



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 03:18 PM EDT

PDB ID : 1S00 / pdb\_00001s00  
Title : PHOTOSYNTHETIC REACTION CENTER DOUBLE MUTANT FROM RHODOBACTER SPHAEROIDES WITH ASP L213 REPLACED WITH ASN AND ARG M233 REPLACED WITH CYS IN THE CHARGE-SEPARATED D+QAQB- STATE  
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Deposited on : 2003-12-29  
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

|                           |   |                                                                  |
|---------------------------|---|------------------------------------------------------------------|
| MolProbity                | : | 4-5-2 with Phenix2.0                                             |
| Mogul                     | : | 2022.3.0, CSD as543be (2022)                                     |
| Xtriage (Phenix)          | : | 2.0                                                              |
| EDS                       | : | 3.0                                                              |
| Buster-report             | : | wwPDB partial adaption of 1.1.7 (2018)                           |
| Percentile statistics     | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| CCP4                      | : | 9.0.015 (Gargrove)                                               |
| Density-Fitness           | : | 1.0.12                                                           |
| Ideal geometry (proteins) | : | Engh & Huber (2001)                                              |

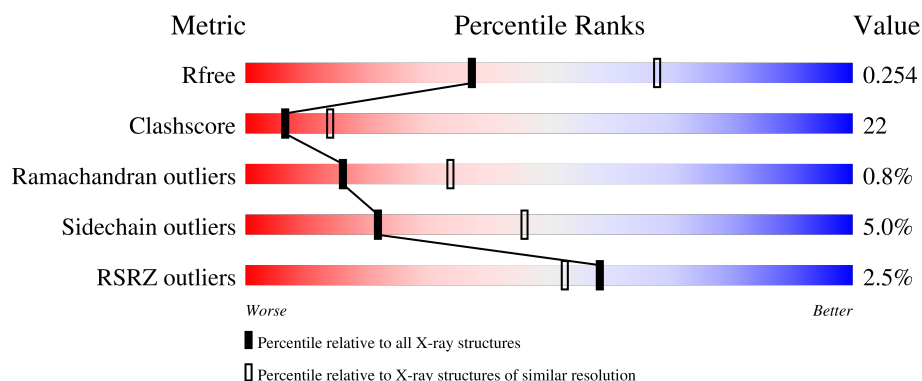
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 4008 (2.60-2.60)                                      |
| Clashscore            | 190562                      | 4347 (2.60-2.60)                                      |
| Ramachandran outliers | 187476                      | 4277 (2.60-2.60)                                      |
| Sidechain outliers    | 187428                      | 4277 (2.60-2.60)                                      |
| RSRZ outliers         | 180081                      | 4008 (2.60-2.60)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain                                                                                             |
|-----|-------|--------|--------------------------------------------------------------------------------------------------------------|
| 1   | L     | 281    | <div> <div>%</div> <div> <div></div> <div>58%</div> <div>37%</div> <div>• •</div> </div> </div>              |
| 1   | R     | 281    | <div> <div>2%</div> <div> <div></div> <div>53%</div> <div>42%</div> <div>5%</div> <div>•</div> </div> </div> |
| 2   | M     | 307    | <div> <div>%</div> <div> <div></div> <div>66%</div> <div>27%</div> <div>• •</div> </div> </div>              |

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.50

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 2   | S     | 307    |                  |
| 3   | H     | 260    |                  |
| 3   | T     | 260    |                  |

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 |
|-----|------|-------|---------|-----------|----------|---------|------------------|
| 4   | BCL  | M     | 1003    | -         | -        | X       | -                |
| 5   | BPH  | L     | 1006    | X         | -        | -       | -                |
| 5   | BPH  | M     | 1005    | X         | -        | -       | -                |
| 5   | BPH  | R     | 2006    | X         | -        | -       | -                |
| 6   | U10  | L     | 1009[A] | -         | -        | -       | X                |
| 6   | U10  | L     | 1009[B] | -         | -        | -       | X                |
| 6   | U10  | R     | 2009[A] | -         | -        | -       | X                |
| 6   | U10  | R     | 2009[B] | -         | -        | -       | X                |

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 14144 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Reaction center protein L chain.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | L     | 281      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2232  | 1507 | 356 | 361 | 8 |         |         |       |
| 1   | R     | 281      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2232  | 1507 | 356 | 361 | 8 |         |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| L     | 213     | ASN      | ASP    | engineered mutation | UNP P02954 |
| R     | 213     | ASN      | ASP    | engineered mutation | UNP P02954 |

- Molecule 2 is a protein called Reaction center protein M chain.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 2   | M     | 301      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2399  | 1602 | 390 | 396 | 11 |         |         |       |
| 2   | S     | 299      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2385  | 1594 | 388 | 392 | 11 |         |         |       |

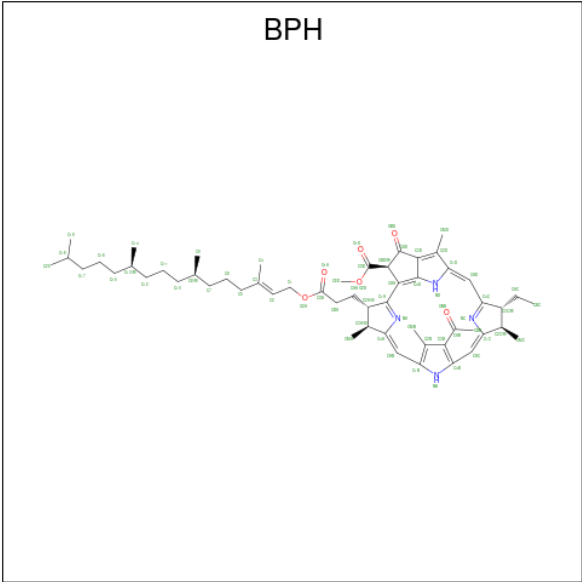
There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| M     | 233     | CYS      | ARG    | engineered mutation | UNP P02953 |
| S     | 233     | CYS      | ARG    | engineered mutation | UNP P02953 |

- Molecule 3 is a protein called Reaction center protein H chain.

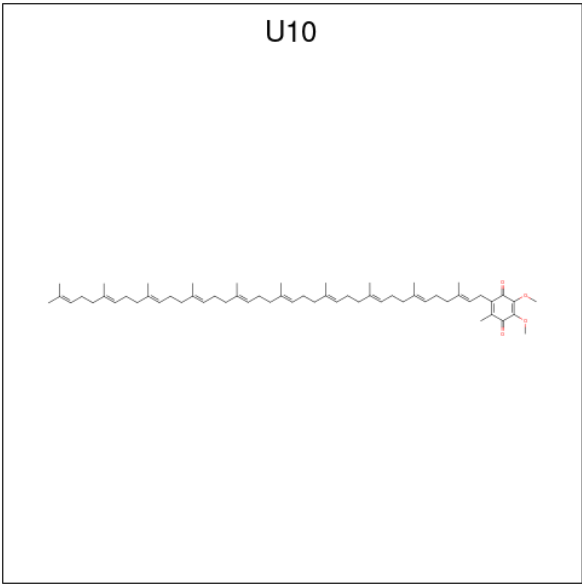
| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 3   | H     | 246      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1869  | 1196 | 320 | 343 | 10 |         |         |       |
| 3   | T     | 246      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1869  | 1196 | 320 | 343 | 10 |         |         |       |





| Mol | Chain | Residues | Atoms |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 5   | L     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 4 | 6 |         |         |
| 5   | M     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 55    | 45 | 4 | 6 |         |         |
| 5   | R     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 65    | 55 | 4 | 6 |         |         |
| 5   | S     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 51    | 41 | 4 | 6 |         |         |

- Molecule 6 is UBIQUINONE-10 (CCD ID: U10) (formula: C<sub>59</sub>H<sub>90</sub>O<sub>4</sub>).

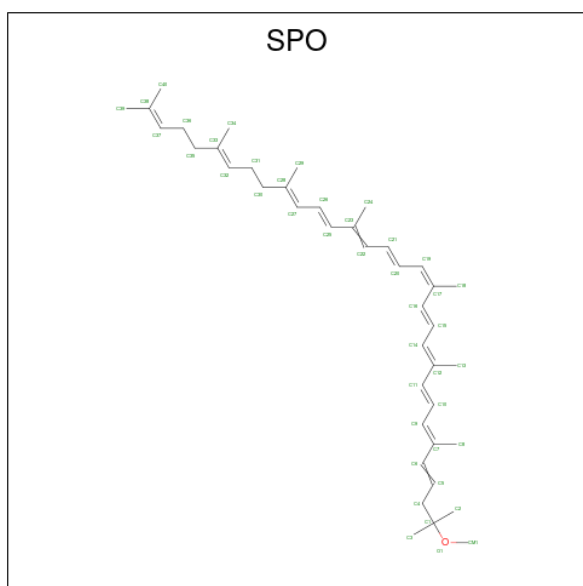


| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 6   | L     | 1        | Total | C  | O | 0       | 1       |
|     |       |          | 60    | 52 | 8 |         |         |
| 6   | M     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 38    | 34 | 4 |         |         |
| 6   | R     | 1        | Total | C  | O | 0       | 1       |
|     |       |          | 36    | 28 | 8 |         |         |
| 6   | S     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 32    | 28 | 4 |         |         |

- Molecule 7 is FE (II) ION (CCD ID: FE2) (formula: Fe).

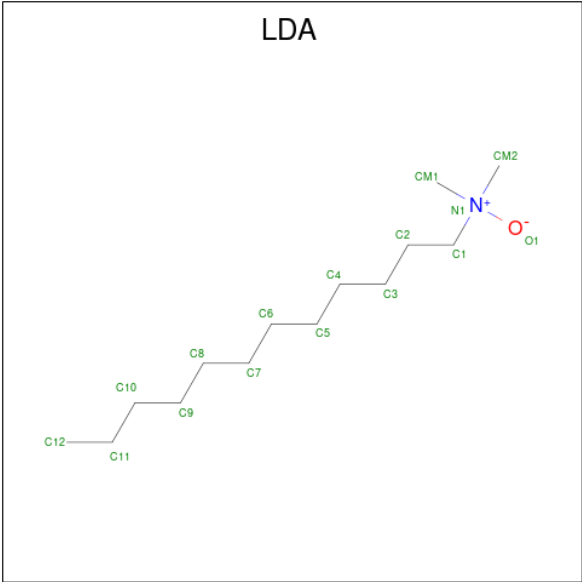
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 7   | M     | 1        | Total | Fe | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 7   | S     | 1        | Total | Fe | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 8 is SPHEROIDENE (CCD ID: SPO) (formula: C<sub>41</sub>H<sub>60</sub>O).



| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 8   | M     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 42    | 41 | 1 |         |         |
| 8   | S     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 42    | 41 | 1 |         |         |

- Molecule 9 is LAURYL DIMETHYLAMINE-N-OXIDE (CCD ID: LDA) (formula: C<sub>14</sub>H<sub>31</sub>NO).



| Mol | Chain | Residues | Atoms |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 9   | M     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 16    | 14 | 1 | 1 |         |         |

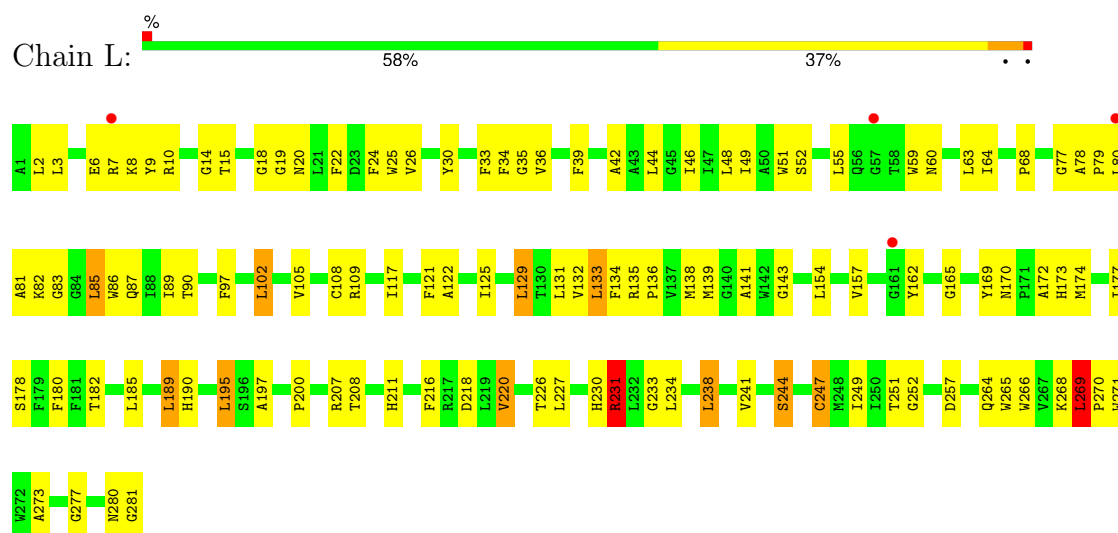
- Molecule 10 is water.

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 10  | L     | 26       | Total | O  | 0       | 0       |
|     |       |          | 26    | 26 |         |         |
| 10  | M     | 42       | Total | O  | 0       | 0       |
|     |       |          | 42    | 42 |         |         |
| 10  | H     | 39       | Total | O  | 0       | 0       |
|     |       |          | 39    | 39 |         |         |
| 10  | R     | 13       | Total | O  | 0       | 0       |
|     |       |          | 13    | 13 |         |         |
| 10  | S     | 24       | Total | O  | 0       | 0       |
|     |       |          | 24    | 24 |         |         |
| 10  | T     | 12       | Total | O  | 0       | 0       |
|     |       |          | 12    | 12 |         |         |

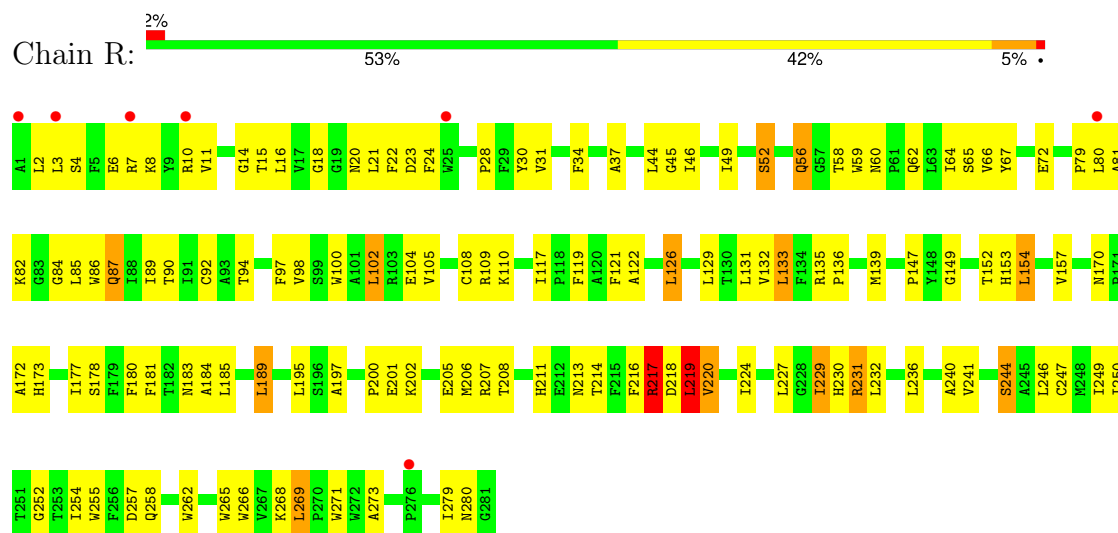
### 3 Residue-property plots [i](#)

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

- Molecule 1: Reaction center protein L chain

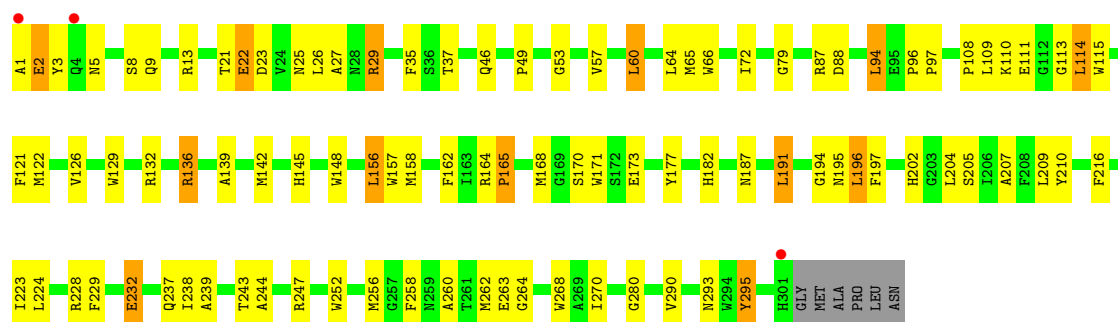


- Molecule 1: Reaction center protein L chain

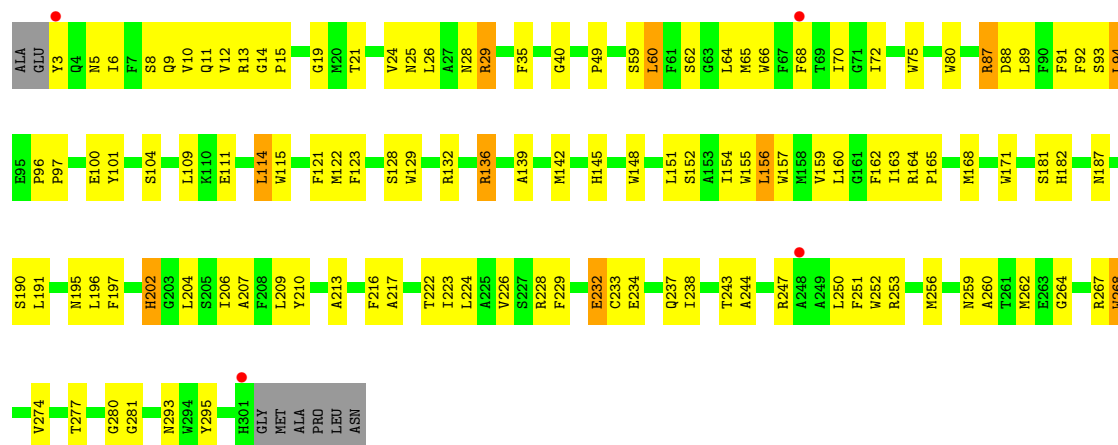


- Molecule 2: Reaction center protein M chain

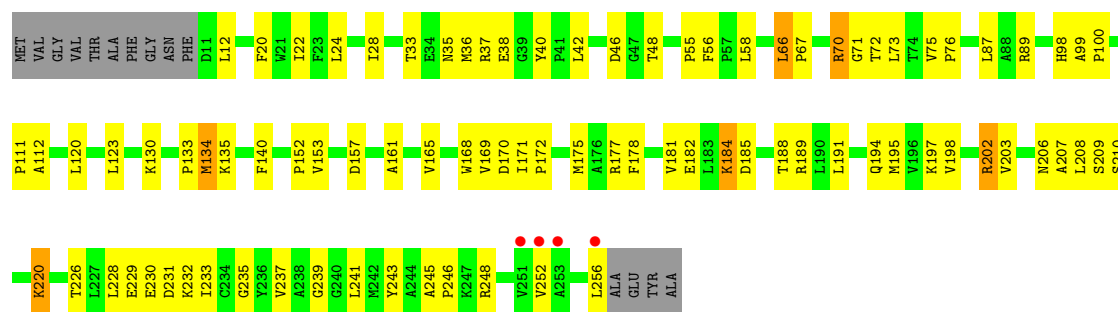




• Molecule 2: Reaction center protein M chain

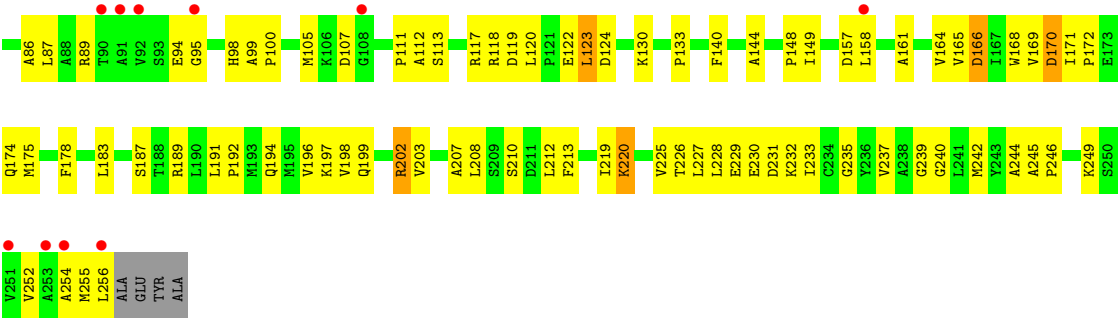


• Molecule 3: Reaction center protein H chain



• Molecule 3: Reaction center protein H chain





## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 43 21 2                                                   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 137.73Å 137.73Å 277.15Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 39.84 – 2.60<br>39.84 – 2.60                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 94.8 (39.84-2.60)<br>94.8 (39.84-2.60)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | 0.09                                                        | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.83 (at 2.61Å)                                             | Xtriage          |
| Refinement program                                                      | CNS                                                         | Depositor        |
| R, $R_{free}$                                                           | 0.226 , 0.268<br>0.210 , 0.254                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 3965 reflections (5.06%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 51.1                                                        | Xtriage          |
| Anisotropy                                                              | 0.363                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.37 , 58.3                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.92                                                        | EDS              |
| Total number of atoms                                                   | 14144                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 49.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LDA, SPO, FE2, U10, BCL, BPH

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   | L     | 0.51         | 0/2320      | 0.92        | 8/3175 (0.3%)   |
| 1   | R     | 0.43         | 0/2320      | 0.96        | 7/3175 (0.2%)   |
| 2   | M     | 0.51         | 0/2491      | 0.94        | 8/3402 (0.2%)   |
| 2   | S     | 0.44         | 0/2477      | 0.91        | 6/3383 (0.2%)   |
| 3   | H     | 0.47         | 0/1917      | 0.92        | 5/2608 (0.2%)   |
| 3   | T     | 0.39         | 0/1917      | 0.90        | 3/2608 (0.1%)   |
| All | All   | 0.46         | 0/13442     | 0.93        | 37/18351 (0.2%) |

There are no bond length outliers.

All (37) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | H     | 22  | ILE  | N-CA-C  | -7.55 | 102.98      | 110.30   |
| 2   | M     | 46  | GLN  | N-CA-C  | 7.31  | 120.43      | 109.25   |
| 1   | R     | 244 | SER  | N-CA-C  | -7.03 | 103.31      | 110.97   |
| 1   | R     | 229 | ILE  | CB-CA-C | -6.77 | 103.15      | 112.02   |
| 1   | R     | 217 | ARG  | N-CA-C  | -6.76 | 103.84      | 111.14   |
| 2   | M     | 210 | TYR  | N-CA-C  | -6.75 | 103.85      | 111.14   |
| 1   | L     | 3   | LEU  | N-CA-C  | -6.68 | 101.72      | 110.53   |
| 2   | S     | 217 | ALA  | N-CA-C  | -5.93 | 104.89      | 111.36   |
| 2   | S     | 268 | TRP  | N-CA-C  | -5.86 | 104.97      | 111.36   |
| 3   | H     | 66  | LEU  | CA-C-N  | 5.82  | 125.75      | 119.76   |
| 3   | H     | 66  | LEU  | C-N-CA  | 5.82  | 125.75      | 119.76   |
| 1   | R     | 56  | GLN  | N-CA-C  | -5.80 | 106.37      | 113.50   |
| 3   | H     | 133 | PRO  | N-CA-C  | -5.69 | 101.60      | 111.32   |
| 3   | T     | 60  | LYS  | N-CA-C  | -5.62 | 102.50      | 109.64   |
| 2   | S     | 267 | ARG  | N-CA-C  | -5.59 | 105.18      | 112.23   |
| 2   | M     | 268 | TRP  | N-CA-C  | -5.59 | 105.09      | 111.07   |
| 2   | S     | 160 | LEU  | N-CA-C  | 5.58  | 117.82      | 111.02   |
| 2   | M     | 202 | HIS  | N-CA-C  | -5.50 | 105.30      | 112.23   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | M     | 37  | THR  | N-CA-C  | -5.50 | 105.83      | 112.54   |
| 1   | L     | 134 | PHE  | N-CA-C  | 5.37  | 116.81      | 111.07   |
| 1   | L     | 244 | SER  | N-CA-C  | -5.36 | 105.35      | 111.14   |
| 3   | H     | 243 | TYR  | N-CA-C  | 5.34  | 119.64      | 113.18   |
| 2   | S     | 89  | LEU  | N-CA-C  | 5.33  | 117.51      | 111.11   |
| 2   | S     | 202 | HIS  | N-CA-C  | -5.22 | 105.67      | 111.36   |
| 2   | M     | 295 | TYR  | N-CA-C  | -5.21 | 105.50      | 111.07   |
| 1   | L     | 269 | LEU  | CA-C-N  | 5.20  | 126.34      | 119.84   |
| 1   | L     | 269 | LEU  | C-N-CA  | 5.20  | 126.34      | 119.84   |
| 1   | L     | 26  | VAL  | N-CA-C  | -5.19 | 98.52       | 107.24   |
| 1   | R     | 271 | TRP  | N-CA-C  | 5.17  | 119.34      | 113.19   |
| 1   | R     | 219 | LEU  | N-CA-C  | 5.16  | 116.99      | 111.36   |
| 3   | T     | 170 | ASP  | N-CA-C  | -5.16 | 98.92       | 107.99   |
| 1   | L     | 35  | GLY  | N-CA-C  | -5.14 | 106.19      | 112.77   |
| 2   | M     | 22  | GLU  | CB-CA-C | -5.13 | 110.64      | 116.54   |
| 1   | R     | 52  | SER  | N-CA-C  | -5.13 | 105.87      | 111.82   |
| 2   | M     | 79  | GLY  | N-CA-C  | -5.12 | 107.01      | 114.90   |
| 1   | L     | 231 | ARG  | N-CA-C  | -5.05 | 105.77      | 111.28   |
| 3   | T     | 169 | VAL  | N-CA-C  | 5.05  | 116.24      | 108.71   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | L     | 2232  | 0        | 2189     | 111     | 0            |
| 1   | R     | 2232  | 0        | 2189     | 131     | 0            |
| 2   | M     | 2399  | 0        | 2310     | 91      | 0            |
| 2   | S     | 2385  | 0        | 2296     | 121     | 0            |
| 3   | H     | 1869  | 0        | 1884     | 78      | 0            |
| 3   | T     | 1869  | 0        | 1884     | 107     | 0            |
| 4   | L     | 183   | 0        | 189      | 27      | 0            |
| 4   | M     | 66    | 0        | 74       | 21      | 0            |
| 4   | R     | 66    | 0        | 74       | 10      | 0            |
| 4   | S     | 183   | 0        | 189      | 29      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 5   | L     | 65    | 0        | 74       | 5       | 0            |
| 5   | M     | 55    | 0        | 53       | 1       | 0            |
| 5   | R     | 65    | 0        | 74       | 9       | 0            |
| 5   | S     | 51    | 0        | 45       | 6       | 0            |
| 6   | L     | 60    | 0        | 70       | 3       | 0            |
| 6   | M     | 38    | 0        | 47       | 0       | 0            |
| 6   | R     | 36    | 0        | 30       | 3       | 0            |
| 6   | S     | 32    | 0        | 39       | 1       | 0            |
| 7   | M     | 1     | 0        | 0        | 0       | 0            |
| 7   | S     | 1     | 0        | 0        | 0       | 0            |
| 8   | M     | 42    | 0        | 60       | 6       | 0            |
| 8   | S     | 42    | 0        | 60       | 2       | 0            |
| 9   | M     | 16    | 0        | 31       | 2       | 0            |
| 10  | H     | 39    | 0        | 0        | 2       | 0            |
| 10  | L     | 26    | 0        | 0        | 4       | 0            |
| 10  | M     | 42    | 0        | 0        | 1       | 0            |
| 10  | R     | 13    | 0        | 0        | 0       | 0            |
| 10  | S     | 24    | 0        | 0        | 2       | 0            |
| 10  | T     | 12    | 0        | 0        | 1       | 0            |
| All | All   | 14144 | 0        | 13861    | 606     | 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 22.

All (606) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:R:200:PRO:HB3  | 1:R:207:ARG:HD3   | 1.42                     | 1.02              |
| 2:S:157:TRP:HB2  | 4:S:2003:BCL:H62  | 1.44                     | 0.99              |
| 1:R:219:LEU:HD13 | 1:R:220:VAL:HG23  | 1.48                     | 0.95              |
| 3:T:226:THR:OG1  | 3:T:229:GLU:HG3   | 1.68                     | 0.93              |
| 3:H:33:THR:HA    | 3:H:36:MET:HE2    | 1.52                     | 0.92              |
| 1:R:208:THR:H    | 1:R:211:HIS:HD2   | 1.18                     | 0.92              |
| 1:R:189:LEU:HG   | 1:R:216:PHE:HZ    | 1.37                     | 0.90              |
| 1:L:241:VAL:HG21 | 5:L:1006:BPH:HAC1 | 1.53                     | 0.89              |
| 2:M:157:TRP:HB2  | 4:M:1003:BCL:H62  | 1.57                     | 0.86              |
| 1:R:208:THR:H    | 1:R:211:HIS:CD2   | 1.94                     | 0.86              |
| 2:M:239:ALA:HB1  | 3:H:66:LEU:HD11   | 1.60                     | 0.83              |
| 1:L:55:LEU:HD13  | 1:L:81:ALA:HB2    | 1.59                     | 0.82              |
| 1:L:77:GLY:HA2   | 1:L:87:GLN:HE22   | 1.44                     | 0.82              |
| 2:S:21:THR:HG23  | 2:S:26:LEU:HD21   | 1.59                     | 0.82              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 3:T:194:GLN:H     | 3:T:194:GLN:NE2    | 1.78                     | 0.81              |
| 1:R:153:HIS:O     | 1:R:157:VAL:HG23   | 1.81                     | 0.81              |
| 2:S:243:THR:O     | 2:S:247:ARG:HG3    | 1.81                     | 0.81              |
| 2:M:13:ARG:HD2    | 2:M:35:PHE:CD2     | 2.16                     | 0.80              |
| 1:L:52:SER:HB2    | 1:L:85:LEU:HD23    | 1.63                     | 0.80              |
| 1:L:189:LEU:HG    | 1:L:216:PHE:HZ     | 1.46                     | 0.79              |
| 3:H:70:ARG:HH11   | 3:H:70:ARG:HG2     | 1.47                     | 0.79              |
| 3:H:228:LEU:HD11  | 3:H:232:LYS:HE3    | 1.63                     | 0.78              |
| 2:S:197:PHE:HZ    | 4:S:2003:BCL:HBB2  | 1.47                     | 0.78              |
| 1:L:79:PRO:HG2    | 1:L:82:LYS:HB2     | 1.66                     | 0.77              |
| 1:L:227:LEU:HD13  | 2:M:232:GLU:HG2    | 1.65                     | 0.77              |
| 2:M:229:PHE:HB2   | 2:M:244:ALA:HB2    | 1.66                     | 0.77              |
| 1:L:257:ASP:HB3   | 10:L:1010:HOH:O    | 1.83                     | 0.77              |
| 1:L:157:VAL:HG11  | 4:M:1003:BCL:HBB1  | 1.67                     | 0.76              |
| 1:R:227:LEU:HD13  | 2:S:232:GLU:HG2    | 1.66                     | 0.76              |
| 3:H:178:PHE:HZ    | 3:H:230:GLU:HG2    | 1.51                     | 0.75              |
| 2:S:13:ARG:HD2    | 2:S:35:PHE:CD2     | 2.21                     | 0.74              |
| 2:M:197:PHE:HZ    | 4:M:1003:BCL:HBB2  | 1.53                     | 0.74              |
| 2:S:228:ARG:HA    | 3:T:194:GLN:CG     | 2.17                     | 0.74              |
| 2:S:268:TRP:HE1   | 3:T:35:ASN:ND2     | 1.85                     | 0.74              |
| 3:H:171:ILE:HB    | 3:H:172:PRO:HD3    | 1.72                     | 0.72              |
| 1:R:189:LEU:HG    | 1:R:216:PHE:CZ     | 2.24                     | 0.72              |
| 3:T:252:VAL:O     | 3:T:256:LEU:HD13   | 1.89                     | 0.72              |
| 1:R:241:VAL:HG21  | 5:R:2006:BPH:HAC1  | 1.70                     | 0.72              |
| 2:S:11:GLN:HB2    | 3:T:144:ALA:HB3    | 1.70                     | 0.72              |
| 3:T:194:GLN:H     | 3:T:194:GLN:CD     | 1.96                     | 0.72              |
| 5:R:2006:BPH:H7C2 | 4:S:2004:BCL:H201  | 1.71                     | 0.72              |
| 1:R:200:PRO:CB    | 1:R:207:ARG:HD3    | 2.18                     | 0.72              |
| 1:L:190:HIS:HA    | 6:L:1009[B]:U10:O2 | 1.89                     | 0.72              |
| 4:R:2002:BCL:HBD  | 4:S:2004:BCL:HBC1  | 1.70                     | 0.72              |
| 1:R:79:PRO:HG2    | 1:R:82:LYS:HB2     | 1.72                     | 0.71              |
| 2:S:101:TYR:O     | 2:S:104:SER:HB3    | 1.91                     | 0.70              |
| 2:S:229:PHE:HB2   | 2:S:244:ALA:HB2    | 1.73                     | 0.70              |
| 2:M:197:PHE:CZ    | 4:M:1003:BCL:HBB2  | 2.26                     | 0.70              |
| 1:R:105:VAL:O     | 1:R:109:ARG:HG3    | 1.90                     | 0.70              |
| 1:R:195:LEU:HB3   | 2:S:145:HIS:CD2    | 2.26                     | 0.70              |
| 3:T:42:LEU:N      | 3:T:53:GLN:HE22    | 1.89                     | 0.70              |
| 2:S:136:ARG:HA    | 2:S:136:ARG:NE     | 2.06                     | 0.70              |
| 3:T:133:PRO:HG3   | 3:T:168:TRP:CE2    | 2.27                     | 0.69              |
| 4:L:1002:BCL:HBD  | 4:L:1004:BCL:CBC   | 2.21                     | 0.69              |
| 2:M:157:TRP:HB2   | 4:M:1003:BCL:C6    | 2.21                     | 0.69              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:R:66:VAL:HG11   | 1:R:89:ILE:HD12  | 1.72                     | 0.69              |
| 1:R:207:ARG:HG3   | 2:S:142:MET:HG2  | 1.74                     | 0.69              |
| 3:T:171:ILE:HB    | 3:T:172:PRO:HD3  | 1.75                     | 0.68              |
| 1:R:4:SER:HB2     | 3:T:79:GLU:CG    | 2.24                     | 0.68              |
| 2:M:97:PRO:HG2    | 2:M:171:TRP:HB2  | 1.76                     | 0.68              |
| 2:S:207:ALA:HA    | 4:S:2004:BCL:O1A | 1.93                     | 0.68              |
| 3:T:119:ASP:O     | 3:T:120:LEU:HD23 | 1.92                     | 0.68              |
| 3:T:112:ALA:HA    | 3:T:235:GLY:O    | 1.94                     | 0.68              |
| 3:T:87:LEU:HD23   | 3:T:100:PRO:HA   | 1.75                     | 0.68              |
| 2:S:152:SER:HB2   | 2:S:274:VAL:HG13 | 1.75                     | 0.67              |
| 1:L:208:THR:H     | 1:L:211:HIS:CD2  | 2.13                     | 0.66              |
| 1:R:60:ASN:O      | 1:R:64:ILE:HG13  | 1.96                     | 0.66              |
| 2:S:9:GLN:NE2     | 3:T:198:VAL:H    | 1.94                     | 0.66              |
| 1:R:52:SER:HB2    | 1:R:85:LEU:HD23  | 1.76                     | 0.66              |
| 2:S:237:GLN:HB2   | 2:S:262:MET:HG2  | 1.78                     | 0.66              |
| 2:M:243:THR:O     | 2:M:247:ARG:HG3  | 1.96                     | 0.66              |
| 2:M:228:ARG:HA    | 3:H:194:GLN:CG   | 2.26                     | 0.66              |
| 4:R:2002:BCL:HBD  | 4:S:2004:BCL:CBC | 2.25                     | 0.66              |
| 1:R:2:LEU:HB3     | 1:R:6:GLU:HB3    | 1.77                     | 0.66              |
| 3:T:189:ARG:HG2   | 3:T:189:ARG:HH11 | 1.60                     | 0.65              |
| 2:M:9:GLN:NE2     | 3:H:198:VAL:H    | 1.95                     | 0.65              |
| 3:H:202:ARG:HG2   | 3:H:203:VAL:N    | 2.10                     | 0.65              |
| 1:L:14:GLY:O      | 1:L:109:ARG:HD3  | 1.97                     | 0.65              |
| 2:S:268:TRP:NE1   | 3:T:35:ASN:HD21  | 1.94                     | 0.65              |
| 3:H:37:ARG:O      | 3:H:38:GLU:HG2   | 1.97                     | 0.65              |
| 1:R:85:LEU:O      | 1:R:89:ILE:HG13  | 1.96                     | 0.65              |
| 3:T:165:VAL:O     | 3:T:166:ASP:HB2  | 1.94                     | 0.65              |
| 1:L:265:TRP:O     | 1:L:269:LEU:HD13 | 1.97                     | 0.64              |
| 2:M:2:GLU:O       | 2:M:3:TYR:HB3    | 1.98                     | 0.64              |
| 2:M:156:LEU:HD13  | 4:M:1003:BCL:H43 | 1.79                     | 0.64              |
| 3:H:226:THR:OG1   | 3:H:229:GLU:HG3  | 1.97                     | 0.64              |
| 1:R:4:SER:HB2     | 3:T:79:GLU:HG2   | 1.79                     | 0.64              |
| 3:H:170:ASP:HB2   | 3:H:177:ARG:HG3  | 1.79                     | 0.63              |
| 1:L:218:ASP:OD1   | 2:M:29:ARG:HD2   | 1.98                     | 0.63              |
| 2:M:53:GLY:O      | 2:M:57:VAL:HG23  | 1.97                     | 0.63              |
| 2:M:228:ARG:HA    | 3:H:194:GLN:HG2  | 1.81                     | 0.63              |
| 1:L:195:LEU:HB3   | 2:M:145:HIS:CD2  | 2.33                     | 0.63              |
| 2:M:9:GLN:HE22    | 3:H:197:LYS:HA   | 1.62                     | 0.63              |
| 2:S:25:ASN:HD22   | 2:S:28:ASN:ND2   | 1.97                     | 0.63              |
| 3:H:112:ALA:HB2   | 3:H:239:GLY:HA3  | 1.80                     | 0.63              |
| 4:L:1001:BCL:HBB3 | 4:M:1003:BCL:H41 | 1.79                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:L:173:HIS:CE1   | 1:L:177:ILE:HD11  | 2.33                     | 0.62              |
| 4:L:1001:BCL:HBC1 | 4:M:1003:BCL:CBD  | 2.29                     | 0.62              |
| 1:R:205:GLU:HG2   | 3:T:65:ILE:HG22   | 1.82                     | 0.62              |
| 3:T:130:LYS:HE3   | 3:T:170:ASP:OD2   | 1.99                     | 0.62              |
| 3:H:194:GLN:CD    | 3:H:194:GLN:H     | 2.08                     | 0.62              |
| 3:H:220:LYS:HB2   | 3:H:220:LYS:NZ    | 2.15                     | 0.62              |
| 1:R:8:LYS:HD2     | 3:T:113:SER:HB3   | 1.82                     | 0.62              |
| 1:L:7:ARG:HH12    | 3:H:87:LEU:HB2    | 1.65                     | 0.62              |
| 3:H:130:LYS:HE3   | 3:H:170:ASP:OD2   | 1.99                     | 0.62              |
| 2:S:109:LEU:HD22  | 2:S:114:LEU:HD13  | 1.81                     | 0.61              |
| 4:L:1002:BCL:HBD  | 4:L:1004:BCL:HBC1 | 1.81                     | 0.61              |
| 1:R:20:ASN:HA     | 1:R:23:ASP:HB2    | 1.82                     | 0.61              |
| 2:S:60:LEU:O      | 2:S:64:LEU:HG     | 2.00                     | 0.61              |
| 1:L:189:LEU:HG    | 1:L:216:PHE:CZ    | 2.33                     | 0.61              |
| 3:T:44:ASN:C      | 3:T:46:ASP:H      | 2.07                     | 0.61              |
| 3:H:87:LEU:HD23   | 3:H:100:PRO:HA    | 1.81                     | 0.61              |
| 2:S:97:PRO:HG2    | 2:S:171:TRP:HB2   | 1.80                     | 0.61              |
| 1:L:208:THR:H     | 1:L:211:HIS:HD2   | 1.47                     | 0.61              |
| 2:S:229:PHE:CE2   | 2:S:247:ARG:HD2   | 2.36                     | 0.61              |
| 4:S:2001:BCL:HBC1 | 4:S:2003:BCL:CAD  | 2.30                     | 0.61              |
| 2:M:109:LEU:HD22  | 2:M:114:LEU:HD13  | 1.83                     | 0.61              |
| 1:L:207:ARG:HG2   | 2:M:142:MET:HG2   | 1.83                     | 0.60              |
| 3:H:70:ARG:HG2    | 3:H:70:ARG:NH1    | 2.14                     | 0.60              |
| 2:M:260:ALA:HB1   | 3:H:35:ASN:OD1    | 2.01                     | 0.60              |
| 3:H:229:GLU:O     | 3:H:233:ILE:HG13  | 2.01                     | 0.60              |
| 1:L:200:PRO:HB3   | 1:L:207:ARG:HD3   | 1.83                     | 0.60              |
| 2:M:280:GLY:HA2   | 4:M:1003:BCL:HED2 | 1.84                     | 0.60              |
| 2:S:9:GLN:HE22    | 3:T:198:VAL:H     | 1.50                     | 0.60              |
| 2:M:195:ASN:HD22  | 2:M:195:ASN:C     | 2.10                     | 0.60              |
| 1:L:33:PHE:O      | 1:L:36:VAL:HG22   | 2.02                     | 0.60              |
| 3:H:161:ALA:HB2   | 3:H:210:SER:HA    | 1.82                     | 0.60              |
| 3:T:60:LYS:HG2    | 3:T:61:PRO:HD2    | 1.83                     | 0.60              |
| 1:L:139:MET:HE3   | 1:L:252:GLY:HA3   | 1.83                     | 0.59              |
| 1:R:86:TRP:CZ2    | 1:R:132:VAL:HG13  | 2.37                     | 0.59              |
| 2:M:136:ARG:NE    | 2:M:136:ARG:HA    | 2.16                     | 0.59              |
| 3:H:112:ALA:HA    | 3:H:235:GLY:O     | 2.03                     | 0.59              |
| 2:M:1:ALA:O       | 2:M:2:GLU:HB2     | 2.02                     | 0.59              |
| 2:M:164:ARG:HB3   | 2:M:165:PRO:HD3   | 1.82                     | 0.59              |
| 1:R:135:ARG:HB3   | 1:R:136:PRO:HD3   | 1.85                     | 0.59              |
| 2:M:168:MET:CB    | 2:M:173:GLU:HG3   | 2.32                     | 0.59              |
| 3:T:33:THR:HA     | 3:T:36:MET:CG     | 2.32                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:S:8:SER:OG      | 3:T:175:MET:HE1   | 2.02                     | 0.59              |
| 1:R:265:TRP:O     | 1:R:269:LEU:HD13  | 2.02                     | 0.59              |
| 3:T:202:ARG:HG2   | 3:T:203:VAL:N     | 2.16                     | 0.59              |
| 4:L:1001:BCL:HBC1 | 4:M:1003:BCL:HBD  | 1.85                     | 0.59              |
| 3:H:66:LEU:HB2    | 3:H:71:GLY:O      | 2.03                     | 0.58              |
| 3:H:152:PRO:HG2   | 3:H:202:ARG:HB2   | 1.85                     | 0.58              |
| 2:S:62:SER:O      | 2:S:121:PHE:HB3   | 2.03                     | 0.58              |
| 2:S:3:TYR:CZ      | 2:S:5:ASN:HA      | 2.39                     | 0.58              |
| 2:S:25:ASN:ND2    | 2:S:28:ASN:ND2    | 2.51                     | 0.58              |
| 3:T:105:MET:HE2   | 3:T:212:LEU:HD13  | 1.86                     | 0.58              |
| 3:T:42:LEU:H      | 3:T:53:GLN:HE22   | 1.51                     | 0.58              |
| 2:M:162:PHE:HB2   | 8:M:1010:SPO:H291 | 1.85                     | 0.58              |
| 3:H:248:ARG:NH1   | 3:H:248:ARG:HB2   | 2.18                     | 0.58              |
| 2:S:268:TRP:NE1   | 3:T:35:ASN:ND2    | 2.52                     | 0.58              |
| 2:S:88:ASP:HB2    | 2:S:92:PHE:CZ     | 2.39                     | 0.58              |
| 3:T:183:LEU:HD21  | 3:T:213:PHE:HB3   | 1.86                     | 0.58              |
| 1:L:34:PHE:CE1    | 1:L:102:LEU:HD23  | 2.38                     | 0.58              |
| 3:H:194:GLN:H     | 3:H:194:GLN:NE2   | 2.01                     | 0.58              |
| 1:R:207:ARG:HD2   | 1:R:207:ARG:N     | 2.18                     | 0.58              |
| 2:S:228:ARG:HA    | 3:T:194:GLN:HG2   | 1.84                     | 0.58              |
| 2:M:9:GLN:HE22    | 3:H:198:VAL:H     | 1.52                     | 0.57              |
| 1:R:178:SER:HA    | 4:S:2001:BCL:HBA2 | 1.86                     | 0.57              |
| 2:S:264:GLY:HA3   | 3:T:35:ASN:OD1    | 2.04                     | 0.57              |
| 1:L:230:HIS:CD2   | 2:M:223:ILE:HG13  | 2.39                     | 0.57              |
| 1:L:241:VAL:CG2   | 5:L:1006:BPH:HAC1 | 2.30                     | 0.57              |
| 2:S:152:SER:CB    | 2:S:274:VAL:HG13  | 2.33                     | 0.57              |
| 1:R:157:VAL:HG11  | 4:S:2003:BCL:HBB1 | 1.86                     | 0.57              |
| 2:S:9:GLN:HE22    | 3:T:197:LYS:HA    | 1.69                     | 0.57              |
| 1:L:277:GLY:O     | 1:L:281:GLY:HA3   | 2.05                     | 0.57              |
| 2:M:8:SER:OG      | 3:H:175:MET:HE1   | 2.05                     | 0.57              |
| 10:L:1032:HOH:O   | 2:M:49:PRO:HG2    | 2.03                     | 0.57              |
| 2:S:197:PHE:CZ    | 4:S:2003:BCL:HBB2 | 2.36                     | 0.57              |
| 3:H:245:ALA:HB3   | 3:H:246:PRO:HD3   | 1.85                     | 0.57              |
| 1:L:49:ILE:CG1    | 1:L:89:ILE:HD13   | 2.35                     | 0.57              |
| 1:L:51:TRP:CE3    | 1:L:85:LEU:HD11   | 2.40                     | 0.56              |
| 1:R:18:GLY:O      | 1:R:21:LEU:HG     | 2.04                     | 0.56              |
| 1:L:44:LEU:O      | 1:L:48:LEU:HG     | 2.04                     | 0.56              |
| 2:S:49:PRO:HG2    | 10:S:2019:HOH:O   | 2.05                     | 0.56              |
| 3:T:44:ASN:O      | 3:T:46:ASP:N      | 2.38                     | 0.56              |
| 2:M:157:TRP:CE3   | 2:M:158:MET:HG2   | 2.40                     | 0.56              |
| 2:M:182:HIS:CG    | 8:M:1010:SPO:H181 | 2.40                     | 0.56              |

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| Atom-1            | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|----------------------|--------------------------|-------------------|
| 4:L:1002:BCL:HBD  | 4:L:1004:BCL:HBC3    | 1.86                     | 0.56              |
| 1:R:230:HIS:CD2   | 2:S:223:ILE:HG13     | 2.41                     | 0.56              |
| 2:S:209:LEU:HD22  | 4:S:2003:BCL:H3A     | 1.88                     | 0.56              |
| 1:L:90:THR:HG23   | 1:L:132:VAL:HG11     | 1.88                     | 0.56              |
| 3:T:12:LEU:N      | 3:T:12:LEU:HD22      | 2.21                     | 0.56              |
| 3:T:133:PRO:HG3   | 3:T:168:TRP:CZ2      | 2.41                     | 0.56              |
| 3:T:168:TRP:HB2   | 3:T:178:PHE:HB2      | 1.88                     | 0.56              |
| 2:S:66:TRP:NE1    | 2:S:70:ILE:HD11      | 2.21                     | 0.55              |
| 4:S:2001:BCL:HBB3 | 4:S:2003:BCL:H61     | 1.89                     | 0.55              |
| 2:S:228:ARG:HA    | 3:T:194:GLN:HG3      | 1.88                     | 0.55              |
| 2:M:195:ASN:ND2   | 2:M:197:PHE:H        | 2.04                     | 0.55              |
| 1:L:49:ILE:HG13   | 1:L:89:ILE:HD13      | 1.88                     | 0.55              |
| 2:S:274:VAL:HA    | 5:S:2005:BPH:HBC1    | 1.88                     | 0.55              |
| 4:L:1002:BCL:H122 | 5:L:1006:BPH:H3A     | 1.88                     | 0.55              |
| 2:S:24:VAL:HG22   | 2:S:139:ALA:HB1      | 1.89                     | 0.55              |
| 2:M:290:VAL:HG11  | 3:H:12:LEU:HB2       | 1.90                     | 0.54              |
| 2:S:210:TYR:HB2   | 4:S:2004:BCL:O1A     | 2.08                     | 0.54              |
| 4:R:2002:BCL:H122 | 5:R:2006:BPH:H3A     | 1.89                     | 0.54              |
| 2:S:202:HIS:CE1   | 2:S:206:ILE:HD11     | 2.42                     | 0.54              |
| 1:R:139:MET:HE3   | 1:R:252:GLY:O        | 2.08                     | 0.54              |
| 3:T:189:ARG:HG2   | 3:T:189:ARG:NH1      | 2.23                     | 0.54              |
| 1:L:189:LEU:HB3   | 6:L:1009[A]:U10:H4M3 | 1.88                     | 0.54              |
| 2:M:94:LEU:HD22   | 2:M:115:TRP:HB2      | 1.89                     | 0.54              |
| 1:R:46:ILE:HG12   | 4:S:2004:BCL:H202    | 1.90                     | 0.54              |
| 1:R:86:TRP:CH2    | 1:R:132:VAL:HG13     | 2.43                     | 0.54              |
| 1:L:182:THR:HG21  | 6:L:1009[B]:U10:H18  | 1.90                     | 0.54              |
| 2:M:66:TRP:CD1    | 2:M:122:MET:HB2      | 2.43                     | 0.54              |
| 3:H:182:GLU:HA    | 3:H:188:THR:HG22     | 1.89                     | 0.53              |
| 1:L:197:ALA:HA    | 1:L:207:ARG:HB2      | 1.90                     | 0.53              |
| 3:T:229:GLU:O     | 3:T:233:ILE:HG13     | 2.08                     | 0.53              |
| 2:M:168:MET:HB2   | 2:M:173:GLU:HG3      | 1.89                     | 0.53              |
| 2:S:70:ILE:HA     | 2:S:94:LEU:HD12      | 1.91                     | 0.53              |
| 1:L:80:LEU:CD2    | 1:L:80:LEU:H         | 2.22                     | 0.53              |
| 2:S:164:ARG:HB3   | 2:S:165:PRO:HD3      | 1.91                     | 0.53              |
| 3:T:75:VAL:HA     | 3:T:76:PRO:C         | 2.33                     | 0.53              |
| 3:H:40:TYR:HB3    | 3:H:58:LEU:HD21      | 1.90                     | 0.52              |
| 1:R:11:VAL:O      | 1:R:110:LYS:NZ       | 2.35                     | 0.52              |
| 3:T:33:THR:HA     | 3:T:36:MET:HG3       | 1.91                     | 0.52              |
| 1:R:185:LEU:HD13  | 5:S:2005:BPH:ND      | 2.24                     | 0.52              |
| 2:S:65:MET:HB3    | 2:S:121:PHE:CD2      | 2.44                     | 0.52              |
| 1:R:131:LEU:HD11  | 4:S:2004:BCL:HBC2    | 1.91                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:T:33:THR:HA     | 3:T:36:MET:HG2    | 1.91                     | 0.52              |
| 3:T:228:LEU:O     | 3:T:232:LYS:HG3   | 2.09                     | 0.52              |
| 2:S:10:VAL:HG21   | 3:T:148:PRO:HD3   | 1.90                     | 0.52              |
| 3:T:86:ALA:HB3    | 3:T:107:ASP:HB3   | 1.92                     | 0.52              |
| 3:T:44:ASN:HB2    | 3:T:46:ASP:OD1    | 2.10                     | 0.52              |
| 3:T:178:PHE:HZ    | 3:T:230:GLU:HG3   | 1.73                     | 0.52              |
| 2:M:237:GLN:HB2   | 2:M:262:MET:HG2   | 1.90                     | 0.52              |
| 3:T:164:VAL:HG21  | 3:T:203:VAL:HG21  | 1.92                     | 0.52              |
| 1:R:219:LEU:HD22  | 1:R:219:LEU:O     | 2.09                     | 0.52              |
| 1:R:22:PHE:HA     | 1:R:24:PHE:CE2    | 2.45                     | 0.52              |
| 1:L:15:THR:HG22   | 1:L:30:TYR:OH     | 2.10                     | 0.51              |
| 5:R:2006:BPH:H152 | 4:S:2004:BCL:HBB3 | 1.93                     | 0.51              |
| 2:M:232:GLU:OE1   | 2:M:232:GLU:N     | 2.39                     | 0.51              |
| 2:S:204:LEU:HD13  | 3:T:20:PHE:CE2    | 2.45                     | 0.51              |
| 1:L:170:ASN:HB3   | 1:L:173:HIS:HB2   | 1.91                     | 0.51              |
| 1:R:100:TRP:O     | 1:R:104:GLU:HG3   | 2.10                     | 0.51              |
| 1:R:246:LEU:O     | 1:R:250:ILE:HG12  | 2.10                     | 0.51              |
| 2:S:280:GLY:HA2   | 4:S:2003:BCL:HED2 | 1.93                     | 0.51              |
| 4:L:1002:BCL:HAA2 | 4:L:1004:BCL:HBC1 | 1.93                     | 0.51              |
| 1:L:80:LEU:H      | 1:L:80:LEU:HD22   | 1.76                     | 0.51              |
| 2:M:60:LEU:CD2    | 2:M:64:LEU:HG     | 2.41                     | 0.51              |
| 4:L:1001:BCL:HBB2 | 8:M:1010:SPO:H243 | 1.92                     | 0.51              |
| 2:S:233:CYS:O     | 2:S:237:GLN:HG2   | 2.10                     | 0.51              |
| 1:L:117:ILE:HD13  | 2:M:252:TRP:CZ2   | 2.46                     | 0.51              |
| 2:M:72:ILE:HD12   | 8:M:1010:SPO:HM11 | 1.93                     | 0.51              |
| 1:L:211:HIS:HE1   | 2:M:22:GLU:OE1    | 1.93                     | 0.51              |
| 1:R:244:SER:HB3   | 4:R:2002:BCL:O1A  | 2.10                     | 0.51              |
| 3:T:36:MET:HB2    | 3:T:59:PRO:HD3    | 1.92                     | 0.50              |
| 1:L:135:ARG:NH1   | 1:L:251:THR:O     | 2.45                     | 0.50              |
| 3:H:37:ARG:C      | 3:H:38:GLU:HG2    | 2.36                     | 0.50              |
| 1:R:200:PRO:HG3   | 1:R:205:GLU:O     | 2.10                     | 0.50              |
| 2:S:148:TRP:HA    | 2:S:148:TRP:CE3   | 2.46                     | 0.50              |
| 2:S:148:TRP:HA    | 2:S:148:TRP:HE3   | 1.76                     | 0.50              |
| 1:L:135:ARG:HB3   | 1:L:136:PRO:HD3   | 1.92                     | 0.50              |
| 2:S:64:LEU:O      | 2:S:68:PHE:HB2    | 2.11                     | 0.50              |
| 2:S:232:GLU:O     | 2:S:234:GLU:HG3   | 2.12                     | 0.50              |
| 3:T:45:GLU:CD     | 3:T:95:GLY:H      | 2.20                     | 0.50              |
| 2:M:65:MET:HB3    | 2:M:121:PHE:CD2   | 2.47                     | 0.50              |
| 3:T:122:GLU:OE1   | 3:T:227:LEU:HD11  | 2.12                     | 0.50              |
| 2:M:209:LEU:HD22  | 4:M:1003:BCL:H3A  | 1.94                     | 0.50              |
| 3:H:165:VAL:HG11  | 3:H:182:GLU:HB2   | 1.94                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:R:45:GLY:O      | 1:R:49:ILE:HG13   | 2.11                     | 0.50              |
| 1:L:233:GLY:HA3   | 2:M:216:PHE:CE1   | 2.48                     | 0.49              |
| 1:L:180:PHE:CD2   | 4:L:1002:BCL:HMA3 | 2.47                     | 0.49              |
| 3:H:87:LEU:HA     | 3:H:99:ALA:O      | 2.13                     | 0.49              |
| 3:H:252:VAL:O     | 3:H:256:LEU:HD13  | 2.12                     | 0.49              |
| 1:R:66:VAL:HG12   | 1:R:86:TRP:HB2    | 1.93                     | 0.49              |
| 1:R:122:ALA:O     | 1:R:126:LEU:HD22  | 2.11                     | 0.49              |
| 2:S:25:ASN:HD22   | 2:S:28:ASN:HD21   | 1.58                     | 0.49              |
| 1:R:255:TRP:HZ2   | 1:R:258:GLN:O     | 1.96                     | 0.49              |
| 2:S:21:THR:CG2    | 2:S:26:LEU:HD21   | 2.37                     | 0.49              |
| 2:S:24:VAL:HG22   | 2:S:139:ALA:CB    | 2.41                     | 0.49              |
| 1:L:226:THR:HG23  | 1:L:227:LEU:N     | 2.27                     | 0.49              |
| 1:L:18:GLY:O      | 1:L:19:GLY:C      | 2.55                     | 0.49              |
| 2:S:3:TYR:CE1     | 2:S:9:GLN:HG3     | 2.47                     | 0.49              |
| 1:L:162:TYR:HA    | 1:L:165:GLY:O     | 2.13                     | 0.49              |
| 3:T:18:TYR:O      | 3:T:22:ILE:HG12   | 2.13                     | 0.49              |
| 1:R:72:GLU:H      | 1:R:72:GLU:CD     | 2.21                     | 0.49              |
| 2:M:177:TYR:HE1   | 8:M:1010:SPO:H22  | 1.77                     | 0.49              |
| 2:S:293:ASN:OD1   | 2:S:295:TYR:HB3   | 2.12                     | 0.49              |
| 3:T:59:PRO:HG2    | 3:T:76:PRO:HD3    | 1.95                     | 0.49              |
| 3:T:220:LYS:HG3   | 3:T:229:GLU:OE2   | 2.13                     | 0.49              |
| 1:L:86:TRP:CH2    | 1:L:132:VAL:HG13  | 2.48                     | 0.49              |
| 1:R:180:PHE:CD2   | 4:R:2002:BCL:HMA3 | 2.48                     | 0.49              |
| 2:S:100:GLU:H     | 2:S:100:GLU:CD    | 2.20                     | 0.49              |
| 2:S:222:THR:O     | 2:S:226:VAL:HG22  | 2.13                     | 0.48              |
| 3:T:12:LEU:HD22   | 3:T:12:LEU:H      | 1.75                     | 0.48              |
| 1:L:105:VAL:O     | 1:L:109:ARG:HG3   | 2.14                     | 0.48              |
| 4:L:1001:BCL:HBC1 | 4:M:1003:BCL:CAD  | 2.43                     | 0.48              |
| 3:H:55:PRO:HG2    | 3:H:56:PHE:CD2    | 2.48                     | 0.48              |
| 3:H:220:LYS:HB2   | 3:H:220:LYS:HZ2   | 1.77                     | 0.48              |
| 4:L:1004:BCL:O1A  | 2:M:207:ALA:HA    | 2.14                     | 0.48              |
| 3:T:207:ALA:HB1   | 3:T:237:VAL:O     | 2.12                     | 0.48              |
| 2:S:123:PHE:HA    | 2:S:157:TRP:HH2   | 1.79                     | 0.48              |
| 3:T:45:GLU:HG3    | 3:T:94:GLU:OE1    | 2.13                     | 0.48              |
| 1:L:60:ASN:ND2    | 1:L:63:LEU:HD23   | 2.28                     | 0.48              |
| 1:L:138:MET:SD    | 1:L:249:ILE:HD11  | 2.54                     | 0.48              |
| 1:L:170:ASN:HB3   | 1:L:173:HIS:CB    | 2.43                     | 0.48              |
| 1:R:241:VAL:HG21  | 5:R:2006:BPH:CAC  | 2.42                     | 0.48              |
| 1:R:241:VAL:CG2   | 5:R:2006:BPH:HAC1 | 2.43                     | 0.48              |
| 4:L:1004:BCL:H202 | 5:L:1006:BPH:H7C2 | 1.96                     | 0.48              |
| 1:R:44:LEU:HD23   | 1:R:92:CYS:SG     | 2.53                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:S:59:SER:HB2    | 2:S:128:SER:OG    | 2.14                     | 0.48              |
| 4:L:1001:BCL:HBB2 | 4:L:1001:BCL:HHC  | 1.96                     | 0.48              |
| 3:H:228:LEU:CD1   | 3:H:232:LYS:HE3   | 2.39                     | 0.48              |
| 1:R:268:LYS:HA    | 1:R:273:ALA:HB2   | 1.94                     | 0.48              |
| 4:S:2001:BCL:HBC1 | 4:S:2003:BCL:CB D | 2.44                     | 0.48              |
| 1:L:42:ALA:O      | 1:L:46:ILE:HG13   | 2.13                     | 0.47              |
| 1:R:218:ASP:OD1   | 2:S:29:ARG:HD2    | 2.13                     | 0.47              |
| 1:R:119:PHE:O     | 1:R:122:ALA:HB3   | 2.14                     | 0.47              |
| 1:L:172:ALA:HB3   | 1:L:247:CYS:HA    | 1.95                     | 0.47              |
| 2:M:122:MET:O     | 2:M:126:VAL:HG23  | 2.14                     | 0.47              |
| 2:M:256:MET:HE3   | 2:M:258:PHE:CE1   | 2.49                     | 0.47              |
| 4:R:2002:BCL:NC   | 4:S:2003:BCL:HBB3 | 2.29                     | 0.47              |
| 3:T:208:LEU:HD12  | 3:T:240:GLY:HA3   | 1.96                     | 0.47              |
| 1:L:97:PHE:CE1    | 4:L:1002:BCL:H121 | 2.49                     | 0.47              |
| 1:L:234:LEU:O     | 1:L:238:LEU:HB2   | 2.15                     | 0.47              |
| 3:H:170:ASP:HB2   | 3:H:177:ARG:CG    | 2.44                     | 0.47              |
| 3:H:195:MET:CE    | 3:H:207:ALA:HB2   | 2.44                     | 0.47              |
| 1:R:246:LEU:HA    | 1:R:249:ILE:HG22  | 1.96                     | 0.47              |
| 2:S:164:ARG:O     | 2:S:168:MET:HG2   | 2.14                     | 0.47              |
| 1:L:60:ASN:CG     | 1:L:63:LEU:HD23   | 2.39                     | 0.47              |
| 1:R:139:MET:HE3   | 1:R:252:GLY:HA3   | 1.96                     | 0.47              |
| 2:S:60:LEU:O      | 2:S:60:LEU:HD22   | 2.15                     | 0.47              |
| 2:S:65:MET:HB3    | 2:S:121:PHE:CE2   | 2.50                     | 0.47              |
| 3:T:12:LEU:H      | 3:T:12:LEU:CD2    | 2.28                     | 0.47              |
| 1:L:22:PHE:HA     | 1:L:24:PHE:CE2    | 2.50                     | 0.47              |
| 1:L:55:LEU:CD1    | 1:L:81:ALA:HB2    | 2.38                     | 0.47              |
| 2:M:25:ASN:OD1    | 2:M:27:ALA:HB3    | 2.15                     | 0.47              |
| 1:R:157:VAL:CG1   | 4:S:2003:BCL:HBB1 | 2.45                     | 0.47              |
| 1:R:183:ASN:ND2   | 2:S:213:ALA:HA    | 2.30                     | 0.47              |
| 1:R:213:ASN:O     | 1:R:217:ARG:HB2   | 2.14                     | 0.47              |
| 1:R:250:ILE:HB    | 1:R:254:ILE:HD11  | 1.97                     | 0.47              |
| 3:T:79:GLU:OE1    | 3:T:79:GLU:HA     | 2.15                     | 0.47              |
| 1:R:3:LEU:HD12    | 2:S:250:LEU:HD21  | 1.96                     | 0.47              |
| 3:T:44:ASN:C      | 3:T:46:ASP:N      | 2.72                     | 0.47              |
| 1:L:86:TRP:CZ2    | 1:L:132:VAL:HG13  | 2.50                     | 0.47              |
| 1:L:125:ILE:O     | 1:L:129:LEU:HB2   | 2.14                     | 0.47              |
| 2:S:60:LEU:HA     | 5:S:2005:BPH:H4C2 | 1.97                     | 0.47              |
| 2:S:87:ARG:HG3    | 2:S:88:ASP:N      | 2.30                     | 0.47              |
| 1:L:227:LEU:HD11  | 2:M:5:ASN:HD21    | 1.79                     | 0.46              |
| 3:H:111:PRO:HB2   | 3:H:239:GLY:HA2   | 1.96                     | 0.46              |
| 4:R:2002:BCL:H2C  | 4:S:2003:BCL:H2C  | 1.96                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:L:8:LYS:HE2     | 1:L:9:TYR:CZ      | 2.50                     | 0.46              |
| 2:M:194:GLY:O     | 2:M:195:ASN:HB3   | 2.16                     | 0.46              |
| 5:R:2006:BPH:CMC  | 2:S:213:ALA:HB3   | 2.46                     | 0.46              |
| 1:L:59:TRP:HA     | 1:L:59:TRP:CE3    | 2.51                     | 0.46              |
| 1:L:80:LEU:HD22   | 1:L:80:LEU:N      | 2.30                     | 0.46              |
| 2:S:75:TRP:HB3    | 2:S:80:TRP:CE3    | 2.49                     | 0.46              |
| 1:L:241:VAL:HG21  | 5:L:1006:BPH:H2C  | 1.97                     | 0.46              |
| 4:L:1001:BCL:HBB3 | 4:M:1003:BCL:C4   | 2.44                     | 0.46              |
| 2:M:22:GLU:HB3    | 2:M:139:ALA:O     | 2.15                     | 0.46              |
| 2:M:229:PHE:CB    | 2:M:244:ALA:HB2   | 2.40                     | 0.46              |
| 2:S:157:TRP:HB2   | 4:S:2003:BCL:C6   | 2.32                     | 0.46              |
| 3:T:70:ARG:NH2    | 3:T:123:LEU:HD13  | 2.31                     | 0.46              |
| 1:L:169:TYR:HA    | 1:L:174:MET:HE3   | 1.98                     | 0.46              |
| 1:L:268:LYS:C     | 1:L:273:ALA:HB2   | 2.41                     | 0.46              |
| 1:L:280:ASN:ND2   | 2:M:88:ASP:OD1    | 2.40                     | 0.46              |
| 1:R:129:LEU:O     | 1:R:133:LEU:HB3   | 2.16                     | 0.46              |
| 2:S:162:PHE:C     | 2:S:165:PRO:HD2   | 2.40                     | 0.46              |
| 1:L:178:SER:HA    | 4:L:1001:BCL:O1A  | 2.16                     | 0.46              |
| 1:L:207:ARG:HA    | 1:L:207:ARG:HD2   | 1.67                     | 0.46              |
| 1:L:220:VAL:O     | 1:L:220:VAL:CG1   | 2.62                     | 0.46              |
| 1:L:266:TRP:HE1   | 2:M:87:ARG:HA     | 1.80                     | 0.46              |
| 2:M:195:ASN:HD22  | 2:M:196:LEU:N     | 2.14                     | 0.46              |
| 3:H:153:VAL:HG21  | 3:H:181:VAL:HG22  | 1.98                     | 0.46              |
| 3:H:206:ASN:ND2   | 3:H:248:ARG:HD3   | 2.30                     | 0.46              |
| 1:R:97:PHE:CE1    | 4:R:2002:BCL:H121 | 2.51                     | 0.46              |
| 3:T:42:LEU:H      | 3:T:53:GLN:NE2    | 2.14                     | 0.46              |
| 3:T:170:ASP:O     | 3:T:174:GLN:N     | 2.48                     | 0.46              |
| 2:M:205:SER:OG    | 4:M:1003:BCL:HMA3 | 2.16                     | 0.46              |
| 1:R:15:THR:HG22   | 1:R:30:TYR:OH     | 2.16                     | 0.46              |
| 1:R:181:PHE:CE1   | 4:S:2003:BCL:O1A  | 2.68                     | 0.46              |
| 1:R:2:LEU:N       | 1:R:2:LEU:HD12    | 2.30                     | 0.45              |
| 2:M:13:ARG:O      | 3:H:140:PHE:HA    | 2.15                     | 0.45              |
| 4:M:1003:BCL:H193 | 5:M:1005:BPH:HMA2 | 1.98                     | 0.45              |
| 1:R:207:ARG:HB3   | 1:R:211:HIS:CG    | 2.51                     | 0.45              |
| 4:R:2002:BCL:H52  | 5:R:2006:BPH:HBB2 | 1.97                     | 0.45              |
| 1:R:67:TYR:CD2    | 1:R:147:PRO:HB3   | 2.52                     | 0.45              |
| 2:S:274:VAL:HA    | 5:S:2005:BPH:CBC  | 2.47                     | 0.45              |
| 4:L:1001:BCL:CBC  | 4:M:1003:BCL:CAD  | 2.94                     | 0.45              |
| 2:S:3:TYR:CE2     | 3:T:194:GLN:HA    | 2.52                     | 0.45              |
| 3:T:37:ARG:HH11   | 3:T:37:ARG:HG2    | 1.81                     | 0.45              |
| 2:M:3:TYR:CE1     | 2:M:9:GLN:HG3     | 2.52                     | 0.45              |

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| Atom-1           | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|----------------------|--------------------------|-------------------|
| 2:S:156:LEU:HD12 | 2:S:277:THR:HG22     | 1.97                     | 0.45              |
| 3:H:24:LEU:O     | 3:H:28:ILE:HG13      | 2.16                     | 0.45              |
| 1:R:56:GLN:NE2   | 1:R:58:THR:HG21      | 2.30                     | 0.45              |
| 1:R:197:ALA:HA   | 1:R:207:ARG:HG2      | 1.99                     | 0.45              |
| 1:R:214:THR:O    | 1:R:218:ASP:HB2      | 2.16                     | 0.45              |
| 3:T:161:ALA:HB2  | 3:T:210:SER:HA       | 1.99                     | 0.45              |
| 3:T:199:GLN:HB2  | 3:T:202:ARG:O        | 2.16                     | 0.45              |
| 1:L:39:PHE:CD1   | 1:L:39:PHE:C         | 2.95                     | 0.45              |
| 1:L:157:VAL:CG1  | 4:M:1003:BCL:HBB1    | 2.43                     | 0.45              |
| 2:M:256:MET:HE3  | 2:M:258:PHE:CZ       | 2.51                     | 0.45              |
| 3:T:245:ALA:HB3  | 3:T:246:PRO:HD3      | 1.99                     | 0.45              |
| 3:H:46:ASP:HB3   | 10:H:266:HOH:O       | 2.16                     | 0.45              |
| 1:L:68:PRO:HB3   | 1:L:86:TRP:CD2       | 2.52                     | 0.45              |
| 3:H:66:LEU:HA    | 3:H:67:PRO:HD3       | 1.79                     | 0.45              |
| 3:H:70:ARG:NH1   | 3:H:70:ARG:CG        | 2.80                     | 0.45              |
| 3:H:140:PHE:CD2  | 3:H:169:VAL:HG11     | 2.52                     | 0.45              |
| 1:R:6:GLU:OE2    | 1:R:10:ARG:NH1       | 2.50                     | 0.45              |
| 1:R:14:GLY:O     | 1:R:109:ARG:HD3      | 2.17                     | 0.45              |
| 2:S:155:TRP:NE1  | 2:S:281:GLY:HA3      | 2.32                     | 0.45              |
| 3:H:209:SER:O    | 3:H:210:SER:C        | 2.60                     | 0.44              |
| 1:R:3:LEU:HB2    | 1:R:6:GLU:HB2        | 1.99                     | 0.44              |
| 1:L:7:ARG:HG2    | 1:L:7:ARG:HH11       | 1.81                     | 0.44              |
| 3:H:40:TYR:CE2   | 3:H:42:LEU:HD21      | 2.53                     | 0.44              |
| 3:H:184:LYS:HD3  | 3:H:184:LYS:N        | 2.33                     | 0.44              |
| 1:R:224:ILE:HG22 | 6:R:2009[A]:U10:H3M3 | 1.99                     | 0.44              |
| 1:L:49:ILE:HG12  | 1:L:89:ILE:HD13      | 1.99                     | 0.44              |
| 1:R:170:ASN:HB3  | 1:R:173:HIS:CB       | 2.48                     | 0.44              |
| 1:R:232:LEU:O    | 1:R:236:LEU:HG       | 2.18                     | 0.44              |
| 2:S:3:TYR:CD2    | 3:T:194:GLN:HA       | 2.52                     | 0.44              |
| 2:S:94:LEU:HD22  | 2:S:115:TRP:HB2      | 1.99                     | 0.44              |
| 3:T:183:LEU:HD12 | 3:T:189:ARG:NH1      | 2.33                     | 0.44              |
| 3:T:207:ALA:O    | 3:T:240:GLY:HA3      | 2.17                     | 0.44              |
| 3:T:157:ASP:CG   | 3:T:210:SER:H        | 2.26                     | 0.44              |
| 2:M:238:ILE:HD13 | 2:M:263:GLU:HB2      | 1.99                     | 0.44              |
| 1:R:94:THR:O     | 1:R:98:VAL:HG23      | 2.17                     | 0.44              |
| 1:L:60:ASN:O     | 1:L:64:ILE:HG13      | 2.18                     | 0.44              |
| 1:L:80:LEU:HD12  | 1:L:85:LEU:CD1       | 2.48                     | 0.44              |
| 1:L:105:VAL:O    | 1:L:108:CYS:HB2      | 2.17                     | 0.44              |
| 1:L:139:MET:HE3  | 1:L:252:GLY:CA       | 2.47                     | 0.44              |
| 1:R:79:PRO:C     | 1:R:81:ALA:H         | 2.25                     | 0.44              |
| 1:R:224:ILE:N    | 6:R:2009[B]:U10:O5   | 2.51                     | 0.44              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:R:279:ILE:HD12 | 2:S:91:PHE:C      | 2.42                     | 0.44              |
| 1:L:90:THR:CG2   | 1:L:132:VAL:HG11  | 2.48                     | 0.44              |
| 2:M:148:TRP:HA   | 2:M:148:TRP:CE3   | 2.53                     | 0.44              |
| 1:R:265:TRP:CG   | 1:R:266:TRP:N     | 2.85                     | 0.44              |
| 2:S:129:TRP:O    | 2:S:132:ARG:HB3   | 2.17                     | 0.44              |
| 1:R:173:HIS:CE1  | 1:R:177:ILE:HD11  | 2.52                     | 0.44              |
| 3:T:111:PRO:HG2  | 3:T:242:MET:SD    | 2.58                     | 0.44              |
| 3:T:187:SER:HB2  | 10:T:269:HOH:O    | 2.17                     | 0.44              |
| 1:L:14:GLY:C     | 1:L:109:ARG:HH11  | 2.25                     | 0.43              |
| 1:R:22:PHE:HA    | 1:R:24:PHE:HE2    | 1.82                     | 0.43              |
| 1:L:231:ARG:HD2  | 2:M:5:ASN:O       | 2.17                     | 0.43              |
| 3:H:153:VAL:HG21 | 3:H:181:VAL:CG2   | 2.47                     | 0.43              |
| 3:H:185:ASP:OD1  | 3:H:185:ASP:C     | 2.60                     | 0.43              |
| 1:R:213:ASN:HB3  | 1:R:217:ARG:NH2   | 2.33                     | 0.43              |
| 1:R:268:LYS:C    | 1:R:273:ALA:HB2   | 2.44                     | 0.43              |
| 2:S:187:ASN:HA   | 4:S:2003:BCL:CBC  | 2.49                     | 0.43              |
| 2:S:251:PHE:CD2  | 2:S:251:PHE:C     | 2.96                     | 0.43              |
| 2:S:253:ARG:HB2  | 2:S:259:ASN:OD1   | 2.18                     | 0.43              |
| 3:T:255:MET:C    | 3:T:256:LEU:HD12  | 2.43                     | 0.43              |
| 1:L:141:ALA:C    | 1:L:143:GLY:N     | 2.76                     | 0.43              |
| 2:M:87:ARG:HG3   | 2:M:88:ASP:N      | 2.33                     | 0.43              |
| 1:R:105:VAL:O    | 1:R:108:CYS:HB2   | 2.18                     | 0.43              |
| 2:S:11:GLN:OE1   | 2:S:40:GLY:HA3    | 2.17                     | 0.43              |
| 3:T:87:LEU:HD22  | 3:T:98:HIS:O      | 2.18                     | 0.43              |
| 3:T:111:PRO:HB2  | 3:T:239:GLY:HA2   | 2.00                     | 0.43              |
| 3:T:191:LEU:O    | 3:T:192:PRO:C     | 2.60                     | 0.43              |
| 2:M:129:TRP:O    | 2:M:132:ARG:HB3   | 2.19                     | 0.43              |
| 2:M:148:TRP:HA   | 2:M:148:TRP:HE3   | 1.83                     | 0.43              |
| 2:S:10:VAL:HG21  | 3:T:148:PRO:CD    | 2.47                     | 0.43              |
| 3:T:117:ARG:O    | 3:T:118:ARG:C     | 2.62                     | 0.43              |
| 3:H:40:TYR:CZ    | 3:H:42:LEU:HD21   | 2.54                     | 0.43              |
| 1:R:184:ALA:HB3  | 5:S:2005:BPH:CMC  | 2.49                     | 0.43              |
| 1:L:2:LEU:HB3    | 1:L:6:GLU:HB3     | 2.01                     | 0.43              |
| 1:L:226:THR:CG2  | 1:L:227:LEU:N     | 2.81                     | 0.43              |
| 4:L:1002:BCL:NC  | 4:M:1003:BCL:HBB3 | 2.34                     | 0.43              |
| 2:M:204:LEU:HD13 | 3:H:20:PHE:CE2    | 2.54                     | 0.43              |
| 1:R:231:ARG:NE   | 2:S:6:ILE:O       | 2.52                     | 0.43              |
| 3:T:117:ARG:O    | 3:T:228:LEU:HB2   | 2.18                     | 0.43              |
| 1:L:244:SER:HB3  | 4:L:1002:BCL:O1A  | 2.18                     | 0.43              |
| 1:L:6:GLU:O      | 1:L:7:ARG:C       | 2.62                     | 0.43              |
| 4:L:1002:BCL:H2C | 4:M:1003:BCL:H2C  | 2.00                     | 0.43              |

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| Atom-1               | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|-------------------|--------------------------|-------------------|
| 3:H:178:PHE:CZ       | 3:H:230:GLU:HG2   | 2.40                     | 0.43              |
| 1:L:268:LYS:HA       | 1:L:268:LYS:HD3   | 1.71                     | 0.43              |
| 3:H:134:MET:O        | 3:H:135:LYS:C     | 2.61                     | 0.43              |
| 3:H:189:ARG:HG2      | 3:H:189:ARG:HH11  | 1.83                     | 0.43              |
| 1:R:219:LEU:CD1      | 1:R:220:VAL:HG23  | 2.33                     | 0.43              |
| 2:S:256:MET:HE1      | 6:S:2008:U10:H13  | 2.01                     | 0.43              |
| 4:L:1004:BCL:C2      | 4:L:1004:BCL:H71  | 2.48                     | 0.42              |
| 1:R:85:LEU:HD12      | 1:R:85:LEU:HA     | 1.89                     | 0.42              |
| 2:S:157:TRP:HD1      | 4:S:2001:BCL:HBB1 | 1.84                     | 0.42              |
| 3:T:36:MET:HB3       | 3:T:58:LEU:HD23   | 2.01                     | 0.42              |
| 3:H:241:LEU:HB2      | 10:H:276:HOH:O    | 2.19                     | 0.42              |
| 1:R:7:ARG:HH12       | 3:T:87:LEU:HB2    | 1.84                     | 0.42              |
| 1:R:65:SER:CB        | 1:R:152:THR:HG21  | 2.49                     | 0.42              |
| 1:R:102:LEU:O        | 1:R:105:VAL:HB    | 2.18                     | 0.42              |
| 6:R:2009[B]:U10:H3M1 | 10:S:2023:HOH:O   | 2.18                     | 0.42              |
| 2:M:191:LEU:HD12     | 2:M:191:LEU:HA    | 1.89                     | 0.42              |
| 3:H:40:TYR:CB        | 3:H:58:LEU:HD21   | 2.49                     | 0.42              |
| 1:R:97:PHE:HE1       | 4:R:2002:BCL:H121 | 1.85                     | 0.42              |
| 1:R:172:ALA:HB3      | 1:R:247:CYS:HA    | 2.01                     | 0.42              |
| 2:S:15:PRO:HD2       | 3:T:140:PHE:CE1   | 2.54                     | 0.42              |
| 2:S:159:VAL:HA       | 2:S:163:ILE:HB    | 2.00                     | 0.42              |
| 3:T:58:LEU:HD23      | 3:T:58:LEU:HA     | 1.90                     | 0.42              |
| 1:L:269:LEU:HG       | 1:L:271:TRP:CH2   | 2.54                     | 0.42              |
| 4:L:1001:BCL:HBC2    | 4:L:1001:BCL:H2C  | 1.79                     | 0.42              |
| 2:M:2:GLU:O          | 2:M:3:TYR:CB      | 2.64                     | 0.42              |
| 2:M:96:PRO:HB3       | 2:M:115:TRP:CE2   | 2.55                     | 0.42              |
| 8:M:1010:SPO:HM12    | 8:M:1010:SPO:H42  | 1.94                     | 0.42              |
| 3:H:157:ASP:OD1      | 3:H:157:ASP:N     | 2.53                     | 0.42              |
| 1:R:84:GLY:HA2       | 1:R:87:GLN:HE21   | 1.84                     | 0.42              |
| 2:S:96:PRO:HA        | 2:S:115:TRP:CG    | 2.55                     | 0.42              |
| 3:H:89:ARG:HG2       | 3:H:98:HIS:CE1    | 2.54                     | 0.42              |
| 3:H:168:TRP:HB2      | 3:H:178:PHE:HB2   | 2.01                     | 0.42              |
| 1:R:16:LEU:HD11      | 1:R:105:VAL:HG11  | 2.02                     | 0.42              |
| 2:S:196:LEU:HD12     | 2:S:196:LEU:HA    | 1.87                     | 0.42              |
| 1:L:121:PHE:O        | 1:L:122:ALA:C     | 2.61                     | 0.42              |
| 1:R:60:ASN:OD1       | 1:R:62:GLN:N      | 2.53                     | 0.42              |
| 2:S:97:PRO:CG        | 2:S:171:TRP:HB2   | 2.46                     | 0.42              |
| 3:T:37:ARG:HG2       | 3:T:37:ARG:NH1    | 2.35                     | 0.42              |
| 1:L:131:LEU:HD11     | 4:L:1004:BCL:HBC2 | 2.01                     | 0.42              |
| 2:M:21:THR:O         | 2:M:22:GLU:C      | 2.61                     | 0.42              |
| 2:S:13:ARG:O         | 3:T:140:PHE:HA    | 2.19                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:S:66:TRP:CZ2    | 2:S:122:MET:HE3   | 2.54                     | 0.42              |
| 2:S:260:ALA:HA    | 3:T:35:ASN:HB3    | 2.00                     | 0.42              |
| 1:L:10:ARG:NH2    | 1:L:25:TRP:HB2    | 2.35                     | 0.42              |
| 2:S:190:SER:HB2   | 4:S:2003:BCL:H3C  | 2.00                     | 0.42              |
| 3:T:69:GLY:C      | 3:T:71:GLY:H      | 2.28                     | 0.42              |
| 1:R:220:VAL:HG21  | 5:S:2005:BPH:HED3 | 2.00                     | 0.42              |
| 1:R:280:ASN:HB2   | 2:S:88:ASP:OD1    | 2.20                     | 0.42              |
| 2:S:14:GLY:HA3    | 3:T:140:PHE:CZ    | 2.55                     | 0.42              |
| 1:L:180:PHE:CE2   | 4:L:1002:BCL:HMA3 | 2.54                     | 0.42              |
| 1:L:185:LEU:CD1   | 1:L:189:LEU:HD22  | 2.49                     | 0.42              |
| 1:R:79:PRO:O      | 1:R:81:ALA:N      | 2.53                     | 0.42              |
| 1:R:149:GLY:HA3   | 1:R:152:THR:OG1   | 2.20                     | 0.42              |
| 2:S:224:LEU:HD23  | 2:S:224:LEU:HA    | 1.89                     | 0.42              |
| 2:S:232:GLU:O     | 2:S:234:GLU:N     | 2.52                     | 0.42              |
| 3:T:219:ILE:CG2   | 3:T:225:VAL:HG23  | 2.50                     | 0.42              |
| 1:L:208:THR:OG1   | 1:L:211:HIS:HD2   | 2.03                     | 0.41              |
| 2:M:110:LYS:C     | 2:M:111:GLU:HG3   | 2.45                     | 0.41              |
| 3:H:46:ASP:OD1    | 3:H:48:THR:OG1    | 2.36                     | 0.41              |
| 1:R:28:PRO:HB3    | 2:S:253:ARG:HH11  | 1.85                     | 0.41              |
| 1:L:280:ASN:HB2   | 2:M:87:ARG:HE     | 1.84                     | 0.41              |
| 5:R:2006:BPH:HMC1 | 2:S:213:ALA:HB3   | 2.02                     | 0.41              |
| 1:L:264:GLN:OE1   | 1:L:268:LYS:HE2   | 2.20                     | 0.41              |
| 3:H:241:LEU:O     | 3:H:248:ARG:NH2   | 2.53                     | 0.41              |
| 3:H:248:ARG:HB2   | 3:H:248:ARG:CZ    | 2.49                     | 0.41              |
| 1:R:90:THR:HG23   | 1:R:132:VAL:HG11  | 2.02                     | 0.41              |
| 1:R:121:PHE:O     | 1:R:122:ALA:C     | 2.61                     | 0.41              |
| 1:R:206:MET:HE2   | 1:R:206:MET:HB3   | 1.88                     | 0.41              |
| 3:T:17:ILE:O      | 3:T:21:TRP:CD1    | 2.73                     | 0.41              |
| 3:T:158:LEU:HG    | 3:T:249:LYS:HG3   | 2.02                     | 0.41              |
| 1:R:7:ARG:NH2     | 3:T:98:HIS:HD2    | 2.19                     | 0.41              |
| 1:R:16:LEU:HD11   | 1:R:105:VAL:CG1   | 2.50                     | 0.41              |
| 1:R:180:PHE:CD2   | 1:R:240:ALA:HB1   | 2.54                     | 0.41              |
| 1:R:189:LEU:HD12  | 1:R:189:LEU:HA    | 1.93                     | 0.41              |
| 1:R:268:LYS:HA    | 1:R:273:ALA:CB    | 2.49                     | 0.41              |
| 2:S:234:GLU:O     | 2:S:238:ILE:HG13  | 2.20                     | 0.41              |
| 2:M:5:ASN:HD22    | 2:M:224:LEU:HD22  | 1.84                     | 0.41              |
| 3:H:66:LEU:HD23   | 3:H:72:THR:HA     | 2.02                     | 0.41              |
| 1:R:34:PHE:HA     | 1:R:37:ALA:HB3    | 2.02                     | 0.41              |
| 1:R:72:GLU:CD     | 1:R:72:GLU:N      | 2.78                     | 0.41              |
| 1:R:200:PRO:O     | 1:R:201:GLU:C     | 2.64                     | 0.41              |
| 1:L:133:LEU:HD23  | 1:L:133:LEU:C     | 2.44                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:22:GLU:HB3    | 2:M:23:ASP:H      | 1.65                     | 0.41              |
| 2:M:109:LEU:HA    | 2:M:113:GLY:HA3   | 2.01                     | 0.41              |
| 2:M:264:GLY:HA3   | 3:H:35:ASN:OD1    | 2.21                     | 0.41              |
| 2:M:293:ASN:OD1   | 2:M:295:TYR:HB3   | 2.21                     | 0.41              |
| 1:R:79:PRO:C      | 1:R:81:ALA:N      | 2.78                     | 0.41              |
| 1:R:117:ILE:HD13  | 2:S:252:TRP:CZ2   | 2.55                     | 0.41              |
| 1:R:246:LEU:O     | 1:R:249:ILE:HG22  | 2.21                     | 0.41              |
| 3:T:36:MET:HE3    | 3:T:58:LEU:HD23   | 2.03                     | 0.41              |
| 3:T:99:ALA:HA     | 3:T:100:PRO:HD3   | 1.84                     | 0.41              |
| 1:L:85:LEU:O      | 1:L:89:ILE:HG13   | 2.21                     | 0.41              |
| 1:L:102:LEU:HD12  | 1:L:102:LEU:HA    | 1.84                     | 0.41              |
| 3:H:165:VAL:CG1   | 3:H:182:GLU:HB2   | 2.50                     | 0.41              |
| 4:S:2001:BCL:HHC  | 4:S:2001:BCL:HBB2 | 2.01                     | 0.41              |
| 3:T:212:LEU:CD1   | 3:T:244:ALA:HB2   | 2.51                     | 0.41              |
| 1:L:51:TRP:CZ3    | 1:L:85:LEU:HD11   | 2.55                     | 0.41              |
| 1:R:280:ASN:HB2   | 2:S:87:ARG:HE     | 1.86                     | 0.41              |
| 2:S:151:LEU:O     | 2:S:155:TRP:N     | 2.49                     | 0.41              |
| 4:S:2001:BCL:HBB2 | 8:S:2010:SPO:H243 | 2.03                     | 0.41              |
| 3:T:199:GLN:OE1   | 3:T:202:ARG:HD2   | 2.21                     | 0.41              |
| 10:L:1032:HOH:O   | 2:M:29:ARG:HD2    | 2.21                     | 0.41              |
| 4:M:1003:BCL:H62  | 4:M:1003:BCL:H92  | 1.93                     | 0.41              |
| 3:H:120:LEU:N     | 3:H:226:THR:HB    | 2.36                     | 0.41              |
| 2:S:21:THR:HG23   | 2:S:26:LEU:CD2    | 2.42                     | 0.41              |
| 2:S:93:SER:HB2    | 2:S:181:SER:HB3   | 2.03                     | 0.41              |
| 2:S:182:HIS:CG    | 8:S:2010:SPO:H181 | 2.56                     | 0.41              |
| 3:T:149:ILE:CD1   | 3:T:166:ASP:HA    | 2.51                     | 0.41              |
| 1:L:78:ALA:HB1    | 1:L:79:PRO:HD2    | 2.02                     | 0.41              |
| 1:L:83:GLY:O      | 1:L:87:GLN:HG3    | 2.21                     | 0.41              |
| 2:M:170:SER:HB2   | 10:M:1041:HOH:O   | 2.21                     | 0.41              |
| 2:S:151:LEU:HA    | 2:S:154:ILE:HB    | 2.02                     | 0.41              |
| 1:L:20:ASN:HB3    | 10:L:1018:HOH:O   | 2.21                     | 0.40              |
| 2:M:9:GLN:HE22    | 3:H:198:VAL:N     | 2.17                     | 0.40              |
| 1:L:60:ASN:HB3    | 1:L:63:LEU:HB2    | 2.03                     | 0.40              |
| 1:L:80:LEU:HB3    | 1:L:85:LEU:HD13   | 2.02                     | 0.40              |
| 2:M:145:HIS:CE1   | 9:M:1011:LDA:HM13 | 2.56                     | 0.40              |
| 1:R:3:LEU:HD12    | 2:S:250:LEU:CD2   | 2.51                     | 0.40              |
| 1:L:129:LEU:HD12  | 1:L:129:LEU:HA    | 1.89                     | 0.40              |
| 3:H:207:ALA:HB1   | 3:H:237:VAL:O     | 2.22                     | 0.40              |
| 1:R:59:TRP:HA     | 1:R:59:TRP:CE3    | 2.57                     | 0.40              |
| 1:R:133:LEU:C     | 1:R:136:PRO:HD2   | 2.46                     | 0.40              |
| 1:R:201:GLU:O     | 1:R:202:LYS:C     | 2.64                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:S:75:TRP:HB3    | 2:S:80:TRP:CZ3    | 2.56                     | 0.40              |
| 3:T:60:LYS:CG     | 3:T:61:PRO:HD2    | 2.50                     | 0.40              |
| 3:T:254:ALA:C     | 3:T:256:LEU:H     | 2.29                     | 0.40              |
| 4:L:1001:BCL:HHC  | 4:L:1001:BCL:CBB  | 2.50                     | 0.40              |
| 4:L:1004:BCL:H161 | 4:L:1004:BCL:H141 | 1.90                     | 0.40              |
| 2:M:108:PRO:O     | 2:M:109:LEU:C     | 2.65                     | 0.40              |
| 2:M:187:ASN:HA    | 4:M:1003:BCL:CBC  | 2.52                     | 0.40              |
| 2:M:195:ASN:C     | 2:M:195:ASN:ND2   | 2.77                     | 0.40              |
| 3:H:75:VAL:HA     | 3:H:76:PRO:C      | 2.46                     | 0.40              |
| 1:R:6:GLU:HG3     | 2:S:250:LEU:HD22  | 2.02                     | 0.40              |
| 1:R:177:ILE:HD13  | 4:S:2001:BCL:HMD2 | 2.02                     | 0.40              |
| 1:R:230:HIS:NE2   | 2:S:223:ILE:HG13  | 2.37                     | 0.40              |
| 1:R:262:TRP:O     | 1:R:265:TRP:HD1   | 2.05                     | 0.40              |
| 1:R:269:LEU:HD12  | 1:R:269:LEU:HA    | 1.91                     | 0.40              |
| 2:M:270:ILE:HD13  | 9:M:1011:LDA:H32  | 2.04                     | 0.40              |
| 1:R:154:LEU:O     | 1:R:157:VAL:HB    | 2.21                     | 0.40              |
| 2:S:123:PHE:HA    | 2:S:157:TRP:CH2   | 2.57                     | 0.40              |
| 3:T:192:PRO:CB    | 3:T:194:GLN:HE21  | 2.35                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1   | L     | 279/281 (99%) | 262 (94%) | 16 (6%) | 1 (0%)   | 30          | 51  |
| 1   | R     | 279/281 (99%) | 264 (95%) | 12 (4%) | 3 (1%)   | 11          | 25  |
| 2   | M     | 299/307 (97%) | 280 (94%) | 18 (6%) | 1 (0%)   | 36          | 58  |
| 2   | S     | 297/307 (97%) | 284 (96%) | 11 (4%) | 2 (1%)   | 18          | 38  |
| 3   | H     | 244/260 (94%) | 233 (96%) | 11 (4%) | 0        | 100         | 100 |
| 3   | T     | 244/260 (94%) | 223 (91%) | 15 (6%) | 6 (2%)   | 4           | 8   |

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| Mol | Chain | Analysed        | Favoured   | Allowed | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|---------|----------|-------------|----|
| All | All   | 1642/1696 (97%) | 1546 (94%) | 83 (5%) | 13 (1%)  | 16          | 34 |

All (13) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | M     | 2   | GLU  |
| 3   | T     | 45  | GLU  |
| 3   | T     | 220 | LYS  |
| 1   | R     | 80  | LEU  |
| 1   | R     | 257 | ASP  |
| 2   | S     | 195 | ASN  |
| 3   | T     | 70  | ARG  |
| 3   | T     | 124 | ASP  |
| 1   | L     | 270 | PRO  |
| 3   | T     | 89  | ARG  |
| 3   | T     | 166 | ASP  |
| 1   | R     | 31  | VAL  |
| 2   | S     | 19  | GLY  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1   | L     | 220/220 (100%)  | 208 (94%)  | 12 (6%)  | 19          | 41 |
| 1   | R     | 220/220 (100%)  | 208 (94%)  | 12 (6%)  | 19          | 41 |
| 2   | M     | 236/240 (98%)   | 225 (95%)  | 11 (5%)  | 23          | 48 |
| 2   | S     | 235/240 (98%)   | 222 (94%)  | 13 (6%)  | 19          | 41 |
| 3   | H     | 199/208 (96%)   | 189 (95%)  | 10 (5%)  | 22          | 46 |
| 3   | T     | 199/208 (96%)   | 192 (96%)  | 7 (4%)   | 32          | 59 |
| All | All   | 1309/1336 (98%) | 1244 (95%) | 65 (5%)  | 22          | 46 |

All (65) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | L     | 85  | LEU  |
| 1   | L     | 102 | LEU  |
| 1   | L     | 129 | LEU  |
| 1   | L     | 133 | LEU  |
| 1   | L     | 154 | LEU  |
| 1   | L     | 189 | LEU  |
| 1   | L     | 195 | LEU  |
| 1   | L     | 220 | VAL  |
| 1   | L     | 231 | ARG  |
| 1   | L     | 238 | LEU  |
| 1   | L     | 247 | CYS  |
| 1   | L     | 269 | LEU  |
| 2   | M     | 26  | LEU  |
| 2   | M     | 29  | ARG  |
| 2   | M     | 60  | LEU  |
| 2   | M     | 94  | LEU  |
| 2   | M     | 114 | LEU  |
| 2   | M     | 136 | ARG  |
| 2   | M     | 156 | LEU  |
| 2   | M     | 165 | PRO  |
| 2   | M     | 191 | LEU  |
| 2   | M     | 196 | LEU  |
| 2   | M     | 232 | GLU  |
| 3   | H     | 70  | ARG  |
| 3   | H     | 73  | LEU  |
| 3   | H     | 123 | LEU  |
| 3   | H     | 134 | MET  |
| 3   | H     | 184 | LYS  |
| 3   | H     | 191 | LEU  |
| 3   | H     | 202 | ARG  |
| 3   | H     | 208 | LEU  |
| 3   | H     | 220 | LYS  |
| 3   | H     | 231 | ASP  |
| 1   | R     | 87  | GLN  |
| 1   | R     | 102 | LEU  |
| 1   | R     | 126 | LEU  |
| 1   | R     | 133 | LEU  |
| 1   | R     | 154 | LEU  |
| 1   | R     | 189 | LEU  |
| 1   | R     | 217 | ARG  |
| 1   | R     | 219 | LEU  |
| 1   | R     | 220 | VAL  |
| 1   | R     | 229 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | R     | 231 | ARG  |
| 1   | R     | 269 | LEU  |
| 2   | S     | 12  | VAL  |
| 2   | S     | 29  | ARG  |
| 2   | S     | 60  | LEU  |
| 2   | S     | 72  | ILE  |
| 2   | S     | 87  | ARG  |
| 2   | S     | 94  | LEU  |
| 2   | S     | 111 | GLU  |
| 2   | S     | 114 | LEU  |
| 2   | S     | 136 | ARG  |
| 2   | S     | 156 | LEU  |
| 2   | S     | 191 | LEU  |
| 2   | S     | 216 | PHE  |
| 2   | S     | 232 | GLU  |
| 3   | T     | 73  | LEU  |
| 3   | T     | 79  | GLU  |
| 3   | T     | 82  | ASP  |
| 3   | T     | 123 | LEU  |
| 3   | T     | 196 | VAL  |
| 3   | T     | 202 | ARG  |
| 3   | T     | 231 | ASP  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | L     | 87  | GLN  |
| 1   | L     | 211 | HIS  |
| 1   | L     | 274 | ASN  |
| 2   | M     | 5   | ASN  |
| 2   | M     | 9   | GLN  |
| 2   | M     | 44  | ASN  |
| 2   | M     | 195 | ASN  |
| 3   | H     | 98  | HIS  |
| 3   | H     | 126 | HIS  |
| 3   | H     | 129 | ASN  |
| 3   | H     | 194 | GLN  |
| 3   | H     | 206 | ASN  |
| 1   | R     | 87  | GLN  |
| 1   | R     | 211 | HIS  |
| 2   | S     | 5   | ASN  |
| 2   | S     | 9   | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | S     | 28  | ASN  |
| 2   | S     | 44  | ASN  |
| 2   | S     | 195 | ASN  |
| 3   | T     | 35  | ASN  |
| 3   | T     | 44  | ASN  |
| 3   | T     | 53  | GLN  |
| 3   | T     | 174 | GLN  |
| 3   | T     | 194 | 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 23 ligands modelled in this entry, 2 are monoatomic - leaving 21 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 | $\# Z  > 2$ |
| 5   | BPH  | R     | 2006    | -    | 59,70,70     | 2.11 | 14 (23%)    | 59,101,101  | 2.85 | 21 (35%)    |
| 6   | U10  | R     | 2009[A] | -    | 18,18,63     | 2.17 | 6 (33%)     | 24,25,79    | 2.20 | 7 (29%)     |
| 4   | BCL  | L     | 1002    | 1    | 69,74,74     | 1.79 | 12 (17%)    | 79,115,115  | 1.90 | 22 (27%)    |
| 5   | BPH  | M     | 1005    | -    | 49,60,70     | 2.20 | 15 (30%)    | 47,89,101   | 3.06 | 21 (44%)    |
| 5   | BPH  | S     | 2005    | -    | 45,56,70     | 2.32 | 15 (33%)    | 41,84,101   | 3.29 | 19 (46%)    |

| Mol | Type | Chain | Res     | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|---------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |         |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 8   | SPO  | M     | 1010    | -    | 41,41,41     | 3.09 | 21 (51%) | 47,50,50    | 2.44 | 15 (31%) |
| 9   | LDA  | M     | 1011    | -    | 13,15,15     | 1.85 | 1 (7%)   | 14,17,17    | 1.62 | 4 (28%)  |
| 4   | BCL  | S     | 2003    | 2    | 69,74,74     | 1.79 | 12 (17%) | 79,115,115  | 1.88 | 23 (29%) |
| 8   | SPO  | S     | 2010    | -    | 41,41,41     | 3.08 | 22 (53%) | 47,50,50    | 2.47 | 17 (36%) |
| 4   | BCL  | L     | 1001    | 2    | 54,59,74     | 2.04 | 15 (27%) | 61,97,115   | 2.02 | 15 (24%) |
| 5   | BPH  | L     | 1006    | -    | 59,70,70     | 2.16 | 14 (23%) | 59,101,101  | 2.82 | 22 (37%) |
| 6   | U10  | L     | 1009[B] | -    | 30,30,63     | 2.02 | 9 (30%)  | 37,39,79    | 2.01 | 11 (29%) |
| 4   | BCL  | S     | 2001    | 2    | 54,59,74     | 2.09 | 16 (29%) | 61,97,115   | 1.95 | 17 (27%) |
| 6   | U10  | S     | 2008    | -    | 32,32,63     | 1.96 | 10 (31%) | 40,41,79    | 1.90 | 10 (25%) |
| 4   | BCL  | R     | 2002    | 1    | 69,74,74     | 1.81 | 11 (15%) | 79,115,115  | 1.88 | 20 (25%) |
| 4   | BCL  | M     | 1003    | 2    | 69,74,74     | 1.74 | 14 (20%) | 79,115,115  | 1.91 | 25 (31%) |
| 4   | BCL  | L     | 1004    | 1    | 69,74,74     | 1.79 | 13 (18%) | 79,115,115  | 1.77 | 18 (22%) |
| 6   | U10  | M     | 1008    | -    | 38,38,63     | 2.05 | 13 (34%) | 48,49,79    | 1.80 | 13 (27%) |
| 6   | U10  | R     | 2009[B] | -    | 18,18,63     | 2.14 | 6 (33%)  | 24,25,79    | 2.15 | 7 (29%)  |
| 6   | U10  | L     | 1009[A] | -    | 30,30,63     | 2.12 | 11 (36%) | 37,39,79    | 2.08 | 11 (29%) |
| 4   | BCL  | S     | 2004    | 1    | 69,74,74     | 1.83 | 17 (24%) | 79,115,115  | 1.87 | 19 (24%) |

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

| Mol | Type | Chain | Res     | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|---------|------|-----------|---------------|---------|
| 5   | BPH  | R     | 2006    | -    | 2/2/18/22 | 9/37/105/105  | 0/5/6/6 |
| 6   | U10  | R     | 2009[A] | -    | -         | 1/9/33/87     | 0/1/1/1 |
| 4   | BCL  | L     | 1002    | 1    | -         | 4/41/137/137  | -       |
| 5   | BPH  | M     | 1005    | -    | 1/1/16/22 | 6/25/93/105   | 0/5/6/6 |
| 5   | BPH  | S     | 2005    | -    | -         | 9/21/89/105   | 0/5/6/6 |
| 8   | SPO  | M     | 1010    | -    | -         | 13/47/47/47   | -       |
| 9   | LDA  | M     | 1011    | -    | -         | 7/13/13/13    | -       |
| 4   | BCL  | S     | 2003    | 2    | -         | 10/41/137/137 | -       |
| 8   | SPO  | S     | 2010    | -    | -         | 12/47/47/47   | -       |
| 4   | BCL  | L     | 1001    | 2    | -         | 0/23/119/137  | -       |
| 5   | BPH  | L     | 1006    | -    | 2/2/18/22 | 8/37/105/105  | 0/5/6/6 |
| 6   | U10  | L     | 1009[B] | -    | -         | 5/24/48/87    | 0/1/1/1 |
| 4   | BCL  | S     | 2001    | 2    | -         | 8/23/119/137  | -       |

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| Mol | Type | Chain | Res     | Link | Chirals | Torsions     | Rings   |
|-----|------|-------|---------|------|---------|--------------|---------|
| 6   | U10  | S     | 2008    | -    | -       | 4/26/50/87   | 0/1/1/1 |
| 4   | BCL  | R     | 2002    | 1    | -       | 7/41/137/137 | -       |
| 4   | BCL  | L     | 1004    | 1    | -       | 9/41/137/137 | -       |
| 4   | BCL  | M     | 1003    | 2    | -       | 9/41/137/137 | -       |
| 6   | U10  | M     | 1008    | -    | -       | 4/33/57/87   | 0/1/1/1 |
| 6   | U10  | R     | 2009[B] | -    | -       | 0/9/33/87    | 0/1/1/1 |
| 6   | U10  | L     | 1009[A] | -    | -       | 9/24/48/87   | 0/1/1/1 |
| 4   | BCL  | S     | 2004    | 1    | -       | 9/41/137/137 | -       |

All (267) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 8   | M     | 1010 | SPO  | C15-C16 | 7.96  | 1.55        | 1.34     |
| 8   | S     | 2010 | SPO  | C6-C5   | 7.91  | 1.54        | 1.32     |
| 8   | S     | 2010 | SPO  | C10-C11 | 7.73  | 1.54        | 1.34     |
| 8   | M     | 1010 | SPO  | C6-C5   | 7.73  | 1.53        | 1.32     |
| 8   | M     | 1010 | SPO  | C10-C11 | 7.58  | 1.54        | 1.34     |
| 8   | S     | 2010 | SPO  | C15-C16 | 7.34  | 1.53        | 1.34     |
| 5   | M     | 1005 | BPH  | C2C-C3C | -7.26 | 1.48        | 1.54     |
| 5   | S     | 2005 | BPH  | C2C-C3C | -7.10 | 1.48        | 1.54     |
| 5   | R     | 2006 | BPH  | C2C-C3C | -7.06 | 1.48        | 1.54     |
| 4   | S     | 2003 | BCL  | C3B-C4B | 6.97  | 1.54        | 1.41     |
| 4   | R     | 2002 | BCL  | C3B-C4B | 6.76  | 1.54        | 1.41     |
| 4   | M     | 1003 | BCL  | C3B-C4B | 6.73  | 1.54        | 1.41     |
| 4   | L     | 1002 | BCL  | C3B-C4B | 6.52  | 1.54        | 1.41     |
| 4   | S     | 2001 | BCL  | C3B-C4B | 6.41  | 1.53        | 1.41     |
| 5   | L     | 1006 | BPH  | C1D-C2D | 6.40  | 1.46        | 1.39     |
| 4   | L     | 1004 | BCL  | C3B-C4B | 6.36  | 1.53        | 1.41     |
| 9   | M     | 1011 | LDA  | O1-N1   | -6.24 | 1.26        | 1.42     |
| 4   | S     | 2004 | BCL  | C3B-C4B | 6.11  | 1.53        | 1.41     |
| 4   | L     | 1001 | BCL  | C3B-C4B | 5.97  | 1.52        | 1.41     |
| 5   | R     | 2006 | BPH  | C1D-C2D | 5.87  | 1.46        | 1.39     |
| 4   | R     | 2002 | BCL  | MG-ND   | 5.81  | 2.17        | 2.05     |
| 4   | L     | 1002 | BCL  | MG-NB   | -5.77 | 1.94        | 2.05     |
| 4   | S     | 2001 | BCL  | MG-NB   | -5.76 | 1.94        | 2.05     |
| 4   | S     | 2004 | BCL  | MG-NB   | -5.75 | 1.94        | 2.05     |
| 5   | S     | 2005 | BPH  | C1D-C2D | 5.74  | 1.45        | 1.39     |
| 4   | S     | 2003 | BCL  | MG-NB   | -5.74 | 1.94        | 2.05     |
| 4   | L     | 1001 | BCL  | MG-NB   | -5.74 | 1.94        | 2.05     |
| 4   | L     | 1002 | BCL  | MG-ND   | 5.63  | 2.16        | 2.05     |
| 5   | L     | 1006 | BPH  | C11-C10 | -5.60 | 1.28        | 1.52     |

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| Mol | Chain | Res     | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|---------|------|---------|-------|-------------|----------|
| 5   | M     | 1005    | BPH  | C1B-C2B | 5.59  | 1.45        | 1.39     |
| 5   | M     | 1005    | BPH  | C1D-C2D | 5.58  | 1.45        | 1.39     |
| 6   | M     | 1008    | U10  | O4-C4   | 5.57  | 1.50        | 1.36     |
| 4   | S     | 2001    | BCL  | MG-ND   | 5.55  | 2.16        | 2.05     |
| 5   | L     | 1006    | BPH  | C1B-C2B | 5.52  | 1.45        | 1.39     |
| 5   | R     | 2006    | BPH  | C11-C10 | -5.51 | 1.29        | 1.52     |
| 4   | L     | 1004    | BCL  | MG-NB   | -5.46 | 1.95        | 2.05     |
| 4   | S     | 2003    | BCL  | MG-ND   | 5.34  | 2.16        | 2.05     |
| 5   | L     | 1006    | BPH  | C2C-C3C | -5.33 | 1.50        | 1.54     |
| 5   | S     | 2005    | BPH  | C1B-C2B | 5.15  | 1.45        | 1.39     |
| 4   | M     | 1003    | BCL  | MG-NB   | -5.14 | 1.95        | 2.05     |
| 4   | R     | 2002    | BCL  | MG-NB   | -5.14 | 1.95        | 2.05     |
| 6   | S     | 2008    | U10  | O4-C4   | 5.05  | 1.48        | 1.36     |
| 4   | S     | 2004    | BCL  | MG-ND   | 5.01  | 2.15        | 2.05     |
| 5   | R     | 2006    | BPH  | C1B-C2B | 4.92  | 1.45        | 1.39     |
| 8   | M     | 1010    | SPO  | C21-C20 | 4.92  | 1.49        | 1.36     |
| 4   | M     | 1003    | BCL  | MG-ND   | 4.89  | 2.15        | 2.05     |
| 4   | L     | 1004    | BCL  | MG-ND   | 4.85  | 2.15        | 2.05     |
| 6   | R     | 2009[A] | U10  | O4-C4   | 4.85  | 1.48        | 1.36     |
| 8   | S     | 2010    | SPO  | C26-C25 | 4.79  | 1.47        | 1.34     |
| 6   | L     | 1009[A] | U10  | O4-C4   | 4.79  | 1.48        | 1.36     |
| 6   | R     | 2009[B] | U10  | O4-C4   | 4.79  | 1.48        | 1.36     |
| 8   | S     | 2010    | SPO  | C21-C20 | 4.79  | 1.49        | 1.36     |
| 4   | L     | 1001    | BCL  | MG-ND   | 4.78  | 2.15        | 2.05     |
| 8   | M     | 1010    | SPO  | C26-C25 | 4.78  | 1.47        | 1.34     |
| 6   | L     | 1009[B] | U10  | O4-C4   | 4.69  | 1.48        | 1.36     |
| 6   | L     | 1009[A] | U10  | C13-C14 | 4.35  | 1.43        | 1.33     |
| 8   | S     | 2010    | SPO  | O1-CM1  | 4.34  | 1.56        | 1.43     |
| 4   | L     | 1001    | BCL  | C3C-C4C | -4.31 | 1.46        | 1.51     |
| 5   | S     | 2005    | BPH  | O2A-CGA | 4.29  | 1.45        | 1.33     |
| 5   | L     | 1006    | BPH  | C3A-C2A | -4.28 | 1.51        | 1.54     |
| 6   | L     | 1009[B] | U10  | C13-C14 | 4.25  | 1.42        | 1.33     |
| 5   | L     | 1006    | BPH  | O2D-CGD | 4.24  | 1.43        | 1.33     |
| 8   | M     | 1010    | SPO  | O1-CM1  | 4.18  | 1.56        | 1.43     |
| 5   | R     | 2006    | BPH  | O2A-CGA | 4.16  | 1.45        | 1.33     |
| 5   | L     | 1006    | BPH  | C3B-C4B | 3.99  | 1.47        | 1.41     |
| 5   | L     | 1006    | BPH  | O2A-CGA | 3.94  | 1.44        | 1.33     |
| 6   | S     | 2008    | U10  | C13-C14 | 3.94  | 1.42        | 1.33     |
| 4   | L     | 1004    | BCL  | C1B-C2B | 3.80  | 1.52        | 1.43     |
| 5   | S     | 2005    | BPH  | O2D-CGD | 3.77  | 1.42        | 1.33     |
| 4   | L     | 1001    | BCL  | MG-NC   | -3.77 | 1.97        | 2.06     |
| 5   | M     | 1005    | BPH  | O2D-CGD | 3.72  | 1.42        | 1.33     |

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| Mol | Chain | Res     | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|---------|------|---------|-------|-------------|----------|
| 5   | R     | 2006    | BPH  | O2D-CGD | 3.70  | 1.42        | 1.33     |
| 6   | M     | 1008    | U10  | C13-C14 | 3.69  | 1.41        | 1.33     |
| 6   | M     | 1008    | U10  | C7-C8   | -3.67 | 1.44        | 1.50     |
| 5   | S     | 2005    | BPH  | CHA-CBD | 3.64  | 1.55        | 1.51     |
| 4   | S     | 2004    | BCL  | C1B-C2B | 3.63  | 1.51        | 1.43     |
| 4   | S     | 2001    | BCL  | C3C-C4C | -3.57 | 1.47        | 1.51     |
| 6   | L     | 1009[A] | U10  | C8-C9   | 3.55  | 1.41        | 1.33     |
| 4   | M     | 1003    | BCL  | MG-NA   | 3.55  | 2.14        | 2.06     |
| 4   | R     | 2002    | BCL  | CBB-CAB | 3.53  | 1.57        | 1.50     |
| 6   | R     | 2009[A] | U10  | O3-C3   | 3.52  | 1.45        | 1.36     |
| 6   | L     | 1009[A] | U10  | C6-C1   | 3.51  | 1.41        | 1.35     |
| 6   | M     | 1008    | U10  | C23-C24 | 3.49  | 1.41        | 1.33     |
| 6   | L     | 1009[A] | U10  | O3-C3   | 3.48  | 1.45        | 1.36     |
| 4   | R     | 2002    | BCL  | MG-NA   | 3.45  | 2.14        | 2.06     |
| 6   | R     | 2009[B] | U10  | O3-C3M  | -3.42 | 1.37        | 1.45     |
| 6   | L     | 1009[B] | U10  | O3-C3M  | -3.41 | 1.37        | 1.45     |
| 4   | S     | 2001    | BCL  | MG-NC   | -3.40 | 1.98        | 2.06     |
| 5   | S     | 2005    | BPH  | C3B-C4B | 3.35  | 1.46        | 1.41     |
| 5   | M     | 1005    | BPH  | O2A-CGA | 3.33  | 1.43        | 1.33     |
| 4   | L     | 1002    | BCL  | MG-NA   | 3.33  | 2.14        | 2.06     |
| 8   | M     | 1010    | SPO  | C4-C1   | 3.31  | 1.58        | 1.52     |
| 6   | R     | 2009[B] | U10  | O3-C3   | 3.28  | 1.44        | 1.36     |
| 6   | R     | 2009[A] | U10  | C6-C1   | 3.27  | 1.41        | 1.35     |
| 6   | L     | 1009[B] | U10  | C8-C9   | 3.23  | 1.40        | 1.33     |
| 4   | S     | 2003    | BCL  | MG-NA   | 3.22  | 2.13        | 2.06     |
| 8   | S     | 2010    | SPO  | C37-C38 | 3.22  | 1.42        | 1.32     |
| 4   | L     | 1004    | BCL  | C3C-C4C | -3.18 | 1.47        | 1.51     |
| 4   | L     | 1001    | BCL  | C1B-C2B | 3.17  | 1.50        | 1.43     |
| 6   | R     | 2009[A] | U10  | C7-C8   | -3.16 | 1.45        | 1.50     |
| 5   | L     | 1006    | BPH  | C2-C3   | 3.12  | 1.40        | 1.33     |
| 4   | L     | 1004    | BCL  | MG-NC   | -3.12 | 1.98        | 2.06     |
| 6   | S     | 2008    | U10  | O3-C3   | 3.10  | 1.44        | 1.36     |
| 6   | L     | 1009[B] | U10  | O3-C3   | 3.10  | 1.44        | 1.36     |
| 6   | L     | 1009[A] | U10  | O3-C3M  | -3.10 | 1.38        | 1.45     |
| 6   | S     | 2008    | U10  | O3-C3M  | -3.10 | 1.38        | 1.45     |
| 6   | M     | 1008    | U10  | C18-C19 | 3.09  | 1.40        | 1.33     |
| 5   | R     | 2006    | BPH  | C1A-C2A | 3.08  | 1.55        | 1.51     |
| 5   | M     | 1005    | BPH  | CAA-C2A | 3.07  | 1.60        | 1.54     |
| 8   | M     | 1010    | SPO  | C6-C7   | -3.07 | 1.39        | 1.46     |
| 6   | R     | 2009[B] | U10  | C6-C1   | 3.06  | 1.40        | 1.35     |
| 5   | R     | 2006    | BPH  | C4D-ND  | -3.04 | 1.34        | 1.38     |
| 8   | M     | 1010    | SPO  | C10-C9  | 3.02  | 1.52        | 1.43     |

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| Mol | Chain | Res     | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|---------|------|---------|-------|-------------|----------|
| 6   | R     | 2009[A] | U10  | O3-C3M  | -3.01 | 1.38        | 1.45     |
| 8   | S     | 2010    | SPO  | C4-C1   | 3.00  | 1.58        | 1.52     |
| 4   | S     | 2004    | BCL  | MG-NC   | -3.00 | 1.99        | 2.06     |
| 8   | S     | 2010    | SPO  | C11-C12 | -2.99 | 1.39        | 1.46     |
| 6   | S     | 2008    | U10  | C7-C8   | -2.99 | 1.45        | 1.50     |
| 5   | R     | 2006    | BPH  | O2D-CED | -2.96 | 1.38        | 1.45     |
| 6   | M     | 1008    | U10  | O3-C3M  | -2.96 | 1.38        | 1.45     |
| 6   | M     | 1008    | U10  | O3-C3   | 2.96  | 1.43        | 1.36     |
| 8   | S     | 2010    | SPO  | C25-C23 | -2.96 | 1.39        | 1.46     |
| 4   | S     | 2001    | BCL  | C1B-C2B | 2.95  | 1.50        | 1.43     |
| 5   | R     | 2006    | BPH  | C2-C3   | 2.95  | 1.39        | 1.33     |
| 4   | S     | 2004    | BCL  | CAA-C2A | 2.95  | 1.59        | 1.54     |
| 4   | S     | 2004    | BCL  | MG-NA   | 2.93  | 2.13        | 2.06     |
| 4   | S     | 2001    | BCL  | CBB-CAB | 2.92  | 1.55        | 1.50     |
| 4   | L     | 1002    | BCL  | CBB-CAB | 2.91  | 1.55        | 1.50     |
| 5   | S     | 2005    | BPH  | C4D-ND  | -2.91 | 1.34        | 1.38     |
| 4   | S     | 2003    | BCL  | C3D-C4D | -2.91 | 1.37        | 1.44     |
| 6   | R     | 2009[B] | U10  | C7-C8   | -2.90 | 1.46        | 1.50     |
| 6   | S     | 2008    | U10  | C18-C19 | 2.89  | 1.39        | 1.33     |
| 8   | M     | 1010    | SPO  | C32-C33 | 2.88  | 1.39        | 1.33     |
| 4   | L     | 1002    | BCL  | C1B-C2B | 2.87  | 1.49        | 1.43     |
| 8   | S     | 2010    | SPO  | C10-C9  | 2.87  | 1.52        | 1.43     |
| 5   | S     | 2005    | BPH  | C1A-C2A | 2.87  | 1.55        | 1.51     |
| 4   | S     | 2001    | BCL  | C3D-C4D | -2.86 | 1.37        | 1.44     |
| 8   | M     | 1010    | SPO  | C25-C23 | -2.86 | 1.39        | 1.46     |
| 6   | L     | 1009[B] | U10  | C18-C19 | 2.85  | 1.39        | 1.33     |
| 8   | S     | 2010    | SPO  | O1-C1   | 2.85  | 1.57        | 1.41     |
| 8   | M     | 1010    | SPO  | C37-C38 | 2.84  | 1.41        | 1.32     |
| 6   | S     | 2008    | U10  | C8-C9   | 2.83  | 1.39        | 1.33     |
| 4   | S     | 2004    | BCL  | C3C-C4C | -2.82 | 1.48        | 1.51     |
| 8   | S     | 2010    | SPO  | C32-C33 | 2.81  | 1.39        | 1.33     |
| 8   | M     | 1010    | SPO  | C11-C12 | -2.81 | 1.39        | 1.46     |
| 6   | S     | 2008    | U10  | C6-C1   | 2.80  | 1.40        | 1.35     |
| 4   | S     | 2003    | BCL  | CHD-C1D | 2.80  | 1.43        | 1.38     |
| 5   | L     | 1006    | BPH  | O2D-CED | -2.80 | 1.39        | 1.45     |
| 6   | L     | 1009[B] | U10  | C6-C1   | 2.79  | 1.40        | 1.35     |
| 6   | L     | 1009[A] | U10  | C18-C19 | 2.79  | 1.39        | 1.33     |
| 4   | S     | 2001    | BCL  | CAA-C2A | 2.78  | 1.59        | 1.54     |
| 5   | M     | 1005    | BPH  | O2D-CED | -2.77 | 1.39        | 1.45     |
| 4   | R     | 2002    | BCL  | C1B-C2B | 2.77  | 1.49        | 1.43     |
| 4   | S     | 2001    | BCL  | MG-NA   | 2.77  | 2.12        | 2.06     |
| 4   | L     | 1002    | BCL  | CHD-C1D | 2.76  | 1.43        | 1.38     |

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| Mol | Chain | Res     | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|---------|------|---------|-------|-------------|----------|
| 5   | M     | 1005    | BPH  | C3B-C4B | 2.75  | 1.45        | 1.41     |
| 5   | M     | 1005    | BPH  | C2-C3   | 2.74  | 1.39        | 1.33     |
| 5   | S     | 2005    | BPH  | C2-C3   | 2.74  | 1.39        | 1.33     |
| 8   | M     | 1010    | SPO  | C8-C7   | 2.73  | 1.56        | 1.50     |
| 6   | R     | 2009[B] | U10  | C8-C9   | 2.73  | 1.40        | 1.32     |
| 5   | S     | 2005    | BPH  | CAA-C2A | 2.72  | 1.59        | 1.54     |
| 4   | L     | 1001    | BCL  | C3D-C4D | -2.72 | 1.38        | 1.44     |
| 4   | M     | 1003    | BCL  | C1B-C2B | 2.71  | 1.49        | 1.43     |
| 8   | S     | 2010    | SPO  | C26-C27 | 2.70  | 1.51        | 1.43     |
| 4   | S     | 2004    | BCL  | CBB-CAB | 2.70  | 1.55        | 1.50     |
| 6   | L     | 1009[B] | U10  | C7-C8   | -2.70 | 1.46        | 1.50     |
| 4   | M     | 1003    | BCL  | CHD-C1D | 2.69  | 1.43        | 1.38     |
| 5   | S     | 2005    | BPH  | O2D-CED | -2.69 | 1.39        | 1.45     |
| 4   | R     | 2002    | BCL  | CHD-C1D | 2.69  | 1.43        | 1.38     |
| 5   | M     | 1005    | BPH  | C3A-C2A | -2.68 | 1.52        | 1.54     |
| 8   | S     | 2010    | SPO  | C6-C7   | -2.68 | 1.40        | 1.46     |
| 8   | M     | 1010    | SPO  | C26-C27 | 2.67  | 1.51        | 1.43     |
| 8   | M     | 1010    | SPO  | O1-C1   | 2.67  | 1.56        | 1.41     |
| 6   | L     | 1009[A] | U10  | C7-C8   | -2.67 | 1.46        | 1.50     |
| 4   | L     | 1001    | BCL  | C1D-C2D | -2.66 | 1.40        | 1.45     |
| 5   | L     | 1006    | BPH  | CHA-CBD | 2.64  | 1.54        | 1.51     |
| 8   | M     | 1010    | SPO  | C13-C12 | 2.63  | 1.56        | 1.50     |
| 6   | M     | 1008    | U10  | C6-C1   | 2.62  | 1.39        | 1.35     |
| 8   | S     | 2010    | SPO  | C8-C7   | 2.60  | 1.56        | 1.50     |
| 4   | S     | 2004    | BCL  | C3D-C4D | -2.59 | 1.38        | 1.44     |
| 8   | M     | 1010    | SPO  | C15-C14 | 2.54  | 1.51        | 1.43     |
| 4   | L     | 1004    | BCL  | CBB-CAB | 2.51  | 1.55        | 1.50     |
| 4   | M     | 1003    | BCL  | C3D-C4D | -2.51 | 1.38        | 1.44     |
| 5   | M     | 1005    | BPH  | CBD-CGD | -2.51 | 1.49        | 1.52     |
| 5   | M     | 1005    | BPH  | C3B-C2B | -2.51 | 1.35        | 1.39     |
| 4   | S     | 2003    | BCL  | CMD-C2D | 2.50  | 1.55        | 1.50     |
| 4   | S     | 2004    | BCL  | C4-C3   | 2.50  | 1.56        | 1.50     |
| 6   | L     | 1009[A] | U10  | C7-C6   | 2.50  | 1.56        | 1.51     |
| 6   | R     | 2009[A] | U10  | C8-C9   | 2.48  | 1.39        | 1.32     |
| 4   | L     | 1001    | BCL  | CAA-C2A | 2.48  | 1.58        | 1.54     |
| 4   | S     | 2003    | BCL  | C1B-C2B | 2.48  | 1.48        | 1.43     |
| 4   | L     | 1002    | BCL  | C3C-C4C | -2.47 | 1.48        | 1.51     |
| 8   | M     | 1010    | SPO  | C24-C23 | 2.46  | 1.55        | 1.50     |
| 6   | L     | 1009[A] | U10  | C15-C14 | 2.44  | 1.56        | 1.50     |
| 4   | L     | 1001    | BCL  | CAA-CBA | 2.44  | 1.60        | 1.52     |
| 4   | M     | 1003    | BCL  | C4B-NB  | -2.44 | 1.34        | 1.37     |
| 6   | M     | 1008    | U10  | C27-C28 | -2.43 | 1.43        | 1.50     |

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| Mol | Chain | Res     | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|---------|------|---------|-------|-------------|----------|
| 8   | S     | 2010    | SPO  | C13-C12 | 2.42  | 1.55        | 1.50     |
| 6   | M     | 1008    | U10  | C15-C14 | 2.41  | 1.56        | 1.50     |
| 4   | L     | 1002    | BCL  | C3D-C4D | -2.38 | 1.38        | 1.44     |
| 4   | S     | 2004    | BCL  | CAA-CBA | 2.38  | 1.60        | 1.52     |
| 5   | R     | 2006    | BPH  | C3D-C2D | -2.38 | 1.35        | 1.39     |
| 8   | S     | 2010    | SPO  | C35-C33 | 2.37  | 1.56        | 1.51     |
| 6   | M     | 1008    | U10  | C8-C9   | 2.37  | 1.38        | 1.33     |
| 6   | L     | 1009[B] | U10  | C15-C14 | 2.37  | 1.56        | 1.50     |
| 4   | R     | 2002    | BCL  | CMD-C2D | 2.36  | 1.55        | 1.50     |
| 4   | M     | 1003    | BCL  | C3C-C4C | -2.36 | 1.48        | 1.51     |
| 8   | M     | 1010    | SPO  | C14-C12 | 2.36  | 1.41        | 1.35     |
| 4   | L     | 1002    | BCL  | CMD-C2D | 2.35  | 1.55        | 1.50     |
| 4   | L     | 1004    | BCL  | C3D-C4D | -2.35 | 1.38        | 1.44     |
| 5   | R     | 2006    | BPH  | CAA-C2A | 2.33  | 1.58        | 1.54     |
| 5   | R     | 2006    | BPH  | C3B-C4B | 2.33  | 1.45        | 1.41     |
| 4   | L     | 1004    | BCL  | MG-NA   | 2.31  | 2.11        | 2.06     |
| 4   | S     | 2001    | BCL  | C1-C2   | 2.31  | 1.55        | 1.49     |
| 8   | S     | 2010    | SPO  | C24-C23 | 2.30  | 1.55        | 1.50     |
| 8   | S     | 2010    | SPO  | C19-C17 | 2.30  | 1.41        | 1.35     |
| 8   | S     | 2010    | SPO  | C15-C14 | 2.30  | 1.50        | 1.43     |
| 5   | S     | 2005    | BPH  | C3B-C2B | -2.30 | 1.35        | 1.39     |
| 4   | L     | 1002    | BCL  | C4-C3   | 2.29  | 1.56        | 1.50     |
| 4   | M     | 1003    | BCL  | OBB-CAB | -2.28 | 1.18        | 1.23     |
| 4   | L     | 1004    | BCL  | C6-C5   | 2.27  | 1.60        | 1.52     |
| 4   | L     | 1001    | BCL  | C4B-NB  | -2.26 | 1.34        | 1.37     |
| 5   | L     | 1006    | BPH  | C1A-C2A | 2.26  | 1.54        | 1.51     |
| 5   | L     | 1006    | BPH  | C4D-ND  | -2.25 | 1.35        | 1.38     |
| 4   | R     | 2002    | BCL  | OBB-CAB | -2.25 | 1.18        | 1.23     |
| 5   | L     | 1006    | BPH  | CAA-C2A | 2.24  | 1.58        | 1.54     |
| 4   | S     | 2004    | BCL  | CMD-C2D | 2.23  | 1.55        | 1.50     |
| 4   | R     | 2002    | BCL  | C3D-C4D | -2.23 | 1.39        | 1.44     |
| 4   | S     | 2004    | BCL  | C4B-NB  | -2.22 | 1.34        | 1.37     |
| 4   | L     | 1001    | BCL  | MG-NA   | 2.22  | 2.11        | 2.06     |
| 4   | M     | 1003    | BCL  | CMD-C2D | 2.20  | 1.55        | 1.50     |
| 6   | S     | 2008    | U10  | C15-C14 | 2.20  | 1.56        | 1.50     |
| 4   | S     | 2001    | BCL  | CAA-CBA | 2.20  | 1.59        | 1.52     |
| 4   | M     | 1003    | BCL  | MG-NC   | -2.20 | 2.01        | 2.06     |
| 4   | R     | 2002    | BCL  | C4-C3   | 2.20  | 1.56        | 1.50     |
| 4   | S     | 2001    | BCL  | C1D-C2D | -2.19 | 1.41        | 1.45     |
| 4   | S     | 2003    | BCL  | C4-C3   | 2.18  | 1.56        | 1.50     |
| 4   | S     | 2003    | BCL  | CBB-CAB | 2.18  | 1.54        | 1.50     |
| 4   | L     | 1004    | BCL  | C4-C3   | 2.17  | 1.56        | 1.50     |

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| Mol | Chain | Res     | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|---------|------|---------|-------|-------------|----------|
| 5   | M     | 1005    | BPH  | C4D-ND  | -2.16 | 1.35        | 1.38     |
| 6   | S     | 2008    | U10  | C20-C19 | 2.15  | 1.56        | 1.50     |
| 4   | S     | 2003    | BCL  | C4B-NB  | -2.15 | 1.35        | 1.37     |
| 4   | S     | 2004    | BCL  | C1D-C2D | -2.14 | 1.41        | 1.45     |
| 4   | L     | 1001    | BCL  | C4-C3   | 2.13  | 1.56        | 1.50     |
| 8   | S     | 2010    | SPO  | C14-C12 | 2.12  | 1.40        | 1.35     |
| 4   | S     | 2004    | BCL  | OBG-CAB | -2.12 | 1.18        | 1.23     |
| 6   | L     | 1009[A] | U10  | C20-C19 | 2.11  | 1.55        | 1.50     |
| 5   | M     | 1005    | BPH  | C1A-C2A | 2.10  | 1.54        | 1.51     |
| 4   | S     | 2001    | BCL  | OBG-CAD | -2.10 | 1.18        | 1.22     |
| 5   | R     | 2006    | BPH  | C3A-C2A | -2.08 | 1.52        | 1.54     |
| 4   | S     | 2001    | BCL  | C4B-NB  | -2.08 | 1.35        | 1.37     |
| 4   | L     | 1001    | BCL  | OBG-CAB | -2.08 | 1.18        | 1.23     |
| 4   | M     | 1003    | BCL  | CBB-CAB | 2.07  | 1.54        | 1.50     |
| 4   | L     | 1004    | BCL  | C1D-C2D | -2.07 | 1.41        | 1.45     |
| 4   | L     | 1004    | BCL  | CMD-C2D | 2.06  | 1.55        | 1.50     |
| 5   | M     | 1005    | BPH  | CMB-C2B | 2.05  | 1.55        | 1.51     |
| 8   | M     | 1010    | SPO  | C19-C17 | 2.04  | 1.40        | 1.35     |
| 4   | S     | 2003    | BCL  | MG-NC   | -2.03 | 2.01        | 2.06     |
| 6   | M     | 1008    | U10  | C30-C29 | 2.03  | 1.55        | 1.50     |
| 4   | S     | 2001    | BCL  | C4-C3   | 2.03  | 1.55        | 1.50     |
| 4   | L     | 1001    | BCL  | CMD-C2D | 2.03  | 1.54        | 1.50     |
| 6   | M     | 1008    | U10  | C20-C19 | 2.02  | 1.55        | 1.50     |
| 5   | S     | 2005    | BPH  | C3A-C2A | -2.02 | 1.53        | 1.54     |
| 4   | L     | 1002    | BCL  | OBG-CAB | -2.01 | 1.18        | 1.23     |
| 4   | S     | 2004    | BCL  | CHD-C1D | 2.01  | 1.42        | 1.38     |
| 5   | S     | 2005    | BPH  | O1D-CGD | 2.01  | 1.26        | 1.21     |
| 4   | M     | 1003    | BCL  | C2-C3   | -2.00 | 1.28        | 1.33     |

All (337) bond angle outliers are listed below:

| Mol | Chain | Res     | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-------------|-------|-------------|----------|
| 5   | S     | 2005    | BPH  | O2D-CGD-CBD | 14.28 | 126.64      | 110.95   |
| 5   | R     | 2006    | BPH  | O2D-CGD-CBD | 13.97 | 126.30      | 110.95   |
| 5   | L     | 1006    | BPH  | O2D-CGD-CBD | 13.54 | 125.83      | 110.95   |
| 5   | M     | 1005    | BPH  | O2D-CGD-CBD | 13.51 | 125.80      | 110.95   |
| 8   | S     | 2010    | SPO  | C15-C14-C12 | -6.63 | 117.98      | 127.28   |
| 6   | L     | 1009[A] | U10  | C3M-O3-C3   | 6.50  | 139.32      | 116.47   |
| 6   | R     | 2009[A] | U10  | C3M-O3-C3   | 6.48  | 139.25      | 116.47   |
| 5   | R     | 2006    | BPH  | C1-C2-C3    | 6.40  | 136.69      | 126.20   |
| 6   | R     | 2009[B] | U10  | C3M-O3-C3   | 6.37  | 138.86      | 116.47   |
| 8   | S     | 2010    | SPO  | C20-C21-C22 | -6.32 | 110.59      | 123.52   |

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| Mol | Chain | Res     | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-------------|-------|-------------|----------|
| 4   | R     | 2002    | BCL  | C4A-NA-C1A  | -6.31 | 103.80      | 106.68   |
| 6   | S     | 2008    | U10  | C3M-O3-C3   | 6.20  | 138.27      | 116.47   |
| 4   | L     | 1002    | BCL  | C4A-NA-C1A  | -6.19 | 103.85      | 106.68   |
| 6   | L     | 1009[B] | U10  | C3M-O3-C3   | 6.08  | 137.85      | 116.47   |
| 8   | M     | 1010    | SPO  | C20-C21-C22 | -6.06 | 111.12      | 123.52   |
| 4   | L     | 1001    | BCL  | CBC-CAC-C3C | -6.00 | 100.68      | 113.41   |
| 5   | L     | 1006    | BPH  | C1-C2-C3    | 5.95  | 135.95      | 126.20   |
| 6   | M     | 1008    | U10  | C3M-O3-C3   | 5.85  | 137.03      | 116.47   |
| 5   | S     | 2005    | BPH  | C1-C2-C3    | 5.81  | 135.72      | 126.20   |
| 8   | M     | 1010    | SPO  | C15-C14-C12 | -5.77 | 119.19      | 127.28   |
| 4   | S     | 2001    | BCL  | C4A-NA-C1A  | -5.61 | 104.12      | 106.68   |
| 4   | S     | 2004    | BCL  | C4A-NA-C1A  | -5.58 | 104.13      | 106.68   |
| 4   | S     | 2001    | BCL  | CBC-CAC-C3C | -5.57 | 101.59      | 113.41   |
| 5   | L     | 1006    | BPH  | CBC-CAC-C3C | 5.53  | 124.65      | 113.78   |
| 5   | M     | 1005    | BPH  | C1-C2-C3    | 5.53  | 135.25      | 126.20   |
| 4   | S     | 2003    | BCL  | C4A-NA-C1A  | -5.46 | 104.19      | 106.68   |
| 5   | R     | 2006    | BPH  | CBC-CAC-C3C | 5.34  | 124.27      | 113.78   |
| 4   | M     | 1003    | BCL  | C4A-NA-C1A  | -5.31 | 104.26      | 106.68   |
| 8   | M     | 1010    | SPO  | C26-C27-C28 | -5.30 | 120.23      | 127.69   |
| 4   | L     | 1001    | BCL  | C1-C2-C3    | -5.21 | 118.34      | 126.76   |
| 8   | S     | 2010    | SPO  | C25-C23-C22 | -5.07 | 111.03      | 119.01   |
| 5   | L     | 1006    | BPH  | O1D-CGD-CBD | -5.03 | 117.10      | 124.72   |
| 8   | M     | 1010    | SPO  | C25-C23-C22 | -5.00 | 111.14      | 119.01   |
| 5   | S     | 2005    | BPH  | O1D-CGD-CBD | -5.00 | 117.15      | 124.72   |
| 5   | R     | 2006    | BPH  | O1D-CGD-CBD | -4.94 | 117.22      | 124.72   |
| 5   | M     | 1005    | BPH  | O1D-CGD-CBD | -4.94 | 117.24      | 124.72   |
| 5   | R     | 2006    | BPH  | C4D-CHA-CBD | -4.83 | 106.14      | 108.45   |
| 4   | S     | 2003    | BCL  | C1D-ND-C4D  | 4.80  | 109.68      | 106.31   |
| 8   | S     | 2010    | SPO  | C26-C27-C28 | -4.77 | 120.98      | 127.69   |
| 4   | L     | 1001    | BCL  | C4A-NA-C1A  | -4.67 | 104.55      | 106.68   |
| 5   | M     | 1005    | BPH  | CBC-CAC-C3C | 4.65  | 122.93      | 113.78   |
| 6   | M     | 1008    | U10  | C27-C28-C29 | 4.62  | 143.06      | 127.64   |
| 4   | L     | 1004    | BCL  | C4A-NA-C1A  | -4.57 | 104.59      | 106.68   |
| 4   | S     | 2004    | BCL  | C1D-ND-C4D  | 4.55  | 109.50      | 106.31   |
| 5   | L     | 1006    | BPH  | C6-C5-C3    | 4.54  | 124.53      | 113.47   |
| 4   | M     | 1003    | BCL  | C1D-ND-C4D  | 4.48  | 109.46      | 106.31   |
| 5   | L     | 1006    | BPH  | CED-O2D-CGD | 4.48  | 126.07      | 115.92   |
| 4   | L     | 1002    | BCL  | C1D-ND-C4D  | 4.46  | 109.44      | 106.31   |
| 5   | M     | 1005    | BPH  | CED-O2D-CGD | 4.40  | 125.90      | 115.92   |
| 5   | S     | 2005    | BPH  | C4D-CHA-CBD | -4.39 | 106.35      | 108.45   |
| 4   | L     | 1001    | BCL  | C1D-ND-C4D  | 4.29  | 109.32      | 106.31   |
| 8   | M     | 1010    | SPO  | C24-C23-C25 | 4.27  | 124.61      | 118.09   |

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| Mol | Chain | Res     | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-------------|-------|-------------|----------|
| 4   | M     | 1003    | BCL  | C11-C12-C13 | -4.27 | 101.78      | 115.97   |
| 4   | S     | 2001    | BCL  | C1D-ND-C4D  | 4.24  | 109.29      | 106.31   |
| 4   | S     | 2003    | BCL  | C11-C12-C13 | -4.23 | 101.91      | 115.97   |
| 4   | L     | 1004    | BCL  | C1D-ND-C4D  | 4.22  | 109.28      | 106.31   |
| 4   | R     | 2002    | BCL  | C1D-ND-C4D  | 4.17  | 109.23      | 106.31   |
| 8   | S     | 2010    | SPO  | C4-C5-C6    | -4.15 | 119.09      | 124.91   |
| 8   | S     | 2010    | SPO  | C24-C23-C25 | 4.08  | 124.33      | 118.09   |
| 5   | R     | 2006    | BPH  | C6-C5-C3    | 4.06  | 123.35      | 113.47   |
| 5   | S     | 2005    | BPH  | CED-O2D-CGD | 4.05  | 125.11      | 115.92   |
| 4   | M     | 1003    | BCL  | C4D-CHA-C1A | 4.03  | 126.05      | 121.24   |
| 4   | L     | 1004    | BCL  | C1-O2A-CGA  | 4.01  | 126.37      | 116.65   |
| 4   | R     | 2002    | BCL  | C7-C6-C5    | -4.01 | 102.57      | 113.26   |
| 5   | R     | 2006    | BPH  | CED-O2D-CGD | 3.98  | 124.95      | 115.92   |
| 5   | S     | 2005    | BPH  | O2D-CGD-O1D | -3.92 | 116.21      | 123.85   |
| 4   | L     | 1002    | BCL  | C7-C6-C5    | -3.88 | 102.93      | 113.26   |
| 5   | M     | 1005    | BPH  | C6-C5-C3    | 3.86  | 122.87      | 113.47   |
| 4   | L     | 1002    | BCL  | C4D-CHA-C1A | 3.84  | 125.82      | 121.24   |
| 4   | S     | 2003    | BCL  | C4D-CHA-C1A | 3.83  | 125.82      | 121.24   |
| 5   | R     | 2006    | BPH  | O2D-CGD-O1D | -3.81 | 116.43      | 123.85   |
| 4   | L     | 1001    | BCL  | CAC-C3C-C4C | -3.78 | 104.20      | 112.58   |
| 4   | L     | 1002    | BCL  | C1-C2-C3    | -3.76 | 120.03      | 126.20   |
| 5   | R     | 2006    | BPH  | C11-C10-C8  | 3.76  | 128.46      | 115.97   |
| 8   | M     | 1010    | SPO  | C3-C1-C2    | 3.76  | 117.29      | 110.43   |
| 6   | R     | 2009[A] | U10  | O5-C5-C6    | -3.75 | 114.53      | 121.79   |
| 6   | L     | 1009[B] | U10  | O2-C2-C3    | -3.74 | 113.11      | 121.03   |
| 4   | S     | 2004    | BCL  | C4D-CHA-C1A | 3.73  | 125.70      | 121.24   |
| 8   | S     | 2010    | SPO  | C6-C7-C9    | -3.73 | 113.14      | 119.01   |
| 6   | L     | 1009[A] | U10  | O5-C5-C6    | -3.72 | 114.59      | 121.79   |
| 8   | S     | 2010    | SPO  | C15-C16-C17 | -3.71 | 116.18      | 126.36   |
| 5   | S     | 2005    | BPH  | CBC-CAC-C3C | 3.71  | 121.08      | 113.78   |
| 4   | S     | 2004    | BCL  | CBB-CAB-C3B | 3.70  | 128.21      | 120.40   |
| 4   | L     | 1001    | BCL  | C4D-CHA-C1A | 3.69  | 125.65      | 121.24   |
| 4   | M     | 1003    | BCL  | CBB-CAB-C3B | 3.67  | 128.14      | 120.40   |
| 4   | S     | 2004    | BCL  | C11-C12-C13 | -3.67 | 103.77      | 115.97   |
| 4   | L     | 1004    | BCL  | C4D-CHA-C1A | 3.65  | 125.60      | 121.24   |
| 6   | S     | 2008    | U10  | O5-C5-C6    | -3.63 | 114.76      | 121.79   |
| 4   | S     | 2003    | BCL  | OBB-CAB-CBB | -3.63 | 111.64      | 119.77   |
| 5   | L     | 1006    | BPH  | C4D-CHA-CBD | -3.62 | 106.72      | 108.45   |
| 4   | L     | 1004    | BCL  | CBB-CAB-C3B | 3.62  | 128.03      | 120.40   |
| 4   | L     | 1004    | BCL  | OBB-CAB-CBB | -3.62 | 111.67      | 119.77   |
| 4   | S     | 2004    | BCL  | CBC-CAC-C3C | -3.61 | 105.75      | 113.41   |
| 4   | M     | 1003    | BCL  | CAA-CBA-CGA | -3.60 | 103.00      | 113.21   |

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| Mol | Chain | Res     | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-------------|-------|-------------|----------|
| 6   | R     | 2009[B] | U10  | O5-C5-C6    | -3.60 | 114.83      | 121.79   |
| 8   | M     | 1010    | SPO  | C15-C16-C17 | -3.59 | 116.52      | 126.36   |
| 4   | L     | 1004    | BCL  | CAC-C3C-C4C | -3.58 | 104.63      | 112.58   |
| 4   | R     | 2002    | BCL  | C4D-CHA-C1A | 3.57  | 125.50      | 121.24   |
| 5   | S     | 2005    | BPH  | C1C-C2C-C3C | 3.57  | 106.23      | 102.84   |
| 4   | S     | 2001    | BCL  | C4D-CHA-C1A | 3.55  | 125.48      | 121.24   |
| 5   | L     | 1006    | BPH  | C11-C10-C8  | 3.54  | 127.72      | 115.97   |
| 5   | M     | 1005    | BPH  | O2D-CGD-O1D | -3.54 | 116.96      | 123.85   |
| 6   | L     | 1009[B] | U10  | O5-C5-C6    | -3.52 | 114.99      | 121.79   |
| 4   | M     | 1003    | BCL  | OBb-CAB-CBB | -3.51 | 111.90      | 119.77   |
| 6   | M     | 1008    | U10  | O5-C5-C6    | -3.51 | 115.00      | 121.79   |
| 8   | S     | 2010    | SPO  | C3-C1-C2    | 3.51  | 116.84      | 110.43   |
| 4   | L     | 1001    | BCL  | OBb-CAB-CBB | -3.50 | 111.93      | 119.77   |
| 5   | L     | 1006    | BPH  | O2D-CGD-O1D | -3.50 | 117.04      | 123.85   |
| 5   | M     | 1005    | BPH  | CMA-C3A-C4A | -3.48 | 107.11      | 114.61   |
| 5   | R     | 2006    | BPH  | C1C-C2C-C3C | 3.48  | 106.15      | 102.84   |
| 4   | M     | 1003    | BCL  | C4-C3-C5    | 3.47  | 121.26      | 115.23   |
| 4   | S     | 2003    | BCL  | CBB-CAB-C3B | 3.45  | 127.68      | 120.40   |
| 5   | M     | 1005    | BPH  | C1C-C2C-C3C | 3.45  | 106.12      | 102.84   |
| 4   | S     | 2004    | BCL  | OBb-CAB-CBB | -3.45 | 112.05      | 119.77   |
| 8   | M     | 1010    | SPO  | C4-C5-C6    | -3.44 | 120.08      | 124.91   |
| 4   | L     | 1004    | BCL  | CBC-CAC-C3C | -3.42 | 106.16      | 113.41   |
| 5   | L     | 1006    | BPH  | C1C-C2C-C3C | 3.42  | 106.09      | 102.84   |
| 4   | R     | 2002    | BCL  | C11-C12-C13 | -3.40 | 104.67      | 115.97   |
| 6   | R     | 2009[B] | U10  | O2-C2-C3    | -3.39 | 113.84      | 121.03   |
| 4   | L     | 1001    | BCL  | C2C-C3C-C4C | 3.38  | 106.39      | 101.34   |
| 6   | R     | 2009[A] | U10  | O2-C2-C3    | -3.37 | 113.89      | 121.03   |
| 6   | L     | 1009[A] | U10  | O2-C2-C3    | -3.35 | 113.94      | 121.03   |
| 8   | M     | 1010    | SPO  | C8-C7-C6    | 3.34  | 123.19      | 118.09   |
| 8   | S     | 2010    | SPO  | C8-C7-C6    | 3.32  | 123.17      | 118.09   |
| 9   | M     | 1011    | LDA  | CM1-N1-C1   | -3.32 | 103.26      | 110.23   |
| 4   | L     | 1001    | BCL  | CAA-C2A-C3A | -3.29 | 104.11      | 113.00   |
| 4   | R     | 2002    | BCL  | OBb-CAB-CBB | -3.29 | 112.41      | 119.77   |
| 4   | L     | 1002    | BCL  | O2D-CGD-CBD | -3.28 | 105.50      | 111.23   |
| 4   | R     | 2002    | BCL  | CBB-CAB-C3B | 3.28  | 127.31      | 120.40   |
| 4   | S     | 2004    | BCL  | CAA-C2A-C3A | -3.27 | 104.16      | 113.00   |
| 8   | M     | 1010    | SPO  | C18-C17-C19 | -3.25 | 117.55      | 122.82   |
| 4   | S     | 2001    | BCL  | C2C-C3C-C4C | 3.25  | 106.20      | 101.34   |
| 6   | L     | 1009[A] | U10  | C1-C6-C5    | -3.24 | 116.47      | 119.62   |
| 8   | M     | 1010    | SPO  | C6-C7-C9    | -3.24 | 113.92      | 119.01   |
| 4   | S     | 2003    | BCL  | C4-C3-C5    | 3.23  | 120.83      | 115.23   |
| 4   | S     | 2001    | BCL  | CAA-C2A-C3A | -3.21 | 104.32      | 113.00   |

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| Mol | Chain | Res     | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-------------|-------|-------------|----------|
| 4   | L     | 1001    | BCL  | CBB-CAB-C3B | 3.19  | 127.12      | 120.40   |
| 5   | S     | 2005    | BPH  | C4-C3-C5    | 3.18  | 119.87      | 116.13   |
| 4   | L     | 1002    | BCL  | OBG-CAB-CBB | -3.17 | 112.66      | 119.77   |
| 4   | L     | 1004    | BCL  | O2A-C1-C2   | -3.17 | 95.91       | 108.11   |
| 4   | L     | 1002    | BCL  | CBB-CAB-C3B | 3.17  | 127.08      | 120.40   |
| 6   | S     | 2008    | U10  | O2-C2-C3    | -3.14 | 114.37      | 121.03   |
| 4   | S     | 2001    | BCL  | OBG-CAB-CBB | -3.14 | 112.74      | 119.77   |
| 4   | S     | 2004    | BCL  | C16-C15-C13 | -3.13 | 105.57      | 115.97   |
| 5   | S     | 2005    | BPH  | CMA-C3A-C4A | -3.12 | 107.88      | 114.61   |
| 4   | S     | 2004    | BCL  | C1-C2-C3    | -3.12 | 121.09      | 126.20   |
| 6   | M     | 1008    | U10  | O2-C2-C3    | -3.12 | 114.43      | 121.03   |
| 4   | L     | 1004    | BCL  | C2C-C3C-C4C | 3.11  | 106.00      | 101.34   |
| 4   | S     | 2004    | BCL  | CAC-C3C-C4C | -3.10 | 105.69      | 112.58   |
| 6   | L     | 1009[B] | U10  | C1-C6-C5    | -3.09 | 116.61      | 119.62   |
| 5   | M     | 1005    | BPH  | C4D-CHA-CBD | -3.09 | 106.97      | 108.45   |
| 5   | S     | 2005    | BPH  | C4C-C3C-C2C | 3.09  | 105.78      | 102.84   |
| 4   | S     | 2001    | BCL  | CBB-CAB-C3B | 3.08  | 126.89      | 120.40   |
| 4   | S     | 2004    | BCL  | CHA-C1A-NA  | -3.06 | 119.47      | 126.39   |
| 4   | L     | 1004    | BCL  | C11-C12-C13 | -3.05 | 105.83      | 115.97   |
| 4   | S     | 2004    | BCL  | C2C-C3C-C4C | 3.04  | 105.90      | 101.34   |
| 5   | R     | 2006    | BPH  | CMA-C3A-C4A | -3.03 | 108.09      | 114.61   |
| 4   | M     | 1003    | BCL  | CHA-C1A-NA  | -3.01 | 119.56      | 126.39   |
| 6   | M     | 1008    | U10  | C20-C19-C21 | -3.01 | 110.00      | 115.23   |
| 5   | L     | 1006    | BPH  | C4C-C3C-C2C | 3.01  | 105.70      | 102.84   |
| 4   | M     | 1003    | BCL  | CBA-CAA-C2A | 2.99  | 122.69      | 113.79   |
| 4   | L     | 1002    | BCL  | O1D-CGD-CBD | 2.97  | 130.38      | 124.52   |
| 4   | R     | 2002    | BCL  | CHD-C1D-ND  | -2.96 | 120.64      | 124.80   |
| 8   | S     | 2010    | SPO  | C20-C19-C17 | -2.95 | 123.14      | 127.28   |
| 4   | S     | 2003    | BCL  | CAA-CBA-CGA | -2.94 | 104.85      | 113.21   |
| 5   | L     | 1006    | BPH  | C7-C6-C5    | -2.93 | 105.45      | 113.26   |
| 5   | L     | 1006    | BPH  | CMA-C3A-C4A | -2.91 | 108.35      | 114.61   |
| 6   | R     | 2009[A] | U10  | C1-C6-C5    | -2.89 | 116.81      | 119.62   |
| 8   | M     | 1010    | SPO  | C10-C9-C7   | -2.88 | 123.24      | 127.28   |
| 4   | S     | 2003    | BCL  | CHA-C1A-NA  | -2.87 | 119.89      | 126.39   |
| 4   | S     | 2001    | BCL  | CHD-C1D-ND  | -2.87 | 120.77      | 124.80   |
| 4   | R     | 2002    | BCL  | CAA-C2A-C3A | -2.87 | 105.25      | 113.00   |
| 4   | L     | 1002    | BCL  | C16-C15-C13 | -2.87 | 106.44      | 115.97   |
| 6   | R     | 2009[B] | U10  | C1-C6-C5    | -2.85 | 116.85      | 119.62   |
| 4   | R     | 2002    | BCL  | CAC-C3C-C4C | -2.84 | 106.27      | 112.58   |
| 4   | L     | 1001    | BCL  | CHA-C1A-NA  | -2.84 | 119.95      | 126.39   |
| 6   | L     | 1009[B] | U10  | C20-C19-C21 | -2.84 | 110.31      | 115.23   |
| 5   | S     | 2005    | BPH  | C2B-C1B-NB  | 2.83  | 111.48      | 109.43   |

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| Mol | Chain | Res     | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-------------|-------|-------------|----------|
| 5   | L     | 1006    | BPH  | CMB-C2B-C3B | 2.83  | 130.34      | 124.68   |
| 4   | R     | 2002    | BCL  | CHA-C1A-NA  | -2.83 | 119.98      | 126.39   |
| 9   | M     | 1011    | LDA  | O1-N1-C1    | 2.82  | 116.20      | 109.27   |
| 5   | R     | 2006    | BPH  | C4C-C3C-C2C | 2.82  | 105.52      | 102.84   |
| 8   | S     | 2010    | SPO  | C18-C17-C19 | -2.82 | 118.25      | 122.82   |
| 4   | S     | 2001    | BCL  | CBA-CAA-C2A | 2.78  | 122.06      | 113.79   |
| 4   | L     | 1002    | BCL  | CHA-C1A-NA  | -2.78 | 120.10      | 126.39   |
| 5   | M     | 1005    | BPH  | C1B-NB-C4B  | -2.77 | 104.78      | 108.82   |
| 4   | L     | 1002    | BCL  | C4D-C3D-CAD | -2.76 | 105.10      | 108.11   |
| 4   | L     | 1001    | BCL  | CHD-C1D-ND  | -2.76 | 120.92      | 124.80   |
| 4   | L     | 1004    | BCL  | CHD-C1D-ND  | -2.76 | 120.92      | 124.80   |
| 4   | M     | 1003    | BCL  | CBC-CAC-C3C | -2.76 | 107.56      | 113.41   |
| 4   | S     | 2001    | BCL  | CHA-C1A-NA  | -2.75 | 120.15      | 126.39   |
| 6   | L     | 1009[A] | U10  | C20-C19-C21 | -2.74 | 110.46      | 115.23   |
| 4   | L     | 1002    | BCL  | CHD-C1D-ND  | -2.74 | 120.94      | 124.80   |
| 5   | M     | 1005    | BPH  | CMB-C2B-C3B | 2.74  | 130.15      | 124.68   |
| 4   | M     | 1003    | BCL  | CHD-C1D-ND  | -2.73 | 120.96      | 124.80   |
| 6   | S     | 2008    | U10  | C1-C6-C5    | -2.73 | 116.97      | 119.62   |
| 5   | L     | 1006    | BPH  | C2B-C1B-NB  | 2.72  | 111.40      | 109.43   |
| 4   | L     | 1002    | BCL  | CAC-C3C-C4C | -2.72 | 106.54      | 112.58   |
| 4   | S     | 2003    | BCL  | C4D-C3D-CAD | -2.72 | 105.15      | 108.11   |
| 5   | M     | 1005    | BPH  | CAA-C2A-C3A | -2.71 | 105.68      | 113.00   |
| 4   | L     | 1002    | BCL  | C11-C12-C13 | -2.69 | 107.01      | 115.97   |
| 4   | R     | 2002    | BCL  | C1-C2-C3    | -2.69 | 121.79      | 126.20   |
| 6   | L     | 1009[B] | U10  | C17-C18-C19 | 2.68  | 133.76      | 127.62   |
| 5   | M     | 1005    | BPH  | C2B-C1B-NB  | 2.67  | 111.36      | 109.43   |
| 6   | L     | 1009[B] | U10  | C16-C14-C13 | 2.67  | 127.15      | 121.17   |
| 6   | L     | 1009[A] | U10  | C16-C14-C13 | 2.65  | 127.12      | 121.17   |
| 6   | S     | 2008    | U10  | C20-C19-C21 | -2.64 | 110.64      | 115.23   |
| 4   | S     | 2004    | BCL  | CHD-C1D-ND  | -2.64 | 121.08      | 124.80   |
| 4   | M     | 1003    | BCL  | CGD-CBD-CAD | -2.64 | 102.31      | 110.85   |
| 4   | L     | 1004    | BCL  | CHA-C1A-NA  | -2.64 | 120.42      | 126.39   |
| 5   | M     | 1005    | BPH  | O2A-CGA-O1A | -2.63 | 117.04      | 123.63   |
| 4   | S     | 2003    | BCL  | CHD-C1D-ND  | -2.63 | 121.10      | 124.80   |
| 4   | S     | 2003    | BCL  | CBC-CAC-C3C | -2.63 | 107.83      | 113.41   |
| 5   | R     | 2006    | BPH  | CMB-C2B-C3B | 2.63  | 129.93      | 124.68   |
| 4   | R     | 2002    | BCL  | O1D-CGD-CBD | 2.62  | 129.69      | 124.52   |
| 4   | L     | 1002    | BCL  | CAA-C2A-C3A | -2.62 | 105.92      | 113.00   |
| 5   | R     | 2006    | BPH  | O2A-CGA-O1A | -2.60 | 117.12      | 123.63   |
| 4   | R     | 2002    | BCL  | O2D-CGD-CBD | -2.59 | 106.71      | 111.23   |
| 6   | L     | 1009[A] | U10  | C8-C7-C6    | 2.58  | 118.45      | 112.08   |
| 5   | S     | 2005    | BPH  | CAA-C2A-C3A | -2.58 | 106.03      | 113.00   |

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| Mol | Chain | Res     | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-------------|-------|-------------|----------|
| 5   | L     | 1006    | BPH  | O2A-CGA-O1A | -2.58 | 117.18      | 123.63   |
| 5   | S     | 2005    | BPH  | C1B-NB-C4B  | -2.57 | 105.08      | 108.82   |
| 6   | L     | 1009[A] | U10  | C7-C6-C5    | -2.55 | 115.55      | 118.52   |
| 4   | S     | 2004    | BCL  | C4D-C3D-CAD | -2.55 | 105.34      | 108.11   |
| 5   | L     | 1006    | BPH  | OBD-CAD-CBD | -2.54 | 122.09      | 125.82   |
| 6   | S     | 2008    | U10  | C17-C18-C19 | 2.54  | 133.44      | 127.62   |
| 4   | R     | 2002    | BCL  | C4D-C3D-CAD | -2.54 | 105.35      | 108.11   |
| 5   | M     | 1005    | BPH  | C4C-C3C-C2C | 2.54  | 105.25      | 102.84   |
| 6   | M     | 1008    | U10  | C1-C6-C5    | -2.52 | 117.17      | 119.62   |
| 5   | M     | 1005    | BPH  | CMD-C2D-C3D | 2.49  | 129.67      | 124.68   |
| 4   | S     | 2004    | BCL  | C7-C6-C5    | -2.49 | 106.64      | 113.26   |
| 5   | S     | 2005    | BPH  | CMB-C2B-C3B | 2.48  | 129.64      | 124.68   |
| 5   | R     | 2006    | BPH  | C7-C6-C5    | -2.48 | 106.65      | 113.26   |
| 8   | M     | 1010    | SPO  | C20-C19-C17 | -2.48 | 123.80      | 127.28   |
| 5   | R     | 2006    | BPH  | C1B-NB-C4B  | -2.48 | 105.21      | 108.82   |
| 4   | S     | 2001    | BCL  | C4D-C3D-CAD | -2.47 | 105.42      | 108.11   |
| 4   | S     | 2003    | BCL  | C2C-C3C-C4C | 2.46  | 105.02      | 101.34   |
| 6   | S     | 2008    | U10  | C16-C14-C13 | 2.45  | 126.66      | 121.17   |
| 6   | S     | 2008    | U10  | C6-C1-C2    | 2.43  | 121.09      | 119.17   |
| 5   | L     | 1006    | BPH  | CMA-C3A-C2A | -2.43 | 104.75      | 114.13   |
| 4   | S     | 2001    | BCL  | CAC-C3C-C4C | -2.42 | 107.21      | 112.58   |
| 6   | L     | 1009[A] | U10  | C17-C18-C19 | 2.42  | 133.17      | 127.62   |
| 4   | L     | 1002    | BCL  | C2C-C3C-C4C | 2.42  | 104.96      | 101.34   |
| 6   | M     | 1008    | U10  | C6-C1-C2    | 2.42  | 121.08      | 119.17   |
| 5   | M     | 1005    | BPH  | OBD-CAD-CBD | -2.42 | 122.28      | 125.82   |
| 4   | R     | 2002    | BCL  | C16-C15-C13 | -2.41 | 107.95      | 115.97   |
| 5   | L     | 1006    | BPH  | CAA-C2A-C3A | -2.40 | 106.51      | 113.00   |
| 4   | M     | 1003    | BCL  | C2C-C3C-C4C | 2.39  | 104.92      | 101.34   |
| 4   | M     | 1003    | BCL  | C11-C10-C8  | -2.39 | 108.02      | 115.97   |
| 4   | L     | 1002    | BCL  | C12-C11-C10 | -2.37 | 102.65      | 113.28   |
| 4   | S     | 2001    | BCL  | C1-C2-C3    | -2.36 | 122.94      | 126.76   |
| 4   | S     | 2003    | BCL  | CGD-CBD-CAD | -2.36 | 103.21      | 110.85   |
| 4   | R     | 2002    | BCL  | CBC-CAC-C3C | -2.35 | 108.43      | 113.41   |
| 4   | M     | 1003    | BCL  | C4D-C3D-CAD | -2.34 | 105.56      | 108.11   |
| 5   | S     | 2005    | BPH  | CMD-C2D-C3D | 2.34  | 129.35      | 124.68   |
| 6   | R     | 2009[A] | U10  | C6-C1-C2    | 2.34  | 121.01      | 119.17   |
| 4   | M     | 1003    | BCL  | CHD-C1D-C2D | 2.33  | 130.34      | 125.49   |
| 6   | R     | 2009[B] | U10  | C6-C1-C2    | 2.32  | 121.00      | 119.17   |
| 4   | S     | 2003    | BCL  | CAA-C2A-C3A | -2.32 | 106.73      | 113.00   |
| 4   | L     | 1004    | BCL  | C4D-C3D-CAD | -2.31 | 105.59      | 108.11   |
| 4   | L     | 1004    | BCL  | C12-C11-C10 | -2.30 | 102.95      | 113.28   |
| 4   | S     | 2003    | BCL  | CHD-C1D-C2D | 2.29  | 130.25      | 125.49   |

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| Mol | Chain | Res     | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-------------|-------|-------------|----------|
| 5   | M     | 1005    | BPH  | C4A-C3A-C2A | 2.29  | 105.01      | 102.84   |
| 5   | M     | 1005    | BPH  | CMA-C3A-C2A | -2.28 | 105.31      | 114.13   |
| 5   | R     | 2006    | BPH  | CAA-C2A-C3A | -2.28 | 106.84      | 113.00   |
| 4   | S     | 2004    | BCL  | CMD-C2D-C3D | 2.28  | 132.91      | 127.69   |
| 4   | R     | 2002    | BCL  | C2C-C3C-C4C | 2.27  | 104.74      | 101.34   |
| 4   | L     | 1002    | BCL  | CMA-C3A-C2A | -2.26 | 105.22      | 113.98   |
| 5   | S     | 2005    | BPH  | OBD-CAD-CBD | -2.25 | 122.53      | 125.82   |
| 4   | R     | 2002    | BCL  | CHD-C1D-C2D | 2.24  | 130.15      | 125.49   |
| 6   | R     | 2009[A] | U10  | C4-C3-C2    | -2.24 | 116.59      | 120.69   |
| 5   | S     | 2005    | BPH  | O2A-CGA-O1A | -2.23 | 118.04      | 123.63   |
| 4   | L     | 1001    | BCL  | C4D-C3D-CAD | -2.23 | 105.68      | 108.11   |
| 4   | L     | 1001    | BCL  | CMD-C2D-C3D | 2.22  | 132.78      | 127.69   |
| 5   | R     | 2006    | BPH  | CMD-C2D-C3D | 2.22  | 129.12      | 124.68   |
| 4   | M     | 1003    | BCL  | O2A-CGA-O1A | -2.21 | 118.11      | 123.63   |
| 4   | R     | 2002    | BCL  | C4-C3-C5    | 2.21  | 119.06      | 115.23   |
| 5   | L     | 1006    | BPH  | C1B-NB-C4B  | -2.20 | 105.61      | 108.82   |
| 4   | M     | 1003    | BCL  | C7-C6-C5    | -2.20 | 107.41      | 113.26   |
| 4   | S     | 2001    | BCL  | CHD-C1D-C2D | 2.19  | 130.05      | 125.49   |
| 4   | S     | 2003    | BCL  | CAC-C3C-C4C | -2.19 | 107.73      | 112.58   |
| 5   | M     | 1005    | BPH  | C7-C6-C5    | -2.18 | 107.45      | 113.26   |
| 4   | M     | 1003    | BCL  | CAC-C3C-C4C | -2.18 | 107.75      | 112.58   |
| 4   | L     | 1002    | BCL  | CBC-CAC-C3C | -2.18 | 108.80      | 113.41   |
| 4   | S     | 2003    | BCL  | C11-C10-C8  | -2.18 | 108.73      | 115.97   |
| 4   | M     | 1003    | BCL  | CAA-C2A-C3A | -2.17 | 107.13      | 113.00   |
| 6   | R     | 2009[A] | U10  | C7-C6-C5    | -2.17 | 116.00      | 118.52   |
| 6   | L     | 1009[A] | U10  | C4-C3-C2    | -2.16 | 116.72      | 120.69   |
| 8   | M     | 1010    | SPO  | C1-C4-C5    | 2.16  | 118.58      | 112.98   |
| 8   | M     | 1010    | SPO  | C5-C6-C7    | -2.16 | 122.63      | 125.89   |
| 5   | L     | 1006    | BPH  | CMD-C2D-C3D | 2.15  | 128.97      | 124.68   |
| 6   | S     | 2008    | U10  | C4-C3-C2    | -2.14 | 116.76      | 120.69   |
| 6   | M     | 1008    | U10  | C16-C14-C13 | 2.14  | 125.97      | 121.17   |
| 4   | L     | 1004    | BCL  | CMD-C2D-C3D | 2.14  | 132.60      | 127.69   |
| 4   | S     | 2003    | BCL  | C7-C6-C5    | -2.14 | 107.56      | 113.26   |
| 6   | L     | 1009[A] | U10  | C6-C1-C2    | 2.14  | 120.86      | 119.17   |
| 6   | L     | 1009[B] | U10  | C3-C2-C1    | 2.13  | 122.32      | 118.10   |
| 4   | M     | 1003    | BCL  | O1D-CGD-CBD | 2.13  | 128.73      | 124.52   |
| 4   | S     | 2001    | BCL  | CAA-C2A-C1A | 2.13  | 118.96      | 111.97   |
| 4   | S     | 2003    | BCL  | C16-C15-C13 | -2.13 | 108.89      | 115.97   |
| 4   | S     | 2003    | BCL  | CBA-CAA-C2A | 2.13  | 120.13      | 113.79   |
| 8   | S     | 2010    | SPO  | C1-C4-C5    | 2.13  | 118.51      | 112.98   |
| 8   | S     | 2010    | SPO  | C9-C10-C11  | -2.12 | 117.06      | 123.20   |
| 4   | M     | 1003    | BCL  | C16-C15-C13 | -2.11 | 108.94      | 115.97   |

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| Mol | Chain | Res     | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|---------|------|-------------|-------|-------------|----------|
| 9   | M     | 1011    | LDA  | C9-C8-C7    | -2.11 | 103.72      | 114.37   |
| 4   | L     | 1001    | BCL  | C3D-C2D-C1D | -2.10 | 102.96      | 105.83   |
| 4   | L     | 1002    | BCL  | CMD-C2D-C3D | 2.09  | 132.49      | 127.69   |
| 4   | L     | 1004    | BCL  | C16-C15-C13 | -2.09 | 109.01      | 115.97   |
| 6   | L     | 1009[B] | U10  | C6-C1-C2    | 2.09  | 120.82      | 119.17   |
| 4   | S     | 2004    | BCL  | C12-C11-C10 | -2.09 | 103.92      | 113.28   |
| 6   | M     | 1008    | U10  | C17-C18-C19 | 2.08  | 132.39      | 127.62   |
| 5   | S     | 2005    | BPH  | C6-C5-C3    | 2.08  | 123.57      | 113.70   |
| 4   | S     | 2001    | BCL  | CMD-C2D-C3D | 2.08  | 132.45      | 127.69   |
| 9   | M     | 1011    | LDA  | CM2-N1-C1   | 2.08  | 114.59      | 110.23   |
| 6   | R     | 2009[B] | U10  | C4-C3-C2    | -2.07 | 116.89      | 120.69   |
| 6   | M     | 1008    | U10  | C21-C19-C18 | 2.07  | 125.81      | 121.17   |
| 6   | M     | 1008    | U10  | C3-C2-C1    | 2.06  | 122.17      | 118.10   |
| 5   | R     | 2006    | BPH  | C2B-C1B-NB  | 2.05  | 110.91      | 109.43   |
| 4   | M     | 1003    | BCL  | O2A-CGA-CBA | 2.05  | 118.07      | 111.83   |
| 8   | S     | 2010    | SPO  | C13-C12-C11 | 2.04  | 121.20      | 118.09   |
| 4   | S     | 2003    | BCL  | O1D-CGD-CBD | 2.04  | 128.53      | 124.52   |
| 4   | S     | 2003    | BCL  | C12-C11-C10 | -2.03 | 104.17      | 113.28   |
| 4   | L     | 1002    | BCL  | CHD-C1D-C2D | 2.03  | 129.71      | 125.49   |
| 8   | S     | 2010    | SPO  | C27-C26-C25 | -2.03 | 117.31      | 123.20   |
| 5   | L     | 1006    | BPH  | C4A-C3A-C2A | 2.03  | 104.77      | 102.84   |
| 6   | M     | 1008    | U10  | C4-C3-C2    | -2.03 | 116.97      | 120.69   |
| 4   | M     | 1003    | BCL  | C3D-C2D-C1D | -2.03 | 103.06      | 105.83   |
| 6   | R     | 2009[B] | U10  | C1M-C1-C6   | -2.03 | 121.12      | 124.45   |
| 6   | S     | 2008    | U10  | C21-C19-C18 | 2.03  | 125.72      | 121.17   |
| 6   | L     | 1009[B] | U10  | C4-C3-C2    | -2.02 | 116.98      | 120.69   |
| 5   | R     | 2006    | BPH  | OBD-CAD-CBD | -2.02 | 122.86      | 125.82   |
| 4   | S     | 2004    | BCL  | CHD-C1D-C2D | 2.02  | 129.68      | 125.49   |
| 6   | M     | 1008    | U10  | C31-C29-C30 | -2.02 | 109.95      | 114.59   |
| 5   | R     | 2006    | BPH  | C5-C3-C2    | -2.01 | 116.65      | 121.17   |
| 4   | L     | 1004    | BCL  | C7-C6-C5    | -2.01 | 107.90      | 113.26   |
| 8   | S     | 2010    | SPO  | O1-C1-C2    | 2.01  | 122.80      | 108.97   |
| 6   | L     | 1009[B] | U10  | C7-C8-C9    | 2.00  | 130.28      | 126.83   |

All (5) chirality outliers are listed below:

| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 5   | L     | 1006 | BPH  | C13  |
| 5   | L     | 1006 | BPH  | C8   |
| 5   | M     | 1005 | BPH  | C8   |
| 5   | R     | 2006 | BPH  | C13  |
| 5   | R     | 2006 | BPH  | C8   |

All (143) torsion outliers are listed below:

| Mol | Chain | Res     | Type | Atoms           |
|-----|-------|---------|------|-----------------|
| 4   | L     | 1004    | BCL  | C1A-C2A-CAA-CBA |
| 4   | L     | 1004    | BCL  | C3A-C2A-CAA-CBA |
| 4   | S     | 2001    | BCL  | C1A-C2A-CAA-CBA |
| 5   | L     | 1006    | BPH  | C4C-C3C-CAC-CBC |
| 5   | R     | 2006    | BPH  | CBD-CGD-O2D-CED |
| 5   | S     | 2005    | BPH  | C1-C2-C3-C5     |
| 8   | M     | 1010    | SPO  | C3-C1-O1-CM1    |
| 8   | M     | 1010    | SPO  | C4-C5-C6-C7     |
| 8   | M     | 1010    | SPO  | C36-C37-C38-C39 |
| 8   | M     | 1010    | SPO  | C36-C37-C38-C40 |
| 8   | S     | 2010    | SPO  | C3-C1-O1-CM1    |
| 8   | S     | 2010    | SPO  | C4-C5-C6-C7     |
| 8   | S     | 2010    | SPO  | C36-C37-C38-C39 |
| 8   | S     | 2010    | SPO  | C36-C37-C38-C40 |
| 5   | S     | 2005    | BPH  | CBD-CGD-O2D-CED |
| 5   | R     | 2006    | BPH  | O1D-CGD-O2D-CED |
| 4   | R     | 2002    | BCL  | C4-C3-C5-C6     |
| 4   | R     | 2002    | BCL  | C2-C3-C5-C6     |
| 5   | M     | 1005    | BPH  | CBD-CGD-O2D-CED |
| 4   | M     | 1003    | BCL  | C4-C3-C5-C6     |
| 4   | S     | 2003    | BCL  | C4-C3-C5-C6     |
| 6   | L     | 1009[B] | U10  | C9-C11-C12-C13  |
| 6   | L     | 1009[B] | U10  | C14-C16-C17-C18 |
| 6   | M     | 1008    | U10  | C24-C26-C27-C28 |
| 8   | M     | 1010    | SPO  | C33-C35-C36-C37 |
| 4   | M     | 1003    | BCL  | C2-C3-C5-C6     |
| 4   | S     | 2003    | BCL  | C2-C3-C5-C6     |
| 4   | S     | 2003    | BCL  | C15-C16-C17-C18 |
| 8   | S     | 2010    | SPO  | C33-C35-C36-C37 |
| 5   | L     | 1006    | BPH  | C8-C10-C11-C12  |
| 5   | L     | 1006    | BPH  | C10-C11-C12-C13 |
| 5   | S     | 2005    | BPH  | O1D-CGD-O2D-CED |
| 5   | R     | 2006    | BPH  | C10-C11-C12-C13 |
| 4   | L     | 1002    | BCL  | C15-C16-C17-C18 |
| 5   | M     | 1005    | BPH  | O1D-CGD-O2D-CED |
| 5   | S     | 2005    | BPH  | O2A-C1-C2-C3    |
| 5   | R     | 2006    | BPH  | C8-C10-C11-C12  |
| 4   | S     | 2001    | BCL  | C3A-C2A-CAA-CBA |
| 4   | M     | 1003    | BCL  | C3-C5-C6-C7     |
| 9   | M     | 1011    | LDA  | C4-C5-C6-C7     |
| 8   | M     | 1010    | SPO  | C1-C4-C5-C6     |
| 8   | S     | 2010    | SPO  | C1-C4-C5-C6     |

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| Mol | Chain | Res     | Type | Atoms           |
|-----|-------|---------|------|-----------------|
| 5   | M     | 1005    | BPH  | C4-C3-C5-C6     |
| 5   | L     | 1006    | BPH  | C2C-C3C-CAC-CBC |
| 4   | L     | 1004    | BCL  | C2A-CAA-CBA-CGA |
| 4   | S     | 2004    | BCL  | C1A-C2A-CAA-CBA |
| 4   | M     | 1003    | BCL  | C11-C10-C8-C7   |
| 4   | S     | 2003    | BCL  | C11-C10-C8-C7   |
| 4   | S     | 2004    | BCL  | C12-C13-C15-C16 |
| 5   | R     | 2006    | BPH  | C12-C13-C15-C16 |
| 5   | R     | 2006    | BPH  | C14-C13-C15-C16 |
| 5   | M     | 1005    | BPH  | C2-C3-C5-C6     |
| 4   | S     | 2004    | BCL  | C15-C16-C17-C18 |
| 5   | L     | 1006    | BPH  | O2A-C1-C2-C3    |
| 5   | M     | 1005    | BPH  | O2A-C1-C2-C3    |
| 5   | R     | 2006    | BPH  | O2A-C1-C2-C3    |
| 4   | S     | 2003    | BCL  | C13-C15-C16-C17 |
| 4   | S     | 2003    | BCL  | C11-C12-C13-C14 |
| 4   | S     | 2004    | BCL  | C14-C13-C15-C16 |
| 4   | L     | 1002    | BCL  | C12-C13-C15-C16 |
| 4   | R     | 2002    | BCL  | C12-C13-C15-C16 |
| 4   | S     | 2003    | BCL  | C11-C12-C13-C15 |
| 5   | L     | 1006    | BPH  | C12-C13-C15-C16 |
| 8   | M     | 1010    | SPO  | C19-C20-C21-C22 |
| 6   | L     | 1009[A] | U10  | C14-C16-C17-C18 |
| 8   | S     | 2010    | SPO  | C20-C21-C22-C23 |
| 9   | M     | 1011    | LDA  | C2-C3-C4-C5     |
| 5   | M     | 1005    | BPH  | C5-C6-C7-C8     |
| 9   | M     | 1011    | LDA  | C1-C2-C3-C4     |
| 6   | S     | 2008    | U10  | C5-C4-O4-C4M    |
| 6   | L     | 1009[A] | U10  | C12-C11-C9-C10  |
| 6   | L     | 1009[A] | U10  | C15-C14-C16-C17 |
| 6   | L     | 1009[A] | U10  | C5-C6-C7-C8     |
| 4   | L     | 1004    | BCL  | C11-C10-C8-C9   |
| 4   | R     | 2002    | BCL  | C14-C13-C15-C16 |
| 5   | L     | 1006    | BPH  | C14-C13-C15-C16 |
| 9   | M     | 1011    | LDA  | C2-C1-N1-CM1    |
| 9   | M     | 1011    | LDA  | C2-C1-N1-CM2    |
| 6   | L     | 1009[A] | U10  | C13-C14-C16-C17 |
| 5   | S     | 2005    | BPH  | C2-C3-C5-C6     |
| 4   | L     | 1004    | BCL  | C11-C10-C8-C7   |
| 4   | M     | 1003    | BCL  | C11-C12-C13-C15 |
| 4   | S     | 2004    | BCL  | C11-C10-C8-C7   |
| 4   | S     | 2004    | BCL  | C11-C12-C13-C15 |

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| Mol | Chain | Res     | Type | Atoms           |
|-----|-------|---------|------|-----------------|
| 4   | S     | 2003    | BCL  | C3-C5-C6-C7     |
| 4   | L     | 1002    | BCL  | C14-C13-C15-C16 |
| 4   | S     | 2004    | BCL  | C11-C10-C8-C9   |
| 9   | M     | 1011    | LDA  | C2-C1-N1-O1     |
| 8   | S     | 2010    | SPO  | C4-C1-O1-CM1    |
| 4   | L     | 1004    | BCL  | CHA-CBD-CGD-O2D |
| 6   | L     | 1009[A] | U10  | C12-C11-C9-C8   |
| 8   | M     | 1010    | SPO  | C20-C21-C22-C23 |
| 4   | L     | 1004    | BCL  | C13-C15-C16-C17 |
| 4   | S     | 2004    | BCL  | C11-C12-C13-C14 |
| 6   | S     | 2008    | U10  | C20-C19-C21-C22 |
| 6   | L     | 1009[B] | U10  | C2-C3-O3-C3M    |
| 8   | M     | 1010    | SPO  | C17-C19-C20-C21 |
| 4   | M     | 1003    | BCL  | C11-C12-C13-C14 |
| 5   | R     | 2006    | BPH  | C16-C17-C18-C20 |
| 6   | S     | 2008    | U10  | C21-C22-C23-C24 |
| 4   | S     | 2003    | BCL  | C5-C6-C7-C8     |
| 4   | R     | 2002    | BCL  | C15-C16-C17-C18 |
| 6   | S     | 2008    | U10  | C18-C19-C21-C22 |
| 8   | M     | 1010    | SPO  | C18-C17-C19-C20 |
| 8   | S     | 2010    | SPO  | C18-C17-C19-C20 |
| 9   | M     | 1011    | LDA  | C6-C7-C8-C9     |
| 5   | S     | 2005    | BPH  | C4-C3-C5-C6     |
| 6   | L     | 1009[B] | U10  | C15-C14-C16-C17 |
| 6   | L     | 1009[A] | U10  | C2-C3-O3-C3M    |
| 6   | M     | 1008    | U10  | C5-C4-O4-C4M    |
| 4   | M     | 1003    | BCL  | C11-C10-C8-C9   |
| 4   | S     | 2003    | BCL  | C11-C10-C8-C9   |
| 4   | S     | 2001    | BCL  | C2B-C3B-CAB-OB  |
| 4   | S     | 2001    | BCL  | C2B-C3B-CAB-CB  |
| 5   | S     | 2005    | BPH  | C1-C2-C3-C4     |
| 4   | M     | 1003    | BCL  | C13-C15-C16-C17 |
| 8   | M     | 1010    | SPO  | C16-C17-C19-C20 |
| 8   | S     | 2010    | SPO  | C16-C17-C19-C20 |
| 4   | M     | 1003    | BCL  | C5-C6-C7-C8     |
| 4   | L     | 1002    | BCL  | C2A-CAA-CBA-CGA |
| 6   | L     | 1009[B] | U10  | C13-C14-C16-C17 |
| 6   | M     | 1008    | U10  | C20-C19-C21-C22 |
| 4   | R     | 2002    | BCL  | C8-C10-C11-C12  |
| 5   | R     | 2006    | BPH  | C16-C17-C18-C19 |
| 5   | S     | 2005    | BPH  | CHA-CBD-CGD-O1D |
| 6   | L     | 1009[A] | U10  | C20-C19-C21-C22 |

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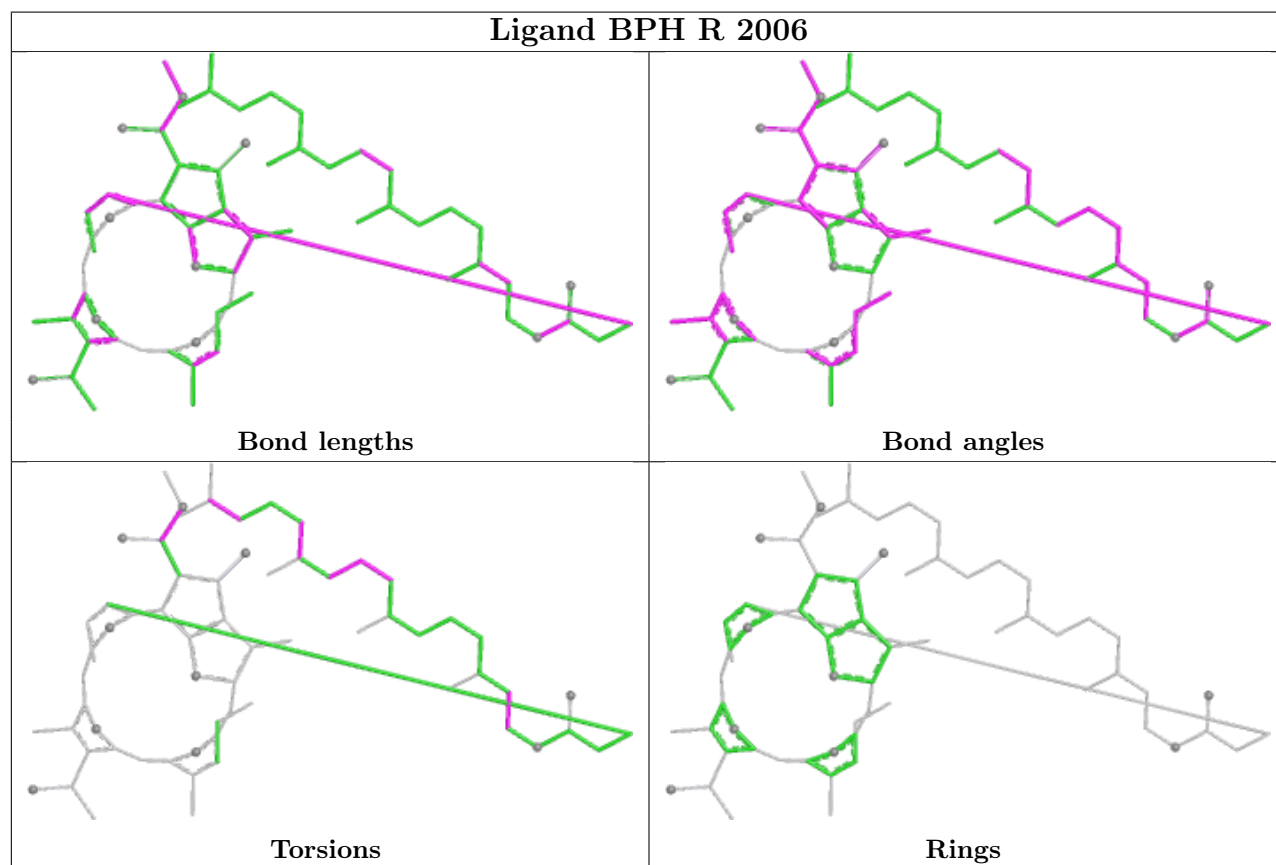
| Mol | Chain | Res     | Type | Atoms           |
|-----|-------|---------|------|-----------------|
| 8   | S     | 2010    | SPO  | C17-C19-C20-C21 |
| 4   | S     | 2001    | BCL  | C4B-C3B-CAB-OB  |
| 4   | S     | 2001    | BCL  | C4B-C3B-CAB-CB  |
| 5   | L     | 1006    | BPH  | C6-C7-C8-C9     |
| 4   | S     | 2001    | BCL  | CAA-CBA-CGA-O2A |
| 4   | S     | 2004    | BCL  | C5-C6-C7-C8     |
| 5   | S     | 2005    | BPH  | C2A-CAA-CBA-CGA |
| 4   | R     | 2002    | BCL  | C2A-CAA-CBA-CGA |
| 8   | S     | 2010    | SPO  | C30-C31-C32-C33 |
| 6   | L     | 1009[A] | U10  | C1-C6-C7-C8     |
| 4   | S     | 2001    | BCL  | CAA-CBA-CGA-O1A |
| 6   | M     | 1008    | U10  | C14-C16-C17-C18 |
| 8   | M     | 1010    | SPO  | C30-C31-C32-C33 |
| 4   | L     | 1004    | BCL  | CAD-CBD-CGD-O2D |
| 8   | M     | 1010    | SPO  | C4-C1-O1-CM1    |
| 4   | L     | 1004    | BCL  | C5-C6-C7-C8     |
| 6   | R     | 2009[A] | U10  | C2-C3-O3-C3M    |

There are no ring outliers.

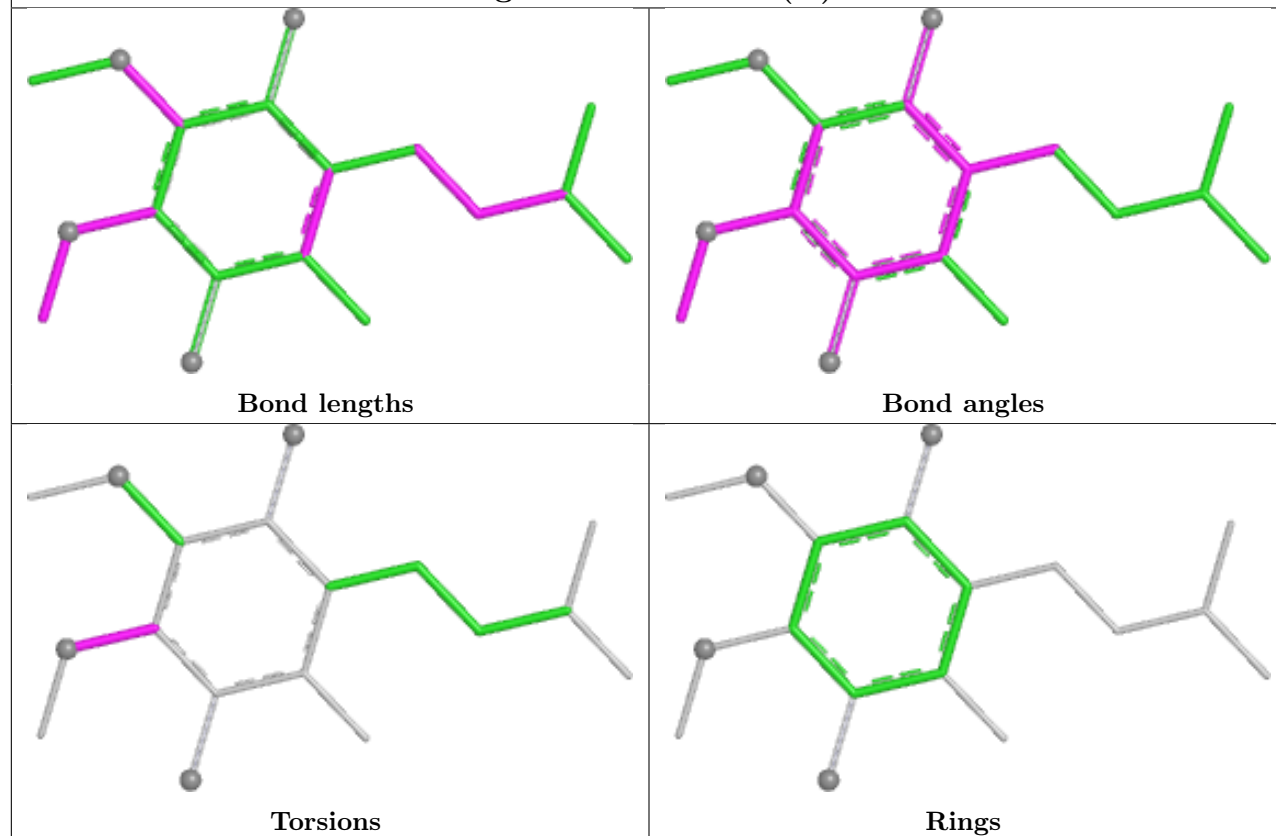
20 monomers are involved in 104 short contacts:

| Mol | Chain | Res     | Type | Clashes | Symm-Clashes |
|-----|-------|---------|------|---------|--------------|
| 5   | R     | 2006    | BPH  | 9       | 0            |
| 6   | R     | 2009[A] | U10  | 1       | 0            |
| 4   | L     | 1002    | BCL  | 11      | 0            |
| 5   | M     | 1005    | BPH  | 1       | 0            |
| 5   | S     | 2005    | BPH  | 6       | 0            |
| 8   | M     | 1010    | SPO  | 6       | 0            |
| 9   | M     | 1011    | LDA  | 2       | 0            |
| 4   | S     | 2003    | BCL  | 16      | 0            |
| 8   | S     | 2010    | SPO  | 2       | 0            |
| 4   | L     | 1001    | BCL  | 11      | 0            |
| 5   | L     | 1006    | BPH  | 5       | 0            |
| 6   | L     | 1009[B] | U10  | 2       | 0            |
| 4   | S     | 2001    | BCL  | 8       | 0            |
| 6   | S     | 2008    | U10  | 1       | 0            |
| 4   | R     | 2002    | BCL  | 10      | 0            |
| 4   | M     | 1003    | BCL  | 21      | 0            |
| 4   | L     | 1004    | BCL  | 9       | 0            |
| 6   | R     | 2009[B] | U10  | 2       | 0            |
| 6   | L     | 1009[A] | U10  | 1       | 0            |
| 4   | S     | 2004    | BCL  | 8       | 0            |

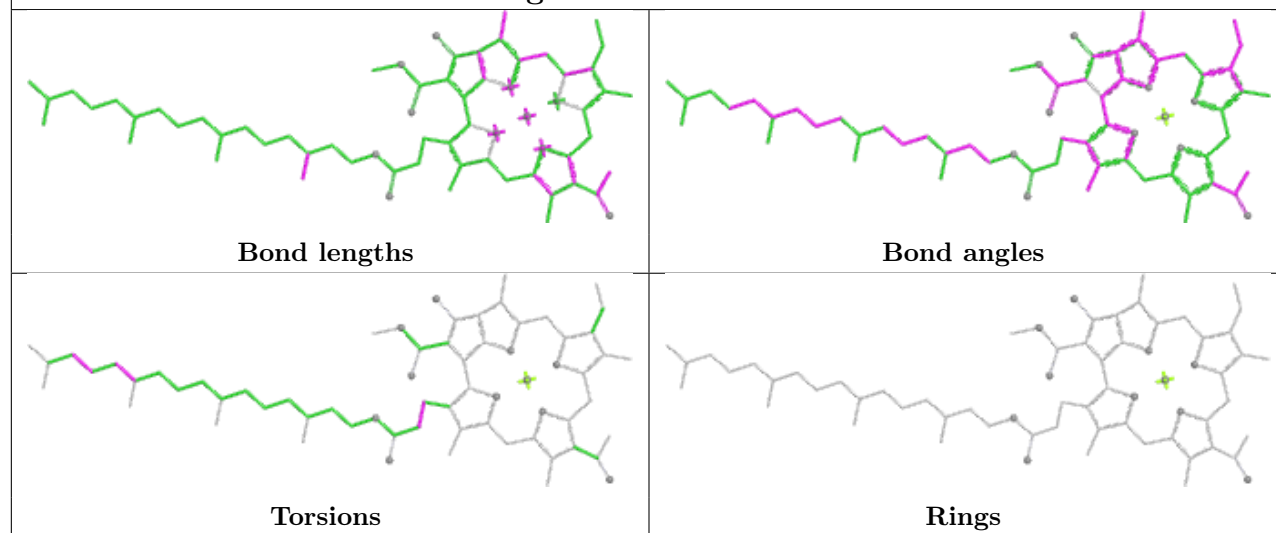
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



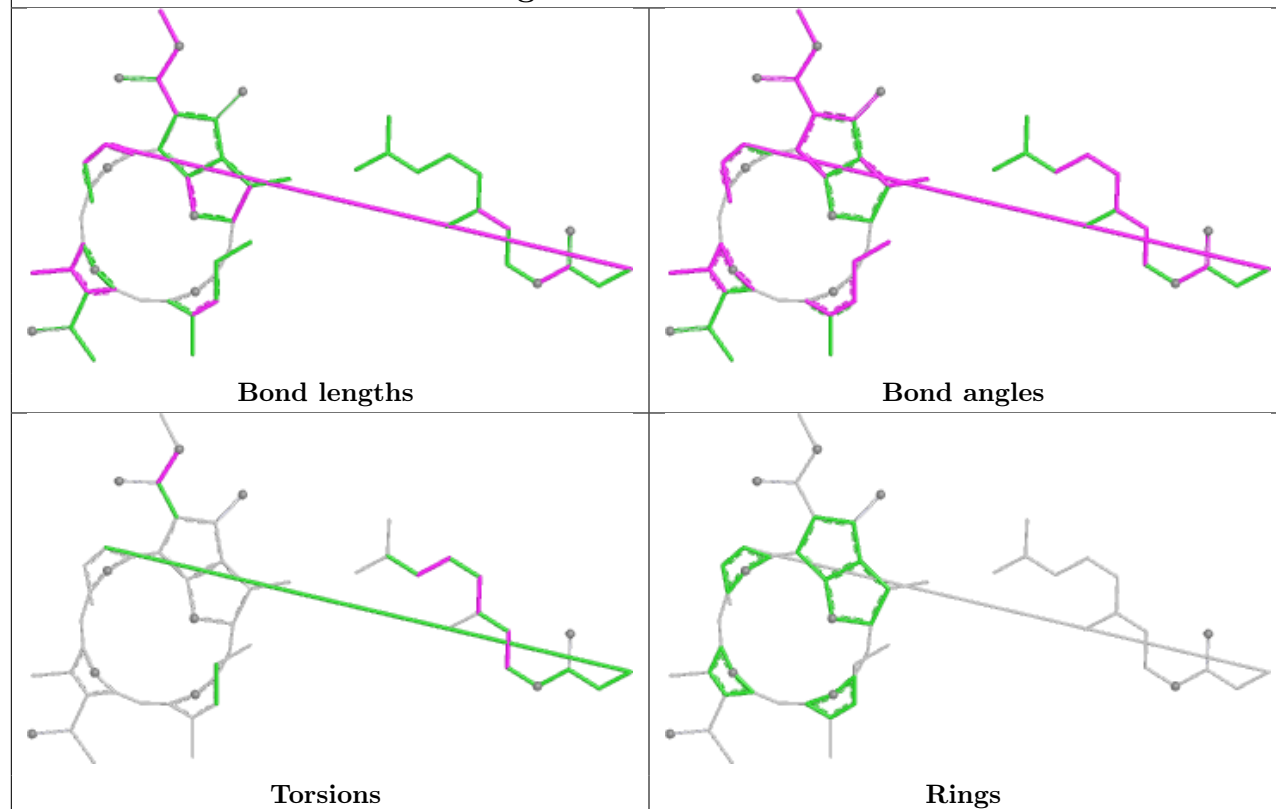
## Ligand U10 R 2009 (A)



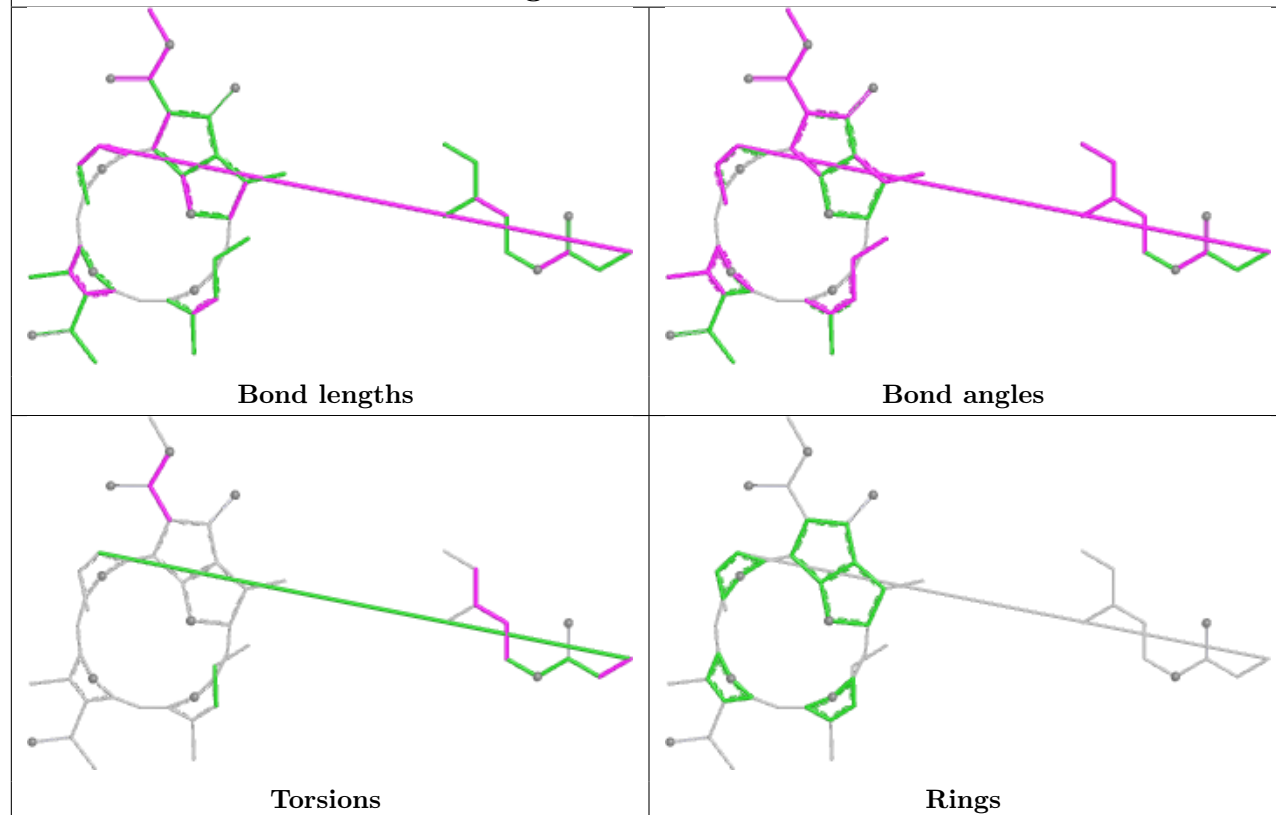
## Ligand BCL L 1002

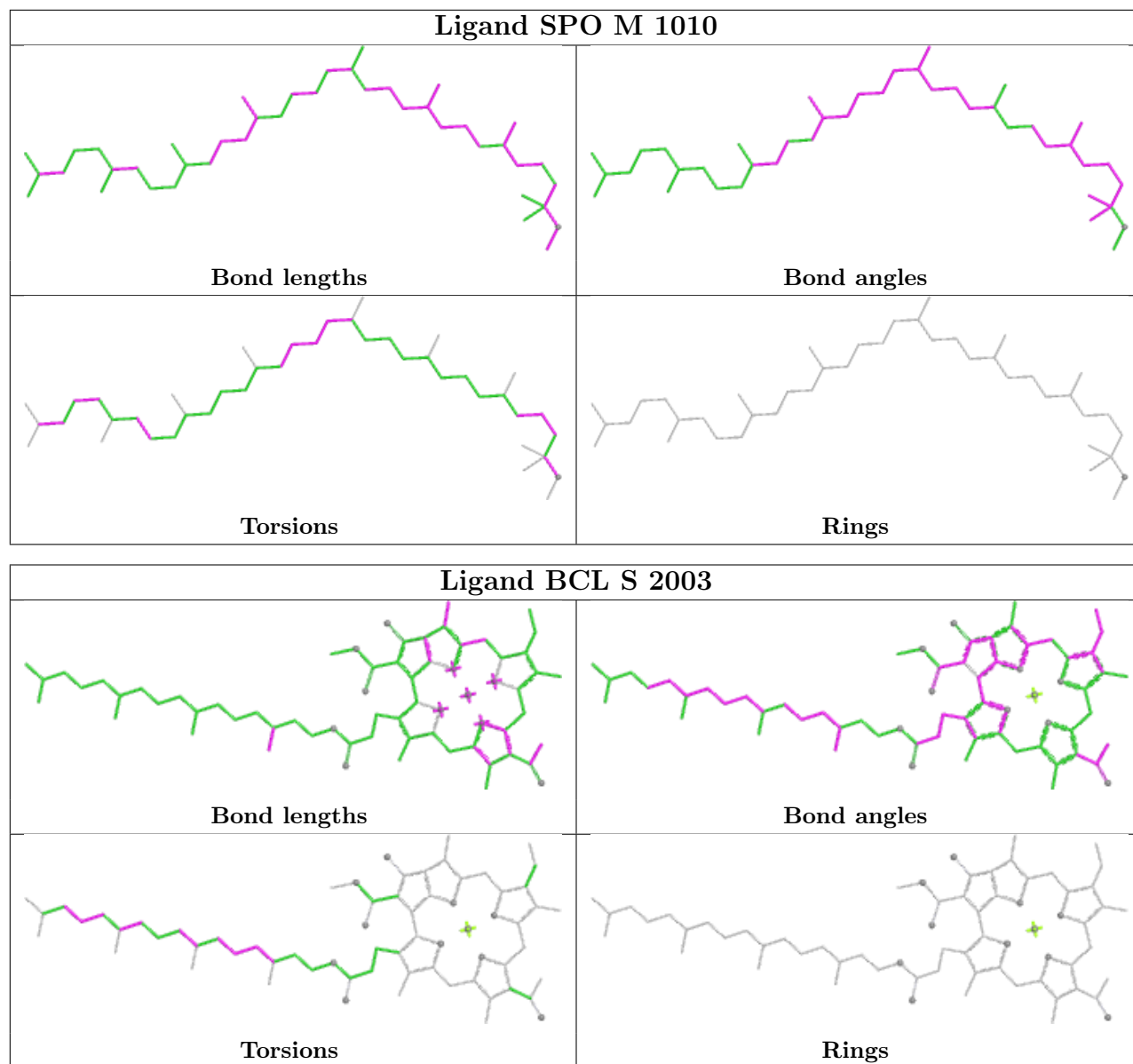


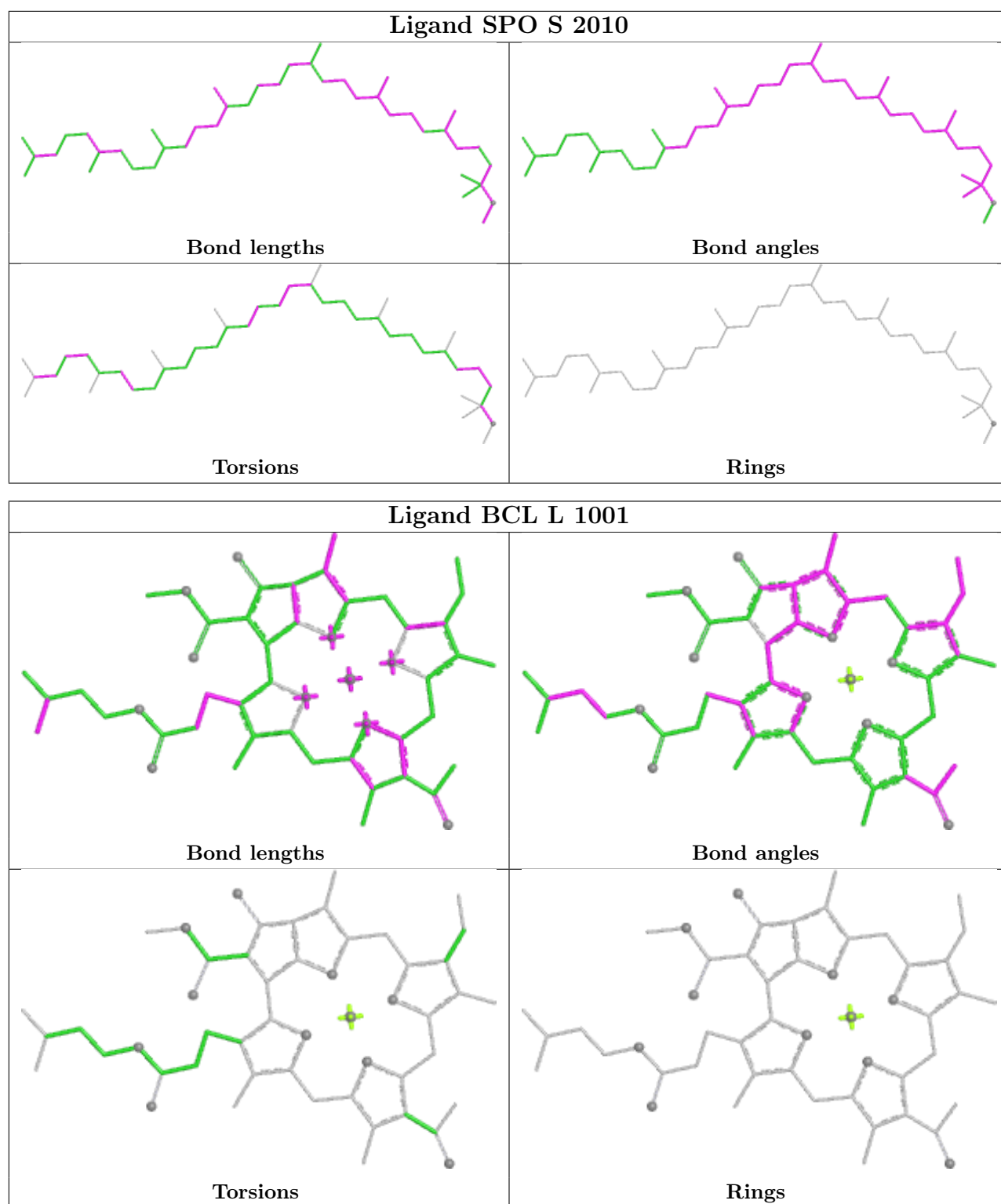
## Ligand BPH M 1005

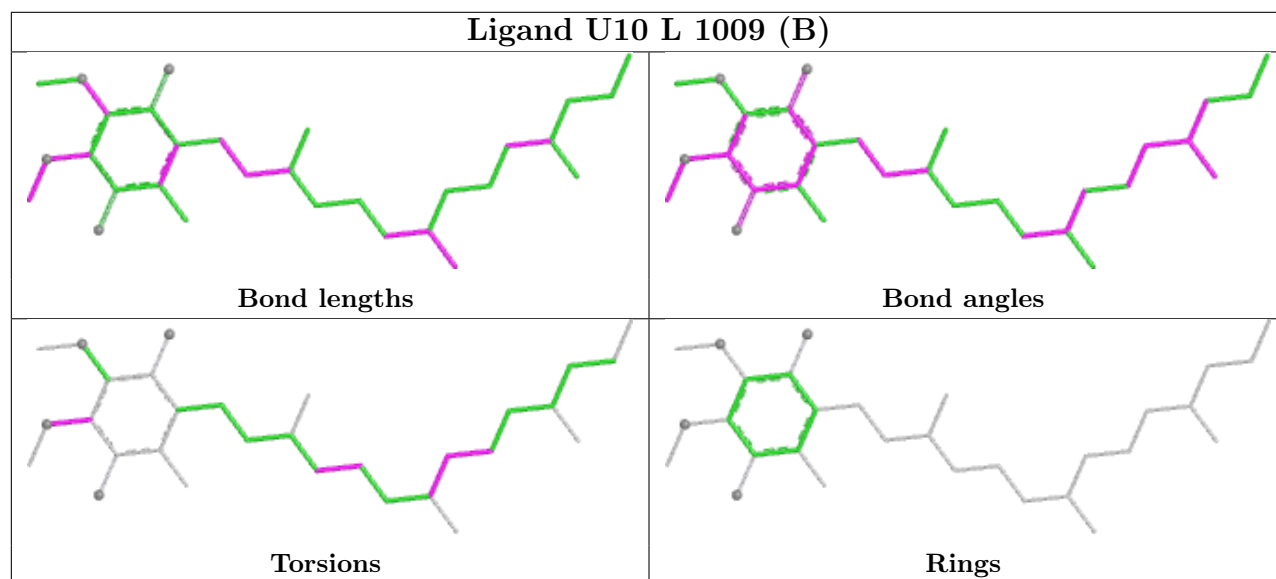
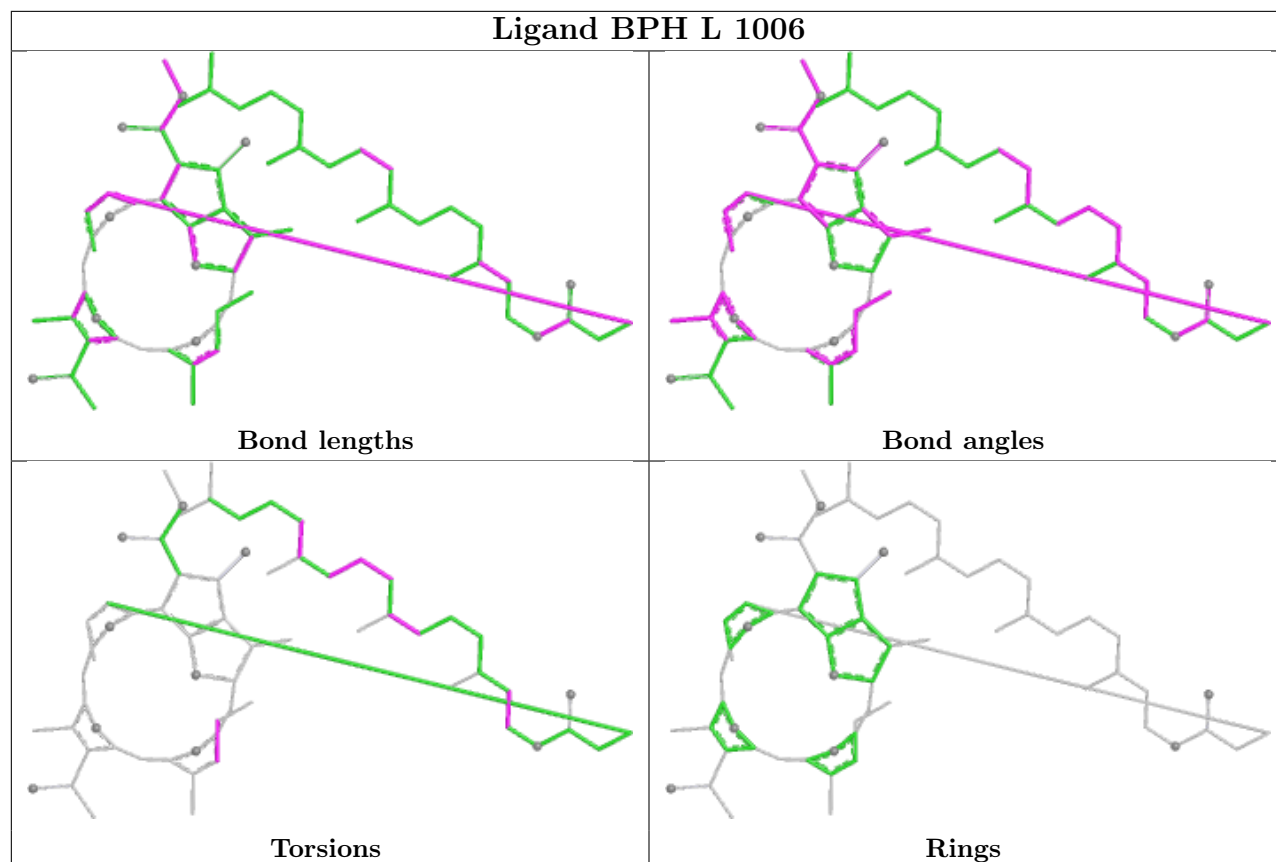


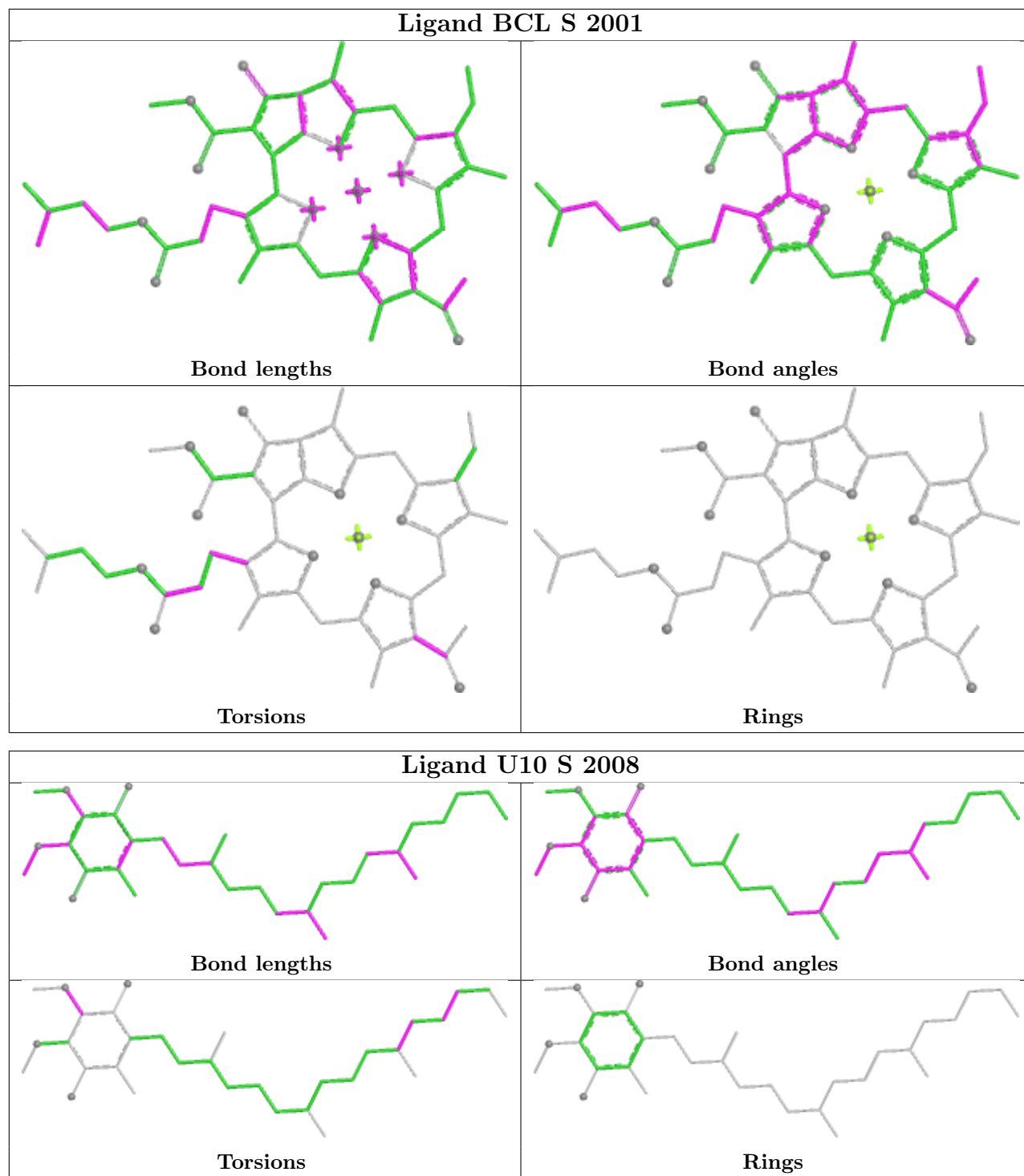
## Ligand BPH S 2005

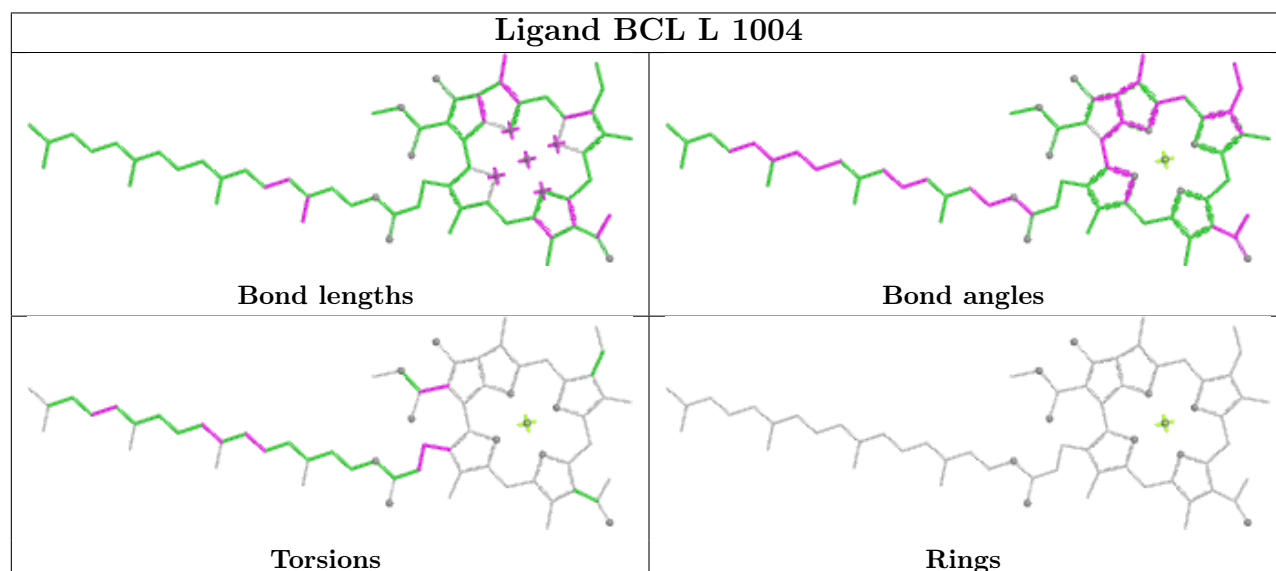
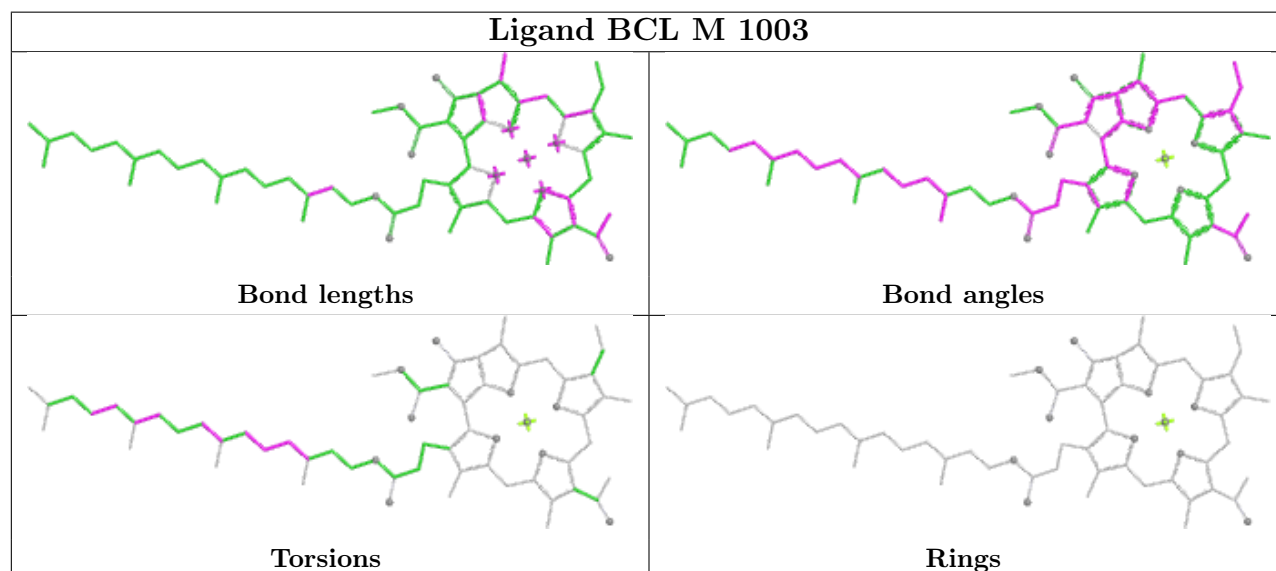
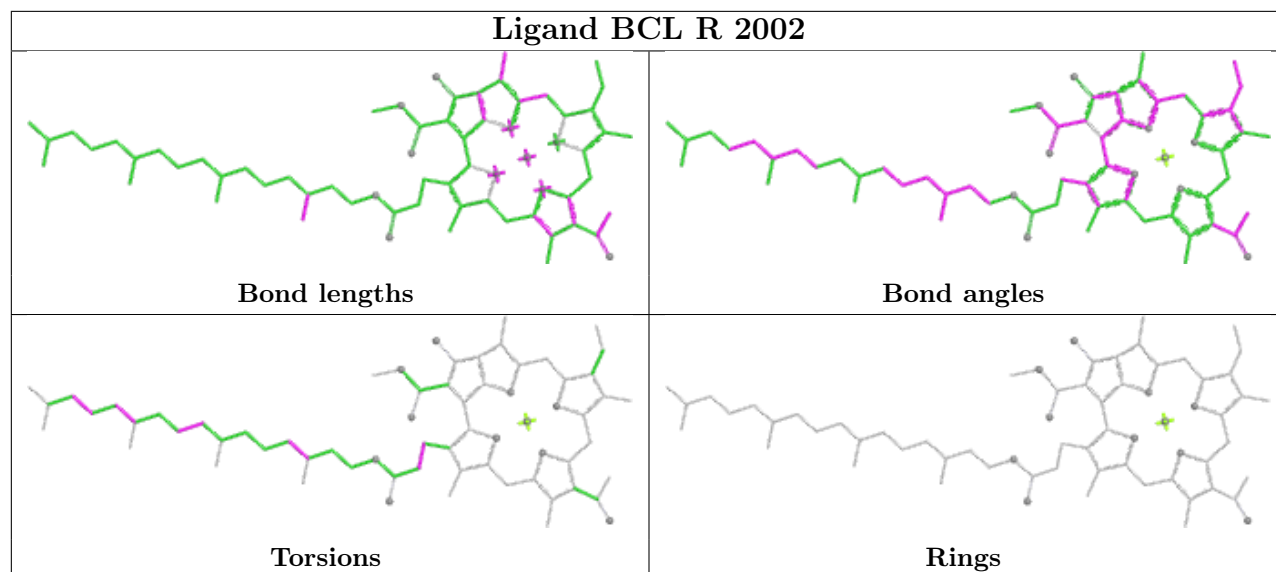


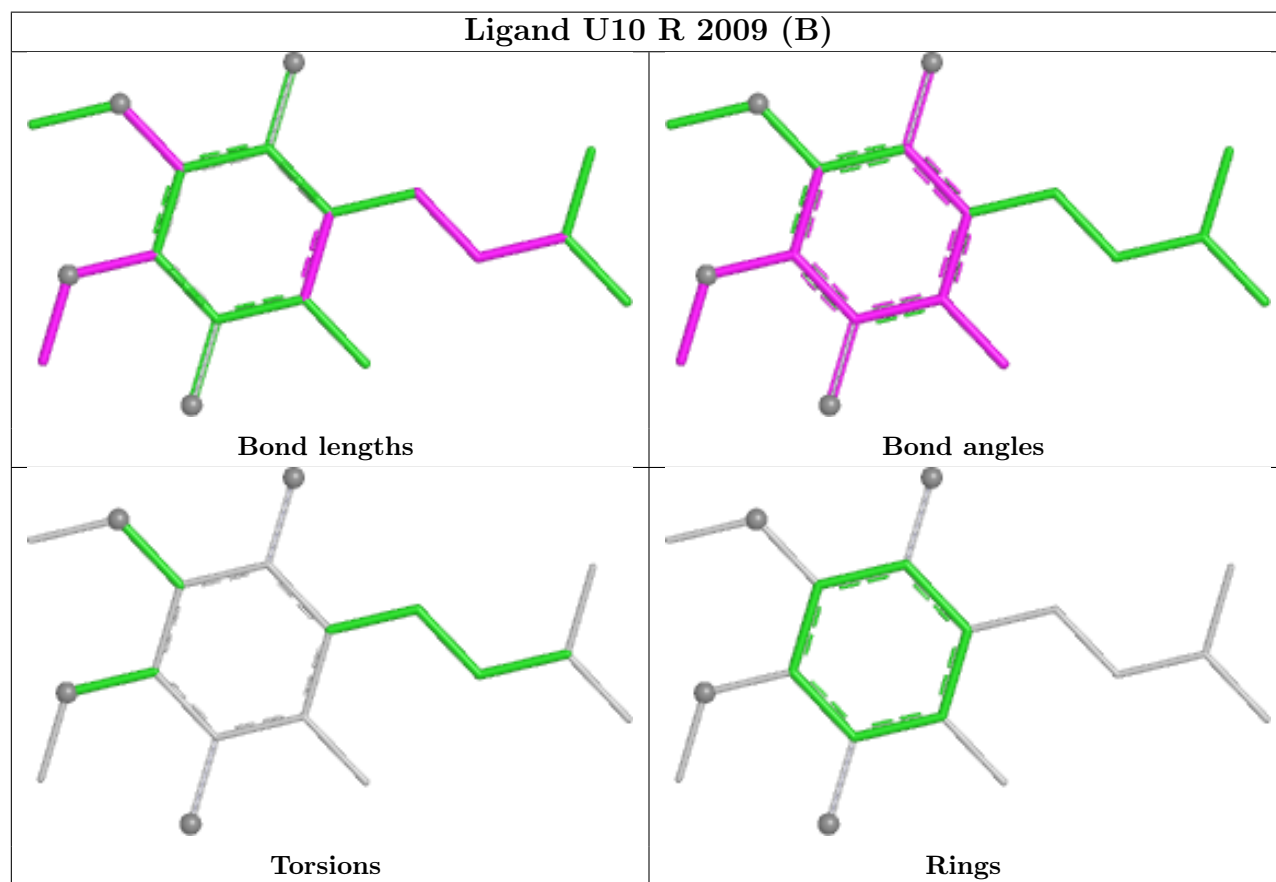
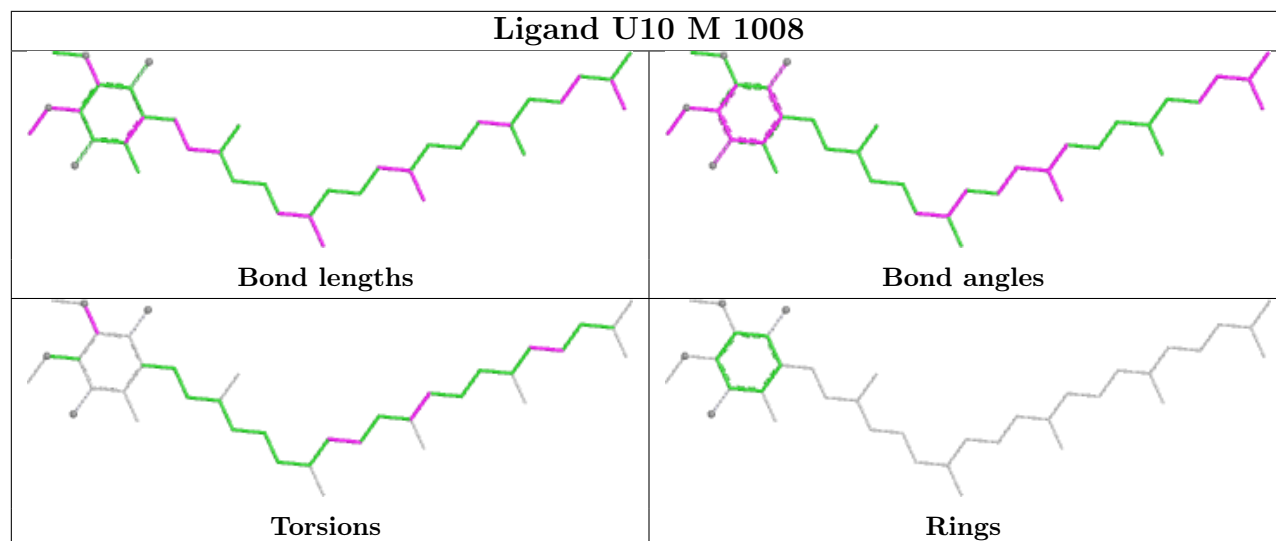


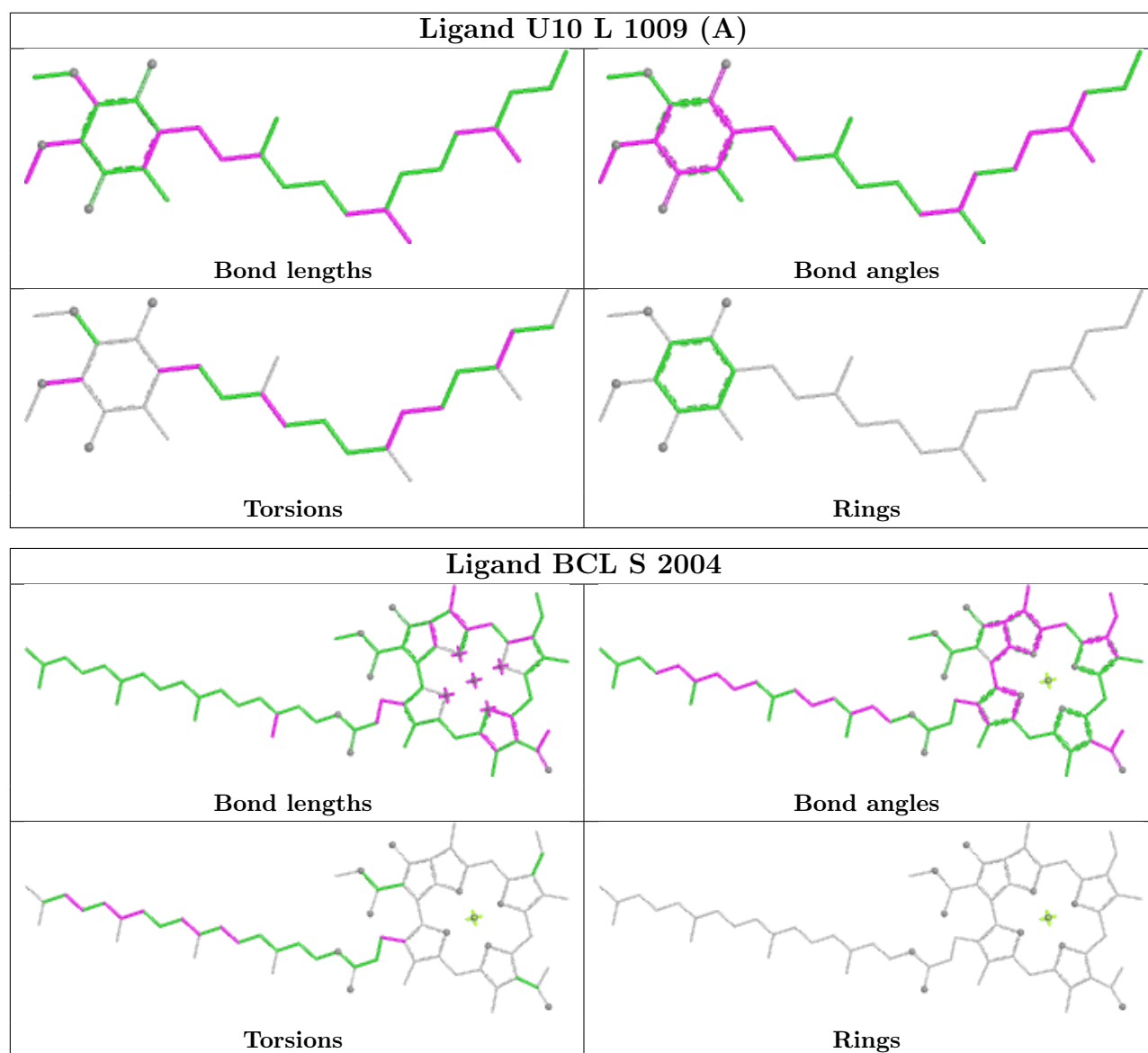












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1   | L     | 281/281 (100%)  | 0.01   | 4 (1%) 73 69  | 23, 42, 61, 77        | 0     |
| 1   | R     | 281/281 (100%)  | 0.42   | 7 (2%) 58 52  | 35, 56, 73, 82        | 0     |
| 2   | M     | 301/307 (98%)   | -0.18  | 3 (0%) 79 76  | 26, 38, 53, 85        | 0     |
| 2   | S     | 299/307 (97%)   | 0.10   | 4 (1%) 75 71  | 37, 50, 59, 89        | 0     |
| 3   | H     | 246/260 (94%)   | 0.02   | 4 (1%) 70 66  | 28, 44, 65, 97        | 0     |
| 3   | T     | 246/260 (94%)   | 0.68   | 19 (7%) 19 15 | 47, 62, 84, 99        | 0     |
| All | All   | 1654/1696 (97%) | 0.16   | 41 (2%) 58 52 | 23, 49, 74, 99        | 0     |

All (41) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | R     | 1   | ALA  | 5.1  |
| 2   | M     | 1   | ALA  | 4.0  |
| 2   | M     | 301 | HIS  | 3.9  |
| 3   | H     | 256 | LEU  | 3.6  |
| 3   | T     | 254 | ALA  | 3.6  |
| 3   | T     | 256 | LEU  | 3.4  |
| 3   | T     | 55  | PRO  | 3.1  |
| 3   | T     | 78  | PRO  | 3.1  |
| 3   | T     | 90  | THR  | 2.9  |
| 2   | S     | 3   | TYR  | 2.9  |
| 3   | T     | 91  | ALA  | 2.9  |
| 3   | T     | 251 | VAL  | 2.8  |
| 3   | T     | 54  | GLY  | 2.7  |
| 2   | S     | 68  | PHE  | 2.7  |
| 3   | T     | 69  | GLY  | 2.7  |
| 3   | T     | 79  | GLU  | 2.6  |
| 3   | T     | 158 | LEU  | 2.5  |
| 3   | H     | 252 | VAL  | 2.5  |
| 1   | L     | 80  | LEU  | 2.5  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 3   | H     | 251 | VAL  | 2.4  |
| 1   | R     | 7   | ARG  | 2.4  |
| 1   | R     | 276 | PRO  | 2.3  |
| 3   | T     | 92  | VAL  | 2.3  |
| 2   | S     | 301 | HIS  | 2.3  |
| 3   | T     | 80  | SER  | 2.3  |
| 1   | L     | 7   | ARG  | 2.3  |
| 2   | M     | 4   | GLN  | 2.3  |
| 1   | R     | 10  | ARG  | 2.2  |
| 1   | L     | 161 | GLY  | 2.2  |
| 1   | R     | 80  | LEU  | 2.2  |
| 3   | H     | 253 | ALA  | 2.2  |
| 1   | R     | 3   | LEU  | 2.2  |
| 3   | T     | 38  | GLU  | 2.2  |
| 3   | T     | 73  | LEU  | 2.2  |
| 2   | S     | 248 | ALA  | 2.1  |
| 1   | R     | 25  | TRP  | 2.1  |
| 3   | T     | 49  | PRO  | 2.1  |
| 1   | L     | 57  | GLY  | 2.1  |
| 3   | T     | 253 | ALA  | 2.1  |
| 3   | T     | 95  | GLY  | 2.0  |
| 3   | T     | 108 | GLY  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res     | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|---------|-------|------|------|----------------------------|-------|
| 6   | U10  | L     | 1009[A] | 30/63 | 0.68 | 0.50 | 54,67,69,70                | 30    |

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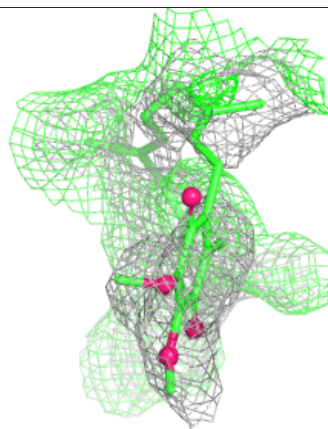
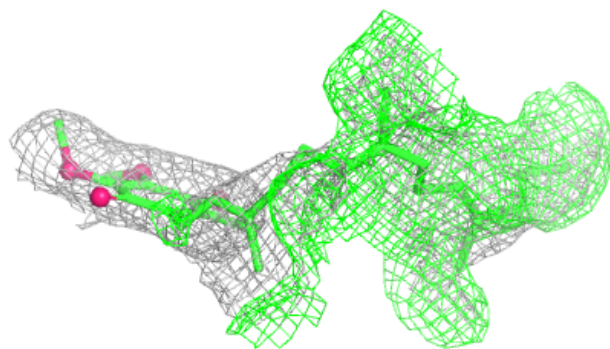
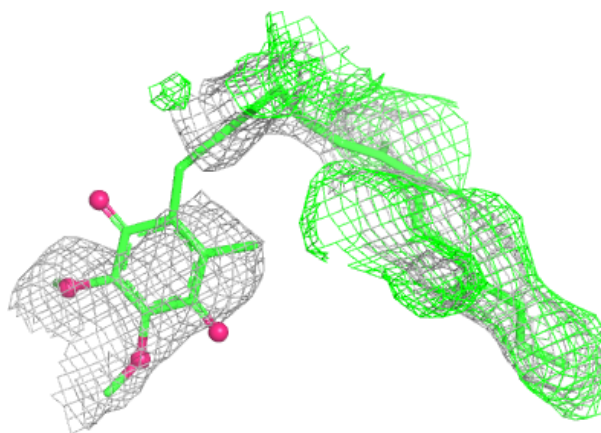
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| Mol | Type | Chain | Res     | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|---------|-------|------|------|----------------------------|-------|
| 6   | U10  | L     | 1009[B] | 30/63 | 0.68 | 0.50 | 44,54,65,66                | 30    |
| 6   | U10  | R     | 2009[A] | 18/63 | 0.68 | 0.51 | 94,96,97,98                | 18    |
| 6   | U10  | R     | 2009[B] | 18/63 | 0.68 | 0.51 | 95,96,97,97                | 18    |
| 9   | LDA  | M     | 1011    | 16/16 | 0.81 | 0.22 | 49,61,78,78                | 0     |
| 6   | U10  | S     | 2008    | 32/63 | 0.87 | 0.16 | 56,58,64,66                | 0     |
| 4   | BCL  | S     | 2001    | 51/66 | 0.87 | 0.15 | 38,45,58,61                | 0     |
| 4   | BCL  | S     | 2004    | 66/66 | 0.88 | 0.16 | 44,52,74,75                | 0     |
| 8   | SPO  | S     | 2010    | 42/42 | 0.89 | 0.16 | 38,49,64,66                | 0     |
| 4   | BCL  | R     | 2002    | 66/66 | 0.90 | 0.14 | 42,53,56,56                | 0     |
| 4   | BCL  | L     | 1001    | 51/66 | 0.90 | 0.12 | 26,32,45,48                | 0     |
| 4   | BCL  | S     | 2003    | 66/66 | 0.91 | 0.14 | 44,49,62,71                | 0     |
| 4   | BCL  | L     | 1002    | 66/66 | 0.91 | 0.13 | 31,36,44,52                | 0     |
| 8   | SPO  | M     | 1010    | 42/42 | 0.91 | 0.14 | 31,36,59,61                | 0     |
| 6   | U10  | M     | 1008    | 38/63 | 0.91 | 0.14 | 36,42,63,64                | 0     |
| 5   | BPH  | R     | 2006    | 65/65 | 0.91 | 0.13 | 47,56,61,62                | 0     |
| 4   | BCL  | L     | 1004    | 66/66 | 0.92 | 0.12 | 28,34,57,59                | 0     |
| 4   | BCL  | M     | 1003    | 66/66 | 0.92 | 0.12 | 24,38,47,49                | 0     |
| 5   | BPH  | M     | 1005    | 55/65 | 0.94 | 0.09 | 26,32,43,46                | 0     |
| 5   | BPH  | L     | 1006    | 65/65 | 0.94 | 0.10 | 24,35,41,43                | 0     |
| 5   | BPH  | S     | 2005    | 51/65 | 0.94 | 0.09 | 35,42,51,52                | 0     |
| 7   | FE2  | S     | 2007    | 1/1   | 0.99 | 0.02 | 51,51,51,51                | 0     |
| 7   | FE2  | M     | 1007    | 1/1   | 0.99 | 0.02 | 33,33,33,33                | 0     |

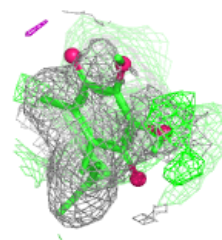
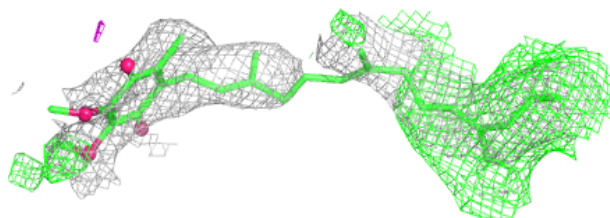
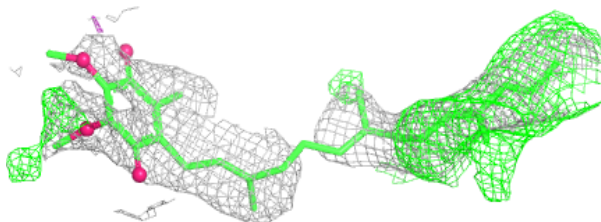
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around U10 L 1009 (A):**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

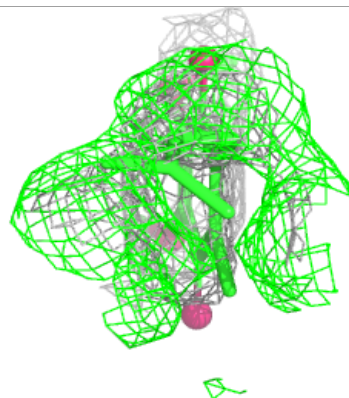
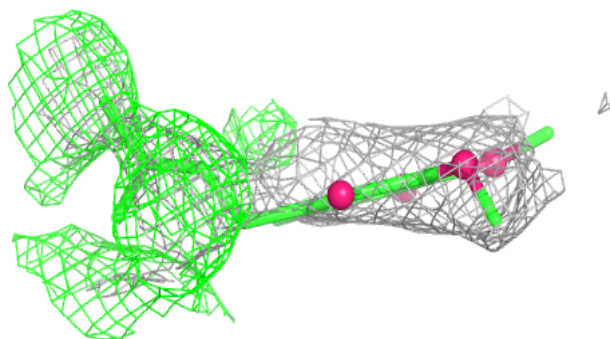
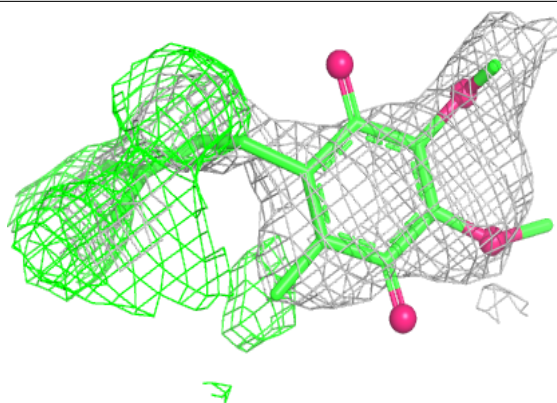
**Electron density around U10 L 1009 (B):**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

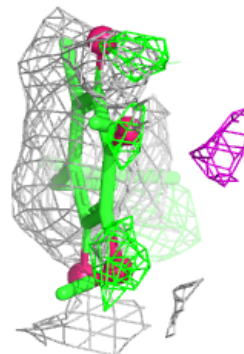
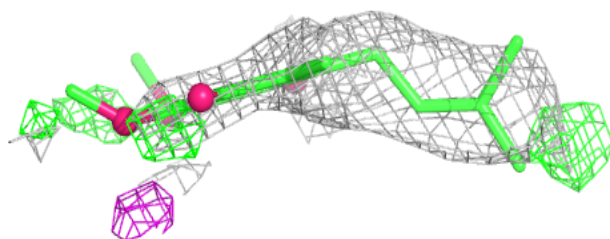
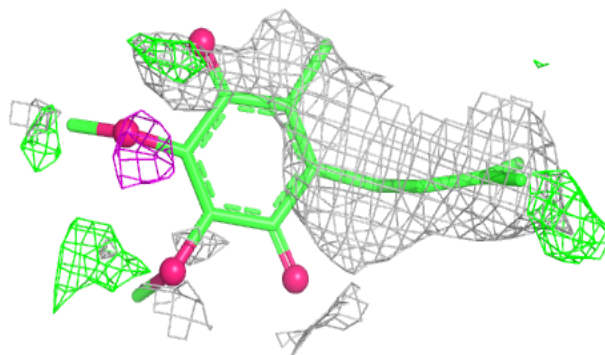


**Electron density around U10 R 2009 (A):**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

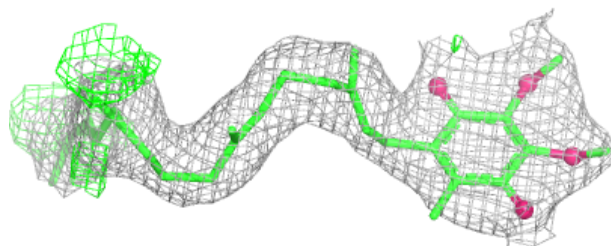
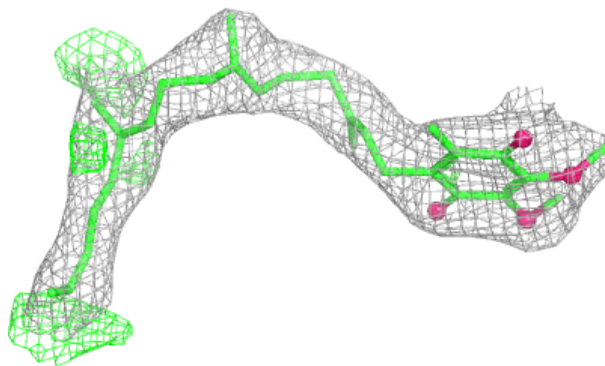
**Electron density around U10 R 2009 (B):**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



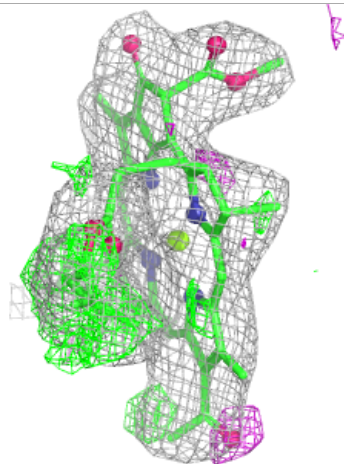
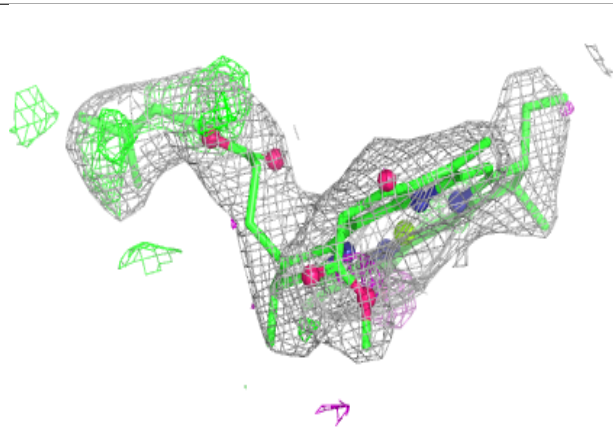
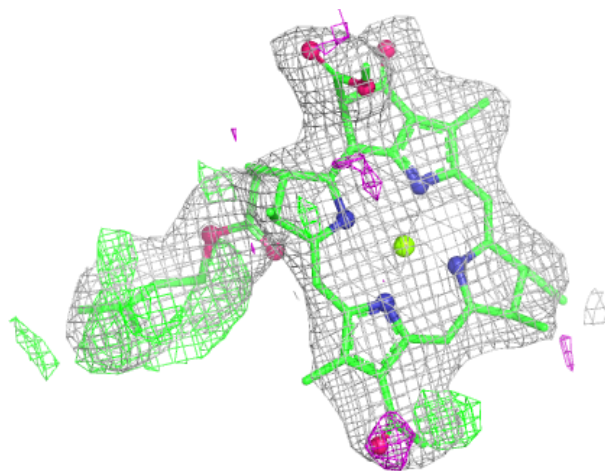
**Electron density around U10 S 2008:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



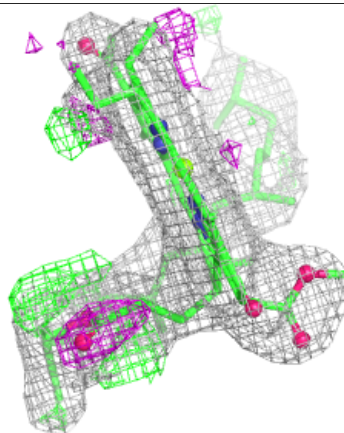
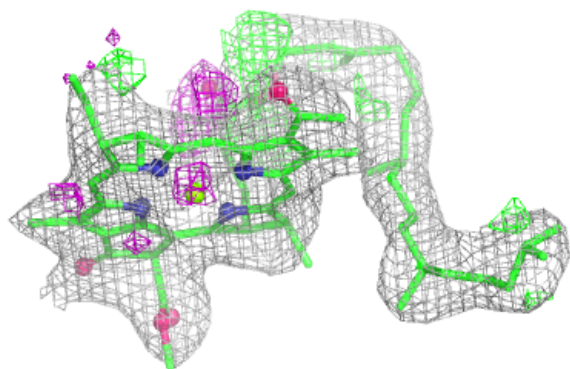
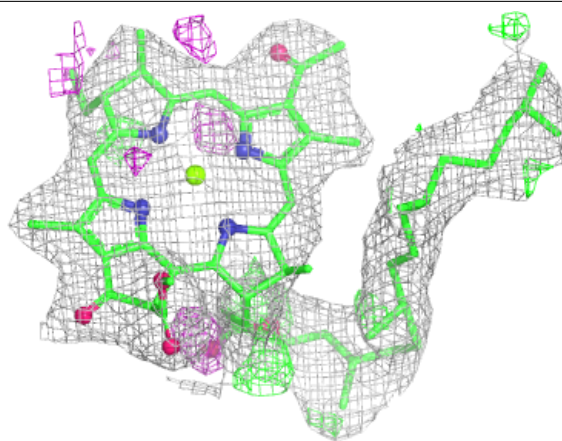
**Electron density around BCL S 2001:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

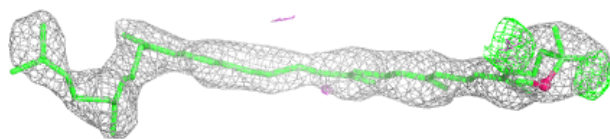
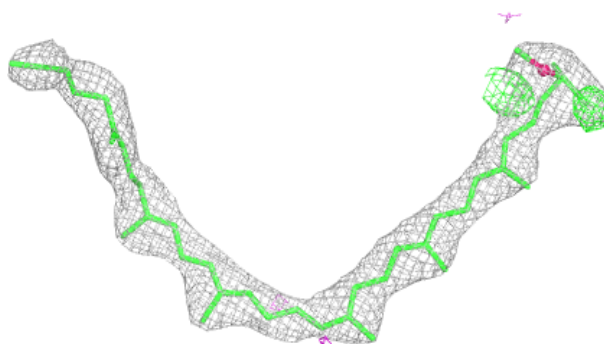


**Electron density around BCL S 2004:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

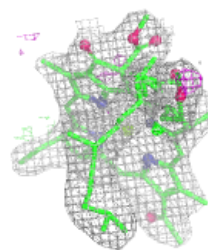
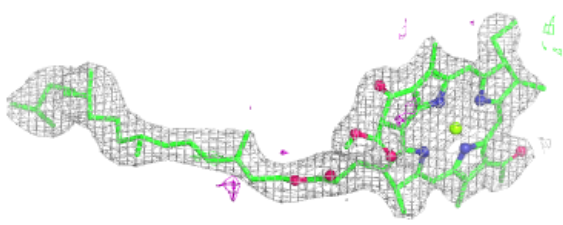
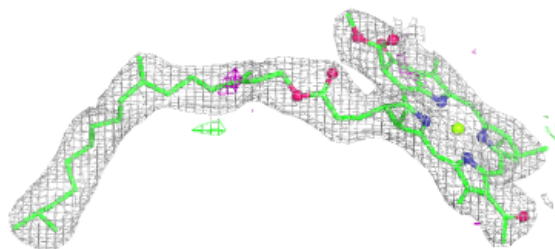
**Electron density around SPO S 2010:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



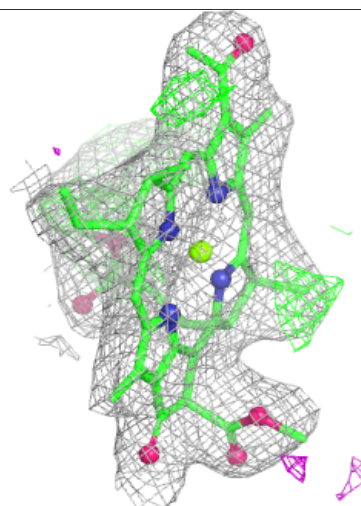
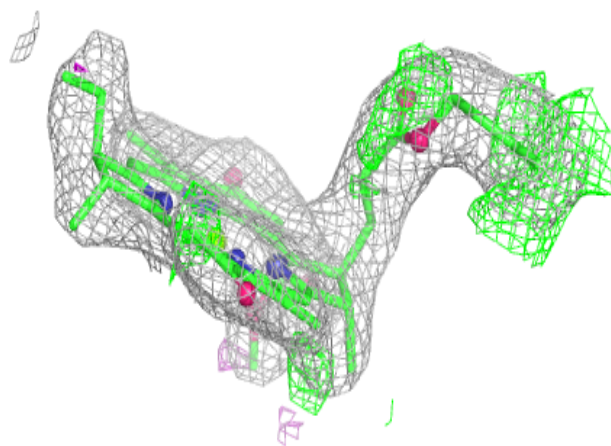
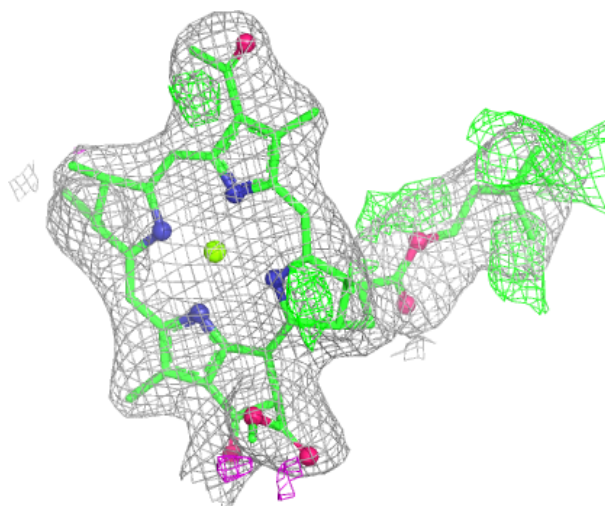
**Electron density around BCL R 2002:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



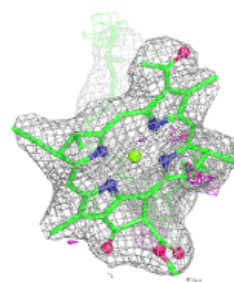
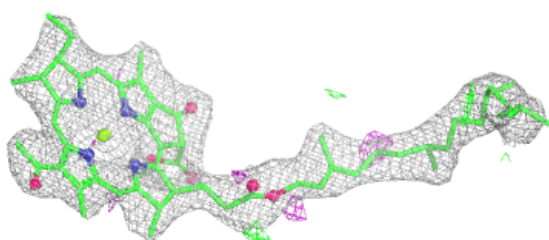
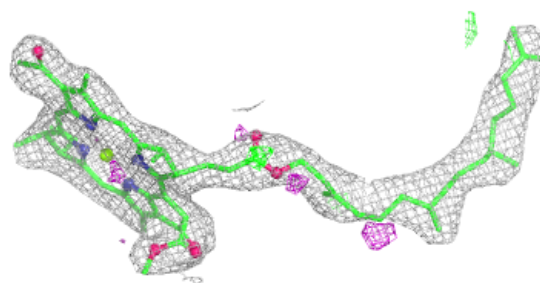
**Electron density around BCL L 1001:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

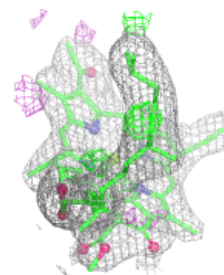
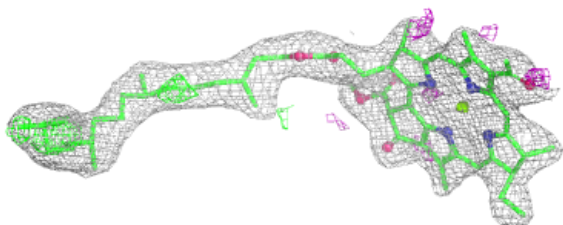
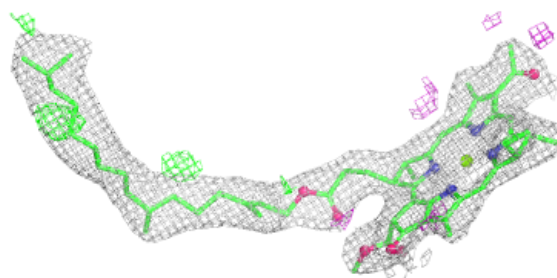


**Electron density around BCL S 2003:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

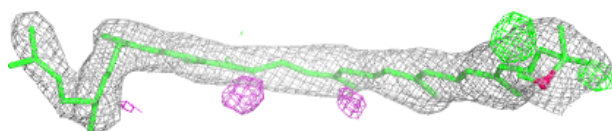
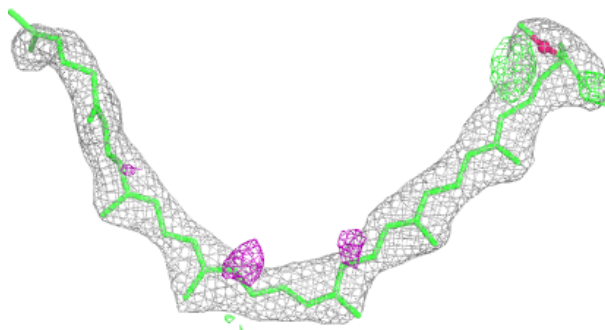
**Electron density around BCL L 1002:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

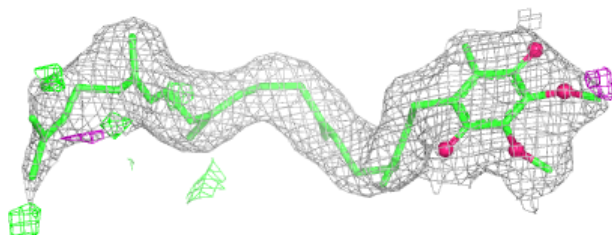
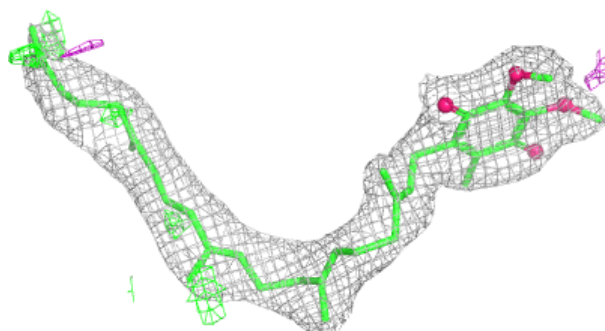


**Electron density around SPO M 1010:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

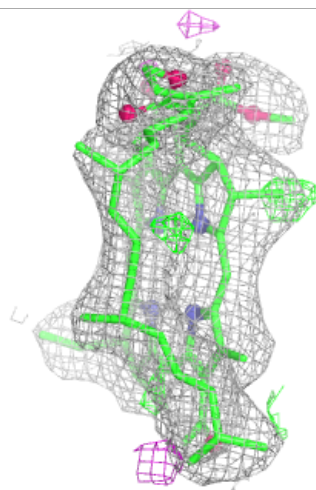
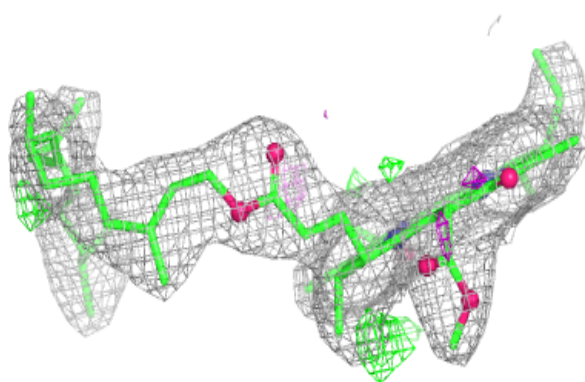
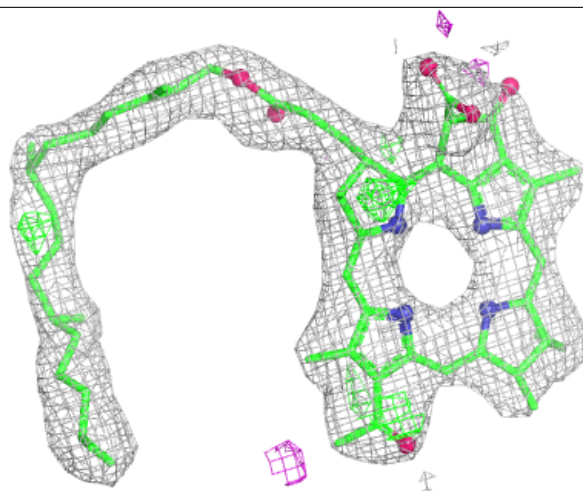
**Electron density around U10 M 1008:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



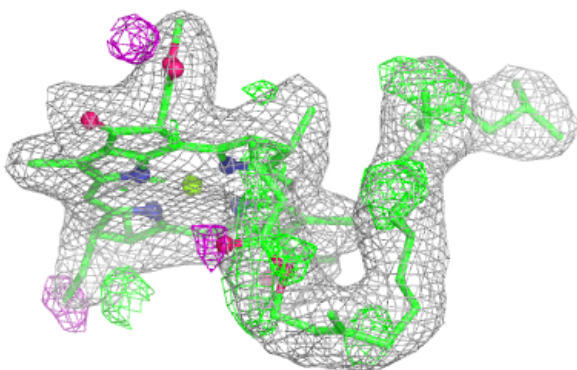
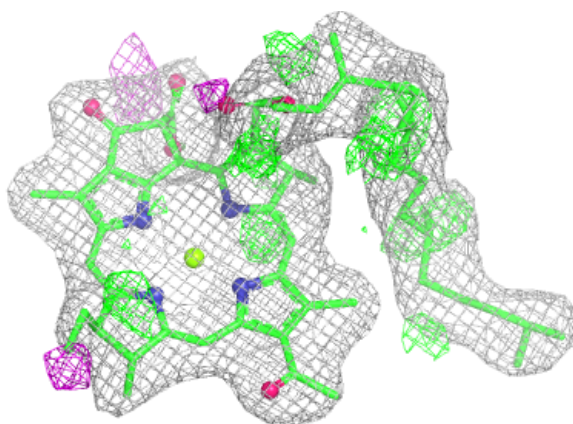
**Electron density around BPH R 2006:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

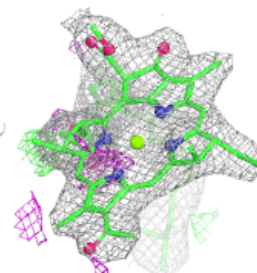
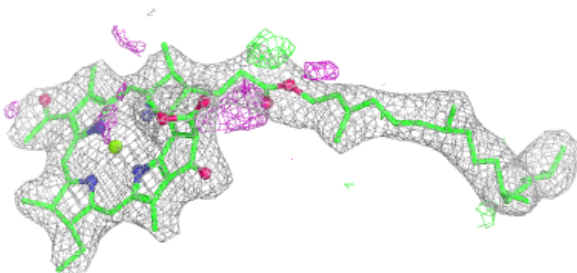
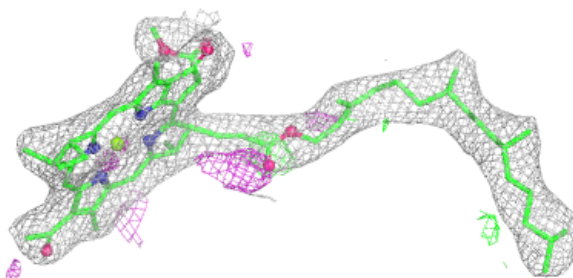


**Electron density around BCL L 1004:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

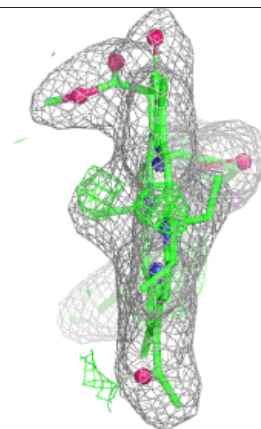
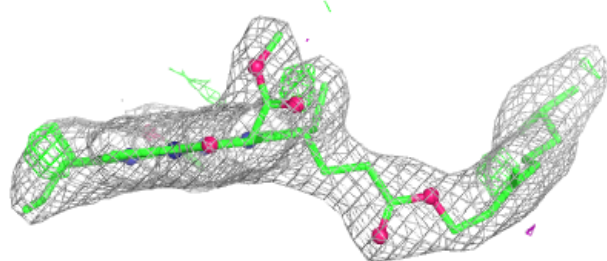
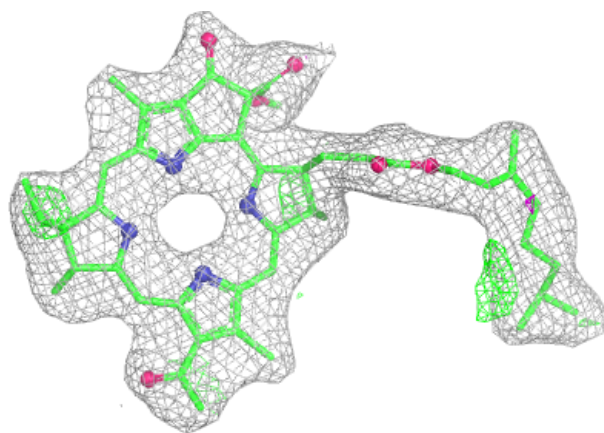
**Electron density around BCL M 1003:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



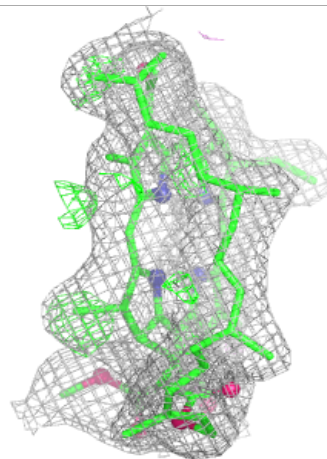
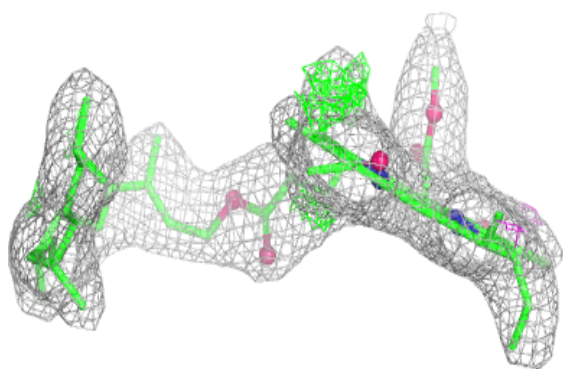
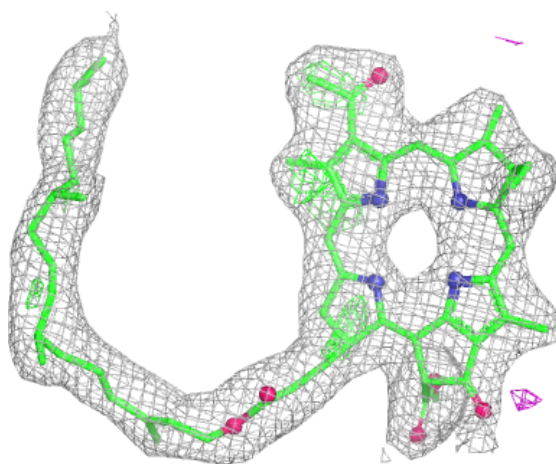
**Electron density around BPH M 1005:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



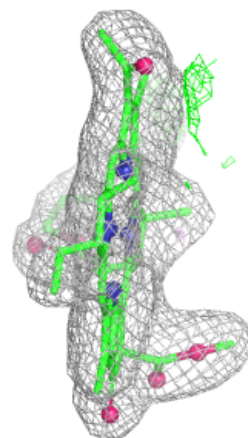
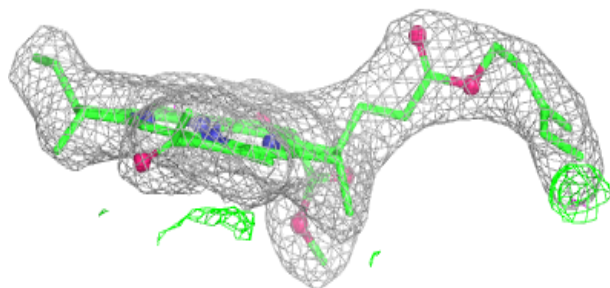
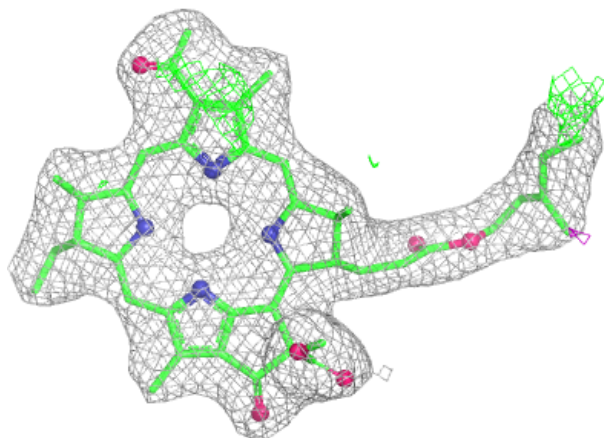
**Electron density around BPH L 1006:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around BPH S 2005:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.