



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:58 PM UTC

PDB ID : 7TLF / pdb\_00007tlf  
Title : Structure of the photoacclimated Light Harvesting Complex PE545 from *Proteomonas sulcata*  
Authors : Jeffrey, P.D.; Spangler, L.C.; Scholes, G.D.  
Deposited on : 2022-01-18  
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

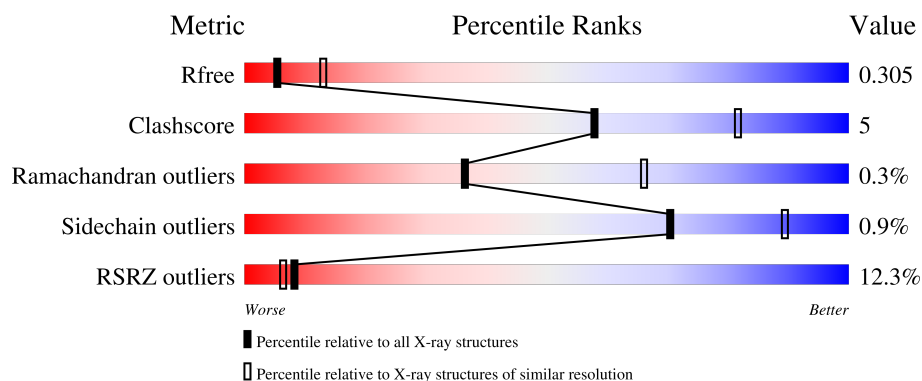
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 3866 (2.80-2.80)                                      |
| Clashscore            | 190562                      | 4276 (2.80-2.80)                                      |
| Ramachandran outliers | 187476                      | 4196 (2.80-2.80)                                      |
| Sidechain outliers    | 187428                      | 4198 (2.80-2.80)                                      |
| RSRZ outliers         | 180081                      | 3869 (2.80-2.80)                                      |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 76     |                  |
| 1   | E     | 76     |                  |
| 1   | I     | 76     |                  |
| 1   | M     | 76     |                  |
| 2   | B     | 177    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 2   | D     | 177    |                  |
| 2   | F     | 177    |                  |
| 2   | H     | 177    |                  |
| 2   | J     | 177    |                  |
| 2   | L     | 177    |                  |
| 2   | N     | 177    |                  |
| 2   | P     | 177    |                  |
| 3   | C     | 67     |                  |
| 3   | G     | 67     |                  |
| 3   | K     | 67     |                  |
| 3   | O     | 67     |                  |

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15397 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 Phycoerythrin alpha-subunit 1.

| Mol | Chain | Residues | Atoms |     |    |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|---|---------|---------|-------|
| 1   | A     | 72       | Total | C   | N  | O   | S | 0       | 0       | 0     |
|     |       |          | 528   | 326 | 91 | 108 | 3 |         |         |       |
| 1   | E     | 74       | Total | C   | N  | O   | S | 0       | 0       | 0     |
|     |       |          | 544   | 337 | 94 | 110 | 3 |         |         |       |
| 1   | I     | 75       | Total | C   | N  | O   | S | 0       | 0       | 0     |
|     |       |          | 553   | 343 | 96 | 111 | 3 |         |         |       |
| 1   | M     | 74       | Total | C   | N  | O   | S | 0       | 0       | 0     |
|     |       |          | 544   | 337 | 94 | 110 | 3 |         |         |       |

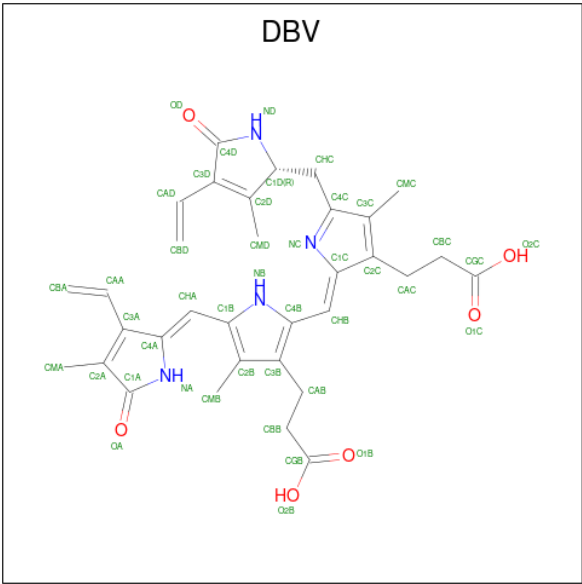
- Molecule 2 is a protein called Phycoerythrin beta-subunit.

| Mol | Chain | Residues | Atoms |     |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 2   | B     | 162      | Total | C   | N   | O   | S  | 0       | 1       | 0     |
|     |       |          | 1180  | 728 | 206 | 236 | 10 |         |         |       |
| 2   | D     | 173      | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1262  | 776 | 220 | 256 | 10 |         |         |       |
| 2   | F     | 166      | Total | C   | N   | O   | S  | 0       | 1       | 0     |
|     |       |          | 1207  | 743 | 209 | 245 | 10 |         |         |       |
| 2   | H     | 170      | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1231  | 759 | 211 | 251 | 10 |         |         |       |
| 2   | J     | 170      | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1241  | 765 | 217 | 249 | 10 |         |         |       |
| 2   | L     | 172      | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1253  | 771 | 219 | 253 | 10 |         |         |       |
| 2   | N     | 170      | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1239  | 765 | 217 | 247 | 10 |         |         |       |
| 2   | P     | 173      | Total | C   | N   | O   | S  | 0       | 1       | 0     |
|     |       |          | 1261  | 777 | 220 | 254 | 10 |         |         |       |

- Molecule 3 is a protein called Phycoerythrin alpha-subunit 2.

| Mol | Chain | Residues | Atoms |     |    |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|---|---------|---------|-------|
| 3   | C     | 60       | Total | C   | N  | O   | S | 0       | 0       | 0     |
|     |       |          | 445   | 274 | 78 | 89  | 4 |         |         |       |
| 3   | G     | 67       | Total | C   | N  | O   | S | 0       | 0       | 0     |
|     |       |          | 496   | 304 | 87 | 100 | 5 |         |         |       |
| 3   | K     | 67       | Total | C   | N  | O   | S | 0       | 0       | 0     |
|     |       |          | 496   | 304 | 87 | 100 | 5 |         |         |       |
| 3   | O     | 67       | Total | C   | N  | O   | S | 0       | 0       | 0     |
|     |       |          | 496   | 304 | 87 | 100 | 5 |         |         |       |

- Molecule 4 is 15,16-DIHYDROBILIVERDIN (CCD ID: DBV) (formula: C<sub>33</sub>H<sub>36</sub>N<sub>4</sub>O<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



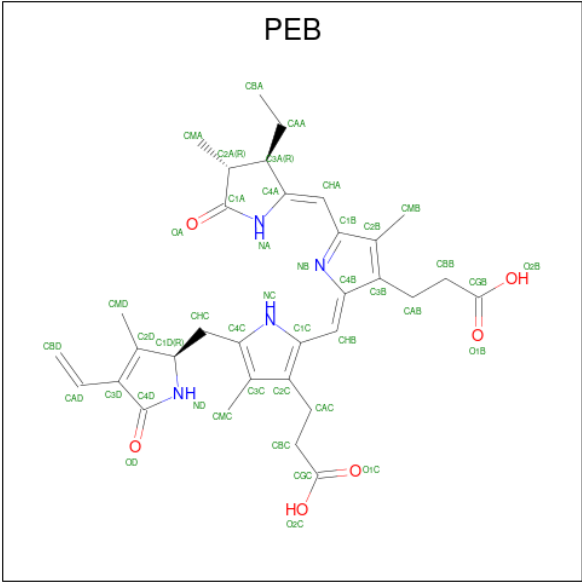
| Mol | Chain | Residues | Atoms |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 4   | A     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 43    | 33 | 4 | 6 |         |         |
| 4   | C     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 43    | 33 | 4 | 6 |         |         |
| 4   | E     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 43    | 33 | 4 | 6 |         |         |
| 4   | G     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 43    | 33 | 4 | 6 |         |         |
| 4   | I     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 43    | 33 | 4 | 6 |         |         |
| 4   | K     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 43    | 33 | 4 | 6 |         |         |
| 4   | M     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 43    | 33 | 4 | 6 |         |         |

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

- Molecule 5 is PHYCOERYTHROBILIN (CCD ID: PEB) (formula: C<sub>33</sub>H<sub>40</sub>N<sub>4</sub>O<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 5   | B     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 43    | 33 | 4 | 6 |         |         |
| 5   | B     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 43    | 33 | 4 | 6 |         |         |
| 5   | B     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 43    | 33 | 4 | 6 |         |         |
| 5   | D     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 43    | 33 | 4 | 6 |         |         |
| 5   | D     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 43    | 33 | 4 | 6 |         |         |
| 5   | D     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 43    | 33 | 4 | 6 |         |         |
| 5   | F     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 43    | 33 | 4 | 6 |         |         |
| 5   | F     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 43    | 33 | 4 | 6 |         |         |
| 5   | F     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 43    | 33 | 4 | 6 |         |         |
| 5   | H     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 43    | 33 | 4 | 6 |         |         |

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| Mol | Chain | Residues | Atoms |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 5   | H     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 43    | 33 | 4 | 6 |         |         |
| 5   | H     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 43    | 33 | 4 | 6 |         |         |
| 5   | J     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 43    | 33 | 4 | 6 |         |         |
| 5   | J     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 43    | 33 | 4 | 6 |         |         |
| 5   | J     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 43    | 33 | 4 | 6 |         |         |
| 5   | L     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 43    | 33 | 4 | 6 |         |         |
| 5   | L     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 43    | 33 | 4 | 6 |         |         |
| 5   | L     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 43    | 33 | 4 | 6 |         |         |
| 5   | N     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 43    | 33 | 4 | 6 |         |         |
| 5   | N     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 43    | 33 | 4 | 6 |         |         |
| 5   | N     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 43    | 33 | 4 | 6 |         |         |
| 5   | P     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 43    | 33 | 4 | 6 |         |         |
| 5   | P     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 43    | 33 | 4 | 6 |         |         |
| 5   | P     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 43    | 33 | 4 | 6 |         |         |

- Molecule 6 is water.

| Mol | Chain | Residues | Atoms |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 6   | B     | 2        | Total | O | 0       | 0       |
|     |       |          | 2     | 2 |         |         |
| 6   | C     | 2        | Total | O | 0       | 0       |
|     |       |          | 2     | 2 |         |         |
| 6   | D     | 4        | Total | O | 0       | 0       |
|     |       |          | 4     | 4 |         |         |
| 6   | E     | 4        | Total | O | 0       | 0       |
|     |       |          | 4     | 4 |         |         |
| 6   | G     | 2        | Total | O | 0       | 0       |
|     |       |          | 2     | 2 |         |         |

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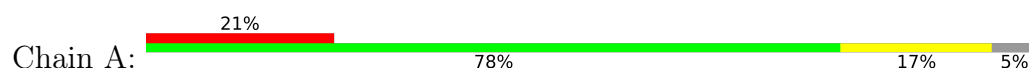
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| Mol | Chain | Residues | Atoms      |        | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|---------|---------|
| 6   | F     | 5        | Total<br>5 | O<br>5 | 0       | 0       |
| 6   | H     | 8        | Total<br>8 | O<br>8 | 0       | 0       |
| 6   | I     | 4        | Total<br>4 | O<br>4 | 0       | 0       |
| 6   | K     | 2        | Total<br>2 | O<br>2 | 0       | 0       |
| 6   | J     | 3        | Total<br>3 | O<br>3 | 0       | 0       |
| 6   | L     | 2        | Total<br>2 | O<br>2 | 0       | 0       |
| 6   | M     | 2        | Total<br>2 | O<br>2 | 0       | 0       |
| 6   | O     | 1        | Total<br>1 | O<br>1 | 0       | 0       |
| 6   | N     | 1        | Total<br>1 | O<br>1 | 0       | 0       |
| 6   | P     | 3        | Total<br>3 | O<br>3 | 0       | 0       |

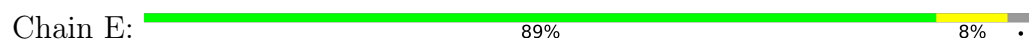
### 3 Residue-property plots [i](#)

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.

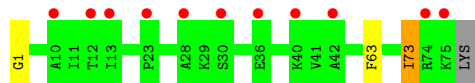
- Molecule 1: Phycoerythrin alpha-subunit 1



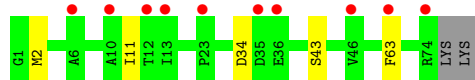
- Molecule 1: Phycoerythrin alpha-subunit 1



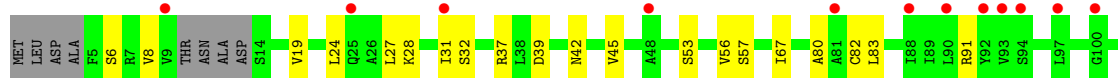
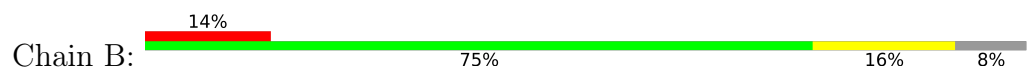
- Molecule 1: Phycoerythrin alpha-subunit 1



- Molecule 1: Phycoerythrin alpha-subunit 1

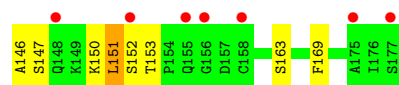
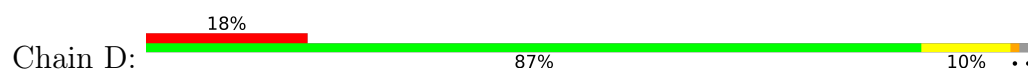


- Molecule 2: Phycoerythrin beta-subunit

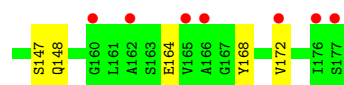
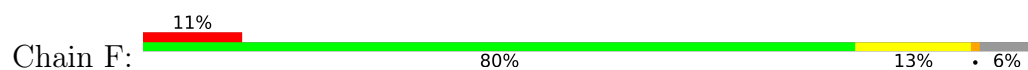




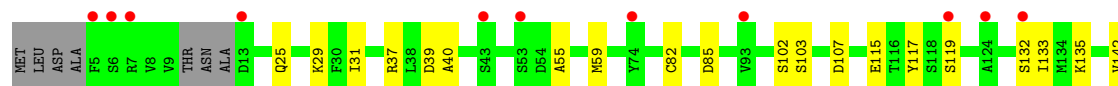
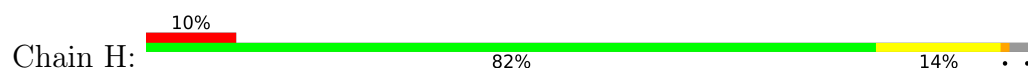
• Molecule 2: Phycoerythrin beta-subunit



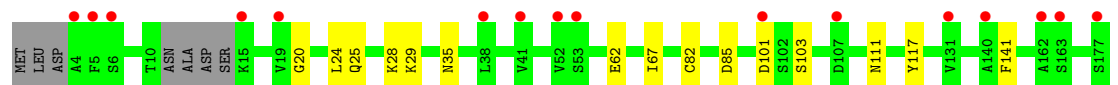
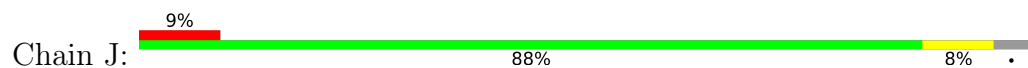
• Molecule 2: Phycoerythrin beta-subunit



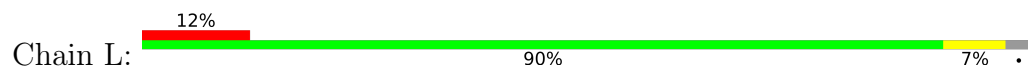
• Molecule 2: Phycoerythrin beta-subunit



• Molecule 2: Phycoerythrin beta-subunit



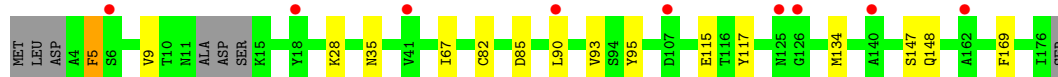
• Molecule 2: Phycoerythrin beta-subunit



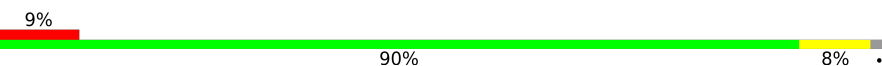
S177

- Molecule 2: Phycoerythrin beta-subunit

Chain N: 



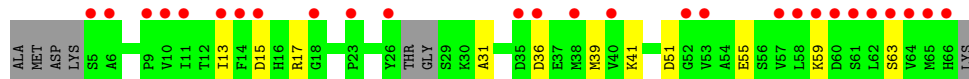
- Molecule 2: Phycoerythrin beta-subunit

Chain P: 

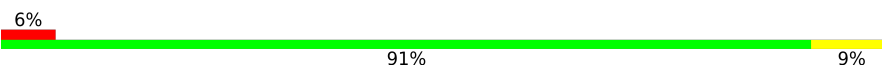


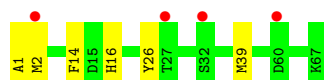
- Molecule 3: Phycoerythrin alpha-subunit 2

Chain C: 

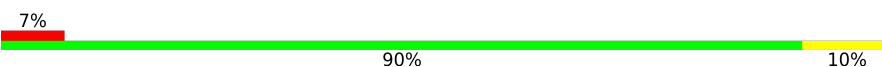


- Molecule 3: Phycoerythrin alpha-subunit 2

Chain G: 

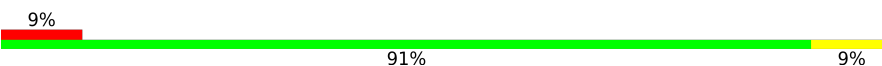


- Molecule 3: Phycoerythrin alpha-subunit 2

Chain K: 



- Molecule 3: Phycoerythrin alpha-subunit 2

Chain O: 



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 1 21 1                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 88.25Å 132.24Å 93.41Å<br>90.00° 116.92° 90.00°              | Depositor        |
| Resolution (Å)                                                          | 29.35 – 2.80<br>29.35 – 2.80                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.0 (29.35-2.80)<br>99.1 (29.35-2.80)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.24                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 0.96 (at 2.76Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX 1.17_3644                                            | Depositor        |
| R, $R_{free}$                                                           | 0.245 , 0.306<br>0.246 , 0.305                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 2457 reflections (5.10%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 42.6                                                        | Xtriage          |
| Anisotropy                                                              | 0.620                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.34 , 60.2                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$ | Xtriage          |
| Estimated twinning fraction                                             | 0.000 for h,-k,-h-l                                         | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.90                                                        | EDS              |
| Total number of atoms                                                   | 15397                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 55.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.06 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.2086e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths |         | Bond angles |                |
|-----|-------|--------------|---------|-------------|----------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5        |
| 1   | A     | 0.30         | 0/533   | 0.68        | 2/711 (0.3%)   |
| 1   | E     | 0.22         | 0/549   | 0.52        | 0/732          |
| 1   | I     | 0.20         | 0/558   | 0.48        | 0/743          |
| 1   | M     | 0.20         | 0/549   | 0.46        | 0/732          |
| 2   | B     | 0.23         | 0/1191  | 0.48        | 0/1607         |
| 2   | D     | 0.21         | 0/1274  | 0.45        | 0/1720         |
| 2   | F     | 0.22         | 0/1221  | 0.48        | 0/1649         |
| 2   | H     | 0.30         | 0/1243  | 0.60        | 0/1678         |
| 2   | J     | 0.22         | 0/1253  | 0.45        | 0/1690         |
| 2   | L     | 0.20         | 0/1265  | 0.44        | 0/1706         |
| 2   | N     | 0.22         | 0/1251  | 0.44        | 0/1689         |
| 2   | P     | 0.20         | 0/1276  | 0.42        | 0/1723         |
| 3   | C     | 0.21         | 0/449   | 0.47        | 0/600          |
| 3   | G     | 0.20         | 0/501   | 0.47        | 0/668          |
| 3   | K     | 0.19         | 0/501   | 0.48        | 0/668          |
| 3   | O     | 0.17         | 0/501   | 0.43        | 0/668          |
| All | All   | 0.22         | 0/14115 | 0.48        | 2/18984 (0.0%) |

There are no bond length outliers.

All (2) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1   | A     | 5   | SER  | CA-C-N | 5.13 | 131.33      | 121.54   |
| 1   | A     | 5   | SER  | C-N-CA | 5.13 | 131.33      | 121.54   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 528   | 0        | 533      | 12      | 0            |
| 1   | E     | 544   | 0        | 555      | 7       | 0            |
| 1   | I     | 553   | 0        | 568      | 3       | 0            |
| 1   | M     | 544   | 0        | 555      | 5       | 0            |
| 2   | B     | 1180  | 0        | 1171     | 19      | 0            |
| 2   | D     | 1262  | 0        | 1257     | 15      | 0            |
| 2   | F     | 1207  | 0        | 1206     | 19      | 0            |
| 2   | H     | 1231  | 0        | 1219     | 16      | 0            |
| 2   | J     | 1241  | 0        | 1244     | 13      | 0            |
| 2   | L     | 1253  | 0        | 1248     | 7       | 0            |
| 2   | N     | 1239  | 0        | 1241     | 14      | 0            |
| 2   | P     | 1261  | 0        | 1257     | 9       | 0            |
| 3   | C     | 445   | 0        | 447      | 6       | 0            |
| 3   | G     | 496   | 0        | 505      | 5       | 0            |
| 3   | K     | 496   | 0        | 505      | 6       | 0            |
| 3   | O     | 496   | 0        | 505      | 4       | 0            |
| 4   | A     | 43    | 0        | 33       | 1       | 0            |
| 4   | C     | 43    | 0        | 32       | 2       | 0            |
| 4   | E     | 43    | 0        | 33       | 1       | 0            |
| 4   | G     | 43    | 0        | 32       | 2       | 0            |
| 4   | I     | 43    | 0        | 32       | 0       | 0            |
| 4   | K     | 43    | 0        | 32       | 2       | 0            |
| 4   | M     | 43    | 0        | 32       | 2       | 0            |
| 4   | O     | 43    | 0        | 32       | 1       | 0            |
| 5   | B     | 129   | 0        | 110      | 2       | 0            |
| 5   | D     | 129   | 0        | 109      | 1       | 0            |
| 5   | F     | 129   | 0        | 110      | 1       | 0            |
| 5   | H     | 129   | 0        | 110      | 2       | 0            |
| 5   | J     | 129   | 0        | 110      | 3       | 0            |
| 5   | L     | 129   | 0        | 110      | 0       | 0            |
| 5   | N     | 129   | 0        | 109      | 2       | 0            |
| 5   | P     | 129   | 0        | 110      | 0       | 0            |
| 6   | B     | 2     | 0        | 0        | 0       | 0            |
| 6   | C     | 2     | 0        | 0        | 0       | 0            |
| 6   | D     | 4     | 0        | 0        | 1       | 0            |
| 6   | E     | 4     | 0        | 0        | 0       | 0            |
| 6   | F     | 5     | 0        | 0        | 1       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 6   | G     | 2     | 0        | 0        | 0       | 0            |
| 6   | H     | 8     | 0        | 0        | 0       | 0            |
| 6   | I     | 4     | 0        | 0        | 0       | 0            |
| 6   | J     | 3     | 0        | 0        | 0       | 0            |
| 6   | K     | 2     | 0        | 0        | 0       | 0            |
| 6   | L     | 2     | 0        | 0        | 0       | 0            |
| 6   | M     | 2     | 0        | 0        | 0       | 0            |
| 6   | N     | 1     | 0        | 0        | 0       | 0            |
| 6   | O     | 1     | 0        | 0        | 0       | 0            |
| 6   | P     | 3     | 0        | 0        | 0       | 0            |
| All | All   | 15397 | 0        | 15152    | 138     | 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 5.

All (138) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 2:D:31:ILE:HD12 | 2:D:37:ARG:HD2   | 1.68                     | 0.76              |
| 3:G:1:ALA:N     | 2:H:107:ASP:O    | 2.21                     | 0.73              |
| 2:B:31:ILE:HD12 | 2:B:37:ARG:HD2   | 1.72                     | 0.71              |
| 2:H:146:ALA:HB1 | 2:H:150:LYS:HG3  | 1.74                     | 0.70              |
| 2:H:31:ILE:HD12 | 2:H:37:ARG:HD2   | 1.74                     | 0.68              |
| 2:H:102:SER:OG  | 2:H:171:LYS:NZ   | 2.22                     | 0.66              |
| 2:H:25:GLN:HG2  | 2:H:29:LYS:HE3   | 1.80                     | 0.64              |
| 2:D:146:ALA:HB1 | 2:D:150:LYS:HG3  | 1.80                     | 0.63              |
| 2:B:32:SER:HB3  | 2:B:37:ARG:HH21  | 1.62                     | 0.63              |
| 1:E:64:LYS:NZ   | 2:H:39:ASP:OD1   | 2.28                     | 0.62              |
| 2:F:31:ILE:HD12 | 2:F:37:ARG:HD2   | 1.80                     | 0.61              |
| 3:O:65:MET:HE1  | 2:P:67:ILE:HD11  | 1.83                     | 0.61              |
| 1:I:73:ILE:HD12 | 2:J:62:GLU:HB2   | 1.86                     | 0.57              |
| 2:F:56:VAL:HG21 | 2:F:83:LEU:HD23  | 1.86                     | 0.57              |
| 2:D:147:SER:HB3 | 2:D:150:LYS:HG2  | 1.87                     | 0.56              |
| 2:N:115:GLU:N   | 2:N:115:GLU:OE1  | 2.38                     | 0.56              |
| 1:A:56:LYS:HE2  | 2:B:53:SER:HB2   | 1.87                     | 0.55              |
| 2:F:101:ASP:OD2 | 2:F:103:SER:OG   | 2.25                     | 0.54              |
| 2:N:147:SER:OG  | 2:N:148:GLN:OE1  | 2.24                     | 0.54              |
| 2:L:148:GLN:O   | 2:L:148:GLN:NE2  | 2.41                     | 0.54              |
| 3:K:21:ARG:NH2  | 3:K:24:LYS:HE2   | 2.24                     | 0.53              |
| 2:H:115:GLU:OE1 | 2:H:115:GLU:N    | 2.37                     | 0.52              |
| 1:E:73:ILE:HG21 | 2:F:129:ARG:HH21 | 1.74                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:67:ILE:HG13  | 4:C:101:DBV:HMB3 | 1.92                     | 0.52              |
| 1:I:1:GLY:HA2    | 2:J:111:ASN:HB3  | 1.90                     | 0.52              |
| 1:I:63:PHE:CZ    | 2:J:67:ILE:HD11  | 2.45                     | 0.52              |
| 2:F:147:SER:OG   | 2:F:148:GLN:OE1  | 2.24                     | 0.52              |
| 2:J:85:ASP:OD2   | 2:J:117:TYR:OH   | 2.26                     | 0.51              |
| 1:A:65:GLU:CD    | 2:D:152:SER:HG   | 2.18                     | 0.51              |
| 2:L:3:ASP:O      | 2:L:5:PHE:N      | 2.44                     | 0.51              |
| 3:G:26:TYR:HB2   | 3:G:39:MET:HE1   | 1.93                     | 0.51              |
| 1:E:43:SER:HB2   | 2:F:9:VAL:HA     | 1.92                     | 0.51              |
| 2:P:31:ILE:HD12  | 2:P:37:ARG:HD2   | 1.92                     | 0.51              |
| 3:C:15:ASP:OD1   | 3:C:17:ARG:HG3   | 2.11                     | 0.50              |
| 1:A:11:ILE:O     | 2:B:45:VAL:HG11  | 2.12                     | 0.50              |
| 2:P:115:GLU:N    | 2:P:115:GLU:OE1  | 2.40                     | 0.50              |
| 2:B:42:ASN:OD1   | 3:C:63:SER:HB2   | 2.12                     | 0.50              |
| 1:A:63:PHE:CZ    | 2:B:67:ILE:HD11  | 2.46                     | 0.49              |
| 2:N:93:VAL:HG11  | 2:N:169:PHE:CE2  | 2.48                     | 0.49              |
| 2:B:56:VAL:HG21  | 2:B:83:LEU:HD23  | 1.95                     | 0.49              |
| 2:D:91:ARG:NH2   | 6:D:302:HOH:O    | 2.45                     | 0.49              |
| 2:B:107:ASP:O    | 2:B:111:ASN:HB3  | 2.13                     | 0.49              |
| 2:J:35:ASN:HB3   | 5:J:202:PEB:C1C  | 2.43                     | 0.48              |
| 1:E:63:PHE:CZ    | 2:F:64:PRO:HB3   | 2.49                     | 0.48              |
| 2:B:114:LYS:HB2  | 2:B:176:ILE:HA   | 1.96                     | 0.47              |
| 3:C:51:ASP:O     | 3:C:55:GLU:HG3   | 2.13                     | 0.47              |
| 2:F:101:ASP:CG   | 2:F:103:SER:H    | 2.22                     | 0.47              |
| 2:N:85:ASP:OD2   | 2:N:117:TYR:OH   | 2.32                     | 0.47              |
| 2:D:82:CYS:HA    | 5:D:203:PEB:HAA1 | 1.76                     | 0.47              |
| 1:E:60:PHE:CE1   | 2:F:57:SER:HB2   | 2.49                     | 0.47              |
| 1:A:9:PRO:O      | 2:B:91:ARG:HB3   | 2.14                     | 0.47              |
| 2:D:151:LEU:HD23 | 2:D:153:THR:O    | 2.14                     | 0.47              |
| 1:E:73:ILE:HG21  | 2:F:129:ARG:NH2  | 2.29                     | 0.47              |
| 2:N:90:LEU:HB2   | 2:N:134:MET:CE   | 2.44                     | 0.47              |
| 2:J:25:GLN:HG2   | 2:J:29:LYS:HE3   | 1.97                     | 0.47              |
| 2:H:132:SER:O    | 2:H:135:LYS:HB3  | 2.14                     | 0.47              |
| 3:K:65:MET:HE1   | 2:L:67:ILE:HD11  | 1.98                     | 0.46              |
| 2:F:164:GLU:HG2  | 2:F:168:TYR:CE2  | 2.51                     | 0.46              |
| 1:M:43:SER:HB2   | 2:N:9:VAL:HA     | 1.97                     | 0.46              |
| 1:A:56:LYS:NZ    | 1:A:59:GLU:OE1   | 2.37                     | 0.46              |
| 2:H:85:ASP:OD2   | 2:H:117:TYR:OH   | 2.27                     | 0.46              |
| 1:A:41:VAL:HG12  | 2:B:8:VAL:HG11   | 1.98                     | 0.46              |
| 2:F:101:ASP:OD1  | 2:F:103:SER:HB3  | 2.16                     | 0.46              |
| 2:B:19:VAL:HG11  | 2:B:27:LEU:HD22  | 1.97                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:O:39:MET:HE3   | 3:O:41:LYS:HB2   | 1.98                     | 0.46              |
| 2:N:90:LEU:HB2   | 2:N:134:MET:HE1  | 1.98                     | 0.46              |
| 2:J:24:LEU:HG    | 2:J:28:LYS:HE2   | 1.98                     | 0.45              |
| 2:J:25:GLN:O     | 2:J:29:LYS:HG3   | 2.16                     | 0.45              |
| 1:M:2:MET:HE3    | 1:M:2:MET:HB3    | 1.90                     | 0.45              |
| 2:L:74:TYR:O     | 2:L:75:THR:OG1   | 2.30                     | 0.45              |
| 2:D:146:ALA:HB3  | 2:D:151:LEU:HD12 | 1.99                     | 0.45              |
| 4:M:101:DBV:HMB3 | 2:P:67:ILE:HG13  | 1.97                     | 0.45              |
| 1:A:60:PHE:CE1   | 2:B:57:SER:HB2   | 2.52                     | 0.45              |
| 4:K:101:DBV:HMB3 | 2:J:67:ILE:HG13  | 1.99                     | 0.45              |
| 1:A:11:ILE:HG12  | 1:A:41:VAL:HG22  | 1.98                     | 0.45              |
| 1:A:48:VAL:O     | 2:B:80:ALA:HB1   | 2.17                     | 0.45              |
| 4:G:101:DBV:CMB  | 4:G:101:DBV:HNA  | 2.30                     | 0.45              |
| 2:P:9:VAL:O      | 2:P:108:ARG:NH1  | 2.50                     | 0.45              |
| 2:B:24:LEU:HG    | 2:B:28:LYS:HE2   | 1.98                     | 0.44              |
| 4:A:101:DBV:CMB  | 4:A:101:DBV:HNA  | 2.29                     | 0.44              |
| 4:G:101:DBV:HMB3 | 2:F:67:ILE:HG13  | 1.99                     | 0.44              |
| 2:F:110:LEU:HD21 | 2:F:172:VAL:HG22 | 1.99                     | 0.44              |
| 2:H:40:ALA:HB1   | 2:H:142:VAL:HG22 | 2.00                     | 0.44              |
| 2:N:35:ASN:HB3   | 5:N:202:PEB:C1C  | 2.48                     | 0.44              |
| 2:D:93:VAL:HG11  | 2:D:169:PHE:CE2  | 2.53                     | 0.43              |
| 2:P:74:TYR:O     | 2:P:75:THR:OG1   | 2.31                     | 0.43              |
| 2:D:5:PHE:HB3    | 2:D:95:TYR:OH    | 2.18                     | 0.43              |
| 3:G:14:PHE:HD2   | 3:G:16:HIS:CE1   | 2.36                     | 0.43              |
| 2:L:101:ASP:OD1  | 2:L:103:SER:N    | 2.32                     | 0.43              |
| 2:P:167:GLY:O    | 2:P:171:LYS:HG3  | 2.19                     | 0.43              |
| 2:H:148:GLN:HA   | 2:H:151:LEU:HB2  | 2.01                     | 0.43              |
| 2:D:147:SER:O    | 2:D:151:LEU:N    | 2.52                     | 0.42              |
| 2:F:24:LEU:HG    | 2:F:28:LYS:HE2   | 2.01                     | 0.42              |
| 5:F:202:PEB:HBB1 | 5:F:202:PEB:HAB1 | 1.85                     | 0.42              |
| 2:L:33:GLU:OE2   | 2:L:36:LYS:NZ    | 2.38                     | 0.42              |
| 2:N:5:PHE:HD1    | 2:N:5:PHE:HA     | 1.70                     | 0.42              |
| 3:C:13:ILE:HB    | 2:D:42:ASN:CG    | 2.45                     | 0.42              |
| 1:A:6:ALA:HB3    | 1:A:45:LYS:HG3   | 2.02                     | 0.42              |
| 1:E:2:MET:HE3    | 1:E:2:MET:HB3    | 1.90                     | 0.42              |
| 2:H:82:CYS:HA    | 5:H:203:PEB:HAA1 | 1.79                     | 0.42              |
| 2:J:101:ASP:OD1  | 2:J:103:SER:OG   | 2.36                     | 0.42              |
| 2:H:25:GLN:O     | 2:H:29:LYS:HG3   | 2.19                     | 0.42              |
| 3:G:26:TYR:HB2   | 3:G:39:MET:CE    | 2.49                     | 0.42              |
| 2:J:82:CYS:HA    | 5:J:203:PEB:HAA1 | 1.85                     | 0.42              |
| 2:F:101:ASP:OD1  | 2:F:103:SER:CB   | 2.68                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:N:90:LEU:HD22  | 2:N:134:MET:HE2  | 2.02                     | 0.41              |
| 4:M:101:DBV:CMB  | 4:M:101:DBV:HNA  | 2.33                     | 0.41              |
| 1:A:65:GLU:OE1   | 2:D:152:SER:OG   | 2.32                     | 0.41              |
| 1:M:63:PHE:CZ    | 2:N:67:ILE:HD11  | 2.55                     | 0.41              |
| 2:P:51:ILE:HG12  | 2:P:137:CYS:HB3  | 2.01                     | 0.41              |
| 3:K:26:TYR:HB2   | 3:K:39:MET:HE2   | 2.02                     | 0.41              |
| 1:M:11:ILE:HD11  | 2:N:95:TYR:HA    | 2.03                     | 0.41              |
| 2:B:39:ASP:OD1   | 5:B:202:PEB:HMD1 | 2.20                     | 0.41              |
| 2:F:15:LYS:N     | 6:F:301:HOH:O    | 2.52                     | 0.41              |
| 2:B:82:CYS:HA    | 5:B:203:PEB:HAA1 | 1.90                     | 0.41              |
| 3:G:2:MET:HE3    | 3:G:2:MET:HB3    | 1.75                     | 0.41              |
| 2:H:59:MET:HE2   | 2:H:59:MET:HB3   | 1.99                     | 0.41              |
| 2:J:141:PHE:HZ   | 5:J:201:PEB:HMA2 | 1.84                     | 0.41              |
| 3:K:3:ASP:OD2    | 2:L:108:ARG:NH2  | 2.53                     | 0.41              |
| 2:N:82:CYS:HA    | 5:N:203:PEB:HAA1 | 1.87                     | 0.41              |
| 3:O:26:TYR:HB3   | 4:O:101:DBV:HBD1 | 2.02                     | 0.41              |
| 2:B:105:LEU:O    | 2:B:109:CYS:HB3  | 2.20                     | 0.41              |
| 3:C:39:MET:HE3   | 3:C:41:LYS:HB2   | 2.03                     | 0.41              |
| 2:F:38:LEU:HA    | 2:F:38:LEU:HD23  | 1.84                     | 0.41              |
| 2:H:39:ASP:OD1   | 5:H:202:PEB:HMD1 | 2.20                     | 0.41              |
| 1:M:34:ASP:OD1   | 2:N:28:LYS:NZ    | 2.47                     | 0.41              |
| 3:O:30:LYS:HA    | 3:O:30:LYS:HD3   | 1.94                     | 0.41              |
| 2:P:151:LEU:HD12 | 2:P:151:LEU:HA   | 1.88                     | 0.41              |
| 4:C:101:DBV:HNA  | 4:C:101:DBV:CMB  | 2.34                     | 0.40              |
| 2:D:113:LEU:HD12 | 2:D:113:LEU:HA   | 1.92                     | 0.40              |
| 3:K:2:MET:HE3    | 3:K:2:MET:HB3    | 1.99                     | 0.40              |
| 2:H:55:ALA:HA    | 2:H:133:ILE:HG21 | 2.04                     | 0.40              |
| 3:C:31:ALA:N     | 3:C:36:ASP:OD1   | 2.48                     | 0.40              |
| 4:E:101:DBV:CMB  | 4:E:101:DBV:HNA  | 2.34                     | 0.40              |
| 3:K:26:TYR:HB3   | 4:K:101:DBV:HBD1 | 2.03                     | 0.40              |
| 2:D:146:ALA:HB1  | 2:D:150:LYS:HE3  | 2.02                     | 0.40              |
| 2:F:125:ASN:OD1  | 2:F:126:GLY:N    | 2.52                     | 0.40              |
| 2:J:20:GLY:HA2   | 2:J:24:LEU:HB2   | 2.03                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|---------|----------|-------------|-----|
| 1   | A     | 70/76 (92%)     | 65 (93%)   | 5 (7%)  | 0        | 100         | 100 |
| 1   | E     | 72/76 (95%)     | 69 (96%)   | 3 (4%)  | 0        | 100         | 100 |
| 1   | I     | 73/76 (96%)     | 69 (94%)   | 4 (6%)  | 0        | 100         | 100 |
| 1   | M     | 72/76 (95%)     | 70 (97%)   | 2 (3%)  | 0        | 100         | 100 |
| 2   | B     | 156/177 (88%)   | 152 (97%)  | 2 (1%)  | 2 (1%)   | 9           | 31  |
| 2   | D     | 169/177 (96%)   | 163 (96%)  | 5 (3%)  | 1 (1%)   | 21          | 51  |
| 2   | F     | 163/177 (92%)   | 161 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 2   | H     | 166/177 (94%)   | 164 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 2   | J     | 166/177 (94%)   | 163 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 2   | L     | 168/177 (95%)   | 163 (97%)  | 4 (2%)  | 1 (1%)   | 21          | 51  |
| 2   | N     | 166/177 (94%)   | 163 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 2   | P     | 170/177 (96%)   | 165 (97%)  | 4 (2%)  | 1 (1%)   | 21          | 51  |
| 3   | C     | 56/67 (84%)     | 54 (96%)   | 2 (4%)  | 0        | 100         | 100 |
| 3   | G     | 65/67 (97%)     | 63 (97%)   | 2 (3%)  | 0        | 100         | 100 |
| 3   | K     | 65/67 (97%)     | 63 (97%)   | 2 (3%)  | 0        | 100         | 100 |
| 3   | O     | 65/67 (97%)     | 63 (97%)   | 1 (2%)  | 1 (2%)   | 8           | 28  |
| All | All   | 1862/1988 (94%) | 1810 (97%) | 46 (2%) | 6 (0%)   | 36          | 66  |

All (6) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | L     | 4   | ALA  |
| 2   | B     | 6   | SER  |
| 2   | B     | 144 | ASN  |
| 2   | D     | 9   | VAL  |
| 3   | O     | 24  | LYS  |
| 2   | P     | 4   | ALA  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 1   | A     | 57/62 (92%)     | 56 (98%)   | 1 (2%)   | 51          | 82  |
| 1   | E     | 59/62 (95%)     | 59 (100%)  | 0        | 100         | 100 |
| 1   | I     | 60/62 (97%)     | 59 (98%)   | 1 (2%)   | 53          | 83  |
| 1   | M     | 59/62 (95%)     | 59 (100%)  | 0        | 100         | 100 |
| 2   | B     | 130/143 (91%)   | 128 (98%)  | 2 (2%)   | 57          | 84  |
| 2   | D     | 140/143 (98%)   | 137 (98%)  | 3 (2%)   | 47          | 79  |
| 2   | F     | 134/143 (94%)   | 132 (98%)  | 2 (2%)   | 57          | 84  |
| 2   | H     | 136/143 (95%)   | 133 (98%)  | 3 (2%)   | 45          | 78  |
| 2   | J     | 137/143 (96%)   | 137 (100%) | 0        | 100         | 100 |
| 2   | L     | 138/143 (96%)   | 138 (100%) | 0        | 100         | 100 |
| 2   | N     | 136/143 (95%)   | 135 (99%)  | 1 (1%)   | 76          | 91  |
| 2   | P     | 139/143 (97%)   | 139 (100%) | 0        | 100         | 100 |
| 3   | C     | 50/55 (91%)     | 49 (98%)   | 1 (2%)   | 48          | 80  |
| 3   | G     | 55/55 (100%)    | 55 (100%)  | 0        | 100         | 100 |
| 3   | K     | 55/55 (100%)    | 55 (100%)  | 0        | 100         | 100 |
| 3   | O     | 55/55 (100%)    | 55 (100%)  | 0        | 100         | 100 |
| All | All   | 1540/1612 (96%) | 1526 (99%) | 14 (1%)  | 70          | 89  |

All (14) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 7   | LYS  |
| 2   | B     | 135 | LYS  |
| 2   | B     | 152 | SER  |
| 3   | C     | 59  | LYS  |
| 2   | D     | 145 | THR  |
| 2   | D     | 151 | LEU  |
| 2   | D     | 163 | SER  |
| 2   | F     | 43  | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | F     | 101 | ASP  |
| 2   | H     | 103 | SER  |
| 2   | H     | 119 | SER  |
| 2   | H     | 151 | LEU  |
| 1   | I     | 73  | ILE  |
| 2   | N     | 5   | PHE  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | G     | 34  | GLN  |
| 1   | M     | 33  | 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](#)

32 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 5   | PEB  | H     | 201 | 2    | 46,46,46     | 1.52 | 8 (17%)     | 56,67,67    | 1.71 | 11 (19%)    |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 4   | DBV  | C     | 101 | 3    | 46,46,46     | 2.30 | 10 (21%) | 56,67,67    | 1.89 | 18 (32%) |
| 5   | PEB  | L     | 202 | 2    | 46,46,46     | 1.56 | 6 (13%)  | 56,67,67    | 1.61 | 11 (19%) |
| 5   | PEB  | L     | 201 | 2    | 46,46,46     | 1.52 | 6 (13%)  | 56,67,67    | 1.82 | 14 (25%) |
| 5   | PEB  | N     | 202 | 2    | 46,46,46     | 1.67 | 11 (23%) | 56,67,67    | 1.54 | 11 (19%) |
| 5   | PEB  | H     | 203 | 2    | 46,46,46     | 1.51 | 6 (13%)  | 56,67,67    | 1.74 | 14 (25%) |
| 5   | PEB  | B     | 202 | 2    | 46,46,46     | 1.52 | 8 (17%)  | 56,67,67    | 1.56 | 10 (17%) |
| 5   | PEB  | J     | 202 | 2    | 46,46,46     | 1.57 | 7 (15%)  | 56,67,67    | 1.57 | 9 (16%)  |
| 5   | PEB  | L     | 203 | 2    | 46,46,46     | 1.55 | 7 (15%)  | 56,67,67    | 1.71 | 12 (21%) |
| 4   | DBV  | K     | 101 | 3    | 46,46,46     | 2.14 | 11 (23%) | 56,67,67    | 1.90 | 17 (30%) |
| 4   | DBV  | E     | 101 | 1    | 46,46,46     | 2.10 | 11 (23%) | 56,67,67    | 1.87 | 16 (28%) |
| 5   | PEB  | D     | 202 | 2    | 46,46,46     | 1.55 | 10 (21%) | 56,67,67    | 1.70 | 11 (19%) |
| 5   | PEB  | N     | 203 | 2    | 46,46,46     | 1.48 | 8 (17%)  | 56,67,67    | 1.72 | 13 (23%) |
| 5   | PEB  | B     | 203 | 2    | 46,46,46     | 1.49 | 10 (21%) | 56,67,67    | 1.76 | 16 (28%) |
| 5   | PEB  | J     | 201 | 2    | 46,46,46     | 1.48 | 6 (13%)  | 56,67,67    | 1.78 | 14 (25%) |
| 5   | PEB  | P     | 202 | 2    | 46,46,46     | 1.62 | 8 (17%)  | 56,67,67    | 1.61 | 12 (21%) |
| 5   | PEB  | P     | 201 | 2    | 46,46,46     | 1.54 | 6 (13%)  | 56,67,67    | 1.80 | 15 (26%) |
| 4   | DBV  | A     | 101 | 1    | 46,46,46     | 2.21 | 10 (21%) | 56,67,67    | 1.85 | 16 (28%) |
| 5   | PEB  | D     | 201 | 2    | 46,46,46     | 1.46 | 5 (10%)  | 56,67,67    | 1.95 | 15 (26%) |
| 5   | PEB  | F     | 203 | 2    | 46,46,46     | 1.48 | 7 (15%)  | 56,67,67    | 1.71 | 9 (16%)  |
| 5   | PEB  | B     | 201 | 2    | 46,46,46     | 1.48 | 5 (10%)  | 56,67,67    | 1.64 | 12 (21%) |
| 5   | PEB  | J     | 203 | 2    | 46,46,46     | 1.57 | 7 (15%)  | 56,67,67    | 1.76 | 13 (23%) |
| 4   | DBV  | O     | 101 | 3    | 46,46,46     | 2.21 | 12 (26%) | 56,67,67    | 1.97 | 19 (33%) |
| 4   | DBV  | M     | 101 | 1    | 46,46,46     | 2.33 | 11 (23%) | 56,67,67    | 1.84 | 15 (26%) |
| 4   | DBV  | G     | 101 | 3    | 46,46,46     | 2.13 | 10 (21%) | 56,67,67    | 1.87 | 17 (30%) |
| 5   | PEB  | H     | 202 | 2    | 46,46,46     | 1.60 | 8 (17%)  | 56,67,67    | 1.57 | 12 (21%) |
| 5   | PEB  | N     | 201 | 2    | 46,46,46     | 1.48 | 6 (13%)  | 56,67,67    | 1.62 | 11 (19%) |
| 5   | PEB  | P     | 203 | 2    | 46,46,46     | 1.46 | 6 (13%)  | 56,67,67    | 1.76 | 11 (19%) |
| 4   | DBV  | I     | 101 | 1    | 46,46,46     | 2.35 | 11 (23%) | 56,67,67    | 1.80 | 15 (26%) |
| 5   | PEB  | F     | 202 | 2    | 46,46,46     | 1.58 | 8 (17%)  | 56,67,67    | 1.67 | 11 (19%) |
| 5   | PEB  | F     | 201 | 2    | 46,46,46     | 1.65 | 7 (15%)  | 56,67,67    | 1.79 | 16 (28%) |
| 5   | PEB  | D     | 203 | 2    | 46,46,46     | 1.57 | 7 (15%)  | 56,67,67    | 1.75 | 14 (25%) |

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   | PEB  | H     | 201 | 2    | -       | 6/26/74/74  | 0/4/4/4 |
| 4   | DBV  | C     | 101 | 3    | -       | 12/26/74/74 | 0/4/4/4 |
| 5   | PEB  | L     | 202 | 2    | -       | 11/26/74/74 | 0/4/4/4 |
| 5   | PEB  | L     | 201 | 2    | -       | 6/26/74/74  | 0/4/4/4 |
| 5   | PEB  | N     | 202 | 2    | -       | 8/26/74/74  | 0/4/4/4 |
| 5   | PEB  | H     | 203 | 2    | -       | 4/26/74/74  | 0/4/4/4 |
| 5   | PEB  | B     | 202 | 2    | -       | 9/26/74/74  | 0/4/4/4 |
| 5   | PEB  | J     | 202 | 2    | -       | 8/26/74/74  | 0/4/4/4 |
| 5   | PEB  | L     | 203 | 2    | -       | 4/26/74/74  | 0/4/4/4 |
| 4   | DBV  | K     | 101 | 3    | -       | 6/26/74/74  | 0/4/4/4 |
| 4   | DBV  | E     | 101 | 1    | -       | 6/26/74/74  | 0/4/4/4 |
| 5   | PEB  | D     | 202 | 2    | -       | 9/26/74/74  | 0/4/4/4 |
| 5   | PEB  | N     | 203 | 2    | -       | 4/26/74/74  | 0/4/4/4 |
| 5   | PEB  | B     | 203 | 2    | -       | 6/26/74/74  | 0/4/4/4 |
| 5   | PEB  | J     | 201 | 2    | -       | 6/26/74/74  | 0/4/4/4 |
| 5   | PEB  | P     | 202 | 2    | -       | 8/26/74/74  | 0/4/4/4 |
| 5   | PEB  | P     | 201 | 2    | -       | 4/26/74/74  | 0/4/4/4 |
| 4   | DBV  | A     | 101 | 1    | -       | 6/26/74/74  | 0/4/4/4 |
| 5   | PEB  | D     | 201 | 2    | -       | 6/26/74/74  | 0/4/4/4 |
| 5   | PEB  | F     | 203 | 2    | -       | 6/26/74/74  | 0/4/4/4 |
| 5   | PEB  | B     | 201 | 2    | -       | 6/26/74/74  | 0/4/4/4 |
| 5   | PEB  | J     | 203 | 2    | -       | 6/26/74/74  | 0/4/4/4 |
| 4   | DBV  | O     | 101 | 3    | -       | 7/26/74/74  | 0/4/4/4 |
| 4   | DBV  | M     | 101 | 1    | -       | 7/26/74/74  | 0/4/4/4 |
| 4   | DBV  | G     | 101 | 3    | -       | 7/26/74/74  | 0/4/4/4 |
| 5   | PEB  | H     | 202 | 2    | -       | 7/26/74/74  | 0/4/4/4 |
| 5   | PEB  | N     | 201 | 2    | -       | 4/26/74/74  | 0/4/4/4 |
| 5   | PEB  | P     | 203 | 2    | -       | 4/26/74/74  | 0/4/4/4 |
| 4   | DBV  | I     | 101 | 1    | -       | 9/26/74/74  | 0/4/4/4 |
| 5   | PEB  | F     | 202 | 2    | -       | 6/26/74/74  | 0/4/4/4 |
| 5   | PEB  | F     | 201 | 2    | -       | 6/26/74/74  | 0/4/4/4 |
| 5   | PEB  | D     | 203 | 2    | -       | 4/26/74/74  | 0/4/4/4 |

All (259) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 4   | M     | 101 | DBV  | C4B-C3B | 7.46 | 1.59        | 1.42     |
| 4   | I     | 101 | DBV  | C4B-C3B | 6.61 | 1.57        | 1.42     |
| 4   | C     | 101 | DBV  | CHA-C1B | 6.34 | 1.54        | 1.40     |
| 4   | O     | 101 | DBV  | C4B-C3B | 6.16 | 1.56        | 1.42     |
| 4   | A     | 101 | DBV  | C4B-C3B | 6.12 | 1.56        | 1.42     |
| 4   | I     | 101 | DBV  | CHA-C1B | 6.01 | 1.54        | 1.40     |
| 4   | O     | 101 | DBV  | CHA-C1B | 6.00 | 1.53        | 1.40     |
| 4   | G     | 101 | DBV  | CHA-C1B | 5.95 | 1.53        | 1.40     |
| 4   | K     | 101 | DBV  | C4B-C3B | 5.93 | 1.55        | 1.42     |
| 4   | C     | 101 | DBV  | C4B-C3B | 5.89 | 1.55        | 1.42     |
| 4   | M     | 101 | DBV  | CHB-C4B | 5.89 | 1.53        | 1.40     |
| 4   | I     | 101 | DBV  | CHB-C4B | 5.81 | 1.53        | 1.40     |
| 4   | K     | 101 | DBV  | CHA-C1B | 5.72 | 1.53        | 1.40     |
| 4   | A     | 101 | DBV  | CHB-C4B | 5.71 | 1.53        | 1.40     |
| 4   | O     | 101 | DBV  | CHB-C4B | 5.64 | 1.53        | 1.40     |
| 4   | C     | 101 | DBV  | CHB-C4B | 5.58 | 1.53        | 1.40     |
| 4   | E     | 101 | DBV  | CHA-C1B | 5.55 | 1.52        | 1.40     |
| 4   | O     | 101 | DBV  | C1B-NB  | 5.55 | 1.47        | 1.37     |
| 5   | L     | 203 | PEB  | C4C-C3C | 5.51 | 1.45        | 1.38     |
| 4   | I     | 101 | DBV  | C1B-NB  | 5.46 | 1.47        | 1.37     |
| 4   | E     | 101 | DBV  | CHB-C4B | 5.39 | 1.52        | 1.40     |
| 4   | A     | 101 | DBV  | CHA-C1B | 5.36 | 1.52        | 1.40     |
| 5   | B     | 202 | PEB  | C4C-C3C | 5.31 | 1.45        | 1.38     |
| 4   | K     | 101 | DBV  | CHB-C4B | 5.27 | 1.52        | 1.40     |
| 4   | E     | 101 | DBV  | C4B-C3B | 5.25 | 1.54        | 1.42     |
| 4   | C     | 101 | DBV  | C1B-NB  | 5.24 | 1.46        | 1.37     |
| 5   | H     | 201 | PEB  | C4C-C3C | 5.24 | 1.45        | 1.38     |
| 4   | M     | 101 | DBV  | C1B-NB  | 5.21 | 1.46        | 1.37     |
| 5   | B     | 201 | PEB  | C4C-C3C | 5.20 | 1.45        | 1.38     |
| 5   | L     | 202 | PEB  | C4C-C3C | 5.16 | 1.45        | 1.38     |
| 4   | M     | 101 | DBV  | CHA-C1B | 5.15 | 1.52        | 1.40     |
| 5   | P     | 202 | PEB  | C4C-C3C | 5.13 | 1.45        | 1.38     |
| 4   | K     | 101 | DBV  | C1B-NB  | 5.09 | 1.46        | 1.37     |
| 5   | J     | 202 | PEB  | C4C-C3C | 5.06 | 1.45        | 1.38     |
| 5   | F     | 201 | PEB  | C4C-C3C | 5.04 | 1.45        | 1.38     |
| 5   | P     | 201 | PEB  | C4C-C3C | 5.01 | 1.45        | 1.38     |
| 5   | N     | 202 | PEB  | C4C-C3C | 5.01 | 1.45        | 1.38     |
| 5   | D     | 201 | PEB  | C4C-C3C | 5.00 | 1.45        | 1.38     |
| 5   | F     | 202 | PEB  | C4C-C3C | 4.96 | 1.45        | 1.38     |
| 5   | L     | 201 | PEB  | C4C-C3C | 4.95 | 1.45        | 1.38     |
| 4   | G     | 101 | DBV  | C1B-NB  | 4.84 | 1.46        | 1.37     |
| 4   | G     | 101 | DBV  | CHB-C4B | 4.83 | 1.51        | 1.40     |
| 5   | D     | 203 | PEB  | C4C-C3C | 4.83 | 1.44        | 1.38     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 5   | J     | 201 | PEB  | C4C-C3C | 4.82  | 1.44        | 1.38     |
| 5   | B     | 203 | PEB  | C4C-C3C | 4.80  | 1.44        | 1.38     |
| 5   | P     | 203 | PEB  | C4C-C3C | 4.79  | 1.44        | 1.38     |
| 5   | N     | 201 | PEB  | C4C-C3C | 4.77  | 1.44        | 1.38     |
| 5   | H     | 203 | PEB  | C4C-C3C | 4.76  | 1.44        | 1.38     |
| 4   | G     | 101 | DBV  | C4B-C3B | 4.76  | 1.53        | 1.42     |
| 5   | J     | 203 | PEB  | C4C-C3C | 4.75  | 1.44        | 1.38     |
| 5   | F     | 203 | PEB  | C4C-C3C | 4.74  | 1.44        | 1.38     |
| 5   | D     | 202 | PEB  | C4C-C3C | 4.72  | 1.44        | 1.38     |
| 5   | H     | 202 | PEB  | C4C-C3C | 4.61  | 1.44        | 1.38     |
| 5   | N     | 203 | PEB  | C4C-C3C | 4.58  | 1.44        | 1.38     |
| 4   | I     | 101 | DBV  | CBC-CGC | 4.53  | 1.61        | 1.50     |
| 4   | C     | 101 | DBV  | CBC-CGC | 4.37  | 1.60        | 1.50     |
| 4   | A     | 101 | DBV  | CBB-CGB | 4.31  | 1.60        | 1.50     |
| 5   | N     | 202 | PEB  | CBB-CGB | -4.21 | 1.40        | 1.50     |
| 4   | C     | 101 | DBV  | CBB-CGB | 4.07  | 1.60        | 1.50     |
| 5   | F     | 201 | PEB  | CHB-C1C | 4.03  | 1.49        | 1.40     |
| 4   | I     | 101 | DBV  | CBB-CGB | 3.96  | 1.59        | 1.50     |
| 5   | P     | 202 | PEB  | CHB-C1C | 3.94  | 1.49        | 1.40     |
| 4   | A     | 101 | DBV  | CBC-CGC | 3.94  | 1.59        | 1.50     |
| 5   | J     | 201 | PEB  | C4C-NC  | 3.93  | 1.45        | 1.37     |
| 4   | G     | 101 | DBV  | CBC-CGC | 3.91  | 1.59        | 1.50     |
| 4   | E     | 101 | DBV  | CBB-CGB | 3.89  | 1.59        | 1.50     |
| 4   | A     | 101 | DBV  | C1B-NB  | 3.87  | 1.44        | 1.37     |
| 5   | P     | 201 | PEB  | CHB-C1C | 3.84  | 1.49        | 1.40     |
| 4   | A     | 101 | DBV  | C4B-NB  | -3.82 | 1.31        | 1.37     |
| 4   | M     | 101 | DBV  | CBC-CGC | 3.73  | 1.59        | 1.50     |
| 4   | M     | 101 | DBV  | CBB-CGB | 3.71  | 1.59        | 1.50     |
| 5   | F     | 202 | PEB  | C4C-NC  | 3.60  | 1.45        | 1.37     |
| 5   | F     | 201 | PEB  | C4C-NC  | 3.59  | 1.44        | 1.37     |
| 5   | H     | 203 | PEB  | CHB-C1C | 3.58  | 1.48        | 1.40     |
| 5   | P     | 202 | PEB  | C4C-NC  | 3.58  | 1.44        | 1.37     |
| 5   | H     | 201 | PEB  | CBB-CGB | -3.58 | 1.42        | 1.50     |
| 4   | E     | 101 | DBV  | C4B-NB  | -3.55 | 1.31        | 1.37     |
| 5   | L     | 201 | PEB  | CHB-C1C | 3.52  | 1.48        | 1.40     |
| 4   | O     | 101 | DBV  | C4B-NB  | -3.50 | 1.31        | 1.37     |
| 5   | P     | 201 | PEB  | C4C-NC  | 3.49  | 1.44        | 1.37     |
| 4   | G     | 101 | DBV  | C4B-NB  | -3.47 | 1.31        | 1.37     |
| 5   | J     | 202 | PEB  | CBB-CGB | -3.45 | 1.42        | 1.50     |
| 4   | C     | 101 | DBV  | C1B-C2B | 3.45  | 1.49        | 1.41     |
| 4   | C     | 101 | DBV  | C4B-NB  | -3.44 | 1.31        | 1.37     |
| 5   | D     | 203 | PEB  | CBB-CGB | -3.44 | 1.42        | 1.50     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4   | E     | 101 | DBV  | CBC-CGC | 3.43  | 1.58        | 1.50     |
| 4   | M     | 101 | DBV  | C4B-NB  | -3.41 | 1.32        | 1.37     |
| 4   | E     | 101 | DBV  | C1B-NB  | 3.40  | 1.43        | 1.37     |
| 4   | K     | 101 | DBV  | C4B-NB  | -3.40 | 1.32        | 1.37     |
| 5   | F     | 201 | PEB  | CHC-C4C | 3.39  | 1.54        | 1.50     |
| 4   | G     | 101 | DBV  | C1B-C2B | 3.38  | 1.49        | 1.41     |
| 5   | H     | 203 | PEB  | C4C-NC  | 3.37  | 1.44        | 1.37     |
| 5   | P     | 203 | PEB  | CHB-C1C | 3.33  | 1.47        | 1.40     |
| 4   | K     | 101 | DBV  | CBC-CGC | 3.28  | 1.58        | 1.50     |
| 5   | H     | 202 | PEB  | CHC-C1D | -3.27 | 1.46        | 1.53     |
| 5   | D     | 203 | PEB  | CHB-C1C | 3.26  | 1.47        | 1.40     |
| 5   | N     | 201 | PEB  | C4C-NC  | 3.25  | 1.44        | 1.37     |
| 4   | I     | 101 | DBV  | C4B-NB  | -3.25 | 1.32        | 1.37     |
| 5   | L     | 202 | PEB  | CHB-C1C | 3.19  | 1.47        | 1.40     |
| 4   | K     | 101 | DBV  | C1B-C2B | 3.17  | 1.49        | 1.41     |
| 4   | O     | 101 | DBV  | C1B-C2B | 3.17  | 1.49        | 1.41     |
| 5   | D     | 201 | PEB  | C4C-NC  | 3.14  | 1.44        | 1.37     |
| 4   | E     | 101 | DBV  | C1B-C2B | 3.13  | 1.48        | 1.41     |
| 4   | G     | 101 | DBV  | CBB-CGB | 3.12  | 1.57        | 1.50     |
| 5   | H     | 202 | PEB  | CHB-C1C | 3.11  | 1.47        | 1.40     |
| 4   | A     | 101 | DBV  | C3A-C2A | 3.10  | 1.43        | 1.37     |
| 4   | I     | 101 | DBV  | C1B-C2B | 3.07  | 1.48        | 1.41     |
| 5   | H     | 203 | PEB  | CBB-CGB | -3.07 | 1.43        | 1.50     |
| 5   | L     | 202 | PEB  | C4C-NC  | 3.07  | 1.43        | 1.37     |
| 5   | J     | 202 | PEB  | C4C-NC  | 3.05  | 1.43        | 1.37     |
| 5   | J     | 203 | PEB  | CHC-C1D | -3.05 | 1.47        | 1.53     |
| 4   | M     | 101 | DBV  | C1B-C2B | 3.04  | 1.48        | 1.41     |
| 4   | A     | 101 | DBV  | C1B-C2B | 3.03  | 1.48        | 1.41     |
| 4   | O     | 101 | DBV  | C1C-NC  | -3.02 | 1.32        | 1.38     |
| 5   | H     | 202 | PEB  | C4C-NC  | 3.00  | 1.43        | 1.37     |
| 5   | F     | 201 | PEB  | CBC-CGC | -2.99 | 1.43        | 1.50     |
| 4   | C     | 101 | DBV  | C3A-C2A | 2.98  | 1.43        | 1.37     |
| 5   | B     | 202 | PEB  | C4C-NC  | 2.98  | 1.43        | 1.37     |
| 4   | G     | 101 | DBV  | C3A-C2A | 2.98  | 1.43        | 1.37     |
| 5   | L     | 201 | PEB  | C4C-NC  | 2.97  | 1.43        | 1.37     |
| 5   | P     | 203 | PEB  | C4C-NC  | 2.97  | 1.43        | 1.37     |
| 5   | N     | 203 | PEB  | CHB-C1C | 2.94  | 1.47        | 1.40     |
| 5   | D     | 203 | PEB  | C4C-NC  | 2.92  | 1.43        | 1.37     |
| 4   | M     | 101 | DBV  | C3A-C2A | 2.90  | 1.43        | 1.37     |
| 5   | H     | 202 | PEB  | CMD-C2D | -2.89 | 1.45        | 1.50     |
| 5   | D     | 202 | PEB  | C4C-NC  | 2.87  | 1.43        | 1.37     |
| 5   | N     | 202 | PEB  | C4C-NC  | 2.81  | 1.43        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4   | E     | 101 | DBV  | C3A-C2A | 2.78  | 1.42        | 1.37     |
| 5   | L     | 203 | PEB  | C4C-NC  | 2.78  | 1.43        | 1.37     |
| 5   | J     | 203 | PEB  | C1C-NC  | -2.77 | 1.33        | 1.37     |
| 5   | J     | 202 | PEB  | CHB-C1C | 2.77  | 1.46        | 1.40     |
| 5   | F     | 203 | PEB  | CBC-CGC | -2.76 | 1.44        | 1.50     |
| 5   | B     | 201 | PEB  | CBB-CGB | -2.76 | 1.44        | 1.50     |
| 4   | I     | 101 | DBV  | C3A-C2A | 2.73  | 1.42        | 1.37     |
| 5   | J     | 203 | PEB  | CBC-CGC | -2.70 | 1.44        | 1.50     |
| 4   | I     | 101 | DBV  | C1C-NC  | -2.70 | 1.32        | 1.38     |
| 5   | L     | 203 | PEB  | CHC-C1D | -2.69 | 1.48        | 1.53     |
| 5   | H     | 201 | PEB  | C4C-NC  | 2.64  | 1.42        | 1.37     |
| 5   | F     | 201 | PEB  | CBB-CGB | -2.62 | 1.44        | 1.50     |
| 5   | F     | 202 | PEB  | CHC-C1D | -2.62 | 1.48        | 1.53     |
| 5   | F     | 202 | PEB  | C1C-NC  | -2.62 | 1.33        | 1.37     |
| 5   | J     | 201 | PEB  | CHB-C1C | 2.62  | 1.46        | 1.40     |
| 5   | D     | 201 | PEB  | CHB-C1C | 2.62  | 1.46        | 1.40     |
| 5   | P     | 202 | PEB  | CBC-CGC | -2.62 | 1.44        | 1.50     |
| 5   | D     | 203 | PEB  | CMD-C2D | -2.60 | 1.46        | 1.50     |
| 5   | N     | 202 | PEB  | CMD-C2D | -2.60 | 1.46        | 1.50     |
| 5   | N     | 202 | PEB  | C1C-NC  | -2.60 | 1.33        | 1.37     |
| 5   | F     | 203 | PEB  | C4C-NC  | 2.59  | 1.42        | 1.37     |
| 4   | O     | 101 | DBV  | CBB-CGB | 2.56  | 1.56        | 1.50     |
| 5   | P     | 203 | PEB  | CMD-C2D | -2.56 | 1.46        | 1.50     |
| 5   | D     | 202 | PEB  | CHC-C1D | -2.55 | 1.48        | 1.53     |
| 5   | P     | 201 | PEB  | C1C-NC  | -2.55 | 1.33        | 1.37     |
| 5   | L     | 201 | PEB  | CBB-CGB | -2.54 | 1.44        | 1.50     |
| 5   | F     | 202 | PEB  | C4B-NB  | -2.54 | 1.33        | 1.38     |
| 5   | B     | 201 | PEB  | C4C-NC  | 2.53  | 1.42        | 1.37     |
| 5   | D     | 203 | PEB  | CBC-CGC | -2.53 | 1.44        | 1.50     |
| 5   | N     | 202 | PEB  | CHA-C4A | -2.53 | 1.32        | 1.36     |
| 5   | B     | 202 | PEB  | CBC-CGC | -2.52 | 1.44        | 1.50     |
| 5   | H     | 202 | PEB  | CBC-CGC | -2.52 | 1.44        | 1.50     |
| 5   | D     | 202 | PEB  | CMD-C2D | -2.49 | 1.46        | 1.50     |
| 4   | M     | 101 | DBV  | C1C-NC  | -2.49 | 1.33        | 1.38     |
| 5   | J     | 202 | PEB  | C4B-C3B | -2.48 | 1.41        | 1.45     |
| 4   | K     | 101 | DBV  | C1C-NC  | -2.48 | 1.33        | 1.38     |
| 5   | H     | 202 | PEB  | C1C-NC  | -2.48 | 1.33        | 1.37     |
| 5   | P     | 202 | PEB  | C4B-NB  | -2.46 | 1.33        | 1.38     |
| 5   | N     | 202 | PEB  | C4B-C3B | -2.46 | 1.41        | 1.45     |
| 5   | B     | 203 | PEB  | CBB-CGB | -2.44 | 1.44        | 1.50     |
| 5   | H     | 201 | PEB  | CHB-C1C | 2.44  | 1.45        | 1.40     |
| 5   | L     | 202 | PEB  | CMD-C2D | -2.44 | 1.46        | 1.50     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 5   | P     | 203 | PEB  | CBB-CGB | -2.43 | 1.45        | 1.50     |
| 4   | K     | 101 | DBV  | C3A-C2A | 2.42  | 1.42        | 1.37     |
| 5   | B     | 201 | PEB  | CHB-C1C | 2.42  | 1.45        | 1.40     |
| 5   | F     | 203 | PEB  | CHB-C1C | 2.41  | 1.45        | 1.40     |
| 4   | C     | 101 | DBV  | C1C-NC  | -2.41 | 1.33        | 1.38     |
| 5   | N     | 201 | PEB  | CBB-CGB | -2.39 | 1.45        | 1.50     |
| 4   | K     | 101 | DBV  | CBB-CGB | 2.38  | 1.56        | 1.50     |
| 5   | F     | 203 | PEB  | C4B-NB  | -2.37 | 1.33        | 1.38     |
| 5   | L     | 203 | PEB  | CHB-C1C | 2.36  | 1.45        | 1.40     |
| 5   | P     | 202 | PEB  | CHC-C1D | -2.36 | 1.48        | 1.53     |
| 5   | N     | 203 | PEB  | CBB-CGB | -2.36 | 1.45        | 1.50     |
| 5   | L     | 203 | PEB  | CBB-CGB | -2.35 | 1.45        | 1.50     |
| 5   | J     | 202 | PEB  | C1C-NC  | -2.35 | 1.33        | 1.37     |
| 5   | N     | 201 | PEB  | C4B-NB  | -2.35 | 1.33        | 1.38     |
| 5   | B     | 202 | PEB  | CBB-CGB | -2.35 | 1.45        | 1.50     |
| 5   | D     | 202 | PEB  | CBB-CGB | -2.34 | 1.45        | 1.50     |
| 5   | J     | 203 | PEB  | CHB-C1C | 2.34  | 1.45        | 1.40     |
| 5   | N     | 202 | PEB  | CHB-C1C | 2.34  | 1.45        | 1.40     |
| 5   | B     | 202 | PEB  | C4B-NB  | -2.34 | 1.33        | 1.38     |
| 5   | D     | 201 | PEB  | CBB-CGB | -2.33 | 1.45        | 1.50     |
| 5   | N     | 203 | PEB  | C1C-NC  | -2.33 | 1.33        | 1.37     |
| 5   | B     | 203 | PEB  | C4B-NB  | -2.33 | 1.33        | 1.38     |
| 5   | F     | 202 | PEB  | CHB-C1C | 2.31  | 1.45        | 1.40     |
| 5   | L     | 203 | PEB  | C2D-C3D | 2.31  | 1.37        | 1.34     |
| 5   | D     | 202 | PEB  | C1C-NC  | -2.29 | 1.33        | 1.37     |
| 5   | N     | 203 | PEB  | CHC-C1D | -2.29 | 1.48        | 1.53     |
| 5   | N     | 203 | PEB  | C4C-NC  | 2.29  | 1.42        | 1.37     |
| 5   | J     | 201 | PEB  | CBC-CGC | -2.29 | 1.45        | 1.50     |
| 5   | D     | 203 | PEB  | C1C-NC  | -2.29 | 1.33        | 1.37     |
| 5   | P     | 201 | PEB  | C4B-NB  | -2.29 | 1.33        | 1.38     |
| 5   | J     | 202 | PEB  | CMD-C2D | -2.28 | 1.46        | 1.50     |
| 5   | F     | 203 | PEB  | C1C-NC  | -2.28 | 1.33        | 1.37     |
| 5   | N     | 201 | PEB  | CHB-C1C | 2.28  | 1.45        | 1.40     |
| 5   | B     | 203 | PEB  | CMC-C3C | -2.28 | 1.46        | 1.50     |
| 5   | F     | 202 | PEB  | CMD-C2D | -2.26 | 1.46        | 1.50     |
| 5   | H     | 201 | PEB  | C4B-C3B | -2.26 | 1.42        | 1.45     |
| 5   | B     | 203 | PEB  | C4C-NC  | 2.25  | 1.42        | 1.37     |
| 4   | E     | 101 | DBV  | C1C-NC  | -2.25 | 1.33        | 1.38     |
| 5   | J     | 201 | PEB  | CHC-C4C | 2.24  | 1.52        | 1.50     |
| 5   | N     | 201 | PEB  | CBC-CGC | -2.22 | 1.45        | 1.50     |
| 4   | O     | 101 | DBV  | C3A-C2A | 2.22  | 1.41        | 1.37     |
| 5   | N     | 203 | PEB  | CBC-CGC | -2.22 | 1.45        | 1.50     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 5   | L     | 202 | PEB  | C4B-NB  | -2.22 | 1.33        | 1.38     |
| 5   | D     | 202 | PEB  | CHA-C1B | 2.21  | 1.45        | 1.40     |
| 4   | O     | 101 | DBV  | CBC-CGC | 2.21  | 1.55        | 1.50     |
| 5   | F     | 202 | PEB  | CBB-CGB | -2.21 | 1.45        | 1.50     |
| 5   | L     | 202 | PEB  | CHC-C1D | -2.20 | 1.49        | 1.53     |
| 5   | P     | 201 | PEB  | CBB-CGB | -2.20 | 1.45        | 1.50     |
| 5   | B     | 201 | PEB  | C4B-NB  | -2.19 | 1.33        | 1.38     |
| 5   | P     | 203 | PEB  | CHC-C1D | -2.19 | 1.49        | 1.53     |
| 5   | B     | 203 | PEB  | CBC-CGC | -2.18 | 1.45        | 1.50     |
| 5   | J     | 201 | PEB  | CBB-CGB | -2.17 | 1.45        | 1.50     |
| 5   | B     | 203 | PEB  | C1C-NC  | -2.17 | 1.34        | 1.37     |
| 5   | H     | 201 | PEB  | C1C-NC  | -2.17 | 1.34        | 1.37     |
| 5   | L     | 201 | PEB  | C1C-NC  | -2.17 | 1.34        | 1.37     |
| 5   | D     | 202 | PEB  | CHB-C1C | 2.17  | 1.45        | 1.40     |
| 5   | B     | 203 | PEB  | CHC-C1D | -2.16 | 1.49        | 1.53     |
| 4   | I     | 101 | DBV  | C1A-C2A | -2.16 | 1.43        | 1.48     |
| 5   | B     | 203 | PEB  | CMD-C2D | -2.15 | 1.47        | 1.50     |
| 5   | H     | 202 | PEB  | C4B-NB  | -2.15 | 1.34        | 1.38     |
| 4   | O     | 101 | DBV  | CAD-C3D | 2.15  | 1.53        | 1.47     |
| 5   | J     | 203 | PEB  | CBB-CGB | -2.15 | 1.45        | 1.50     |
| 5   | B     | 202 | PEB  | CHB-C1C | 2.15  | 1.45        | 1.40     |
| 5   | L     | 201 | PEB  | CBC-CGC | -2.14 | 1.45        | 1.50     |
| 5   | F     | 201 | PEB  | C4B-NB  | -2.12 | 1.34        | 1.38     |
| 5   | D     | 202 | PEB  | C4B-C3B | -2.12 | 1.42        | 1.45     |
| 4   | A     | 101 | DBV  | C1C-NC  | -2.11 | 1.34        | 1.38     |
| 5   | H     | 203 | PEB  | CAA-C3A | -2.10 | 1.50        | 1.54     |
| 5   | H     | 201 | PEB  | C4B-NB  | -2.10 | 1.34        | 1.38     |
| 5   | D     | 201 | PEB  | C4B-C3B | -2.09 | 1.42        | 1.45     |
| 5   | D     | 202 | PEB  | C4B-NB  | -2.09 | 1.34        | 1.38     |
| 4   | G     | 101 | DBV  | C1C-NC  | -2.09 | 1.34        | 1.38     |
| 4   | E     | 101 | DBV  | C4D-ND  | 2.09  | 1.37        | 1.35     |
| 5   | P     | 202 | PEB  | CMD-C2D | -2.08 | 1.47        | 1.50     |
| 5   | J     | 203 | PEB  | CMC-C3C | -2.08 | 1.46        | 1.50     |
| 4   | K     | 101 | DBV  | CHB-C1C | -2.08 | 1.34        | 1.38     |
| 5   | B     | 202 | PEB  | O2C-CGC | -2.07 | 1.24        | 1.30     |
| 5   | L     | 203 | PEB  | C4B-NB  | -2.07 | 1.34        | 1.38     |
| 5   | P     | 202 | PEB  | CBB-CGB | -2.07 | 1.45        | 1.50     |
| 5   | N     | 202 | PEB  | CHC-C1D | -2.06 | 1.49        | 1.53     |
| 5   | H     | 203 | PEB  | CBC-CGC | -2.05 | 1.45        | 1.50     |
| 5   | B     | 202 | PEB  | C1C-NC  | -2.05 | 1.34        | 1.37     |
| 5   | N     | 202 | PEB  | CBC-CGC | -2.04 | 1.45        | 1.50     |
| 5   | B     | 203 | PEB  | CMB-C2B | -2.04 | 1.46        | 1.50     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 5   | F     | 203 | PEB  | CMB-C2B | -2.04 | 1.46        | 1.50     |
| 4   | M     | 101 | DBV  | CMC-C3C | -2.01 | 1.46        | 1.50     |
| 5   | N     | 203 | PEB  | C4B-NB  | -2.01 | 1.34        | 1.38     |
| 5   | N     | 202 | PEB  | CAB-C3B | -2.01 | 1.46        | 1.51     |
| 5   | H     | 201 | PEB  | CMD-C2D | -2.01 | 1.47        | 1.50     |
| 4   | O     | 101 | DBV  | CHB-C1C | -2.00 | 1.34        | 1.38     |

All (430) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 4   | O     | 101 | DBV  | C1D-ND-C4D  | -6.46 | 103.48      | 113.42   |
| 5   | P     | 201 | PEB  | CMC-C3C-C4C | -6.12 | 120.40      | 126.97   |
| 5   | P     | 203 | PEB  | CMC-C3C-C4C | -6.04 | 120.49      | 126.97   |
| 5   | D     | 202 | PEB  | CMC-C3C-C4C | -5.95 | 120.58      | 126.97   |
| 4   | M     | 101 | DBV  | C1D-ND-C4D  | -5.74 | 104.59      | 113.42   |
| 5   | D     | 203 | PEB  | CMC-C3C-C4C | -5.70 | 120.85      | 126.97   |
| 4   | K     | 101 | DBV  | C1D-ND-C4D  | -5.65 | 104.73      | 113.42   |
| 4   | I     | 101 | DBV  | C1D-ND-C4D  | -5.56 | 104.87      | 113.42   |
| 5   | N     | 203 | PEB  | CMC-C3C-C4C | -5.56 | 121.01      | 126.97   |
| 4   | G     | 101 | DBV  | C1D-ND-C4D  | -5.52 | 104.94      | 113.42   |
| 4   | C     | 101 | DBV  | C1D-ND-C4D  | -5.50 | 104.95      | 113.42   |
| 5   | H     | 201 | PEB  | CMC-C3C-C4C | -5.48 | 121.09      | 126.97   |
| 5   | F     | 201 | PEB  | CMC-C3C-C4C | -5.46 | 121.11      | 126.97   |
| 5   | L     | 201 | PEB  | CMC-C3C-C4C | -5.44 | 121.13      | 126.97   |
| 5   | H     | 203 | PEB  | CMC-C3C-C4C | -5.39 | 121.18      | 126.97   |
| 5   | J     | 202 | PEB  | CMC-C3C-C4C | -5.37 | 121.21      | 126.97   |
| 5   | L     | 203 | PEB  | CMC-C3C-C4C | -5.36 | 121.21      | 126.97   |
| 5   | B     | 203 | PEB  | CMC-C3C-C4C | -5.30 | 121.28      | 126.97   |
| 5   | D     | 201 | PEB  | CMC-C3C-C4C | -5.25 | 121.33      | 126.97   |
| 4   | A     | 101 | DBV  | C1D-ND-C4D  | -5.22 | 105.40      | 113.42   |
| 4   | E     | 101 | DBV  | C1D-ND-C4D  | -5.11 | 105.56      | 113.42   |
| 5   | F     | 202 | PEB  | CMC-C3C-C4C | -5.07 | 121.53      | 126.97   |
| 5   | L     | 202 | PEB  | CMC-C3C-C4C | -5.04 | 121.56      | 126.97   |
| 5   | N     | 202 | PEB  | CMC-C3C-C4C | -5.04 | 121.56      | 126.97   |
| 5   | J     | 201 | PEB  | CMC-C3C-C4C | -5.01 | 121.60      | 126.97   |
| 5   | F     | 201 | PEB  | C3C-C4C-NC  | -4.99 | 104.28      | 108.31   |
| 5   | N     | 201 | PEB  | CMC-C3C-C4C | -4.92 | 121.69      | 126.97   |
| 5   | B     | 201 | PEB  | CMC-C3C-C4C | -4.89 | 121.72      | 126.97   |
| 5   | F     | 203 | PEB  | CMC-C3C-C4C | -4.83 | 121.78      | 126.97   |
| 5   | J     | 203 | PEB  | CMC-C3C-C4C | -4.81 | 121.81      | 126.97   |
| 5   | H     | 202 | PEB  | CMC-C3C-C4C | -4.75 | 121.88      | 126.97   |
| 5   | J     | 201 | PEB  | C3C-C4C-NC  | -4.65 | 104.55      | 108.31   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 5   | P     | 202 | PEB  | CMC-C3C-C4C | -4.45 | 122.19      | 126.97   |
| 4   | O     | 101 | DBV  | C1D-CHC-C4C | 4.42  | 124.09      | 113.74   |
| 5   | B     | 202 | PEB  | CMC-C3C-C4C | -4.32 | 122.34      | 126.97   |
| 4   | K     | 101 | DBV  | C4A-NA-C1A  | -4.18 | 105.53      | 110.66   |
| 4   | I     | 101 | DBV  | C4A-NA-C1A  | -4.18 | 105.53      | 110.66   |
| 5   | L     | 201 | PEB  | C2A-C3A-C4A | 4.15  | 107.55      | 101.34   |
| 4   | O     | 101 | DBV  | C4A-NA-C1A  | -4.08 | 105.65      | 110.66   |
| 4   | M     | 101 | DBV  | C4A-NA-C1A  | -4.05 | 105.69      | 110.66   |
| 5   | J     | 202 | PEB  | C3C-C4C-NC  | -4.03 | 105.05      | 108.31   |
| 5   | L     | 201 | PEB  | C2A-C1A-NA  | 4.02  | 111.63      | 108.29   |
| 5   | D     | 201 | PEB  | C2A-C1A-NA  | 4.00  | 111.62      | 108.29   |
| 5   | J     | 203 | PEB  | C1B-CHA-C4A | 4.00  | 135.37      | 127.25   |
| 4   | E     | 101 | DBV  | C4A-NA-C1A  | -3.99 | 105.76      | 110.66   |
| 5   | F     | 203 | PEB  | C2A-C1A-NA  | 3.96  | 111.58      | 108.29   |
| 5   | J     | 203 | PEB  | C2A-C1A-NA  | 3.88  | 111.52      | 108.29   |
| 5   | B     | 203 | PEB  | C2C-C1C-NC  | 3.88  | 112.43      | 107.57   |
| 4   | A     | 101 | DBV  | C1D-CHC-C4C | 3.78  | 122.59      | 113.74   |
| 5   | P     | 201 | PEB  | C2A-C3A-C4A | 3.78  | 107.00      | 101.34   |
| 5   | L     | 203 | PEB  | C2C-C1C-NC  | 3.76  | 112.29      | 107.57   |
| 5   | D     | 201 | PEB  | C2A-C3A-C4A | 3.76  | 106.97      | 101.34   |
| 4   | C     | 101 | DBV  | C4A-NA-C1A  | -3.75 | 106.06      | 110.66   |
| 5   | H     | 203 | PEB  | C1B-CHA-C4A | 3.73  | 134.82      | 127.25   |
| 5   | P     | 203 | PEB  | C2A-C1A-NA  | 3.71  | 111.38      | 108.29   |
| 4   | A     | 101 | DBV  | C4A-NA-C1A  | -3.70 | 106.12      | 110.66   |
| 5   | H     | 203 | PEB  | C2A-C3A-C4A | 3.69  | 106.86      | 101.34   |
| 5   | N     | 201 | PEB  | C2A-C1A-NA  | 3.67  | 111.34      | 108.29   |
| 5   | F     | 203 | PEB  | C3C-C4C-NC  | -3.67 | 105.34      | 108.31   |
| 4   | K     | 101 | DBV  | C1D-CHC-C4C | 3.65  | 122.28      | 113.74   |
| 5   | D     | 203 | PEB  | C2A-C3A-C4A | 3.64  | 106.79      | 101.34   |
| 5   | P     | 201 | PEB  | C2A-C1A-NA  | 3.59  | 111.27      | 108.29   |
| 5   | L     | 203 | PEB  | C2A-C3A-C4A | 3.59  | 106.71      | 101.34   |
| 5   | D     | 201 | PEB  | CHC-C4C-NC  | 3.57  | 125.88      | 121.10   |
| 5   | B     | 201 | PEB  | C2A-C1A-NA  | 3.57  | 111.26      | 108.29   |
| 5   | F     | 202 | PEB  | C2C-C1C-NC  | 3.57  | 112.04      | 107.57   |
| 5   | L     | 201 | PEB  | OA-C1A-C2A  | -3.56 | 123.34      | 126.17   |
| 5   | B     | 202 | PEB  | C2C-C1C-NC  | 3.56  | 112.03      | 107.57   |
| 5   | H     | 201 | PEB  | C2A-C1A-NA  | 3.55  | 111.25      | 108.29   |
| 5   | D     | 202 | PEB  | C2C-C1C-NC  | 3.54  | 112.01      | 107.57   |
| 5   | B     | 203 | PEB  | C2A-C1A-NA  | 3.54  | 111.23      | 108.29   |
| 5   | B     | 201 | PEB  | C3C-C4C-NC  | -3.53 | 105.45      | 108.31   |
| 4   | G     | 101 | DBV  | C4A-NA-C1A  | -3.53 | 106.33      | 110.66   |
| 5   | N     | 201 | PEB  | C3C-C4C-NC  | -3.52 | 105.47      | 108.31   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 5   | L     | 201 | PEB  | C1D-ND-C4D  | -3.51 | 108.02      | 113.42   |
| 5   | J     | 203 | PEB  | C2A-C3A-C4A | 3.50  | 106.59      | 101.34   |
| 5   | H     | 201 | PEB  | C2C-C1C-NC  | 3.49  | 111.94      | 107.57   |
| 5   | P     | 203 | PEB  | C2A-C3A-C4A | 3.48  | 106.56      | 101.34   |
| 5   | L     | 203 | PEB  | C2A-C1A-NA  | 3.48  | 111.18      | 108.29   |
| 5   | D     | 201 | PEB  | C1B-CHA-C4A | 3.47  | 134.30      | 127.25   |
| 4   | C     | 101 | DBV  | C1C-C2C-C3C | -3.45 | 103.00      | 106.73   |
| 5   | D     | 201 | PEB  | C2C-C1C-NC  | 3.40  | 111.83      | 107.57   |
| 4   | O     | 101 | DBV  | C3D-C4D-ND  | 3.39  | 113.68      | 107.33   |
| 5   | D     | 203 | PEB  | C1B-CHA-C4A | 3.39  | 134.13      | 127.25   |
| 5   | H     | 201 | PEB  | C2A-C3A-C4A | 3.35  | 106.35      | 101.34   |
| 5   | F     | 201 | PEB  | CHC-C4C-NC  | 3.34  | 125.57      | 121.10   |
| 4   | A     | 101 | DBV  | CHA-C1B-NB  | -3.33 | 117.77      | 125.29   |
| 5   | D     | 203 | PEB  | C3C-C4C-NC  | -3.33 | 105.62      | 108.31   |
| 5   | P     | 202 | PEB  | C1B-CHA-C4A | 3.32  | 134.00      | 127.25   |
| 5   | L     | 202 | PEB  | C3C-C4C-NC  | -3.28 | 105.66      | 108.31   |
| 5   | D     | 201 | PEB  | CHC-C1D-ND  | -3.27 | 109.71      | 113.73   |
| 5   | N     | 201 | PEB  | C2C-C1C-NC  | 3.27  | 111.67      | 107.57   |
| 4   | A     | 101 | DBV  | CHA-C1B-C2B | 3.27  | 135.53      | 127.53   |
| 5   | N     | 202 | PEB  | C3C-C4C-NC  | -3.27 | 105.67      | 108.31   |
| 5   | F     | 203 | PEB  | C2C-C1C-NC  | 3.27  | 111.66      | 107.57   |
| 5   | D     | 201 | PEB  | C3C-C4C-NC  | -3.26 | 105.68      | 108.31   |
| 5   | N     | 203 | PEB  | C2A-C1A-NA  | 3.25  | 111.00      | 108.29   |
| 5   | J     | 201 | PEB  | C2A-C1A-NA  | 3.24  | 110.98      | 108.29   |
| 4   | C     | 101 | DBV  | C3D-C4D-ND  | 3.23  | 113.38      | 107.33   |
| 5   | F     | 201 | PEB  | C2A-C3A-C4A | 3.22  | 106.17      | 101.34   |
| 5   | B     | 202 | PEB  | CHA-C1B-C2B | 3.21  | 133.12      | 124.87   |
| 5   | H     | 203 | PEB  | CHA-C4A-NA  | 3.20  | 129.63      | 125.63   |
| 4   | G     | 101 | DBV  | C1D-CHC-C4C | 3.18  | 121.18      | 113.74   |
| 5   | P     | 202 | PEB  | C3C-C4C-NC  | -3.18 | 105.74      | 108.31   |
| 5   | F     | 203 | PEB  | C2A-C3A-C4A | 3.18  | 106.09      | 101.34   |
| 4   | K     | 101 | DBV  | C3D-C4D-ND  | 3.16  | 113.25      | 107.33   |
| 4   | I     | 101 | DBV  | CMD-C2D-C3D | -3.16 | 125.47      | 129.95   |
| 5   | B     | 201 | PEB  | C2C-C1C-NC  | 3.16  | 111.53      | 107.57   |
| 5   | D     | 201 | PEB  | OA-C1A-C2A  | -3.15 | 123.67      | 126.17   |
| 5   | F     | 202 | PEB  | C3C-C4C-NC  | -3.13 | 105.78      | 108.31   |
| 4   | C     | 101 | DBV  | CHA-C1B-C2B | 3.13  | 135.20      | 127.53   |
| 4   | E     | 101 | DBV  | C2A-C1A-NA  | 3.13  | 113.56      | 106.55   |
| 5   | H     | 202 | PEB  | C3C-C4C-NC  | -3.12 | 105.79      | 108.31   |
| 5   | J     | 203 | PEB  | C2C-C1C-NC  | 3.12  | 111.48      | 107.57   |
| 5   | P     | 203 | PEB  | C3C-C4C-NC  | -3.11 | 105.79      | 108.31   |
| 4   | M     | 101 | DBV  | CHA-C1B-NB  | -3.10 | 118.28      | 125.29   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 4   | M     | 101 | DBV  | C3D-C4D-ND  | 3.10  | 113.14      | 107.33   |
| 4   | M     | 101 | DBV  | C2A-C1A-NA  | 3.08  | 113.45      | 106.55   |
| 5   | N     | 203 | PEB  | C2A-C3A-C4A | 3.07  | 105.94      | 101.34   |
| 5   | N     | 203 | PEB  | C2C-C1C-NC  | 3.07  | 111.41      | 107.57   |
| 5   | P     | 201 | PEB  | C1D-ND-C4D  | -3.06 | 108.71      | 113.42   |
| 4   | M     | 101 | DBV  | C4B-C3B-C2B | -3.06 | 104.06      | 107.62   |
| 4   | A     | 101 | DBV  | C3D-C4D-ND  | 3.06  | 113.06      | 107.33   |
| 4   | I     | 101 | DBV  | C3D-C4D-ND  | 3.05  | 113.05      | 107.33   |
| 4   | K     | 101 | DBV  | C2A-C1A-NA  | 3.04  | 113.36      | 106.55   |
| 4   | G     | 101 | DBV  | C2A-C1A-NA  | 3.03  | 113.33      | 106.55   |
| 5   | F     | 201 | PEB  | C2A-C1A-NA  | 3.03  | 110.81      | 108.29   |
| 5   | L     | 203 | PEB  | C1B-CHA-C4A | 3.02  | 133.40      | 127.25   |
| 5   | L     | 203 | PEB  | C3C-C4C-NC  | -3.02 | 105.87      | 108.31   |
| 4   | E     | 101 | DBV  | C4B-C3B-C2B | -3.02 | 104.11      | 107.62   |
| 4   | E     | 101 | DBV  | C1C-C2C-C3C | -3.02 | 103.46      | 106.73   |
| 5   | N     | 203 | PEB  | C1B-CHA-C4A | 3.02  | 133.38      | 127.25   |
| 4   | O     | 101 | DBV  | C2A-C1A-NA  | 3.01  | 113.30      | 106.55   |
| 5   | P     | 203 | PEB  | C2C-C1C-NC  | 3.01  | 111.35      | 107.57   |
| 5   | P     | 201 | PEB  | C3C-C4C-NC  | -3.01 | 105.88      | 108.31   |
| 5   | D     | 202 | PEB  | CHA-C1B-C2B | 3.01  | 132.60      | 124.87   |
| 4   | I     | 101 | DBV  | C1C-C2C-C3C | -3.00 | 103.48      | 106.73   |
| 5   | J     | 201 | PEB  | C2A-C3A-C4A | 2.99  | 105.82      | 101.34   |
| 4   | E     | 101 | DBV  | C3D-C4D-ND  | 2.99  | 112.93      | 107.33   |
| 4   | C     | 101 | DBV  | CHA-C1B-NB  | -2.98 | 118.56      | 125.29   |
| 5   | P     | 203 | PEB  | C1B-CHA-C4A | 2.98  | 133.30      | 127.25   |
| 5   | F     | 203 | PEB  | C1B-CHA-C4A | 2.98  | 133.30      | 127.25   |
| 5   | H     | 201 | PEB  | C3C-C4C-NC  | -2.98 | 105.90      | 108.31   |
| 4   | A     | 101 | DBV  | C4B-C3B-C2B | -2.97 | 104.16      | 107.62   |
| 4   | E     | 101 | DBV  | CHA-C1B-C2B | 2.97  | 134.81      | 127.53   |
| 5   | B     | 203 | PEB  | CHA-C1B-C2B | 2.97  | 132.49      | 124.87   |
| 5   | L     | 201 | PEB  | C3C-C4C-NC  | -2.96 | 105.92      | 108.31   |
| 5   | H     | 203 | PEB  | C2A-C1A-NA  | 2.95  | 110.74      | 108.29   |
| 4   | E     | 101 | DBV  | CHA-C1B-NB  | -2.95 | 118.63      | 125.29   |
| 5   | J     | 203 | PEB  | C1D-ND-C4D  | -2.95 | 108.89      | 113.42   |
| 4   | C     | 101 | DBV  | C1D-CHC-C4C | 2.95  | 120.64      | 113.74   |
| 5   | J     | 201 | PEB  | C1B-CHA-C4A | 2.94  | 133.24      | 127.25   |
| 4   | I     | 101 | DBV  | C2A-C1A-NA  | 2.94  | 113.14      | 106.55   |
| 5   | N     | 202 | PEB  | C2C-C1C-NC  | 2.94  | 111.25      | 107.57   |
| 5   | F     | 203 | PEB  | CHA-C1B-C2B | 2.94  | 132.43      | 124.87   |
| 4   | A     | 101 | DBV  | C1C-C2C-C3C | -2.94 | 103.55      | 106.73   |
| 5   | P     | 201 | PEB  | CHA-C1B-C2B | 2.93  | 132.41      | 124.87   |
| 4   | K     | 101 | DBV  | CMD-C2D-C3D | -2.93 | 125.79      | 129.95   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 5   | P     | 202 | PEB  | C1C-CHB-C4B | 2.93  | 134.61      | 128.22   |
| 4   | E     | 101 | DBV  | CHA-C4A-NA  | -2.93 | 119.82      | 126.06   |
| 5   | H     | 202 | PEB  | C2A-C1A-NA  | 2.92  | 110.71      | 108.29   |
| 4   | M     | 101 | DBV  | C1C-C2C-C3C | -2.91 | 103.58      | 106.73   |
| 5   | P     | 202 | PEB  | C2A-C3A-C4A | 2.91  | 105.70      | 101.34   |
| 5   | L     | 203 | PEB  | C1D-ND-C4D  | -2.91 | 108.95      | 113.42   |
| 4   | C     | 101 | DBV  | C2A-C1A-NA  | 2.91  | 113.06      | 106.55   |
| 5   | B     | 201 | PEB  | C1D-ND-C4D  | -2.90 | 108.95      | 113.42   |
| 5   | B     | 202 | PEB  | C3C-C4C-NC  | -2.90 | 105.97      | 108.31   |
| 4   | G     | 101 | DBV  | CHA-C4A-NA  | -2.90 | 119.88      | 126.06   |
| 4   | E     | 101 | DBV  | CMD-C2D-C3D | -2.89 | 125.84      | 129.95   |
| 4   | K     | 101 | DBV  | C1C-C2C-C3C | -2.89 | 103.60      | 106.73   |
| 4   | K     | 101 | DBV  | C4B-C3B-C2B | -2.89 | 104.26      | 107.62   |
| 4   | G     | 101 | DBV  | C3D-C4D-ND  | 2.88  | 112.74      | 107.33   |
| 5   | L     | 202 | PEB  | C2C-C1C-NC  | 2.88  | 111.18      | 107.57   |
| 4   | I     | 101 | DBV  | C4B-C3B-C2B | -2.88 | 104.27      | 107.62   |
| 5   | D     | 203 | PEB  | CHA-C4A-NA  | 2.87  | 129.21      | 125.63   |
| 5   | B     | 203 | PEB  | C2A-C3A-C4A | 2.87  | 105.64      | 101.34   |
| 5   | F     | 202 | PEB  | CHA-C1B-C2B | 2.86  | 132.22      | 124.87   |
| 5   | L     | 203 | PEB  | CHA-C1B-C2B | 2.86  | 132.21      | 124.87   |
| 4   | A     | 101 | DBV  | C2A-C1A-NA  | 2.85  | 112.94      | 106.55   |
| 4   | M     | 101 | DBV  | C1D-CHC-C4C | 2.85  | 120.42      | 113.74   |
| 5   | D     | 203 | PEB  | C2A-C1A-NA  | 2.85  | 110.66      | 108.29   |
| 4   | C     | 101 | DBV  | OD-C4D-C3D  | -2.85 | 122.84      | 129.71   |
| 5   | H     | 202 | PEB  | C1C-CHB-C4B | 2.84  | 134.42      | 128.22   |
| 4   | O     | 101 | DBV  | CHC-C1D-ND  | 2.83  | 117.22      | 113.73   |
| 5   | J     | 202 | PEB  | C2C-C1C-NC  | 2.83  | 111.11      | 107.57   |
| 4   | O     | 101 | DBV  | C1C-C2C-C3C | -2.82 | 103.67      | 106.73   |
| 5   | P     | 203 | PEB  | CHA-C1B-C2B | 2.82  | 132.10      | 124.87   |
| 5   | D     | 202 | PEB  | C2A-C3A-C4A | 2.81  | 105.56      | 101.34   |
| 5   | L     | 202 | PEB  | CHA-C1B-C2B | 2.80  | 132.08      | 124.87   |
| 5   | F     | 202 | PEB  | C2A-C3A-C4A | 2.80  | 105.53      | 101.34   |
| 5   | H     | 202 | PEB  | C1D-ND-C4D  | -2.80 | 109.12      | 113.42   |
| 5   | L     | 201 | PEB  | C2C-C1C-NC  | 2.79  | 111.07      | 107.57   |
| 5   | F     | 203 | PEB  | C1D-ND-C4D  | -2.79 | 109.13      | 113.42   |
| 5   | B     | 203 | PEB  | C3C-C4C-NC  | -2.79 | 106.06      | 108.31   |
| 5   | H     | 202 | PEB  | CBC-CAC-C2C | 2.79  | 120.24      | 112.53   |
| 4   | G     | 101 | DBV  | C1C-C2C-C3C | -2.78 | 103.71      | 106.73   |
| 4   | E     | 101 | DBV  | C1D-CHC-C4C | 2.78  | 120.25      | 113.74   |
| 4   | C     | 101 | DBV  | C4B-C3B-C2B | -2.78 | 104.38      | 107.62   |
| 5   | J     | 203 | PEB  | OA-C1A-C2A  | -2.75 | 123.98      | 126.17   |
| 5   | F     | 202 | PEB  | C1C-CHB-C4B | 2.75  | 134.23      | 128.22   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 5   | D     | 203 | PEB  | C2C-C1C-NC  | 2.75  | 111.02      | 107.57   |
| 5   | H     | 203 | PEB  | C3C-C4C-NC  | -2.75 | 106.09      | 108.31   |
| 4   | I     | 101 | DBV  | OD-C4D-ND   | -2.74 | 122.25      | 126.02   |
| 5   | J     | 201 | PEB  | C2C-C1C-NC  | 2.73  | 110.99      | 107.57   |
| 4   | G     | 101 | DBV  | OD-C4D-ND   | -2.73 | 122.27      | 126.02   |
| 5   | J     | 202 | PEB  | C1D-ND-C4D  | -2.73 | 109.23      | 113.42   |
| 5   | D     | 202 | PEB  | O1C-CGC-CBC | -2.72 | 114.46      | 123.09   |
| 4   | M     | 101 | DBV  | CHA-C4A-NA  | -2.72 | 120.26      | 126.06   |
| 4   | M     | 101 | DBV  | OD-C4D-ND   | -2.72 | 122.28      | 126.02   |
| 4   | K     | 101 | DBV  | CHA-C1B-NB  | -2.71 | 119.16      | 125.29   |
| 5   | H     | 203 | PEB  | CHA-C1B-C2B | 2.71  | 131.84      | 124.87   |
| 5   | N     | 201 | PEB  | C2A-C3A-C4A | 2.71  | 105.39      | 101.34   |
| 5   | H     | 203 | PEB  | C1D-ND-C4D  | -2.71 | 109.26      | 113.42   |
| 4   | E     | 101 | DBV  | OD-C4D-C3D  | -2.70 | 123.18      | 129.71   |
| 4   | K     | 101 | DBV  | CHA-C1B-C2B | 2.70  | 134.15      | 127.53   |
| 5   | L     | 201 | PEB  | OD-C4D-C3D  | -2.70 | 123.20      | 129.71   |
| 4   | M     | 101 | DBV  | CHA-C1B-C2B | 2.69  | 134.11      | 127.53   |
| 5   | D     | 202 | PEB  | C3C-C4C-NC  | -2.69 | 106.14      | 108.31   |
| 5   | N     | 202 | PEB  | CHC-C1D-ND  | -2.68 | 110.44      | 113.73   |
| 5   | J     | 203 | PEB  | CHA-C1B-C2B | 2.67  | 131.74      | 124.87   |
| 5   | N     | 203 | PEB  | C1D-CHC-C4C | -2.67 | 108.83      | 113.32   |
| 5   | P     | 202 | PEB  | CHA-C1B-C2B | 2.67  | 131.72      | 124.87   |
| 4   | G     | 101 | DBV  | CHA-C1B-C2B | 2.66  | 134.05      | 127.53   |
| 5   | H     | 202 | PEB  | C2A-C3A-C4A | 2.66  | 105.32      | 101.34   |
| 5   | F     | 201 | PEB  | C2C-C1C-NC  | 2.65  | 110.89      | 107.57   |
| 5   | N     | 203 | PEB  | CHA-C1B-C2B | 2.64  | 131.65      | 124.87   |
| 5   | N     | 203 | PEB  | C3C-C4C-NC  | -2.64 | 106.18      | 108.31   |
| 5   | H     | 201 | PEB  | CHA-C1B-C2B | 2.64  | 131.64      | 124.87   |
| 4   | A     | 101 | DBV  | CHA-C4A-NA  | -2.63 | 120.45      | 126.06   |
| 5   | N     | 201 | PEB  | C1B-CHA-C4A | 2.63  | 132.59      | 127.25   |
| 5   | J     | 201 | PEB  | CHC-C4C-NC  | 2.63  | 124.61      | 121.10   |
| 5   | B     | 201 | PEB  | C2A-C3A-C4A | 2.63  | 105.27      | 101.34   |
| 5   | B     | 202 | PEB  | C2A-C1A-NA  | 2.62  | 110.47      | 108.29   |
| 4   | O     | 101 | DBV  | C4B-C3B-C2B | -2.62 | 104.57      | 107.62   |
| 5   | D     | 202 | PEB  | C2A-C1A-NA  | 2.61  | 110.46      | 108.29   |
| 5   | P     | 203 | PEB  | C1D-ND-C4D  | -2.61 | 109.41      | 113.42   |
| 4   | O     | 101 | DBV  | OD-C4D-C3D  | -2.60 | 123.42      | 129.71   |
| 4   | G     | 101 | DBV  | C3B-C4B-NB  | 2.59  | 110.81      | 107.57   |
| 5   | J     | 201 | PEB  | OD-C4D-C3D  | -2.59 | 123.47      | 129.71   |
| 5   | H     | 203 | PEB  | C2C-C1C-NC  | 2.58  | 110.81      | 107.57   |
| 4   | I     | 101 | DBV  | C1D-CHC-C4C | 2.58  | 119.78      | 113.74   |
| 4   | C     | 101 | DBV  | CMD-C2D-C3D | -2.58 | 126.29      | 129.95   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 4   | O     | 101 | DBV  | CHA-C4A-NA  | -2.58 | 120.56      | 126.06   |
| 5   | D     | 201 | PEB  | CHA-C4A-NA  | 2.57  | 128.84      | 125.63   |
| 5   | H     | 201 | PEB  | C1B-CHA-C4A | 2.56  | 132.46      | 127.25   |
| 5   | J     | 201 | PEB  | CHC-C1D-ND  | -2.56 | 110.59      | 113.73   |
| 5   | D     | 203 | PEB  | CHA-C1B-C2B | 2.55  | 131.43      | 124.87   |
| 5   | L     | 202 | PEB  | C2A-C3A-C4A | 2.55  | 105.16      | 101.34   |
| 4   | K     | 101 | DBV  | OD-C4D-C3D  | -2.55 | 123.55      | 129.71   |
| 5   | J     | 202 | PEB  | C1C-CHB-C4B | 2.55  | 133.78      | 128.22   |
| 5   | P     | 202 | PEB  | OA-C1A-C2A  | -2.55 | 124.15      | 126.17   |
| 5   | B     | 202 | PEB  | CHA-C1B-NB  | -2.54 | 119.47      | 124.95   |
| 4   | I     | 101 | DBV  | CHA-C1B-NB  | -2.54 | 119.56      | 125.29   |
| 5   | H     | 202 | PEB  | C2C-C1C-NC  | 2.54  | 110.75      | 107.57   |
| 4   | O     | 101 | DBV  | CHA-C1B-NB  | -2.54 | 119.56      | 125.29   |
| 5   | P     | 201 | PEB  | C2C-C1C-NC  | 2.53  | 110.74      | 107.57   |
| 5   | D     | 201 | PEB  | O1B-CGB-CBB | -2.53 | 115.07      | 123.09   |
| 5   | L     | 201 | PEB  | C1B-CHA-C4A | 2.53  | 132.39      | 127.25   |
| 5   | B     | 203 | PEB  | C1B-CHA-C4A | 2.51  | 132.36      | 127.25   |
| 5   | L     | 202 | PEB  | O1C-CGC-CBC | -2.51 | 115.14      | 123.09   |
| 5   | D     | 201 | PEB  | CHA-C1B-C2B | 2.50  | 131.30      | 124.87   |
| 5   | N     | 203 | PEB  | CHC-C1D-ND  | 2.50  | 116.80      | 113.73   |
| 5   | P     | 202 | PEB  | C1D-ND-C4D  | -2.50 | 109.58      | 113.42   |
| 4   | G     | 101 | DBV  | CHA-C1B-NB  | -2.49 | 119.66      | 125.29   |
| 5   | L     | 201 | PEB  | CHA-C1B-C2B | 2.49  | 131.26      | 124.87   |
| 5   | P     | 202 | PEB  | O1C-CGC-CBC | -2.49 | 115.20      | 123.09   |
| 5   | H     | 202 | PEB  | CHA-C1B-C2B | 2.49  | 131.26      | 124.87   |
| 5   | J     | 203 | PEB  | CHA-C4A-NA  | 2.48  | 128.73      | 125.63   |
| 4   | I     | 101 | DBV  | CHA-C1B-C2B | 2.48  | 133.60      | 127.53   |
| 4   | O     | 101 | DBV  | CHA-C1B-C2B | 2.47  | 133.58      | 127.53   |
| 5   | P     | 201 | PEB  | C1C-CHB-C4B | 2.47  | 133.61      | 128.22   |
| 4   | A     | 101 | DBV  | OD-C4D-C3D  | -2.46 | 123.77      | 129.71   |
| 5   | L     | 202 | PEB  | C1C-CHB-C4B | 2.45  | 133.58      | 128.22   |
| 5   | H     | 203 | PEB  | O1B-CGB-CBB | -2.45 | 115.31      | 123.09   |
| 4   | M     | 101 | DBV  | C3A-C4A-NA  | 2.45  | 110.64      | 106.64   |
| 5   | F     | 202 | PEB  | O1C-CGC-CBC | -2.44 | 115.35      | 123.09   |
| 5   | J     | 201 | PEB  | C1D-ND-C4D  | -2.44 | 109.67      | 113.42   |
| 5   | L     | 202 | PEB  | O1B-CGB-CBB | -2.44 | 115.36      | 123.09   |
| 4   | G     | 101 | DBV  | O1C-CGC-CBC | -2.44 | 115.37      | 123.09   |
| 5   | B     | 202 | PEB  | C2A-C3A-C4A | 2.43  | 104.98      | 101.34   |
| 4   | A     | 101 | DBV  | CMD-C2D-C3D | -2.43 | 126.50      | 129.95   |
| 5   | P     | 201 | PEB  | CMC-C3C-C2C | 2.43  | 130.77      | 125.62   |
| 5   | B     | 201 | PEB  | OD-C4D-C3D  | -2.43 | 123.85      | 129.71   |
| 5   | N     | 201 | PEB  | CHC-C4C-NC  | 2.42  | 124.34      | 121.10   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 5   | P     | 202 | PEB  | O1B-CGB-CBB | -2.42 | 115.42      | 123.09   |
| 4   | E     | 101 | DBV  | C3A-C4A-NA  | 2.41  | 110.57      | 106.64   |
| 5   | B     | 203 | PEB  | C1D-ND-C4D  | -2.41 | 109.72      | 113.42   |
| 5   | P     | 202 | PEB  | C2C-C1C-NC  | 2.39  | 110.56      | 107.57   |
| 5   | F     | 202 | PEB  | C2A-C1A-NA  | 2.39  | 110.27      | 108.29   |
| 5   | N     | 203 | PEB  | C1D-ND-C4D  | -2.38 | 109.76      | 113.42   |
| 4   | K     | 101 | DBV  | CHA-C4A-NA  | -2.38 | 120.99      | 126.06   |
| 5   | N     | 201 | PEB  | OD-C4D-C3D  | -2.37 | 123.98      | 129.71   |
| 4   | G     | 101 | DBV  | CAB-C3B-C2B | 2.37  | 132.38      | 127.07   |
| 4   | C     | 101 | DBV  | CHA-C4A-NA  | -2.36 | 121.02      | 126.06   |
| 5   | P     | 202 | PEB  | C2A-C1A-NA  | 2.36  | 110.25      | 108.29   |
| 5   | D     | 201 | PEB  | OD-C4D-C3D  | -2.36 | 124.01      | 129.71   |
| 4   | C     | 101 | DBV  | C3B-C4B-NB  | 2.36  | 110.53      | 107.57   |
| 5   | L     | 202 | PEB  | C2A-C1A-NA  | 2.36  | 110.25      | 108.29   |
| 5   | B     | 202 | PEB  | C1D-ND-C4D  | -2.36 | 109.79      | 113.42   |
| 5   | F     | 201 | PEB  | C1B-CHA-C4A | 2.36  | 132.04      | 127.25   |
| 4   | O     | 101 | DBV  | CBA-CAA-C3A | -2.36 | 115.76      | 127.53   |
| 5   | J     | 203 | PEB  | O1B-CGB-CBB | -2.35 | 115.64      | 123.09   |
| 4   | A     | 101 | DBV  | C3A-C4A-NA  | 2.35  | 110.47      | 106.64   |
| 5   | B     | 201 | PEB  | O1B-CGB-CBB | -2.34 | 115.66      | 123.09   |
| 5   | P     | 201 | PEB  | O1C-CGC-CBC | -2.34 | 115.68      | 123.09   |
| 4   | O     | 101 | DBV  | CHB-C4B-C3B | -2.33 | 122.22      | 127.22   |
| 5   | D     | 203 | PEB  | C1D-ND-C4D  | -2.32 | 109.85      | 113.42   |
| 5   | P     | 201 | PEB  | C1B-CHA-C4A | 2.32  | 131.97      | 127.25   |
| 4   | G     | 101 | DBV  | CMD-C2D-C3D | -2.32 | 126.65      | 129.95   |
| 5   | L     | 201 | PEB  | O1B-CGB-CBB | -2.32 | 115.74      | 123.09   |
| 4   | K     | 101 | DBV  | C3B-C4B-NB  | 2.31  | 110.47      | 107.57   |
| 5   | J     | 202 | PEB  | CHA-C1B-C2B | 2.31  | 130.81      | 124.87   |
| 4   | G     | 101 | DBV  | C4B-C3B-C2B | -2.31 | 104.94      | 107.62   |
| 5   | F     | 202 | PEB  | C1D-ND-C4D  | -2.31 | 109.88      | 113.42   |
| 5   | D     | 203 | PEB  | O1B-CGB-CBB | -2.30 | 115.80      | 123.09   |
| 5   | H     | 201 | PEB  | C1D-ND-C4D  | -2.28 | 109.91      | 113.42   |
| 5   | J     | 203 | PEB  | C3C-C4C-NC  | -2.28 | 106.47      | 108.31   |
| 5   | F     | 202 | PEB  | O1B-CGB-CBB | -2.28 | 115.87      | 123.09   |
| 5   | H     | 201 | PEB  | OD-C4D-C3D  | -2.27 | 124.22      | 129.71   |
| 5   | B     | 202 | PEB  | O1B-CGB-CBB | -2.27 | 115.89      | 123.09   |
| 5   | D     | 202 | PEB  | O1B-CGB-CBB | -2.27 | 115.89      | 123.09   |
| 5   | B     | 203 | PEB  | CHC-C1D-ND  | 2.27  | 116.53      | 113.73   |
| 5   | L     | 202 | PEB  | C1B-CHA-C4A | 2.27  | 131.87      | 127.25   |
| 5   | N     | 202 | PEB  | O1C-CGC-CBC | -2.27 | 115.89      | 123.09   |
| 4   | O     | 101 | DBV  | OD-C4D-ND   | -2.27 | 122.90      | 126.02   |
| 5   | B     | 201 | PEB  | CHA-C1B-C2B | 2.26  | 130.68      | 124.87   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 5   | H     | 201 | PEB  | C1C-C2C-C3C | -2.26 | 104.99      | 107.62   |
| 5   | N     | 201 | PEB  | O1B-CGB-CBB | -2.26 | 115.93      | 123.09   |
| 5   | H     | 203 | PEB  | C1C-CHB-C4B | 2.26  | 133.15      | 128.22   |
| 5   | B     | 203 | PEB  | C1C-C2C-C3C | -2.25 | 105.00      | 107.62   |
| 5   | J     | 202 | PEB  | O1C-CGC-CBC | -2.25 | 115.94      | 123.09   |
| 5   | P     | 201 | PEB  | CHC-C1D-ND  | -2.25 | 110.97      | 113.73   |
| 4   | I     | 101 | DBV  | C3A-C4A-NA  | 2.25  | 110.30      | 106.64   |
| 5   | F     | 201 | PEB  | OD-C4D-C3D  | -2.25 | 124.29      | 129.71   |
| 5   | B     | 201 | PEB  | C1B-CHA-C4A | 2.24  | 131.80      | 127.25   |
| 5   | L     | 201 | PEB  | O1C-CGC-CBC | -2.24 | 116.00      | 123.09   |
| 5   | L     | 202 | PEB  | C1D-ND-C4D  | -2.23 | 109.98      | 113.42   |
| 5   | J     | 201 | PEB  | CMA-C2A-C1A | 2.23  | 117.22      | 112.40   |
| 5   | B     | 203 | PEB  | O1C-CGC-CBC | -2.23 | 116.01      | 123.09   |
| 5   | H     | 201 | PEB  | O1B-CGB-CBB | -2.23 | 116.03      | 123.09   |
| 5   | J     | 201 | PEB  | CAA-C3A-C4A | 2.23  | 118.39      | 112.67   |
| 5   | D     | 202 | PEB  | CHC-C4C-NC  | 2.23  | 124.08      | 121.10   |
| 5   | N     | 202 | PEB  | CHA-C1B-C2B | 2.22  | 130.58      | 124.87   |
| 4   | A     | 101 | DBV  | O1C-CGC-CBC | -2.22 | 116.05      | 123.09   |
| 4   | G     | 101 | DBV  | CBA-CAA-C3A | -2.22 | 116.45      | 127.53   |
| 5   | F     | 201 | PEB  | CHA-C1B-C2B | 2.21  | 130.56      | 124.87   |
| 5   | N     | 203 | PEB  | O1B-CGB-CBB | -2.21 | 116.08      | 123.09   |
| 5   | N     | 202 | PEB  | O1B-CGB-CBB | -2.21 | 116.09      | 123.09   |
| 5   | P     | 203 | PEB  | CMC-C3C-C2C | 2.21  | 130.30      | 125.62   |
| 4   | E     | 101 | DBV  | C3B-C4B-NB  | 2.20  | 110.33      | 107.57   |
| 4   | C     | 101 | DBV  | C3A-C4A-NA  | 2.20  | 110.23      | 106.64   |
| 5   | L     | 201 | PEB  | C1C-CHB-C4B | 2.20  | 133.03      | 128.22   |
| 5   | B     | 201 | PEB  | O1C-CGC-CBC | -2.20 | 116.12      | 123.09   |
| 5   | B     | 203 | PEB  | C1D-CHC-C4C | -2.20 | 109.62      | 113.32   |
| 5   | B     | 203 | PEB  | CMB-C2B-C1B | 2.19  | 128.51      | 125.10   |
| 5   | P     | 201 | PEB  | C3D-C4D-ND  | 2.19  | 111.44      | 107.33   |
| 5   | L     | 201 | PEB  | C3D-C4D-ND  | 2.19  | 111.43      | 107.33   |
| 5   | D     | 203 | PEB  | OA-C1A-C2A  | -2.19 | 124.43      | 126.17   |
| 5   | F     | 201 | PEB  | O1B-CGB-CBB | -2.19 | 116.16      | 123.09   |
| 5   | N     | 203 | PEB  | O1C-CGC-CBC | -2.19 | 116.16      | 123.09   |
| 5   | N     | 202 | PEB  | C1D-ND-C4D  | -2.18 | 110.06      | 113.42   |
| 4   | O     | 101 | DBV  | C3B-C4B-NB  | 2.18  | 110.30      | 107.57   |
| 5   | D     | 201 | PEB  | O1C-CGC-CBC | -2.18 | 116.19      | 123.09   |
| 5   | D     | 202 | PEB  | CMC-C3C-C2C | 2.17  | 130.24      | 125.62   |
| 4   | E     | 101 | DBV  | CBA-CAA-C3A | -2.16 | 116.72      | 127.53   |
| 5   | H     | 203 | PEB  | OA-C1A-C2A  | -2.16 | 124.46      | 126.17   |
| 5   | L     | 203 | PEB  | O1B-CGB-CBB | -2.16 | 116.25      | 123.09   |
| 4   | K     | 101 | DBV  | CBA-CAA-C3A | -2.15 | 116.77      | 127.53   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 5   | J     | 201 | PEB  | CHA-C1B-C2B | 2.15  | 130.39      | 124.87   |
| 5   | J     | 203 | PEB  | C1C-CHB-C4B | 2.14  | 132.90      | 128.22   |
| 4   | M     | 101 | DBV  | CBA-CAA-C3A | -2.14 | 116.84      | 127.53   |
| 5   | H     | 202 | PEB  | O1B-CGB-CBB | -2.14 | 116.31      | 123.09   |
| 5   | F     | 201 | PEB  | OA-C1A-C2A  | -2.13 | 124.48      | 126.17   |
| 5   | D     | 202 | PEB  | C1D-ND-C4D  | -2.13 | 110.14      | 113.42   |
| 5   | F     | 201 | PEB  | CHA-C4A-NA  | 2.13  | 128.29      | 125.63   |
| 5   | J     | 202 | PEB  | C2A-C3A-C4A | 2.13  | 104.53      | 101.34   |
| 4   | M     | 101 | DBV  | OD-C4D-C3D  | -2.13 | 124.57      | 129.71   |
| 5   | P     | 201 | PEB  | OD-C4D-C3D  | -2.12 | 124.58      | 129.71   |
| 5   | J     | 201 | PEB  | O1B-CGB-CBB | -2.12 | 116.36      | 123.09   |
| 5   | P     | 201 | PEB  | CHA-C1B-NB  | -2.12 | 120.38      | 124.95   |
| 5   | F     | 201 | PEB  | C3D-C4D-ND  | 2.12  | 111.30      | 107.33   |
| 5   | N     | 201 | PEB  | O1C-CGC-CBC | -2.12 | 116.38      | 123.09   |
| 4   | E     | 101 | DBV  | C1B-CHA-C4A | -2.12 | 124.73      | 130.82   |
| 5   | B     | 203 | PEB  | CHA-C1B-NB  | -2.11 | 120.39      | 124.95   |
| 5   | D     | 203 | PEB  | O1C-CGC-CBC | -2.11 | 116.40      | 123.09   |
| 4   | O     | 101 | DBV  | C3A-C4A-NA  | 2.11  | 110.08      | 106.64   |
| 5   | F     | 201 | PEB  | C1C-CHB-C4B | 2.11  | 132.82      | 128.22   |
| 5   | N     | 202 | PEB  | CMB-C2B-C1B | 2.11  | 128.37      | 125.10   |
| 5   | H     | 203 | PEB  | O1C-CGC-CBC | -2.10 | 116.43      | 123.09   |
| 4   | A     | 101 | DBV  | CAB-CBB-CGB | 2.10  | 119.23      | 113.67   |
| 4   | G     | 101 | DBV  | CHB-C4B-C3B | -2.09 | 122.72      | 127.22   |
| 5   | F     | 203 | PEB  | OA-C1A-C2A  | -2.08 | 124.52      | 126.17   |
| 5   | N     | 202 | PEB  | CBC-CAC-C2C | 2.08  | 118.28      | 112.53   |
| 4   | C     | 101 | DBV  | O1C-CGC-CBC | -2.08 | 116.50      | 123.09   |
| 4   | C     | 101 | DBV  | CBC-CAC-C2C | 2.08  | 118.28      | 112.53   |
| 5   | J     | 203 | PEB  | C1C-C2C-C3C | -2.08 | 105.20      | 107.62   |
| 5   | P     | 203 | PEB  | CHA-C1B-NB  | -2.08 | 120.47      | 124.95   |
| 5   | P     | 203 | PEB  | O1B-CGB-CBB | -2.08 | 116.51      | 123.09   |
| 4   | C     | 101 | DBV  | CBA-CAA-C3A | -2.08 | 117.16      | 127.53   |
| 4   | I     | 101 | DBV  | OD-C4D-C3D  | -2.07 | 124.70      | 129.71   |
| 5   | H     | 202 | PEB  | C1B-CHA-C4A | 2.07  | 131.46      | 127.25   |
| 5   | B     | 201 | PEB  | C3D-C4D-ND  | 2.07  | 111.21      | 107.33   |
| 5   | N     | 202 | PEB  | C2A-C3A-C4A | 2.07  | 104.44      | 101.34   |
| 4   | A     | 101 | DBV  | OD-C4D-ND   | -2.07 | 123.17      | 126.02   |
| 5   | F     | 201 | PEB  | C1D-ND-C4D  | -2.06 | 110.25      | 113.42   |
| 4   | K     | 101 | DBV  | CAC-C2C-C3C | 2.06  | 131.72      | 127.87   |
| 4   | K     | 101 | DBV  | OD-C4D-ND   | -2.06 | 123.19      | 126.02   |
| 5   | B     | 203 | PEB  | OD-C4D-ND   | -2.06 | 123.19      | 126.02   |
| 5   | F     | 201 | PEB  | O1C-CGC-CBC | -2.05 | 116.59      | 123.09   |
| 5   | D     | 203 | PEB  | C1C-CHB-C4B | 2.05  | 132.70      | 128.22   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 5   | H     | 202 | PEB  | O1C-CGC-CBC | -2.05 | 116.59      | 123.09   |
| 5   | N     | 201 | PEB  | CHA-C1B-C2B | 2.05  | 130.13      | 124.87   |
| 4   | O     | 101 | DBV  | O1C-CGC-CBC | -2.05 | 116.60      | 123.09   |
| 4   | K     | 101 | DBV  | C3A-C4A-NA  | 2.05  | 109.98      | 106.64   |
| 5   | L     | 203 | PEB  | O1C-CGC-CBC | -2.05 | 116.60      | 123.09   |
| 5   | B     | 202 | PEB  | O1C-CGC-CBC | -2.04 | 116.63      | 123.09   |
| 4   | I     | 101 | DBV  | CBA-CAA-C3A | -2.03 | 117.39      | 127.53   |
| 5   | N     | 203 | PEB  | C1C-C2C-C3C | -2.03 | 105.26      | 107.62   |
| 5   | D     | 201 | PEB  | CAA-C3A-C4A | 2.03  | 117.87      | 112.67   |
| 4   | I     | 101 | DBV  | CHA-C4A-NA  | -2.02 | 121.75      | 126.06   |
| 5   | J     | 202 | PEB  | C2A-C1A-NA  | 2.02  | 109.97      | 108.29   |
| 5   | L     | 203 | PEB  | CHA-C1B-NB  | -2.02 | 120.60      | 124.95   |
| 5   | H     | 203 | PEB  | CHA-C1B-NB  | -2.01 | 120.61      | 124.95   |
| 5   | D     | 203 | PEB  | CHC-C1D-ND  | -2.01 | 111.27      | 113.73   |
| 5   | B     | 203 | PEB  | C3D-C4D-ND  | 2.01  | 111.09      | 107.33   |
| 4   | M     | 101 | DBV  | CMD-C2D-C3D | -2.01 | 127.10      | 129.95   |
| 4   | O     | 101 | DBV  | CMD-C2D-C3D | -2.01 | 127.10      | 129.95   |
| 5   | F     | 202 | PEB  | CAA-C3A-C4A | 2.01  | 117.83      | 112.67   |
| 5   | L     | 203 | PEB  | CMC-C3C-C2C | 2.00  | 129.88      | 125.62   |
| 4   | C     | 101 | DBV  | CAC-CBC-CGC | 2.00  | 118.98      | 113.67   |

There are no chirality outliers.

All (208) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 4   | A     | 101 | DBV  | C2A-C3A-CAA-CBA |
| 4   | C     | 101 | DBV  | C2A-C3A-CAA-CBA |
| 4   | C     | 101 | DBV  | C3B-CAB-CBB-CGB |
| 4   | E     | 101 | DBV  | C2A-C3A-CAA-CBA |
| 4   | I     | 101 | DBV  | C2A-C3A-CAA-CBA |
| 4   | K     | 101 | DBV  | C2A-C3A-CAA-CBA |
| 4   | M     | 101 | DBV  | C2A-C3A-CAA-CBA |
| 4   | O     | 101 | DBV  | C2A-C3A-CAA-CBA |
| 5   | B     | 201 | PEB  | C2D-C3D-CAD-CBD |
| 5   | B     | 201 | PEB  | NB-C1B-CHA-C4A  |
| 5   | B     | 201 | PEB  | C2B-C1B-CHA-C4A |
| 5   | B     | 202 | PEB  | C2A-C3A-CAA-CBA |
| 5   | B     | 202 | PEB  | C4A-C3A-CAA-CBA |
| 5   | B     | 202 | PEB  | NA-C4A-CHA-C1B  |
| 5   | B     | 203 | PEB  | NB-C1B-CHA-C4A  |
| 5   | B     | 203 | PEB  | C2B-C1B-CHA-C4A |
| 5   | D     | 201 | PEB  | C2D-C3D-CAD-CBD |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 5   | D     | 201 | PEB  | NB-C1B-CHA-C4A  |
| 5   | D     | 201 | PEB  | C2B-C1B-CHA-C4A |
| 5   | D     | 202 | PEB  | C2A-C3A-CAA-CBA |
| 5   | D     | 202 | PEB  | C4A-C3A-CAA-CBA |
| 5   | D     | 202 | PEB  | NB-C1B-CHA-C4A  |
| 5   | D     | 202 | PEB  | C2B-C1B-CHA-C4A |
| 5   | D     | 203 | PEB  | NB-C1B-CHA-C4A  |
| 5   | D     | 203 | PEB  | C2B-C1B-CHA-C4A |
| 5   | F     | 201 | PEB  | C2D-C3D-CAD-CBD |
| 5   | F     | 201 | PEB  | NB-C1B-CHA-C4A  |
| 5   | F     | 201 | PEB  | C2B-C1B-CHA-C4A |
| 5   | F     | 202 | PEB  | C2A-C3A-CAA-CBA |
| 5   | F     | 202 | PEB  | NB-C1B-CHA-C4A  |
| 5   | F     | 202 | PEB  | C2B-C1B-CHA-C4A |
| 5   | F     | 203 | PEB  | NB-C1B-CHA-C4A  |
| 5   | H     | 201 | PEB  | NB-C1B-CHA-C4A  |
| 5   | H     | 201 | PEB  | C2B-C1B-CHA-C4A |
| 5   | H     | 202 | PEB  | C2A-C3A-CAA-CBA |
| 5   | H     | 202 | PEB  | C4A-C3A-CAA-CBA |
| 5   | H     | 202 | PEB  | NB-C1B-CHA-C4A  |
| 5   | H     | 202 | PEB  | C2B-C1B-CHA-C4A |
| 5   | H     | 203 | PEB  | NB-C1B-CHA-C4A  |
| 5   | H     | 203 | PEB  | C2B-C1B-CHA-C4A |
| 5   | J     | 201 | PEB  | C2D-C3D-CAD-CBD |
| 5   | J     | 201 | PEB  | NB-C1B-CHA-C4A  |
| 5   | J     | 201 | PEB  | C2B-C1B-CHA-C4A |
| 5   | J     | 202 | PEB  | NB-C1B-CHA-C4A  |
| 5   | J     | 202 | PEB  | C2B-C1B-CHA-C4A |
| 5   | J     | 203 | PEB  | NB-C1B-CHA-C4A  |
| 5   | L     | 201 | PEB  | C2D-C3D-CAD-CBD |
| 5   | L     | 201 | PEB  | NB-C1B-CHA-C4A  |
| 5   | L     | 201 | PEB  | C2B-C1B-CHA-C4A |
| 5   | L     | 202 | PEB  | C2A-C3A-CAA-CBA |
| 5   | L     | 202 | PEB  | NA-C4A-CHA-C1B  |
| 5   | L     | 202 | PEB  | NB-C1B-CHA-C4A  |
| 5   | L     | 203 | PEB  | NB-C1B-CHA-C4A  |
| 5   | N     | 201 | PEB  | C2D-C3D-CAD-CBD |
| 5   | N     | 201 | PEB  | NB-C1B-CHA-C4A  |
| 5   | N     | 201 | PEB  | C2B-C1B-CHA-C4A |
| 5   | N     | 202 | PEB  | C2A-C3A-CAA-CBA |
| 5   | N     | 202 | PEB  | NB-C1B-CHA-C4A  |
| 5   | N     | 202 | PEB  | C2B-C1B-CHA-C4A |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 5   | N     | 203 | PEB  | NB-C1B-CHA-C4A  |
| 5   | N     | 203 | PEB  | C2B-C1B-CHA-C4A |
| 5   | P     | 201 | PEB  | C2D-C3D-CAD-CBD |
| 5   | P     | 201 | PEB  | NB-C1B-CHA-C4A  |
| 5   | P     | 201 | PEB  | C2B-C1B-CHA-C4A |
| 5   | P     | 202 | PEB  | C2A-C3A-CAA-CBA |
| 5   | P     | 202 | PEB  | NA-C4A-CHA-C1B  |
| 5   | P     | 202 | PEB  | NB-C1B-CHA-C4A  |
| 5   | P     | 203 | PEB  | NB-C1B-CHA-C4A  |
| 5   | P     | 203 | PEB  | C2B-C1B-CHA-C4A |
| 4   | A     | 101 | DBV  | NB-C1B-CHA-C4A  |
| 4   | C     | 101 | DBV  | NB-C1B-CHA-C4A  |
| 4   | E     | 101 | DBV  | NB-C1B-CHA-C4A  |
| 4   | G     | 101 | DBV  | NB-C1B-CHA-C4A  |
| 4   | I     | 101 | DBV  | NB-C1B-CHA-C4A  |
| 4   | K     | 101 | DBV  | NB-C1B-CHA-C4A  |
| 4   | M     | 101 | DBV  | NB-C1B-CHA-C4A  |
| 4   | O     | 101 | DBV  | NB-C1B-CHA-C4A  |
| 4   | E     | 101 | DBV  | C2B-C1B-CHA-C4A |
| 4   | G     | 101 | DBV  | C2B-C1B-CHA-C4A |
| 4   | I     | 101 | DBV  | C2B-C1B-CHA-C4A |
| 4   | K     | 101 | DBV  | C2B-C1B-CHA-C4A |
| 4   | M     | 101 | DBV  | C2B-C1B-CHA-C4A |
| 4   | O     | 101 | DBV  | C2B-C1B-CHA-C4A |
| 5   | F     | 203 | PEB  | C2B-C1B-CHA-C4A |
| 5   | J     | 203 | PEB  | C2B-C1B-CHA-C4A |
| 5   | L     | 202 | PEB  | C2B-C1B-CHA-C4A |
| 5   | L     | 203 | PEB  | C2B-C1B-CHA-C4A |
| 5   | P     | 202 | PEB  | C2B-C1B-CHA-C4A |
| 4   | A     | 101 | DBV  | C2B-C1B-CHA-C4A |
| 4   | C     | 101 | DBV  | C2B-C1B-CHA-C4A |
| 5   | H     | 202 | PEB  | C2C-CAC-CBC-CGC |
| 5   | B     | 202 | PEB  | NB-C1B-CHA-C4A  |
| 5   | B     | 201 | PEB  | C3B-CAB-CBB-CGB |
| 5   | B     | 202 | PEB  | C2B-C1B-CHA-C4A |
| 5   | B     | 201 | PEB  | C4D-C3D-CAD-CBD |
| 5   | F     | 201 | PEB  | C4D-C3D-CAD-CBD |
| 5   | J     | 201 | PEB  | C4D-C3D-CAD-CBD |
| 5   | N     | 201 | PEB  | C4D-C3D-CAD-CBD |
| 4   | G     | 101 | DBV  | C2A-C3A-CAA-CBA |
| 5   | H     | 201 | PEB  | C2D-C3D-CAD-CBD |
| 4   | C     | 101 | DBV  | C4A-C3A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 4   | I     | 101 | DBV  | C4A-C3A-CAA-CBA |
| 4   | K     | 101 | DBV  | C4A-C3A-CAA-CBA |
| 4   | M     | 101 | DBV  | C4A-C3A-CAA-CBA |
| 5   | L     | 202 | PEB  | C3B-CAB-CBB-CGB |
| 4   | M     | 101 | DBV  | C3B-CAB-CBB-CGB |
| 5   | D     | 201 | PEB  | C4D-C3D-CAD-CBD |
| 5   | L     | 201 | PEB  | C4D-C3D-CAD-CBD |
| 5   | P     | 201 | PEB  | C4D-C3D-CAD-CBD |
| 5   | B     | 201 | PEB  | C4A-C3A-CAA-CBA |
| 5   | F     | 202 | PEB  | C4A-C3A-CAA-CBA |
| 5   | H     | 203 | PEB  | C4A-C3A-CAA-CBA |
| 5   | L     | 202 | PEB  | C4A-C3A-CAA-CBA |
| 5   | N     | 202 | PEB  | C4A-C3A-CAA-CBA |
| 5   | P     | 202 | PEB  | C4A-C3A-CAA-CBA |
| 5   | D     | 201 | PEB  | C3B-CAB-CBB-CGB |
| 4   | C     | 101 | DBV  | C2D-C3D-CAD-CBD |
| 4   | A     | 101 | DBV  | C4A-C3A-CAA-CBA |
| 4   | E     | 101 | DBV  | C4A-C3A-CAA-CBA |
| 4   | G     | 101 | DBV  | C4A-C3A-CAA-CBA |
| 4   | O     | 101 | DBV  | C4A-C3A-CAA-CBA |
| 4   | C     | 101 | DBV  | C4D-C3D-CAD-CBD |
| 5   | H     | 201 | PEB  | C4D-C3D-CAD-CBD |
| 4   | M     | 101 | DBV  | CAB-CBB-CGB-O2B |
| 4   | E     | 101 | DBV  | CAB-CBB-CGB-O1B |
| 5   | D     | 202 | PEB  | CAC-CBC-CGC-O1C |
| 5   | B     | 202 | PEB  | CAC-CBC-CGC-O2C |
| 5   | D     | 202 | PEB  | CAC-CBC-CGC-O2C |
| 5   | B     | 202 | PEB  | CAC-CBC-CGC-O1C |
| 4   | I     | 101 | DBV  | CAB-CBB-CGB-O1B |
| 5   | J     | 202 | PEB  | CAC-CBC-CGC-O2C |
| 5   | J     | 202 | PEB  | CAB-CBB-CGB-O1B |
| 5   | F     | 202 | PEB  | CAC-CBC-CGC-O1C |
| 4   | G     | 101 | DBV  | CAB-CBB-CGB-O1B |
| 4   | A     | 101 | DBV  | CAB-CBB-CGB-O1B |
| 4   | E     | 101 | DBV  | CAB-CBB-CGB-O2B |
| 4   | I     | 101 | DBV  | CAB-CBB-CGB-O2B |
| 4   | O     | 101 | DBV  | CAB-CBB-CGB-O1B |
| 4   | K     | 101 | DBV  | CAB-CBB-CGB-O1B |
| 4   | M     | 101 | DBV  | CAB-CBB-CGB-O1B |
| 5   | L     | 202 | PEB  | CAC-CBC-CGC-O2C |
| 5   | N     | 202 | PEB  | CAB-CBB-CGB-O2B |
| 5   | P     | 202 | PEB  | CAC-CBC-CGC-O2C |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 4   | G     | 101 | DBV  | CAB-CBB-CGB-O2B |
| 5   | F     | 202 | PEB  | CAC-CBC-CGC-O2C |
| 5   | N     | 202 | PEB  | CAB-CBB-CGB-O1B |
| 4   | K     | 101 | DBV  | CAB-CBB-CGB-O2B |
| 5   | J     | 202 | PEB  | CAB-CBB-CGB-O2B |
| 4   | A     | 101 | DBV  | CAB-CBB-CGB-O2B |
| 5   | H     | 202 | PEB  | CAC-CBC-CGC-O2C |
| 5   | P     | 202 | PEB  | CAC-CBC-CGC-O1C |
| 4   | O     | 101 | DBV  | CAB-CBB-CGB-O2B |
| 5   | J     | 202 | PEB  | CAC-CBC-CGC-O1C |
| 5   | L     | 202 | PEB  | CAC-CBC-CGC-O1C |
| 5   | B     | 202 | PEB  | C3A-C4A-CHA-C1B |
| 5   | L     | 202 | PEB  | C3A-C4A-CHA-C1B |
| 5   | P     | 202 | PEB  | C3A-C4A-CHA-C1B |
| 5   | H     | 202 | PEB  | CAC-CBC-CGC-O1C |
| 5   | D     | 202 | PEB  | C2B-C3B-CAB-CBB |
| 4   | I     | 101 | DBV  | C3B-CAB-CBB-CGB |
| 5   | B     | 202 | PEB  | C3B-CAB-CBB-CGB |
| 5   | H     | 201 | PEB  | C4A-C3A-CAA-CBA |
| 5   | J     | 202 | PEB  | C4A-C3A-CAA-CBA |
| 4   | C     | 101 | DBV  | CAC-CBC-CGC-O2C |
| 5   | P     | 203 | PEB  | CAC-CBC-CGC-O2C |
| 5   | B     | 203 | PEB  | CAB-CBB-CGB-O2B |
| 5   | J     | 203 | PEB  | CAB-CBB-CGB-O2B |
| 5   | F     | 203 | PEB  | CAB-CBB-CGB-O2B |
| 5   | N     | 202 | PEB  | CAC-CBC-CGC-O2C |
| 4   | I     | 101 | DBV  | C3B-C4B-CHB-C1C |
| 5   | D     | 203 | PEB  | CAC-CBC-CGC-O2C |
| 5   | L     | 203 | PEB  | CAC-CBC-CGC-O2C |
| 5   | N     | 202 | PEB  | CAC-CBC-CGC-O1C |
| 5   | D     | 202 | PEB  | C4B-C3B-CAB-CBB |
| 5   | J     | 203 | PEB  | CAB-CBB-CGB-O1B |
| 5   | L     | 201 | PEB  | CAB-CBB-CGB-O2B |
| 5   | F     | 203 | PEB  | CAC-CBC-CGC-O2C |
| 5   | L     | 202 | PEB  | CAB-CBB-CGB-O2B |
| 5   | F     | 203 | PEB  | CAB-CBB-CGB-O1B |
| 5   | N     | 203 | PEB  | CAB-CBB-CGB-O2B |
| 5   | P     | 203 | PEB  | CAC-CBC-CGC-O1C |
| 5   | J     | 203 | PEB  | CAC-CBC-CGC-O2C |
| 5   | F     | 203 | PEB  | CAC-CBC-CGC-O1C |
| 5   | J     | 201 | PEB  | CAB-CBB-CGB-O1B |
| 5   | B     | 203 | PEB  | CAB-CBB-CGB-O1B |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 5   | L     | 203 | PEB  | CAC-CBC-CGC-O1C |
| 4   | I     | 101 | DBV  | C2C-CAC-CBC-CGC |
| 5   | F     | 201 | PEB  | C3B-CAB-CBB-CGB |
| 4   | C     | 101 | DBV  | CAB-CBB-CGB-O2B |
| 5   | D     | 203 | PEB  | CAC-CBC-CGC-O1C |
| 4   | C     | 101 | DBV  | CAB-CBB-CGB-O1B |
| 5   | N     | 203 | PEB  | CAB-CBB-CGB-O1B |
| 5   | L     | 202 | PEB  | CAB-CBB-CGB-O1B |
| 4   | C     | 101 | DBV  | CAC-CBC-CGC-O1C |
| 4   | G     | 101 | DBV  | C3B-CAB-CBB-CGB |
| 5   | J     | 201 | PEB  | CAB-CBB-CGB-O2B |
| 5   | J     | 203 | PEB  | CAC-CBC-CGC-O1C |
| 5   | L     | 201 | PEB  | CAB-CBB-CGB-O1B |
| 5   | H     | 201 | PEB  | CAC-CBC-CGC-O2C |
| 5   | B     | 203 | PEB  | CAC-CBC-CGC-O2C |
| 5   | J     | 202 | PEB  | C2A-C3A-CAA-CBA |
| 5   | D     | 201 | PEB  | CAC-CBC-CGC-O2C |
| 5   | H     | 203 | PEB  | CAC-CBC-CGC-O2C |
| 5   | B     | 203 | PEB  | CAC-CBC-CGC-O1C |
| 4   | C     | 101 | DBV  | C2C-CAC-CBC-CGC |
| 4   | O     | 101 | DBV  | C3B-CAB-CBB-CGB |
| 5   | D     | 202 | PEB  | C2C-CAC-CBC-CGC |
| 5   | F     | 201 | PEB  | CAC-CBC-CGC-O2C |

There are no ring outliers.

18 monomers are involved in 22 short contacts:

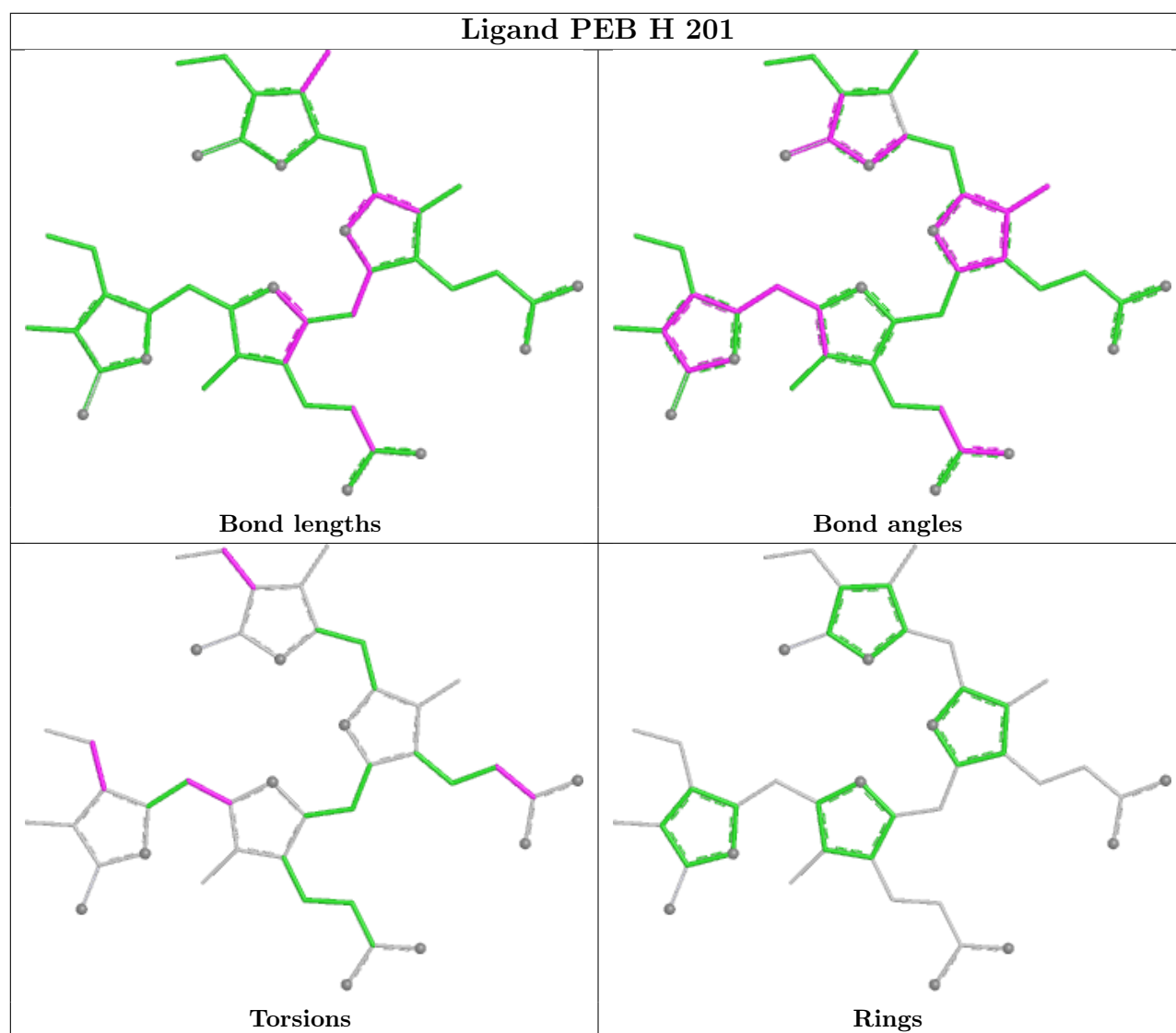
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 4   | C     | 101 | DBV  | 2       | 0            |
| 5   | N     | 202 | PEB  | 1       | 0            |
| 5   | H     | 203 | PEB  | 1       | 0            |
| 5   | B     | 202 | PEB  | 1       | 0            |
| 5   | J     | 202 | PEB  | 1       | 0            |
| 4   | K     | 101 | DBV  | 2       | 0            |
| 4   | E     | 101 | DBV  | 1       | 0            |
| 5   | N     | 203 | PEB  | 1       | 0            |
| 5   | B     | 203 | PEB  | 1       | 0            |
| 5   | J     | 201 | PEB  | 1       | 0            |
| 4   | A     | 101 | DBV  | 1       | 0            |
| 5   | J     | 203 | PEB  | 1       | 0            |
| 4   | O     | 101 | DBV  | 1       | 0            |
| 4   | M     | 101 | DBV  | 2       | 0            |

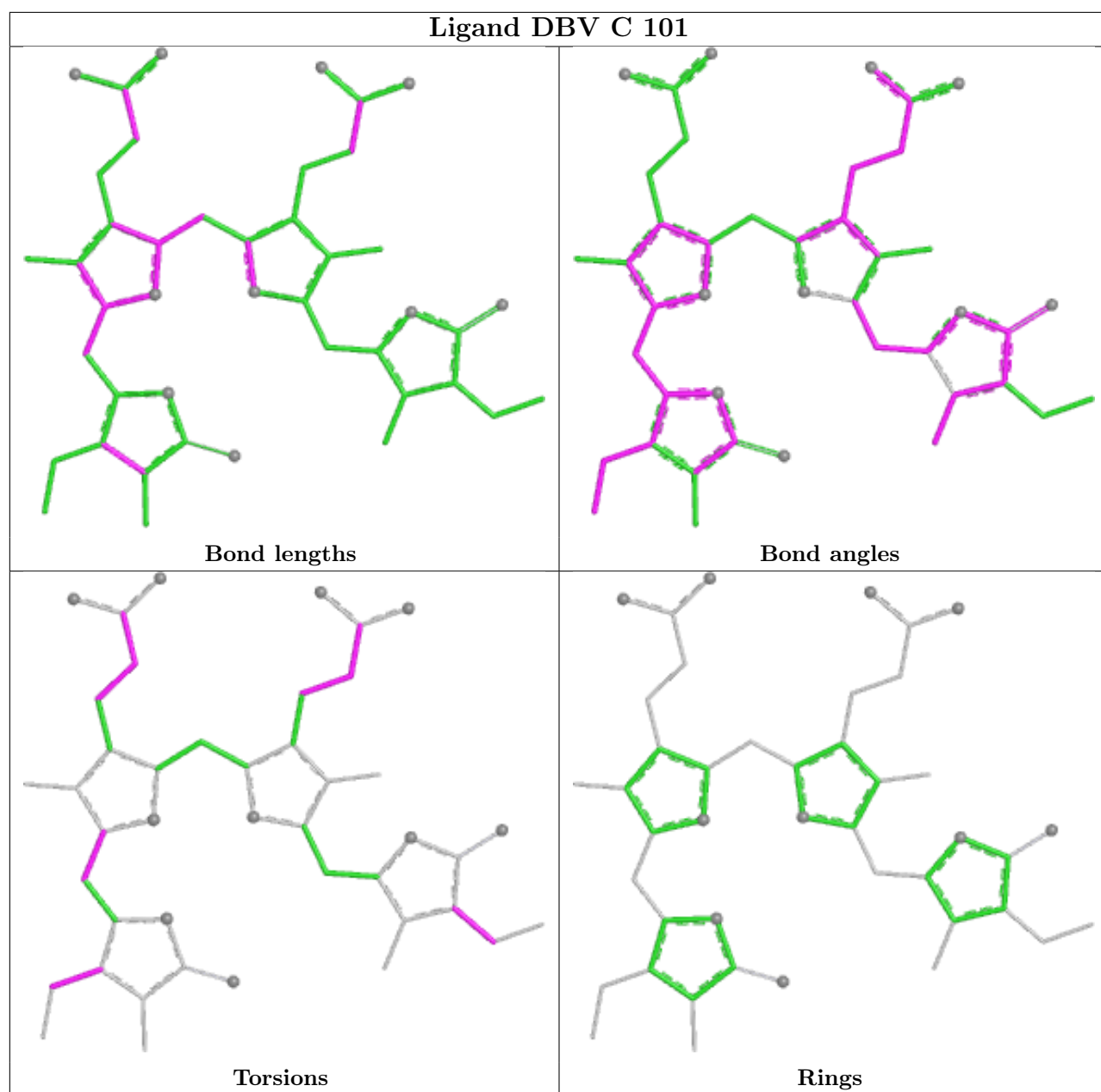
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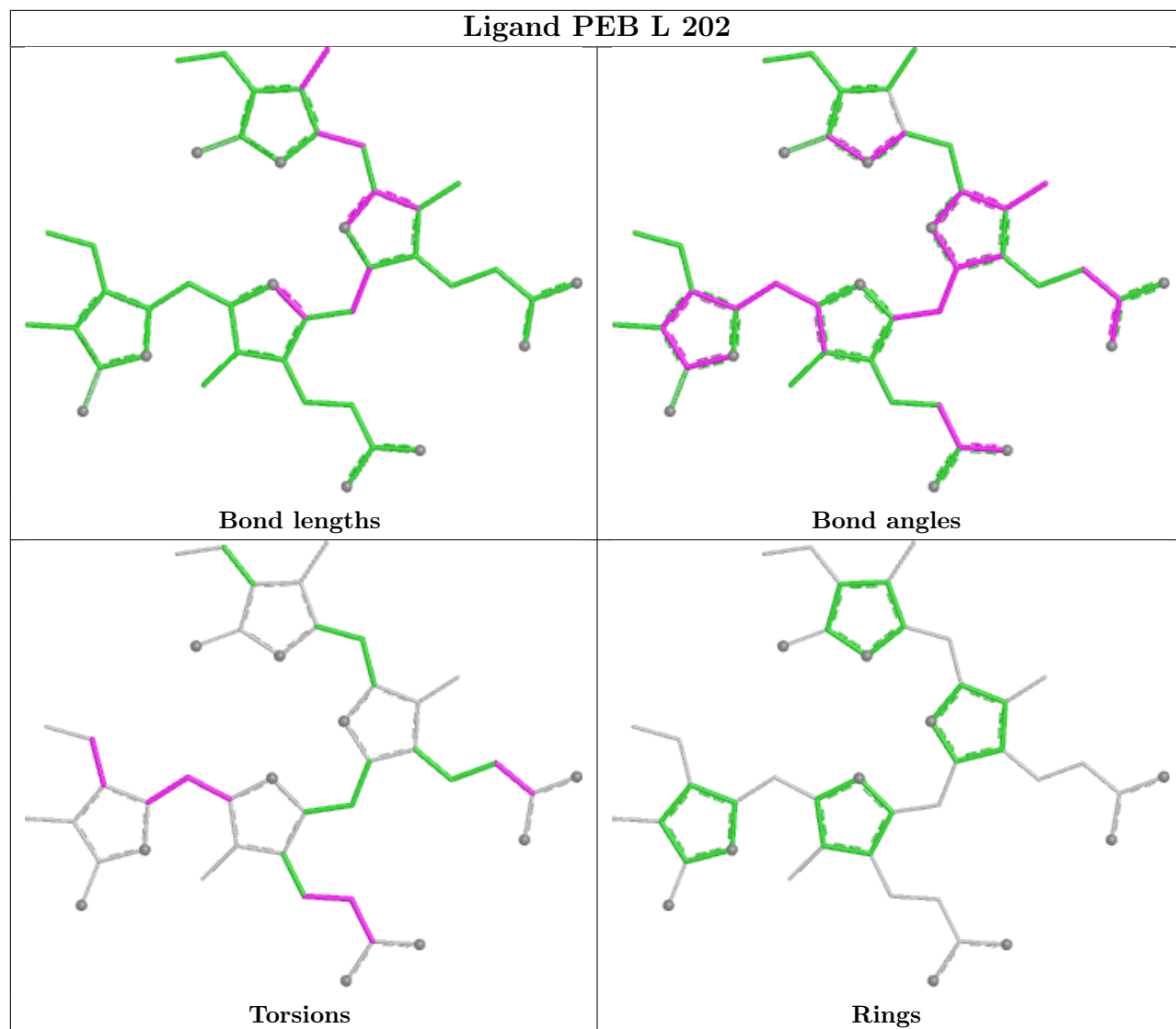
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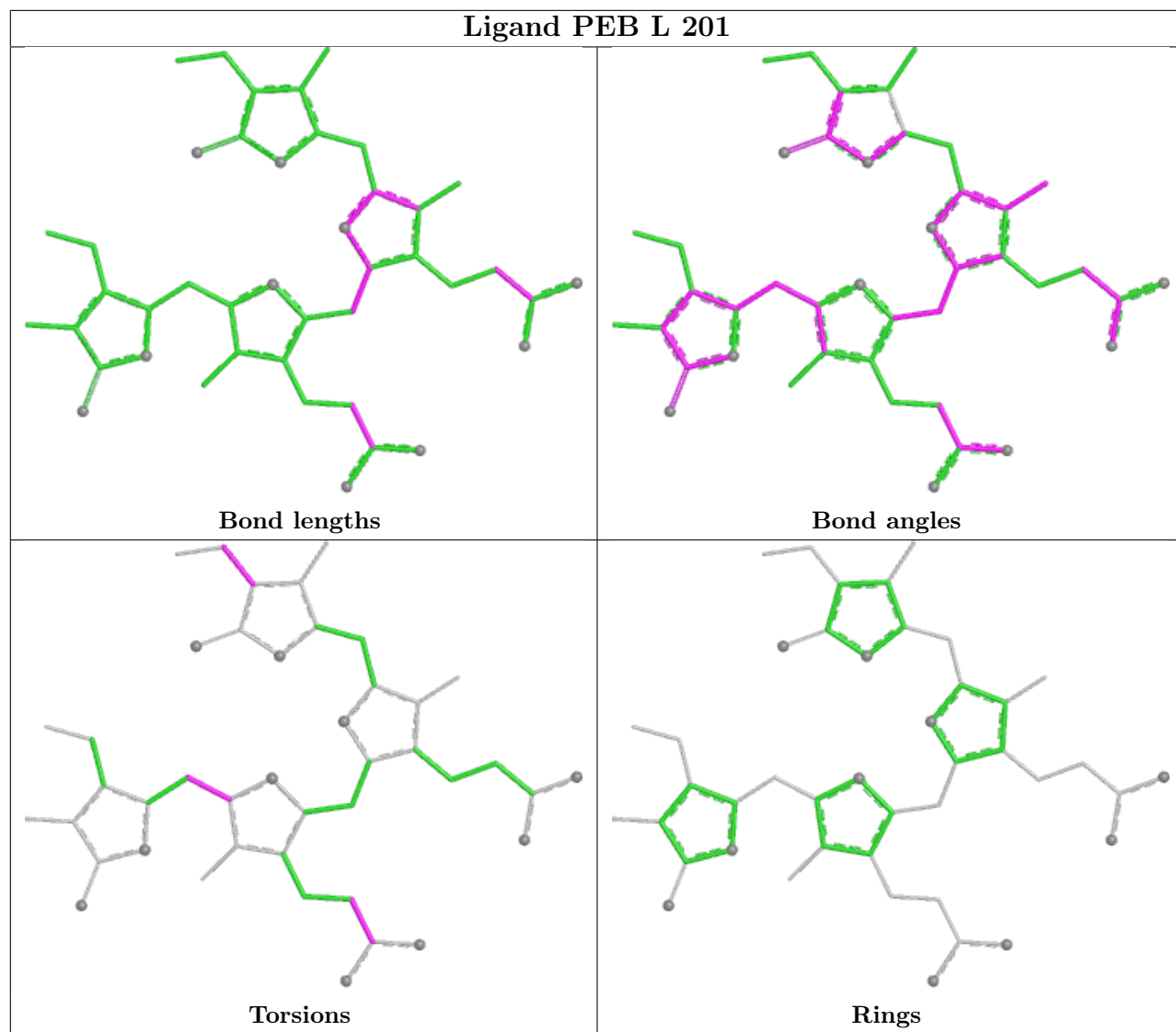
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 4   | G     | 101 | DBV  | 2       | 0            |
| 5   | H     | 202 | PEB  | 1       | 0            |
| 5   | F     | 202 | PEB  | 1       | 0            |
| 5   | D     | 203 | PEB  | 1       | 0            |

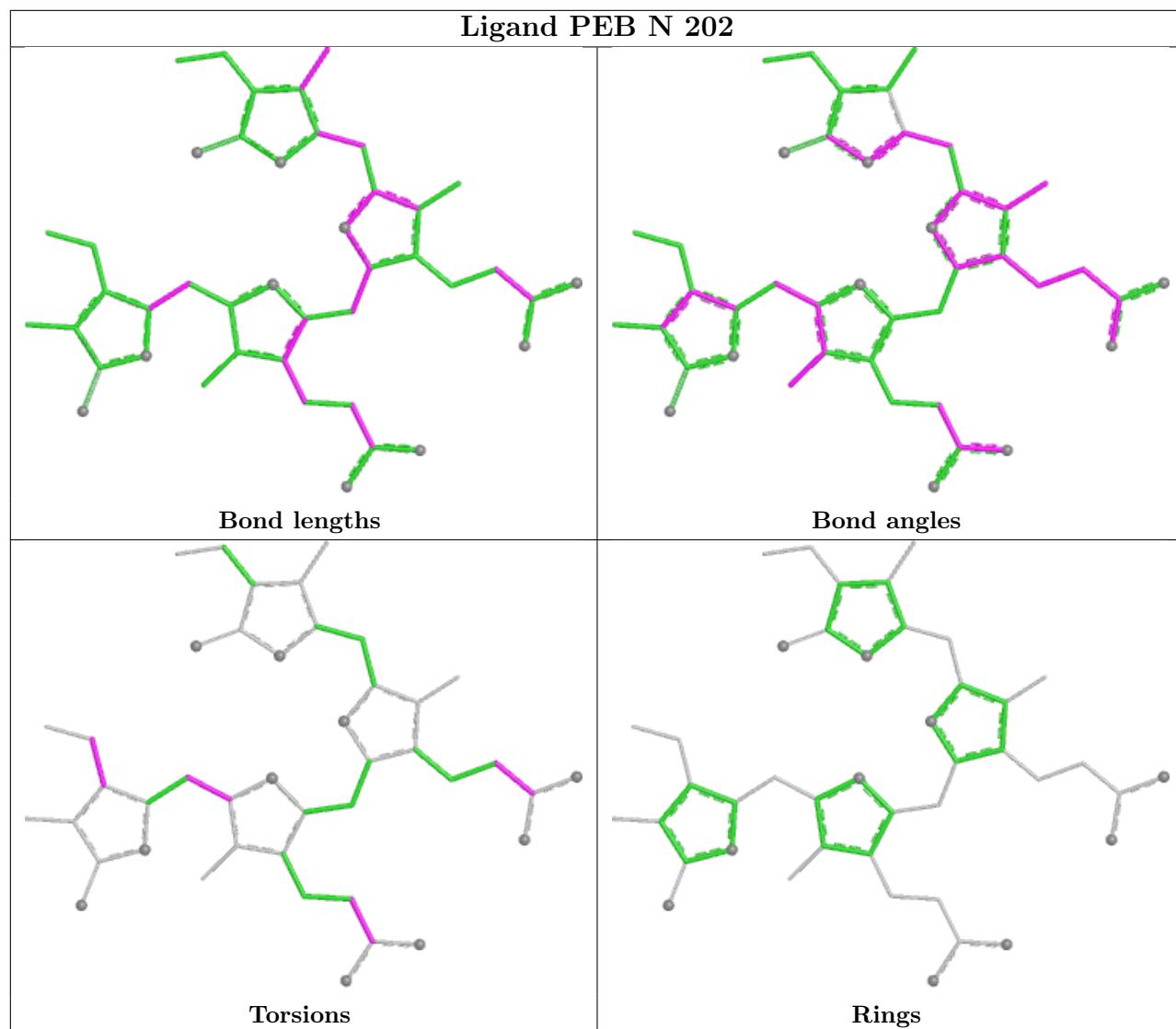
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

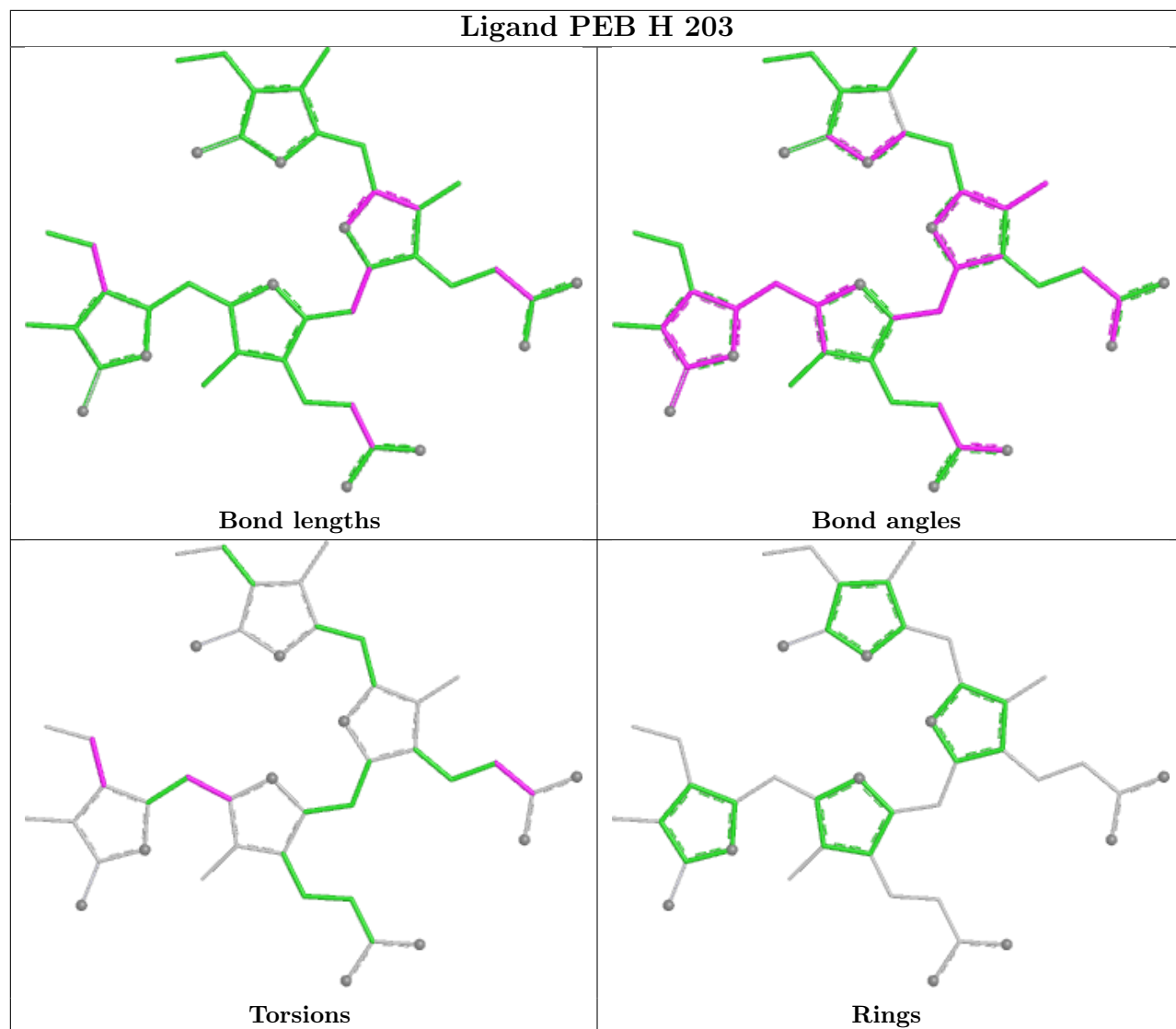


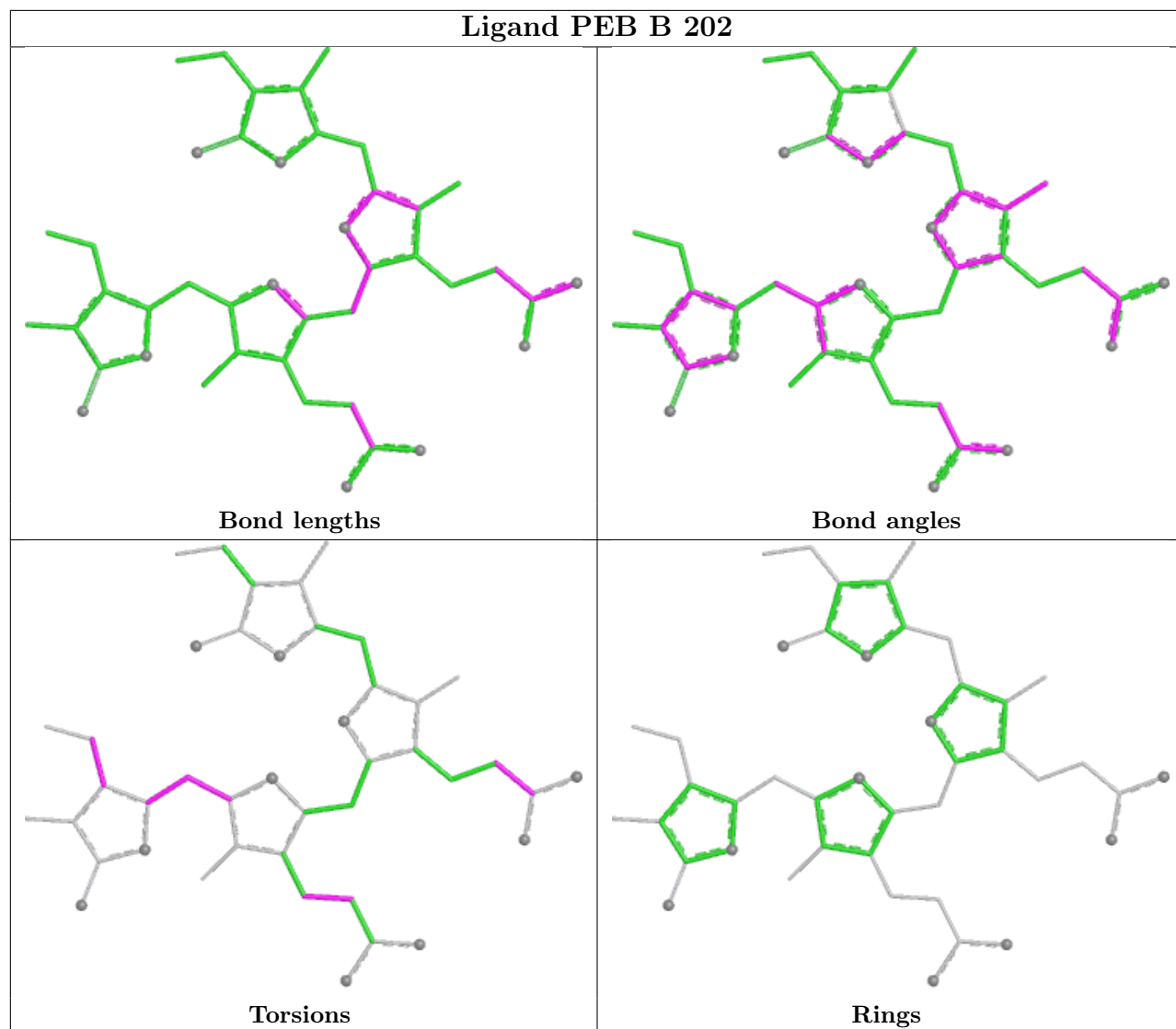




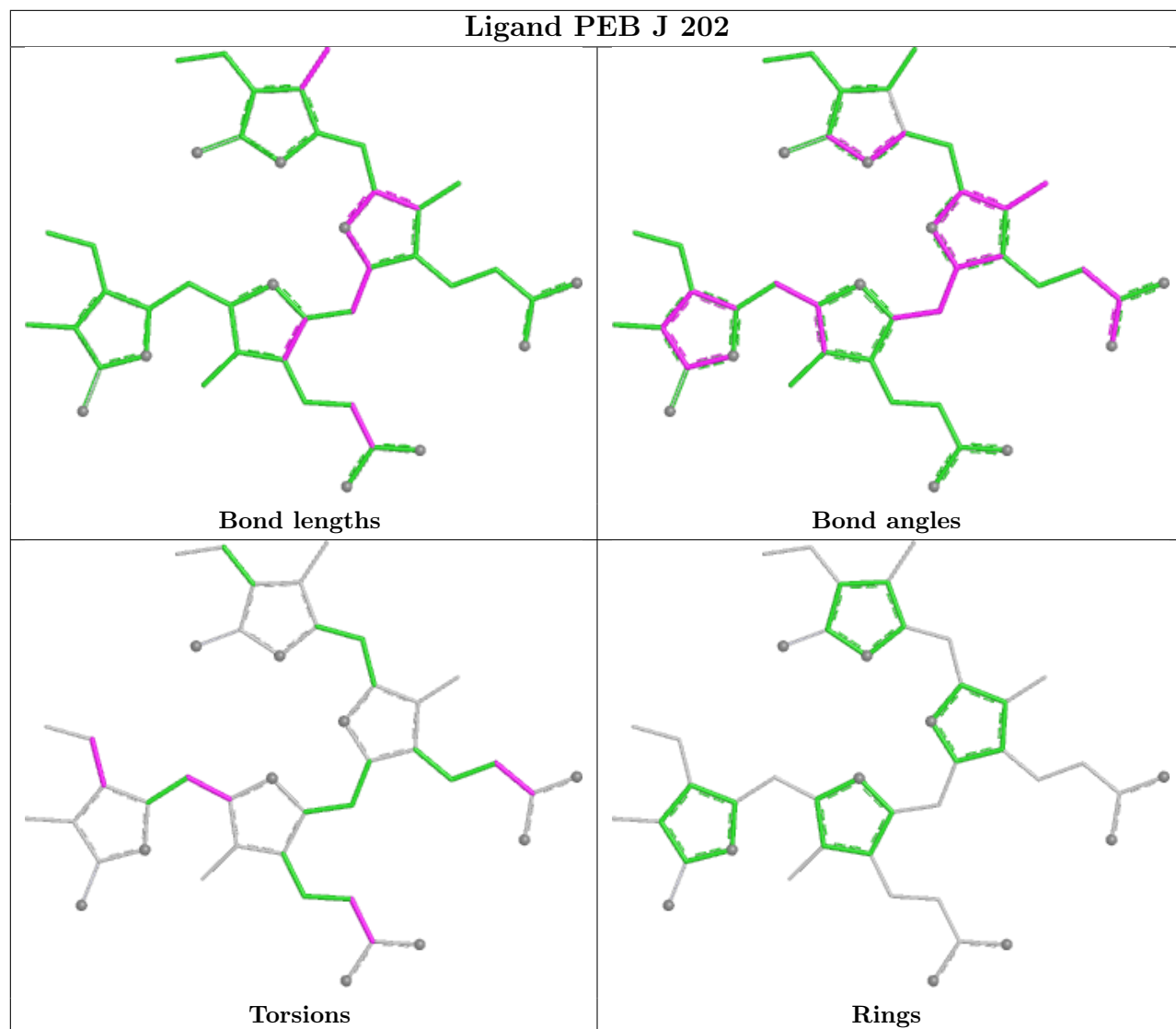




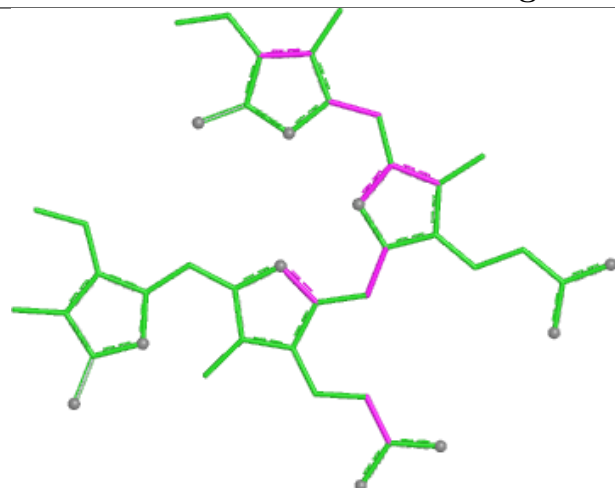




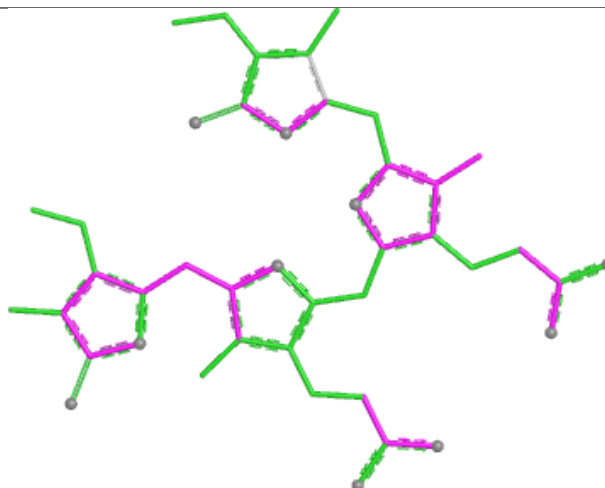
## Ligand PEB J 202



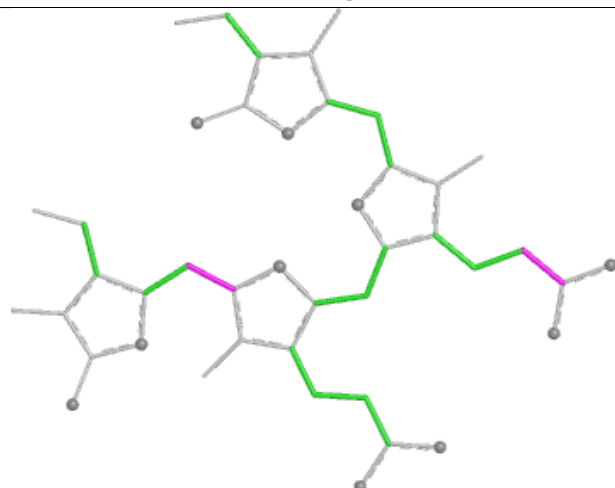
## Ligand PEB L 203



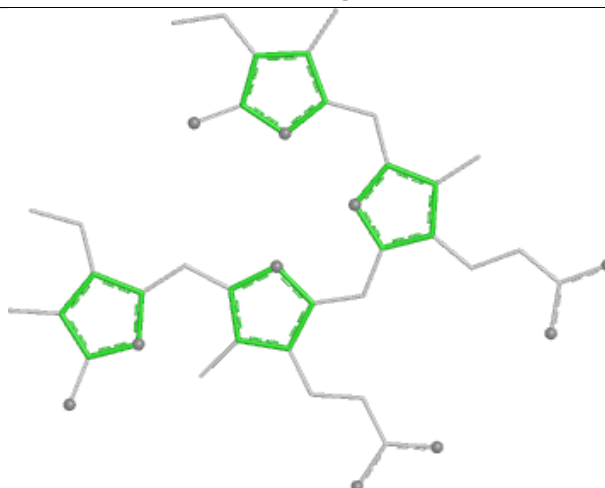
Bond lengths



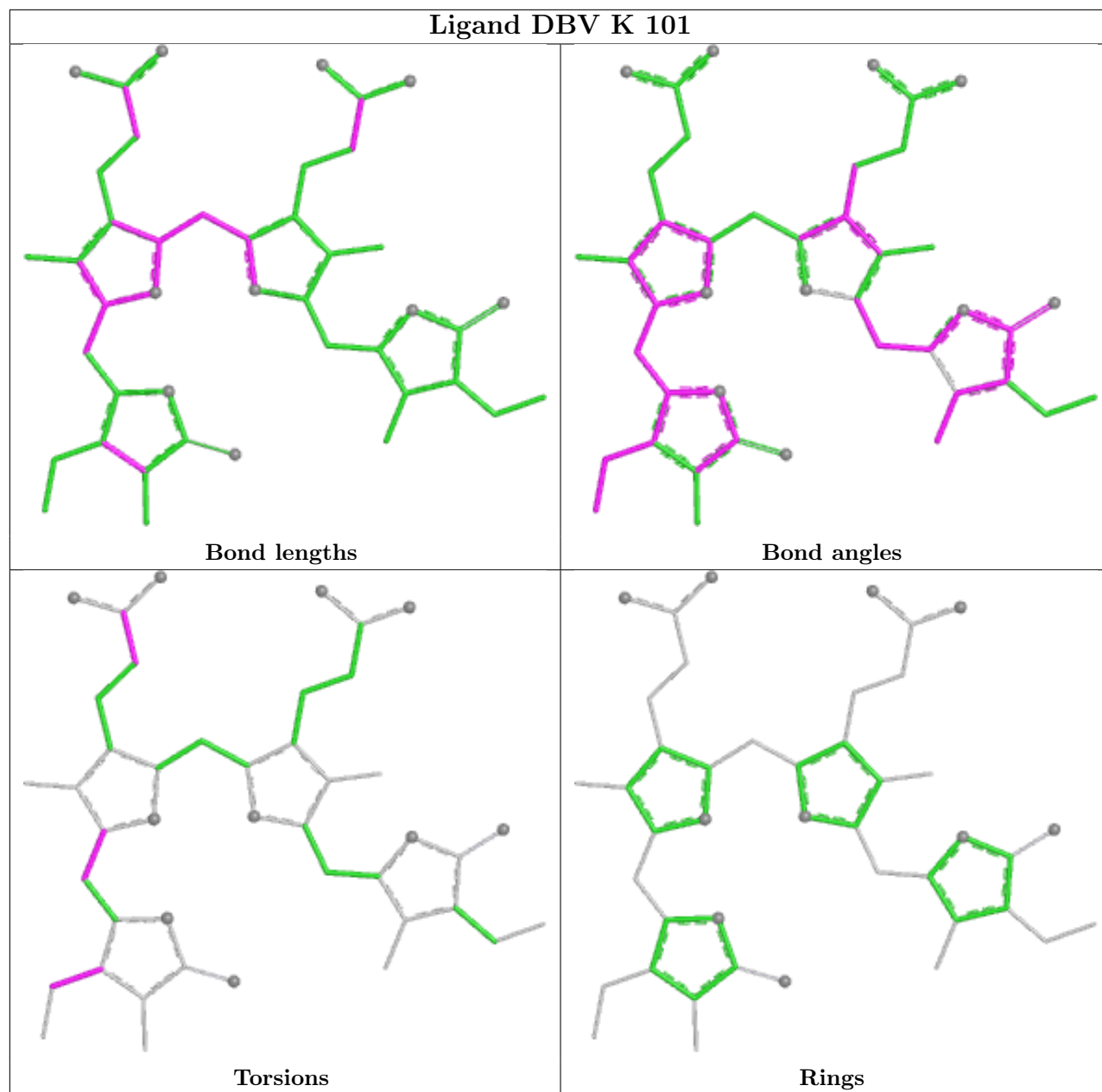
Bond angles



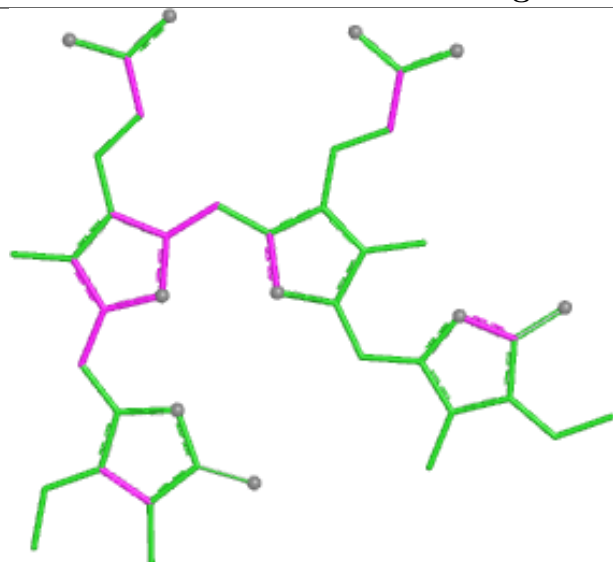
Torsions



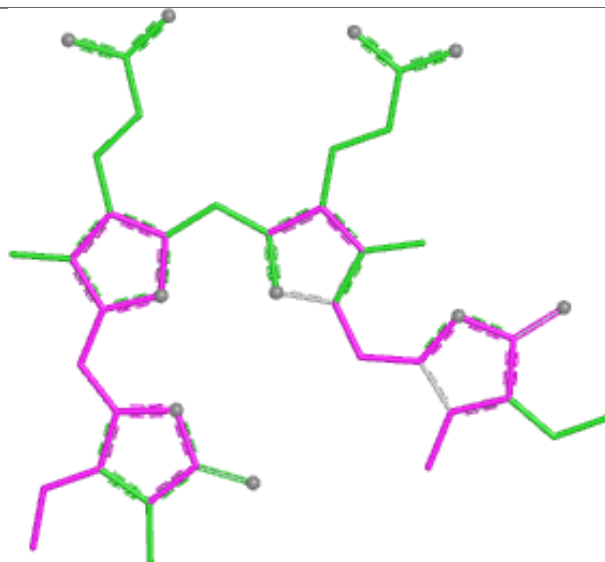
Rings



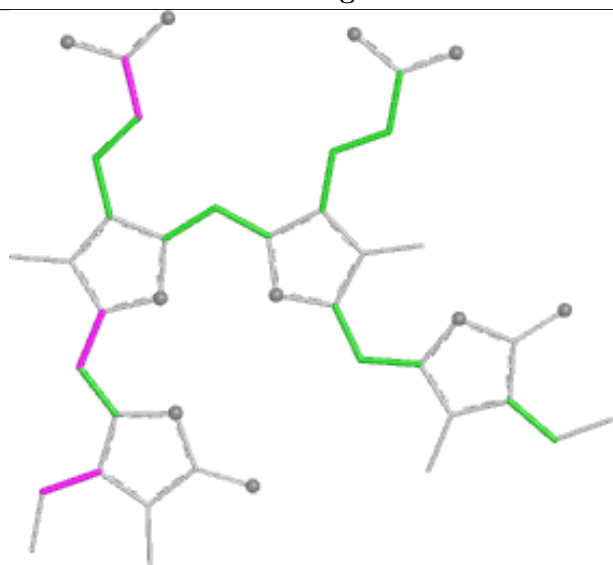
## Ligand DBV E 101



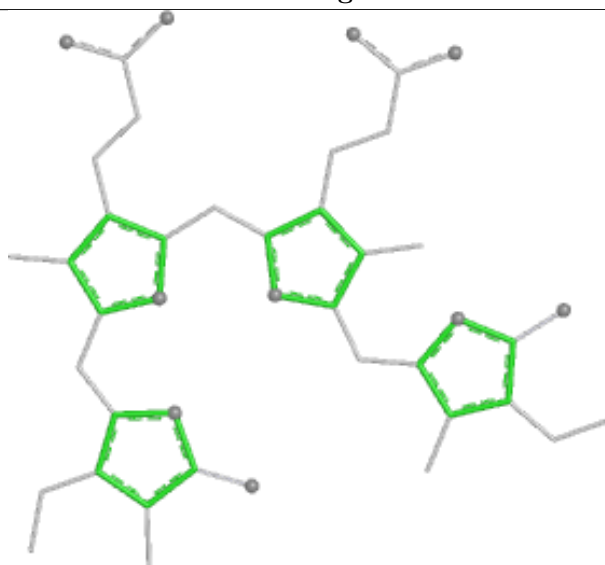
Bond lengths



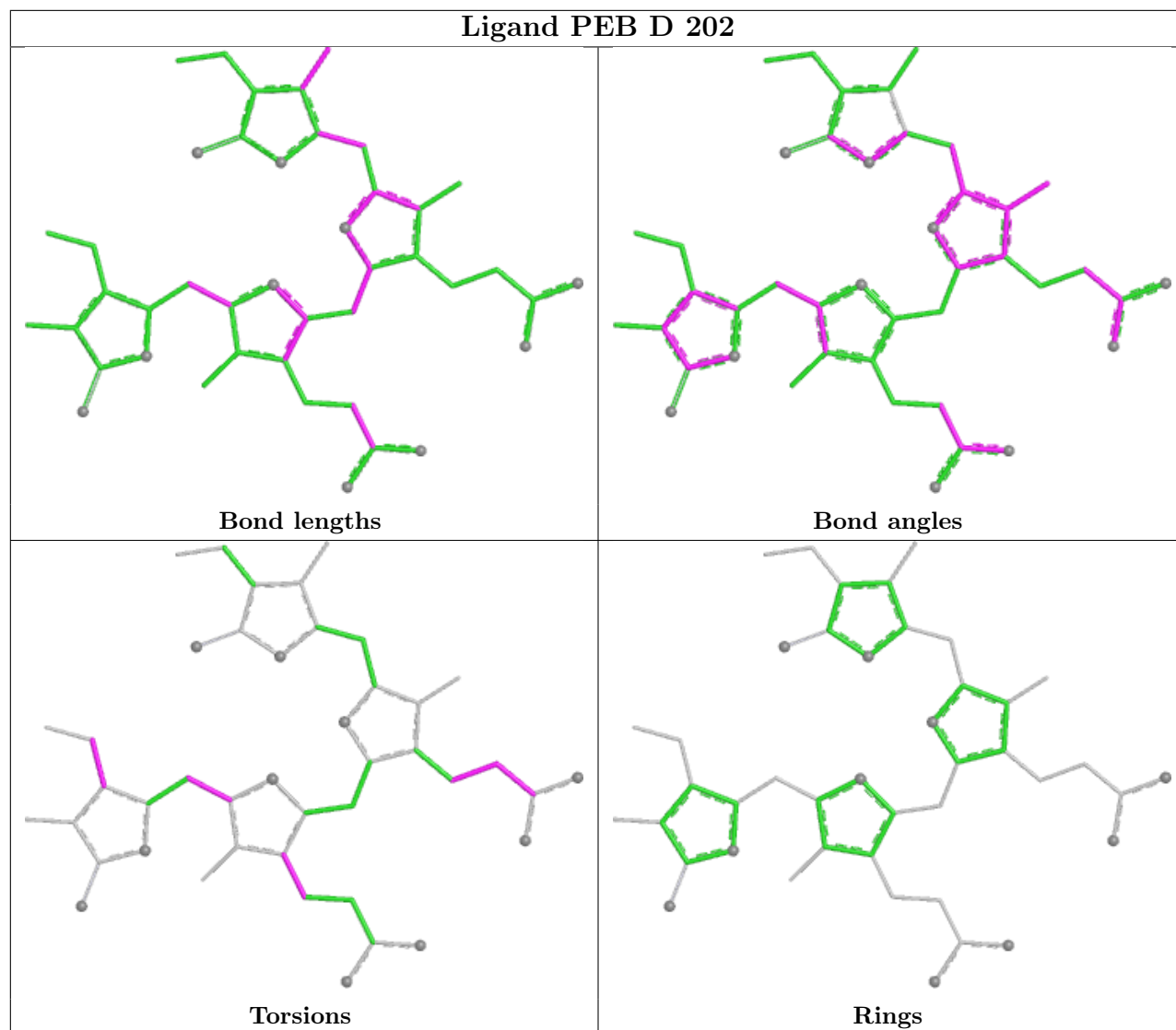
Bond angles

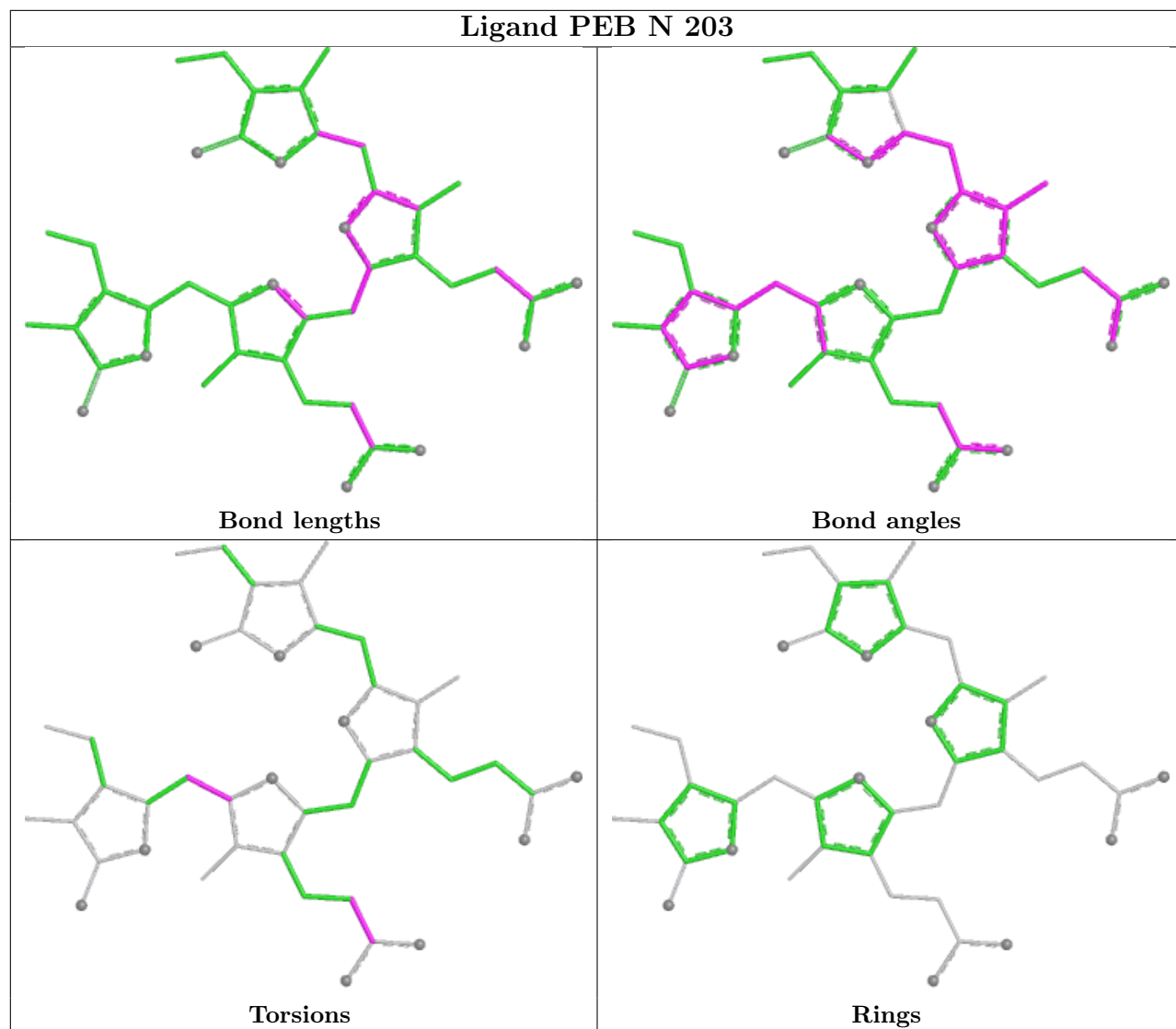


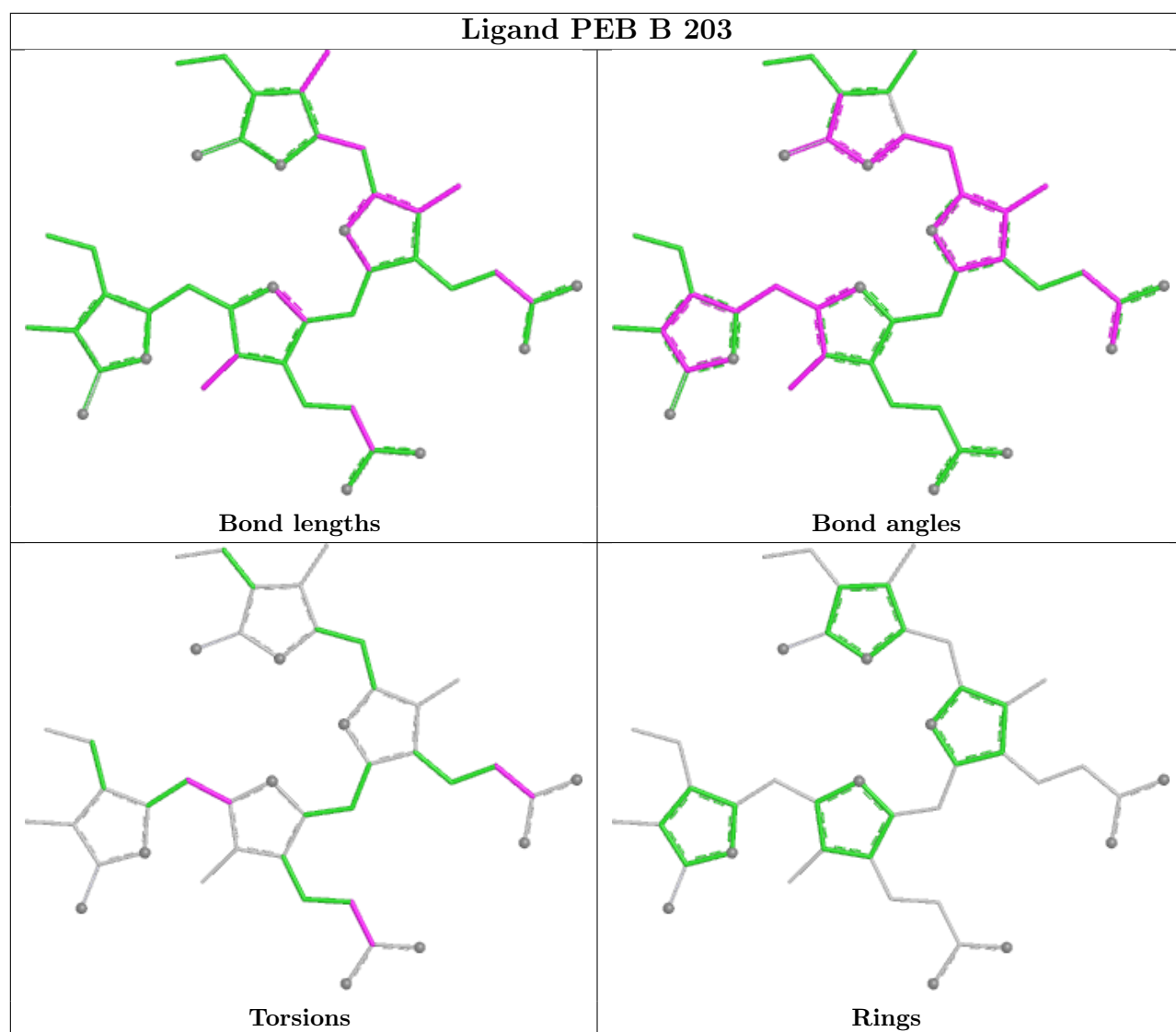
Torsions



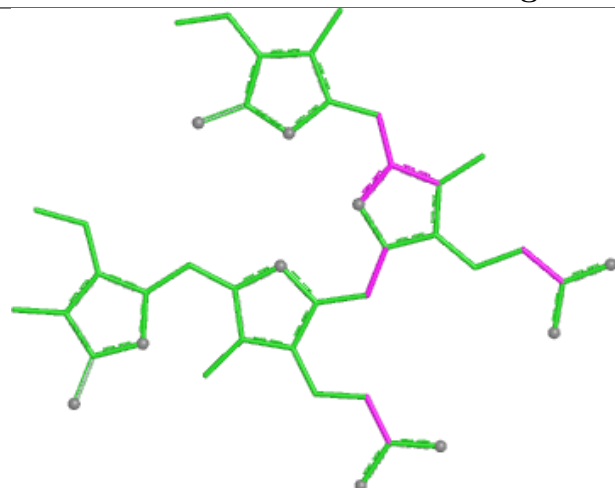
Rings



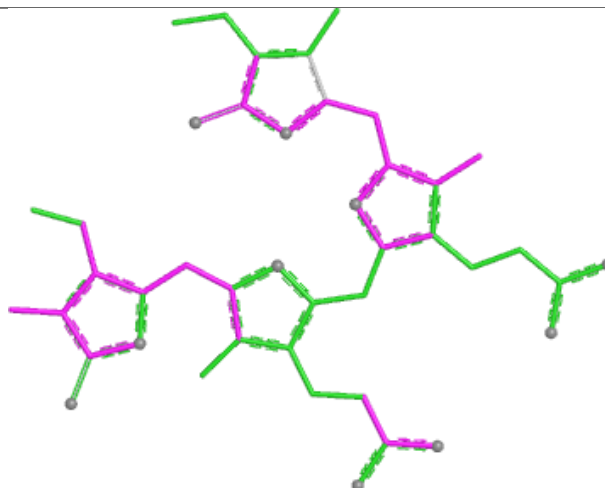




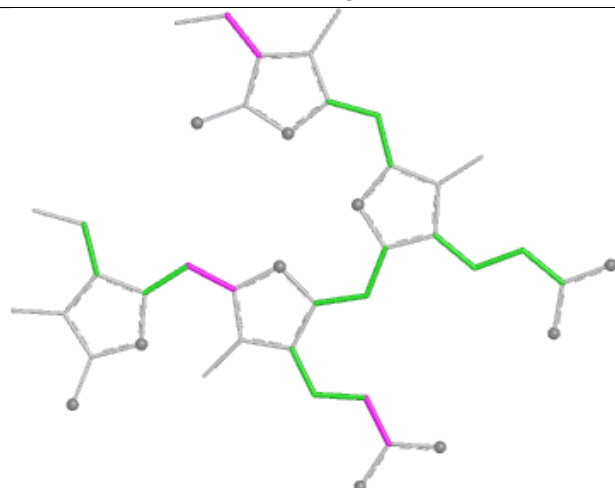
## Ligand PEB J 201



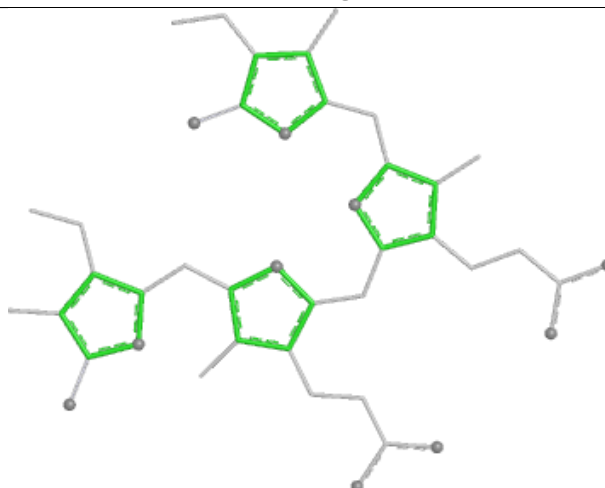
Bond lengths



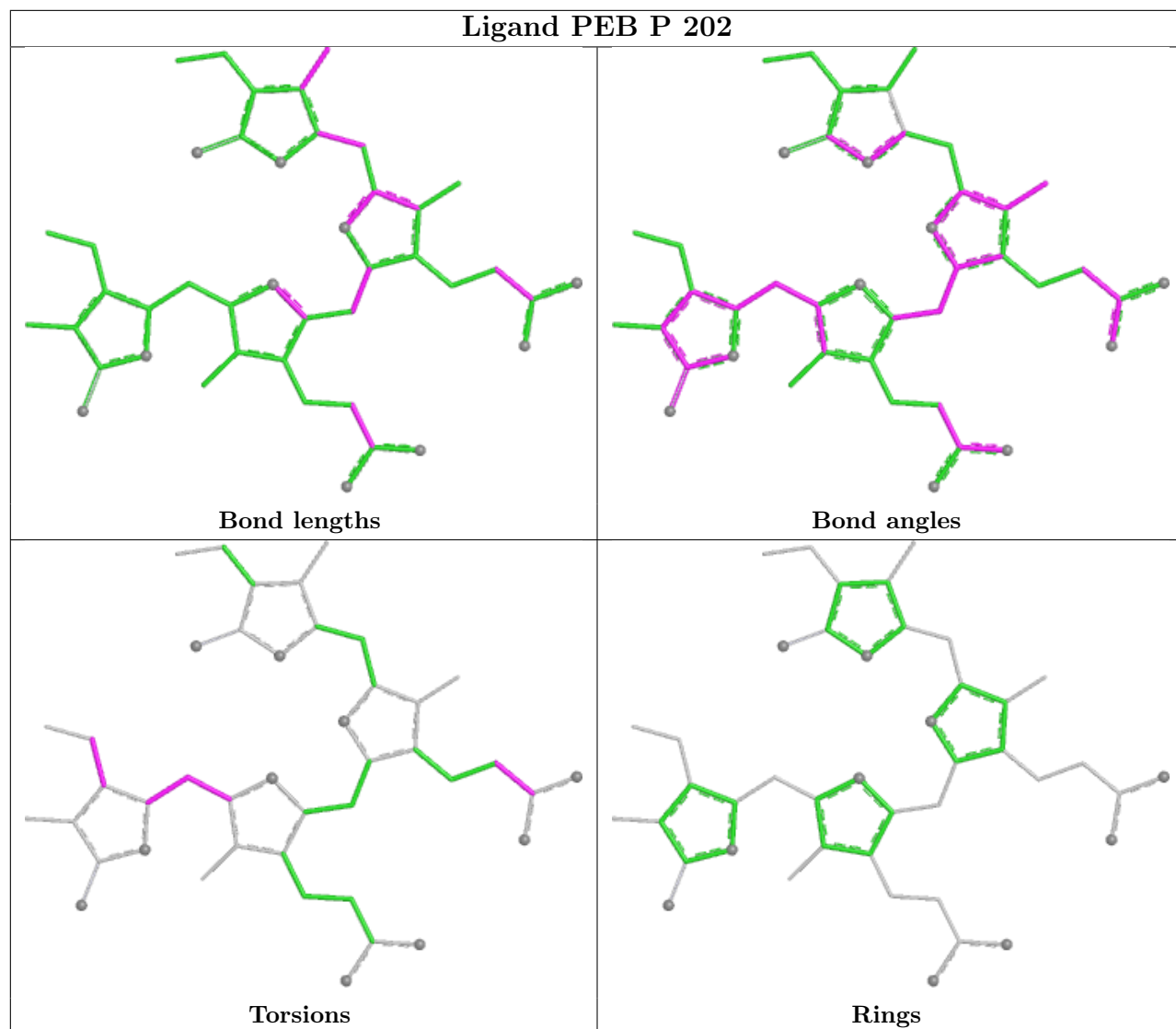
Bond angles

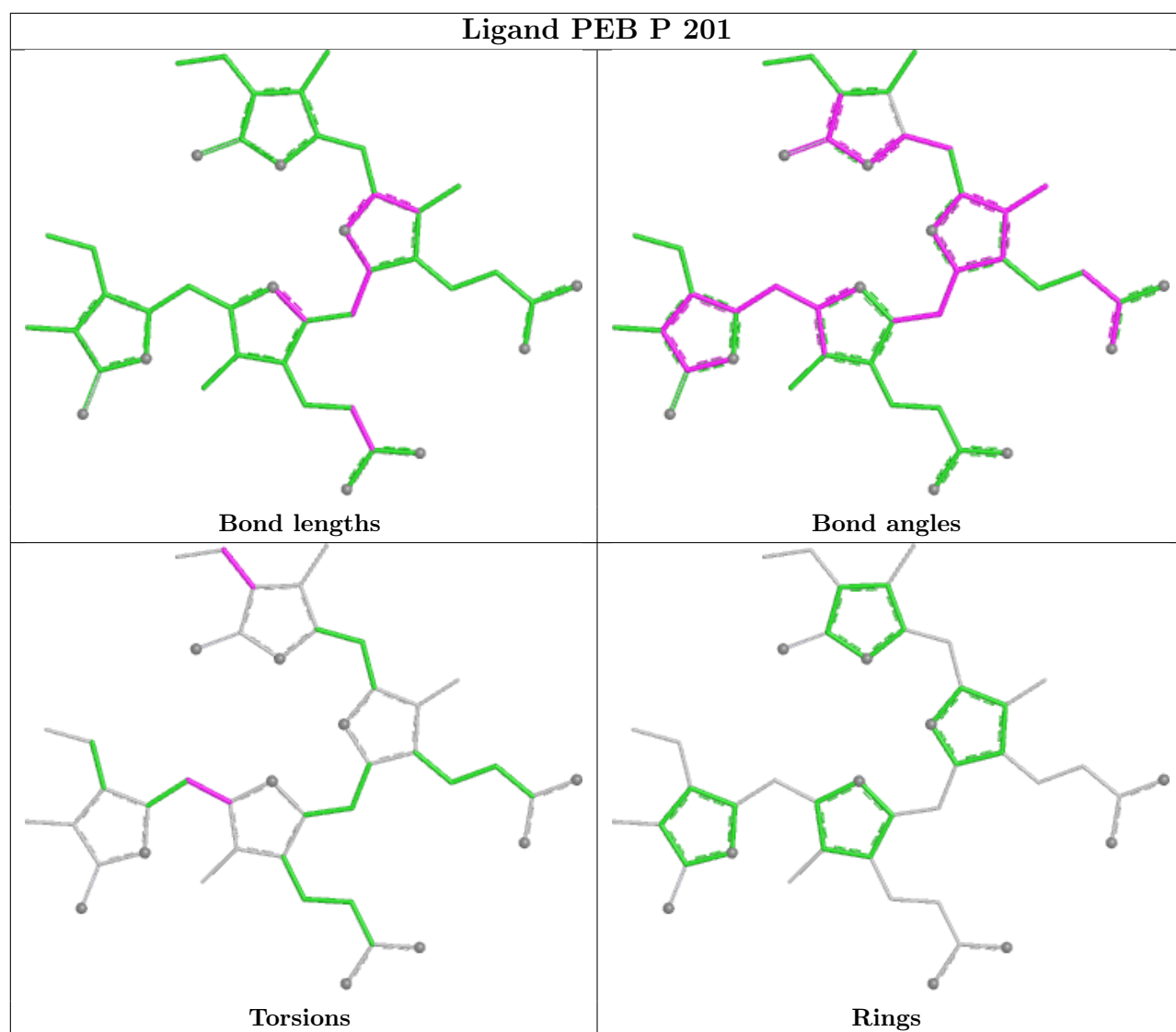


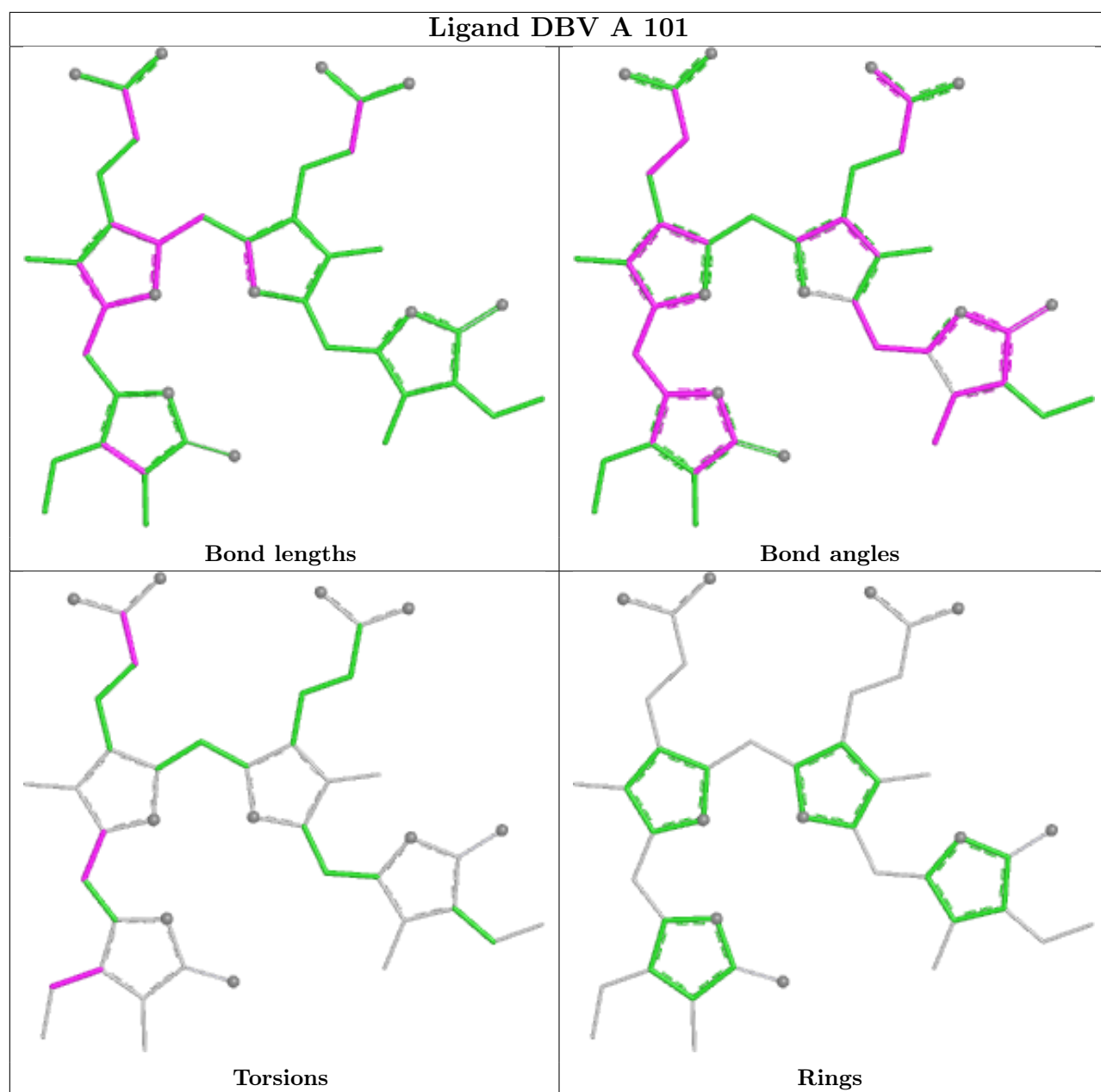
Torsions

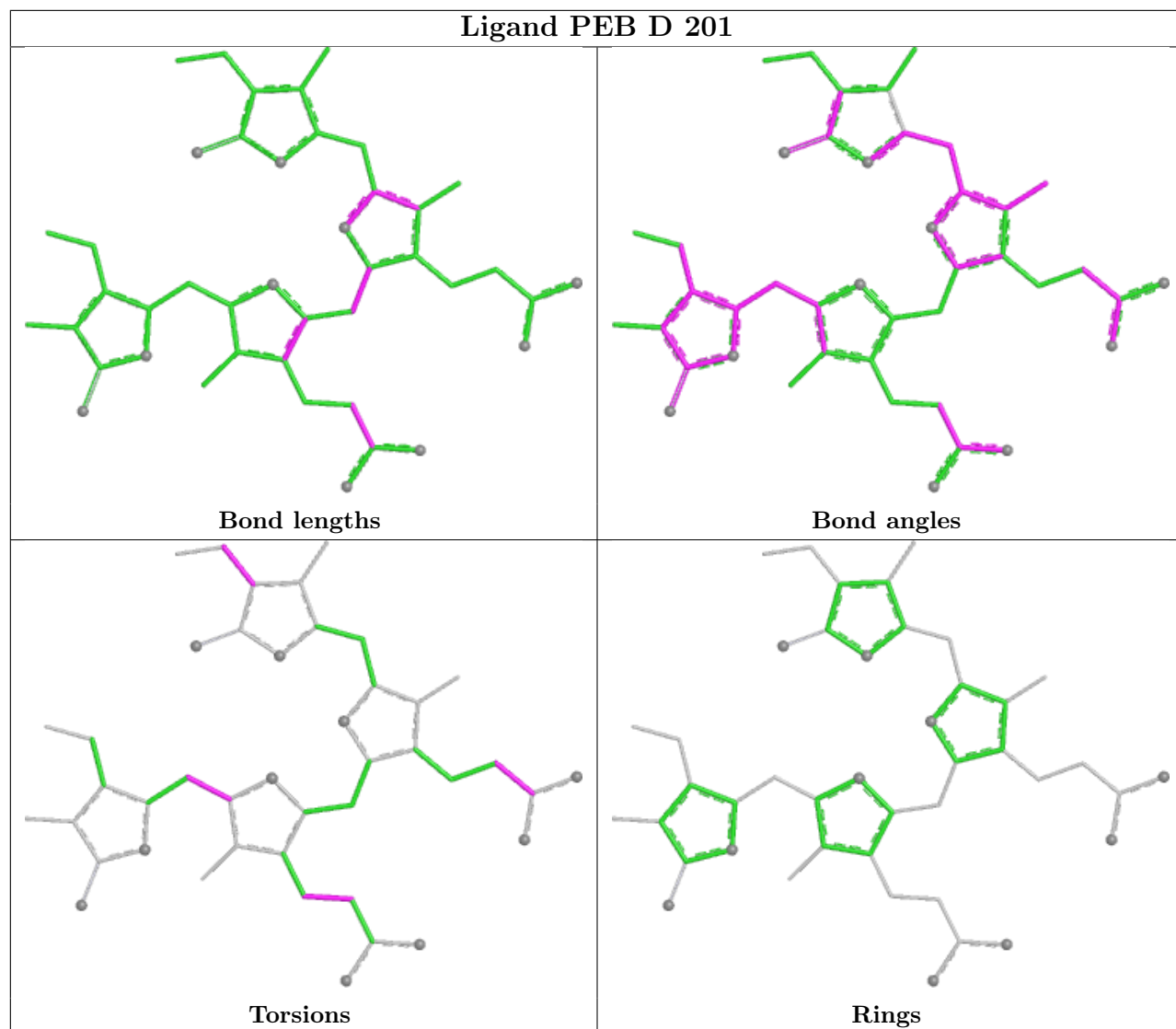


Rings

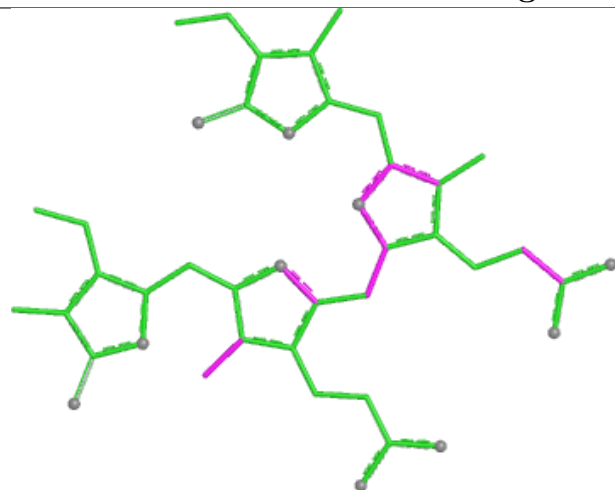




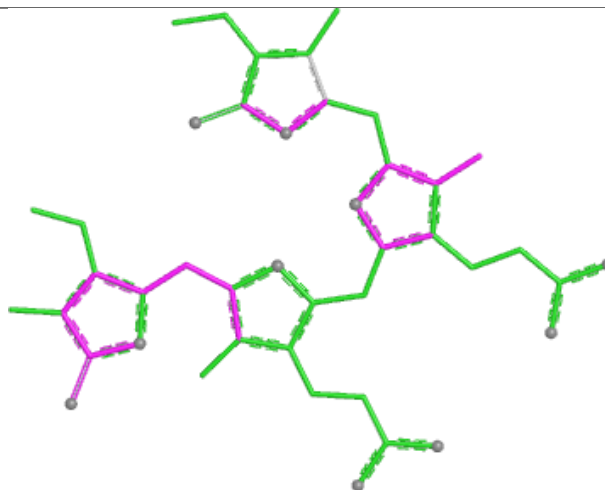




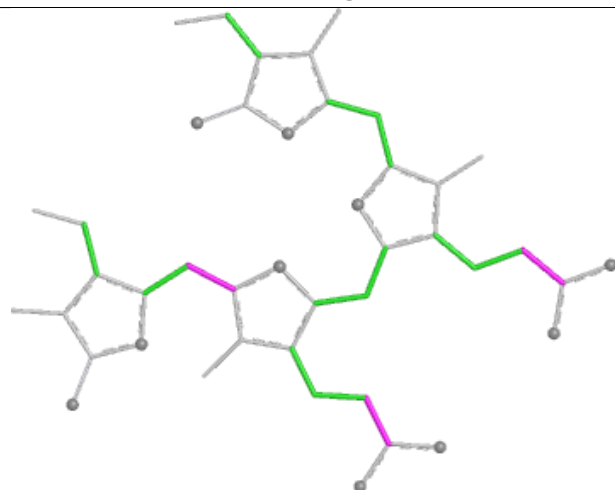
## Ligand PEB F 203



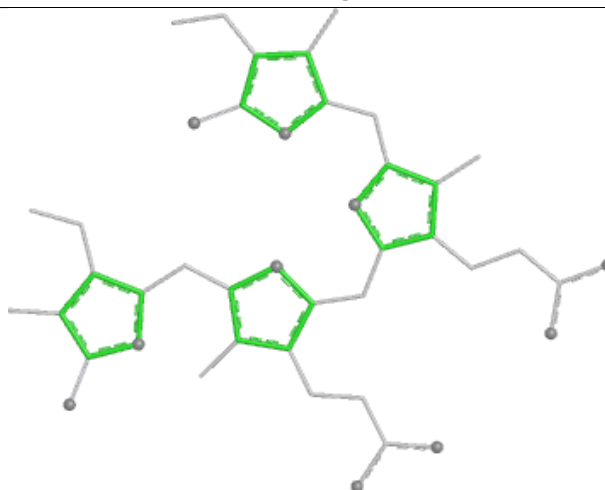
Bond lengths



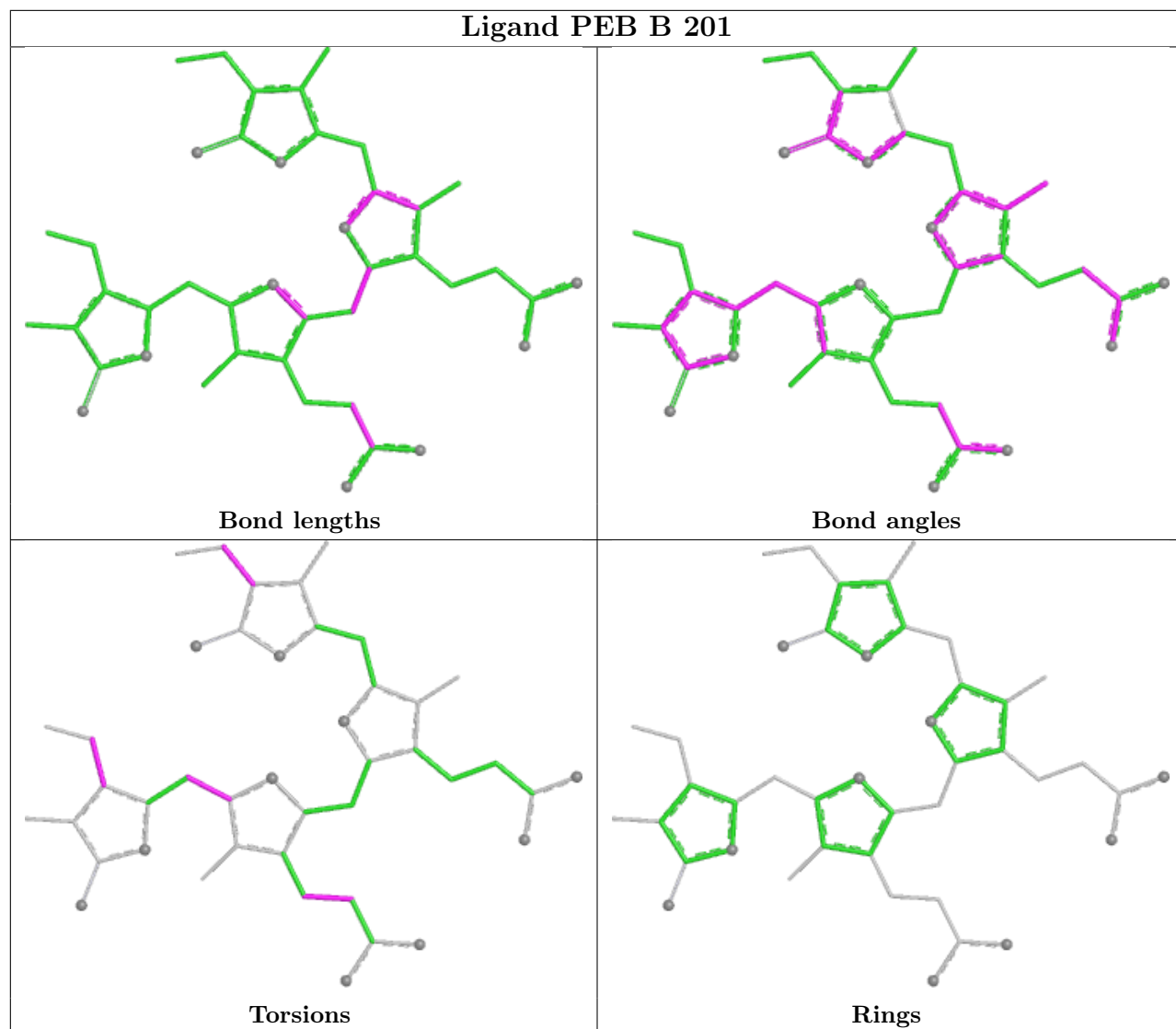
Bond angles



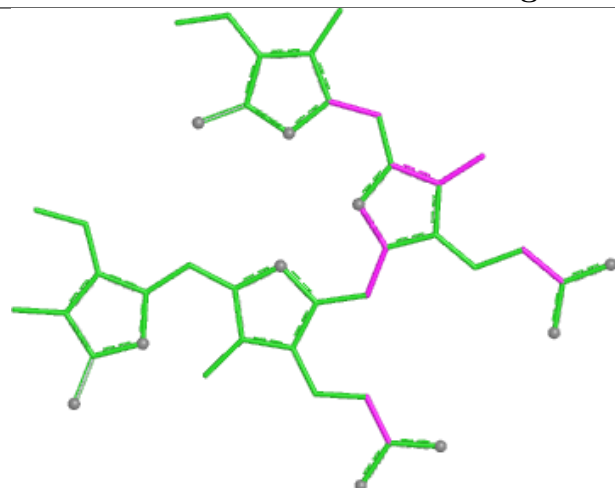
Torsions



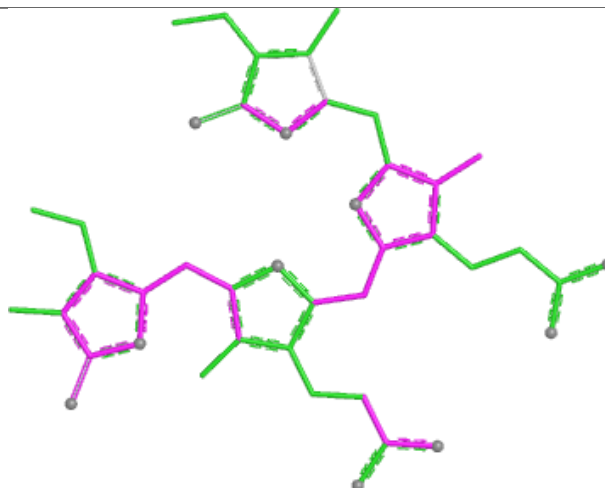
Rings



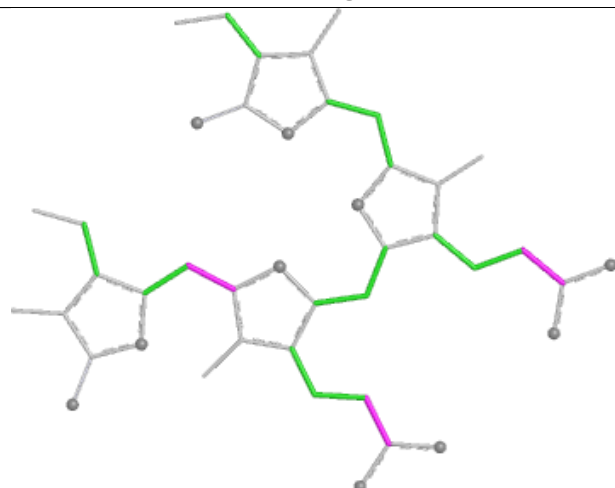
## Ligand PEB J 203



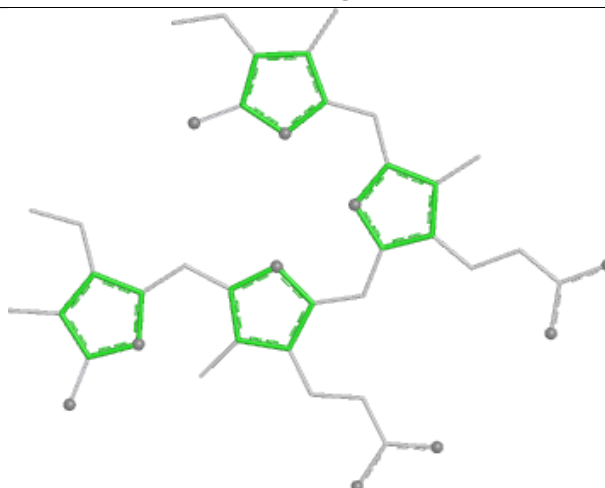
Bond lengths



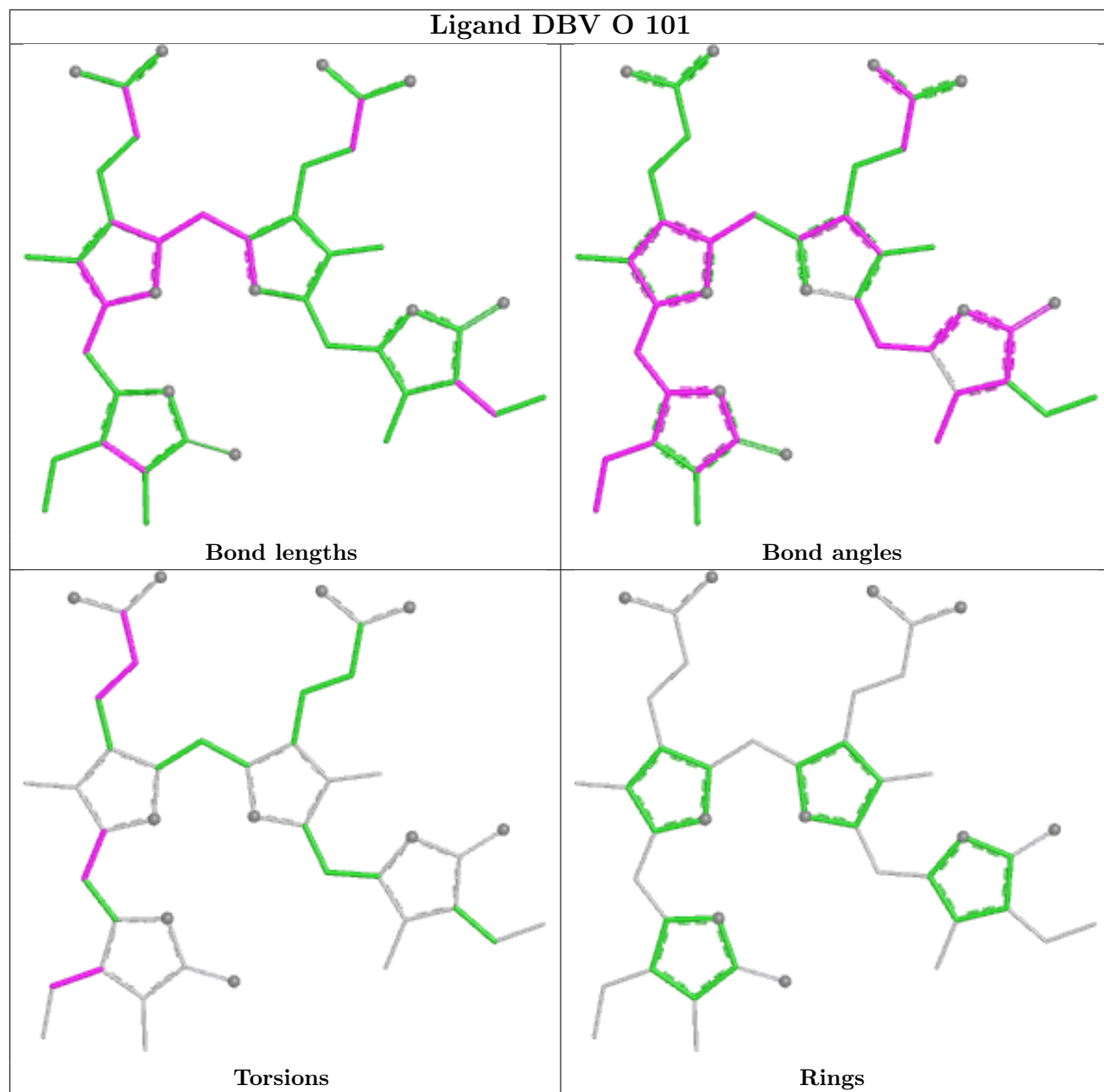
Bond angles

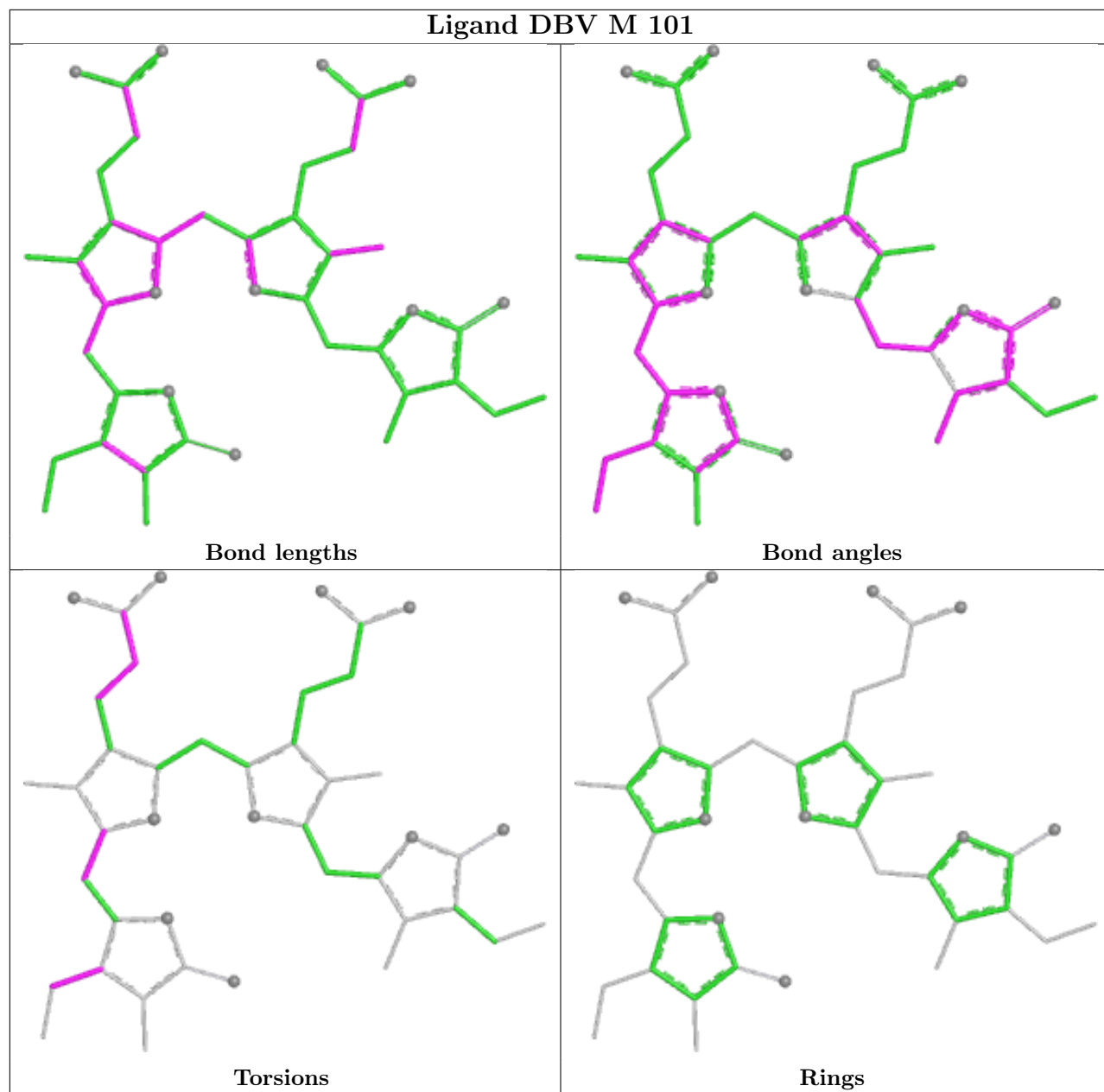


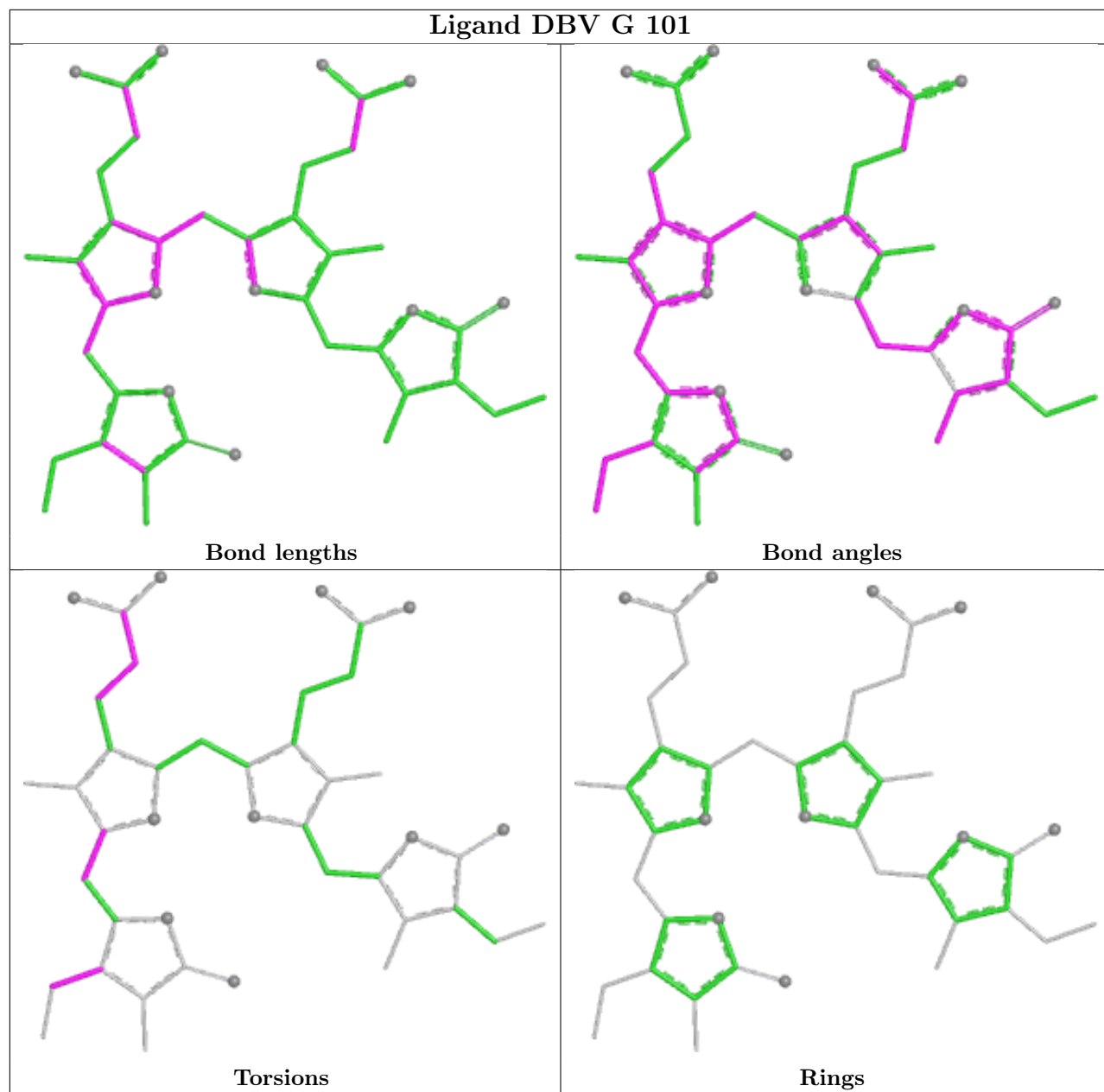
Torsions

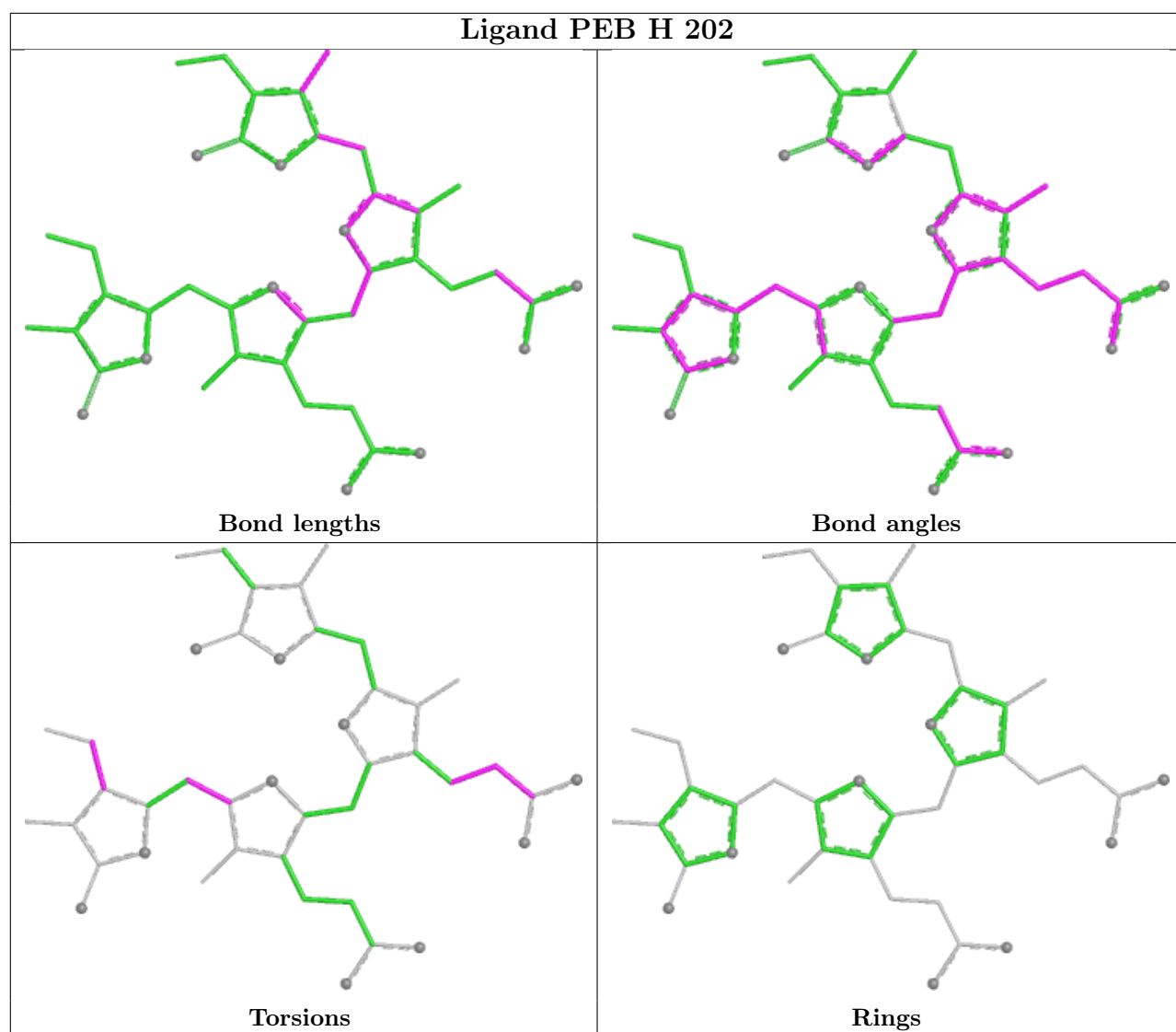


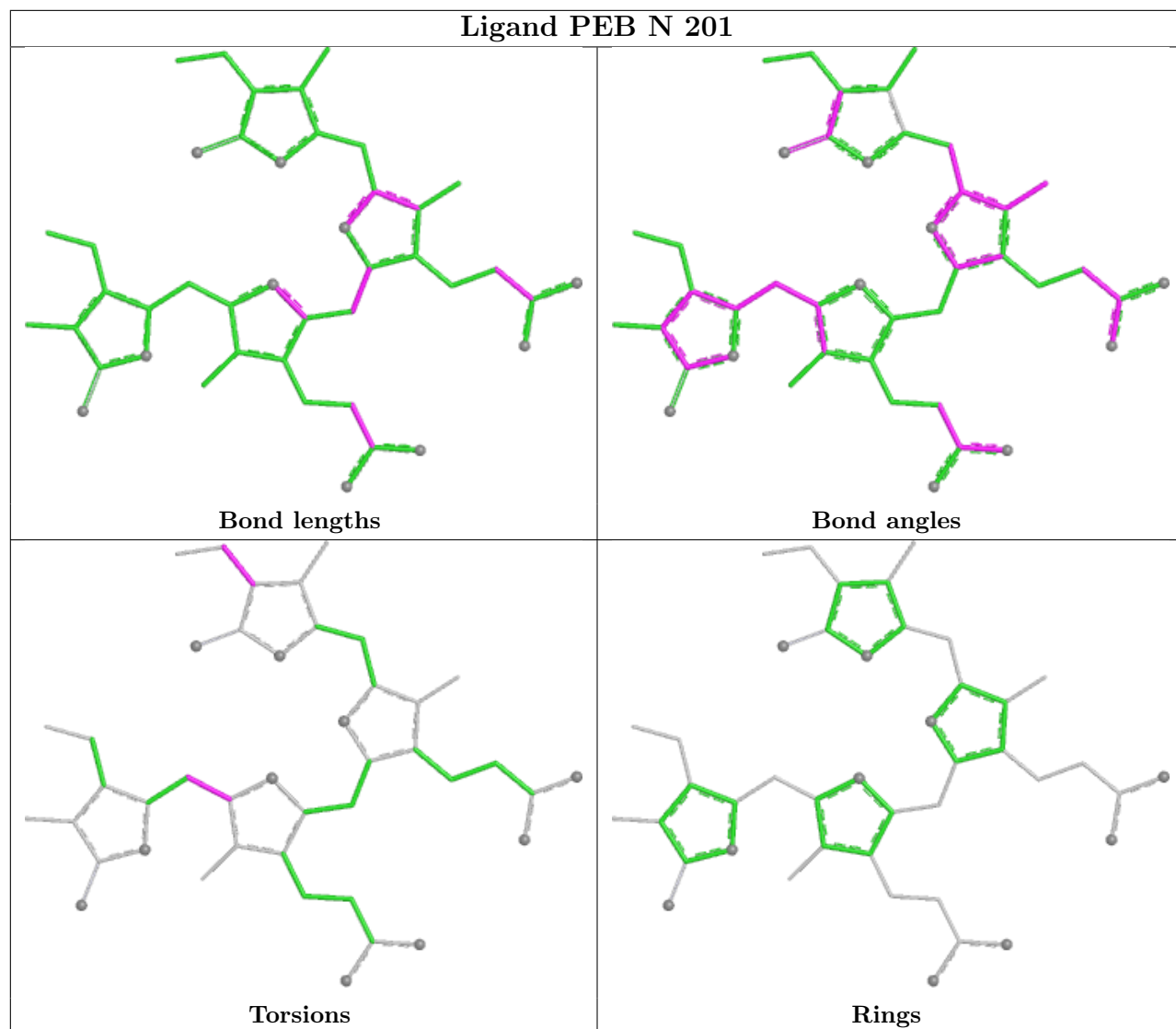
Rings



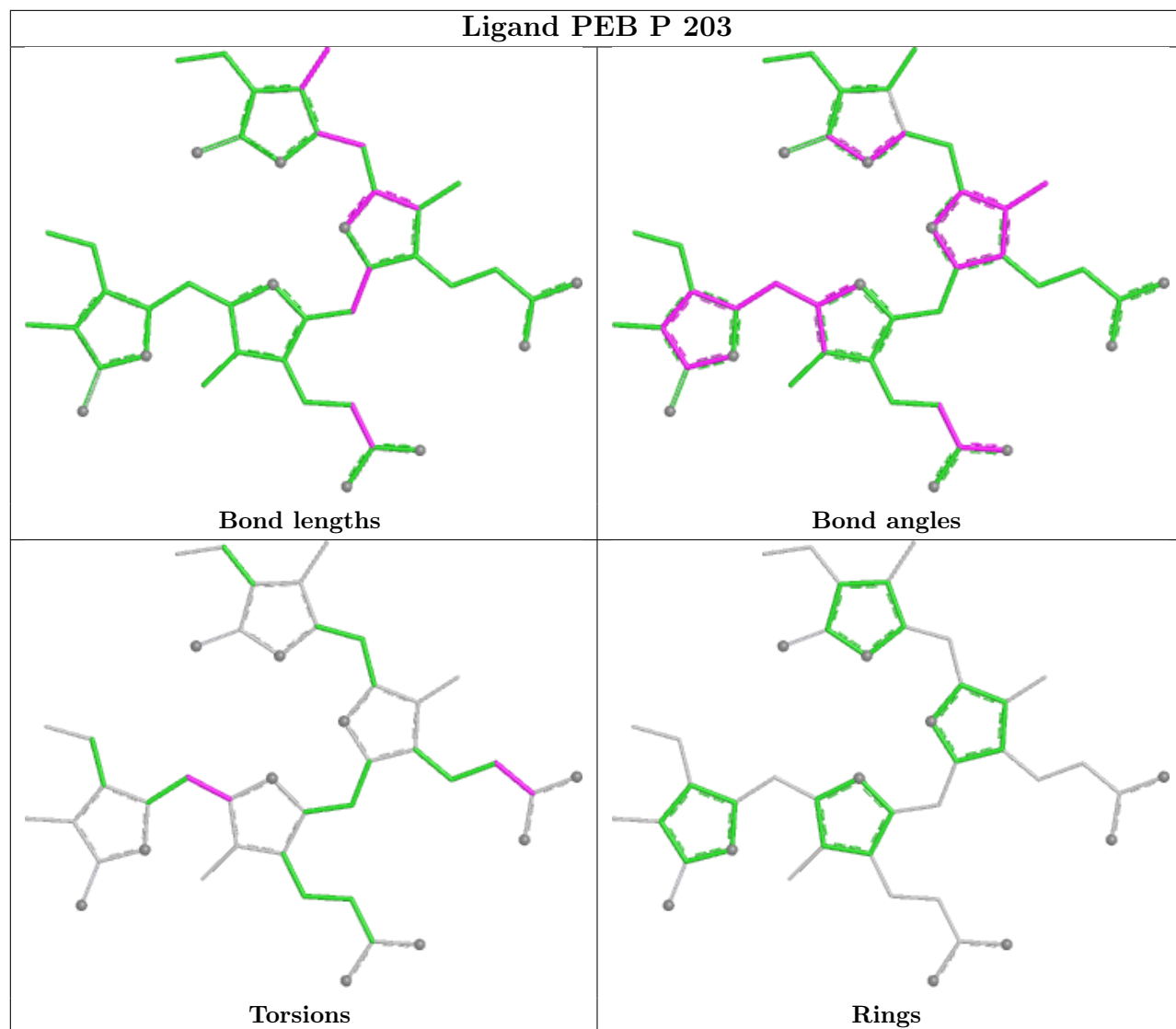




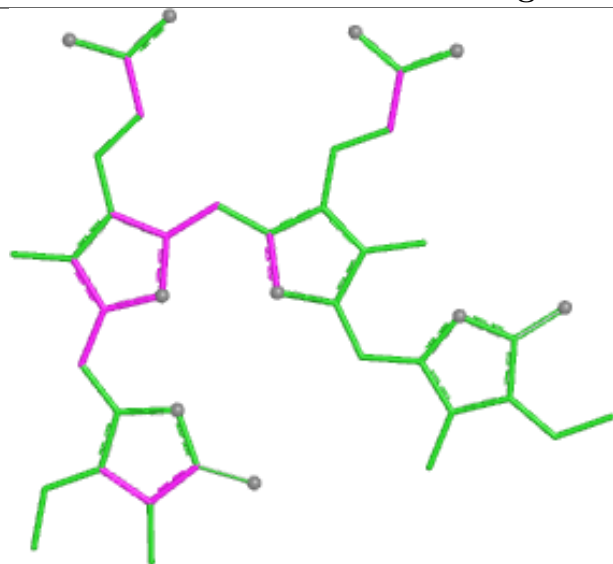




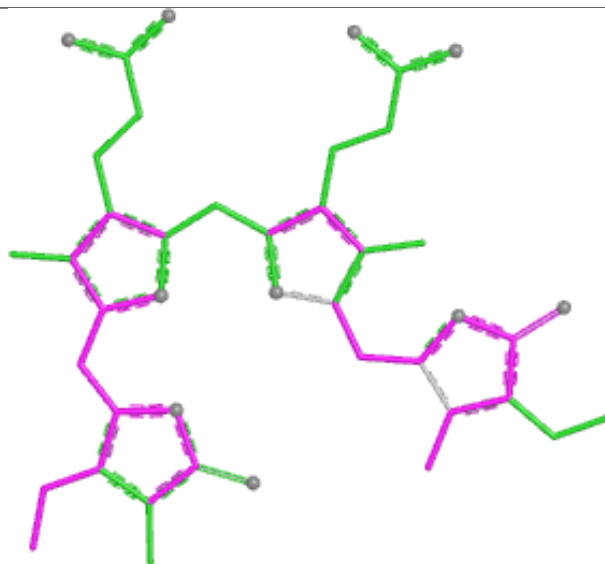
## Ligand PEB P 203



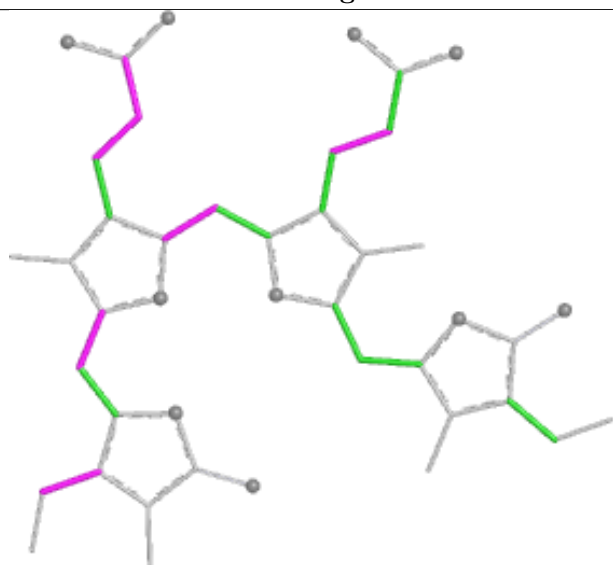
## Ligand DBV I 101



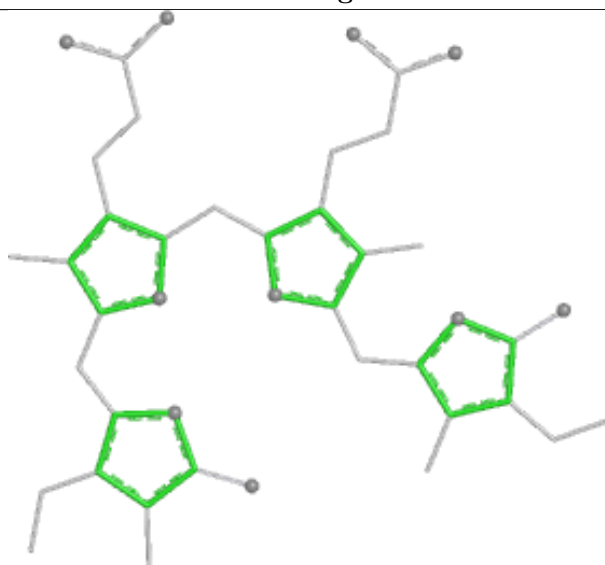
Bond lengths



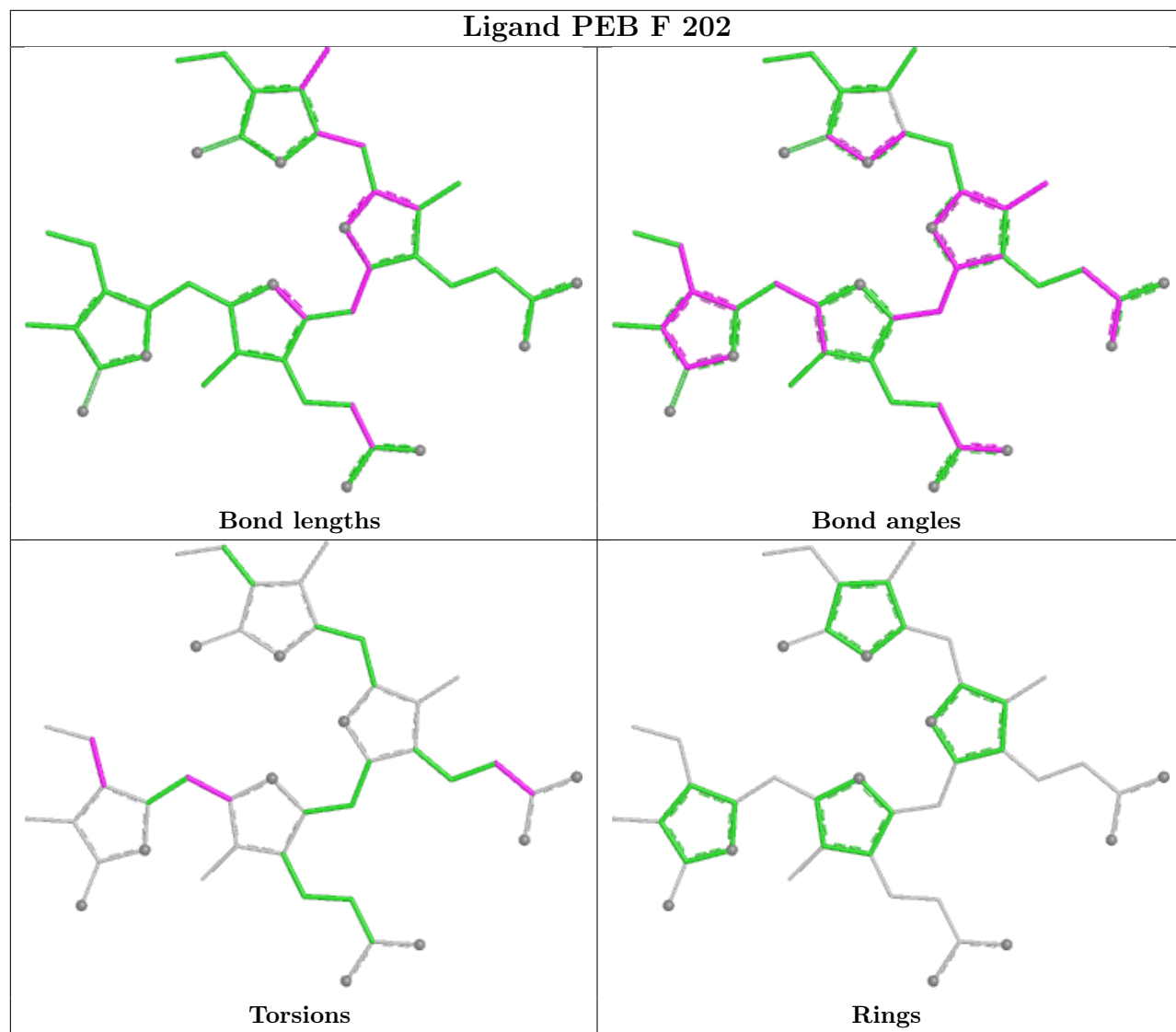
Bond angles

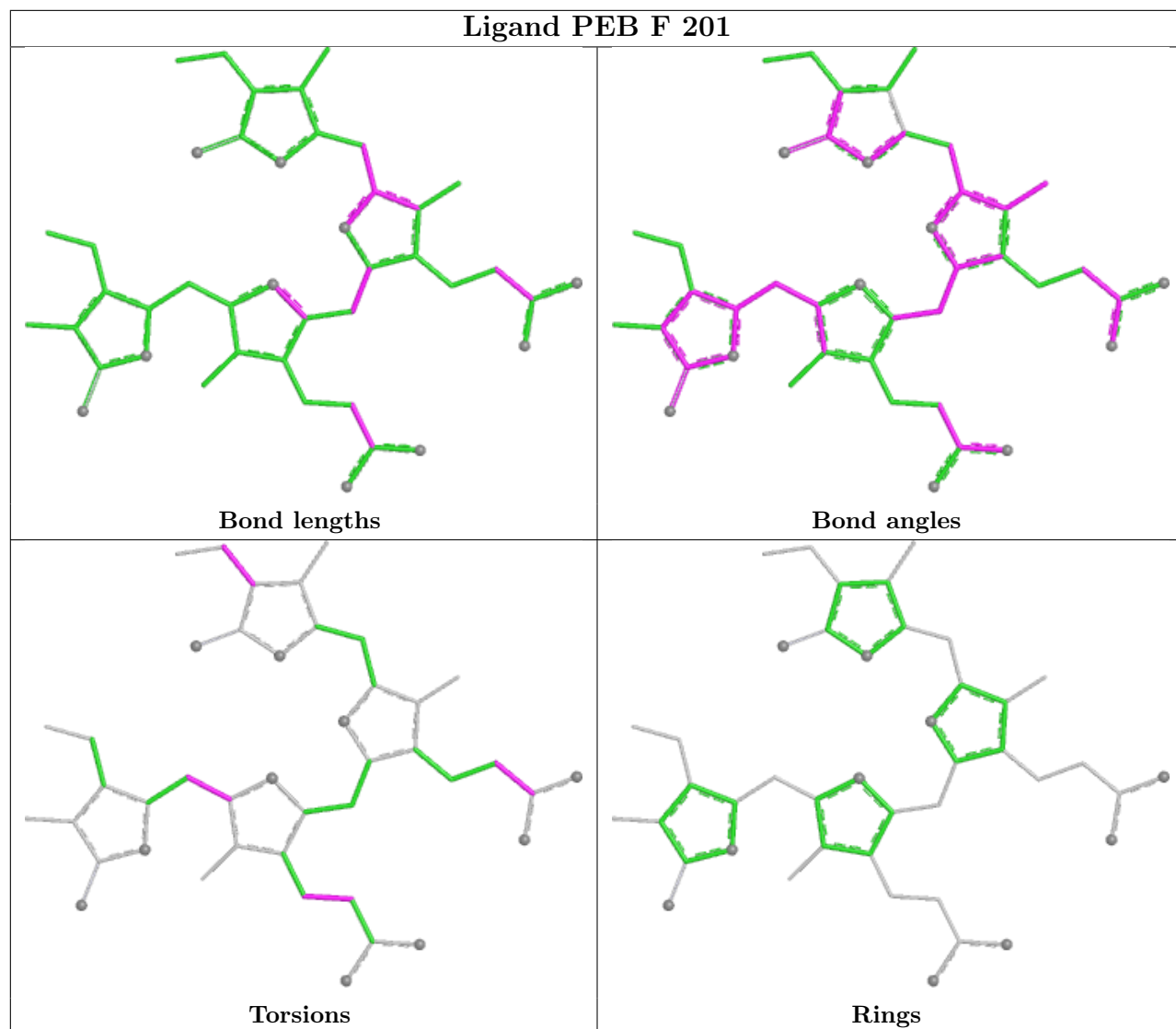


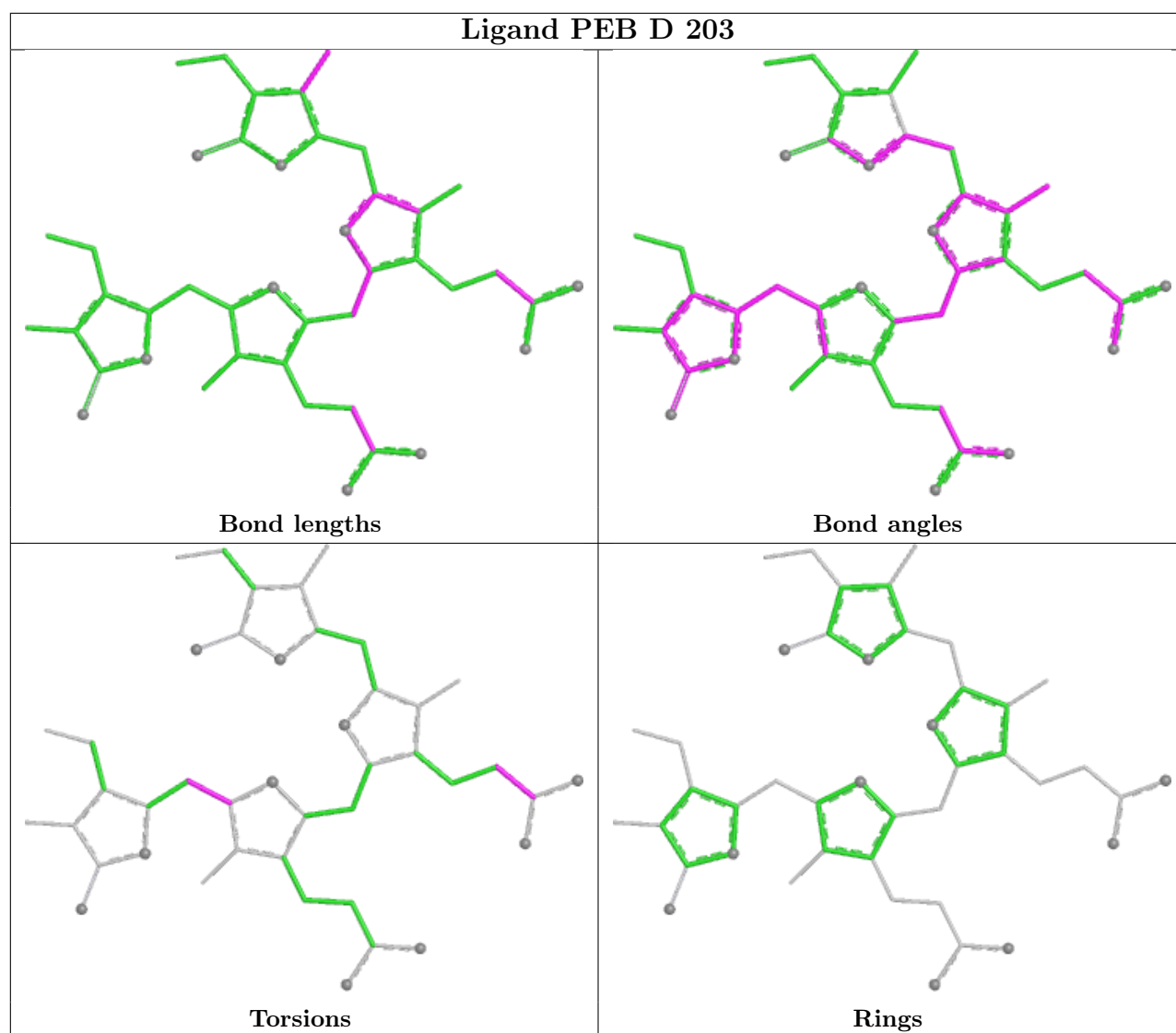
Torsions



Rings







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2                     | OWAB(Å <sup>2</sup> ) | Q<0.9  |
|-----|-------|-----------------|--------|-----------------------------|-----------------------|--------|
| 1   | A     | 72/76 (94%)     | 1.55   | 16 (22%) <b>2</b> <b>1</b>  | 50, 68, 100, 141      | 0      |
| 1   | E     | 74/76 (97%)     | 0.63   | 0 <b>100</b> <b>100</b>     | 28, 45, 64, 68        | 0      |
| 1   | I     | 75/76 (98%)     | 0.94   | 11 (14%) <b>6</b> <b>4</b>  | 32, 54, 75, 113       | 0      |
| 1   | M     | 74/76 (97%)     | 0.93   | 10 (13%) <b>7</b> <b>5</b>  | 38, 58, 74, 93        | 0      |
| 2   | B     | 162/177 (91%)   | 1.23   | 25 (15%) <b>5</b> <b>4</b>  | 32, 59, 89, 116       | 0      |
| 2   | D     | 173/177 (97%)   | 1.24   | 31 (17%) <b>3</b> <b>3</b>  | 32, 56, 107, 143      | 0      |
| 2   | F     | 166/177 (93%)   | 0.90   | 20 (12%) <b>9</b> <b>6</b>  | 30, 47, 82, 98        | 1 (0%) |
| 2   | H     | 170/177 (96%)   | 0.86   | 18 (10%) <b>11</b> <b>8</b> | 27, 45, 78, 150       | 0      |
| 2   | J     | 170/177 (96%)   | 0.90   | 16 (9%) <b>14</b> <b>10</b> | 33, 47, 76, 124       | 0      |
| 2   | L     | 172/177 (97%)   | 1.07   | 21 (12%) <b>8</b> <b>6</b>  | 33, 52, 87, 106       | 0      |
| 2   | N     | 170/177 (96%)   | 0.82   | 9 (5%) <b>32</b> <b>24</b>  | 36, 55, 79, 105       | 0      |
| 2   | P     | 173/177 (97%)   | 0.96   | 16 (9%) <b>14</b> <b>10</b> | 27, 52, 89, 112       | 1 (0%) |
| 3   | C     | 60/67 (89%)     | 2.05   | 27 (45%) <b>0</b> <b>0</b>  | 57, 75, 106, 145      | 0      |
| 3   | G     | 67/67 (100%)    | 0.63   | 4 (5%) <b>27</b> <b>21</b>  | 32, 47, 74, 114       | 0      |
| 3   | K     | 67/67 (100%)    | 0.82   | 5 (7%) <b>20</b> <b>15</b>  | 38, 53, 74, 90        | 0      |
| 3   | O     | 67/67 (100%)    | 1.00   | 6 (8%) <b>15</b> <b>11</b>  | 40, 59, 78, 91        | 0      |
| All | All   | 1912/1988 (96%) | 1.01   | 235 (12%) <b>8</b> <b>6</b> | 27, 53, 89, 150       | 2 (0%) |

All (235) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 30  | SER  | 6.6  |
| 2   | D     | 95  | TYR  | 5.5  |
| 2   | D     | 43  | SER  | 5.4  |
| 1   | A     | 27  | SER  | 5.2  |
| 3   | C     | 18  | GLY  | 5.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 3   | C     | 40  | VAL  | 5.0  |
| 2   | F     | 176 | ILE  | 4.7  |
| 3   | C     | 5   | SER  | 4.6  |
| 1   | A     | 65  | GLU  | 4.6  |
| 2   | J     | 162 | ALA  | 4.5  |
| 2   | L     | 93  | VAL  | 4.4  |
| 2   | H     | 177 | SER  | 4.3  |
| 2   | B     | 107 | ASP  | 4.3  |
| 2   | H     | 119 | SER  | 4.2  |
| 2   | D     | 24  | LEU  | 4.0  |
| 2   | P     | 13  | ASP  | 4.0  |
| 2   | B     | 9   | VAL  | 4.0  |
| 2   | L     | 8   | VAL  | 3.9  |
| 2   | B     | 162 | ALA  | 3.9  |
| 2   | L     | 3   | ASP  | 3.8  |
| 2   | L     | 118 | SER  | 3.8  |
| 1   | M     | 10  | ALA  | 3.8  |
| 1   | A     | 31  | GLY  | 3.7  |
| 2   | D     | 100 | GLY  | 3.7  |
| 2   | P     | 5   | PHE  | 3.7  |
| 2   | H     | 43  | SER  | 3.6  |
| 2   | J     | 4   | ALA  | 3.6  |
| 2   | F     | 8   | VAL  | 3.5  |
| 2   | P     | 93  | VAL  | 3.5  |
| 2   | D     | 30  | PHE  | 3.5  |
| 2   | J     | 5   | PHE  | 3.5  |
| 2   | H     | 124 | ALA  | 3.4  |
| 2   | B     | 165 | VAL  | 3.3  |
| 2   | J     | 41  | VAL  | 3.3  |
| 1   | M     | 63  | PHE  | 3.3  |
| 3   | C     | 14  | PHE  | 3.3  |
| 1   | A     | 6   | ALA  | 3.2  |
| 3   | C     | 61  | SER  | 3.1  |
| 2   | D     | 152 | SER  | 3.1  |
| 2   | B     | 88  | ILE  | 3.1  |
| 2   | B     | 90  | LEU  | 3.1  |
| 1   | I     | 42  | ALA  | 3.1  |
| 2   | D     | 132 | SER  | 3.1  |
| 3   | C     | 60  | ASP  | 3.1  |
| 1   | A     | 28  | ALA  | 3.1  |
| 2   | N     | 162 | ALA  | 3.1  |
| 2   | F     | 165 | VAL  | 3.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 3   | O     | 3   | ASP  | 3.1  |
| 2   | J     | 15  | LYS  | 3.1  |
| 2   | D     | 5   | PHE  | 3.0  |
| 3   | O     | 42  | ALA  | 3.0  |
| 1   | A     | 72  | VAL  | 3.0  |
| 2   | H     | 53  | SER  | 3.0  |
| 1   | A     | 12  | THR  | 3.0  |
| 3   | C     | 13  | ILE  | 3.0  |
| 2   | B     | 115 | GLU  | 3.0  |
| 3   | C     | 63  | SER  | 2.9  |
| 2   | L     | 40  | ALA  | 2.9  |
| 3   | C     | 6   | ALA  | 2.9  |
| 2   | B     | 122 | VAL  | 2.9  |
| 2   | L     | 75  | THR  | 2.9  |
| 2   | F     | 166 | ALA  | 2.9  |
| 3   | G     | 32  | SER  | 2.9  |
| 2   | L     | 120 | LEU  | 2.9  |
| 2   | D     | 13  | ASP  | 2.9  |
| 3   | C     | 57  | VAL  | 2.8  |
| 2   | H     | 5   | PHE  | 2.8  |
| 2   | B     | 161 | LEU  | 2.8  |
| 2   | D     | 38  | LEU  | 2.8  |
| 2   | F     | 34  | GLY  | 2.8  |
| 2   | L     | 41  | VAL  | 2.8  |
| 2   | P     | 176 | ILE  | 2.8  |
| 2   | D     | 39  | ASP  | 2.8  |
| 2   | D     | 148 | GLN  | 2.8  |
| 2   | N     | 107 | ASP  | 2.8  |
| 2   | F     | 94  | SER  | 2.8  |
| 2   | B     | 97  | LEU  | 2.7  |
| 2   | D     | 21  | GLY  | 2.7  |
| 2   | D     | 175 | ALA  | 2.7  |
| 2   | F     | 162 | ALA  | 2.7  |
| 2   | P     | 10  | THR  | 2.7  |
| 3   | C     | 36  | ASP  | 2.7  |
| 2   | P     | 172 | VAL  | 2.7  |
| 2   | L     | 30  | PHE  | 2.7  |
| 2   | H     | 7   | ARG  | 2.7  |
| 2   | H     | 153 | THR  | 2.7  |
| 2   | J     | 140 | ALA  | 2.7  |
| 2   | H     | 152 | SER  | 2.7  |
| 2   | J     | 163 | SER  | 2.7  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 3   | C     | 66  | HIS  | 2.6  |
| 1   | I     | 23  | PRO  | 2.6  |
| 3   | C     | 23  | PRO  | 2.6  |
| 2   | H     | 157 | ASP  | 2.6  |
| 2   | P     | 57  | SER  | 2.6  |
| 2   | D     | 158 | CYS  | 2.6  |
| 3   | C     | 52  | GLY  | 2.6  |
| 2   | B     | 173 | THR  | 2.6  |
| 1   | A     | 14  | PHE  | 2.6  |
| 2   | B     | 81  | ALA  | 2.6  |
| 1   | M     | 74  | ARG  | 2.6  |
| 2   | N     | 18  | TYR  | 2.6  |
| 2   | P     | 9   | VAL  | 2.6  |
| 2   | D     | 177 | SER  | 2.5  |
| 1   | I     | 75  | LYS  | 2.5  |
| 2   | J     | 6   | SER  | 2.5  |
| 1   | M     | 13  | ILE  | 2.5  |
| 3   | C     | 38  | MET  | 2.5  |
| 3   | C     | 26  | TYR  | 2.5  |
| 2   | J     | 177 | SER  | 2.5  |
| 1   | A     | 68  | LEU  | 2.5  |
| 2   | J     | 52  | VAL  | 2.5  |
| 3   | O     | 64  | VAL  | 2.5  |
| 2   | N     | 140 | ALA  | 2.5  |
| 2   | F     | 101 | ASP  | 2.5  |
| 3   | G     | 60  | ASP  | 2.5  |
| 2   | F     | 160 | GLY  | 2.5  |
| 1   | A     | 36  | GLU  | 2.5  |
| 2   | J     | 38  | LEU  | 2.4  |
| 3   | C     | 35  | ASP  | 2.4  |
| 2   | B     | 176 | ILE  | 2.4  |
| 2   | B     | 130 | ALA  | 2.4  |
| 2   | P     | 22  | ALA  | 2.4  |
| 2   | L     | 31  | ILE  | 2.4  |
| 2   | B     | 167 | GLY  | 2.4  |
| 2   | L     | 131 | VAL  | 2.4  |
| 2   | L     | 46  | SER  | 2.4  |
| 1   | A     | 64  | LYS  | 2.4  |
| 1   | I     | 36  | GLU  | 2.4  |
| 3   | G     | 27  | THR  | 2.4  |
| 3   | C     | 59  | LYS  | 2.4  |
| 2   | L     | 86  | ALA  | 2.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | D     | 98  | LEU  | 2.4  |
| 2   | F     | 111 | ASN  | 2.4  |
| 1   | M     | 46  | VAL  | 2.4  |
| 2   | F     | 172 | VAL  | 2.4  |
| 1   | M     | 35  | ASP  | 2.4  |
| 2   | B     | 25  | GLN  | 2.4  |
| 2   | H     | 132 | SER  | 2.4  |
| 2   | L     | 5   | PHE  | 2.3  |
| 3   | O     | 15  | ASP  | 2.3  |
| 2   | P     | 120 | LEU  | 2.3  |
| 1   | I     | 13  | ILE  | 2.3  |
| 1   | I     | 74  | ARG  | 2.3  |
| 2   | N     | 41  | VAL  | 2.3  |
| 3   | G     | 2   | MET  | 2.3  |
| 2   | N     | 6   | SER  | 2.3  |
| 2   | B     | 116 | THR  | 2.3  |
| 2   | D     | 7   | ARG  | 2.3  |
| 3   | C     | 10  | VAL  | 2.3  |
| 2   | B     | 100 | GLY  | 2.3  |
| 2   | L     | 58  | GLY  | 2.3  |
| 2   | N     | 126 | GLY  | 2.3  |
| 2   | P     | 30  | PHE  | 2.3  |
| 2   | F     | 115 | GLU  | 2.3  |
| 2   | D     | 105 | LEU  | 2.3  |
| 2   | F     | 133 | ILE  | 2.3  |
| 2   | H     | 154 | PRO  | 2.3  |
| 2   | D     | 156 | GLY  | 2.3  |
| 2   | F     | 100 | GLY  | 2.3  |
| 2   | J     | 101 | ASP  | 2.3  |
| 2   | J     | 107 | ASP  | 2.3  |
| 2   | P     | 98  | LEU  | 2.3  |
| 2   | F     | 104 | VAL  | 2.3  |
| 2   | J     | 131 | VAL  | 2.3  |
| 3   | C     | 64  | VAL  | 2.3  |
| 1   | A     | 42  | ALA  | 2.2  |
| 1   | M     | 6   | ALA  | 2.2  |
| 2   | D     | 76  | ASN  | 2.2  |
| 3   | K     | 24  | LYS  | 2.2  |
| 2   | H     | 145 | THR  | 2.2  |
| 2   | F     | 177 | SER  | 2.2  |
| 3   | K     | 33  | GLY  | 2.2  |
| 1   | I     | 40  | LYS  | 2.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | L     | 110 | LEU  | 2.2  |
| 2   | B     | 31  | ILE  | 2.2  |
| 3   | K     | 3   | ASP  | 2.2  |
| 2   | B     | 93  | VAL  | 2.2  |
| 2   | D     | 104 | VAL  | 2.2  |
| 3   | C     | 53  | VAL  | 2.2  |
| 3   | O     | 40  | VAL  | 2.2  |
| 2   | B     | 92  | TYR  | 2.2  |
| 2   | D     | 110 | LEU  | 2.2  |
| 2   | L     | 81  | ALA  | 2.2  |
| 2   | H     | 176 | ILE  | 2.2  |
| 2   | D     | 3   | ASP  | 2.2  |
| 2   | H     | 13  | ASP  | 2.2  |
| 1   | A     | 48  | VAL  | 2.2  |
| 1   | M     | 23  | PRO  | 2.2  |
| 2   | B     | 123 | PRO  | 2.2  |
| 1   | A     | 70  | GLY  | 2.2  |
| 2   | L     | 74  | TYR  | 2.2  |
| 3   | K     | 42  | ALA  | 2.2  |
| 2   | F     | 129 | ARG  | 2.2  |
| 2   | F     | 107 | ASP  | 2.2  |
| 2   | P     | 75  | THR  | 2.2  |
| 2   | D     | 74  | TYR  | 2.2  |
| 1   | I     | 28  | ALA  | 2.2  |
| 2   | D     | 115 | GLU  | 2.2  |
| 3   | C     | 15  | ASP  | 2.1  |
| 3   | C     | 65  | MET  | 2.1  |
| 1   | I     | 12  | THR  | 2.1  |
| 1   | M     | 12  | THR  | 2.1  |
| 2   | B     | 124 | ALA  | 2.1  |
| 2   | D     | 4   | ALA  | 2.1  |
| 2   | D     | 86  | ALA  | 2.1  |
| 2   | F     | 132 | SER  | 2.1  |
| 2   | H     | 6   | SER  | 2.1  |
| 2   | P     | 35  | ASN  | 2.1  |
| 3   | C     | 9   | PRO  | 2.1  |
| 2   | L     | 112 | GLY  | 2.1  |
| 2   | B     | 48  | ALA  | 2.1  |
| 1   | M     | 36  | GLU  | 2.1  |
| 3   | K     | 61  | SER  | 2.1  |
| 3   | C     | 58  | LEU  | 2.1  |
| 3   | C     | 62  | LEU  | 2.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | H     | 93  | VAL  | 2.1  |
| 2   | J     | 19  | VAL  | 2.1  |
| 2   | D     | 58  | GLY  | 2.1  |
| 2   | F     | 10  | THR  | 2.1  |
| 3   | C     | 11  | ILE  | 2.1  |
| 2   | B     | 94  | SER  | 2.0  |
| 2   | L     | 99  | SER  | 2.0  |
| 2   | D     | 9   | VAL  | 2.0  |
| 2   | N     | 90  | LEU  | 2.0  |
| 1   | A     | 11  | ILE  | 2.0  |
| 2   | L     | 116 | THR  | 2.0  |
| 2   | P     | 31  | ILE  | 2.0  |
| 1   | I     | 10  | ALA  | 2.0  |
| 1   | I     | 30  | SER  | 2.0  |
| 2   | D     | 155 | GLN  | 2.0  |
| 2   | J     | 53  | SER  | 2.0  |
| 2   | P     | 43  | SER  | 2.0  |
| 2   | N     | 125 | ASN  | 2.0  |
| 3   | O     | 12  | THR  | 2.0  |
| 2   | H     | 74  | TYR  | 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 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 5   | PEB  | D     | 202 | 43/43 | 0.79 | 0.17 | 35,61,102,108              | 0     |
| 5   | PEB  | P     | 203 | 43/43 | 0.81 | 0.15 | 21,59,80,85                | 0     |
| 5   | PEB  | B     | 201 | 43/43 | 0.82 | 0.14 | 16,44,71,73                | 0     |

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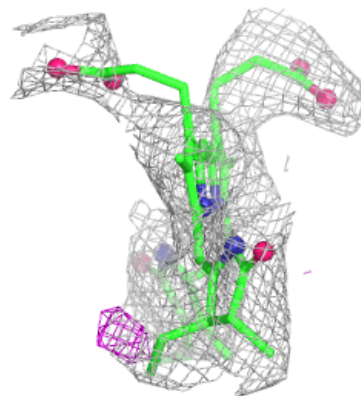
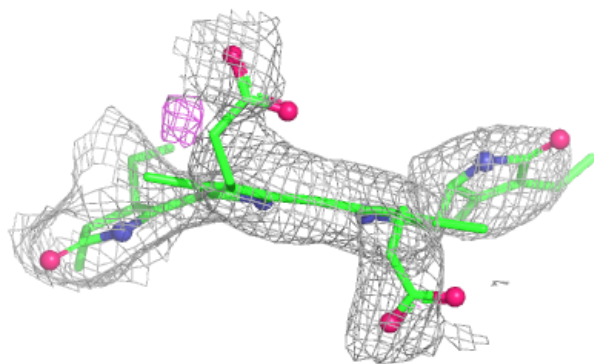
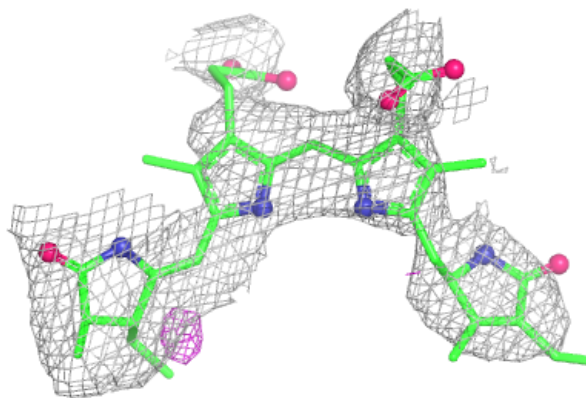
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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 4   | DBV  | C     | 101 | 43/43 | 0.82 | 0.14 | 32,53,67,78                 | 0     |
| 5   | PEB  | L     | 203 | 43/43 | 0.82 | 0.14 | 5,53,69,84                  | 0     |
| 4   | DBV  | I     | 101 | 43/43 | 0.82 | 0.15 | 28,51,70,76                 | 0     |
| 5   | PEB  | P     | 202 | 43/43 | 0.83 | 0.14 | 19,49,73,102                | 0     |
| 5   | PEB  | H     | 202 | 43/43 | 0.84 | 0.15 | 15,54,71,80                 | 0     |
| 5   | PEB  | J     | 201 | 43/43 | 0.84 | 0.12 | 15,36,51,69                 | 0     |
| 5   | PEB  | B     | 202 | 43/43 | 0.84 | 0.13 | 31,51,65,80                 | 0     |
| 4   | DBV  | O     | 101 | 43/43 | 0.84 | 0.12 | 16,40,55,59                 | 0     |
| 5   | PEB  | F     | 202 | 43/43 | 0.84 | 0.13 | 14,41,60,63                 | 0     |
| 5   | PEB  | J     | 203 | 43/43 | 0.85 | 0.12 | 26,41,59,66                 | 0     |
| 5   | PEB  | L     | 202 | 43/43 | 0.85 | 0.13 | 24,56,78,84                 | 0     |
| 4   | DBV  | M     | 101 | 43/43 | 0.85 | 0.15 | 21,52,71,82                 | 0     |
| 5   | PEB  | N     | 201 | 43/43 | 0.85 | 0.12 | 14,34,63,68                 | 0     |
| 5   | PEB  | H     | 203 | 43/43 | 0.85 | 0.13 | 21,45,59,75                 | 0     |
| 5   | PEB  | B     | 203 | 43/43 | 0.85 | 0.12 | 19,48,62,66                 | 0     |
| 4   | DBV  | K     | 101 | 43/43 | 0.86 | 0.13 | 17,46,63,77                 | 0     |
| 5   | PEB  | N     | 202 | 43/43 | 0.86 | 0.12 | 10,39,50,71                 | 0     |
| 4   | DBV  | E     | 101 | 43/43 | 0.86 | 0.14 | 17,42,67,86                 | 0     |
| 5   | PEB  | F     | 203 | 43/43 | 0.86 | 0.12 | 20,38,48,61                 | 0     |
| 5   | PEB  | D     | 201 | 43/43 | 0.87 | 0.12 | 21,45,64,66                 | 0     |
| 5   | PEB  | N     | 203 | 43/43 | 0.87 | 0.12 | 21,48,65,67                 | 0     |
| 5   | PEB  | D     | 203 | 43/43 | 0.88 | 0.11 | 14,40,60,70                 | 0     |
| 5   | PEB  | F     | 201 | 43/43 | 0.88 | 0.10 | 2,28,44,64                  | 0     |
| 4   | DBV  | G     | 101 | 43/43 | 0.88 | 0.11 | 2,32,51,72                  | 0     |
| 5   | PEB  | J     | 202 | 43/43 | 0.88 | 0.12 | 14,36,55,58                 | 0     |
| 4   | DBV  | A     | 101 | 43/43 | 0.88 | 0.13 | 23,39,60,74                 | 0     |
| 5   | PEB  | H     | 201 | 43/43 | 0.88 | 0.10 | 2,36,49,80                  | 0     |
| 5   | PEB  | P     | 201 | 43/43 | 0.89 | 0.10 | 2,30,62,92                  | 0     |
| 5   | PEB  | L     | 201 | 43/43 | 0.90 | 0.10 | 9,32,63,69                  | 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.

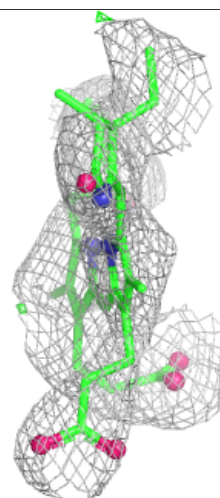
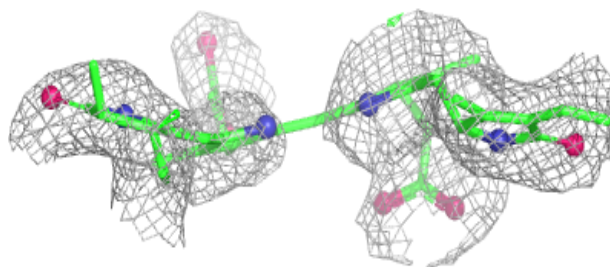
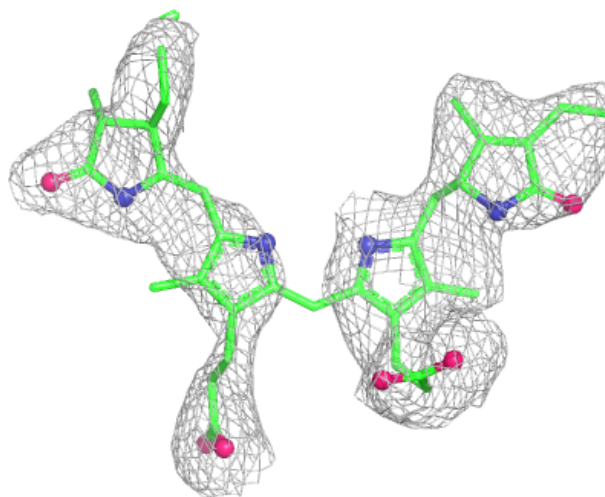
**Electron density around PEB D 202:**

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



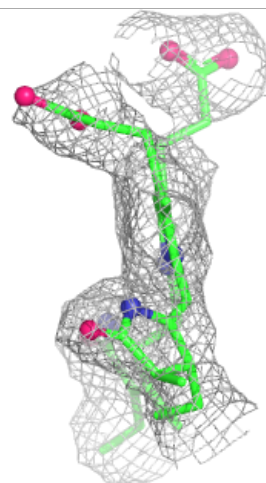
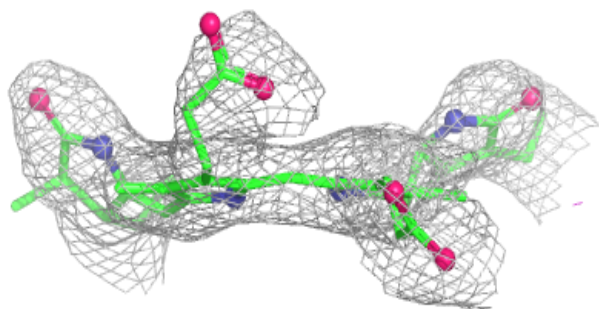
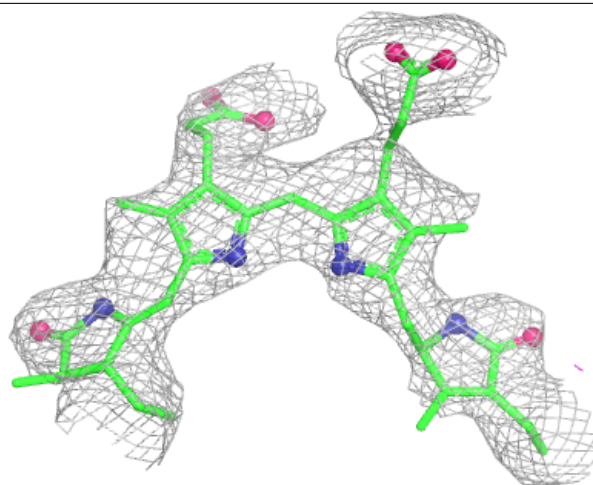
**Electron density around PEB P 203:**

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



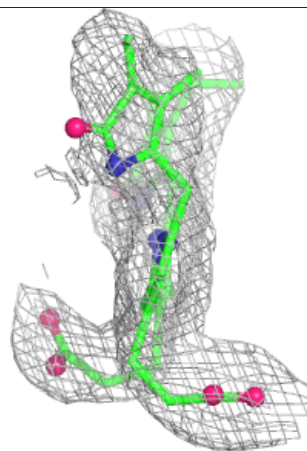
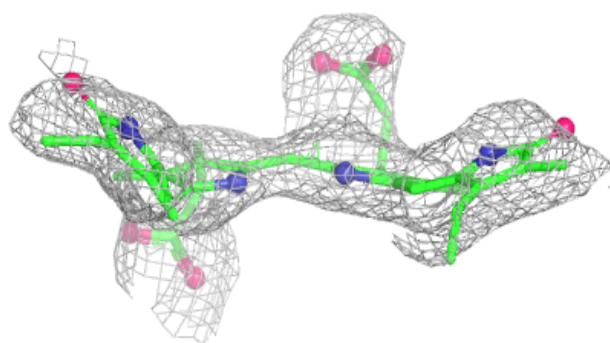
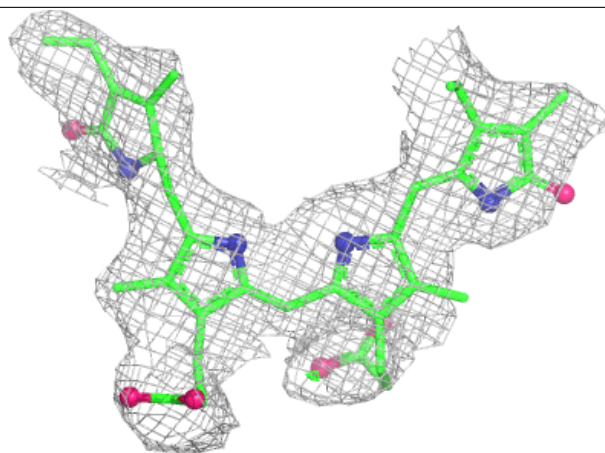
**Electron density around PEB B 201:**

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



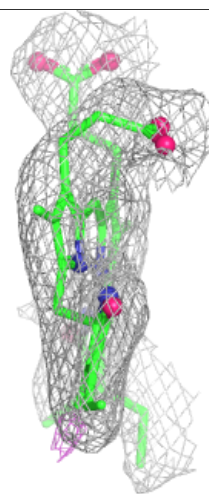
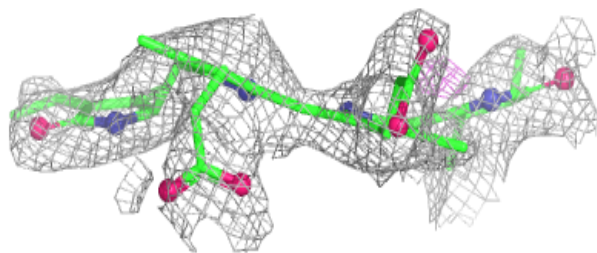
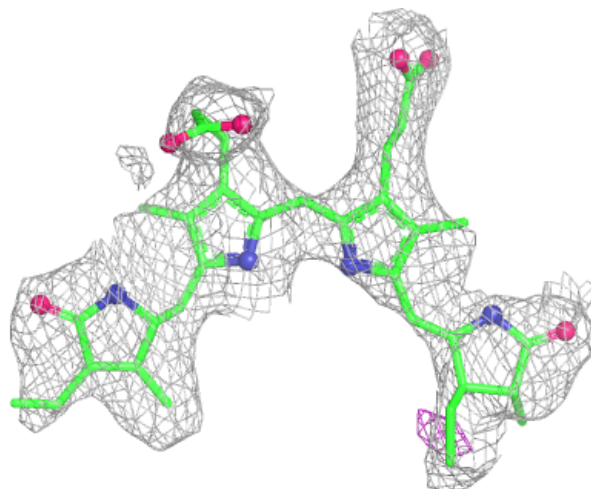
**Electron density around DBV C 101:**

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



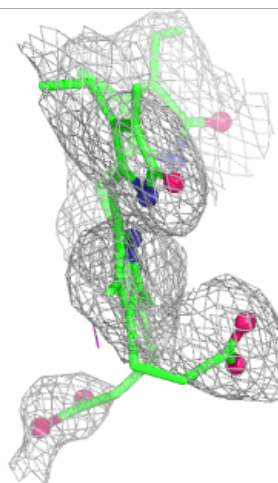
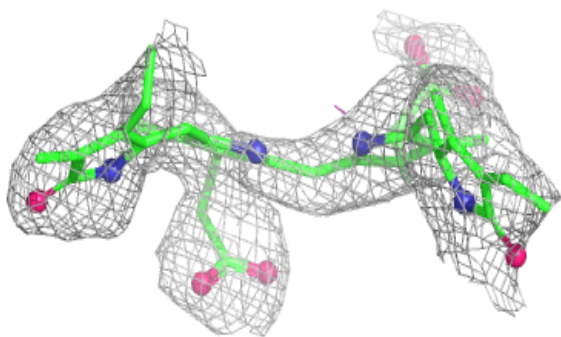
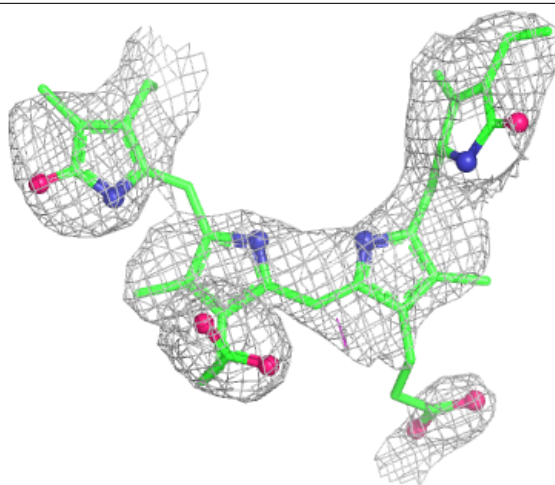
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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



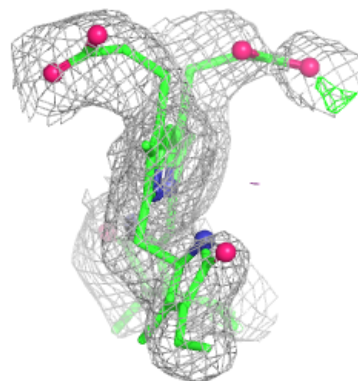
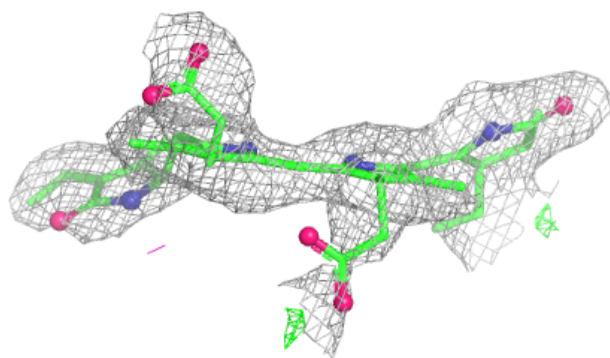
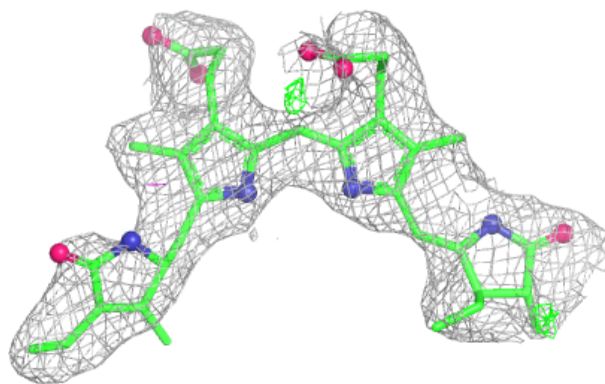
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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



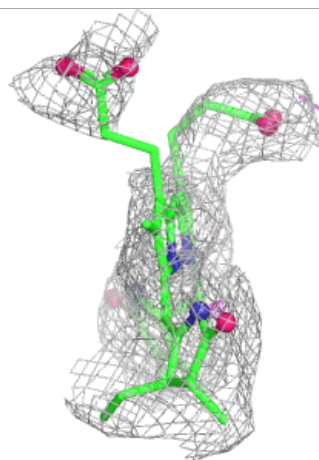
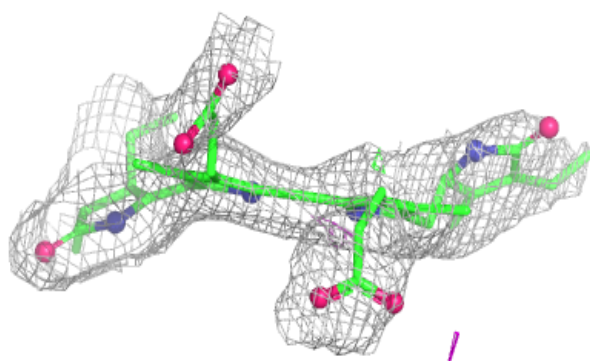
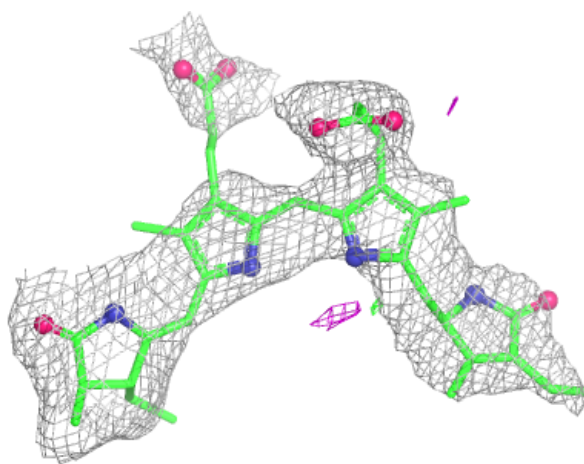
**Electron density around PEB P 202:**

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



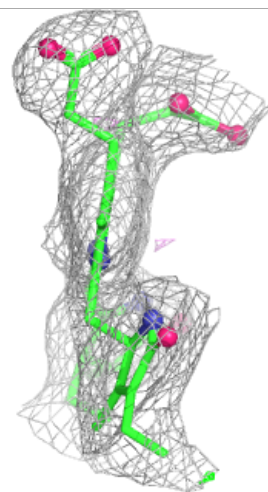
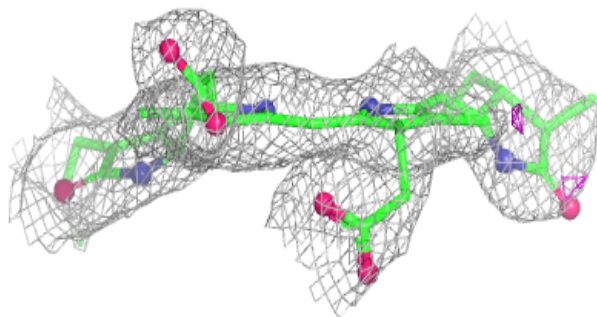
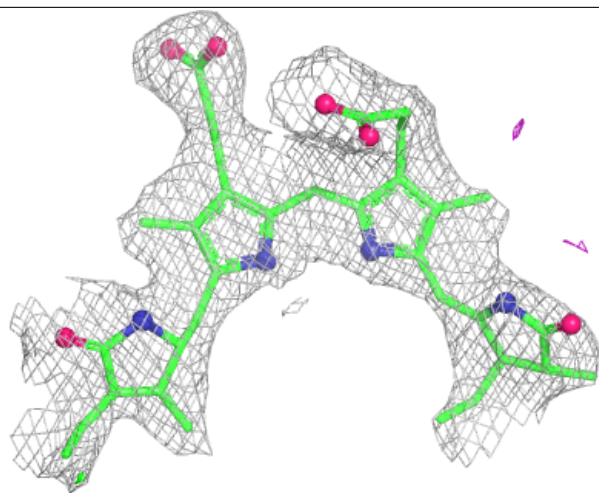
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and green (positive)



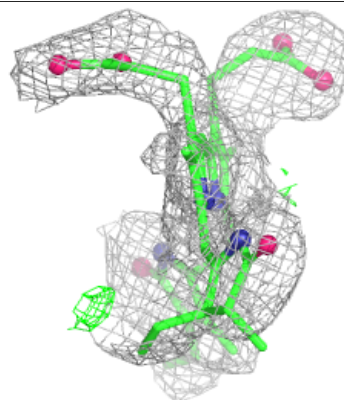
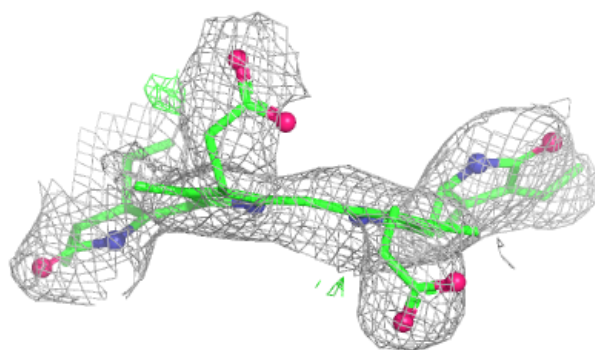
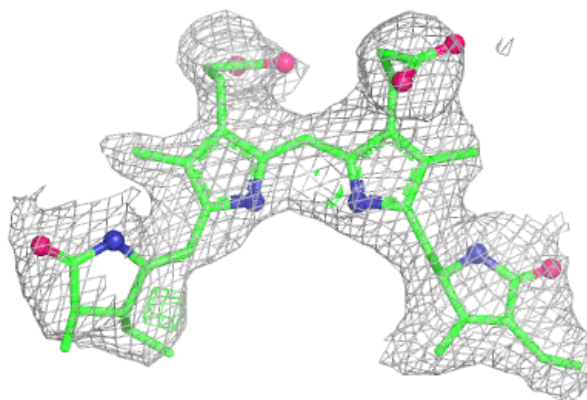
**Electron density around PEB J 201:**

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and green (positive)



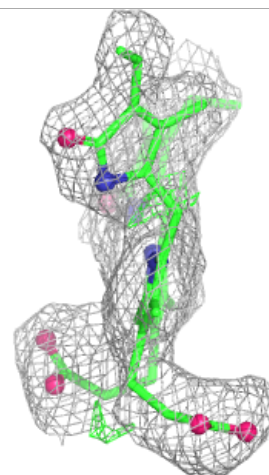
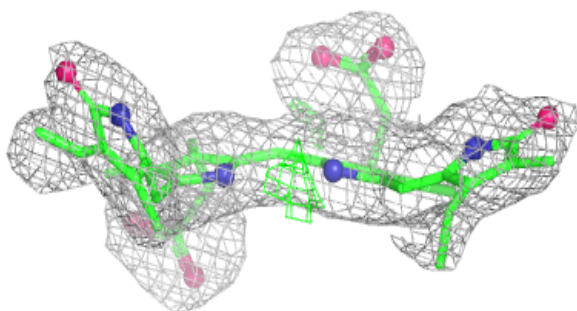
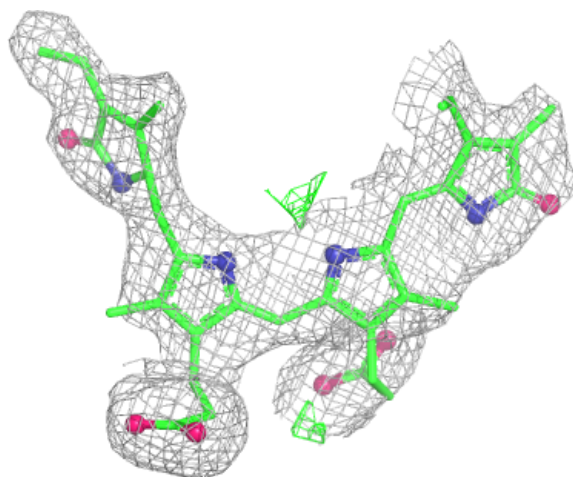
**Electron density around PEB B 202:**

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and green (positive)



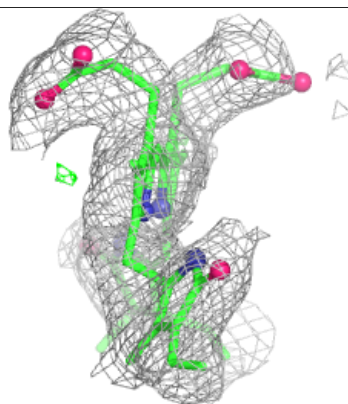
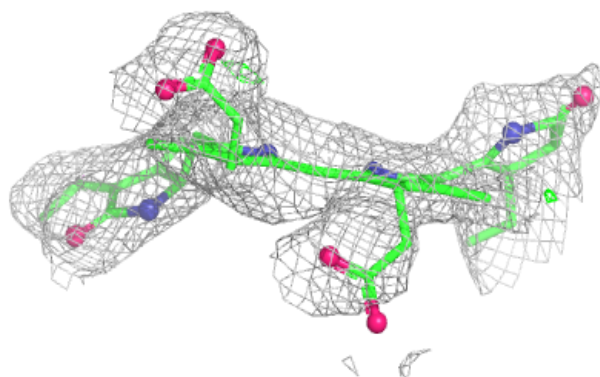
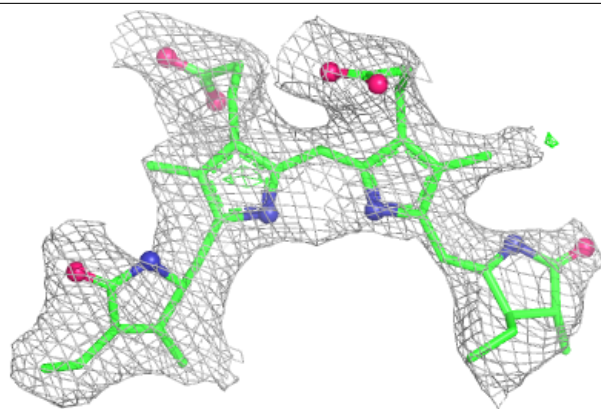
**Electron density around DBV O 101:**

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and green (positive)



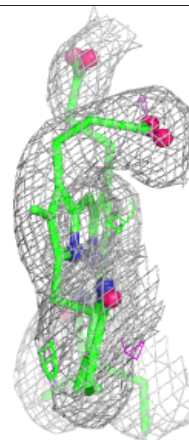
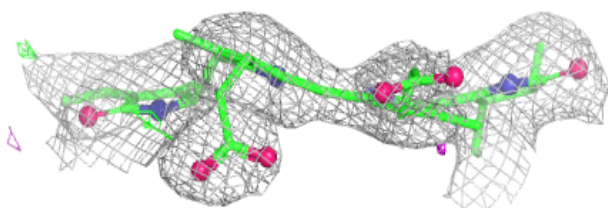
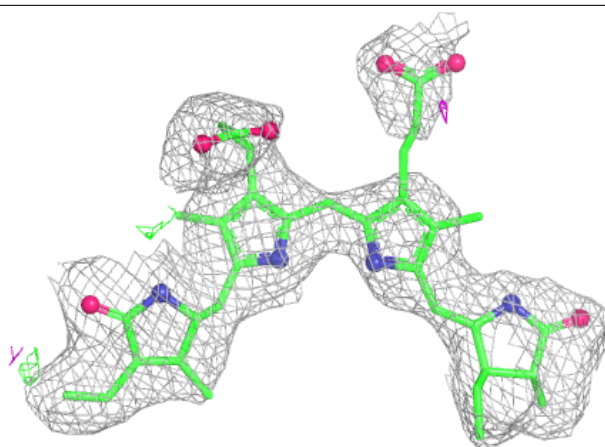
**Electron density around PEB F 202:**

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

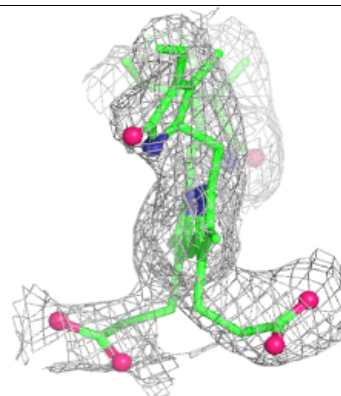
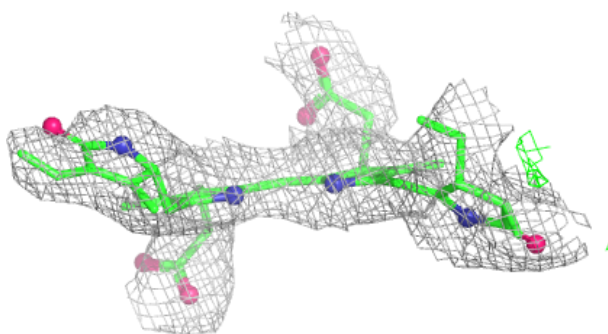
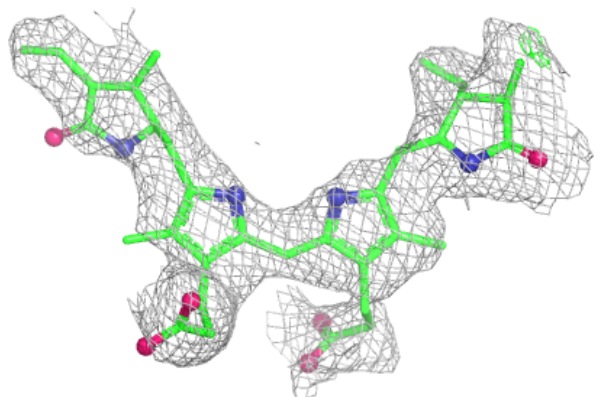


**Electron density around PEB J 203:**

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

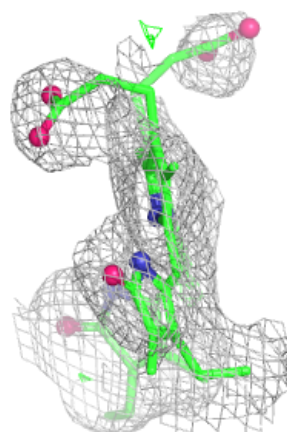
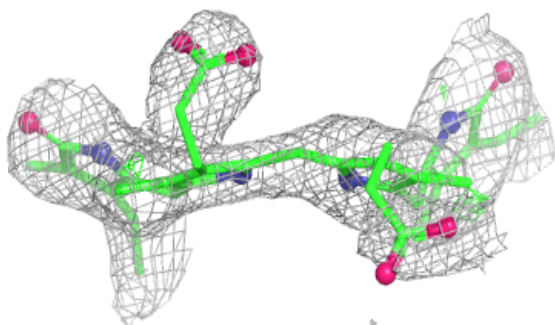
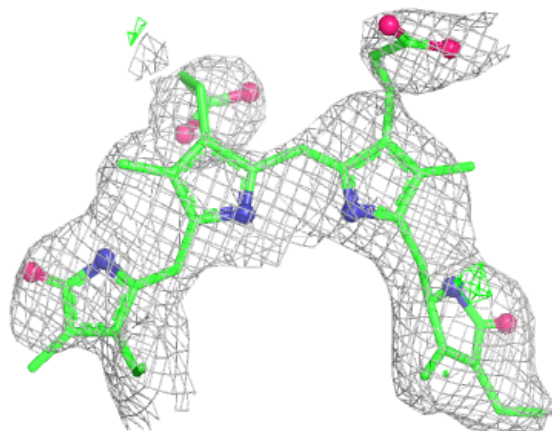
**Electron density around PEB L 202:**

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



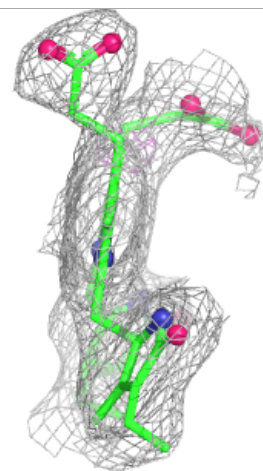
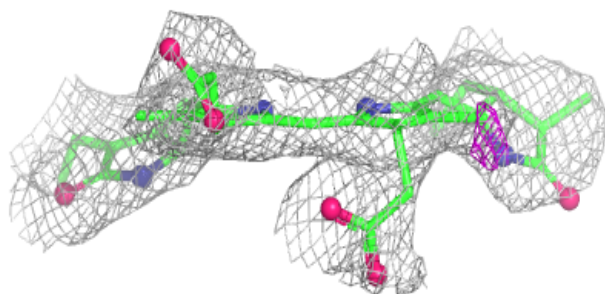
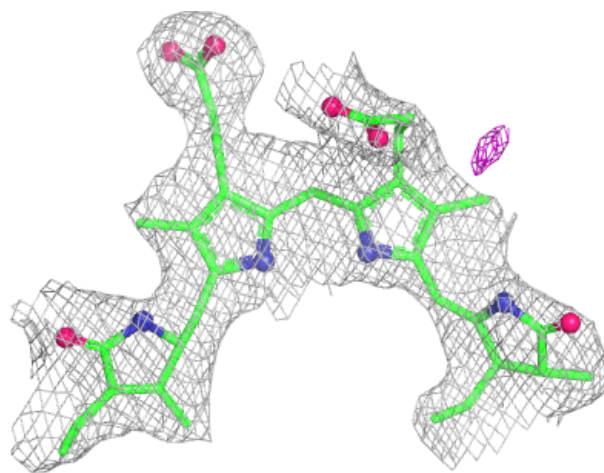
**Electron density around DBV M 101:**

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



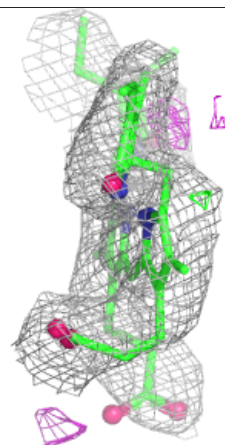
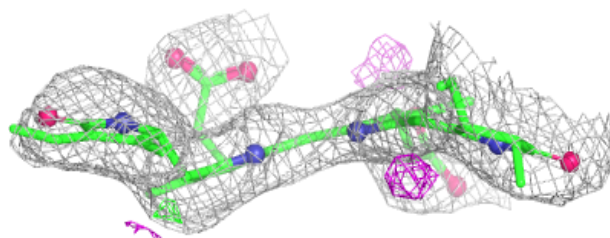
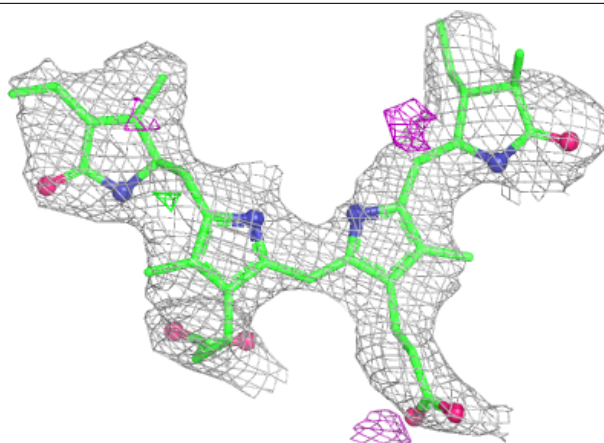
**Electron density around PEB N 201:**

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



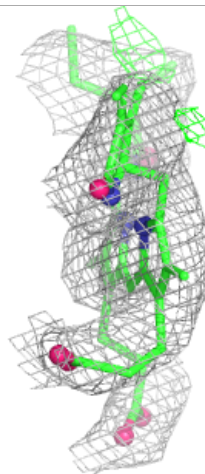
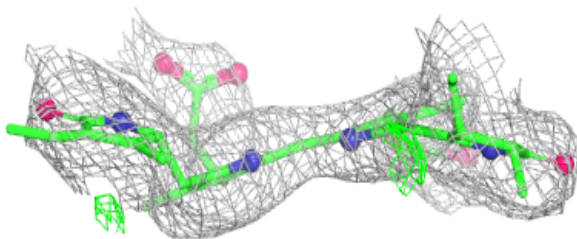
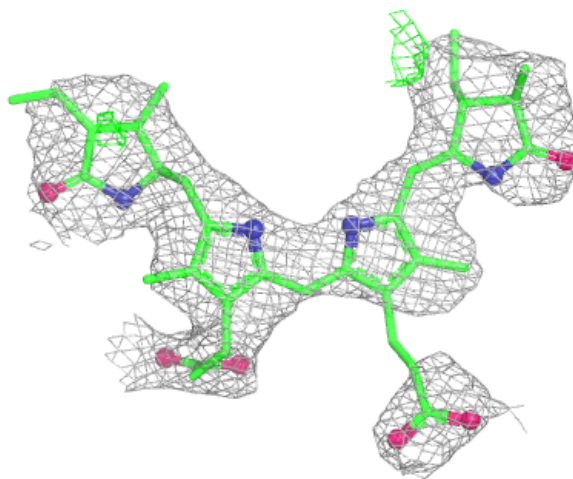
**Electron density around PEB H 203:**

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



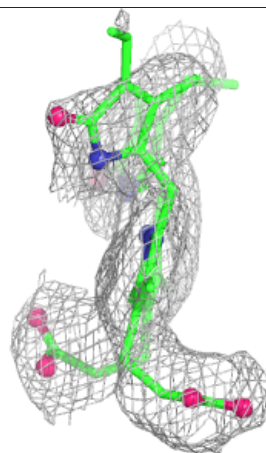
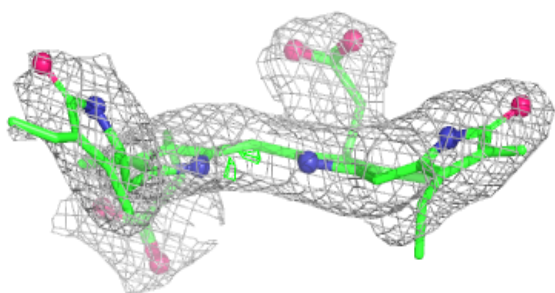
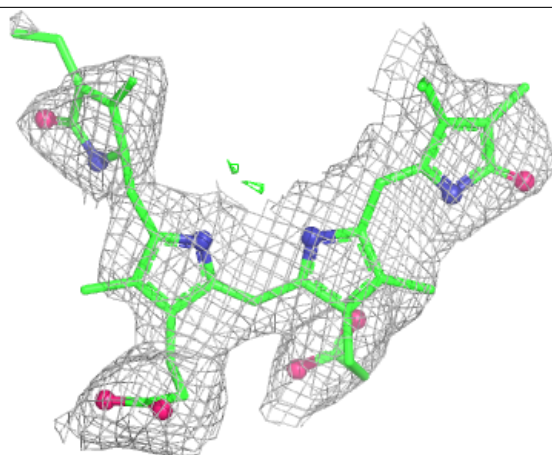
**Electron density around PEB B 203:**

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

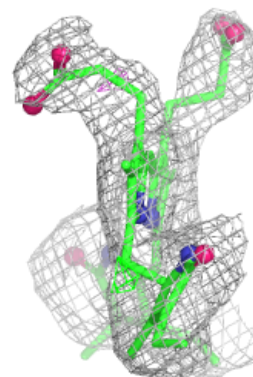
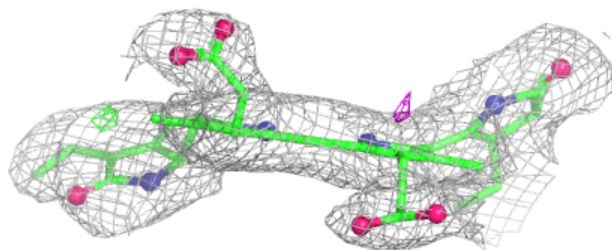
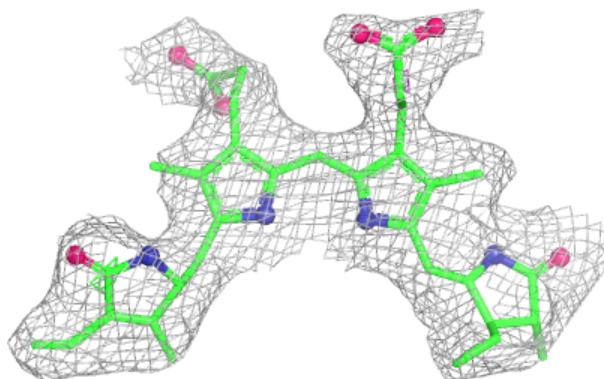


**Electron density around DBV K 101:**

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

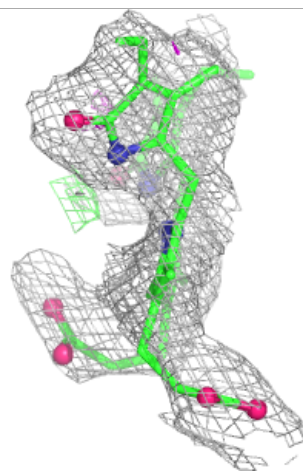
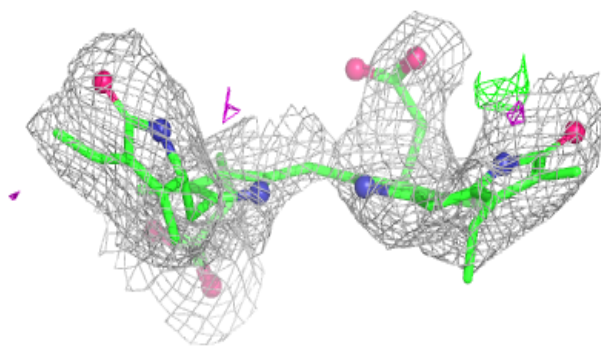
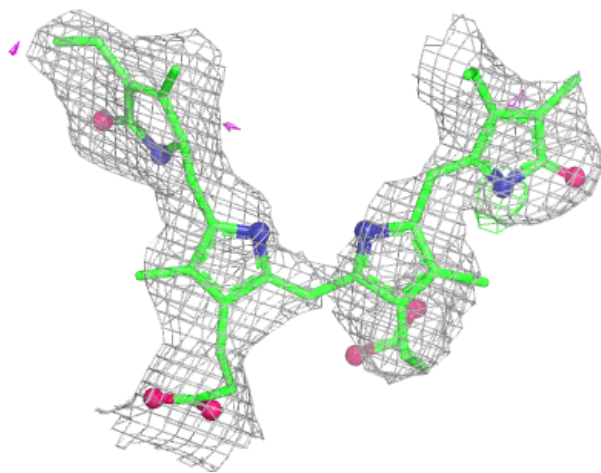
**Electron density around PEB N 202:**

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



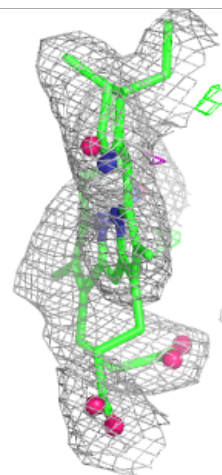
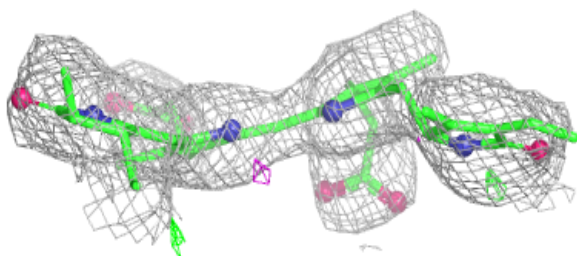
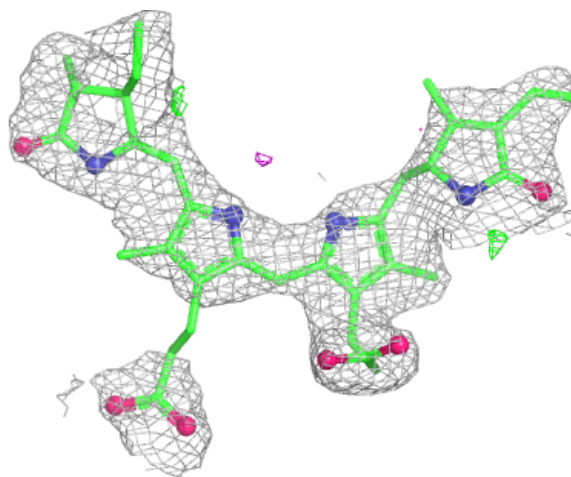
**Electron density around DBV E 101:**

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



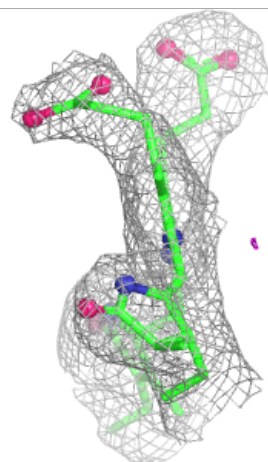
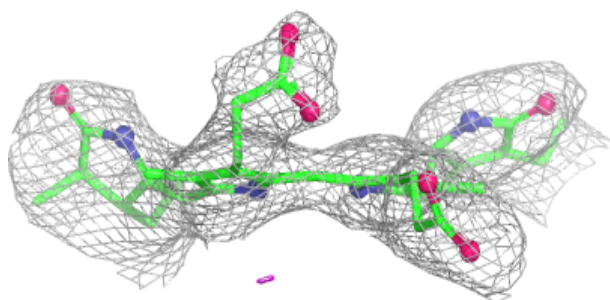
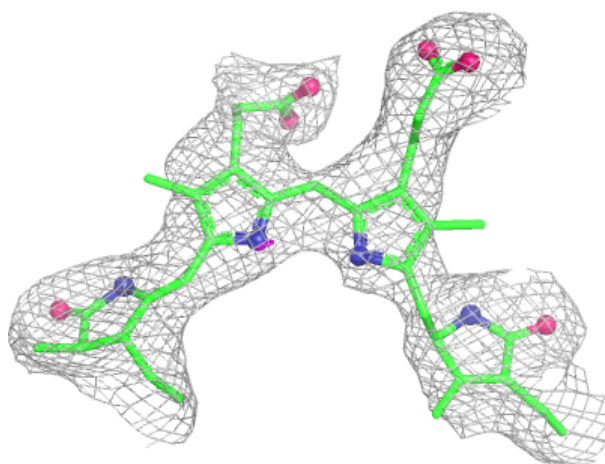
**Electron density around PEB F 203:**

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



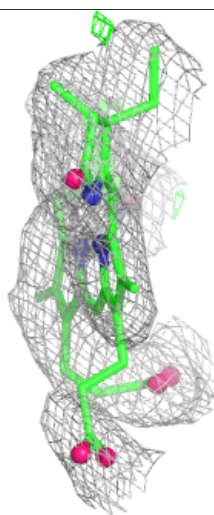
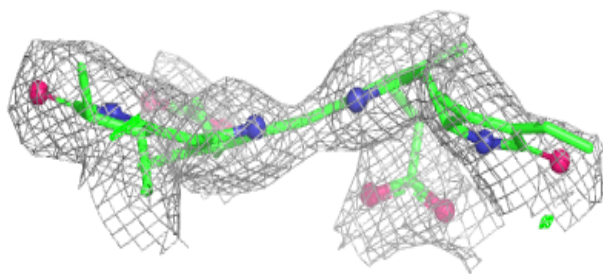
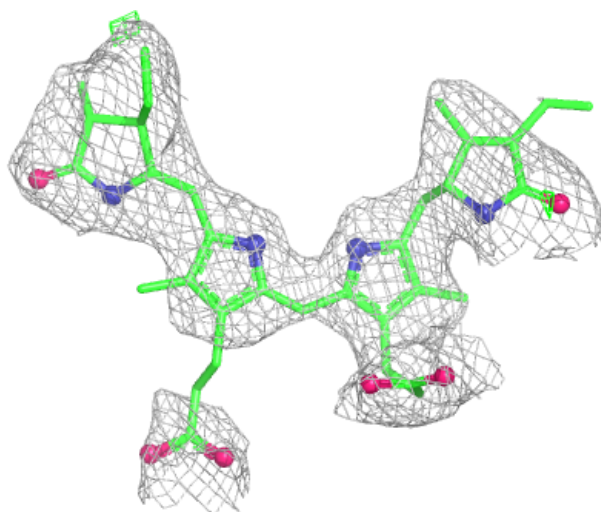
**Electron density around PEB D 201:**

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



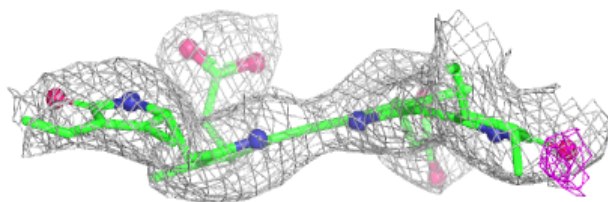
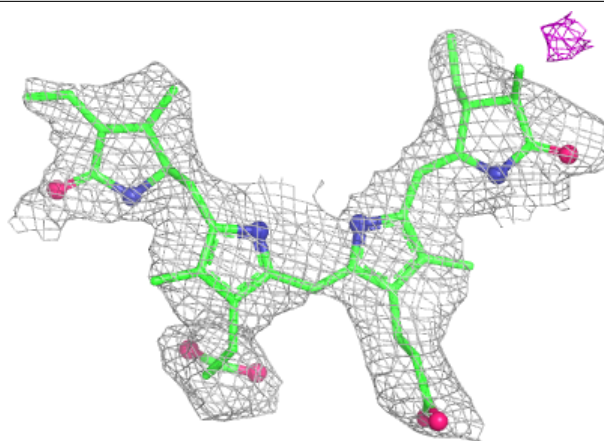
**Electron density around PEB N 203:**

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



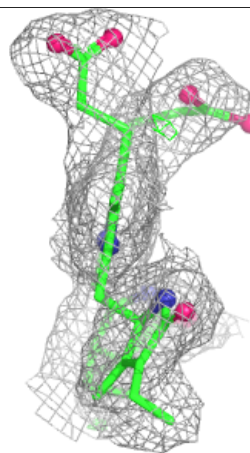
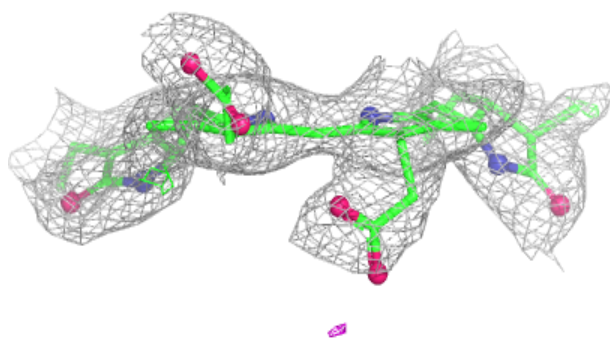
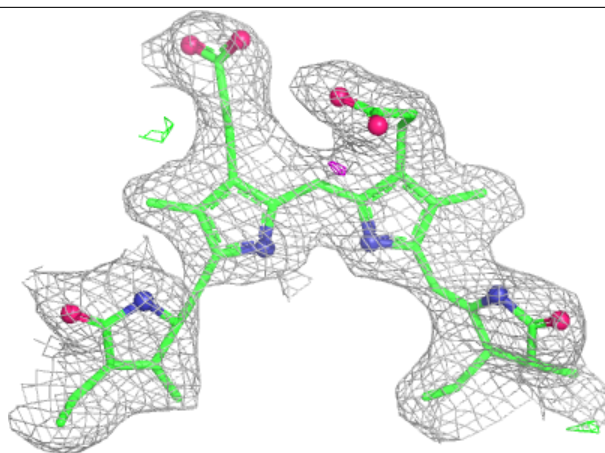
**Electron density around PEB D 203:**

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



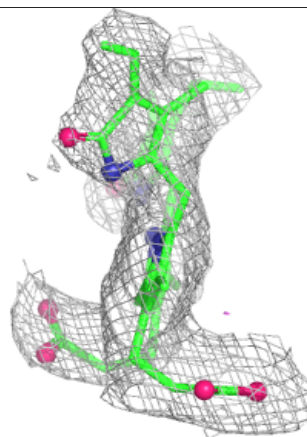
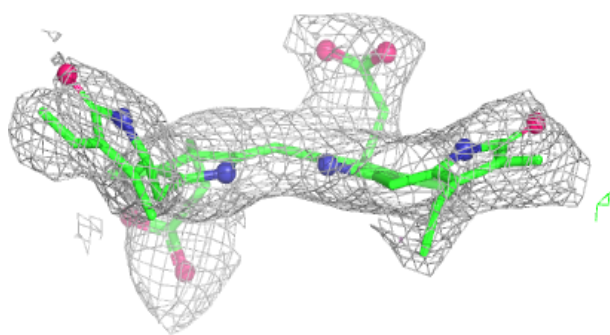
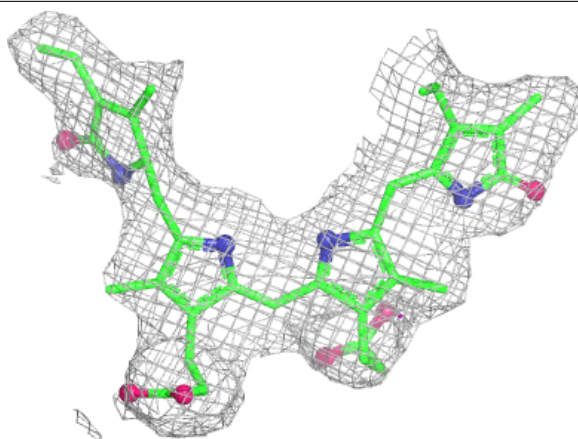
**Electron density around PEB F 201:**

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



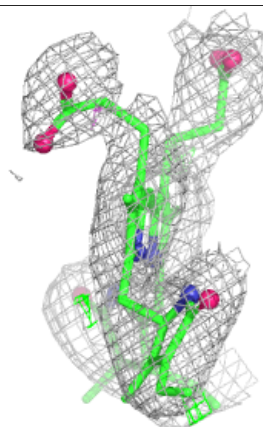
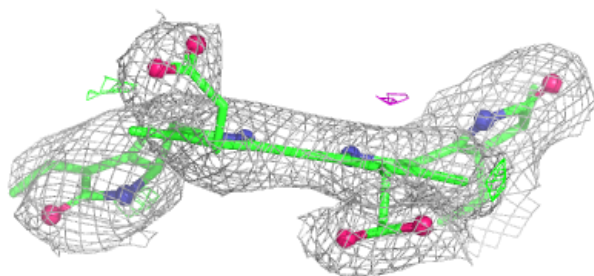
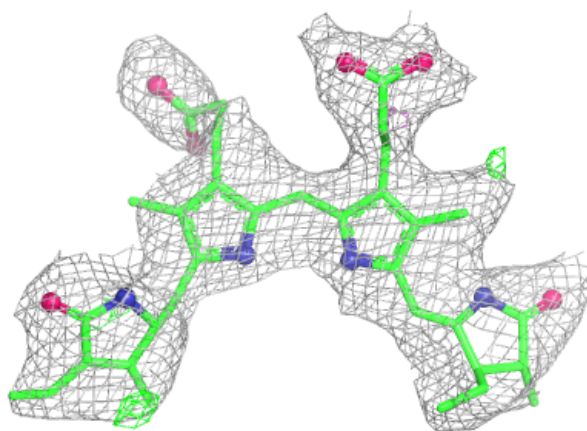
**Electron density around DBV G 101:**

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



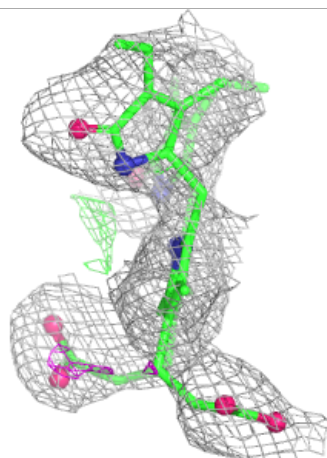
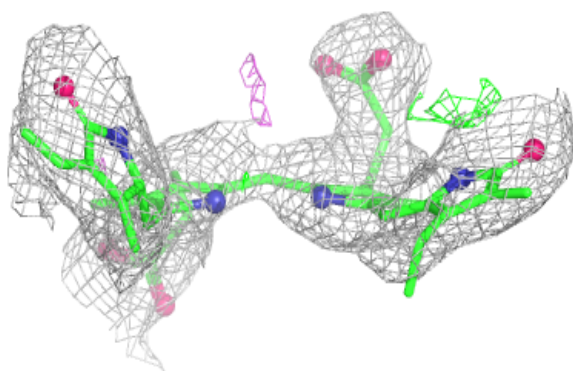
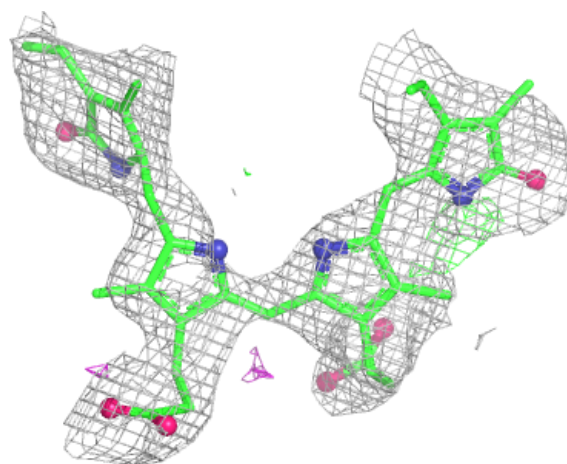
**Electron density around PEB J 202:**

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



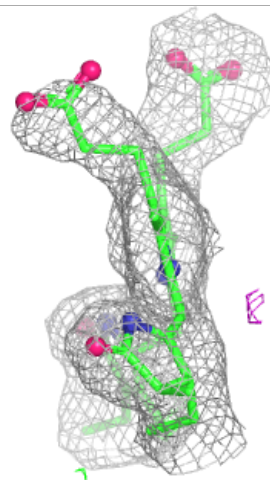
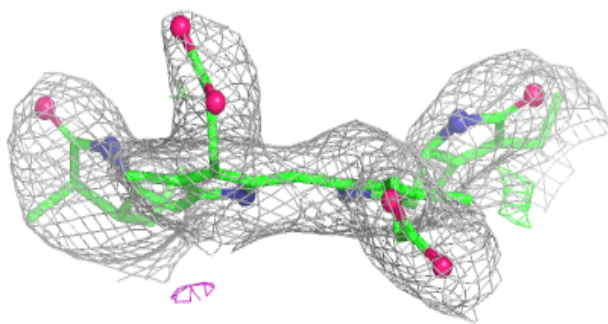
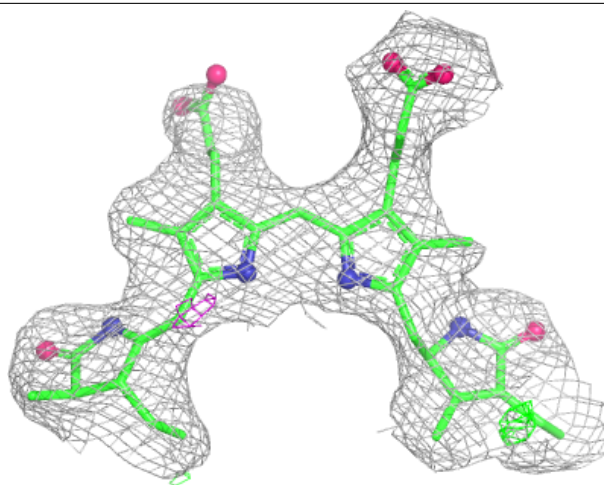
**Electron density around DBV A 101:**

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



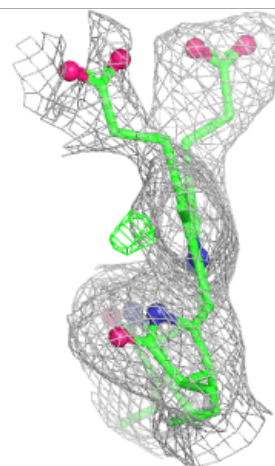
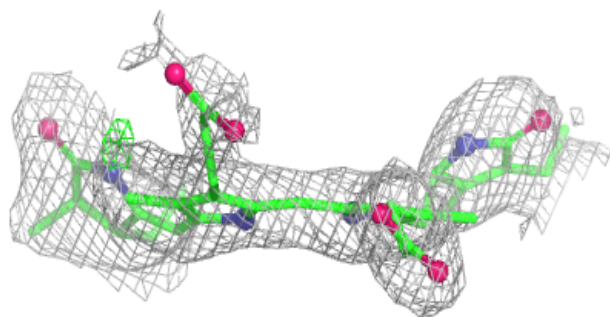
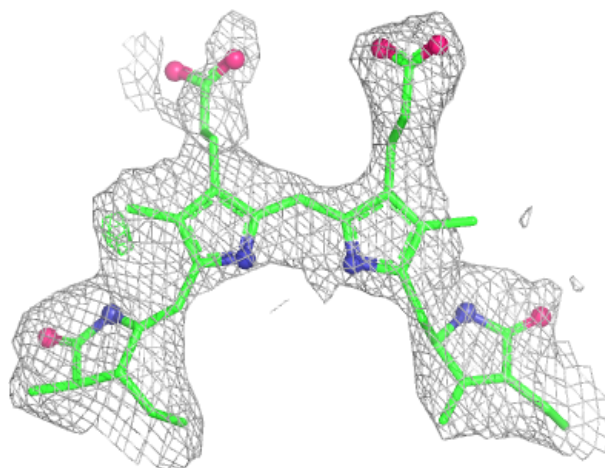
**Electron density around PEB H 201:**

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



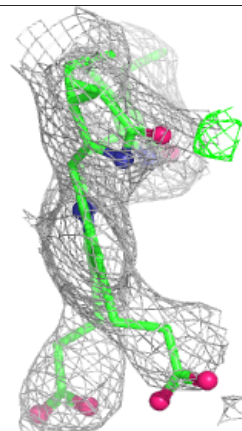
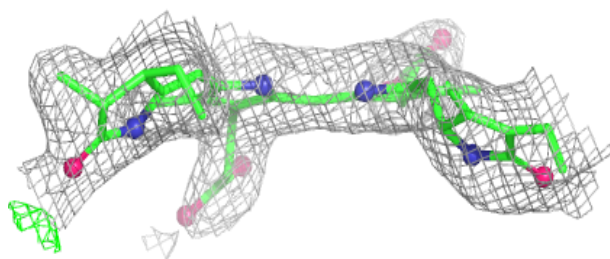
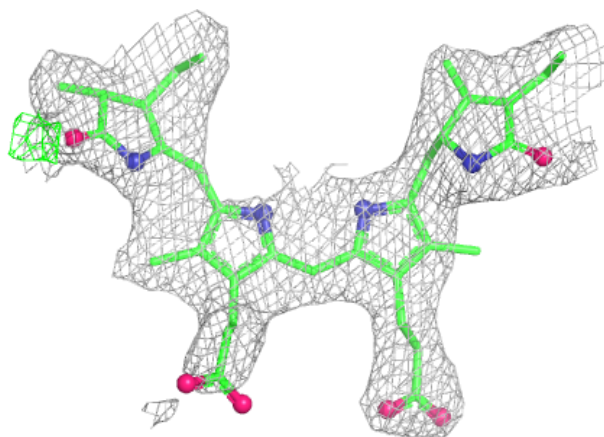
**Electron density around PEB P 201:**

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



**Electron density around PEB L 201:**

$2mF_o - DF_c$  (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.