
| 4   | B     | 807 | POV  | C22-C21-O21-C2      |
| 4   | C     | 808 | POV  | C22-C21-O21-C2      |
| 4   | A     | 808 | POV  | C213-C214-C215-C216 |
| 4   | B     | 807 | POV  | O22-C21-O21-C2      |
| 3   | B     | 805 | PCW  | C16-C17-C18-C19     |
| 3   | C     | 806 | PCW  | C16-C17-C18-C19     |
| 4   | A     | 805 | POV  | C210-C211-C212-C213 |
| 4   | B     | 807 | POV  | C210-C211-C212-C213 |
| 4   | C     | 808 | POV  | C210-C211-C212-C213 |
| 4   | C     | 810 | POV  | C210-C211-C212-C213 |
| 4   | D     | 801 | POV  | C210-C211-C212-C213 |
| 4   | D     | 808 | POV  | C210-C211-C212-C213 |
| 4   | A     | 811 | POV  | C22-C23-C24-C25     |
| 4   | B     | 811 | POV  | C32-C31-O31-C3      |
| 4   | B     | 806 | POV  | C36-C37-C38-C39     |
| 4   | D     | 802 | POV  | C311-C310-C39-C38   |
| 2   | A     | 801 | Y01  | CAJ-CAN-CBA-CAB     |
| 2   | B     | 803 | Y01  | CAJ-CAN-CBA-CAB     |
| 2   | C     | 803 | Y01  | CAJ-CAN-CBA-CAB     |
| 2   | A     | 810 | Y01  | CAX-CAL-CAM-CAY     |
| 2   | C     | 801 | Y01  | CAX-CAL-CAM-CAY     |
| 4   | C     | 802 | POV  | C22-C23-C24-C25     |
| 4   | C     | 808 | POV  | C212-C213-C214-C215 |
| 4   | B     | 802 | POV  | C22-C23-C24-C25     |
| 4   | C     | 808 | POV  | O22-C21-O21-C2      |
| 4   | B     | 807 | POV  | C313-C314-C315-C316 |
| 2   | B     | 804 | Y01  | CAJ-CAN-CBA-CAB     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms               |
|-----|-------|-----|------|---------------------|
| 2   | D     | 804 | Y01  | CAJ-CAN-CBA-CAB     |
| 4   | B     | 807 | POV  | C212-C213-C214-C215 |
| 4   | B     | 807 | POV  | O32-C31-O31-C3      |
| 4   | C     | 808 | POV  | O32-C31-O31-C3      |
| 4   | D     | 803 | POV  | O32-C31-O31-C3      |
| 4   | A     | 805 | POV  | C212-C213-C214-C215 |
| 4   | A     | 808 | POV  | C311-C310-C39-C38   |
| 4   | C     | 811 | POV  | C311-C310-C39-C38   |
| 4   | D     | 801 | POV  | C311-C310-C39-C38   |
| 2   | A     | 810 | Y01  | CAO-CAJ-CAN-CBA     |
| 4   | D     | 808 | POV  | C212-C213-C214-C215 |
| 3   | A     | 803 | PCW  | C16-C17-C18-C19     |
| 4   | B     | 809 | POV  | C210-C211-C212-C213 |
| 4   | D     | 810 | POV  | C210-C211-C212-C213 |
| 4   | B     | 802 | POV  | C32-C31-O31-C3      |
| 4   | A     | 805 | POV  | O32-C31-O31-C3      |
| 4   | B     | 810 | POV  | C311-C310-C39-C38   |
| 4   | D     | 803 | POV  | C22-C23-C24-C25     |
| 4   | A     | 805 | POV  | C313-C314-C315-C316 |
| 4   | C     | 807 | POV  | C36-C37-C38-C39     |
| 4   | D     | 802 | POV  | C36-C37-C38-C39     |
| 4   | D     | 807 | POV  | C32-C33-C34-C35     |
| 4   | D     | 808 | POV  | C313-C314-C315-C316 |
| 4   | D     | 808 | POV  | O22-C21-O21-C2      |
| 4   | D     | 807 | POV  | C36-C37-C38-C39     |
| 2   | B     | 801 | Y01  | CAX-CAL-CAM-CAY     |
| 4   | A     | 805 | POV  | C32-C31-O31-C3      |
| 4   | A     | 808 | POV  | C212-C213-C214-C215 |
| 4   | A     | 809 | POV  | C36-C37-C38-C39     |
| 4   | C     | 808 | POV  | C313-C314-C315-C316 |
| 4   | A     | 804 | POV  | C32-C33-C34-C35     |
| 4   | B     | 811 | POV  | C36-C37-C38-C39     |
| 4   | A     | 805 | POV  | O22-C21-O21-C2      |
| 2   | D     | 805 | Y01  | CAJ-CAN-CBA-CAB     |
| 4   | A     | 808 | POV  | C39-C310-C311-C312  |
| 4   | D     | 801 | POV  | C39-C310-C311-C312  |
| 2   | C     | 805 | Y01  | CAX-CAL-CAM-CAY     |
| 2   | B     | 801 | Y01  | CAO-CBB-CBE-CBI     |
| 2   | C     | 801 | Y01  | CAO-CBB-CBE-CBI     |
| 4   | B     | 810 | POV  | C39-C310-C311-C312  |
| 4   | C     | 811 | POV  | C39-C310-C311-C312  |
| 4   | D     | 808 | POV  | C31-C32-C33-C34     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms               |
|-----|-------|-----|------|---------------------|
| 4   | A     | 811 | POV  | C32-C31-O31-C3      |
| 4   | C     | 802 | POV  | C32-C31-O31-C3      |
| 3   | B     | 805 | PCW  | C19-C20-C21-C22     |
| 4   | B     | 807 | POV  | C22-C23-C24-C25     |
| 4   | D     | 802 | POV  | C32-C33-C34-C35     |
| 4   | A     | 811 | POV  | C1-C2-C3-O31        |
| 4   | B     | 802 | POV  | C1-C2-C3-O31        |
| 4   | C     | 802 | POV  | C1-C2-C3-O31        |
| 4   | A     | 807 | POV  | C210-C211-C212-C213 |
| 4   | C     | 811 | POV  | C210-C211-C212-C213 |
| 4   | C     | 808 | POV  | C22-C23-C24-C25     |
| 4   | D     | 808 | POV  | C32-C31-O31-C3      |
| 4   | B     | 807 | POV  | C31-C32-C33-C34     |
| 4   | B     | 811 | POV  | O32-C31-O31-C3      |
| 4   | B     | 810 | POV  | C212-C213-C214-C215 |
| 4   | C     | 808 | POV  | C31-C32-C33-C34     |
| 4   | B     | 802 | POV  | O32-C31-O31-C3      |
| 2   | D     | 805 | Y01  | CAO-CAJ-CAN-CBA     |
| 4   | A     | 811 | POV  | O32-C31-O31-C3      |
| 2   | B     | 801 | Y01  | CAC-CBB-CBE-CAP     |
| 2   | C     | 801 | Y01  | CAC-CBB-CBE-CAP     |
| 4   | C     | 812 | POV  | C36-C37-C38-C39     |
| 4   | A     | 805 | POV  | C3-C2-O21-C21       |
| 4   | D     | 808 | POV  | C3-C2-O21-C21       |
| 4   | B     | 810 | POV  | C210-C211-C212-C213 |
| 4   | B     | 806 | POV  | C33-C34-C35-C36     |
| 4   | C     | 802 | POV  | O32-C31-O31-C3      |
| 4   | D     | 808 | POV  | O32-C31-O31-C3      |
| 4   | B     | 809 | POV  | C211-C212-C213-C214 |
| 2   | C     | 805 | Y01  | CAO-CBB-CBE-CBI     |
| 2   | C     | 805 | Y01  | CAC-CBB-CBE-CAP     |
| 4   | A     | 804 | POV  | C36-C37-C38-C39     |
| 4   | A     | 805 | POV  | C22-C23-C24-C25     |
| 4   | B     | 806 | POV  | C311-C310-C39-C38   |
| 4   | D     | 801 | POV  | C211-C212-C213-C214 |
| 4   | C     | 802 | POV  | C313-C314-C315-C316 |
| 4   | C     | 808 | POV  | C36-C37-C38-C39     |
| 4   | D     | 808 | POV  | C22-C23-C24-C25     |
| 3   | D     | 806 | PCW  | C19-C20-C21-C22     |
| 4   | B     | 809 | POV  | C29-C210-C211-C212  |
| 2   | A     | 802 | Y01  | CAO-CAJ-CAN-CBA     |
| 4   | D     | 803 | POV  | C313-C314-C315-C316 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms               |
|-----|-------|-----|------|---------------------|
| 4   | B     | 802 | POV  | C313-C314-C315-C316 |
| 4   | B     | 809 | POV  | C213-C214-C215-C216 |
| 4   | A     | 811 | POV  | C39-C310-C311-C312  |
| 4   | C     | 802 | POV  | C39-C310-C311-C312  |
| 4   | D     | 810 | POV  | C213-C214-C215-C216 |
| 4   | B     | 802 | POV  | C39-C310-C311-C312  |
| 4   | D     | 803 | POV  | C39-C310-C311-C312  |
| 2   | C     | 804 | Y01  | CAO-CAJ-CAN-CBA     |
| 4   | C     | 807 | POV  | C311-C310-C39-C38   |
| 4   | A     | 808 | POV  | C210-C211-C212-C213 |
| 4   | D     | 807 | POV  | C311-C310-C39-C38   |
| 4   | A     | 811 | POV  | C313-C314-C315-C316 |
| 4   | A     | 806 | POV  | C213-C214-C215-C216 |
| 4   | A     | 805 | POV  | C31-C32-C33-C34     |
| 2   | C     | 804 | Y01  | CAJ-CAN-CBA-CAA     |
| 4   | D     | 801 | POV  | C212-C213-C214-C215 |
| 4   | C     | 809 | POV  | C213-C214-C215-C216 |
| 4   | C     | 811 | POV  | C212-C213-C214-C215 |
| 4   | D     | 809 | POV  | C213-C214-C215-C216 |
| 4   | C     | 808 | POV  | C21-C22-C23-C24     |
| 4   | B     | 808 | POV  | C213-C214-C215-C216 |
| 4   | B     | 807 | POV  | C21-C22-C23-C24     |
| 4   | B     | 808 | POV  | C211-C212-C213-C214 |
| 4   | D     | 809 | POV  | C211-C212-C213-C214 |
| 2   | C     | 801 | Y01  | CAJ-CAN-CBA-CAB     |
| 4   | B     | 807 | POV  | C311-C312-C313-C314 |
| 4   | A     | 805 | POV  | C35-C36-C37-C38     |
| 2   | D     | 805 | Y01  | CAJ-CAN-CBA-CAA     |
| 4   | C     | 809 | POV  | C211-C212-C213-C214 |
| 4   | D     | 808 | POV  | C311-C312-C313-C314 |
| 4   | C     | 808 | POV  | C35-C36-C37-C38     |
| 4   | A     | 808 | POV  | C29-C210-C211-C212  |
| 4   | A     | 806 | POV  | C211-C212-C213-C214 |
| 4   | A     | 804 | POV  | C311-C310-C39-C38   |
| 2   | A     | 802 | Y01  | CAJ-CAN-CBA-CAA     |
| 2   | A     | 810 | Y01  | CAJ-CAN-CBA-CAB     |
| 2   | B     | 804 | Y01  | CAJ-CAN-CBA-CAA     |
| 2   | C     | 805 | Y01  | CAJ-CAN-CBA-CAB     |
| 4   | A     | 805 | POV  | C36-C37-C38-C39     |
| 2   | B     | 801 | Y01  | CAJ-CAN-CBA-CAB     |
| 4   | C     | 811 | POV  | C211-C212-C213-C214 |
| 4   | B     | 807 | POV  | C36-C37-C38-C39     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms               |
|-----|-------|-----|------|---------------------|
| 2   | D     | 804 | Y01  | CAO-CAJ-CAN-CBA     |
| 2   | A     | 801 | Y01  | CAJ-CAN-CBA-CAA     |
| 2   | B     | 803 | Y01  | CAJ-CAN-CBA-CAA     |
| 2   | D     | 804 | Y01  | CAJ-CAN-CBA-CAA     |
| 4   | A     | 805 | POV  | C311-C312-C313-C314 |
| 4   | D     | 810 | POV  | C29-C210-C211-C212  |
| 2   | A     | 801 | Y01  | CAO-CAJ-CAN-CBA     |
| 2   | C     | 803 | Y01  | CAJ-CAN-CBA-CAA     |
| 4   | B     | 807 | POV  | C35-C36-C37-C38     |
| 4   | D     | 808 | POV  | C35-C36-C37-C38     |
| 4   | C     | 807 | POV  | C33-C34-C35-C36     |
| 2   | B     | 803 | Y01  | CAO-CAJ-CAN-CBA     |
| 2   | A     | 810 | Y01  | CAO-CBB-CBE-CAP     |
| 4   | D     | 809 | POV  | C26-C27-C28-C29     |
| 4   | D     | 803 | POV  | C213-C214-C215-C216 |
| 4   | B     | 810 | POV  | C29-C210-C211-C212  |
| 4   | C     | 802 | POV  | C213-C214-C215-C216 |
| 2   | B     | 804 | Y01  | CAO-CAJ-CAN-CBA     |
| 4   | D     | 803 | POV  | C1-C2-C3-O31        |
| 2   | C     | 803 | Y01  | CAO-CAJ-CAN-CBA     |
| 4   | A     | 811 | POV  | C213-C214-C215-C216 |
| 4   | A     | 811 | POV  | O21-C2-C3-O31       |
| 4   | B     | 802 | POV  | O21-C2-C3-O31       |
| 4   | A     | 804 | POV  | C33-C34-C35-C36     |
| 4   | B     | 802 | POV  | C213-C214-C215-C216 |
| 4   | D     | 808 | POV  | C36-C37-C38-C39     |
| 4   | B     | 807 | POV  | C312-C313-C314-C315 |
| 4   | A     | 811 | POV  | O12-C11-C12-N       |
| 4   | B     | 802 | POV  | O12-C11-C12-N       |
| 4   | C     | 802 | POV  | O12-C11-C12-N       |
| 4   | D     | 803 | POV  | O12-C11-C12-N       |
| 4   | C     | 811 | POV  | C29-C210-C211-C212  |
| 4   | C     | 812 | POV  | C313-C314-C315-C316 |
| 4   | C     | 808 | POV  | C39-C310-C311-C312  |
| 4   | D     | 808 | POV  | C312-C313-C314-C315 |
| 4   | A     | 807 | POV  | C29-C210-C211-C212  |
| 4   | B     | 811 | POV  | C313-C314-C315-C316 |
| 4   | D     | 802 | POV  | C313-C314-C315-C316 |
| 4   | D     | 807 | POV  | C33-C34-C35-C36     |
| 3   | C     | 806 | PCW  | C19-C20-C21-C22     |
| 4   | D     | 808 | POV  | C21-C22-C23-C24     |
| 4   | C     | 808 | POV  | C311-C312-C313-C314 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms               |
|-----|-------|-----|------|---------------------|
| 4   | D     | 801 | POV  | C29-C210-C211-C212  |
| 4   | A     | 809 | POV  | C312-C313-C314-C315 |
| 4   | A     | 811 | POV  | C214-C215-C216-C217 |
| 4   | C     | 802 | POV  | C311-C312-C313-C314 |
| 4   | A     | 805 | POV  | C312-C313-C314-C315 |
| 4   | A     | 807 | POV  | C213-C214-C215-C216 |
| 4   | A     | 805 | POV  | C11-O12-P-O13       |
| 4   | A     | 805 | POV  | C11-O12-P-O14       |
| 4   | A     | 811 | POV  | C11-O12-P-O11       |
| 4   | A     | 811 | POV  | C11-O12-P-O14       |
| 4   | B     | 807 | POV  | C11-O12-P-O14       |
| 4   | C     | 802 | POV  | C11-O12-P-O11       |
| 4   | C     | 802 | POV  | C11-O12-P-O14       |
| 4   | C     | 808 | POV  | C11-O12-P-O14       |
| 4   | D     | 803 | POV  | C11-O12-P-O11       |
| 4   | D     | 803 | POV  | C11-O12-P-O14       |
| 4   | D     | 808 | POV  | C11-O12-P-O14       |
| 4   | B     | 802 | POV  | C311-C312-C313-C314 |
| 4   | B     | 810 | POV  | C211-C212-C213-C214 |
| 4   | B     | 811 | POV  | C312-C313-C314-C315 |
| 4   | C     | 810 | POV  | C213-C214-C215-C216 |
| 4   | B     | 807 | POV  | C39-C310-C311-C312  |
| 4   | A     | 805 | POV  | C39-C310-C311-C312  |
| 2   | B     | 801 | Y01  | CAO-CBB-CBE-CAP     |
| 4   | D     | 803 | POV  | C311-C312-C313-C314 |
| 4   | A     | 809 | POV  | C313-C314-C315-C316 |
| 4   | B     | 809 | POV  | C27-C28-C29-C210    |
| 4   | B     | 807 | POV  | C3-C2-O21-C21       |
| 4   | C     | 808 | POV  | C3-C2-O21-C21       |
| 4   | A     | 808 | POV  | C211-C212-C213-C214 |
| 4   | D     | 803 | POV  | O11-C1-C2-O21       |
| 3   | D     | 806 | PCW  | C15-C16-C17-C18     |
| 2   | C     | 801 | Y01  | CAO-CBB-CBE-CAP     |
| 4   | C     | 802 | POV  | O21-C2-C3-O31       |
| 4   | C     | 812 | POV  | C312-C313-C314-C315 |
| 4   | C     | 802 | POV  | C214-C215-C216-C217 |
| 4   | A     | 811 | POV  | C311-C312-C313-C314 |
| 4   | D     | 802 | POV  | C312-C313-C314-C315 |
| 4   | C     | 808 | POV  | C312-C313-C314-C315 |
| 4   | A     | 809 | POV  | C29-C210-C211-C212  |
| 4   | B     | 811 | POV  | C29-C210-C211-C212  |
| 4   | C     | 810 | POV  | C29-C210-C211-C212  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms               |
|-----|-------|-----|------|---------------------|
| 4   | C     | 812 | POV  | C29-C210-C211-C212  |
| 4   | D     | 802 | POV  | C29-C210-C211-C212  |
| 4   | D     | 810 | POV  | C27-C28-C29-C210    |
| 3   | A     | 803 | PCW  | C19-C20-C21-C22     |
| 2   | C     | 805 | Y01  | CAO-CBB-CBE-CAP     |
| 2   | D     | 804 | Y01  | CAV-CBC-OAW-CAY     |
| 4   | D     | 808 | POV  | C39-C310-C311-C312  |
| 4   | D     | 803 | POV  | C31-C32-C33-C34     |
| 4   | D     | 803 | POV  | O11-C1-C2-C3        |
| 3   | B     | 805 | PCW  | C15-C16-C17-C18     |
| 4   | B     | 802 | POV  | C214-C215-C216-C217 |
| 3   | A     | 803 | PCW  | C21-C22-C23-C24     |
| 3   | C     | 806 | PCW  | C21-C22-C23-C24     |
| 4   | A     | 805 | POV  | C21-C22-C23-C24     |
| 4   | A     | 811 | POV  | O11-C1-C2-O21       |
| 3   | D     | 806 | PCW  | C21-C22-C23-C24     |
| 4   | A     | 811 | POV  | C29-C210-C211-C212  |
| 4   | B     | 802 | POV  | C29-C210-C211-C212  |
| 4   | C     | 802 | POV  | C29-C210-C211-C212  |
| 2   | D     | 804 | Y01  | CAR-CBC-OAW-CAY     |
| 4   | C     | 812 | POV  | C310-C311-C312-C313 |
| 4   | B     | 808 | POV  | C26-C27-C28-C29     |
| 4   | B     | 811 | POV  | C210-C211-C212-C213 |
| 4   | C     | 812 | POV  | C210-C211-C212-C213 |
| 4   | A     | 807 | POV  | C27-C28-C29-C210    |
| 4   | B     | 808 | POV  | C27-C28-C29-C210    |
| 4   | D     | 803 | POV  | C29-C210-C211-C212  |
| 4   | D     | 803 | POV  | C214-C215-C216-C217 |
| 4   | A     | 806 | POV  | C27-C28-C29-C210    |
| 4   | C     | 809 | POV  | C27-C28-C29-C210    |
| 4   | A     | 809 | POV  | C210-C211-C212-C213 |
| 4   | A     | 811 | POV  | C26-C27-C28-C29     |
| 4   | D     | 802 | POV  | C210-C211-C212-C213 |
| 3   | B     | 805 | PCW  | C21-C22-C23-C24     |
| 4   | D     | 809 | POV  | C27-C28-C29-C210    |
| 4   | C     | 810 | POV  | C27-C28-C29-C210    |
| 4   | D     | 803 | POV  | C26-C27-C28-C29     |
| 4   | A     | 811 | POV  | O11-C1-C2-C3        |
| 4   | B     | 802 | POV  | O11-C1-C2-C3        |
| 4   | C     | 802 | POV  | O11-C1-C2-C3        |
| 4   | B     | 802 | POV  | C26-C27-C28-C29     |
| 4   | B     | 808 | POV  | C210-C211-C212-C213 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms               |
|-----|-------|-----|------|---------------------|
| 4   | C     | 802 | POV  | C26-C27-C28-C29     |
| 4   | A     | 808 | POV  | C33-C34-C35-C36     |
| 4   | C     | 811 | POV  | C33-C34-C35-C36     |
| 4   | D     | 801 | POV  | C33-C34-C35-C36     |
| 4   | D     | 803 | POV  | C27-C28-C29-C210    |
| 4   | A     | 809 | POV  | C35-C36-C37-C38     |
| 4   | B     | 802 | POV  | C27-C28-C29-C210    |
| 4   | A     | 806 | POV  | C210-C211-C212-C213 |
| 4   | C     | 809 | POV  | C210-C211-C212-C213 |
| 4   | B     | 811 | POV  | C310-C311-C312-C313 |
| 4   | D     | 802 | POV  | C310-C311-C312-C313 |
| 4   | C     | 802 | POV  | C27-C28-C29-C210    |
| 2   | B     | 801 | Y01  | CAM-CAL-CAX-OAF     |
| 4   | A     | 805 | POV  | C33-C34-C35-C36     |
| 4   | C     | 808 | POV  | C29-C210-C211-C212  |
| 4   | B     | 810 | POV  | C33-C34-C35-C36     |
| 4   | A     | 805 | POV  | C29-C210-C211-C212  |
| 4   | A     | 811 | POV  | C27-C28-C29-C210    |
| 4   | B     | 807 | POV  | C29-C210-C211-C212  |
| 4   | B     | 811 | POV  | C3-C2-O21-C21       |
| 4   | D     | 808 | POV  | C29-C210-C211-C212  |
| 2   | B     | 801 | Y01  | CAM-CAL-CAX-OAH     |

There are no ring outliers.

34 monomers are involved in 178 short contacts:

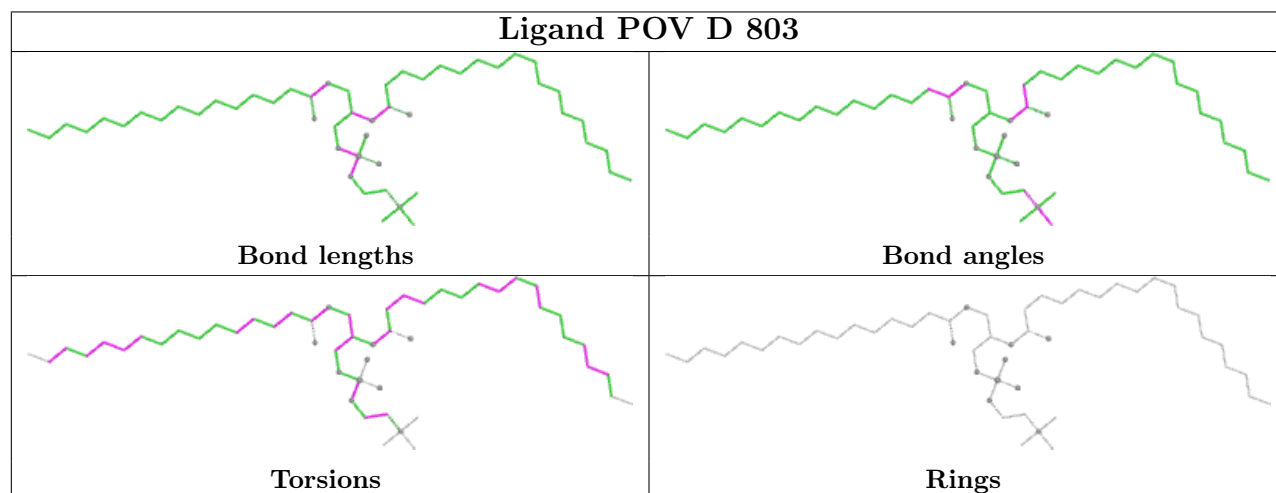
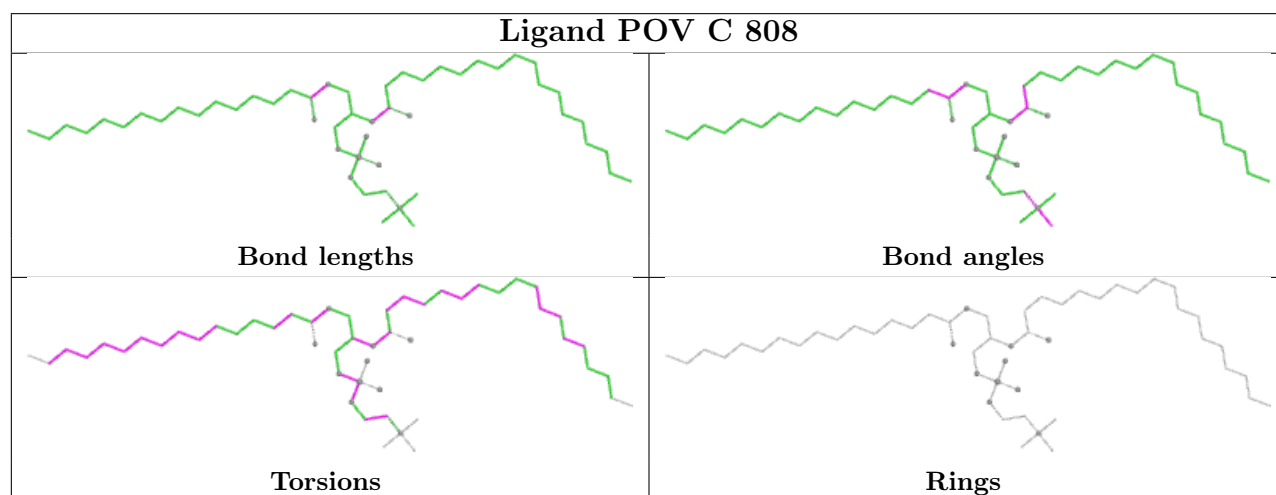
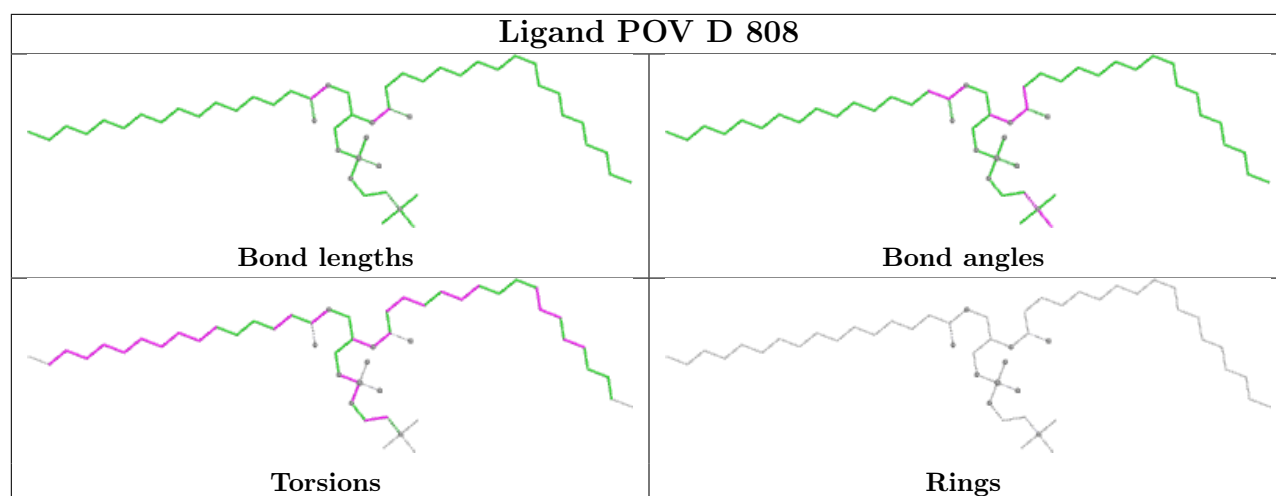
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 4   | D     | 808 | POV  | 1       | 0            |
| 4   | C     | 808 | POV  | 3       | 0            |
| 2   | B     | 801 | Y01  | 14      | 0            |
| 2   | A     | 801 | Y01  | 11      | 0            |
| 2   | C     | 804 | Y01  | 12      | 0            |
| 2   | A     | 802 | Y01  | 14      | 0            |
| 4   | C     | 802 | POV  | 1       | 0            |
| 4   | D     | 802 | POV  | 2       | 0            |
| 4   | D     | 807 | POV  | 1       | 0            |
| 4   | A     | 808 | POV  | 2       | 0            |
| 4   | A     | 806 | POV  | 1       | 0            |
| 2   | A     | 810 | Y01  | 10      | 0            |
| 2   | C     | 803 | Y01  | 10      | 0            |
| 4   | B     | 806 | POV  | 1       | 0            |
| 2   | C     | 801 | Y01  | 13      | 0            |

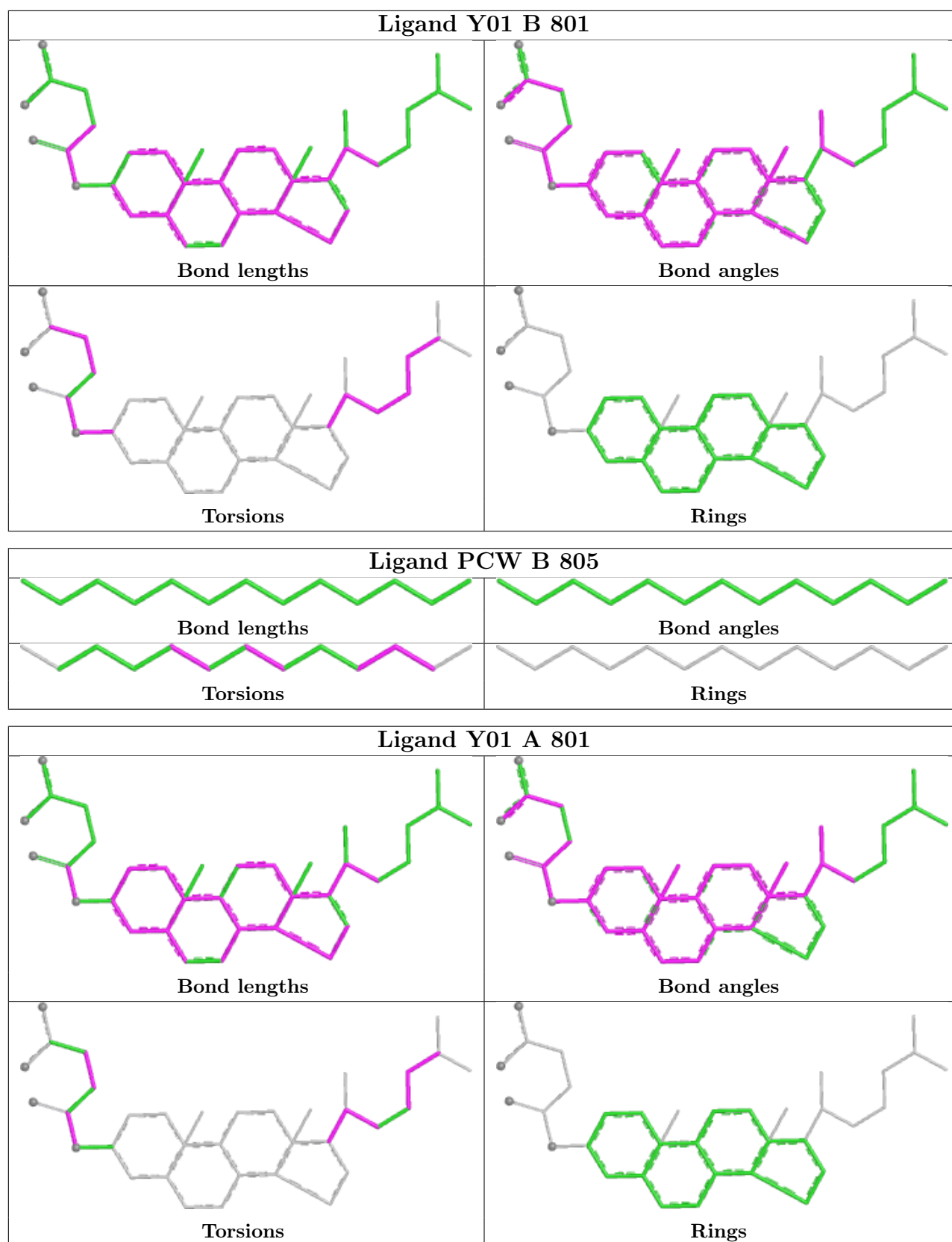
*Continued on next page...*

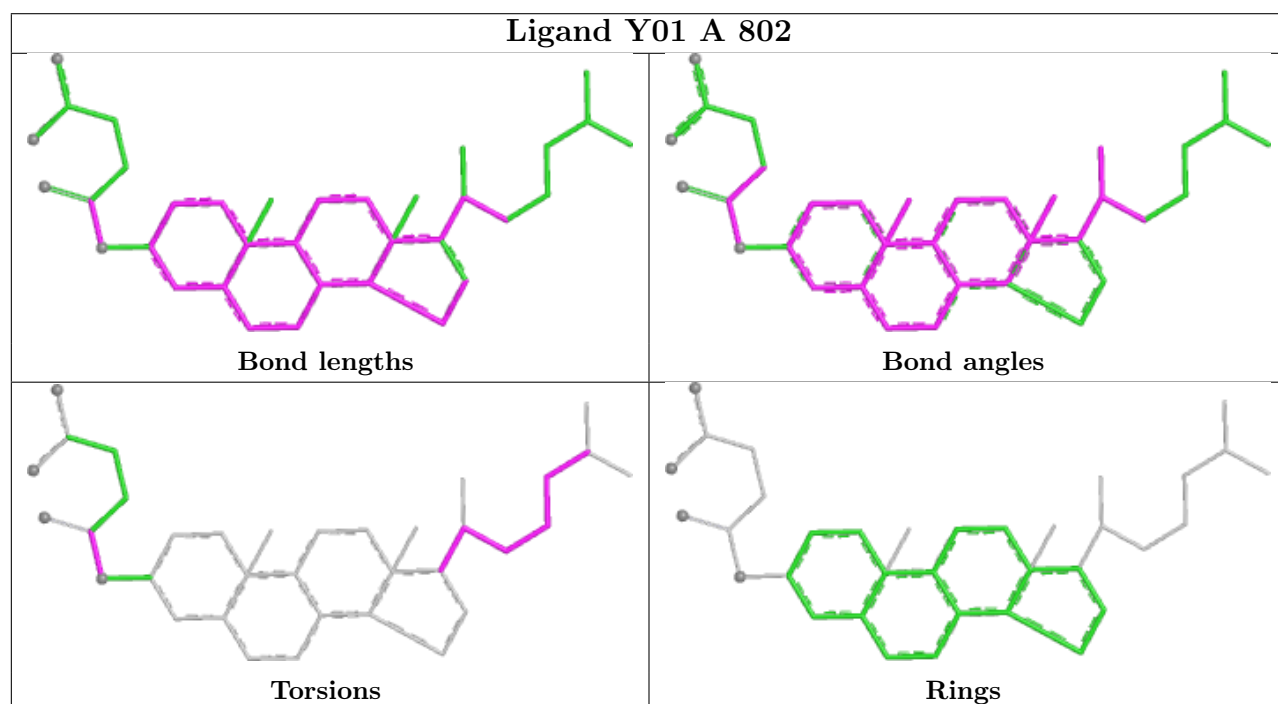
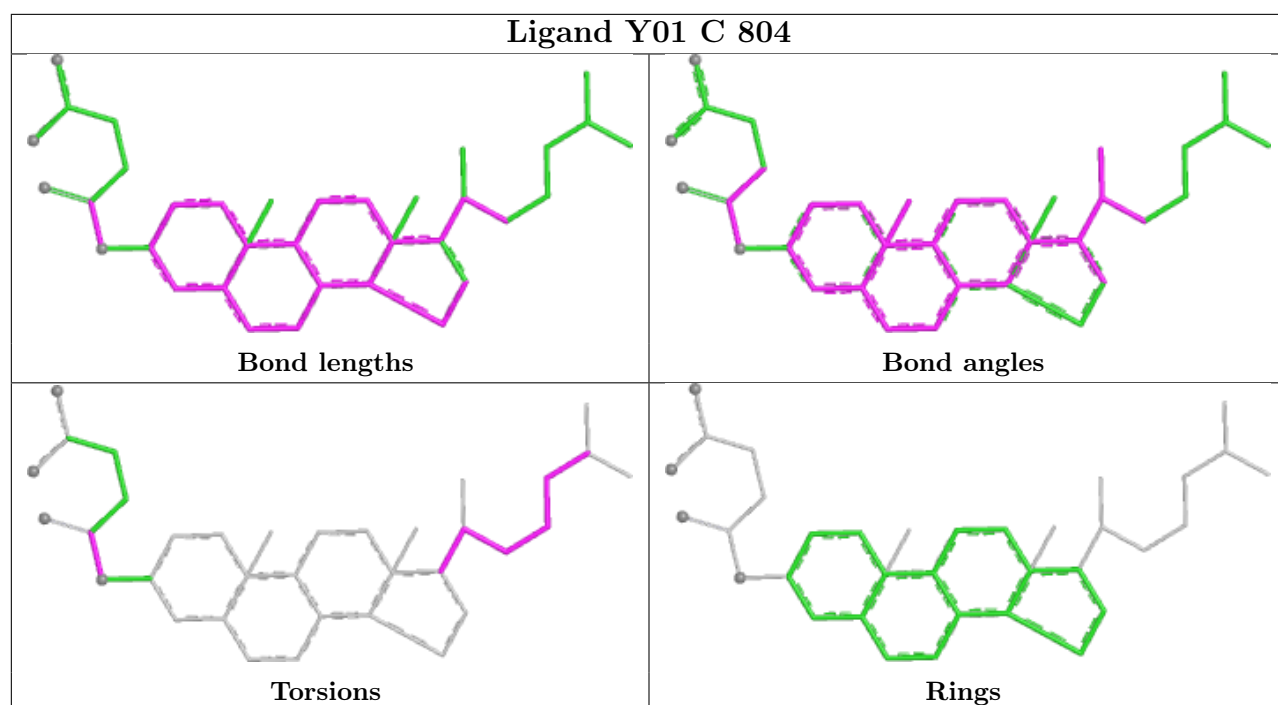
*Continued from previous page...*

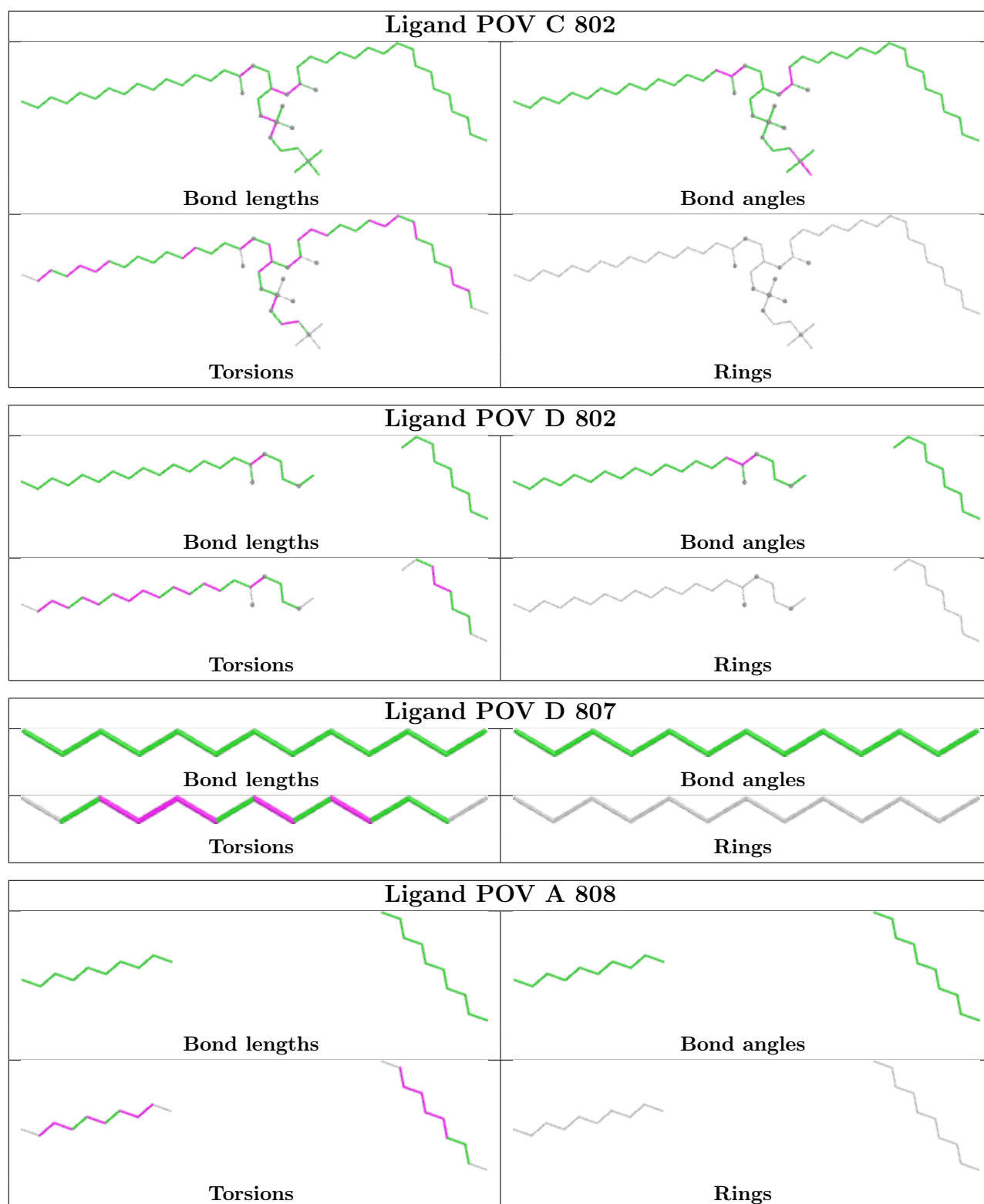
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 4   | A     | 805 | POV  | 3       | 0            |
| 2   | C     | 805 | Y01  | 14      | 0            |
| 2   | B     | 803 | Y01  | 11      | 0            |
| 4   | A     | 811 | POV  | 2       | 0            |
| 4   | B     | 807 | POV  | 2       | 0            |
| 4   | C     | 807 | POV  | 1       | 0            |
| 4   | C     | 812 | POV  | 1       | 0            |
| 2   | D     | 805 | Y01  | 12      | 0            |
| 4   | B     | 810 | POV  | 2       | 0            |
| 4   | D     | 801 | POV  | 2       | 0            |
| 4   | B     | 811 | POV  | 2       | 0            |
| 2   | D     | 804 | Y01  | 9       | 0            |
| 4   | C     | 810 | POV  | 2       | 0            |
| 4   | B     | 809 | POV  | 1       | 0            |
| 2   | B     | 804 | Y01  | 13      | 0            |
| 4   | A     | 809 | POV  | 2       | 0            |
| 4   | D     | 810 | POV  | 2       | 0            |
| 4   | A     | 807 | POV  | 2       | 0            |
| 4   | C     | 811 | POV  | 2       | 0            |

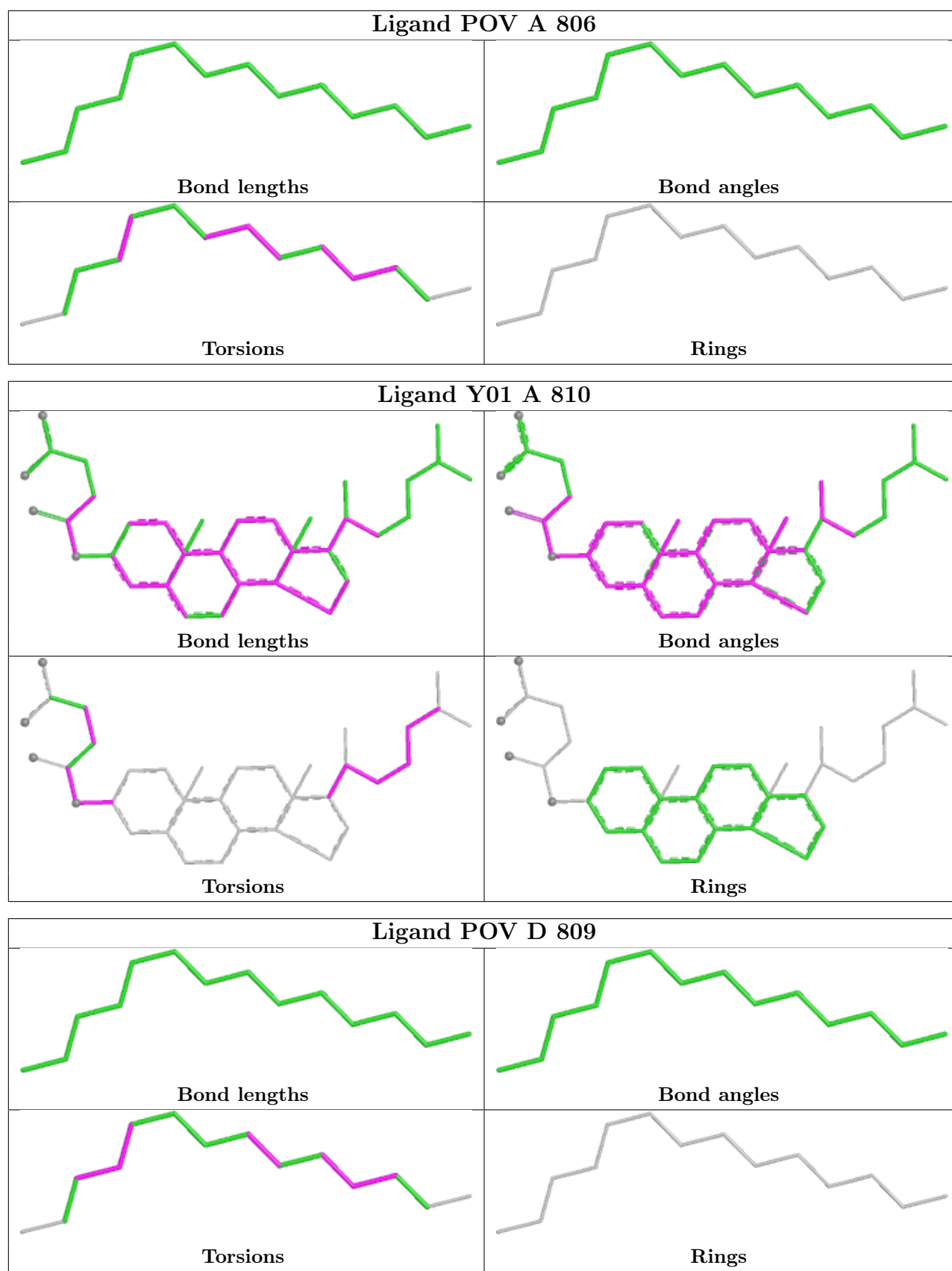
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



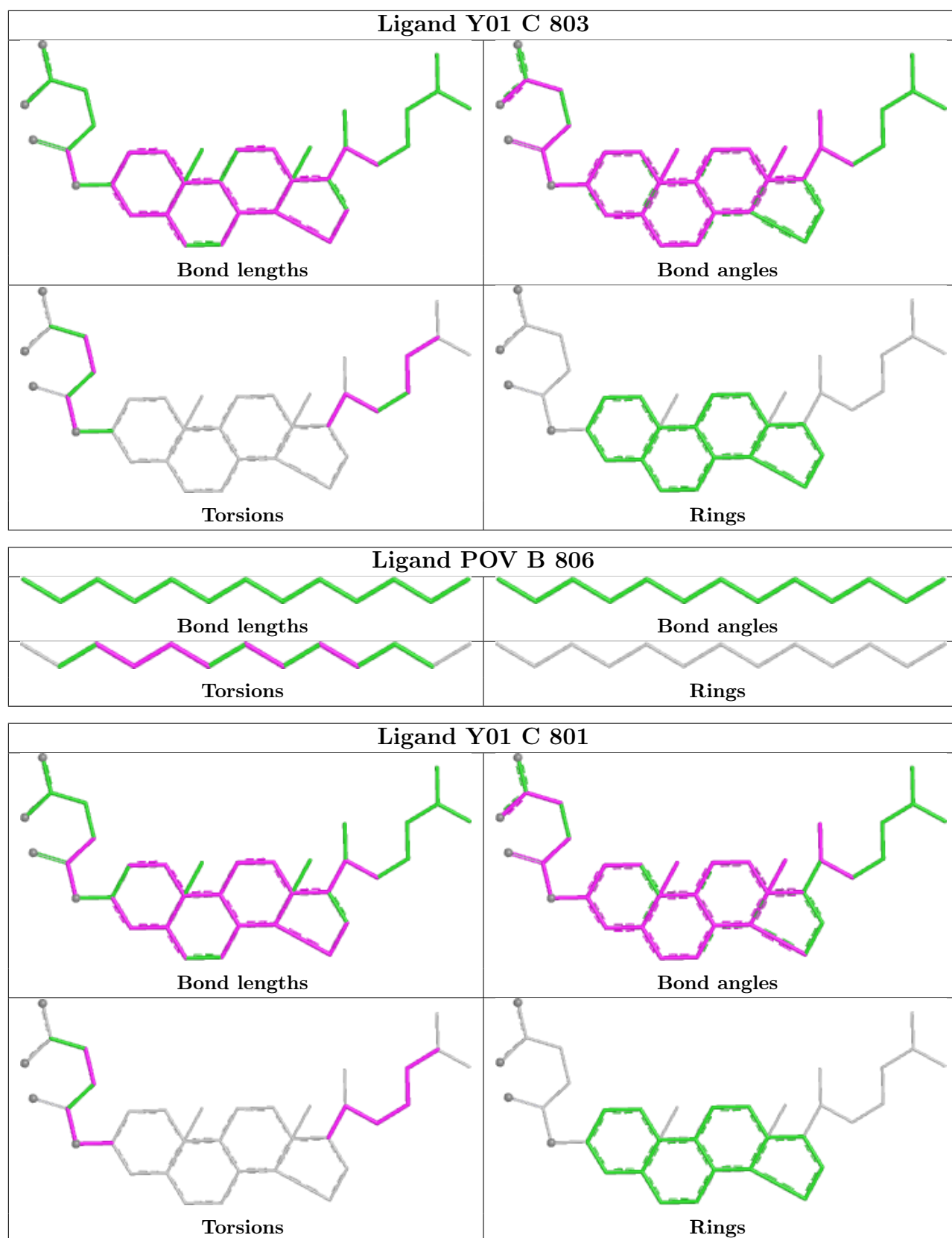


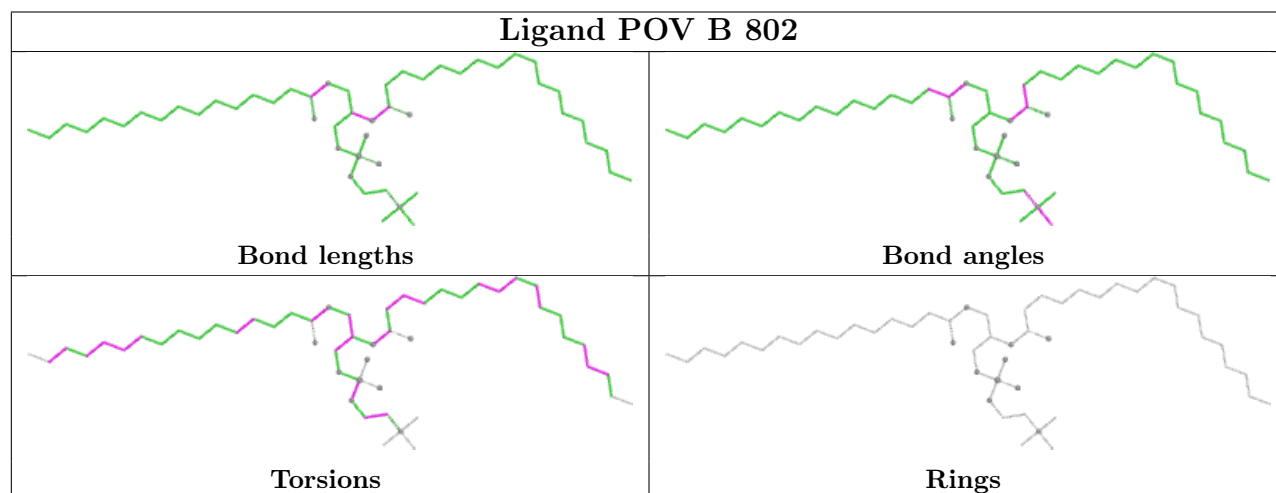
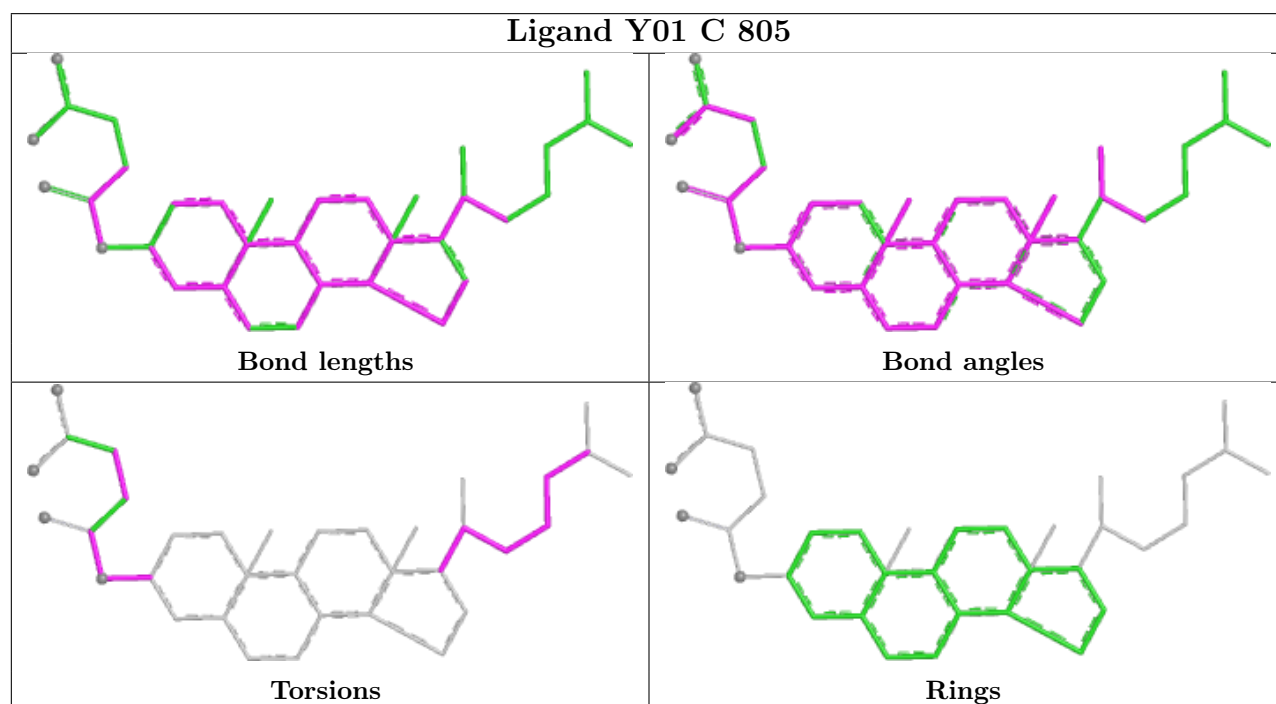
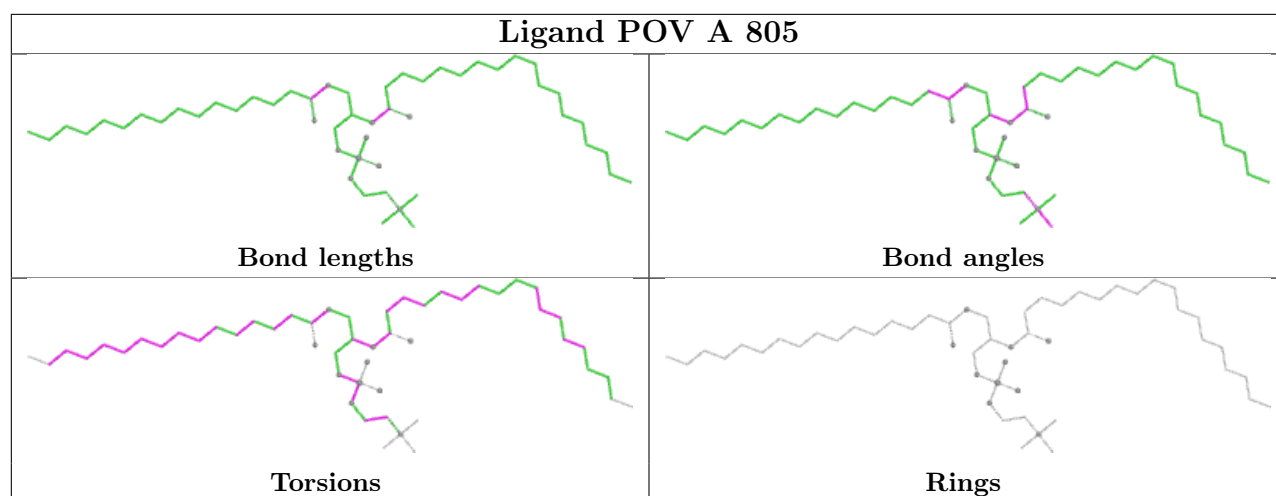


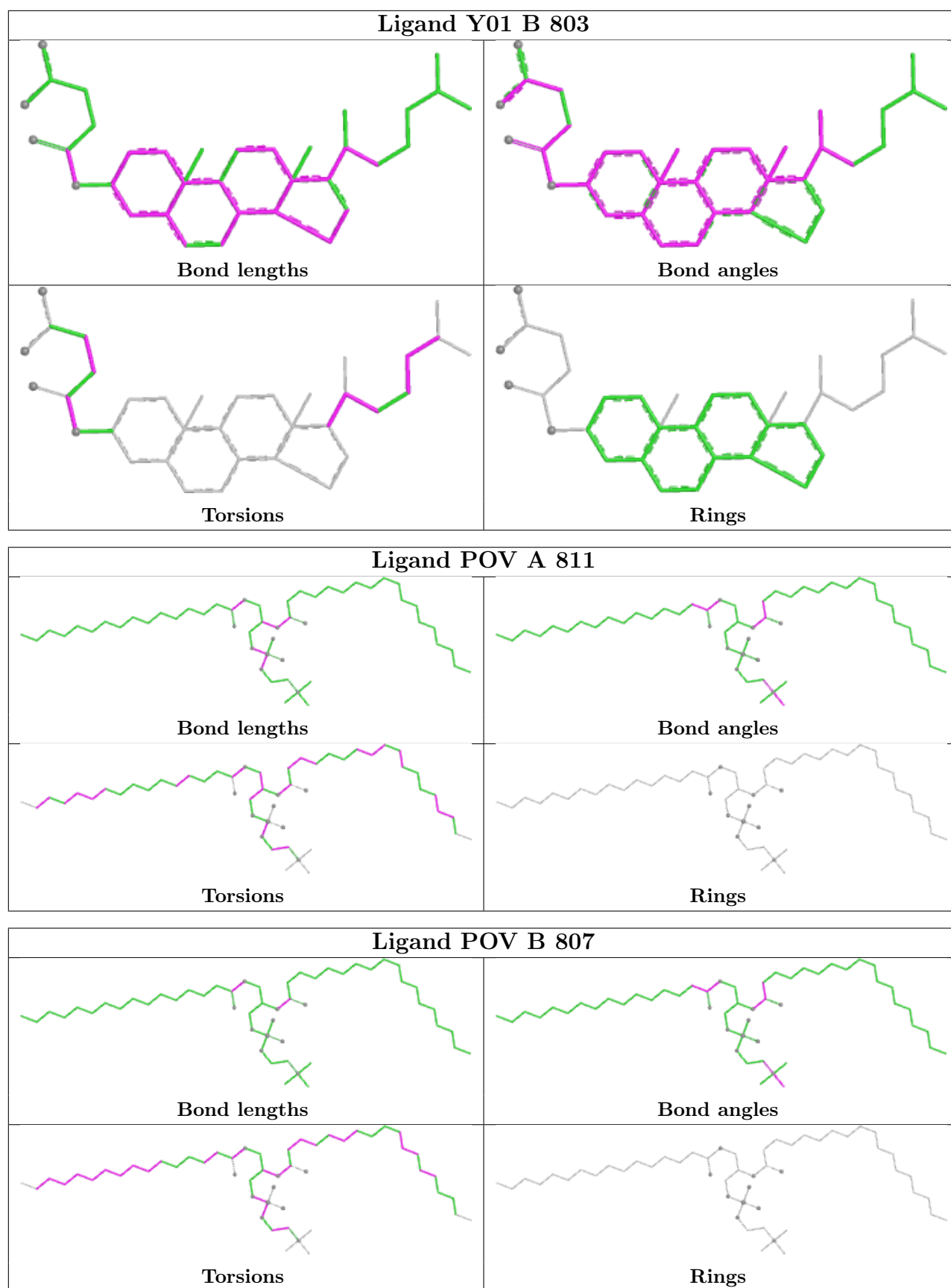


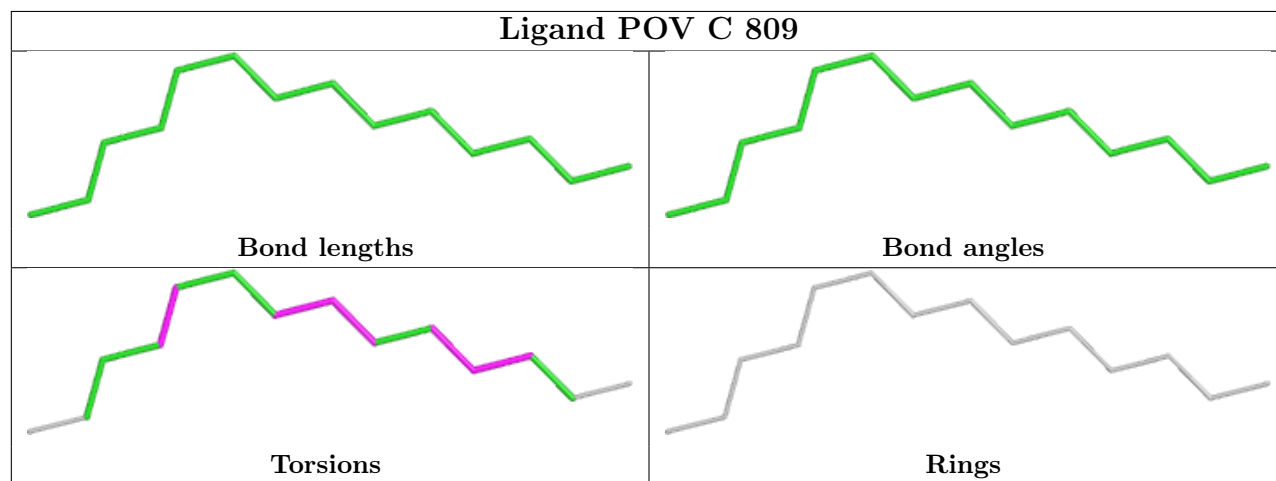
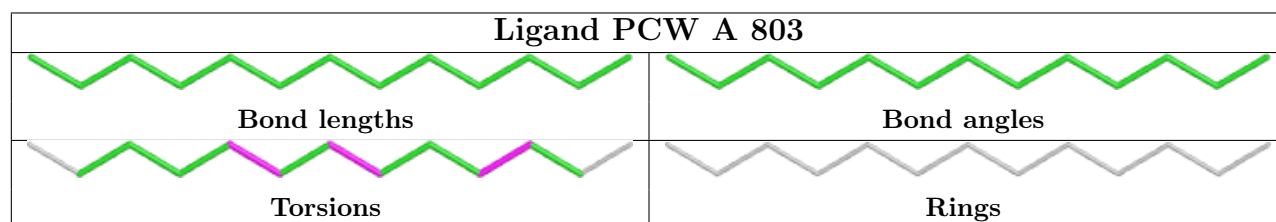
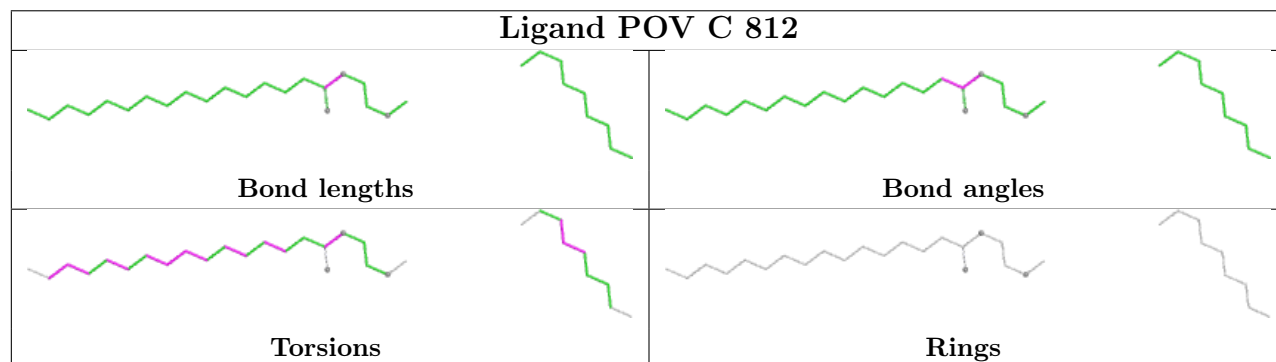
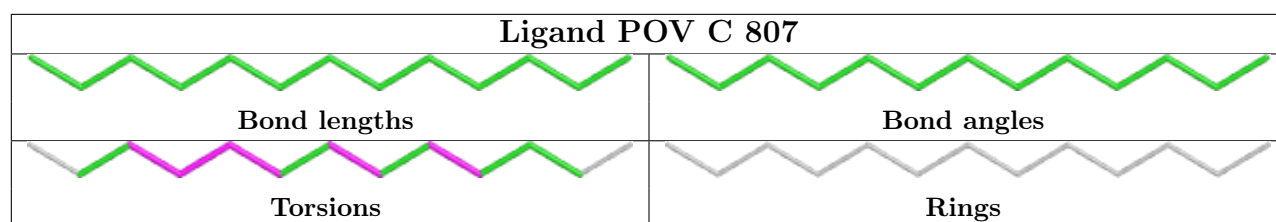


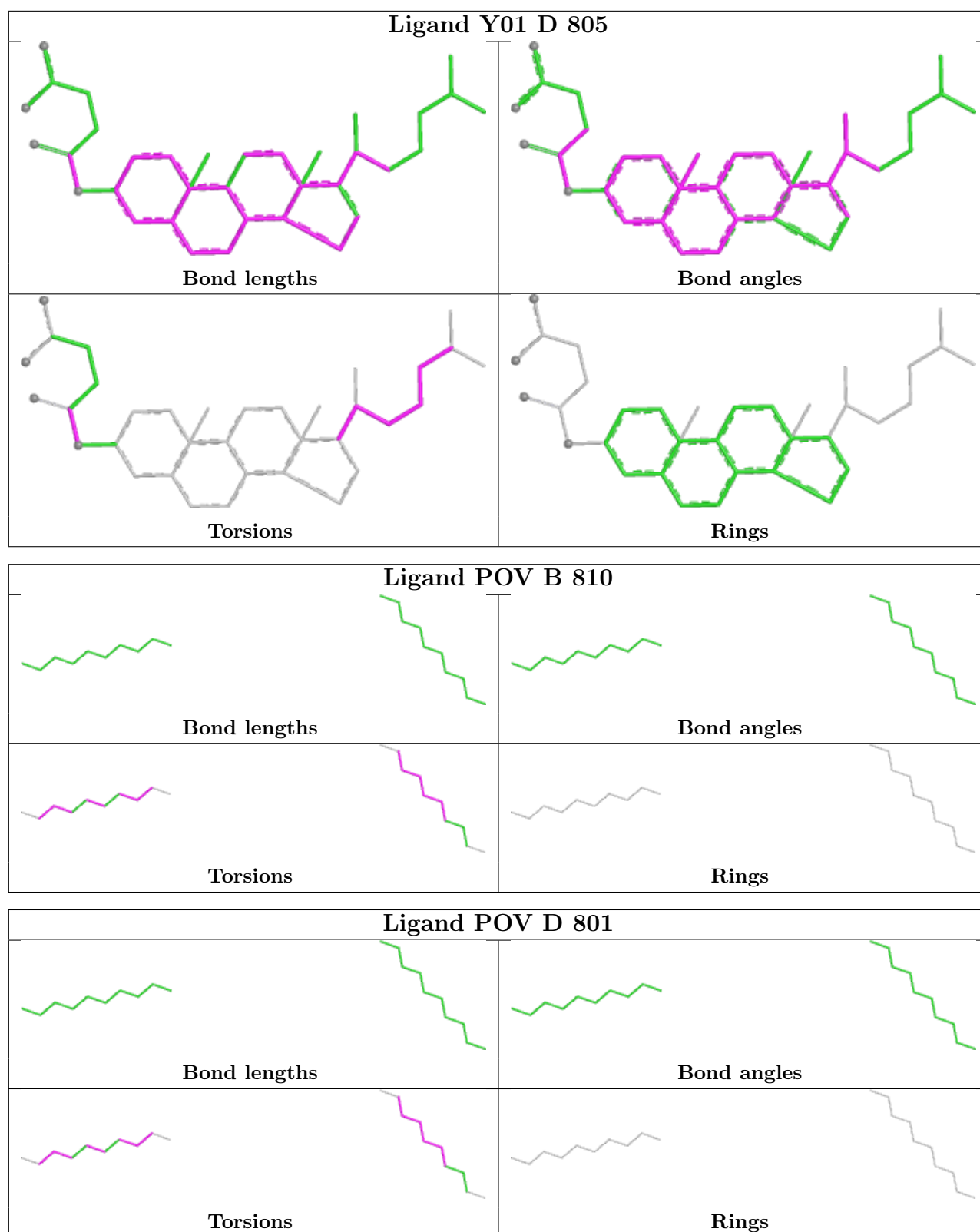


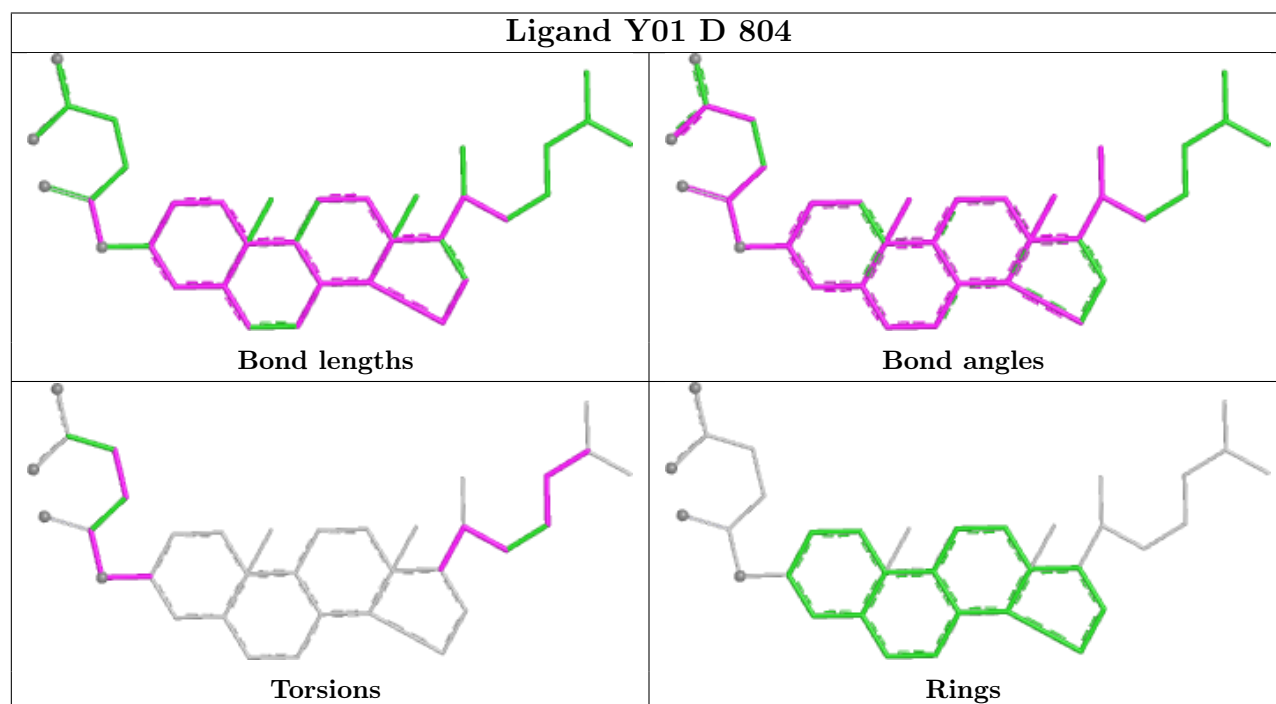
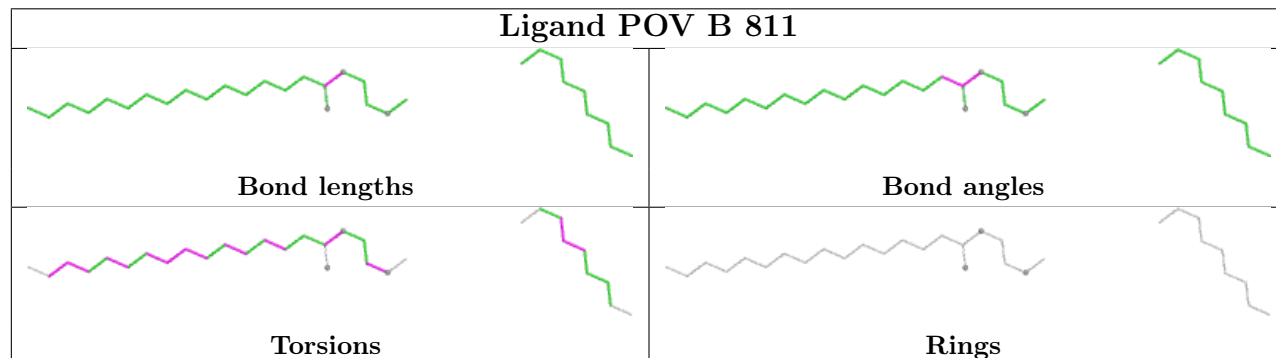
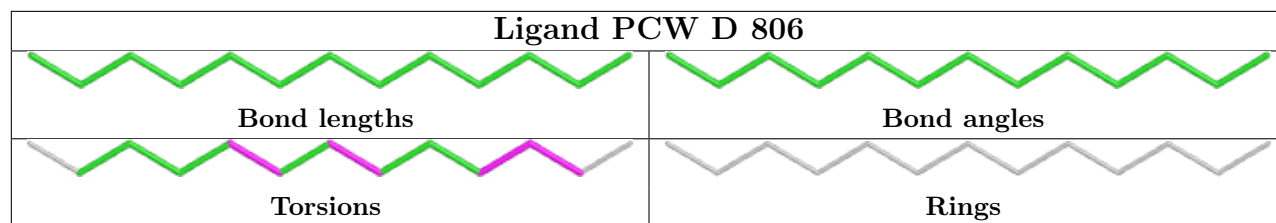


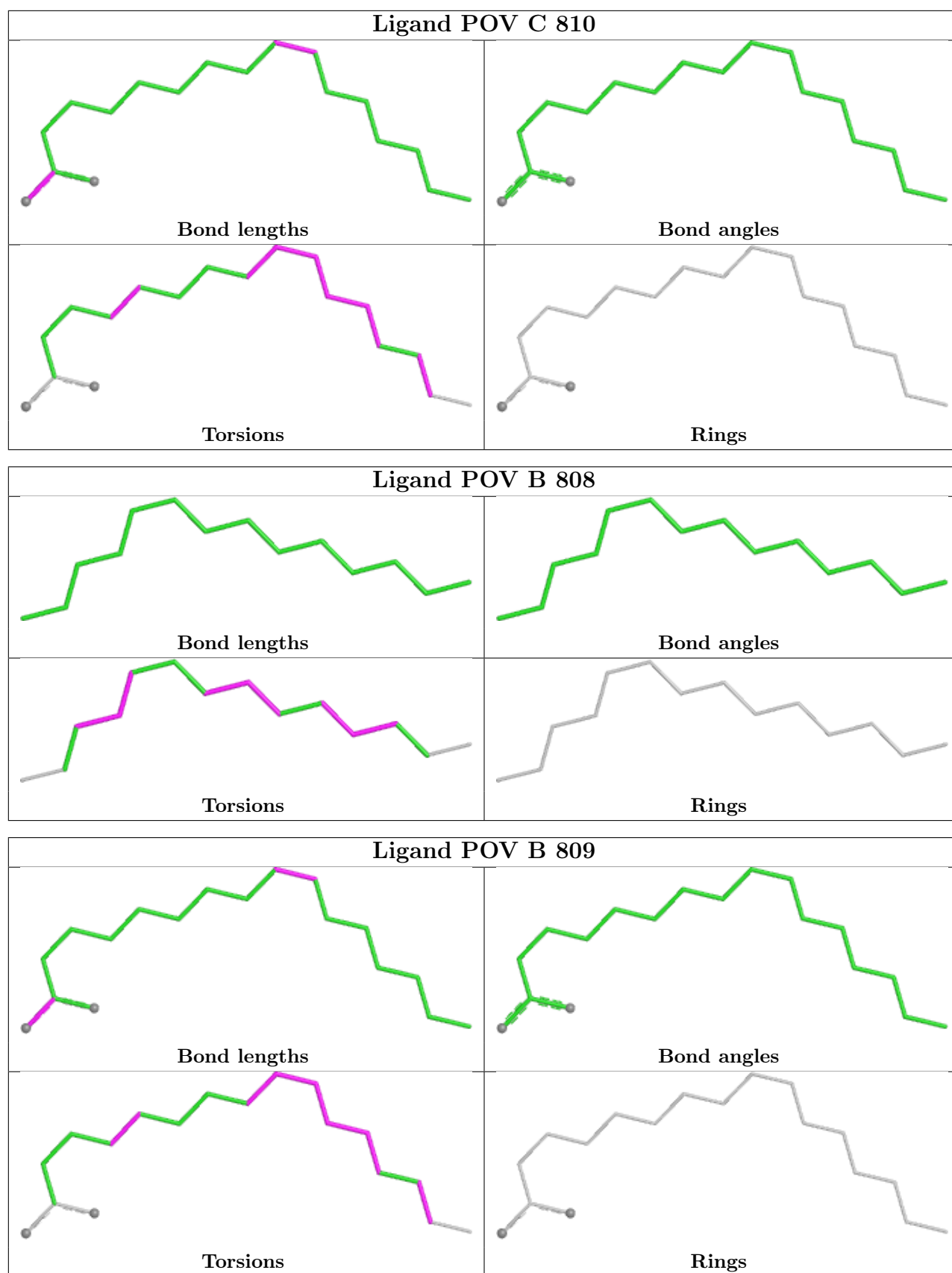


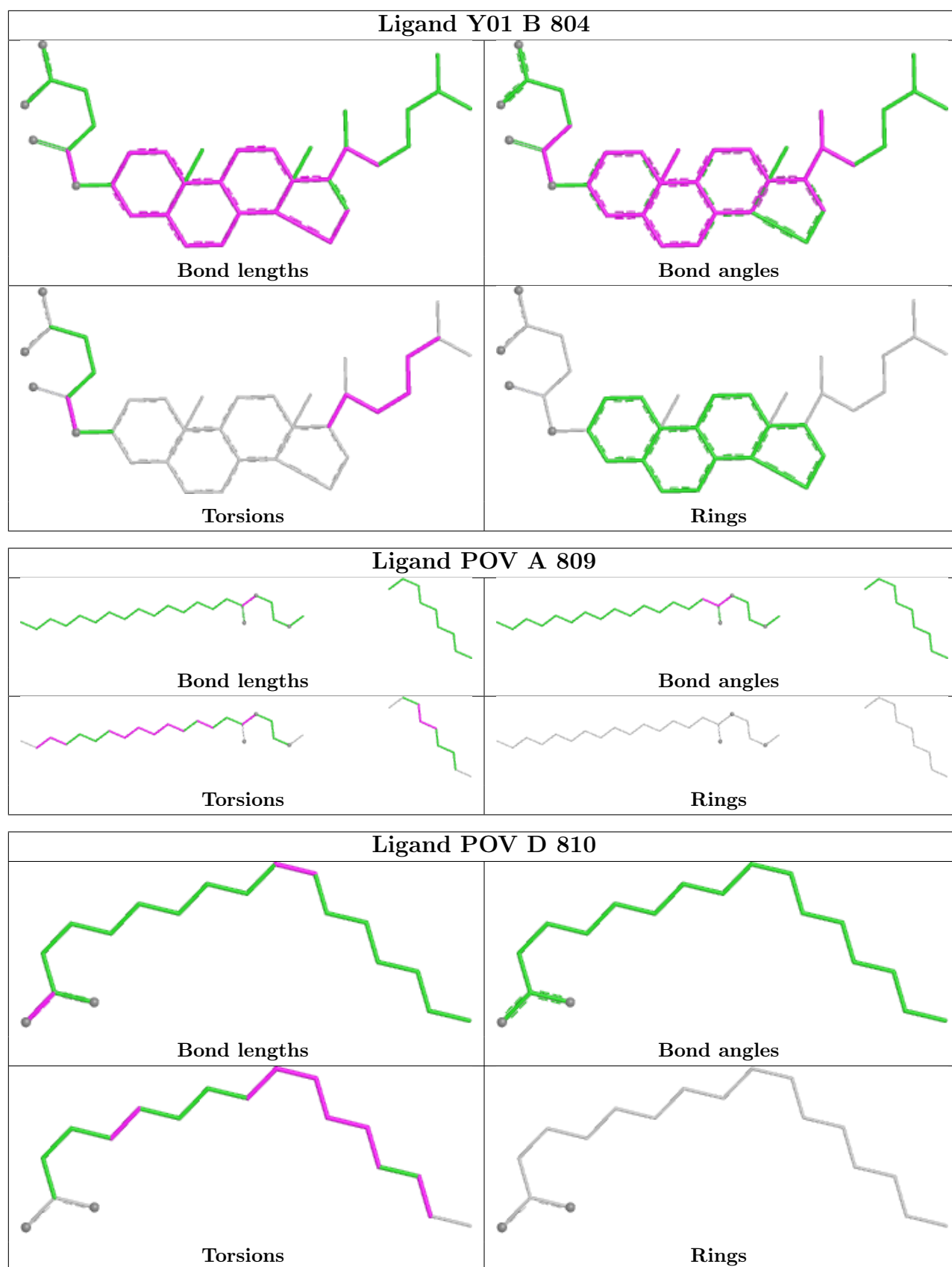




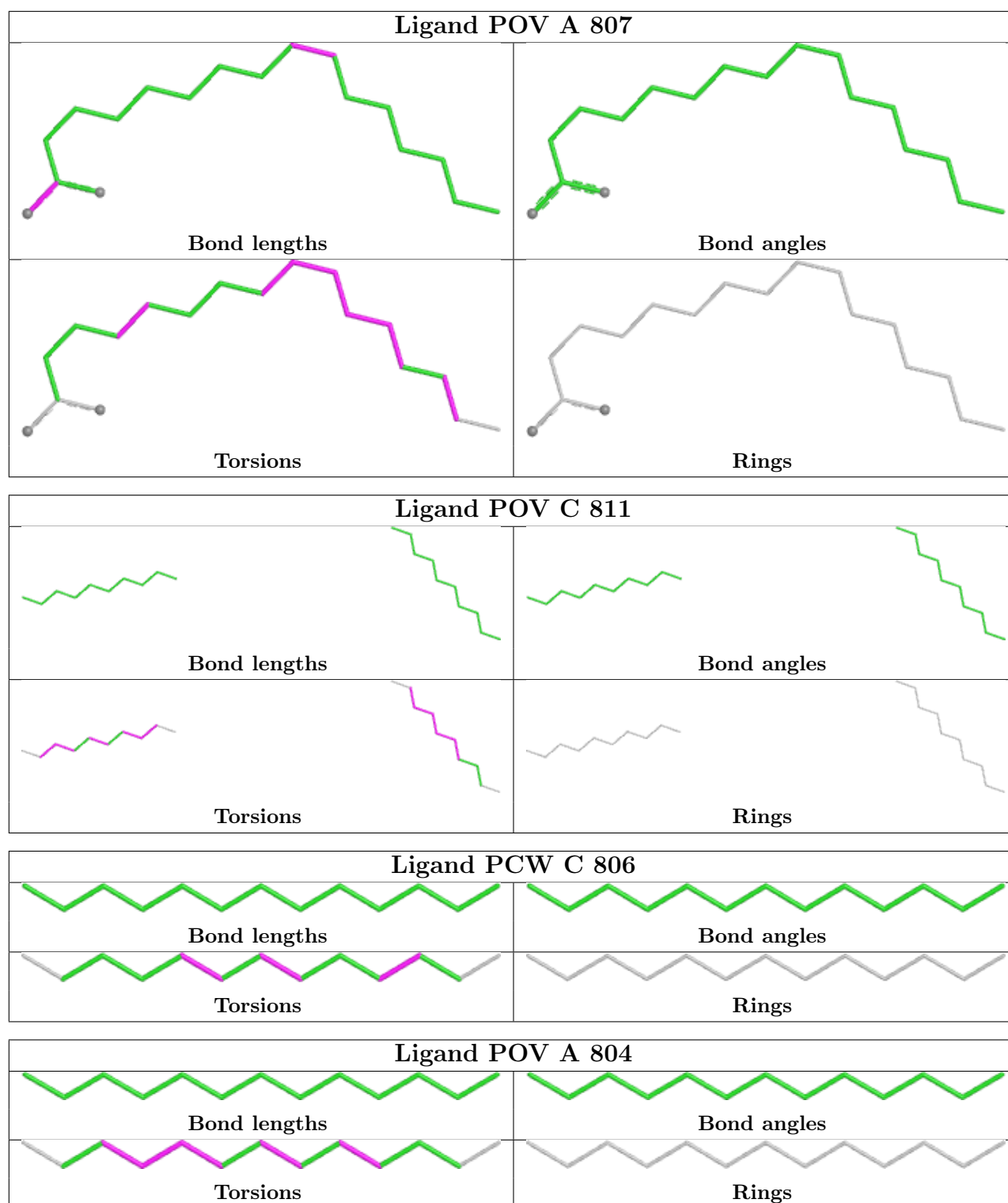












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

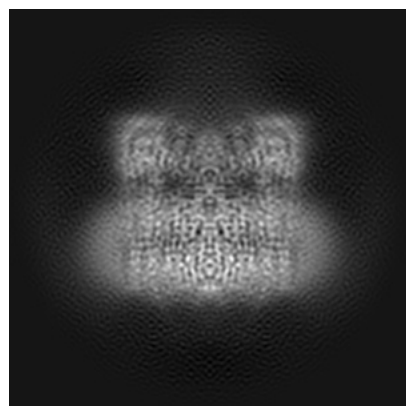
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29344. These allow visual inspection of the internal detail of the map and identification of artifacts.

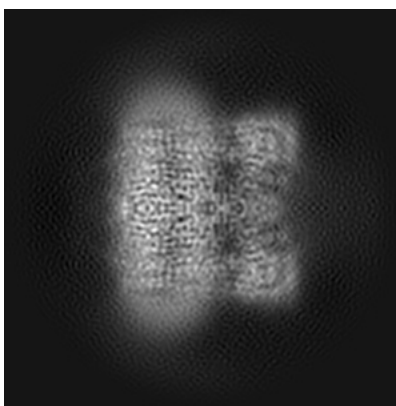
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

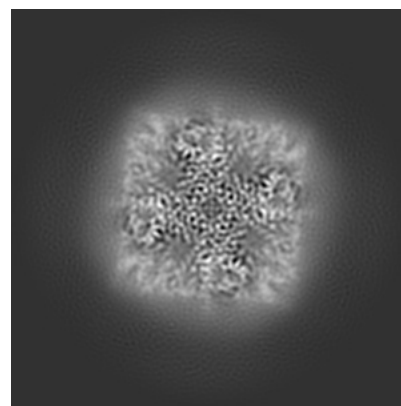
#### 6.1.1 Primary map



X

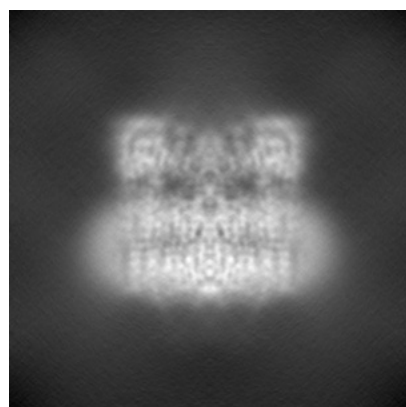


Y

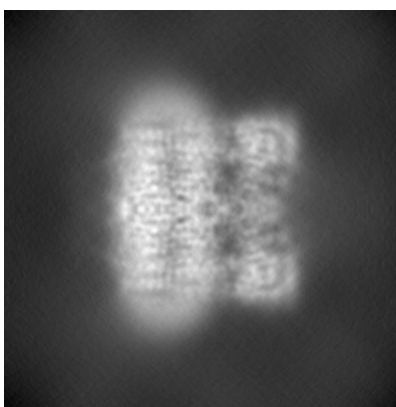


Z

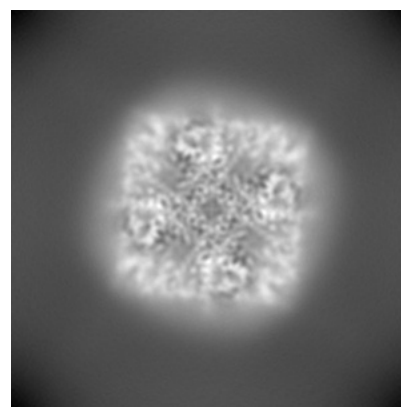
#### 6.1.2 Raw map



X



Y

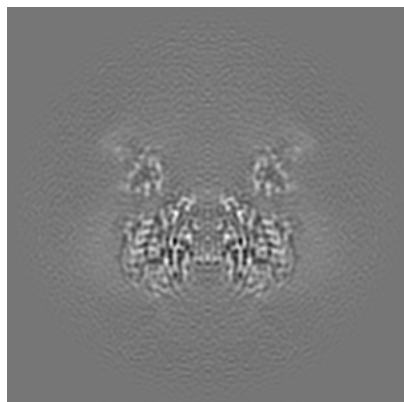


Z

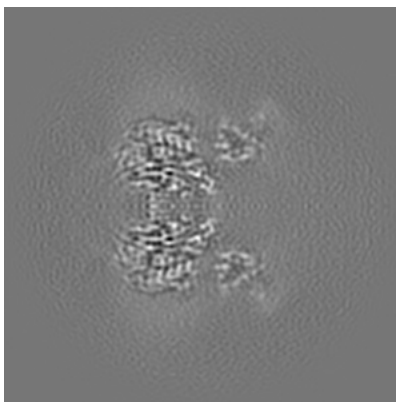
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

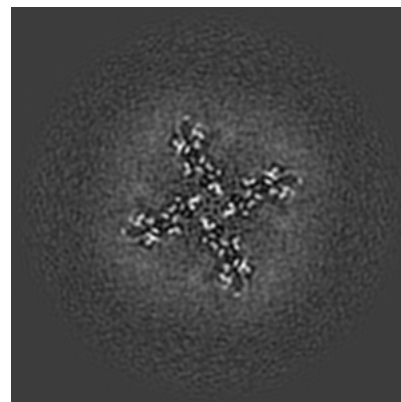
### 6.2.1 Primary map



X Index: 128

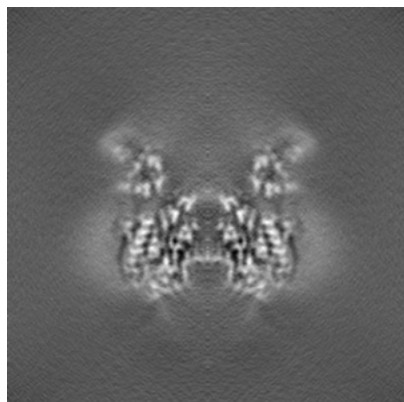


Y Index: 128

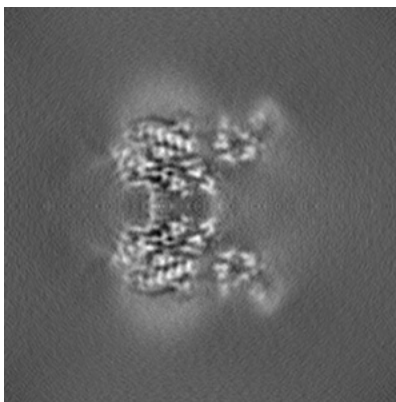


Z Index: 128

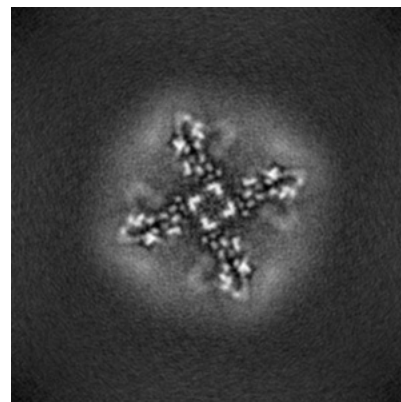
### 6.2.2 Raw map



X Index: 128



Y Index: 128

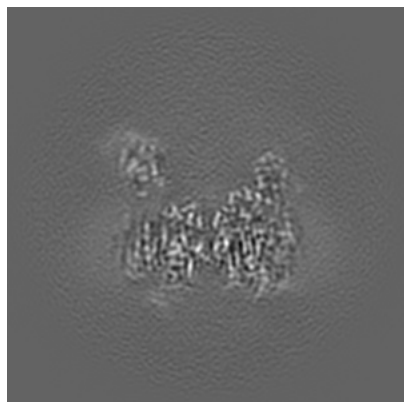


Z Index: 128

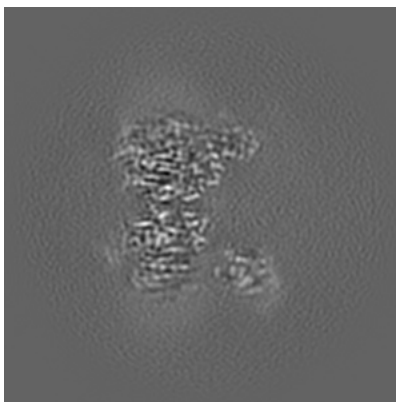
The images above show central slices of the map in three orthogonal directions.

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

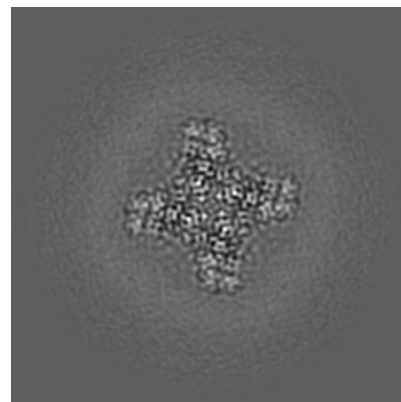
### 6.3.1 Primary map



X Index: 123

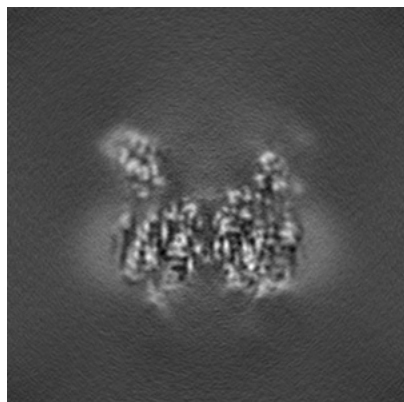


Y Index: 133

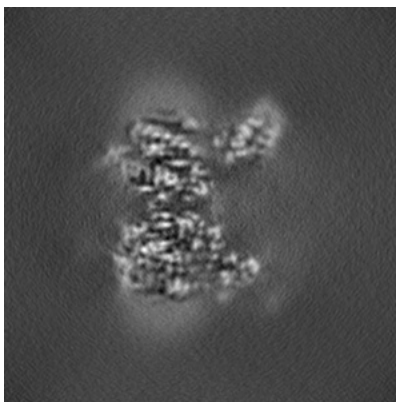


Z Index: 100

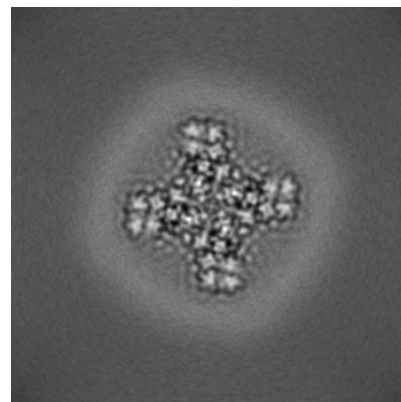
### 6.3.2 Raw map



X Index: 124



Y Index: 124

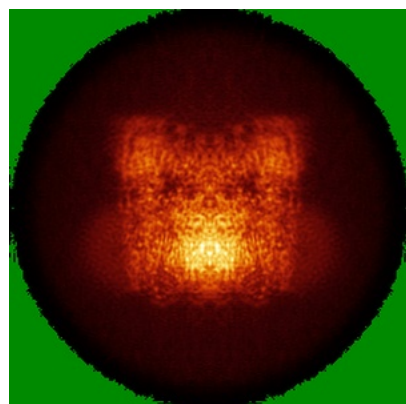


Z Index: 99

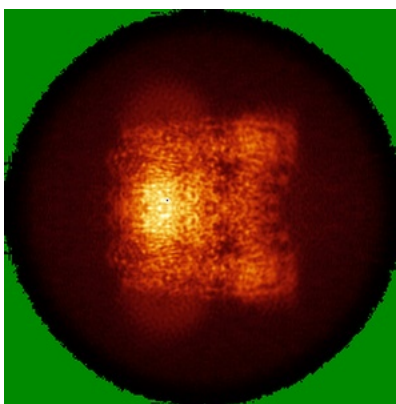
The images above show the largest variance slices of the map in three orthogonal directions.

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

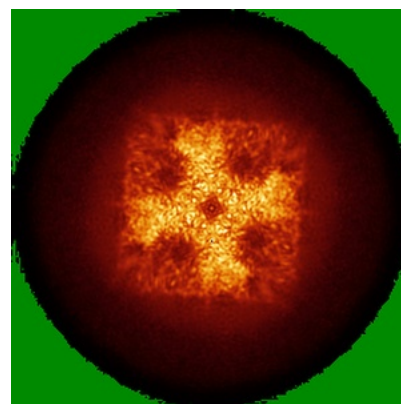
### 6.4.1 Primary map



X

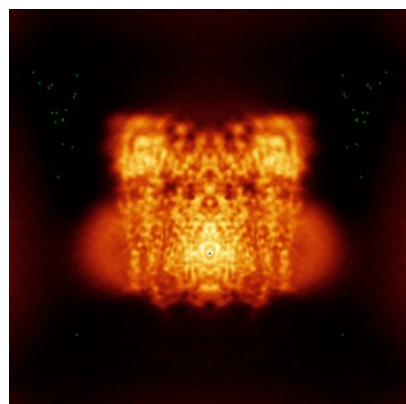


Y

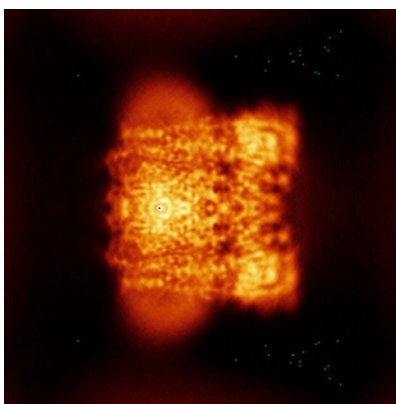


Z

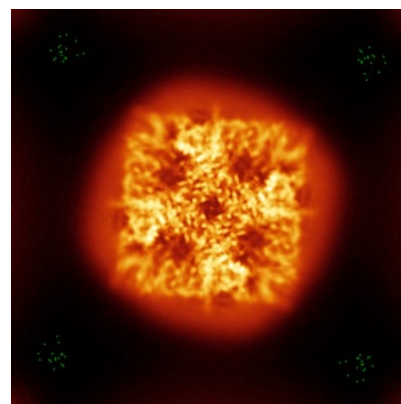
### 6.4.2 Raw map



X



Y



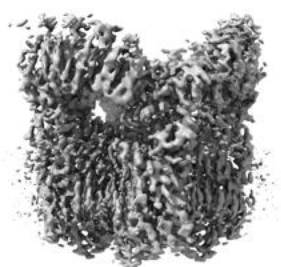
Z

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



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

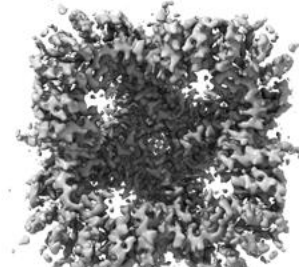
### 6.5.1 Primary map



X



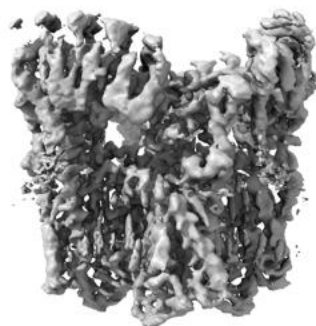
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.51. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

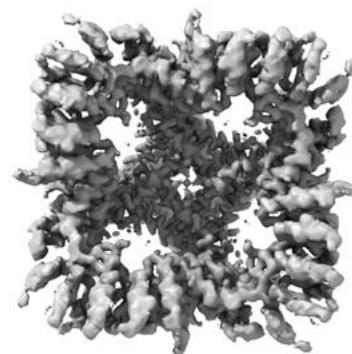
### 6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

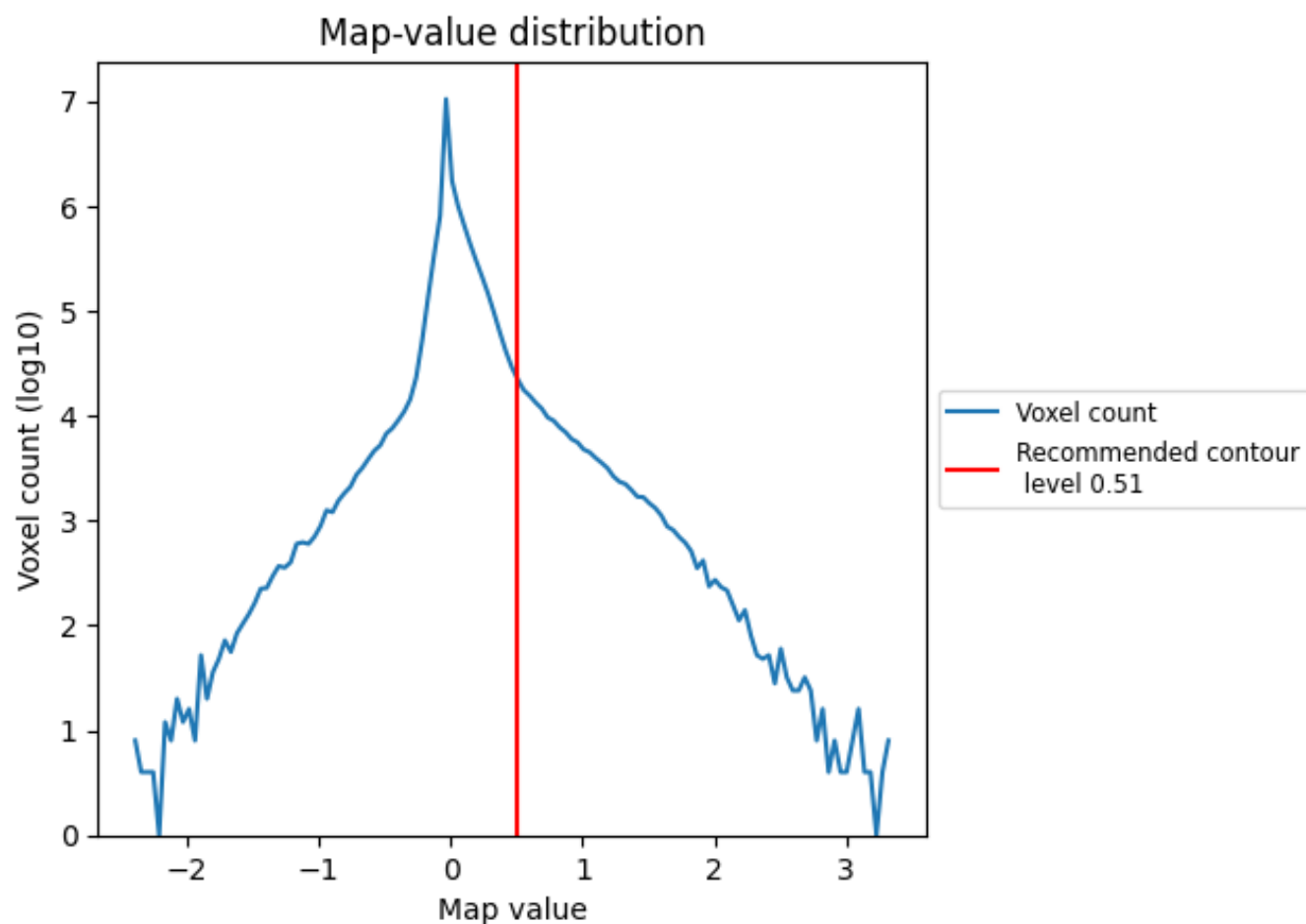
## 6.6 Mask visualisation [i](#)

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.

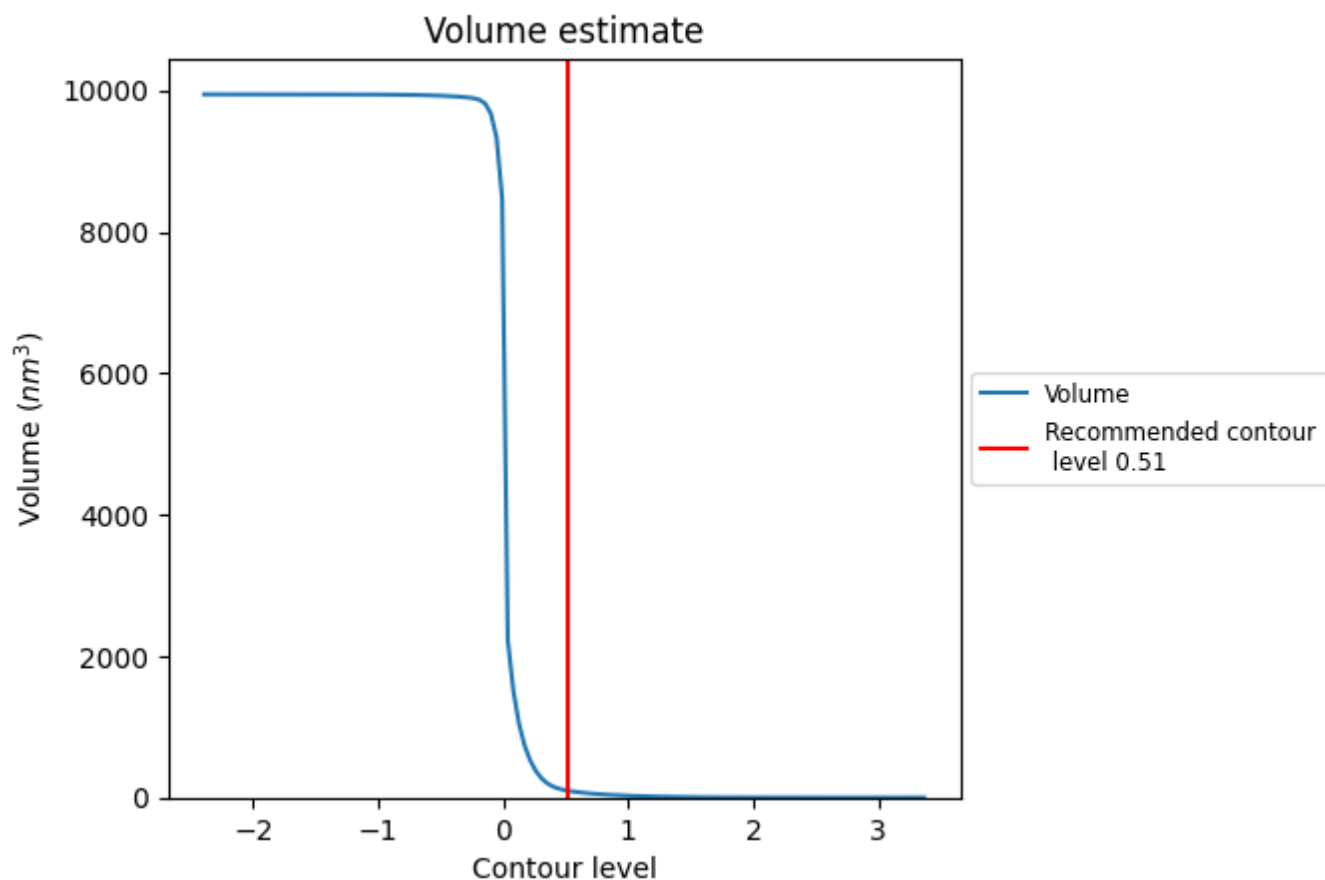
### 7.1 Map-value distribution [i](#)



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.



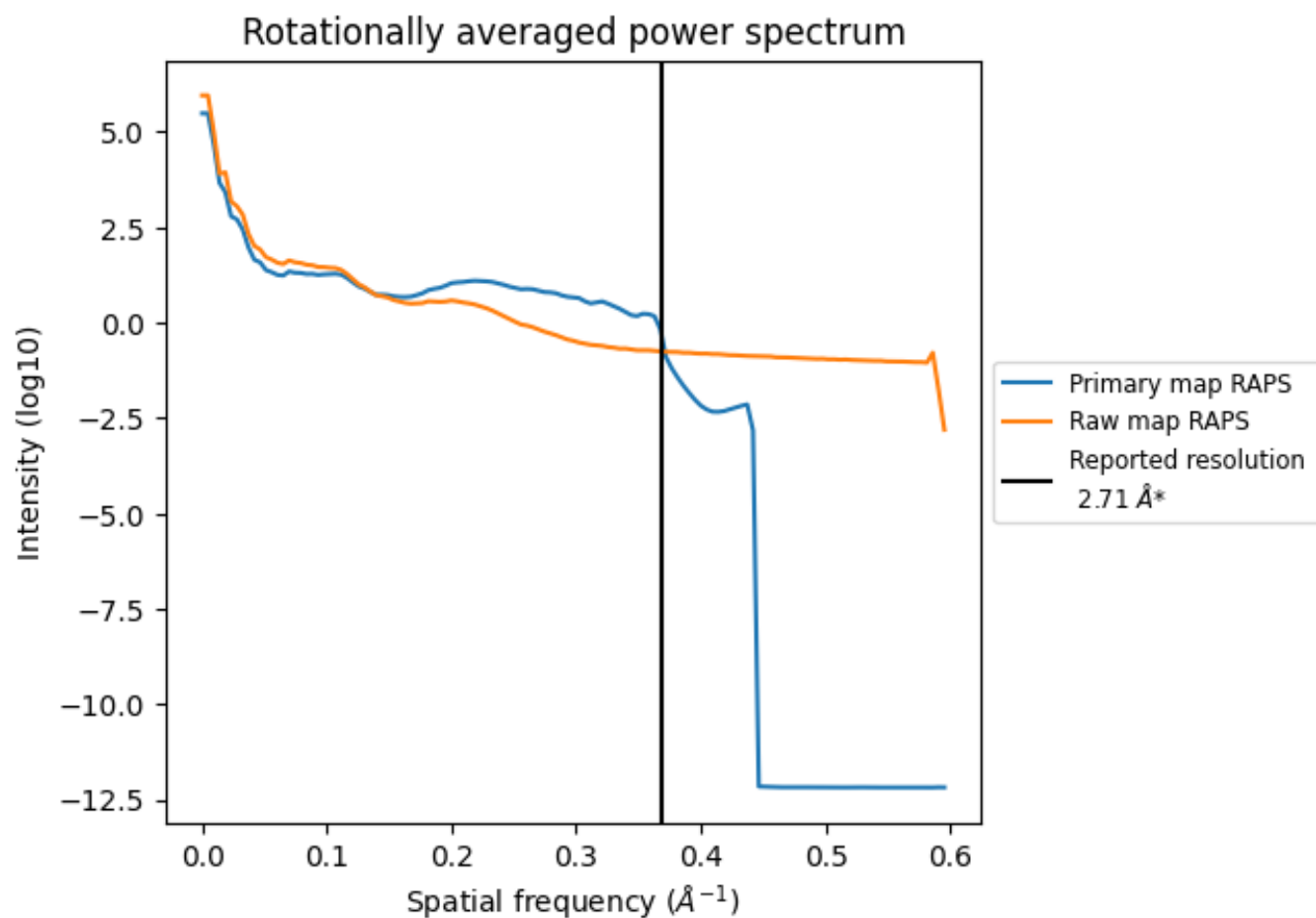
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 100 nm<sup>3</sup>; this corresponds to an approximate mass of 90 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 ⓘ

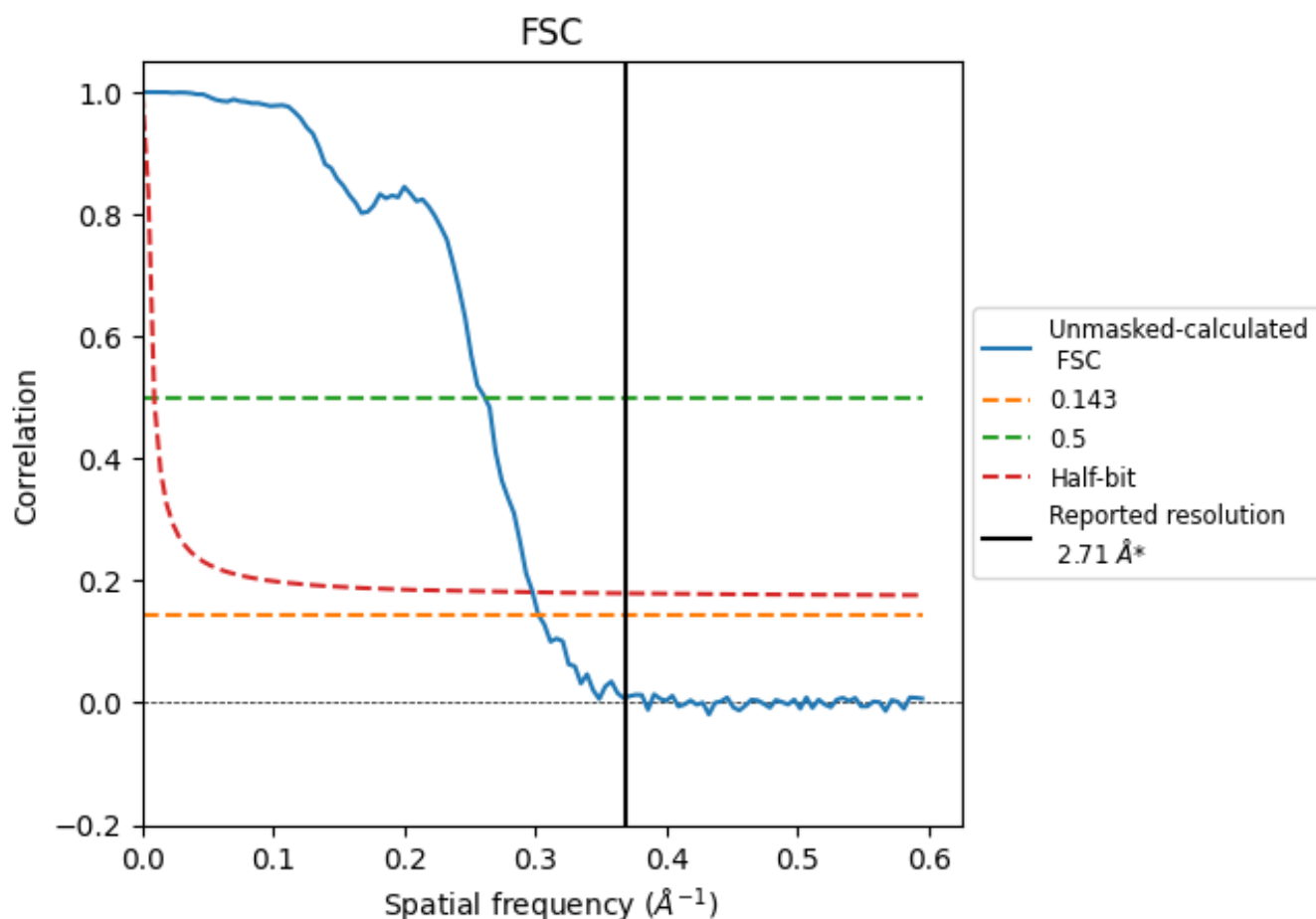


\*Reported resolution corresponds to spatial frequency of 0.369 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.369  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

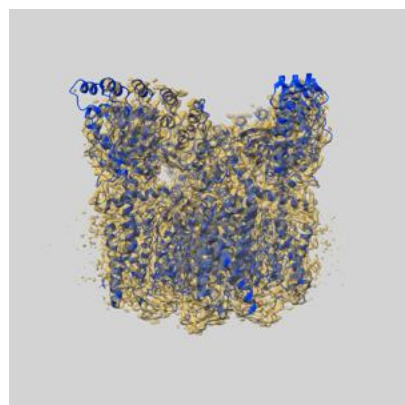
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 2.71                               | -    | -        |
| Author-provided FSC curve | -                                  | -    | -        |
| Unmasked-calculated*      | 3.31                               | 3.83 | 3.36     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.31 differs from the reported value 2.71 by more than 10 %

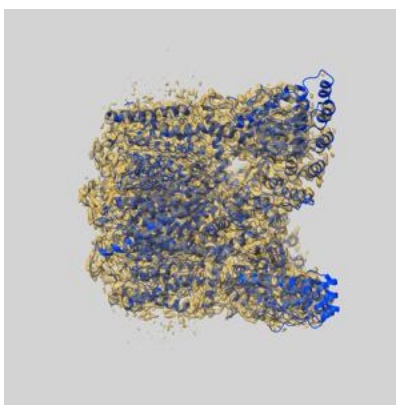
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-29344 and PDB model 8FOB. Per-residue inclusion information can be found in section 3 on page 9.

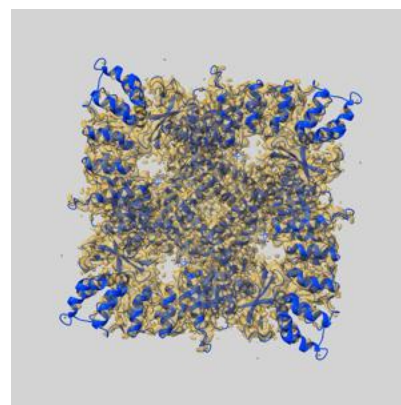
### 9.1 Map-model overlay [i](#)



X



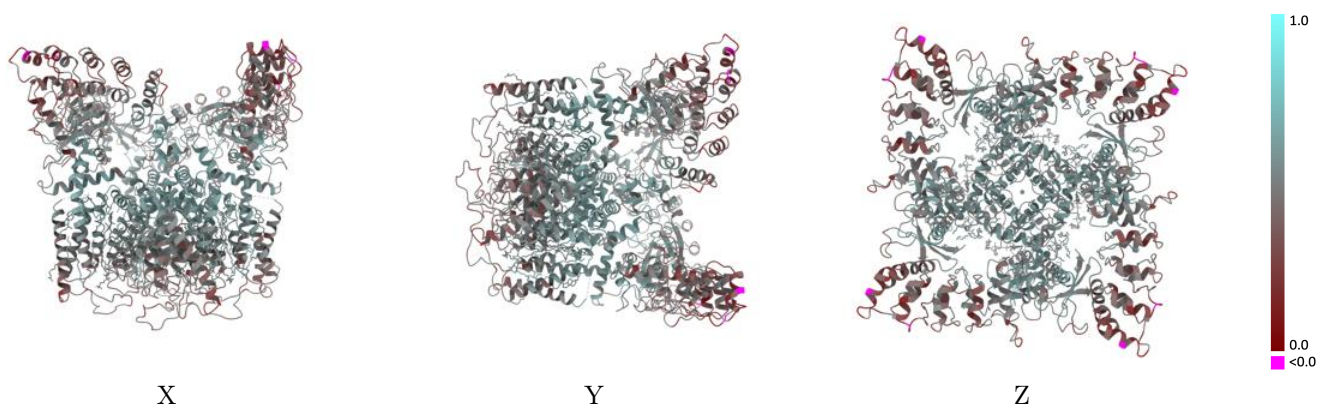
Y



Z

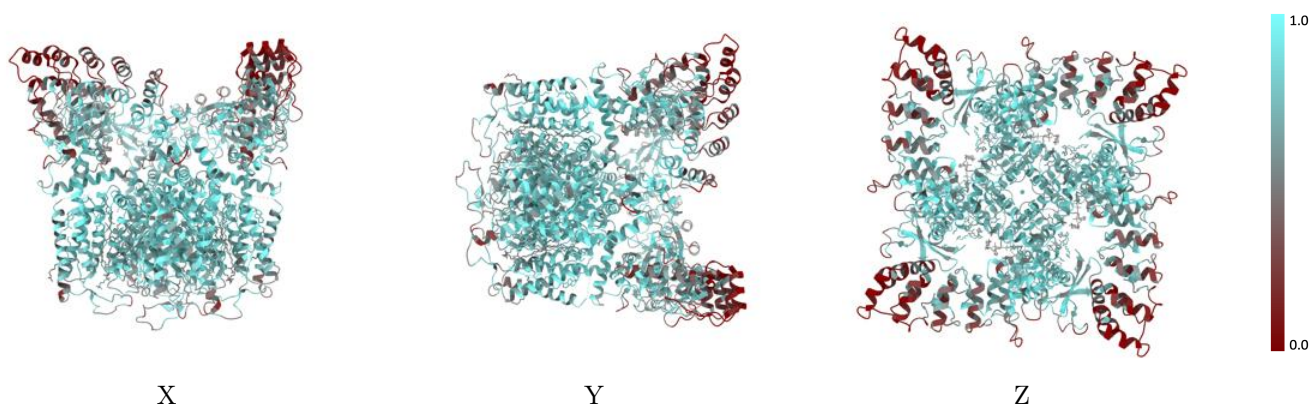
The images above show the 3D surface view of the map at the recommended contour level 0.51 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



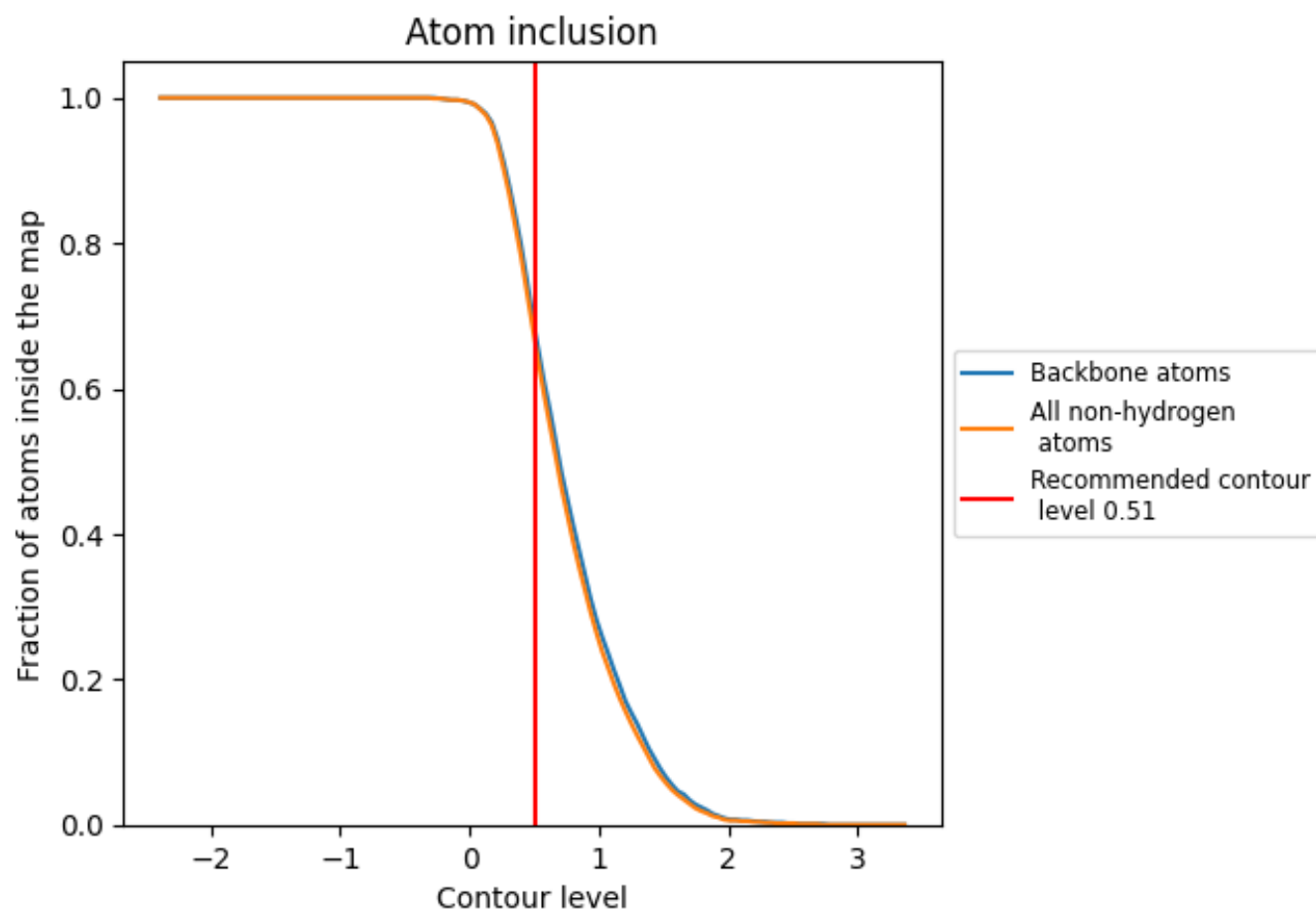
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.51).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 66% 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 (0.51) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion     | Q-score            |
|-------|--------------------|--------------------|
| All   | <div></div> 0.6580 | <div></div> 0.4680 |
| A     | <div></div> 0.6640 | <div></div> 0.4670 |
| B     | <div></div> 0.6660 | <div></div> 0.4690 |
| C     | <div></div> 0.6640 | <div></div> 0.4670 |
| D     | <div></div> 0.6650 | <div></div> 0.4690 |

