



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:34 PM UTC

PDB ID : 1D4C / pdb\_00001d4c  
Title : CRYSTAL STRUCTURE OF THE UNCOMPLEXED FORM OF THE FLAVOCYTOCHROME C FUMARATE REDUCTASE OF SHEWANELLA PUTREFACIENS STRAIN MR-1  
Authors : Leys, D.; Tsapin, A.S.; Meyer, T.E.; Cusanovich, M.A.; Van Beeumen, J.J.  
Deposited on : 1999-10-03  
Resolution : 2.90 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)               | : | NOT EXECUTED                                                     |
| EDS                            | : | NOT EXECUTED                                                     |
| Buster-report                  | : | wwPDB partial adaption of 1.1.7 (2018)                           |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

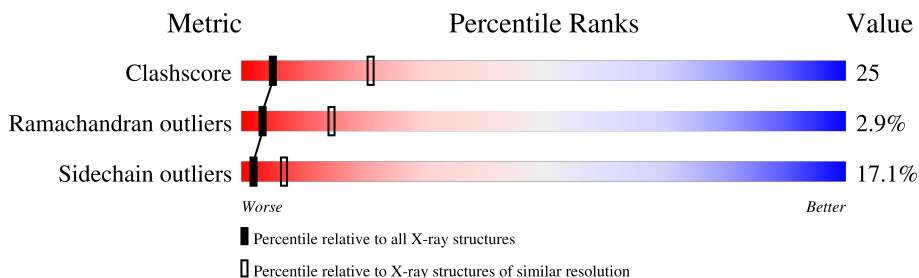
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| Clashscore            | 190562                      | 2690 (2.90-2.90)                                      |
| Ramachandran outliers | 187476                      | 2623 (2.90-2.90)                                      |
| Sidechain outliers    | 187428                      | 2625 (2.90-2.90)                                      |

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  $\leq 5\%$ .

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 572    |                  |
| 1   | B     | 572    |                  |
| 1   | C     | 572    |                  |
| 1   | D     | 572    |                  |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 3   | FAD  | A     | 600 | X         | -        | -       | -                |
| 3   | FAD  | B     | 700 | X         | -        | -       | -                |
| 3   | FAD  | C     | 800 | X         | -        | -       | -                |
| 3   | FAD  | D     | 900 | X         | -        | -       | -                |

## 2 Entry composition [i](#)

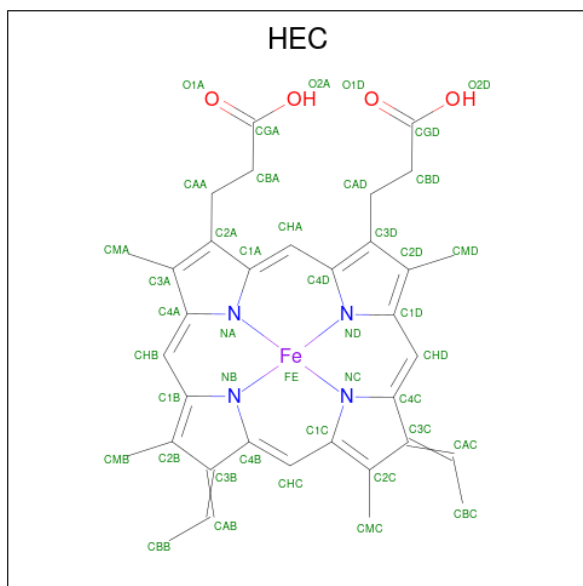
There are 5 unique types of molecules in this entry. The entry contains 17470 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 FLAVOCYTOCHROME C FUMARATE REDUCTASE.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 570      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4124  | 2562 | 736 | 807 | 19 |         |         |       |
| 1   | B     | 566      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4093  | 2542 | 731 | 801 | 19 |         |         |       |
| 1   | C     | 568      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4099  | 2546 | 733 | 801 | 19 |         |         |       |
| 1   | D     | 570      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4113  | 2553 | 734 | 807 | 19 |         |         |       |

- Molecule 2 is HEME C (CCD ID: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ).



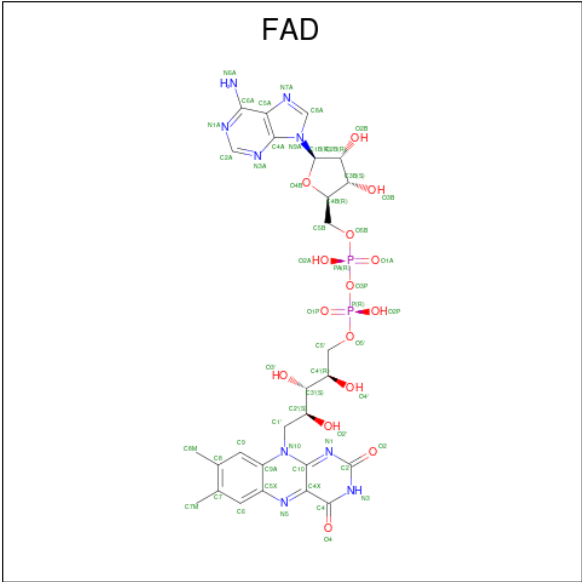
| Mol | Chain | Residues | Atoms |    |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 2   | A     | 1        | Total | C  | Fe | N | O | 0       | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |         |
| 2   | A     | 1        | Total | C  | Fe | N | O | 0       | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |         |

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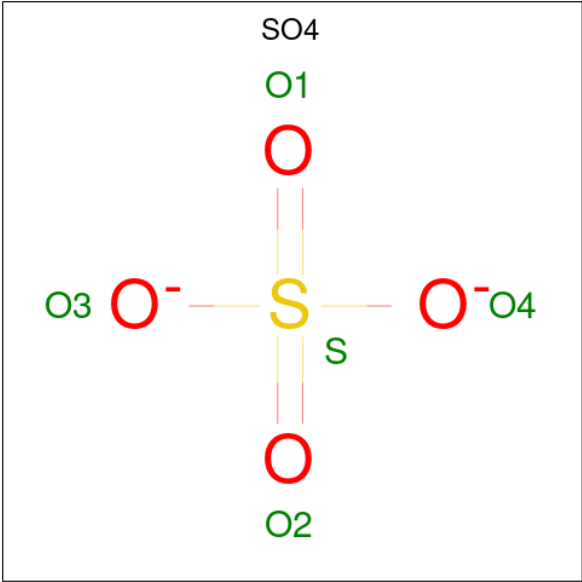
| Mol | Chain | Residues | Atoms       |         |         |        |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 2   | A     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 2   | A     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 2   | B     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 2   | B     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 2   | B     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 2   | B     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 2   | C     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 2   | C     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 2   | C     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 2   | C     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 2   | D     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 2   | D     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 2   | D     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 2   | D     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



| Mol | Chain | Residues | Atoms |    |   |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| 3   | A     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 53    | 27 | 9 | 15 | 2 |         |         |
| 3   | B     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 53    | 27 | 9 | 15 | 2 |         |         |
| 3   | C     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 53    | 27 | 9 | 15 | 2 |         |         |
| 3   | D     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 53    | 27 | 9 | 15 | 2 |         |         |

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



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 4   | B     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | C     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | D     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

- Molecule 5 is water.

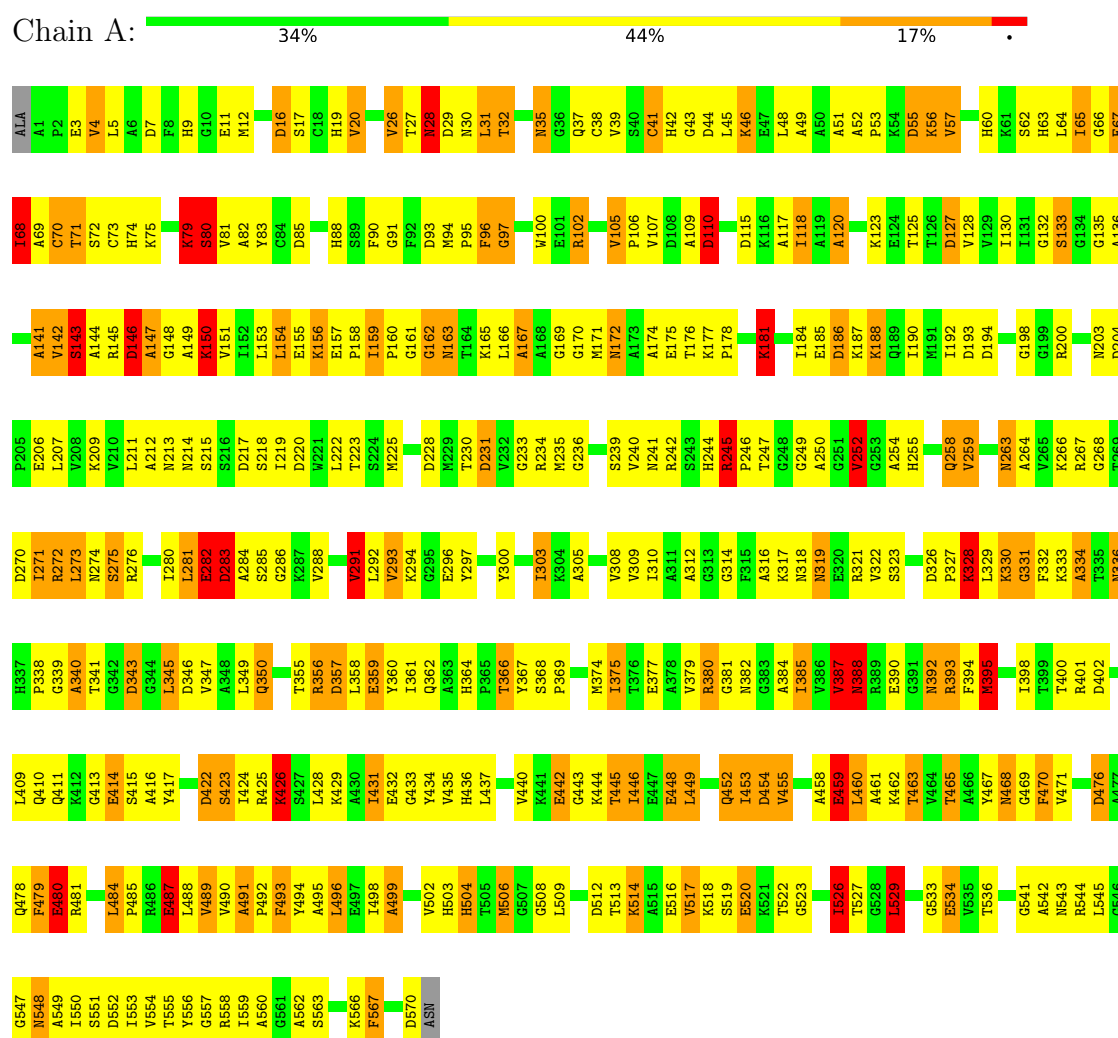
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 5   | A     | 48       | Total | O  | 0       | 0       |
|     |       |          | 48    | 48 |         |         |
| 5   | B     | 29       | Total | O  | 0       | 0       |
|     |       |          | 29    | 29 |         |         |
| 5   | C     | 30       | Total | O  | 0       | 0       |
|     |       |          | 30    | 30 |         |         |
| 5   | D     | 19       | Total | O  | 0       | 0       |
|     |       |          | 19    | 19 |         |         |

### 3 Residue-property plots

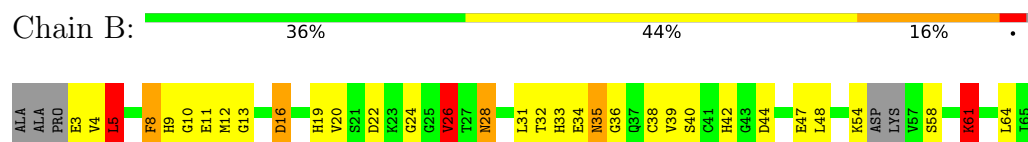
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

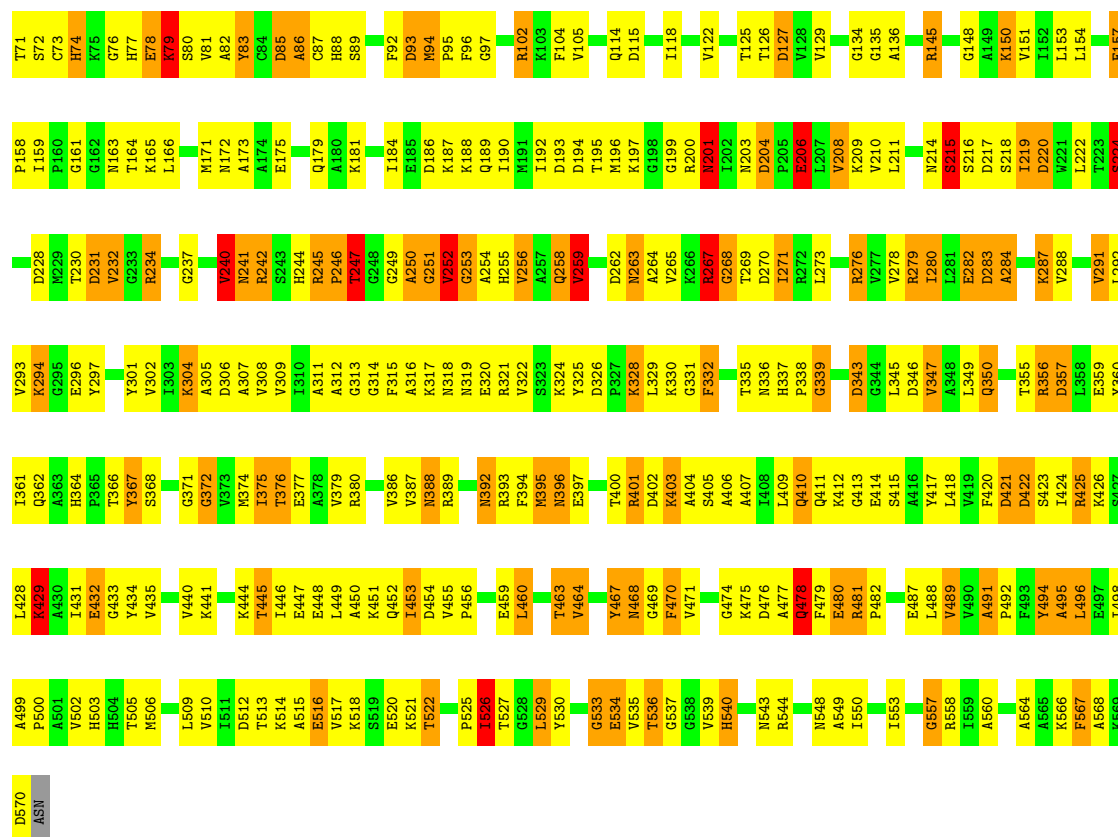
#### • Molecule 1: FLAVOCYTOCHROME C FUMARATE REDUCTASE



#### • Molecule 1: FLAVOCYTOCHROME C FUMARATE REDUCTASE

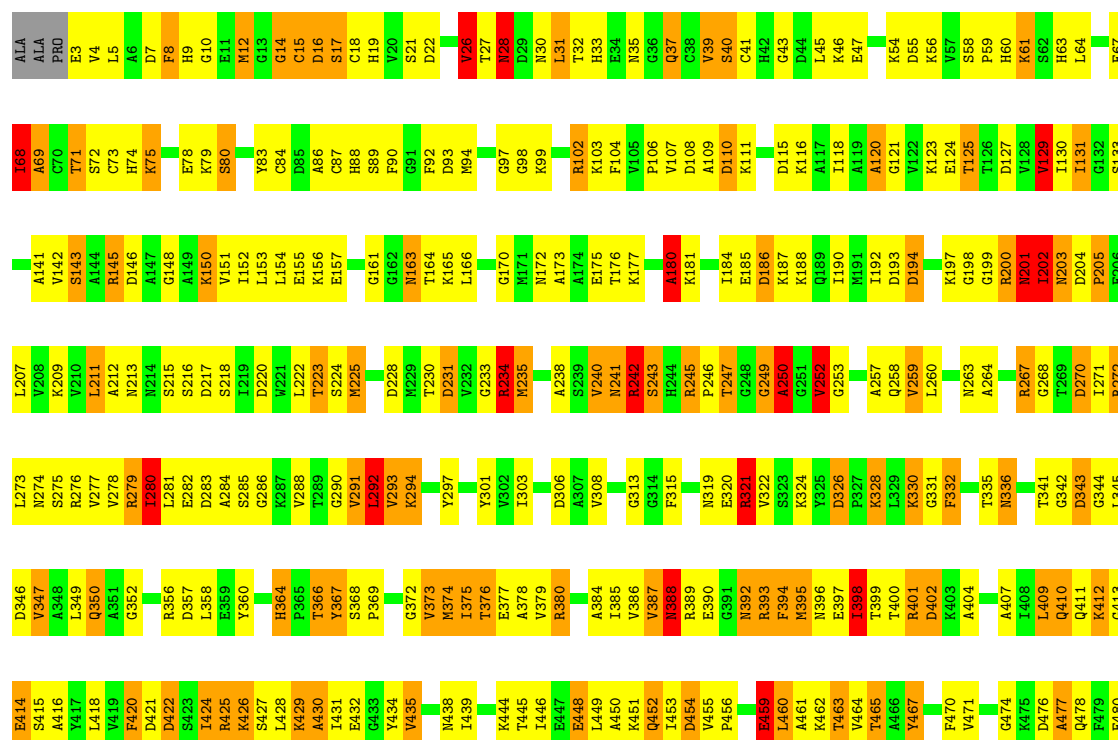


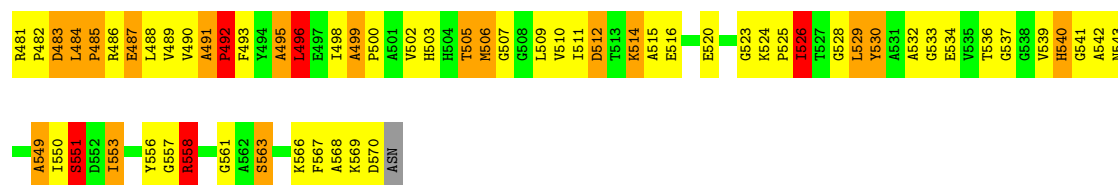




# Molecule 1: FLAVOCYTOCHROME C FUMARATE REDUCTASE

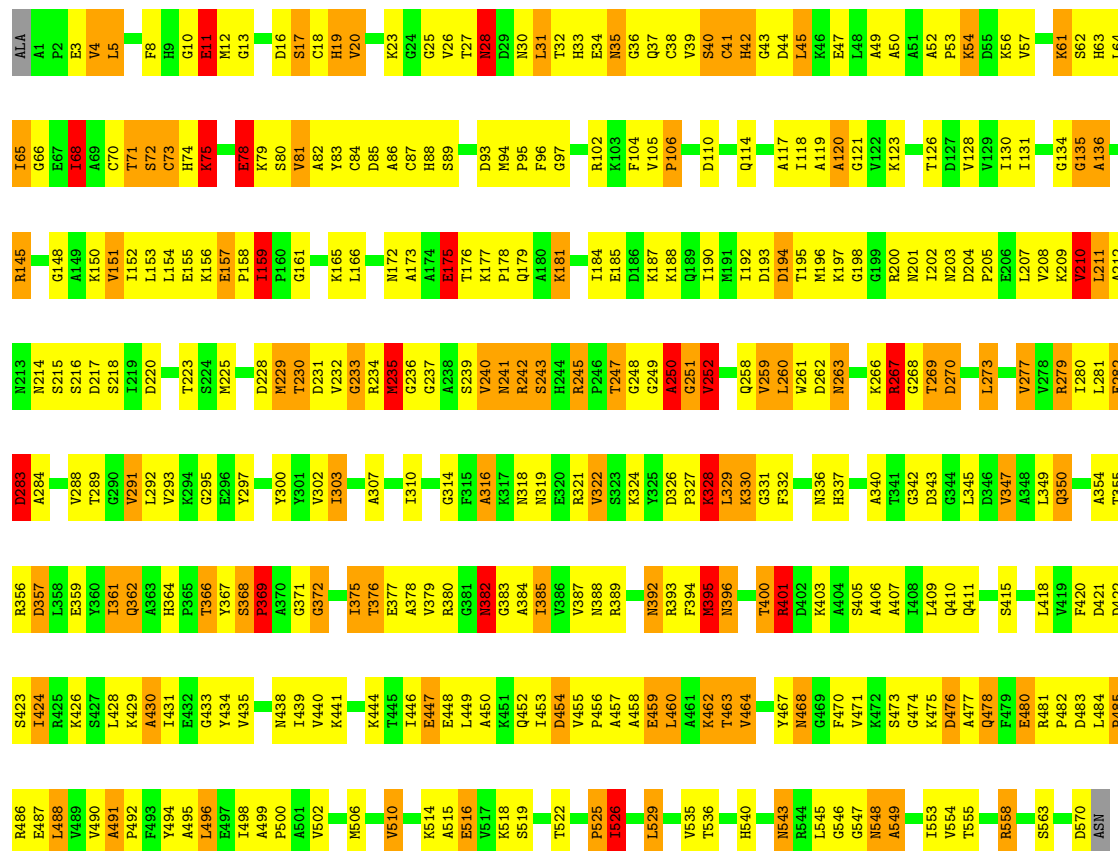
Chain C: 34% 43% 19%





• Molecule 1: FLAVOCYTOCHROME C FUMARATE REDUCTASE

Chain D: 38% 43% 16%



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

| Property                                                 | Value                                           | Source    |
|----------------------------------------------------------|-------------------------------------------------|-----------|
| Space group                                              | P 21 21 2                                       | Depositor |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$ | 109.69Å 216.36Å 112.04Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å)                                           | 15.00 – 2.90                                    | Depositor |
| % Data completeness<br>(in resolution range)             | 93.7 (15.00-2.90)                               | Depositor |
| $R_{merge}$                                              | 0.08                                            | Depositor |
| $R_{sym}$                                                | (Not available)                                 | Depositor |
| Refinement program                                       | REFMAC                                          | Depositor |
| R, $R_{free}$                                            | 0.210 , 0.300                                   | Depositor |
| Estimated twinning fraction                              | No twinning to report.                          | Xtriage   |
| Total number of atoms                                    | 17470                                           | wwPDB-VP  |
| Average B, all atoms (Å <sup>2</sup> )                   | 40.0                                            | wwPDB-VP  |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FAD, HEC, SO4

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     | 1.01         | 1/4192 (0.0%)   | 2.68        | 353/5683 (6.2%)   |
| 1   | B     | 0.97         | 15/4159 (0.4%)  | 2.52        | 288/5637 (5.1%)   |
| 1   | C     | 0.93         | 3/4166 (0.1%)   | 2.56        | 322/5649 (5.7%)   |
| 1   | D     | 0.84         | 1/4179 (0.0%)   | 2.44        | 251/5665 (4.4%)   |
| All | All   | 0.94         | 20/16696 (0.1%) | 2.55        | 1214/22634 (5.4%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 3                   |
| 1   | B     | 0                   | 2                   |
| 1   | C     | 0                   | 3                   |
| 1   | D     | 0                   | 2                   |
| All | All   | 0                   | 10                  |

All (20) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | B     | 476 | ASP  | CG-OD1 | 10.26 | 1.44        | 1.25     |
| 1   | B     | 475 | LYS  | C-O    | 10.05 | 1.36        | 1.23     |
| 1   | C     | 477 | ALA  | C-O    | 9.29  | 1.35        | 1.24     |
| 1   | B     | 477 | ALA  | N-CA   | 7.39  | 1.55        | 1.46     |
| 1   | B     | 469 | GLY  | N-CA   | 7.25  | 1.55        | 1.45     |
| 1   | B     | 468 | ASN  | C-O    | 7.21  | 1.32        | 1.24     |
| 1   | B     | 468 | ASN  | CG-OD1 | 6.85  | 1.36        | 1.23     |
| 1   | B     | 478 | GLN  | N-CA   | 6.77  | 1.54        | 1.46     |
| 1   | D     | 468 | ASN  | CG-ND2 | 6.12  | 1.46        | 1.33     |
| 1   | B     | 476 | ASP  | CG-OD2 | 5.86  | 1.36        | 1.25     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | B     | 480 | GLU  | CD-OE1 | 5.84  | 1.36        | 1.25     |
| 1   | B     | 474 | GLY  | CA-C   | 5.77  | 1.58        | 1.51     |
| 1   | A     | 267 | ARG  | CD-NE  | -5.59 | 1.38        | 1.46     |
| 1   | C     | 459 | GLU  | CD-OE1 | 5.54  | 1.35        | 1.25     |
| 1   | B     | 469 | GLY  | C-N    | 5.51  | 1.41        | 1.33     |
| 1   | B     | 247 | THR  | N-CA   | -5.17 | 1.39        | 1.46     |
| 1   | C     | 459 | GLU  | CD-OE2 | 5.11  | 1.35        | 1.25     |
| 1   | B     | 268 | GLY  | N-CA   | 5.08  | 1.52        | 1.45     |
| 1   | B     | 251 | GLY  | N-CA   | -5.07 | 1.38        | 1.45     |
| 1   | B     | 476 | ASP  | C-N    | 5.04  | 1.40        | 1.33     |

All (1214) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 1   | D     | 245 | ARG  | CD-NE-CZ   | 28.45  | 164.23      | 124.40   |
| 1   | D     | 491 | ALA  | CA-C-O     | -25.02 | 100.19      | 119.46   |
| 1   | C     | 491 | ALA  | CA-C-O     | -23.99 | 95.97       | 119.24   |
| 1   | B     | 570 | ASP  | CA-CB-CG   | 23.53  | 136.13      | 112.60   |
| 1   | A     | 267 | ARG  | CD-NE-CZ   | 23.43  | 157.20      | 124.40   |
| 1   | D     | 401 | ARG  | CD-NE-CZ   | 21.28  | 154.19      | 124.40   |
| 1   | A     | 491 | ALA  | CA-C-O     | -19.91 | 100.00      | 119.51   |
| 1   | A     | 281 | LEU  | CA-C-N     | 19.13  | 157.03      | 121.06   |
| 1   | A     | 281 | LEU  | C-N-CA     | 19.13  | 157.03      | 121.06   |
| 1   | B     | 491 | ALA  | CA-C-O     | -18.86 | 102.03      | 119.75   |
| 1   | B     | 356 | ARG  | CD-NE-CZ   | 18.59  | 150.43      | 124.40   |
| 1   | C     | 267 | ARG  | CD-NE-CZ   | 18.36  | 150.10      | 124.40   |
| 1   | B     | 246 | PRO  | CA-C-N     | 18.07  | 156.06      | 121.54   |
| 1   | B     | 246 | PRO  | C-N-CA     | 18.07  | 156.06      | 121.54   |
| 1   | A     | 7   | ASP  | CA-CB-CG   | 17.71  | 130.31      | 112.60   |
| 1   | C     | 392 | ASN  | CA-CB-CG   | 17.01  | 129.61      | 112.60   |
| 1   | B     | 145 | ARG  | CD-NE-CZ   | 16.17  | 147.04      | 124.40   |
| 1   | D     | 281 | LEU  | CA-C-N     | 16.02  | 147.99      | 121.39   |
| 1   | D     | 281 | LEU  | C-N-CA     | 16.02  | 147.99      | 121.39   |
| 1   | B     | 468 | ASN  | OD1-CG-ND2 | 15.82  | 138.42      | 122.60   |
| 1   | C     | 477 | ALA  | CA-C-O     | -15.59 | 102.05      | 119.97   |
| 1   | A     | 558 | ARG  | CG-CD-NE   | 14.77  | 144.50      | 112.00   |
| 1   | A     | 283 | ASP  | CA-CB-CG   | 14.65  | 127.25      | 112.60   |
| 1   | A     | 245 | ARG  | CB-CG-CD   | 14.40  | 144.42      | 111.30   |
| 1   | C     | 332 | PHE  | CA-CB-CG   | 14.32  | 128.12      | 113.80   |
| 1   | D     | 185 | GLU  | CA-CB-CG   | 14.24  | 142.58      | 114.10   |
| 1   | C     | 16  | ASP  | CA-CB-CG   | 14.24  | 126.84      | 112.60   |
| 1   | D     | 283 | ASP  | CA-CB-CG   | 14.24  | 126.84      | 112.60   |

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| Mol | Chain | Res | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 1   | A     | 102 | ARG  | NE-CZ-NH2  | 14.18  | 131.97      | 119.20   |
| 1   | B     | 252 | VAL  | N-CA-CB    | 14.16  | 125.49      | 110.62   |
| 1   | C     | 328 | LYS  | CA-CB-CG   | 14.02  | 142.13      | 114.10   |
| 1   | B     | 11  | GLU  | CB-CG-CD   | 13.63  | 135.78      | 112.60   |
| 1   | A     | 93  | ASP  | CA-CB-CG   | -13.38 | 99.22       | 112.60   |
| 1   | A     | 319 | ASN  | CA-CB-CG   | 13.31  | 125.91      | 112.60   |
| 1   | C     | 110 | ASP  | CA-CB-CG   | 12.94  | 125.54      | 112.60   |
| 1   | D     | 396 | ASN  | CA-CB-CG   | 12.81  | 125.41      | 112.60   |
| 1   | A     | 380 | ARG  | NE-CZ-NH2  | 12.54  | 130.49      | 119.20   |
| 1   | A     | 558 | ARG  | NE-CZ-NH2  | 12.45  | 130.40      | 119.20   |
| 1   | B     | 246 | PRO  | CA-C-O     | 12.35  | 136.13      | 121.31   |
| 1   | C     | 543 | ASN  | OD1-CG-ND2 | 12.25  | 134.85      | 122.60   |
| 1   | D     | 382 | ASN  | CA-CB-CG   | 12.14  | 124.74      | 112.60   |
| 1   | A     | 186 | ASP  | CA-CB-CG   | 12.11  | 124.71      | 112.60   |
| 1   | D     | 176 | THR  | CA-C-N     | 11.89  | 134.52      | 119.78   |
| 1   | D     | 176 | THR  | C-N-CA     | 11.89  | 134.52      | 119.78   |
| 1   | B     | 343 | ASP  | CA-CB-CG   | 11.79  | 124.39      | 112.60   |
| 1   | C     | 401 | ARG  | CD-NE-CZ   | 11.74  | 140.83      | 124.40   |
| 1   | B     | 267 | ARG  | CA-C-O     | -11.67 | 109.75      | 122.01   |
| 1   | C     | 506 | MET  | CA-C-O     | -11.55 | 108.54      | 120.90   |
| 1   | B     | 16  | ASP  | CA-CB-CG   | 11.49  | 124.09      | 112.60   |
| 1   | B     | 474 | GLY  | O-C-N      | 11.24  | 134.00      | 122.54   |
| 1   | D     | 262 | ASP  | CA-CB-CG   | 11.23  | 123.83      | 112.60   |
| 1   | C     | 156 | LYS  | CA-CB-CG   | 11.22  | 136.55      | 114.10   |
| 1   | B     | 4   | VAL  | N-CA-CB    | 11.17  | 129.68      | 111.36   |
| 1   | B     | 470 | PHE  | N-CA-C     | -11.15 | 99.13       | 111.28   |
| 1   | B     | 250 | ALA  | CA-C-N     | 10.98  | 142.93      | 121.41   |
| 1   | B     | 250 | ALA  | C-N-CA     | 10.98  | 142.93      | 121.41   |
| 1   | B     | 270 | ASP  | CA-CB-CG   | 10.96  | 123.56      | 112.60   |
| 1   | B     | 220 | ASP  | CA-CB-CG   | 10.91  | 123.51      | 112.60   |
| 1   | C     | 102 | ARG  | CD-NE-CZ   | 10.89  | 139.65      | 124.40   |
| 1   | D     | 492 | PRO  | N-CA-CB    | 10.87  | 114.66      | 103.25   |
| 1   | C     | 61  | LYS  | CA-CB-CG   | 10.84  | 135.77      | 114.10   |
| 1   | A     | 3   | GLU  | CA-C-N     | 10.76  | 141.34      | 121.97   |
| 1   | A     | 3   | GLU  | C-N-CA     | 10.76  | 141.34      | 121.97   |
| 1   | A     | 56  | LYS  | CA-C-N     | 10.73  | 141.29      | 121.97   |
| 1   | A     | 56  | LYS  | C-N-CA     | 10.73  | 141.29      | 121.97   |
| 1   | B     | 217 | ASP  | CA-CB-CG   | 10.69  | 123.29      | 112.60   |
| 1   | C     | 478 | GLN  | CB-CG-CD   | -10.64 | 94.51       | 112.60   |
| 1   | C     | 373 | VAL  | CA-C-O     | 10.49  | 134.13      | 121.75   |
| 1   | A     | 481 | ARG  | CD-NE-CZ   | 10.47  | 139.06      | 124.40   |
| 1   | C     | 228 | ASP  | CA-CB-CG   | 10.37  | 122.97      | 112.60   |

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| Mol | Chain | Res | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 1   | A     | 200 | ARG  | CD-NE-CZ   | 10.34  | 138.87      | 124.40   |
| 1   | A     | 281 | LEU  | CA-C-O     | 10.20  | 132.65      | 120.92   |
| 1   | B     | 492 | PRO  | N-CA-CB    | 10.15  | 113.91      | 103.25   |
| 1   | C     | 17  | SER  | CA-C-O     | 10.12  | 132.26      | 120.92   |
| 1   | B     | 252 | VAL  | CA-C-O     | -10.12 | 110.89      | 121.41   |
| 1   | A     | 392 | ASN  | CA-CB-CG   | 10.08  | 122.68      | 112.60   |
| 1   | B     | 161 | GLY  | N-CA-C     | 10.06  | 127.05      | 115.08   |
| 1   | C     | 28  | ASN  | CA-CB-CG   | 10.01  | 122.61      | 112.60   |
| 1   | D     | 242 | ARG  | NE-CZ-NH2  | -9.97  | 110.23      | 119.20   |
| 1   | B     | 251 | GLY  | N-CA-C     | 9.95   | 136.75      | 113.18   |
| 1   | C     | 344 | GLY  | CA-C-O     | -9.94  | 110.81      | 121.05   |
| 1   | A     | 193 | ASP  | CA-CB-CG   | 9.94   | 122.54      | 112.60   |
| 1   | C     | 211 | LEU  | CA-C-O     | 9.94   | 132.00      | 121.07   |
| 1   | C     | 270 | ASP  | CA-CB-CG   | 9.79   | 122.39      | 112.60   |
| 1   | A     | 282 | GLU  | N-CA-C     | 9.79   | 122.45      | 110.41   |
| 1   | C     | 274 | ASN  | OD1-CG-ND2 | 9.71   | 132.31      | 122.60   |
| 1   | B     | 469 | GLY  | CA-C-O     | 9.67   | 130.85      | 120.40   |
| 1   | D     | 25  | GLY  | CA-C-O     | -9.66  | 115.94      | 122.22   |
| 1   | A     | 242 | ARG  | NE-CZ-NH2  | 9.64   | 127.88      | 119.20   |
| 1   | B     | 350 | GLN  | CB-CG-CD   | 9.63   | 128.97      | 112.60   |
| 1   | A     | 16  | ASP  | CA-CB-CG   | 9.60   | 122.20      | 112.60   |
| 1   | A     | 321 | ARG  | O-C-N      | -9.54  | 112.17      | 122.09   |
| 1   | D     | 356 | ARG  | NE-CZ-NH2  | 9.54   | 127.79      | 119.20   |
| 1   | D     | 242 | ARG  | CD-NE-CZ   | 9.52   | 137.72      | 124.40   |
| 1   | C     | 478 | GLN  | OE1-CD-NE2 | 9.51   | 132.11      | 122.60   |
| 1   | D     | 546 | GLY  | CA-C-O     | 9.48   | 129.75      | 121.41   |
| 1   | C     | 259 | VAL  | N-CA-CB    | 9.46   | 121.62      | 110.55   |
| 1   | A     | 258 | GLN  | CA-C-O     | -9.44  | 110.91      | 120.82   |
| 1   | C     | 492 | PRO  | N-CA-CB    | 9.41   | 113.13      | 103.25   |
| 1   | D     | 343 | ASP  | CA-CB-CG   | 9.39   | 121.99      | 112.60   |
| 1   | D     | 16  | ASP  | CA-CB-CG   | 9.34   | 121.94      | 112.60   |
| 1   | D     | 248 | GLY  | O-C-N      | -9.27  | 116.11      | 123.80   |
| 1   | D     | 492 | PRO  | CA-N-CD    | -9.23  | 99.07       | 112.00   |
| 1   | A     | 267 | ARG  | CA-C-O     | -9.23  | 109.97      | 121.50   |
| 1   | B     | 61  | LYS  | CA-CB-CG   | 9.22   | 132.55      | 114.10   |
| 1   | B     | 252 | VAL  | CB-CA-C    | -9.21  | 99.91       | 111.70   |
| 1   | C     | 163 | ASN  | OD1-CG-ND2 | -9.21  | 113.39      | 122.60   |
| 1   | A     | 43  | GLY  | N-CA-C     | -9.20  | 101.20      | 112.33   |
| 1   | A     | 267 | ARG  | NE-CZ-NH1  | -9.19  | 112.31      | 121.50   |
| 1   | B     | 201 | ASN  | CA-CB-CG   | 9.18   | 121.78      | 112.60   |
| 1   | A     | 69  | ALA  | CA-C-N     | 9.15   | 132.73      | 120.65   |
| 1   | A     | 69  | ALA  | C-N-CA     | 9.15   | 132.73      | 120.65   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | D     | 242 | ARG  | NE-CZ-NH1 | 9.15  | 130.65      | 121.50   |
| 1   | D     | 546 | GLY  | O-C-N     | -9.12 | 113.90      | 122.93   |
| 1   | A     | 19  | HIS  | O-C-N     | -9.11 | 112.86      | 123.06   |
| 1   | C     | 301 | TYR  | CA-CB-CG  | 9.09  | 130.25      | 113.90   |
| 1   | B     | 475 | LYS  | O-C-N     | 9.07  | 133.65      | 123.40   |
| 1   | A     | 393 | ARG  | CD-NE-CZ  | 9.07  | 137.09      | 124.40   |
| 1   | C     | 569 | LYS  | CA-C-N    | 9.07  | 138.02      | 121.70   |
| 1   | C     | 569 | LYS  | C-N-CA    | 9.07  | 138.02      | 121.70   |
| 1   | D     | 526 | ILE  | N-CA-CB   | 9.06  | 120.88      | 110.82   |
| 1   | A     | 38  | CYS  | CB-CA-C   | -9.02 | 96.38       | 110.81   |
| 1   | C     | 502 | VAL  | CA-C-O    | -9.02 | 112.30      | 121.59   |
| 1   | B     | 150 | LYS  | CB-CA-C   | 9.01  | 125.27      | 110.22   |
| 1   | A     | 424 | ILE  | N-CA-CB   | 8.99  | 120.49      | 110.51   |
| 1   | C     | 509 | LEU  | CA-C-O    | -8.97 | 111.32      | 121.19   |
| 1   | A     | 242 | ARG  | CD-NE-CZ  | 8.97  | 136.95      | 124.40   |
| 1   | C     | 3   | GLU  | CA-C-N    | 8.96  | 138.11      | 121.97   |
| 1   | C     | 3   | GLU  | C-N-CA    | 8.96  | 138.11      | 121.97   |
| 1   | A     | 329 | LEU  | CA-C-O    | -8.91 | 108.50      | 119.28   |
| 1   | B     | 533 | GLY  | O-C-N     | -8.90 | 114.44      | 122.90   |
| 1   | B     | 259 | VAL  | N-CA-CB   | 8.90  | 123.92      | 110.58   |
| 1   | B     | 19  | HIS  | CA-CB-CG  | -8.84 | 104.96      | 113.80   |
| 1   | A     | 321 | ARG  | NE-CZ-NH1 | 8.81  | 130.31      | 121.50   |
| 1   | A     | 272 | ARG  | NE-CZ-NH2 | -8.79 | 111.29      | 119.20   |
| 1   | A     | 281 | LEU  | O-C-N     | -8.79 | 112.97      | 123.16   |
| 1   | B     | 283 | ASP  | CA-C-N    | 8.78  | 138.30      | 121.54   |
| 1   | B     | 283 | ASP  | C-N-CA    | 8.78  | 138.30      | 121.54   |
| 1   | C     | 141 | ALA  | CA-C-O    | -8.74 | 111.64      | 120.82   |
| 1   | D     | 279 | ARG  | NE-CZ-NH2 | 8.71  | 127.04      | 119.20   |
| 1   | A     | 97  | GLY  | N-CA-C    | 8.70  | 123.38      | 111.54   |
| 1   | D     | 356 | ARG  | CD-NE-CZ  | 8.69  | 136.56      | 124.40   |
| 1   | A     | 526 | ILE  | CB-CA-C   | 8.65  | 121.42      | 110.96   |
| 1   | A     | 570 | ASP  | CA-CB-CG  | 8.63  | 121.23      | 112.60   |
| 1   | A     | 200 | ARG  | NE-CZ-NH1 | 8.62  | 130.12      | 121.50   |
| 1   | D     | 185 | GLU  | CB-CG-CD  | 8.60  | 127.22      | 112.60   |
| 1   | A     | 380 | ARG  | NE-CZ-NH1 | -8.60 | 112.91      | 121.50   |
| 1   | D     | 223 | THR  | O-C-N     | -8.59 | 113.22      | 122.07   |
| 1   | D     | 395 | MET  | CA-CB-CG  | 8.58  | 131.25      | 114.10   |
| 1   | D     | 295 | GLY  | N-CA-C    | -8.54 | 102.11      | 111.93   |
| 1   | A     | 228 | ASP  | CA-CB-CG  | 8.52  | 121.12      | 112.60   |
| 1   | A     | 27  | THR  | N-CA-C    | -8.51 | 103.48      | 114.04   |
| 1   | B     | 276 | ARG  | NE-CZ-NH2 | -8.51 | 111.54      | 119.20   |
| 1   | B     | 401 | ARG  | NE-CZ-NH2 | -8.46 | 111.58      | 119.20   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | C     | 476 | ASP  | CA-CB-CG   | 8.46  | 121.06      | 112.60   |
| 1   | A     | 357 | ASP  | CA-CB-CG   | -8.46 | 104.14      | 112.60   |
| 1   | C     | 558 | ARG  | CG-CD-NE   | 8.45  | 130.59      | 112.00   |
| 1   | D     | 281 | LEU  | CA-C-O     | 8.44  | 130.17      | 120.80   |
| 1   | B     | 252 | VAL  | O-C-N      | 8.44  | 131.07      | 121.96   |
| 1   | C     | 234 | ARG  | NE-CZ-NH1  | 8.42  | 129.92      | 121.50   |
| 1   | A     | 263 | ASN  | CA-C-O     | -8.41 | 111.63      | 120.55   |
| 1   | A     | 328 | LYS  | CB-CA-C    | -8.41 | 96.39       | 110.68   |
| 1   | C     | 223 | THR  | CA-C-O     | 8.41  | 129.46      | 120.55   |
| 1   | A     | 29  | ASP  | CA-CB-CG   | -8.40 | 104.20      | 112.60   |
| 1   | C     | 530 | TYR  | O-C-N      | -8.39 | 112.24      | 123.15   |
| 1   | A     | 434 | TYR  | N-CA-C     | -8.38 | 101.67      | 112.23   |
| 1   | B     | 328 | LYS  | CA-CB-CG   | 8.36  | 130.81      | 114.10   |
| 1   | C     | 503 | HIS  | N-CA-CB    | -8.35 | 97.99       | 111.18   |
| 1   | C     | 356 | ARG  | NE-CZ-NH1  | -8.33 | 113.17      | 121.50   |
| 1   | A     | 105 | VAL  | CA-C-O     | 8.33  | 125.05      | 119.38   |
| 1   | D     | 56  | LYS  | N-CA-C     | 8.33  | 121.82      | 109.24   |
| 1   | A     | 442 | GLU  | CA-CB-CG   | 8.33  | 130.75      | 114.10   |
| 1   | C     | 543 | ASN  | CB-CG-ND2  | -8.30 | 103.94      | 116.40   |
| 1   | A     | 81  | VAL  | CA-C-O     | -8.30 | 111.37      | 120.67   |
| 1   | B     | 129 | VAL  | CA-C-O     | -8.30 | 111.69      | 120.48   |
| 1   | B     | 314 | GLY  | N-CA-C     | 8.29  | 124.85      | 112.41   |
| 1   | A     | 479 | PHE  | CA-CB-CG   | -8.27 | 105.53      | 113.80   |
| 1   | B     | 479 | PHE  | CA-CB-CG   | -8.26 | 105.54      | 113.80   |
| 1   | C     | 540 | HIS  | CA-CB-CG   | -8.26 | 105.54      | 113.80   |
| 1   | C     | 234 | ARG  | NE-CZ-NH2  | -8.22 | 111.80      | 119.20   |
| 1   | C     | 523 | GLY  | CA-C-O     | 8.22  | 128.09      | 118.97   |
| 1   | B     | 567 | PHE  | CA-C-O     | -8.21 | 112.04      | 121.07   |
| 1   | B     | 540 | HIS  | CA-CB-CG   | -8.21 | 105.59      | 113.80   |
| 1   | D     | 543 | ASN  | OD1-CG-ND2 | 8.21  | 130.81      | 122.60   |
| 1   | C     | 204 | ASP  | CA-C-O     | 8.21  | 124.62      | 119.29   |
| 1   | D     | 396 | ASN  | CB-CA-C    | 8.20  | 123.39      | 109.53   |
| 1   | A     | 19  | HIS  | CA-C-O     | 8.18  | 131.18      | 121.36   |
| 1   | B     | 422 | ASP  | CA-CB-CG   | 8.15  | 120.75      | 112.60   |
| 1   | A     | 102 | ARG  | NE-CZ-NH1  | -8.15 | 113.35      | 121.50   |
| 1   | B     | 425 | ARG  | CB-CG-CD   | 8.14  | 130.02      | 111.30   |
| 1   | B     | 157 | GLU  | CA-C-O     | -8.13 | 111.92      | 120.87   |
| 1   | C     | 492 | PRO  | CA-N-CD    | -8.13 | 100.62      | 112.00   |
| 1   | A     | 560 | ALA  | CA-C-O     | -8.10 | 111.88      | 120.63   |
| 1   | D     | 161 | GLY  | N-CA-C     | 8.09  | 126.06      | 115.47   |
| 1   | C     | 161 | GLY  | O-C-N      | -8.07 | 112.53      | 122.46   |
| 1   | A     | 364 | HIS  | CA-CB-CG   | 8.07  | 121.87      | 113.80   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | B     | 318 | ASN  | CA-CB-CG   | 8.06  | 120.66      | 112.60   |
| 1   | D     | 267 | ARG  | NE-CZ-NH1  | -8.04 | 113.46      | 121.50   |
| 1   | A     | 254 | ALA  | CA-C-O     | -8.03 | 112.04      | 120.55   |
| 1   | C     | 133 | SER  | CA-C-N     | 8.03  | 131.31      | 121.83   |
| 1   | C     | 133 | SER  | C-N-CA     | 8.03  | 131.31      | 121.83   |
| 1   | C     | 107 | VAL  | CA-C-N     | 8.01  | 132.49      | 120.31   |
| 1   | C     | 107 | VAL  | C-N-CA     | 8.01  | 132.49      | 120.31   |
| 1   | A     | 4   | VAL  | CA-C-O     | -8.01 | 110.77      | 120.78   |
| 1   | B     | 502 | VAL  | CA-C-O     | -8.00 | 112.67      | 121.23   |
| 1   | B     | 543 | ASN  | CA-CB-CG   | -8.00 | 104.60      | 112.60   |
| 1   | C     | 252 | VAL  | N-CA-CB    | 8.00  | 119.91      | 110.55   |
| 1   | A     | 169 | GLY  | CA-C-O     | -8.00 | 112.96      | 120.80   |
| 1   | C     | 207 | LEU  | CA-C-O     | -8.00 | 112.43      | 120.82   |
| 1   | D     | 263 | ASN  | CA-CB-CG   | -7.99 | 104.61      | 112.60   |
| 1   | A     | 319 | ASN  | OD1-CG-ND2 | -7.98 | 114.62      | 122.60   |
| 1   | C     | 4   | VAL  | CA-C-N     | 7.98  | 131.31      | 120.54   |
| 1   | C     | 4   | VAL  | C-N-CA     | 7.98  | 131.31      | 120.54   |
| 1   | A     | 468 | ASN  | OD1-CG-ND2 | -7.97 | 114.63      | 122.60   |
| 1   | D     | 318 | ASN  | CA-CB-CG   | 7.96  | 120.56      | 112.60   |
| 1   | C     | 4   | VAL  | N-CA-C     | 7.92  | 125.82      | 109.34   |
| 1   | C     | 250 | ALA  | N-CA-C     | 7.92  | 127.68      | 110.80   |
| 1   | C     | 525 | PRO  | CA-C-O     | -7.91 | 112.77      | 121.23   |
| 1   | C     | 121 | GLY  | CA-C-O     | 7.88  | 127.67      | 122.23   |
| 1   | D     | 85  | ASP  | CA-CB-CG   | -7.87 | 104.73      | 112.60   |
| 1   | B     | 70  | CYS  | O-C-N      | 7.87  | 130.46      | 122.12   |
| 1   | C     | 280 | ILE  | CA-C-O     | -7.87 | 110.58      | 121.51   |
| 1   | D     | 328 | LYS  | CA-C-O     | 7.86  | 130.21      | 121.02   |
| 1   | C     | 293 | VAL  | CB-CA-C    | -7.85 | 100.19      | 111.34   |
| 1   | A     | 273 | LEU  | O-C-N      | -7.80 | 113.90      | 122.79   |
| 1   | A     | 148 | GLY  | CA-C-N     | -7.79 | 108.46      | 121.39   |
| 1   | A     | 148 | GLY  | C-N-CA     | -7.79 | 108.46      | 121.39   |
| 1   | A     | 219 | ILE  | CA-C-O     | 7.79  | 130.23      | 120.96   |
| 1   | D     | 4   | VAL  | N-CA-CB    | 7.77  | 125.31      | 111.63   |
| 1   | C     | 71  | THR  | CA-C-O     | -7.76 | 110.45      | 119.61   |
| 1   | D     | 522 | THR  | N-CA-C     | 7.76  | 122.01      | 112.23   |
| 1   | B     | 283 | ASP  | O-C-N      | -7.74 | 116.38      | 122.03   |
| 1   | D     | 220 | ASP  | CA-CB-CG   | 7.73  | 120.33      | 112.60   |
| 1   | B     | 526 | ILE  | N-CA-CB    | 7.72  | 120.26      | 110.99   |
| 1   | D     | 350 | GLN  | CB-CG-CD   | 7.72  | 125.72      | 112.60   |
| 1   | C     | 242 | ARG  | NE-CZ-NH1  | -7.69 | 113.81      | 121.50   |
| 1   | A     | 523 | GLY  | CA-C-O     | 7.68  | 127.67      | 119.07   |
| 1   | A     | 172 | ASN  | CA-CB-CG   | 7.68  | 120.28      | 112.60   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | D     | 41  | CYS  | CA-C-O     | -7.68 | 110.04      | 119.18   |
| 1   | C     | 270 | ASP  | CA-C-O     | 7.67  | 129.13      | 120.84   |
| 1   | C     | 218 | SER  | CB-CA-C    | 7.67  | 125.40      | 110.67   |
| 1   | B     | 179 | GLN  | CA-C-O     | 7.65  | 128.79      | 119.38   |
| 1   | A     | 162 | GLY  | O-C-N      | -7.65 | 112.75      | 122.70   |
| 1   | A     | 150 | LYS  | N-CA-C     | -7.64 | 97.61       | 109.76   |
| 1   | D     | 81  | VAL  | CB-CA-C    | -7.64 | 98.74       | 110.50   |
| 1   | C     | 30  | ASN  | OD1-CG-ND2 | -7.64 | 114.96      | 122.60   |
| 1   | A     | 231 | ASP  | CA-C-N     | -7.63 | 113.14      | 123.14   |
| 1   | A     | 231 | ASP  | C-N-CA     | -7.63 | 113.14      | 123.14   |
| 1   | D     | 362 | GLN  | OE1-CD-NE2 | -7.62 | 114.98      | 122.60   |
| 1   | D     | 74  | HIS  | CA-CB-CG   | 7.61  | 121.41      | 113.80   |
| 1   | A     | 245 | ARG  | CA-C-O     | 7.61  | 126.67      | 120.13   |
| 1   | D     | 217 | ASP  | CA-C-O     | -7.61 | 112.49      | 120.55   |
| 1   | C     | 523 | GLY  | N-CA-C     | -7.60 | 104.05      | 115.00   |
| 1   | A     | 274 | ASN  | OD1-CG-ND2 | 7.60  | 130.20      | 122.60   |
| 1   | C     | 514 | LYS  | CA-C-O     | 7.59  | 128.23      | 119.35   |
| 1   | A     | 522 | THR  | N-CA-C     | 7.59  | 122.60      | 113.12   |
| 1   | D     | 401 | ARG  | NE-CZ-NH2  | -7.57 | 112.39      | 119.20   |
| 1   | A     | 28  | ASN  | O-C-N      | -7.56 | 114.18      | 123.33   |
| 1   | C     | 420 | PHE  | CA-CB-CG   | 7.54  | 121.34      | 113.80   |
| 1   | C     | 401 | ARG  | CA-CB-CG   | 7.53  | 129.17      | 114.10   |
| 1   | B     | 136 | ALA  | CA-C-N     | 7.53  | 128.30      | 119.94   |
| 1   | B     | 136 | ALA  | C-N-CA     | 7.53  | 128.30      | 119.94   |
| 1   | C     | 503 | HIS  | CA-CB-CG   | 7.50  | 121.30      | 113.80   |
| 1   | D     | 151 | VAL  | N-CA-C     | 7.50  | 118.60      | 108.11   |
| 1   | D     | 259 | VAL  | N-CA-CB    | 7.49  | 118.83      | 110.51   |
| 1   | D     | 197 | LYS  | CA-C-O     | -7.48 | 112.49      | 120.42   |
| 1   | A     | 470 | PHE  | CA-CB-CG   | 7.46  | 121.26      | 113.80   |
| 1   | C     | 230 | THR  | CA-C-O     | -7.46 | 110.25      | 119.28   |
| 1   | C     | 99  | LYS  | CA-C-O     | -7.46 | 112.47      | 121.28   |
| 1   | A     | 493 | PHE  | CA-CB-CG   | -7.46 | 106.34      | 113.80   |
| 1   | A     | 491 | ALA  | O-C-N      | 7.45  | 127.80      | 121.31   |
| 1   | A     | 271 | ILE  | O-C-N      | -7.44 | 114.49      | 122.83   |
| 1   | A     | 272 | ARG  | NH1-CZ-NH2 | 7.44  | 128.97      | 119.30   |
| 1   | B     | 145 | ARG  | N-CA-C     | -7.44 | 103.25      | 111.36   |
| 1   | D     | 230 | THR  | CA-C-O     | -7.44 | 110.47      | 119.32   |
| 1   | C     | 86  | ALA  | N-CA-C     | -7.43 | 104.22      | 113.28   |
| 1   | A     | 63  | HIS  | CA-CB-CG   | -7.42 | 106.38      | 113.80   |
| 1   | A     | 275 | SER  | N-CA-CB    | -7.40 | 98.95       | 110.65   |
| 1   | A     | 562 | ALA  | CA-C-O     | 7.40  | 128.40      | 120.55   |
| 1   | B     | 560 | ALA  | CA-C-N     | 7.40  | 128.32      | 120.03   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | B     | 560 | ALA  | C-N-CA     | 7.40  | 128.32      | 120.03   |
| 1   | C     | 19  | HIS  | CA-CB-CG   | -7.39 | 106.41      | 113.80   |
| 1   | B     | 85  | ASP  | CA-C-O     | 7.38  | 128.44      | 120.10   |
| 1   | C     | 41  | CYS  | CA-C-N     | -7.36 | 110.80      | 122.29   |
| 1   | C     | 41  | CYS  | C-N-CA     | -7.36 | 110.80      | 122.29   |
| 1   | A     | 272 | ARG  | CA-C-O     | 7.35  | 128.32      | 120.46   |
| 1   | D     | 359 | GLU  | CA-C-O     | -7.34 | 110.61      | 119.49   |
| 1   | C     | 246 | PRO  | CB-CA-C    | 7.33  | 120.56      | 110.95   |
| 1   | B     | 69  | ALA  | CA-C-O     | 7.33  | 130.37      | 121.87   |
| 1   | B     | 11  | GLU  | CA-CB-CG   | 7.32  | 128.73      | 114.10   |
| 1   | B     | 94  | MET  | CA-C-O     | 7.32  | 125.09      | 119.46   |
| 1   | A     | 231 | ASP  | CA-C-O     | -7.30 | 112.54      | 120.36   |
| 1   | B     | 478 | GLN  | OE1-CD-NE2 | 7.28  | 129.88      | 122.60   |
| 1   | A     | 214 | ASN  | CB-CG-ND2  | 7.28  | 127.31      | 116.40   |
| 1   | C     | 377 | GLU  | CB-CG-CD   | 7.26  | 124.95      | 112.60   |
| 1   | D     | 25  | GLY  | N-CA-C     | -7.26 | 105.06      | 111.95   |
| 1   | B     | 38  | CYS  | CA-C-O     | 7.25  | 128.61      | 121.00   |
| 1   | D     | 223 | THR  | CA-C-O     | 7.25  | 128.43      | 120.82   |
| 1   | D     | 235 | MET  | N-CA-C     | -7.24 | 96.75       | 109.06   |
| 1   | B     | 294 | LYS  | CA-CB-CG   | 7.24  | 128.58      | 114.10   |
| 1   | B     | 492 | PRO  | CA-N-CD    | -7.24 | 101.86      | 112.00   |
| 1   | D     | 400 | THR  | CA-C-N     | 7.24  | 135.36      | 121.54   |
| 1   | D     | 400 | THR  | C-N-CA     | 7.24  | 135.36      | 121.54   |
| 1   | A     | 26  | VAL  | CA-C-O     | -7.24 | 114.77      | 121.72   |
| 1   | C     | 449 | LEU  | N-CA-C     | -7.24 | 102.39      | 112.45   |
| 1   | A     | 217 | ASP  | N-CA-C     | -7.23 | 103.40      | 111.28   |
| 1   | B     | 356 | ARG  | NE-CZ-NH1  | -7.23 | 114.27      | 121.50   |
| 1   | A     | 519 | SER  | N-CA-C     | 7.23  | 121.18      | 110.48   |
| 1   | B     | 534 | GLU  | O-C-N      | -7.22 | 112.82      | 122.43   |
| 1   | D     | 28  | ASN  | CA-C-O     | -7.21 | 113.56      | 121.28   |
| 1   | B     | 104 | PHE  | CA-C-O     | 7.21  | 129.10      | 120.81   |
| 1   | C     | 5   | LEU  | CA-CB-CG   | 7.19  | 141.46      | 116.30   |
| 1   | D     | 201 | ASN  | N-CA-C     | 7.19  | 121.63      | 112.86   |
| 1   | A     | 314 | GLY  | CA-C-O     | -7.18 | 114.36      | 122.33   |
| 1   | B     | 339 | GLY  | O-C-N      | -7.17 | 115.15      | 121.97   |
| 1   | C     | 131 | ILE  | CB-CA-C    | -7.17 | 103.48      | 111.23   |
| 1   | A     | 345 | LEU  | N-CA-C     | -7.17 | 102.87      | 111.69   |
| 1   | A     | 110 | ASP  | CA-CB-CG   | 7.16  | 119.76      | 112.60   |
| 1   | A     | 362 | GLN  | CA-C-O     | -7.16 | 113.14      | 121.16   |
| 1   | C     | 496 | LEU  | N-CA-C     | 7.16  | 120.19      | 108.52   |
| 1   | D     | 200 | ARG  | CA-C-N     | 7.15  | 134.28      | 123.05   |
| 1   | D     | 200 | ARG  | C-N-CA     | 7.15  | 134.28      | 123.05   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | C     | 492 | PRO  | N-CD-CG    | 7.14  | 113.91      | 103.20   |
| 1   | C     | 4   | VAL  | N-CA-CB    | -7.13 | 99.47       | 111.23   |
| 1   | A     | 65  | ILE  | CA-C-O     | -7.12 | 113.59      | 121.92   |
| 1   | A     | 533 | GLY  | O-C-N      | -7.12 | 115.74      | 122.86   |
| 1   | C     | 211 | LEU  | CA-C-N     | 7.12  | 129.69      | 120.44   |
| 1   | C     | 211 | LEU  | C-N-CA     | 7.12  | 129.69      | 120.44   |
| 1   | A     | 88  | HIS  | CA-C-O     | -7.12 | 111.99      | 121.46   |
| 1   | C     | 373 | VAL  | O-C-N      | -7.11 | 115.36      | 122.97   |
| 1   | A     | 35  | ASN  | OD1-CG-ND2 | 7.09  | 129.69      | 122.60   |
| 1   | C     | 165 | LYS  | CA-C-O     | -7.08 | 111.25      | 119.61   |
| 1   | A     | 56  | LYS  | CA-C-O     | 7.07  | 130.16      | 121.89   |
| 1   | D     | 410 | GLN  | CA-CB-CG   | 7.06  | 128.21      | 114.10   |
| 1   | D     | 65  | ILE  | CA-C-O     | -7.04 | 116.12      | 121.68   |
| 1   | A     | 3   | GLU  | N-CA-C     | 7.03  | 122.40      | 107.70   |
| 1   | A     | 330 | LYS  | CA-C-O     | -7.01 | 113.32      | 120.96   |
| 1   | A     | 374 | MET  | CA-C-O     | -6.99 | 113.33      | 121.16   |
| 1   | D     | 357 | ASP  | CA-CB-CG   | -6.99 | 105.61      | 112.60   |
| 1   | A     | 3   | GLU  | CA-C-O     | 6.99  | 130.24      | 120.52   |
| 1   | C     | 336 | ASN  | OD1-CG-ND2 | -6.99 | 115.61      | 122.60   |
| 1   | D     | 282 | GLU  | N-CA-C     | 6.98  | 120.81      | 110.48   |
| 1   | C     | 285 | SER  | CA-C-N     | 6.96  | 135.06      | 121.41   |
| 1   | C     | 285 | SER  | C-N-CA     | 6.96  | 135.06      | 121.41   |
| 1   | C     | 125 | THR  | CA-CB-OG1  | -6.96 | 99.16       | 109.60   |
| 1   | D     | 229 | MET  | CA-C-O     | -6.96 | 113.13      | 121.34   |
| 1   | B     | 11  | GLU  | CA-C-N     | 6.95  | 132.57      | 121.18   |
| 1   | B     | 11  | GLU  | C-N-CA     | 6.95  | 132.57      | 121.18   |
| 1   | C     | 69  | ALA  | N-CA-C     | 6.94  | 119.53      | 110.43   |
| 1   | D     | 68  | ILE  | CB-CA-C    | 6.94  | 122.67      | 111.29   |
| 1   | D     | 10  | GLY  | CA-C-N     | 6.91  | 134.75      | 121.54   |
| 1   | D     | 10  | GLY  | C-N-CA     | 6.91  | 134.75      | 121.54   |
| 1   | B     | 265 | VAL  | O-C-N      | -6.91 | 115.17      | 121.87   |
| 1   | B     | 262 | ASP  | CA-CB-CG   | 6.89  | 119.49      | 112.60   |
| 1   | C     | 336 | ASN  | CA-CB-CG   | 6.88  | 119.48      | 112.60   |
| 1   | C     | 550 | ILE  | CA-C-O     | -6.88 | 113.56      | 120.85   |
| 1   | A     | 282 | GLU  | CA-C-O     | -6.88 | 114.15      | 121.99   |
| 1   | B     | 453 | ILE  | CA-C-N     | 6.87  | 134.67      | 121.54   |
| 1   | B     | 453 | ILE  | C-N-CA     | 6.87  | 134.67      | 121.54   |
| 1   | C     | 68  | ILE  | CA-CB-CG2  | 6.87  | 122.17      | 110.50   |
| 1   | D     | 237 | GLY  | CA-C-O     | 6.87  | 127.21      | 119.59   |
| 1   | B     | 74  | HIS  | O-C-N      | 6.87  | 131.22      | 123.05   |
| 1   | B     | 157 | GLU  | O-C-N      | 6.85  | 128.86      | 121.60   |
| 1   | B     | 271 | ILE  | N-CA-CB    | -6.85 | 103.26      | 110.72   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | C     | 115 | ASP  | CA-C-O     | -6.85 | 113.29      | 120.55   |
| 1   | C     | 123 | LYS  | N-CA-C     | 6.83  | 119.56      | 111.71   |
| 1   | D     | 261 | TRP  | CA-C-O     | 6.83  | 127.82      | 120.24   |
| 1   | D     | 549 | ALA  | CA-C-O     | 6.83  | 127.82      | 120.24   |
| 1   | A     | 318 | ASN  | CA-CB-CG   | 6.82  | 119.42      | 112.60   |
| 1   | A     | 440 | VAL  | CB-CA-C    | -6.81 | 101.65      | 110.98   |
| 1   | D     | 563 | SER  | CA-CB-OG   | 6.81  | 124.72      | 111.10   |
| 1   | B     | 204 | ASP  | CA-C-O     | 6.81  | 124.36      | 119.32   |
| 1   | D     | 510 | VAL  | CA-C-O     | -6.81 | 113.02      | 120.71   |
| 1   | D     | 54  | LYS  | CA-C-O     | 6.80  | 127.27      | 120.88   |
| 1   | D     | 366 | THR  | N-CA-C     | 6.79  | 120.39      | 107.75   |
| 1   | B     | 267 | ARG  | CA-C-N     | -6.79 | 108.10      | 121.41   |
| 1   | B     | 267 | ARG  | C-N-CA     | -6.79 | 108.10      | 121.41   |
| 1   | C     | 46  | LYS  | CA-C-O     | -6.79 | 113.69      | 120.82   |
| 1   | D     | 231 | ASP  | CB-CA-C    | 6.78  | 120.92      | 109.80   |
| 1   | A     | 366 | THR  | CA-C-O     | 6.77  | 133.21      | 121.09   |
| 1   | D     | 516 | GLU  | N-CA-CB    | -6.77 | 99.45       | 109.95   |
| 1   | A     | 359 | GLU  | CA-CB-CG   | 6.76  | 127.63      | 114.10   |
| 1   | A     | 556 | TYR  | CA-C-O     | -6.76 | 113.72      | 120.82   |
| 1   | C     | 422 | ASP  | CA-CB-CG   | -6.74 | 105.86      | 112.60   |
| 1   | A     | 185 | GLU  | CB-CA-C    | 6.74  | 121.47      | 110.22   |
| 1   | C     | 220 | ASP  | CA-C-N     | 6.73  | 129.85      | 120.29   |
| 1   | C     | 220 | ASP  | C-N-CA     | 6.73  | 129.85      | 120.29   |
| 1   | C     | 426 | LYS  | CA-CB-CG   | 6.73  | 127.56      | 114.10   |
| 1   | C     | 240 | VAL  | CA-C-O     | 6.73  | 128.10      | 120.90   |
| 1   | B     | 467 | TYR  | CA-C-O     | 6.72  | 127.67      | 120.55   |
| 1   | C     | 563 | SER  | CA-C-N     | 6.72  | 130.90      | 120.82   |
| 1   | C     | 563 | SER  | C-N-CA     | 6.72  | 130.90      | 120.82   |
| 1   | A     | 552 | ASP  | CA-CB-CG   | 6.72  | 119.32      | 112.60   |
| 1   | B     | 77  | HIS  | CA-CB-CG   | -6.72 | 107.08      | 113.80   |
| 1   | B     | 269 | THR  | CA-C-O     | -6.71 | 113.27      | 120.92   |
| 1   | B     | 491 | ALA  | CA-C-N     | 6.71  | 128.23      | 119.84   |
| 1   | B     | 491 | ALA  | C-N-CA     | 6.71  | 128.23      | 119.84   |
| 1   | C     | 356 | ARG  | NH1-CZ-NH2 | 6.71  | 128.02      | 119.30   |
| 1   | B     | 308 | VAL  | CA-C-O     | -6.69 | 113.51      | 120.27   |
| 1   | C     | 111 | LYS  | CA-CB-CG   | 6.69  | 127.47      | 114.10   |
| 1   | C     | 37  | GLN  | OE1-CD-NE2 | 6.68  | 129.28      | 122.60   |
| 1   | D     | 210 | VAL  | N-CA-C     | -6.68 | 103.82      | 110.30   |
| 1   | B     | 359 | GLU  | CB-CG-CD   | 6.68  | 123.95      | 112.60   |
| 1   | A     | 534 | GLU  | O-C-N      | -6.67 | 113.72      | 122.59   |
| 1   | A     | 184 | ILE  | CA-C-N     | -6.67 | 113.30      | 122.30   |
| 1   | A     | 184 | ILE  | C-N-CA     | -6.67 | 113.30      | 122.30   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | C     | 104 | PHE  | CA-CB-CG | 6.67  | 120.47      | 113.80   |
| 1   | A     | 159 | ILE  | CA-C-N   | 6.67  | 128.18      | 119.84   |
| 1   | A     | 159 | ILE  | C-N-CA   | 6.67  | 128.18      | 119.84   |
| 1   | C     | 247 | THR  | N-CA-CB  | 6.67  | 119.88      | 109.94   |
| 1   | C     | 72  | SER  | CA-CB-OG | -6.66 | 97.78       | 111.10   |
| 1   | A     | 96  | PHE  | CA-C-N   | 6.66  | 127.10      | 120.31   |
| 1   | A     | 96  | PHE  | C-N-CA   | 6.66  | 127.10      | 120.31   |
| 1   | A     | 267 | ARG  | O-C-N    | -6.66 | 113.31      | 121.83   |
| 1   | C     | 491 | ALA  | CA-C-N   | 6.65  | 128.15      | 119.84   |
| 1   | C     | 491 | ALA  | C-N-CA   | 6.65  | 128.15      | 119.84   |
| 1   | A     | 233 | GLY  | O-C-N    | -6.64 | 118.83      | 123.95   |
| 1   | A     | 100 | TRP  | CA-C-O   | -6.64 | 112.88      | 120.58   |
| 1   | C     | 524 | LYS  | CB-CA-C  | 6.62  | 119.04      | 108.91   |
| 1   | B     | 218 | SER  | N-CA-C   | -6.62 | 103.99      | 111.07   |
| 1   | C     | 291 | VAL  | N-CA-C   | 6.62  | 119.64      | 108.86   |
| 1   | B     | 249 | GLY  | N-CA-C   | -6.61 | 97.51       | 113.18   |
| 1   | B     | 309 | VAL  | CA-C-O   | -6.60 | 113.51      | 120.57   |
| 1   | D     | 262 | ASP  | N-CA-C   | -6.60 | 104.01      | 111.14   |
| 1   | D     | 525 | PRO  | CA-C-O   | -6.60 | 114.13      | 121.32   |
| 1   | D     | 23  | LYS  | N-CA-C   | -6.59 | 103.72      | 111.03   |
| 1   | A     | 400 | THR  | CA-C-N   | 6.58  | 130.32      | 120.31   |
| 1   | A     | 400 | THR  | C-N-CA   | 6.58  | 130.32      | 120.31   |
| 1   | C     | 252 | VAL  | CA-C-O   | -6.58 | 114.19      | 121.17   |
| 1   | D     | 135 | GLY  | CA-C-O   | -6.58 | 113.68      | 120.66   |
| 1   | C     | 55  | ASP  | N-CA-C   | 6.58  | 119.29      | 111.33   |
| 1   | D     | 426 | LYS  | CA-CB-CG | 6.58  | 127.25      | 114.10   |
| 1   | D     | 250 | ALA  | CA-C-O   | 6.57  | 129.91      | 120.51   |
| 1   | D     | 375 | ILE  | CA-C-O   | -6.57 | 114.20      | 121.23   |
| 1   | B     | 208 | VAL  | N-CA-C   | -6.57 | 103.84      | 111.00   |
| 1   | A     | 567 | PHE  | CA-C-O   | -6.57 | 113.85      | 121.07   |
| 1   | B     | 76  | GLY  | CA-C-N   | 6.57  | 133.30      | 122.73   |
| 1   | B     | 76  | GLY  | C-N-CA   | 6.57  | 133.30      | 122.73   |
| 1   | D     | 392 | ASN  | CA-CB-CG | 6.56  | 119.16      | 112.60   |
| 1   | A     | 31  | LEU  | N-CA-CB  | -6.56 | 102.23      | 112.13   |
| 1   | D     | 496 | LEU  | N-CA-CB  | -6.55 | 100.89      | 110.84   |
| 1   | C     | 31  | LEU  | N-CA-CB  | -6.54 | 99.43       | 110.49   |
| 1   | B     | 189 | GLN  | CA-C-O   | -6.54 | 113.96      | 120.70   |
| 1   | C     | 341 | THR  | CA-C-O   | -6.54 | 111.54      | 119.32   |
| 1   | C     | 276 | ARG  | CD-NE-CZ | -6.54 | 115.25      | 124.40   |
| 1   | D     | 543 | ASN  | CA-CB-CG | -6.53 | 106.07      | 112.60   |
| 1   | D     | 281 | LEU  | O-C-N    | -6.53 | 115.55      | 123.19   |
| 1   | C     | 161 | GLY  | N-CA-C   | 6.53  | 122.85      | 115.08   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 37  | GLN  | OE1-CD-NE2 | 6.53  | 129.12      | 122.60   |
| 1   | B     | 209 | LYS  | N-CA-CB    | 6.53  | 119.47      | 110.01   |
| 1   | B     | 570 | ASP  | N-CA-CB    | 6.53  | 121.59      | 110.50   |
| 1   | B     | 421 | ASP  | N-CA-CB    | -6.52 | 100.98      | 110.70   |
| 1   | C     | 3   | GLU  | O-C-N      | -6.52 | 112.57      | 123.00   |
| 1   | C     | 401 | ARG  | NE-CZ-NH2  | -6.52 | 113.33      | 119.20   |
| 1   | D     | 241 | ASN  | CB-CG-ND2  | -6.52 | 106.62      | 116.40   |
| 1   | B     | 492 | PRO  | N-CD-CG    | 6.52  | 112.98      | 103.20   |
| 1   | D     | 448 | GLU  | CA-CB-CG   | 6.51  | 127.13      | 114.10   |
| 1   | C     | 47  | GLU  | O-C-N      | -6.50 | 115.33      | 122.09   |
| 1   | B     | 265 | VAL  | CA-C-N     | 6.50  | 128.99      | 120.28   |
| 1   | B     | 265 | VAL  | C-N-CA     | 6.50  | 128.99      | 120.28   |
| 1   | A     | 460 | LEU  | CA-C-O     | 6.50  | 127.64      | 120.82   |
| 1   | B     | 24  | GLY  | CA-C-O     | -6.49 | 115.88      | 122.56   |
| 1   | B     | 426 | LYS  | CG-CD-CE   | 6.49  | 126.23      | 111.30   |
| 1   | D     | 491 | ALA  | CA-C-N     | 6.49  | 127.95      | 119.84   |
| 1   | D     | 491 | ALA  | C-N-CA     | 6.49  | 127.95      | 119.84   |
| 1   | D     | 248 | GLY  | CA-C-O     | 6.49  | 126.16      | 121.04   |
| 1   | B     | 539 | VAL  | CA-C-O     | -6.47 | 113.78      | 120.71   |
| 1   | D     | 197 | LYS  | O-C-N      | 6.47  | 129.52      | 122.15   |
| 1   | A     | 154 | LEU  | O-C-N      | -6.46 | 115.00      | 123.21   |
| 1   | D     | 75  | LYS  | CA-C-O     | -6.46 | 113.66      | 121.28   |
| 1   | D     | 157 | GLU  | CA-C-O     | -6.45 | 113.93      | 120.96   |
| 1   | C     | 103 | LYS  | N-CA-C     | -6.44 | 100.95      | 110.48   |
| 1   | B     | 93  | ASP  | CA-C-O     | 6.43  | 128.78      | 121.58   |
| 1   | D     | 63  | HIS  | CG-CD2-NE2 | 6.43  | 113.63      | 107.20   |
| 1   | A     | 282 | GLU  | N-CA-CB    | -6.43 | 101.58      | 110.38   |
| 1   | A     | 366 | THR  | O-C-N      | -6.42 | 114.47      | 122.82   |
| 1   | A     | 422 | ASP  | CA-C-O     | -6.42 | 112.21      | 119.79   |
| 1   | B     | 328 | LYS  | N-CA-C     | -6.42 | 104.20      | 111.07   |
| 1   | A     | 267 | ARG  | NE-CZ-NH2  | 6.42  | 124.97      | 119.20   |
| 1   | B     | 401 | ARG  | NE-CZ-NH1  | 6.42  | 127.92      | 121.50   |
| 1   | C     | 350 | GLN  | CB-CG-CD   | 6.42  | 123.51      | 112.60   |
| 1   | C     | 98  | GLY  | N-CA-C     | -6.41 | 105.10      | 112.79   |
| 1   | B     | 401 | ARG  | CD-NE-CZ   | 6.41  | 133.37      | 124.40   |
| 1   | A     | 489 | VAL  | N-CA-CB    | -6.41 | 100.66      | 111.23   |
| 1   | B     | 68  | ILE  | CB-CG1-CD1 | -6.39 | 100.39      | 113.80   |
| 1   | A     | 64  | LEU  | CA-C-O     | -6.38 | 114.60      | 121.56   |
| 1   | D     | 36  | GLY  | O-C-N      | -6.37 | 114.42      | 122.70   |
| 1   | D     | 289 | THR  | CA-C-O     | 6.37  | 126.99      | 119.67   |
| 1   | A     | 218 | SER  | CA-CB-OG   | -6.36 | 98.39       | 111.10   |
| 1   | D     | 558 | ARG  | CG-CD-NE   | 6.35  | 125.97      | 112.00   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | C     | 551 | SER  | CB-CA-C    | -6.35 | 100.91      | 110.88   |
| 1   | A     | 212 | ALA  | CA-C-N     | 6.34  | 129.41      | 120.28   |
| 1   | A     | 212 | ALA  | C-N-CA     | 6.34  | 129.41      | 120.28   |
| 1   | A     | 259 | VAL  | N-CA-CB    | 6.34  | 119.16      | 110.54   |
| 1   | D     | 356 | ARG  | CA-C-O     | -6.34 | 114.48      | 121.33   |
| 1   | B     | 491 | ALA  | N-CA-C     | 6.34  | 118.60      | 109.48   |
| 1   | C     | 252 | VAL  | CB-CA-C    | -6.34 | 103.86      | 111.97   |
| 1   | C     | 133 | SER  | O-C-N      | -6.33 | 114.10      | 122.20   |
| 1   | C     | 223 | THR  | O-C-N      | -6.33 | 115.41      | 122.12   |
| 1   | A     | 548 | ASN  | OD1-CG-ND2 | -6.32 | 116.28      | 122.60   |
| 1   | C     | 202 | ILE  | N-CA-C     | -6.32 | 106.54      | 113.43   |
| 1   | B     | 219 | ILE  | O-C-N      | -6.32 | 115.70      | 121.89   |
| 1   | C     | 89  | SER  | CA-CB-OG   | -6.32 | 98.47       | 111.10   |
| 1   | A     | 254 | ALA  | O-C-N      | 6.31  | 128.81      | 122.12   |
| 1   | D     | 159 | ILE  | CA-C-O     | 6.31  | 128.40      | 119.95   |
| 1   | A     | 231 | ASP  | CA-CB-CG   | -6.31 | 106.29      | 112.60   |
| 1   | D     | 282 | GLU  | N-CA-CB    | -6.30 | 100.71      | 110.29   |
| 1   | C     | 234 | ARG  | CA-C-O     | 6.30  | 127.39      | 120.71   |
| 1   | C     | 17  | SER  | CA-C-N     | 6.30  | 132.19      | 122.42   |
| 1   | C     | 17  | SER  | C-N-CA     | 6.30  | 132.19      | 122.42   |
| 1   | A     | 4   | VAL  | N-CA-CB    | 6.30  | 121.62      | 111.23   |
| 1   | A     | 41  | CYS  | N-CA-C     | 6.29  | 120.16      | 112.23   |
| 1   | B     | 163 | ASN  | N-CA-C     | -6.29 | 105.08      | 112.89   |
| 1   | B     | 566 | LYS  | N-CA-CB    | 6.29  | 119.37      | 110.12   |
| 1   | D     | 270 | ASP  | CA-C-O     | 6.28  | 127.29      | 120.58   |
| 1   | D     | 372 | GLY  | N-CA-C     | -6.28 | 106.58      | 115.43   |
| 1   | A     | 118 | ILE  | CA-C-O     | 6.27  | 127.03      | 120.25   |
| 1   | B     | 367 | TYR  | CA-C-O     | 6.27  | 127.13      | 120.36   |
| 1   | C     | 241 | ASN  | OD1-CG-ND2 | 6.27  | 128.87      | 122.60   |
| 1   | C     | 197 | LYS  | N-CA-CB    | 6.27  | 119.16      | 110.07   |
| 1   | C     | 258 | GLN  | CA-C-N     | -6.26 | 112.67      | 120.56   |
| 1   | C     | 258 | GLN  | C-N-CA     | -6.26 | 112.67      | 120.56   |
| 1   | D     | 61  | LYS  | N-CA-CB    | 6.26  | 120.66      | 110.90   |
| 1   | C     | 17  | SER  | O-C-N      | -6.25 | 114.92      | 122.11   |
| 1   | D     | 563 | SER  | N-CA-C     | -6.25 | 105.47      | 113.23   |
| 1   | A     | 212 | ALA  | O-C-N      | -6.25 | 115.34      | 122.09   |
| 1   | A     | 393 | ARG  | CA-C-O     | -6.25 | 114.16      | 121.16   |
| 1   | B     | 22  | ASP  | CA-CB-CG   | 6.25  | 118.85      | 112.60   |
| 1   | D     | 175 | GLU  | N-CA-C     | 6.25  | 120.17      | 111.74   |
| 1   | D     | 474 | GLY  | N-CA-C     | -6.24 | 106.80      | 114.92   |
| 1   | C     | 536 | THR  | CA-CB-OG1  | -6.24 | 100.24      | 109.60   |
| 1   | C     | 567 | PHE  | O-C-N      | -6.23 | 114.08      | 122.43   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | D     | 260 | LEU  | O-C-N      | -6.23 | 114.29      | 122.39   |
| 1   | D     | 95  | PRO  | CA-C-N     | 6.22  | 130.97      | 122.07   |
| 1   | D     | 95  | PRO  | C-N-CA     | 6.22  | 130.97      | 122.07   |
| 1   | B     | 232 | VAL  | CA-C-O     | -6.22 | 113.92      | 120.39   |
| 1   | B     | 126 | THR  | CA-C-O     | -6.22 | 113.98      | 121.32   |
| 1   | A     | 536 | THR  | CA-CB-OG1  | -6.22 | 100.28      | 109.60   |
| 1   | C     | 19  | HIS  | CA-C-O     | -6.21 | 114.48      | 121.81   |
| 1   | C     | 150 | LYS  | CB-CA-C    | 6.20  | 120.45      | 109.72   |
| 1   | A     | 341 | THR  | CA-C-O     | -6.20 | 111.94      | 119.32   |
| 1   | C     | 217 | ASP  | CA-C-O     | 6.20  | 127.10      | 119.97   |
| 1   | A     | 149 | ALA  | CA-C-O     | 6.20  | 128.60      | 121.47   |
| 1   | A     | 169 | GLY  | N-CA-C     | 6.20  | 120.39      | 112.83   |
| 1   | A     | 340 | ALA  | CA-C-O     | -6.20 | 114.90      | 122.64   |
| 1   | C     | 54  | LYS  | CA-C-N     | 6.19  | 128.86      | 120.38   |
| 1   | C     | 54  | LYS  | C-N-CA     | 6.19  | 128.86      | 120.38   |
| 1   | A     | 426 | LYS  | O-C-N      | -6.19 | 114.20      | 122.43   |
| 1   | B     | 481 | ARG  | CA-C-N     | 6.19  | 125.75      | 119.19   |
| 1   | B     | 481 | ARG  | C-N-CA     | 6.19  | 125.75      | 119.19   |
| 1   | B     | 315 | PHE  | CA-C-N     | 6.19  | 129.41      | 120.38   |
| 1   | B     | 315 | PHE  | C-N-CA     | 6.19  | 129.41      | 120.38   |
| 1   | A     | 487 | GLU  | O-C-N      | -6.19 | 114.29      | 122.33   |
| 1   | C     | 352 | GLY  | N-CA-C     | 6.18  | 123.85      | 115.32   |
| 1   | C     | 364 | HIS  | CA-CB-CG   | -6.18 | 107.62      | 113.80   |
| 1   | A     | 356 | ARG  | NE-CZ-NH2  | 6.18  | 124.76      | 119.20   |
| 1   | D     | 57  | VAL  | CB-CA-C    | -6.18 | 103.85      | 111.08   |
| 1   | A     | 107 | VAL  | CA-C-N     | 6.17  | 131.93      | 121.14   |
| 1   | A     | 107 | VAL  | C-N-CA     | 6.17  | 131.93      | 121.14   |
| 1   | B     | 258 | GLN  | CA-C-N     | -6.16 | 111.68      | 120.42   |
| 1   | B     | 258 | GLN  | C-N-CA     | -6.16 | 111.68      | 120.42   |
| 1   | A     | 527 | THR  | N-CA-CB    | 6.16  | 119.11      | 109.69   |
| 1   | B     | 134 | GLY  | O-C-N      | -6.16 | 117.52      | 122.81   |
| 1   | C     | 539 | VAL  | CA-C-O     | -6.16 | 114.22      | 121.05   |
| 1   | C     | 375 | ILE  | N-CA-CB    | 6.14  | 117.23      | 110.53   |
| 1   | B     | 401 | ARG  | CA-CB-CG   | 6.14  | 126.38      | 114.10   |
| 1   | B     | 215 | SER  | O-C-N      | -6.14 | 114.42      | 122.59   |
| 1   | A     | 520 | GLU  | N-CA-C     | -6.13 | 104.15      | 111.69   |
| 1   | A     | 133 | SER  | N-CA-C     | 6.12  | 119.49      | 112.57   |
| 1   | C     | 200 | ARG  | O-C-N      | -6.12 | 114.21      | 122.41   |
| 1   | D     | 241 | ASN  | OD1-CG-ND2 | 6.12  | 128.72      | 122.60   |
| 1   | B     | 537 | GLY  | O-C-N      | -6.11 | 119.24      | 123.95   |
| 1   | C     | 401 | ARG  | NE-CZ-NH1  | 6.11  | 127.61      | 121.50   |
| 1   | C     | 235 | MET  | N-CA-C     | -6.10 | 99.86       | 109.50   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 252 | VAL  | CB-CA-C    | -6.10 | 101.29      | 111.29   |
| 1   | D     | 239 | SER  | CA-C-O     | 6.10  | 125.23      | 118.52   |
| 1   | D     | 429 | LYS  | CA-C-N     | 6.10  | 128.77      | 120.54   |
| 1   | D     | 429 | LYS  | C-N-CA     | 6.10  | 128.77      | 120.54   |
| 1   | C     | 512 | ASP  | N-CA-C     | -6.10 | 100.91      | 109.69   |
| 1   | A     | 214 | ASN  | OD1-CG-ND2 | -6.09 | 116.51      | 122.60   |
| 1   | D     | 324 | LYS  | O-C-N      | -6.09 | 115.75      | 122.09   |
| 1   | B     | 262 | ASP  | N-CA-C     | -6.09 | 104.64      | 111.28   |
| 1   | B     | 283 | ASP  | N-CA-CB    | -6.09 | 105.92      | 111.59   |
| 1   | D     | 251 | GLY  | N-CA-C     | 6.09  | 127.61      | 113.18   |
| 1   | A     | 336 | ASN  | N-CA-C     | 6.09  | 119.53      | 110.52   |
| 1   | B     | 40  | SER  | CA-C-O     | -6.09 | 114.43      | 120.82   |
| 1   | D     | 217 | ASP  | O-C-N      | 6.08  | 128.57      | 122.12   |
| 1   | B     | 79  | LYS  | CA-C-O     | 6.08  | 128.00      | 121.55   |
| 1   | A     | 107 | VAL  | CB-CA-C    | -6.08 | 103.17      | 112.05   |
| 1   | A     | 508 | GLY  | CA-C-N     | 6.07  | 129.75      | 120.82   |
| 1   | A     | 508 | GLY  | C-N-CA     | 6.07  | 129.75      | 120.82   |
| 1   | C     | 349 | LEU  | CB-CA-C    | -6.07 | 100.36      | 110.68   |
| 1   | A     | 143 | SER  | O-C-N      | -6.07 | 114.52      | 122.59   |
| 1   | D     | 236 | GLY  | N-CA-C     | -6.07 | 105.65      | 112.33   |
| 1   | A     | 453 | ILE  | CB-CA-C    | -6.07 | 104.09      | 112.04   |
| 1   | B     | 10  | GLY  | N-CA-C     | -6.06 | 105.25      | 113.37   |
| 1   | D     | 430 | ALA  | CA-C-O     | 6.06  | 127.38      | 120.90   |
| 1   | A     | 563 | SER  | O-C-N      | -6.05 | 115.55      | 122.09   |
| 1   | D     | 185 | GLU  | O-C-N      | -6.05 | 115.57      | 122.84   |
| 1   | A     | 203 | ASN  | CA-CB-CG   | 6.05  | 118.65      | 112.60   |
| 1   | B     | 263 | ASN  | CA-CB-CG   | -6.05 | 106.55      | 112.60   |
| 1   | C     | 567 | PHE  | CA-C-O     | 6.05  | 126.82      | 119.38   |
| 1   | B     | 306 | ASP  | CA-CB-CG   | -6.04 | 106.56      | 112.60   |
| 1   | A     | 213 | ASN  | N-CA-C     | 6.04  | 118.66      | 111.71   |
| 1   | A     | 503 | HIS  | N-CA-C     | 6.04  | 123.66      | 110.80   |
| 1   | B     | 372 | GLY  | CA-C-O     | 6.03  | 125.72      | 119.02   |
| 1   | A     | 490 | VAL  | CA-C-O     | 6.03  | 128.11      | 120.75   |
| 1   | B     | 568 | ALA  | CA-C-O     | -6.03 | 113.45      | 120.20   |
| 1   | C     | 194 | ASP  | CA-CB-CG   | 6.03  | 118.63      | 112.60   |
| 1   | A     | 219 | ILE  | O-C-N      | -6.03 | 114.06      | 121.90   |
| 1   | D     | 357 | ASP  | N-CA-C     | 6.03  | 123.64      | 110.80   |
| 1   | C     | 510 | VAL  | CA-C-O     | 6.03  | 127.52      | 120.71   |
| 1   | D     | 63  | HIS  | CA-CB-CG   | 6.03  | 119.83      | 113.80   |
| 1   | D     | 152 | ILE  | N-CA-CB    | 6.02  | 119.72      | 111.41   |
| 1   | A     | 161 | GLY  | N-CA-C     | 6.01  | 123.96      | 115.30   |
| 1   | A     | 156 | LYS  | CA-C-O     | 6.01  | 126.31      | 119.27   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | D     | 407 | ALA  | CA-C-O     | -6.01 | 114.47      | 120.90   |
| 1   | B     | 560 | ALA  | CA-C-O     | 6.01  | 128.06      | 121.02   |
| 1   | B     | 35  | ASN  | CA-CB-CG   | 6.01  | 118.61      | 112.60   |
| 1   | D     | 535 | VAL  | CA-C-O     | 6.00  | 127.30      | 120.03   |
| 1   | D     | 185 | GLU  | N-CA-CB    | -6.00 | 99.40       | 110.56   |
| 1   | C     | 474 | GLY  | N-CA-C     | -5.99 | 105.25      | 115.08   |
| 1   | C     | 39  | VAL  | CB-CA-C    | 5.99  | 120.22      | 112.14   |
| 1   | A     | 275 | SER  | CA-C-N     | -5.98 | 114.74      | 123.00   |
| 1   | A     | 275 | SER  | C-N-CA     | -5.98 | 114.74      | 123.00   |
| 1   | B     | 520 | GLU  | CA-CB-CG   | 5.98  | 126.06      | 114.10   |
| 1   | A     | 440 | VAL  | CA-C-O     | -5.98 | 114.08      | 120.59   |
| 1   | D     | 252 | VAL  | N-CA-CB    | 5.98  | 121.09      | 111.23   |
| 1   | A     | 480 | GLU  | N-CA-CB    | -5.97 | 101.81      | 110.47   |
| 1   | A     | 563 | SER  | CB-CA-C    | 5.97  | 120.33      | 110.90   |
| 1   | B     | 4   | VAL  | N-CA-C     | -5.97 | 100.47      | 108.35   |
| 1   | B     | 12  | MET  | CB-CA-C    | -5.97 | 99.73       | 110.35   |
| 1   | A     | 270 | ASP  | CA-CB-CG   | 5.96  | 118.56      | 112.60   |
| 1   | B     | 468 | ASN  | CB-CG-OD1  | -5.96 | 108.88      | 120.80   |
| 1   | C     | 216 | SER  | CA-C-O     | -5.96 | 114.23      | 120.55   |
| 1   | B     | 172 | ASN  | OD1-CG-ND2 | 5.96  | 128.56      | 122.60   |
| 1   | C     | 279 | ARG  | CA-C-N     | -5.96 | 111.64      | 122.43   |
| 1   | C     | 279 | ARG  | C-N-CA     | -5.96 | 111.64      | 122.43   |
| 1   | C     | 88  | HIS  | CA-C-O     | -5.96 | 114.28      | 120.89   |
| 1   | C     | 439 | ILE  | CB-CA-C    | -5.96 | 103.82      | 111.20   |
| 1   | D     | 361 | ILE  | O-C-N      | -5.95 | 116.83      | 123.26   |
| 1   | A     | 512 | ASP  | CA-C-O     | -5.95 | 114.59      | 121.49   |
| 1   | C     | 550 | ILE  | CA-C-N     | 5.95  | 128.17      | 120.44   |
| 1   | C     | 550 | ILE  | C-N-CA     | 5.95  | 128.17      | 120.44   |
| 1   | A     | 163 | ASN  | O-C-N      | -5.94 | 114.96      | 122.27   |
| 1   | A     | 312 | ALA  | N-CA-C     | 5.94  | 120.38      | 113.20   |
| 1   | A     | 115 | ASP  | CA-CB-CG   | 5.93  | 118.53      | 112.60   |
| 1   | A     | 388 | ASN  | CB-CG-ND2  | 5.93  | 125.30      | 116.40   |
| 1   | B     | 307 | ALA  | O-C-N      | -5.92 | 115.49      | 123.19   |
| 1   | B     | 516 | GLU  | CA-C-O     | -5.91 | 113.95      | 120.69   |
| 1   | A     | 547 | GLY  | N-CA-C     | -5.91 | 107.26      | 113.58   |
| 1   | B     | 215 | SER  | CA-C-O     | 5.90  | 128.95      | 120.51   |
| 1   | C     | 98  | GLY  | CA-C-O     | -5.90 | 115.67      | 121.93   |
| 1   | B     | 12  | MET  | N-CA-C     | 5.90  | 122.51      | 113.19   |
| 1   | C     | 83  | TYR  | CA-C-N     | 5.90  | 128.99      | 120.38   |
| 1   | C     | 83  | TYR  | C-N-CA     | 5.90  | 128.99      | 120.38   |
| 1   | B     | 315 | PHE  | CA-CB-CG   | 5.90  | 119.70      | 113.80   |
| 1   | D     | 283 | ASP  | O-C-N      | -5.90 | 114.74      | 122.59   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 519 | SER  | O-C-N      | -5.90 | 116.30      | 122.96   |
| 1   | D     | 468 | ASN  | OD1-CG-ND2 | -5.90 | 116.70      | 122.60   |
| 1   | A     | 350 | GLN  | CB-CG-CD   | 5.89  | 122.62      | 112.60   |
| 1   | C     | 222 | LEU  | CA-C-O     | 5.89  | 126.67      | 120.42   |
| 1   | D     | 157 | GLU  | N-CA-CB    | -5.89 | 102.90      | 109.74   |
| 1   | C     | 273 | LEU  | O-C-N      | -5.88 | 114.41      | 122.23   |
| 1   | B     | 476 | ASP  | CA-CB-CG   | 5.88  | 118.48      | 112.60   |
| 1   | D     | 159 | ILE  | O-C-N      | -5.88 | 114.40      | 121.10   |
| 1   | C     | 377 | GLU  | CA-C-O     | 5.88  | 126.72      | 119.79   |
| 1   | C     | 326 | ASP  | CA-CB-CG   | 5.87  | 118.47      | 112.60   |
| 1   | C     | 80  | SER  | CA-C-O     | -5.87 | 114.89      | 121.81   |
| 1   | B     | 536 | THR  | CA-CB-OG1  | -5.86 | 100.80      | 109.60   |
| 1   | A     | 20  | VAL  | CB-CA-C    | -5.86 | 104.36      | 112.04   |
| 1   | C     | 16  | ASP  | CA-C-N     | 5.86  | 129.61      | 120.82   |
| 1   | C     | 16  | ASP  | C-N-CA     | 5.86  | 129.61      | 120.82   |
| 1   | C     | 505 | THR  | O-C-N      | -5.86 | 114.20      | 122.87   |
| 1   | A     | 331 | GLY  | N-CA-C     | 5.86  | 123.44      | 115.30   |
| 1   | A     | 123 | LYS  | CA-C-O     | -5.85 | 112.42      | 119.27   |
| 1   | B     | 356 | ARG  | CA-C-N     | 5.85  | 132.72      | 121.54   |
| 1   | B     | 356 | ARG  | C-N-CA     | 5.85  | 132.72      | 121.54   |
| 1   | C     | 328 | LYS  | O-C-N      | -5.85 | 114.81      | 122.59   |
| 1   | A     | 245 | ARG  | NE-CZ-NH2  | -5.85 | 113.94      | 119.20   |
| 1   | C     | 282 | GLU  | N-CA-C     | 5.85  | 118.77      | 109.65   |
| 1   | B     | 513 | THR  | CA-CB-OG1  | -5.85 | 100.83      | 109.60   |
| 1   | B     | 161 | GLY  | CA-C-N     | 5.84  | 131.47      | 120.07   |
| 1   | B     | 161 | GLY  | C-N-CA     | 5.84  | 131.47      | 120.07   |
| 1   | D     | 424 | ILE  | N-CA-C     | 5.84  | 116.03      | 110.42   |
| 1   | A     | 327 | PRO  | CA-C-N     | 5.84  | 128.38      | 120.38   |
| 1   | A     | 327 | PRO  | C-N-CA     | 5.84  | 128.38      | 120.38   |
| 1   | A     | 28  | ASN  | CA-C-O     | 5.84  | 127.60      | 120.60   |
| 1   | A     | 423 | SER  | CA-C-O     | -5.84 | 114.69      | 120.70   |
| 1   | D     | 242 | ARG  | CA-C-N     | -5.84 | 114.66      | 122.42   |
| 1   | D     | 242 | ARG  | C-N-CA     | -5.84 | 114.66      | 122.42   |
| 1   | A     | 517 | VAL  | N-CA-CB    | 5.83  | 117.65      | 111.00   |
| 1   | A     | 273 | LEU  | CA-C-N     | 5.83  | 130.66      | 122.08   |
| 1   | A     | 273 | LEU  | C-N-CA     | 5.83  | 130.66      | 122.08   |
| 1   | B     | 548 | ASN  | CA-C-O     | -5.83 | 112.77      | 119.60   |
| 1   | B     | 403 | LYS  | CA-CB-CG   | 5.83  | 125.76      | 114.10   |
| 1   | B     | 521 | LYS  | CA-C-O     | -5.83 | 113.51      | 120.10   |
| 1   | C     | 67  | GLU  | CA-C-O     | -5.83 | 114.04      | 120.69   |
| 1   | C     | 152 | ILE  | CB-CG1-CD1 | 5.83  | 126.04      | 113.80   |
| 1   | A     | 276 | ARG  | CA-CB-CG   | 5.83  | 125.75      | 114.10   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | C     | 108 | ASP  | CA-C-N   | 5.82  | 129.03      | 120.82   |
| 1   | C     | 108 | ASP  | C-N-CA   | 5.82  | 129.03      | 120.82   |
| 1   | D     | 354 | ALA  | CA-C-O   | 5.82  | 127.26      | 120.80   |
| 1   | A     | 244 | HIS  | CA-CB-CG | -5.81 | 107.99      | 113.80   |
| 1   | D     | 321 | ARG  | CD-NE-CZ | -5.81 | 116.26      | 124.40   |
| 1   | B     | 224 | SER  | O-C-N    | -5.81 | 114.86      | 122.59   |
| 1   | C     | 525 | PRO  | CB-CA-C  | -5.81 | 104.33      | 111.64   |
| 1   | A     | 285 | SER  | N-CA-CB  | 5.80  | 117.61      | 110.53   |
| 1   | B     | 181 | LYS  | CA-C-O   | -5.80 | 112.94      | 119.79   |
| 1   | C     | 539 | VAL  | CB-CA-C  | -5.80 | 104.42      | 112.02   |
| 1   | B     | 16  | ASP  | N-CA-CB  | 5.80  | 120.18      | 110.32   |
| 1   | D     | 327 | PRO  | CA-C-O   | -5.80 | 110.05      | 120.60   |
| 1   | A     | 242 | ARG  | CA-CB-CG | 5.79  | 125.69      | 114.10   |
| 1   | D     | 202 | ILE  | CA-C-O   | 5.79  | 126.20      | 119.89   |
| 1   | A     | 415 | SER  | CA-C-O   | -5.79 | 114.74      | 121.10   |
| 1   | C     | 553 | ILE  | CA-C-O   | -5.79 | 115.25      | 121.27   |
| 1   | D     | 35  | ASN  | CA-C-O   | -5.79 | 114.36      | 120.55   |
| 1   | D     | 3   | GLU  | N-CA-C   | 5.78  | 118.33      | 110.06   |
| 1   | B     | 470 | PHE  | N-CA-CB  | 5.78  | 118.61      | 110.12   |
| 1   | D     | 212 | ALA  | CA-C-O   | 5.78  | 126.65      | 120.70   |
| 1   | A     | 28  | ASN  | CA-CB-CG | 5.77  | 118.37      | 112.60   |
| 1   | A     | 455 | VAL  | N-CA-CB  | 5.77  | 119.29      | 111.21   |
| 1   | B     | 150 | LYS  | O-C-N    | -5.77 | 116.50      | 123.13   |
| 1   | B     | 197 | LYS  | CA-C-O   | -5.76 | 114.77      | 120.82   |
| 1   | D     | 214 | ASN  | CA-CB-CG | 5.76  | 118.36      | 112.60   |
| 1   | D     | 411 | GLN  | CA-CB-CG | 5.76  | 125.62      | 114.10   |
| 1   | B     | 566 | LYS  | N-CA-C   | -5.75 | 105.01      | 111.28   |
| 1   | B     | 246 | PRO  | O-C-N    | -5.75 | 116.20      | 123.10   |
| 1   | A     | 165 | LYS  | CA-C-O   | -5.75 | 111.86      | 119.10   |
| 1   | A     | 345 | LEU  | CB-CA-C  | 5.75  | 121.21      | 110.70   |
| 1   | A     | 194 | ASP  | CA-CB-CG | 5.74  | 118.34      | 112.60   |
| 1   | D     | 283 | ASP  | CA-C-N   | 5.74  | 132.51      | 121.54   |
| 1   | D     | 283 | ASP  | C-N-CA   | 5.74  | 132.51      | 121.54   |
| 1   | D     | 543 | ASN  | N-CA-C   | 5.74  | 117.74      | 108.32   |
| 1   | A     | 241 | ASN  | CA-CB-CG | -5.74 | 106.86      | 112.60   |
| 1   | D     | 106 | PRO  | CA-C-O   | -5.74 | 114.77      | 121.95   |
| 1   | A     | 291 | VAL  | N-CA-CB  | -5.74 | 101.76      | 111.23   |
| 1   | B     | 42  | HIS  | CA-CB-CG | -5.74 | 108.06      | 113.80   |
| 1   | A     | 355 | THR  | O-C-N    | -5.73 | 115.70      | 123.15   |
| 1   | C     | 151 | VAL  | N-CA-C   | 5.73  | 116.73      | 108.48   |
| 1   | A     | 181 | LYS  | CA-C-O   | -5.72 | 114.45      | 120.63   |
| 1   | B     | 79  | LYS  | O-C-N    | -5.72 | 115.77      | 122.81   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | D     | 480 | GLU  | N-CA-C      | 5.72  | 119.96      | 113.15   |
| 1   | A     | 536 | THR  | CA-CB-CG2   | 5.72  | 120.22      | 110.50   |
| 1   | A     | 70  | CYS  | CA-C-O      | 5.72  | 127.00      | 121.00   |
| 1   | D     | 423 | SER  | CA-C-N      | 5.72  | 127.76      | 120.56   |
| 1   | D     | 423 | SER  | C-N-CA      | 5.72  | 127.76      | 120.56   |
| 1   | A     | 490 | VAL  | O-C-N       | -5.72 | 115.68      | 122.77   |
| 1   | D     | 104 | PHE  | N-CA-CB     | 5.72  | 118.81      | 109.95   |
| 1   | D     | 483 | ASP  | CA-CB-CG    | 5.72  | 118.32      | 112.60   |
| 1   | C     | 33  | HIS  | CA-CB-CG    | -5.71 | 108.09      | 113.80   |
| 1   | D     | 38  | CYS  | N-CA-C      | -5.71 | 104.97      | 111.14   |
| 1   | D     | 210 | VAL  | CB-CA-C     | 5.71  | 118.95      | 111.81   |
| 1   | A     | 504 | HIS  | ND1-CE1-NE2 | -5.71 | 102.69      | 108.40   |
| 1   | B     | 396 | ASN  | CA-CB-CG    | 5.71  | 118.31      | 112.60   |
| 1   | D     | 328 | LYS  | O-C-N       | -5.71 | 115.29      | 122.20   |
| 1   | B     | 192 | ILE  | CB-CA-C     | -5.70 | 104.68      | 111.81   |
| 1   | C     | 568 | ALA  | CA-C-O      | -5.70 | 112.24      | 119.31   |
| 1   | D     | 328 | LYS  | CB-CA-C     | -5.70 | 101.38      | 110.84   |
| 1   | C     | 45  | LEU  | CA-C-O      | -5.70 | 114.51      | 120.55   |
| 1   | D     | 42  | HIS  | CA-CB-CG    | 5.69  | 119.49      | 113.80   |
| 1   | A     | 318 | ASN  | N-CA-CB     | -5.69 | 102.07      | 110.49   |
| 1   | A     | 520 | GLU  | CA-CB-CG    | 5.69  | 125.48      | 114.10   |
| 1   | C     | 271 | ILE  | CA-C-O      | 5.69  | 126.80      | 120.59   |
| 1   | A     | 67  | GLU  | CA-C-N      | -5.69 | 115.13      | 123.10   |
| 1   | A     | 67  | GLU  | C-N-CA      | -5.69 | 115.13      | 123.10   |
| 1   | B     | 494 | TYR  | N-CA-C      | 5.69  | 118.84      | 109.85   |
| 1   | A     | 80  | SER  | CA-CB-OG    | 5.69  | 122.48      | 111.10   |
| 1   | A     | 264 | ALA  | N-CA-CB     | 5.69  | 118.26      | 110.01   |
| 1   | A     | 285 | SER  | CA-C-N      | 5.68  | 132.55      | 121.41   |
| 1   | A     | 285 | SER  | C-N-CA      | 5.68  | 132.55      | 121.41   |
| 1   | C     | 58  | SER  | CB-CA-C     | -5.68 | 100.36      | 108.88   |
| 1   | C     | 186 | ASP  | CA-CB-CG    | 5.67  | 118.27      | 112.60   |
| 1   | A     | 560 | ALA  | CA-C-N      | 5.67  | 126.11      | 119.94   |
| 1   | A     | 560 | ALA  | C-N-CA      | 5.67  | 126.11      | 119.94   |
| 1   | C     | 67  | GLU  | CA-C-N      | -5.67 | 115.39      | 123.10   |
| 1   | C     | 67  | GLU  | C-N-CA      | -5.67 | 115.39      | 123.10   |
| 1   | C     | 247 | THR  | CB-CA-C     | -5.67 | 101.75      | 110.81   |
| 1   | A     | 321 | ARG  | NE-CZ-NH2   | -5.67 | 114.10      | 119.20   |
| 1   | C     | 283 | ASP  | CA-CB-CG    | 5.66  | 118.26      | 112.60   |
| 1   | D     | 194 | ASP  | CA-C-O      | -5.66 | 114.84      | 120.90   |
| 1   | A     | 217 | ASP  | CB-CA-C     | -5.66 | 101.39      | 110.79   |
| 1   | B     | 477 | ALA  | O-C-N       | 5.66  | 128.60      | 122.15   |
| 1   | D     | 88  | HIS  | CA-CB-CG    | 5.66  | 119.46      | 113.80   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | C     | 90  | PHE  | CA-CB-CG   | 5.66  | 119.46      | 113.80   |
| 1   | C     | 68  | ILE  | CB-CA-C    | 5.66  | 118.17      | 111.32   |
| 1   | B     | 72  | SER  | CA-C-O     | 5.65  | 126.39      | 119.05   |
| 1   | C     | 534 | GLU  | CA-CB-CG   | 5.64  | 125.38      | 114.10   |
| 1   | A     | 398 | ILE  | CA-C-O     | 5.64  | 127.83      | 120.78   |
| 1   | B     | 129 | VAL  | CB-CA-C    | -5.64 | 102.43      | 110.83   |
| 1   | D     | 181 | LYS  | CA-C-O     | 5.64  | 126.53      | 120.55   |
| 1   | A     | 328 | LYS  | CA-CB-CG   | 5.63  | 125.37      | 114.10   |
| 1   | B     | 64  | LEU  | CA-C-N     | 5.63  | 130.17      | 122.34   |
| 1   | B     | 64  | LEU  | C-N-CA     | 5.63  | 130.17      | 122.34   |
| 1   | D     | 337 | HIS  | CA-C-N     | 5.63  | 125.10      | 119.24   |
| 1   | D     | 337 | HIS  | C-N-CA     | 5.63  | 125.10      | 119.24   |
| 1   | C     | 292 | LEU  | CB-CA-C    | -5.63 | 102.28      | 111.68   |
| 1   | D     | 314 | GLY  | N-CA-C     | 5.63  | 120.65      | 112.60   |
| 1   | A     | 127 | ASP  | CA-CB-CG   | -5.63 | 106.97      | 112.60   |
| 1   | A     | 559 | ILE  | CA-C-O     | -5.63 | 115.21      | 121.17   |
| 1   | D     | 78  | GLU  | CB-CA-C    | 5.62  | 120.82      | 109.68   |
| 1   | A     | 395 | MET  | CB-CA-C    | -5.62 | 100.15      | 111.17   |
| 1   | A     | 541 | GLY  | CA-C-O     | -5.62 | 113.53      | 121.40   |
| 1   | D     | 71  | THR  | O-C-N      | -5.62 | 115.65      | 122.22   |
| 1   | B     | 74  | HIS  | CA-C-O     | -5.62 | 114.70      | 120.54   |
| 1   | C     | 201 | ASN  | CA-C-N     | -5.62 | 115.08      | 122.16   |
| 1   | C     | 201 | ASN  | C-N-CA     | -5.62 | 115.08      | 122.16   |
| 1   | D     | 63  | HIS  | ND1-CG-CD2 | -5.62 | 100.48      | 106.10   |
| 1   | A     | 567 | PHE  | O-C-N      | 5.61  | 128.09      | 122.08   |
| 1   | A     | 436 | HIS  | CA-C-O     | -5.61 | 112.48      | 119.38   |
| 1   | C     | 202 | ILE  | CA-CB-CG1  | 5.61  | 119.94      | 110.40   |
| 1   | C     | 425 | ARG  | N-CA-CB    | 5.61  | 118.47      | 110.16   |
| 1   | B     | 237 | GLY  | CA-C-O     | 5.61  | 125.42      | 119.03   |
| 1   | B     | 313 | GLY  | CA-C-O     | -5.61 | 115.45      | 122.74   |
| 1   | A     | 548 | ASN  | CB-CG-ND2  | 5.60  | 124.80      | 116.40   |
| 1   | C     | 129 | VAL  | CA-CB-CG1  | 5.59  | 119.90      | 110.40   |
| 1   | A     | 485 | PRO  | N-CA-C     | 5.59  | 120.89      | 113.40   |
| 1   | B     | 296 | GLU  | CA-CB-CG   | -5.59 | 102.92      | 114.10   |
| 1   | B     | 421 | ASP  | N-CA-C     | 5.59  | 118.36      | 110.14   |
| 1   | B     | 502 | VAL  | N-CA-C     | -5.58 | 102.38      | 109.58   |
| 1   | B     | 206 | GLU  | CA-C-O     | -5.58 | 114.63      | 120.55   |
| 1   | C     | 278 | VAL  | CB-CA-C    | -5.58 | 102.14      | 111.29   |
| 1   | B     | 420 | PHE  | CA-C-N     | 5.57  | 133.03      | 123.05   |
| 1   | B     | 420 | PHE  | C-N-CA     | 5.57  | 133.03      | 123.05   |
| 1   | D     | 81  | VAL  | N-CA-C     | 5.57  | 116.76      | 108.46   |
| 1   | A     | 443 | GLY  | N-CA-C     | -5.57 | 101.44      | 111.19   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | A     | 556 | TYR  | CA-CB-CG  | -5.57 | 103.87      | 113.90   |
| 1   | B     | 329 | LEU  | N-CA-C    | 5.57  | 121.05      | 113.37   |
| 1   | B     | 534 | GLU  | CA-C-O    | 5.57  | 126.11      | 119.10   |
| 1   | C     | 566 | LYS  | O-C-N     | -5.57 | 116.30      | 122.09   |
| 1   | C     | 185 | GLU  | CA-C-O    | 5.56  | 127.58      | 120.57   |
| 1   | D     | 369 | PRO  | CA-C-N    | 5.56  | 128.28      | 120.28   |
| 1   | D     | 369 | PRO  | C-N-CA    | 5.56  | 128.28      | 120.28   |
| 1   | A     | 339 | GLY  | O-C-N     | 5.55  | 130.56      | 122.18   |
| 1   | B     | 291 | VAL  | CA-C-O    | 5.54  | 126.90      | 121.19   |
| 1   | D     | 194 | ASP  | CA-CB-CG  | 5.54  | 118.14      | 112.60   |
| 1   | D     | 233 | GLY  | CA-C-O    | -5.54 | 116.05      | 121.93   |
| 1   | C     | 486 | ARG  | CA-C-N    | 5.54  | 129.47      | 120.60   |
| 1   | C     | 486 | ARG  | C-N-CA    | 5.54  | 129.47      | 120.60   |
| 1   | C     | 142 | VAL  | N-CA-CB   | 5.54  | 117.03      | 110.55   |
| 1   | B     | 216 | SER  | CA-C-N    | 5.54  | 127.97      | 120.38   |
| 1   | B     | 216 | SER  | C-N-CA    | 5.54  | 127.97      | 120.38   |
| 1   | B     | 259 | VAL  | CA-C-O    | -5.53 | 114.98      | 120.85   |
| 1   | B     | 312 | ALA  | CA-C-O    | -5.53 | 112.60      | 120.51   |
| 1   | D     | 10  | GLY  | CA-C-O    | 5.52  | 126.97      | 121.00   |
| 1   | B     | 311 | ALA  | N-CA-C    | -5.52 | 105.23      | 112.41   |
| 1   | B     | 364 | HIS  | O-C-N     | 5.52  | 127.47      | 121.23   |
| 1   | B     | 477 | ALA  | N-CA-CB   | -5.52 | 101.99      | 110.16   |
| 1   | A     | 470 | PHE  | N-CA-C    | -5.52 | 105.27      | 111.28   |
| 1   | C     | 449 | LEU  | CA-C-O    | 5.51  | 126.73      | 120.00   |
| 1   | C     | 388 | ASN  | CA-CB-CG  | 5.51  | 118.11      | 112.60   |
| 1   | C     | 510 | VAL  | O-C-N     | -5.51 | 116.67      | 122.95   |
| 1   | B     | 478 | GLN  | N-CA-CB   | -5.50 | 101.19      | 110.49   |
| 1   | C     | 150 | LYS  | N-CA-C    | -5.50 | 100.21      | 109.07   |
| 1   | A     | 156 | LYS  | CA-CB-CG  | 5.50  | 125.10      | 114.10   |
| 1   | B     | 271 | ILE  | O-C-N     | -5.50 | 116.68      | 122.95   |
| 1   | C     | 148 | GLY  | CA-C-O    | -5.50 | 112.22      | 119.25   |
| 1   | B     | 425 | ARG  | NE-CZ-NH2 | 5.50  | 124.15      | 119.20   |
| 1   | B     | 417 | TYR  | CB-CA-C   | -5.49 | 101.36      | 110.14   |
| 1   | C     | 525 | PRO  | O-C-N     | 5.49  | 129.32      | 123.01   |
| 1   | B     | 77  | HIS  | N-CA-C    | 5.49  | 118.98      | 112.72   |
| 1   | A     | 522 | THR  | CA-C-O    | -5.49 | 113.14      | 119.78   |
| 1   | B     | 200 | ARG  | NE-CZ-NH1 | -5.49 | 116.02      | 121.50   |
| 1   | C     | 218 | SER  | N-CA-C    | -5.48 | 105.46      | 111.82   |
| 1   | D     | 93  | ASP  | CA-CB-CG  | 5.48  | 118.08      | 112.60   |
| 1   | C     | 198 | GLY  | CA-C-O    | -5.48 | 115.43      | 120.80   |
| 1   | A     | 514 | LYS  | CG-CD-CE  | 5.47  | 123.89      | 111.30   |
| 1   | B     | 245 | ARG  | CA-CB-CG  | 5.47  | 125.05      | 114.10   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | D     | 396 | ASN  | N-CA-C     | -5.47 | 101.55      | 110.20   |
| 1   | A     | 29  | ASP  | O-C-N      | -5.47 | 115.96      | 122.20   |
| 1   | D     | 235 | MET  | CA-C-O     | -5.47 | 114.04      | 120.60   |
| 1   | C     | 561 | GLY  | N-CA-C     | -5.47 | 105.77      | 112.77   |
| 1   | A     | 411 | GLN  | CA-C-O     | -5.46 | 115.23      | 121.68   |
| 1   | A     | 332 | PHE  | CA-CB-CG   | 5.46  | 119.26      | 113.80   |
| 1   | A     | 141 | ALA  | N-CA-C     | -5.46 | 105.41      | 111.36   |
| 1   | A     | 426 | LYS  | CA-CB-CG   | 5.45  | 125.00      | 114.10   |
| 1   | D     | 519 | SER  | N-CA-C     | 5.45  | 118.55      | 110.48   |
| 1   | A     | 67  | GLU  | CA-C-O     | -5.45 | 114.44      | 120.60   |
| 1   | B     | 254 | ALA  | CA-C-O     | 5.45  | 126.72      | 121.00   |
| 1   | B     | 372 | GLY  | N-CA-C     | -5.45 | 108.11      | 115.36   |
| 1   | C     | 8   | PHE  | CA-C-O     | -5.45 | 114.75      | 120.63   |
| 1   | C     | 212 | ALA  | CA-C-O     | -5.44 | 115.11      | 120.82   |
| 1   | A     | 431 | ILE  | CA-C-N     | 5.44  | 129.39      | 120.63   |
| 1   | A     | 431 | ILE  | C-N-CA     | 5.44  | 129.39      | 120.63   |
| 1   | A     | 459 | GLU  | CB-CA-C    | 5.44  | 119.93      | 110.79   |
| 1   | A     | 228 | ASP  | CB-CA-C    | -5.44 | 102.79      | 111.17   |
| 1   | B     | 262 | ASP  | N-CA-CB    | 5.44  | 118.11      | 110.12   |
| 1   | B     | 93  | ASP  | CB-CA-C    | 5.43  | 120.81      | 111.68   |
| 1   | A     | 333 | LYS  | CB-CA-C    | 5.43  | 118.76      | 109.80   |
| 1   | A     | 481 | ARG  | CA-C-O     | 5.43  | 127.60      | 120.16   |
| 1   | B     | 530 | TYR  | CA-C-O     | -5.43 | 114.98      | 121.11   |
| 1   | C     | 438 | ASN  | N-CA-C     | 5.42  | 119.18      | 112.24   |
| 1   | A     | 385 | ILE  | CA-C-O     | -5.42 | 115.35      | 121.75   |
| 1   | A     | 490 | VAL  | CA-C-N     | 5.42  | 130.73      | 121.35   |
| 1   | A     | 490 | VAL  | C-N-CA     | 5.42  | 130.73      | 121.35   |
| 1   | C     | 102 | ARG  | NE-CZ-NH2  | -5.42 | 114.32      | 119.20   |
| 1   | C     | 335 | THR  | N-CA-C     | -5.42 | 106.34      | 113.17   |
| 1   | B     | 26  | VAL  | CA-C-O     | -5.42 | 115.86      | 121.93   |
| 1   | B     | 276 | ARG  | NH1-CZ-NH2 | 5.42  | 126.34      | 119.30   |
| 1   | D     | 165 | LYS  | CA-C-O     | -5.42 | 112.77      | 120.51   |
| 1   | B     | 38  | CYS  | O-C-N      | -5.41 | 116.40      | 122.03   |
| 1   | C     | 279 | ARG  | CB-CG-CD   | 5.41  | 123.74      | 111.30   |
| 1   | C     | 499 | ALA  | CA-C-N     | 5.41  | 125.41      | 119.89   |
| 1   | C     | 499 | ALA  | C-N-CA     | 5.41  | 125.41      | 119.89   |
| 1   | A     | 309 | VAL  | CB-CA-C    | -5.41 | 103.49      | 110.84   |
| 1   | D     | 382 | ASN  | N-CA-CB    | -5.40 | 101.42      | 110.39   |
| 1   | D     | 468 | ASN  | CB-CG-OD1  | 5.40  | 131.60      | 120.80   |
| 1   | B     | 535 | VAL  | N-CA-C     | -5.40 | 104.20      | 111.44   |
| 1   | A     | 558 | ARG  | NE-CZ-NH1  | -5.40 | 116.10      | 121.50   |
| 1   | A     | 334 | ALA  | CA-C-O     | 5.39  | 128.08      | 121.56   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | B     | 217 | ASP  | CA-C-N    | 5.39  | 127.44      | 120.44   |
| 1   | B     | 217 | ASP  | C-N-CA    | 5.39  | 127.44      | 120.44   |
| 1   | C     | 357 | ASP  | N-CA-CB   | -5.39 | 104.06      | 112.41   |
| 1   | B     | 129 | VAL  | O-C-N     | 5.38  | 128.83      | 123.18   |
| 1   | A     | 169 | GLY  | O-C-N     | 5.38  | 127.39      | 122.17   |
| 1   | B     | 127 | ASP  | N-CA-C    | -5.38 | 104.37      | 111.96   |
| 1   | B     | 525 | PRO  | CA-C-O    | -5.38 | 115.22      | 121.95   |
| 1   | B     | 548 | ASN  | N-CA-C    | -5.38 | 105.85      | 112.90   |
| 1   | D     | 492 | PRO  | N-CD-CG   | 5.38  | 111.27      | 103.20   |
| 1   | C     | 102 | ARG  | NE-CZ-NH1 | 5.38  | 126.88      | 121.50   |
| 1   | B     | 503 | HIS  | N-CA-C    | 5.38  | 120.33      | 113.18   |
| 1   | B     | 3   | GLU  | CA-C-N    | 5.37  | 130.69      | 122.25   |
| 1   | B     | 3   | GLU  | C-N-CA    | 5.37  | 130.69      | 122.25   |
| 1   | A     | 529 | LEU  | CA-C-O    | -5.37 | 114.41      | 120.32   |
| 1   | B     | 332 | PHE  | CA-CB-CG  | 5.37  | 119.17      | 113.80   |
| 1   | C     | 377 | GLU  | N-CA-C    | -5.37 | 105.47      | 112.23   |
| 1   | B     | 245 | ARG  | NE-CZ-NH1 | -5.36 | 116.14      | 121.50   |
| 1   | D     | 220 | ASP  | CA-C-N    | 5.36  | 127.41      | 120.44   |
| 1   | D     | 220 | ASP  | C-N-CA    | 5.36  | 127.41      | 120.44   |
| 1   | D     | 342 | GLY  | CA-C-N    | 5.36  | 127.78      | 120.54   |
| 1   | D     | 342 | GLY  | C-N-CA    | 5.36  | 127.78      | 120.54   |
| 1   | D     | 11  | GLU  | CB-CG-CD  | 5.36  | 121.71      | 112.60   |
| 1   | C     | 64  | LEU  | CA-C-N    | 5.36  | 128.00      | 122.27   |
| 1   | C     | 64  | LEU  | C-N-CA    | 5.36  | 128.00      | 122.27   |
| 1   | C     | 366 | THR  | O-C-N     | -5.36 | 115.46      | 122.43   |
| 1   | B     | 145 | ARG  | CB-CA-C   | 5.36  | 119.96      | 110.85   |
| 1   | D     | 73  | CYS  | CB-CA-C   | -5.36 | 99.76       | 110.42   |
| 1   | A     | 9   | HIS  | CA-C-O    | 5.35  | 125.97      | 119.49   |
| 1   | A     | 470 | PHE  | CA-C-O    | -5.35 | 114.88      | 120.55   |
| 1   | B     | 193 | ASP  | CA-CB-CG  | -5.35 | 107.25      | 112.60   |
| 1   | B     | 291 | VAL  | N-CA-CB   | -5.35 | 101.46      | 111.62   |
| 1   | C     | 84  | CYS  | O-C-N     | -5.35 | 116.11      | 122.20   |
| 1   | C     | 526 | ILE  | N-CA-CB   | 5.35  | 116.36      | 110.53   |
| 1   | D     | 30  | ASN  | CA-CB-CG  | -5.35 | 107.25      | 112.60   |
| 1   | A     | 557 | GLY  | CA-C-O    | -5.34 | 115.55      | 121.05   |
| 1   | B     | 328 | LYS  | N-CA-CB   | 5.34  | 117.76      | 110.01   |
| 1   | C     | 58  | SER  | CA-C-O    | -5.34 | 113.63      | 120.04   |
| 1   | D     | 123 | LYS  | CA-C-O    | -5.34 | 114.06      | 120.10   |
| 1   | D     | 332 | PHE  | CA-CB-CG  | 5.34  | 119.14      | 113.80   |
| 1   | B     | 429 | LYS  | CA-CB-CG  | 5.34  | 124.78      | 114.10   |
| 1   | A     | 349 | LEU  | N-CA-C    | -5.34 | 105.54      | 111.36   |
| 1   | C     | 26  | VAL  | CA-C-O    | -5.34 | 114.63      | 120.72   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | D     | 12  | MET  | CA-CB-CG   | 5.34  | 124.78      | 114.10   |
| 1   | D     | 131 | ILE  | CA-C-O     | -5.34 | 114.55      | 120.74   |
| 1   | C     | 193 | ASP  | CB-CA-C    | 5.34  | 119.33      | 110.90   |
| 1   | A     | 350 | GLN  | N-CA-C     | -5.33 | 106.47      | 112.87   |
| 1   | C     | 222 | LEU  | N-CA-C     | -5.33 | 105.55      | 111.36   |
| 1   | A     | 509 | LEU  | CA-C-O     | -5.33 | 115.69      | 121.44   |
| 1   | D     | 245 | ARG  | N-CA-C     | 5.33  | 113.02      | 108.22   |
| 1   | D     | 86  | ALA  | CA-C-O     | -5.33 | 114.88      | 120.63   |
| 1   | A     | 358 | LEU  | CA-C-O     | -5.32 | 112.83      | 119.38   |
| 1   | A     | 459 | GLU  | N-CA-CB    | -5.32 | 102.26      | 110.13   |
| 1   | A     | 271 | ILE  | N-CA-C     | 5.32  | 116.41      | 108.54   |
| 1   | D     | 150 | LYS  | CB-CA-C    | 5.32  | 118.52      | 109.80   |
| 1   | D     | 316 | ALA  | CA-C-O     | -5.32 | 112.84      | 119.38   |
| 1   | A     | 42  | HIS  | CA-C-O     | -5.31 | 113.00      | 119.32   |
| 1   | A     | 157 | GLU  | N-CA-CB    | -5.31 | 103.49      | 109.49   |
| 1   | A     | 272 | ARG  | O-C-N      | -5.31 | 116.44      | 123.13   |
| 1   | B     | 159 | ILE  | CA-C-N     | 5.31  | 126.48      | 119.84   |
| 1   | B     | 159 | ILE  | C-N-CA     | 5.31  | 126.48      | 119.84   |
| 1   | B     | 255 | HIS  | CA-C-O     | -5.31 | 115.22      | 120.90   |
| 1   | C     | 92  | PHE  | CA-C-O     | -5.31 | 115.31      | 121.15   |
| 1   | A     | 230 | THR  | O-C-N      | -5.31 | 115.04      | 122.37   |
| 1   | B     | 92  | PHE  | O-C-N      | -5.31 | 116.41      | 122.89   |
| 1   | C     | 558 | ARG  | NE-CZ-NH1  | -5.31 | 116.19      | 121.50   |
| 1   | A     | 318 | ASN  | OD1-CG-ND2 | 5.31  | 127.91      | 122.60   |
| 1   | C     | 47  | GLU  | CB-CG-CD   | 5.31  | 121.62      | 112.60   |
| 1   | C     | 12  | MET  | CA-CB-CG   | 5.30  | 124.71      | 114.10   |
| 1   | A     | 43  | GLY  | CA-C-O     | -5.30 | 118.33      | 122.52   |
| 1   | D     | 362 | GLN  | CG-CD-NE2  | 5.30  | 124.35      | 116.40   |
| 1   | C     | 493 | PHE  | CA-CB-CG   | -5.30 | 108.50      | 113.80   |
| 1   | D     | 252 | VAL  | CB-CA-C    | -5.30 | 102.60      | 111.29   |
| 1   | D     | 11  | GLU  | CA-C-N     | 5.30  | 131.66      | 121.54   |
| 1   | D     | 11  | GLU  | C-N-CA     | 5.30  | 131.66      | 121.54   |
| 1   | A     | 492 | PRO  | N-CA-CB    | 5.30  | 108.81      | 103.25   |
| 1   | B     | 209 | LYS  | CB-CA-C    | -5.30 | 102.56      | 110.88   |
| 1   | A     | 526 | ILE  | CA-C-O     | 5.29  | 126.84      | 120.65   |
| 1   | B     | 134 | GLY  | CA-C-N     | 5.29  | 125.97      | 119.99   |
| 1   | B     | 134 | GLY  | C-N-CA     | 5.29  | 125.97      | 119.99   |
| 1   | C     | 108 | ASP  | CA-C-O     | 5.29  | 126.06      | 119.97   |
| 1   | C     | 272 | ARG  | O-C-N      | 5.29  | 129.41      | 123.27   |
| 1   | A     | 303 | ILE  | CA-C-O     | -5.29 | 114.84      | 120.39   |
| 1   | B     | 495 | ALA  | N-CA-C     | 5.29  | 118.07      | 109.24   |
| 1   | A     | 469 | GLY  | O-C-N      | 5.29  | 127.27      | 122.19   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | A     | 146 | ASP  | O-C-N     | -5.29 | 115.56      | 122.59   |
| 1   | B     | 253 | GLY  | CA-C-N    | 5.29  | 127.63      | 120.65   |
| 1   | B     | 253 | GLY  | C-N-CA    | 5.29  | 127.63      | 120.65   |
| 1   | B     | 360 | TYR  | CA-C-O    | 5.28  | 126.01      | 120.36   |
| 1   | C     | 272 | ARG  | CA-C-O    | -5.28 | 114.65      | 120.30   |
| 1   | D     | 216 | SER  | CA-C-N    | 5.28  | 127.36      | 120.28   |
| 1   | D     | 216 | SER  | C-N-CA    | 5.28  | 127.36      | 120.28   |
| 1   | B     | 68  | ILE  | CB-CA-C   | 5.28  | 117.86      | 110.99   |
| 1   | C     | 157 | GLU  | CA-C-N    | 5.28  | 124.97      | 119.64   |
| 1   | C     | 157 | GLU  | C-N-CA    | 5.28  | 124.97      | 119.64   |
| 1   | A     | 338 | PRO  | O-C-N     | -5.27 | 115.42      | 122.22   |
| 1   | C     | 483 | ASP  | CA-CB-CG  | 5.27  | 117.87      | 112.60   |
| 1   | B     | 522 | THR  | CA-C-O    | -5.27 | 112.54      | 118.55   |
| 1   | B     | 64  | LEU  | CA-C-O    | -5.27 | 115.39      | 121.19   |
| 1   | B     | 481 | ARG  | NE-CZ-NH2 | -5.27 | 114.46      | 119.20   |
| 1   | C     | 373 | VAL  | CA-C-N    | 5.27  | 128.83      | 121.24   |
| 1   | C     | 373 | VAL  | C-N-CA    | 5.27  | 128.83      | 121.24   |
| 1   | D     | 279 | ARG  | CD-NE-CZ  | -5.27 | 117.03      | 124.40   |
| 1   | C     | 528 | GLY  | CA-C-O    | -5.27 | 113.79      | 119.27   |
| 1   | A     | 218 | SER  | CB-CA-C   | 5.26  | 120.91      | 110.17   |
| 1   | D     | 438 | ASN  | N-CA-CB   | -5.25 | 104.31      | 112.30   |
| 1   | A     | 499 | ALA  | CA-C-N    | 5.25  | 125.19      | 119.78   |
| 1   | A     | 499 | ALA  | C-N-CA    | 5.25  | 125.19      | 119.78   |
| 1   | A     | 314 | GLY  | O-C-N     | 5.25  | 128.42      | 122.86   |
| 1   | B     | 339 | GLY  | CA-C-O    | 5.25  | 123.81      | 119.04   |
| 1   | C     | 238 | ALA  | N-CA-CB   | 5.25  | 119.18      | 110.52   |
| 1   | A     | 252 | VAL  | CA-CB-CG1 | 5.24  | 119.31      | 110.40   |
| 1   | A     | 381 | GLY  | CA-C-O    | 5.24  | 126.15      | 120.75   |
| 1   | C     | 434 | TYR  | CA-C-N    | 5.24  | 129.31      | 120.29   |
| 1   | C     | 434 | TYR  | C-N-CA    | 5.24  | 129.31      | 120.29   |
| 1   | D     | 343 | ASP  | CA-C-O    | 5.24  | 126.51      | 120.90   |
| 1   | A     | 484 | LEU  | O-C-N     | 5.24  | 126.13      | 121.36   |
| 1   | A     | 563 | SER  | N-CA-CB   | -5.24 | 102.47      | 110.07   |
| 1   | B     | 503 | HIS  | CA-CB-CG  | 5.24  | 119.04      | 113.80   |
| 1   | B     | 47  | GLU  | O-C-N     | -5.24 | 116.64      | 122.09   |
| 1   | B     | 305 | ALA  | CA-C-O    | -5.23 | 115.68      | 121.33   |
| 1   | D     | 356 | ARG  | NE-CZ-NH1 | -5.23 | 116.27      | 121.50   |
| 1   | A     | 107 | VAL  | N-CA-CB   | 5.23  | 118.75      | 110.54   |
| 1   | A     | 200 | ARG  | CG-CD-NE  | 5.23  | 123.51      | 112.00   |
| 1   | B     | 78  | GLU  | CA-C-O    | -5.23 | 115.63      | 121.23   |
| 1   | B     | 372 | GLY  | O-C-N     | -5.23 | 115.75      | 122.39   |
| 1   | A     | 167 | ALA  | CA-C-O    | -5.23 | 113.04      | 120.51   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | C     | 367 | TYR  | CA-C-O     | -5.23 | 115.05      | 120.70   |
| 1   | D     | 19  | HIS  | CA-CB-CG   | -5.23 | 108.57      | 113.80   |
| 1   | D     | 279 | ARG  | NE-CZ-NH1  | -5.23 | 116.27      | 121.50   |
| 1   | A     | 71  | THR  | CA-CB-OG1  | -5.23 | 101.76      | 109.60   |
| 1   | A     | 79  | LYS  | CB-CG-CD   | 5.22  | 123.31      | 111.30   |
| 1   | A     | 506 | MET  | N-CA-C     | 5.22  | 117.72      | 111.71   |
| 1   | D     | 50  | ALA  | N-CA-C     | -5.22 | 105.67      | 111.36   |
| 1   | D     | 231 | ASP  | N-CA-C     | -5.22 | 100.79      | 109.46   |
| 1   | D     | 496 | LEU  | N-CA-C     | 5.22  | 117.31      | 108.02   |
| 1   | D     | 68  | ILE  | CB-CG1-CD1 | -5.22 | 102.84      | 113.80   |
| 1   | A     | 395 | MET  | N-CA-C     | 5.21  | 116.21      | 108.60   |
| 1   | A     | 491 | ALA  | CA-C-N     | 5.21  | 126.35      | 119.84   |
| 1   | A     | 491 | ALA  | C-N-CA     | 5.21  | 126.35      | 119.84   |
| 1   | C     | 401 | ARG  | CA-C-N     | 5.21  | 131.49      | 121.54   |
| 1   | C     | 401 | ARG  | C-N-CA     | 5.21  | 131.49      | 121.54   |
| 1   | B     | 83  | TYR  | CA-C-N     | 5.20  | 127.98      | 120.38   |
| 1   | B     | 83  | TYR  | C-N-CA     | 5.20  | 127.98      | 120.38   |
| 1   | A     | 29  | ASP  | N-CA-CB    | -5.20 | 101.92      | 110.14   |
| 1   | A     | 293 | VAL  | CA-C-N     | -5.20 | 115.28      | 123.13   |
| 1   | A     | 293 | VAL  | C-N-CA     | -5.20 | 115.28      | 123.13   |
| 1   | B     | 241 | ASN  | CB-CG-ND2  | -5.20 | 108.61      | 116.40   |
| 1   | D     | 134 | GLY  | CA-C-O     | -5.20 | 117.08      | 122.28   |
| 1   | D     | 350 | GLN  | CA-CB-CG   | 5.20  | 124.49      | 114.10   |
| 1   | B     | 517 | VAL  | O-C-N      | -5.19 | 117.04      | 122.81   |
| 1   | B     | 242 | ARG  | CD-NE-CZ   | 5.19  | 131.67      | 124.40   |
| 1   | A     | 160 | PRO  | N-CA-C     | 5.19  | 123.16      | 112.47   |
| 1   | B     | 283 | ASP  | N-CA-C     | 5.19  | 115.97      | 108.34   |
| 1   | C     | 152 | ILE  | N-CA-CB    | 5.19  | 118.39      | 111.64   |
| 1   | A     | 242 | ARG  | NE-CZ-NH1  | -5.19 | 116.31      | 121.50   |
| 1   | C     | 341 | THR  | N-CA-C     | 5.19  | 120.25      | 113.30   |
| 1   | A     | 387 | VAL  | CA-C-O     | -5.19 | 115.06      | 120.76   |
| 1   | A     | 467 | TYR  | CA-C-O     | -5.19 | 114.24      | 120.10   |
| 1   | C     | 143 | SER  | O-C-N      | -5.19 | 116.70      | 122.09   |
| 1   | C     | 67  | GLU  | N-CA-C     | -5.18 | 101.52      | 109.76   |
| 1   | C     | 18  | CYS  | N-CA-CB    | -5.18 | 101.00      | 110.27   |
| 1   | C     | 532 | ALA  | O-C-N      | 5.18  | 128.59      | 123.46   |
| 1   | D     | 63  | HIS  | N-CA-C     | -5.18 | 106.65      | 113.17   |
| 1   | B     | 151 | VAL  | N-CA-C     | 5.17  | 116.42      | 108.71   |
| 1   | A     | 309 | VAL  | N-CA-CB    | 5.17  | 117.20      | 110.99   |
| 1   | C     | 543 | ASN  | CA-C-O     | -5.17 | 113.83      | 120.14   |
| 1   | C     | 549 | ALA  | O-C-N      | 5.17  | 127.67      | 122.09   |
| 1   | B     | 304 | LYS  | CA-C-O     | -5.17 | 114.80      | 120.69   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | B     | 557 | GLY  | N-CA-C     | -5.17 | 106.39      | 112.64   |
| 1   | D     | 233 | GLY  | O-C-N      | 5.17  | 127.86      | 122.79   |
| 1   | B     | 86  | ALA  | N-CA-C     | -5.17 | 104.91      | 111.11   |
| 1   | C     | 393 | ARG  | NE-CZ-NH1  | -5.17 | 116.33      | 121.50   |
| 1   | A     | 46  | LYS  | N-CA-CB    | 5.16  | 117.67      | 109.82   |
| 1   | A     | 95  | PRO  | N-CA-C     | -5.16 | 103.08      | 111.03   |
| 1   | B     | 255 | HIS  | N-CA-CB    | 5.16  | 117.64      | 109.94   |
| 1   | C     | 275 | SER  | CA-C-O     | -5.16 | 114.06      | 120.57   |
| 1   | A     | 215 | SER  | CA-C-O     | 5.16  | 125.89      | 120.42   |
| 1   | C     | 276 | ARG  | N-CA-C     | 5.16  | 116.72      | 108.41   |
| 1   | C     | 3   | GLU  | CB-CA-C    | 5.16  | 119.90      | 110.10   |
| 1   | D     | 476 | ASP  | CA-CB-CG   | 5.15  | 117.75      | 112.60   |
| 1   | B     | 5   | LEU  | CA-C-O     | -5.15 | 115.06      | 120.63   |
| 1   | A     | 445 | THR  | CA-C-O     | -5.15 | 115.94      | 121.45   |
| 1   | A     | 492 | PRO  | CA-N-CD    | -5.15 | 104.80      | 112.00   |
| 1   | B     | 67  | GLU  | CA-C-N     | -5.15 | 116.23      | 123.13   |
| 1   | B     | 67  | GLU  | C-N-CA     | -5.15 | 116.23      | 123.13   |
| 1   | B     | 68  | ILE  | CA-CB-CG2  | 5.14  | 119.25      | 110.50   |
| 1   | C     | 200 | ARG  | CA-C-N     | 5.14  | 131.37      | 121.54   |
| 1   | C     | 200 | ARG  | C-N-CA     | 5.14  | 131.37      | 121.54   |
| 1   | B     | 39  | VAL  | CA-C-O     | -5.14 | 115.60      | 120.95   |
| 1   | C     | 130 | ILE  | N-CA-C     | 5.14  | 115.26      | 107.80   |
| 1   | B     | 420 | PHE  | CA-C-O     | 5.14  | 127.27      | 121.51   |
| 1   | B     | 464 | VAL  | N-CA-C     | 5.14  | 115.91      | 110.72   |
| 1   | B     | 279 | ARG  | NE-CZ-NH2  | 5.14  | 123.82      | 119.20   |
| 1   | C     | 283 | ASP  | CA-C-N     | 5.13  | 131.34      | 121.54   |
| 1   | C     | 283 | ASP  | C-N-CA     | 5.13  | 131.34      | 121.54   |
| 1   | C     | 467 | TYR  | CA-C-N     | 5.13  | 127.16      | 120.28   |
| 1   | C     | 467 | TYR  | C-N-CA     | 5.13  | 127.16      | 120.28   |
| 1   | D     | 61  | LYS  | CA-CB-CG   | 5.13  | 124.36      | 114.10   |
| 1   | D     | 318 | ASN  | N-CA-CB    | -5.13 | 103.64      | 110.57   |
| 1   | A     | 3   | GLU  | O-C-N      | -5.13 | 115.19      | 122.99   |
| 1   | A     | 128 | VAL  | O-C-N      | -5.13 | 117.80      | 123.18   |
| 1   | B     | 219 | ILE  | CA-C-O     | 5.13  | 126.39      | 121.05   |
| 1   | D     | 435 | VAL  | CA-C-O     | -5.13 | 115.08      | 120.57   |
| 1   | A     | 68  | ILE  | O-C-N      | -5.13 | 115.44      | 122.62   |
| 1   | C     | 130 | ILE  | CA-C-O     | -5.13 | 115.04      | 120.53   |
| 1   | C     | 259 | VAL  | CG1-CB-CG2 | 5.13  | 122.08      | 110.80   |
| 1   | D     | 8   | PHE  | O-C-N      | -5.13 | 116.22      | 122.22   |
| 1   | D     | 318 | ASN  | CA-C-O     | -5.13 | 116.47      | 122.37   |
| 1   | C     | 176 | THR  | N-CA-C     | 5.12  | 117.67      | 110.14   |
| 1   | A     | 259 | VAL  | CG1-CB-CG2 | 5.12  | 122.07      | 110.80   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | D     | 277 | VAL  | CB-CA-C    | 5.12  | 117.07      | 111.08   |
| 1   | A     | 508 | GLY  | O-C-N      | -5.12 | 118.89      | 123.96   |
| 1   | D     | 27  | THR  | CA-CB-OG1  | 5.12  | 117.28      | 109.60   |
| 1   | A     | 274 | ASN  | CB-CA-C    | -5.12 | 103.63      | 111.66   |
| 1   | C     | 218 | SER  | N-CA-CB    | -5.12 | 102.35      | 110.28   |
| 1   | D     | 548 | ASN  | CA-C-O     | -5.12 | 112.56      | 119.11   |
| 1   | A     | 272 | ARG  | N-CA-C     | 5.11  | 117.04      | 107.99   |
| 1   | C     | 429 | LYS  | O-C-N      | -5.11 | 116.77      | 122.09   |
| 1   | B     | 564 | ALA  | CA-C-O     | -5.11 | 114.09      | 119.97   |
| 1   | C     | 306 | ASP  | CA-C-O     | -5.11 | 114.57      | 120.24   |
| 1   | C     | 46  | LYS  | N-CA-CB    | 5.11  | 117.42      | 110.01   |
| 1   | C     | 249 | GLY  | CA-C-N     | 5.10  | 131.29      | 121.54   |
| 1   | C     | 249 | GLY  | C-N-CA     | 5.10  | 131.29      | 121.54   |
| 1   | D     | 267 | ARG  | CA-C-O     | -5.10 | 113.21      | 120.51   |
| 1   | D     | 184 | ILE  | N-CA-CB    | 5.10  | 116.09      | 110.53   |
| 1   | A     | 382 | ASN  | OD1-CG-ND2 | -5.10 | 117.50      | 122.60   |
| 1   | C     | 14  | GLY  | N-CA-C     | 5.10  | 125.26      | 113.18   |
| 1   | C     | 321 | ARG  | NE-CZ-NH1  | -5.10 | 116.40      | 121.50   |
| 1   | C     | 380 | ARG  | NE-CZ-NH2  | 5.10  | 123.79      | 119.20   |
| 1   | C     | 313 | GLY  | O-C-N      | -5.10 | 117.80      | 123.05   |
| 1   | A     | 359 | GLU  | CB-CG-CD   | 5.09  | 121.26      | 112.60   |
| 1   | B     | 88  | HIS  | CA-CB-CG   | 5.09  | 118.89      | 113.80   |
| 1   | C     | 129 | VAL  | CA-C-N     | -5.09 | 116.50      | 123.12   |
| 1   | C     | 129 | VAL  | C-N-CA     | -5.09 | 116.50      | 123.12   |
| 1   | B     | 256 | VAL  | CA-C-O     | -5.09 | 115.46      | 120.85   |
| 1   | A     | 545 | LEU  | CA-C-O     | -5.09 | 115.25      | 121.05   |
| 1   | A     | 323 | SER  | N-CA-C     | 5.08  | 118.74      | 112.54   |
| 1   | B     | 280 | ILE  | CA-C-O     | -5.08 | 115.09      | 120.48   |
| 1   | D     | 330 | LYS  | N-CA-C     | -5.08 | 102.53      | 110.10   |
| 1   | A     | 333 | LYS  | CB-CG-CD   | 5.08  | 122.99      | 111.30   |
| 1   | B     | 401 | ARG  | N-CA-CB    | 5.08  | 119.08      | 110.49   |
| 1   | C     | 495 | ALA  | N-CA-C     | 5.08  | 116.86      | 108.13   |
| 1   | D     | 269 | THR  | N-CA-C     | 5.08  | 117.83      | 110.42   |
| 1   | C     | 43  | GLY  | N-CA-C     | -5.07 | 106.61      | 112.29   |
| 1   | D     | 429 | LYS  | O-C-N      | -5.07 | 116.42      | 122.20   |
| 1   | A     | 338 | PRO  | N-CA-C     | 5.07  | 120.50      | 113.65   |
| 1   | B     | 269 | THR  | CA-CB-OG1  | -5.07 | 102.00      | 109.60   |
| 1   | A     | 73  | CYS  | O-C-N      | 5.07  | 129.33      | 122.59   |
| 1   | D     | 536 | THR  | CA-C-O     | 5.07  | 127.70      | 121.72   |
| 1   | C     | 5   | LEU  | O-C-N      | -5.06 | 116.82      | 122.09   |
| 1   | A     | 128 | VAL  | CA-C-N     | 5.06  | 129.31      | 122.93   |
| 1   | A     | 128 | VAL  | C-N-CA     | 5.06  | 129.31      | 122.93   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | B     | 301 | TYR  | CA-CB-CG   | 5.06  | 123.01      | 113.90   |
| 1   | A     | 188 | LYS  | N-CA-CB    | 5.06  | 118.01      | 110.22   |
| 1   | B     | 479 | PHE  | CA-C-O     | -5.06 | 115.30      | 121.88   |
| 1   | A     | 271 | ILE  | N-CA-CB    | -5.05 | 105.29      | 110.95   |
| 1   | D     | 302 | VAL  | CA-C-N     | -5.05 | 116.55      | 123.12   |
| 1   | D     | 302 | VAL  | C-N-CA     | -5.05 | 116.55      | 123.12   |
| 1   | B     | 95  | PRO  | CA-C-N     | 5.05  | 129.53      | 122.36   |
| 1   | B     | 95  | PRO  | C-N-CA     | 5.05  | 129.53      | 122.36   |
| 1   | A     | 285 | SER  | N-CA-C     | -5.05 | 102.04      | 109.62   |
| 1   | B     | 379 | VAL  | N-CA-C     | -5.05 | 105.57      | 110.42   |
| 1   | C     | 180 | ALA  | O-C-N      | -5.05 | 115.87      | 122.59   |
| 1   | A     | 267 | ARG  | CA-CB-CG   | -5.05 | 104.00      | 114.10   |
| 1   | C     | 75  | LYS  | CA-C-O     | 5.05  | 127.27      | 121.47   |
| 1   | C     | 17  | SER  | N-CA-CB    | -5.04 | 101.56      | 109.78   |
| 1   | C     | 537 | GLY  | O-C-N      | -5.04 | 119.21      | 123.60   |
| 1   | B     | 22  | ASP  | N-CA-CB    | 5.04  | 118.88      | 110.41   |
| 1   | C     | 73  | CYS  | O-C-N      | 5.04  | 129.29      | 122.59   |
| 1   | C     | 213 | ASN  | OD1-CG-ND2 | 5.04  | 127.64      | 122.60   |
| 1   | C     | 268 | GLY  | CA-C-N     | -5.03 | 113.04      | 120.94   |
| 1   | C     | 268 | GLY  | C-N-CA     | -5.03 | 113.04      | 120.94   |
| 1   | A     | 429 | LYS  | CA-C-O     | -5.03 | 113.40      | 119.49   |
| 1   | B     | 36  | GLY  | CA-C-O     | 5.03  | 125.99      | 120.66   |
| 1   | D     | 240 | VAL  | CB-CA-C    | -5.03 | 101.80      | 110.65   |
| 1   | A     | 30  | ASN  | CA-C-O     | -5.03 | 113.20      | 119.38   |
| 1   | B     | 8   | PHE  | O-C-N      | -5.03 | 116.66      | 122.09   |
| 1   | D     | 357 | ASP  | N-CA-CB    | -5.03 | 101.99      | 110.49   |
| 1   | A     | 51  | ALA  | N-CA-CB    | -5.03 | 103.04      | 110.53   |
| 1   | A     | 308 | VAL  | CA-C-O     | -5.03 | 115.19      | 120.27   |
| 1   | B     | 540 | HIS  | N-CA-C     | 5.02  | 119.09      | 112.92   |
| 1   | C     | 93  | ASP  | CB-CA-C    | 5.02  | 119.74      | 111.31   |
| 1   | D     | 322 | VAL  | N-CA-C     | 5.02  | 115.74      | 110.62   |
| 1   | C     | 345 | LEU  | CB-CA-C    | -5.02 | 102.78      | 110.81   |
| 1   | D     | 38  | CYS  | CA-C-O     | 5.02  | 125.87      | 120.70   |
| 1   | D     | 267 | ARG  | CA-C-N     | -5.02 | 111.58      | 121.41   |
| 1   | D     | 267 | ARG  | C-N-CA     | -5.02 | 111.58      | 121.41   |
| 1   | C     | 427 | SER  | N-CA-C     | 5.01  | 117.40      | 111.33   |
| 1   | D     | 136 | ALA  | CA-C-N     | 5.01  | 125.55      | 119.98   |
| 1   | D     | 136 | ALA  | C-N-CA     | 5.01  | 125.55      | 119.98   |
| 1   | A     | 334 | ALA  | O-C-N      | -5.01 | 116.63      | 123.10   |
| 1   | C     | 380 | ARG  | NH1-CZ-NH2 | -5.01 | 112.79      | 119.30   |
| 1   | D     | 526 | ILE  | CA-C-O     | 5.01  | 127.01      | 120.95   |
| 1   | A     | 520 | GLU  | CB-CA-C    | 5.01  | 119.87      | 110.70   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | C     | 257 | ALA  | CA-C-N   | 5.01  | 126.95      | 120.44   |
| 1   | C     | 257 | ALA  | C-N-CA   | 5.01  | 126.95      | 120.44   |
| 1   | A     | 144 | ALA  | CB-CA-C  | -5.00 | 103.02      | 110.88   |
| 1   | B     | 231 | ASP  | N-CA-C   | -5.00 | 101.80      | 109.76   |
| 1   | C     | 78  | GLU  | N-CA-CB  | -5.00 | 103.30      | 111.66   |
| 1   | A     | 490 | VAL  | N-CA-C   | 5.00  | 115.54      | 107.73   |
| 1   | A     | 9   | HIS  | O-C-N    | -5.00 | 115.89      | 122.39   |
| 1   | A     | 476 | ASP  | CA-CB-CG | 5.00  | 117.60      | 112.60   |
| 1   | C     | 231 | ASP  | CA-C-N   | -5.00 | 116.99      | 123.19   |
| 1   | C     | 231 | ASP  | C-N-CA   | -5.00 | 116.99      | 123.19   |

There are no chirality outliers.

All (10) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group             |
|-----|-------|-----|------|-------------------|
| 1   | A     | 146 | ASP  | Mainchain         |
| 1   | A     | 491 | ALA  | Peptide,Mainchain |
| 1   | B     | 491 | ALA  | Peptide,Mainchain |
| 1   | C     | 477 | ALA  | Mainchain         |
| 1   | C     | 491 | ALA  | Peptide,Mainchain |
| 1   | D     | 491 | ALA  | Peptide,Mainchain |

## 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     | 4124  | 0        | 4013     | 190     | 1            |
| 1   | B     | 4093  | 0        | 3976     | 184     | 0            |
| 1   | C     | 4099  | 0        | 3977     | 202     | 2            |
| 1   | D     | 4113  | 0        | 3988     | 221     | 1            |
| 2   | A     | 172   | 0        | 121      | 14      | 0            |
| 2   | B     | 172   | 0        | 121      | 12      | 0            |
| 2   | C     | 172   | 0        | 120      | 12      | 0            |
| 2   | D     | 172   | 0        | 121      | 18      | 0            |
| 3   | A     | 53    | 0        | 31       | 9       | 0            |
| 3   | B     | 53    | 0        | 31       | 8       | 0            |
| 3   | C     | 53    | 0        | 31       | 12      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3   | D     | 53    | 0        | 30       | 9       | 0            |
| 4   | B     | 5     | 0        | 0        | 1       | 0            |
| 4   | C     | 5     | 0        | 0        | 0       | 0            |
| 4   | D     | 5     | 0        | 0        | 0       | 0            |
| 5   | A     | 48    | 0        | 0        | 2       | 0            |
| 5   | B     | 29    | 0        | 0        | 3       | 0            |
| 5   | C     | 30    | 0        | 0        | 2       | 0            |
| 5   | D     | 19    | 0        | 0        | 2       | 0            |
| All | All   | 17470 | 0        | 16560    | 825     | 2            |

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 25.

All (825) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:18:CYS:SG    | 2:D:603:HEC:HAC  | 1.21                     | 1.71              |
| 3:B:700:FAD:C2'  | 3:B:700:FAD:C1'  | 1.77                     | 1.62              |
| 3:D:900:FAD:C2'  | 3:D:900:FAD:C1'  | 1.78                     | 1.59              |
| 3:A:600:FAD:C1'  | 3:A:600:FAD:C2'  | 1.78                     | 1.57              |
| 3:C:800:FAD:C2'  | 3:C:800:FAD:C1'  | 1.78                     | 1.56              |
| 1:A:41:CYS:SG    | 2:A:604:HEC:HAC  | 1.46                     | 1.55              |
| 1:B:73:CYS:SG    | 2:B:602:HEC:HAC  | 1.48                     | 1.51              |
| 1:D:18:CYS:SG    | 2:D:603:HEC:CAC  | 2.12                     | 1.34              |
| 1:B:73:CYS:SG    | 2:B:602:HEC:CAC  | 2.15                     | 1.33              |
| 1:D:506:MET:HE3  | 1:D:543:ASN:HA   | 1.29                     | 1.14              |
| 1:C:379:VAL:HG11 | 1:C:418:LEU:HD13 | 1.45                     | 0.97              |
| 1:A:288:VAL:HG23 | 1:A:526:ILE:HD11 | 1.46                     | 0.95              |
| 1:D:64:LEU:HD13  | 1:D:159:ILE:HD12 | 1.53                     | 0.91              |
| 1:C:35:ASN:HD21  | 1:C:71:THR:H     | 1.16                     | 0.91              |
| 1:A:66:GLY:H     | 1:A:258:GLN:HE22 | 1.07                     | 0.91              |
| 1:A:319:ASN:HD21 | 1:A:331:GLY:H    | 1.09                     | 0.91              |
| 1:A:452:GLN:HE21 | 1:A:452:GLN:HA   | 1.35                     | 0.91              |
| 1:A:393:ARG:HH11 | 1:A:478:GLN:NE2  | 1.67                     | 0.91              |
| 1:B:166:LEU:HD21 | 2:B:601:HEC:HBC2 | 1.52                     | 0.90              |
| 1:A:35:ASN:HD21  | 1:A:71:THR:H     | 1.18                     | 0.89              |
| 1:B:66:GLY:H     | 1:B:258:GLN:HE22 | 1.19                     | 0.89              |
| 1:C:319:ASN:HD21 | 1:C:331:GLY:H    | 0.94                     | 0.88              |
| 1:D:316:ALA:HB1  | 1:D:502:VAL:HG12 | 1.55                     | 0.88              |
| 1:B:455:VAL:HG21 | 1:B:460:LEU:HD12 | 1.53                     | 0.87              |
| 1:D:447:GLU:HB3  | 1:D:457:ALA:HB1  | 1.57                     | 0.87              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:9:HIS:HA     | 1:C:12:MET:HE3   | 1.57                     | 0.86              |
| 1:C:319:ASN:ND2  | 1:C:331:GLY:H    | 1.75                     | 0.82              |
| 1:D:31:LEU:HD21  | 2:D:603:HEC:HAD1 | 1.62                     | 0.82              |
| 1:C:421:ASP:HB2  | 1:C:488:LEU:HD12 | 1.61                     | 0.81              |
| 1:B:125:THR:HG22 | 1:B:304:LYS:HB3  | 1.63                     | 0.81              |
| 1:D:526:ILE:HG12 | 1:D:529:LEU:HB2  | 1.63                     | 0.81              |
| 1:D:424:ILE:HD13 | 1:D:486:ARG:HD2  | 1.62                     | 0.80              |
| 1:A:66:GLY:H     | 1:A:258:GLN:NE2  | 1.79                     | 0.80              |
| 1:C:392:ASN:HA   | 1:C:463:THR:HG21 | 1.64                     | 0.80              |
| 1:D:362:GLN:HB2  | 1:D:506:MET:HE1  | 1.63                     | 0.80              |
| 1:C:186:ASP:HB2  | 1:C:240:VAL:HG11 | 1.64                     | 0.79              |
| 1:B:409:LEU:HD23 | 1:B:414:GLU:HB3  | 1.64                     | 0.78              |
| 1:C:280:ILE:HD12 | 1:C:347:VAL:HG13 | 1.64                     | 0.77              |
| 1:C:181:LYS:H    | 1:C:181:LYS:HD3  | 1.48                     | 0.77              |
| 1:D:471:VAL:HG22 | 1:D:484:LEU:HB3  | 1.63                     | 0.77              |
| 1:C:175:GLU:OE2  | 1:C:188:LYS:HG3  | 1.84                     | 0.76              |
| 1:D:52:ALA:CA    | 1:D:53:PRO:N     | 2.48                     | 0.76              |
| 1:B:533:GLY:HA2  | 1:B:553:ILE:HG22 | 1.65                     | 0.76              |
| 1:C:233:GLY:HA3  | 1:C:245:ARG:NH2  | 2.01                     | 0.76              |
| 1:D:506:MET:CE   | 1:D:543:ASN:HA   | 2.13                     | 0.75              |
| 1:C:416:ALA:HB3  | 1:C:498:ILE:HD11 | 1.69                     | 0.75              |
| 1:B:366:THR:HG22 | 1:B:498:ILE:HD12 | 1.68                     | 0.75              |
| 1:C:319:ASN:HD21 | 1:C:331:GLY:N    | 1.79                     | 0.74              |
| 1:C:421:ASP:HB3  | 1:C:424:ILE:HG12 | 1.68                     | 0.74              |
| 1:A:322:VAL:HG13 | 1:A:361:ILE:HD13 | 1.69                     | 0.74              |
| 1:A:62:SER:HB3   | 2:A:601:HEC:HBB3 | 1.70                     | 0.73              |
| 1:C:446:ILE:HD13 | 1:C:464:VAL:HG11 | 1.71                     | 0.73              |
| 1:A:145:ARG:HH11 | 1:A:268:GLY:H    | 1.36                     | 0.72              |
| 1:B:68:ILE:HD11  | 2:B:602:HEC:CMC  | 2.19                     | 0.72              |
| 1:B:175:GLU:OE2  | 1:B:188:LYS:HG3  | 1.90                     | 0.72              |
| 1:A:135:GLY:HA3  | 1:A:553:ILE:HD12 | 1.72                     | 0.72              |
| 1:A:177:LYS:HB2  | 1:A:178:PRO:HD3  | 1.71                     | 0.72              |
| 1:D:453:ILE:O    | 1:D:454:ASP:HB2  | 1.89                     | 0.72              |
| 1:D:66:GLY:H     | 1:D:258:GLN:HE22 | 1.36                     | 0.71              |
| 1:B:319:ASN:HD21 | 1:B:331:GLY:H    | 1.36                     | 0.71              |
| 1:A:142:VAL:HG21 | 1:A:225:MET:HE1  | 1.72                     | 0.71              |
| 1:C:452:GLN:HE21 | 1:C:452:GLN:HA   | 1.55                     | 0.71              |
| 1:C:409:LEU:HD22 | 1:C:414:GLU:HB3  | 1.73                     | 0.71              |
| 3:D:900:FAD:C2'  | 3:D:900:FAD:N10  | 2.52                     | 0.71              |
| 1:A:366:THR:HG22 | 1:A:498:ILE:HD13 | 1.72                     | 0.70              |
| 1:D:366:THR:HG21 | 1:D:380:ARG:HE   | 1.56                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:453:ILE:HG22 | 1:D:455:VAL:HG13 | 1.73                     | 0.70              |
| 1:C:194:ASP:OD2  | 1:C:242:ARG:NH2  | 2.24                     | 0.70              |
| 1:D:68:ILE:HD11  | 2:D:602:HEC:HMC1 | 1.73                     | 0.70              |
| 1:A:393:ARG:NH1  | 1:A:478:GLN:NE2  | 2.39                     | 0.70              |
| 1:D:35:ASN:HD21  | 1:D:71:THR:H     | 1.38                     | 0.70              |
| 1:D:225:MET:HE3  | 1:D:263:ASN:CB   | 2.22                     | 0.69              |
| 1:C:181:LYS:H    | 1:C:181:LYS:CD   | 2.00                     | 0.69              |
| 1:D:393:ARG:HD3  | 1:D:478:GLN:HE22 | 1.56                     | 0.69              |
| 1:B:28:ASN:C     | 1:B:28:ASN:HD22  | 2.00                     | 0.69              |
| 1:B:392:ASN:HA   | 1:B:463:THR:HG21 | 1.75                     | 0.68              |
| 1:B:455:VAL:CG2  | 1:B:460:LEU:HD12 | 2.23                     | 0.68              |
| 1:B:550:ILE:HG12 | 3:B:700:FAD:C2   | 2.23                     | 0.68              |
| 1:A:319:ASN:ND2  | 1:A:331:GLY:H    | 1.89                     | 0.68              |
| 1:D:455:VAL:HB   | 1:D:456:PRO:HD2  | 1.75                     | 0.68              |
| 1:A:68:ILE:HD11  | 2:A:602:HEC:HMC1 | 1.76                     | 0.68              |
| 1:A:117:ALA:HA   | 1:A:120:ALA:HB3  | 1.76                     | 0.68              |
| 1:B:68:ILE:HD11  | 2:B:602:HEC:HMC3 | 1.74                     | 0.68              |
| 1:A:186:ASP:HB2  | 1:A:240:VAL:HG11 | 1.74                     | 0.68              |
| 1:D:52:ALA:O     | 1:D:53:PRO:N     | 2.27                     | 0.68              |
| 1:B:460:LEU:O    | 1:B:464:VAL:HG23 | 1.94                     | 0.67              |
| 1:B:549:ALA:HB3  | 3:B:700:FAD:N1   | 2.10                     | 0.67              |
| 1:C:35:ASN:ND2   | 1:C:71:THR:H     | 1.92                     | 0.67              |
| 1:B:58:SER:H     | 1:B:61:LYS:CE    | 2.06                     | 0.67              |
| 1:C:326:ASP:OD2  | 1:C:328:LYS:HB2  | 1.94                     | 0.67              |
| 1:D:310:ILE:HD11 | 1:D:529:LEU:HD21 | 1.76                     | 0.67              |
| 1:C:516:GLU:HG2  | 5:C:843:HOH:O    | 1.94                     | 0.67              |
| 1:C:129:VAL:HB   | 1:C:308:VAL:HG22 | 1.77                     | 0.67              |
| 3:A:600:FAD:C1'  | 3:A:600:FAD:C3'  | 2.71                     | 0.66              |
| 1:B:526:ILE:HG12 | 1:B:529:LEU:HB2  | 1.78                     | 0.66              |
| 1:D:64:LEU:HD13  | 1:D:159:ILE:CD1  | 2.23                     | 0.66              |
| 1:C:549:ALA:HB3  | 3:C:800:FAD:N1   | 2.11                     | 0.66              |
| 1:B:58:SER:H     | 1:B:61:LYS:HE2   | 1.60                     | 0.66              |
| 1:A:393:ARG:HH11 | 1:A:478:GLN:HE21 | 1.42                     | 0.66              |
| 1:C:163:ASN:HD21 | 1:C:336:ASN:ND2  | 1.93                     | 0.66              |
| 1:D:72:SER:HB2   | 1:D:158:PRO:HB2  | 1.78                     | 0.66              |
| 1:A:26:VAL:HG21  | 1:A:297:TYR:HB3  | 1.78                     | 0.66              |
| 1:D:68:ILE:HD11  | 2:D:602:HEC:CMC  | 2.26                     | 0.65              |
| 1:A:393:ARG:NH1  | 1:A:478:GLN:HE21 | 1.95                     | 0.65              |
| 1:B:280:ILE:HG13 | 1:B:347:VAL:HG13 | 1.79                     | 0.65              |
| 1:D:283:ASP:CG   | 1:D:284:ALA:H    | 2.03                     | 0.65              |
| 1:A:319:ASN:HD21 | 1:A:331:GLY:N    | 1.91                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:446:ILE:HG23 | 1:B:460:LEU:HD22 | 1.78                     | 0.65              |
| 1:A:41:CYS:SG    | 2:A:604:HEC:C3C  | 2.84                     | 0.65              |
| 1:B:321:ARG:NH2  | 1:B:346:ASP:OD1  | 2.20                     | 0.65              |
| 1:A:468:ASN:ND2  | 1:A:487:GLU:O    | 2.30                     | 0.65              |
| 1:D:514:LYS:O    | 1:D:515:ALA:HB3  | 1.97                     | 0.65              |
| 1:D:225:MET:HE1  | 1:D:260:LEU:HD23 | 1.77                     | 0.65              |
| 1:B:319:ASN:ND2  | 1:B:331:GLY:H    | 1.94                     | 0.64              |
| 1:D:288:VAL:HG22 | 1:D:526:ILE:HD11 | 1.79                     | 0.64              |
| 1:D:460:LEU:O    | 1:D:464:VAL:HG23 | 1.96                     | 0.64              |
| 1:D:506:MET:HE3  | 1:D:543:ASN:CA   | 2.19                     | 0.64              |
| 1:A:75:LYS:H     | 1:A:80:SER:HB3   | 1.62                     | 0.64              |
| 1:D:45:LEU:HD23  | 2:D:602:HEC:HBB2 | 1.78                     | 0.64              |
| 2:A:601:HEC:HHA  | 2:A:601:HEC:HBA1 | 1.79                     | 0.64              |
| 1:B:389:ARG:NH2  | 1:B:413:GLY:HA3  | 2.13                     | 0.64              |
| 1:A:68:ILE:HD11  | 2:A:602:HEC:CMC  | 2.27                     | 0.64              |
| 1:D:135:GLY:HA3  | 1:D:553:ILE:HD12 | 1.80                     | 0.64              |
| 1:D:393:ARG:NH1  | 1:D:467:TYR:HD2  | 1.94                     | 0.64              |
| 1:D:117:ALA:HA   | 1:D:120:ALA:HB3  | 1.80                     | 0.64              |
| 1:B:471:VAL:HG11 | 1:B:487:GLU:HA   | 1.80                     | 0.64              |
| 1:C:94:MET:HE2   | 2:C:602:HEC:HMD2 | 1.80                     | 0.64              |
| 1:C:530:TYR:CE2  | 1:C:563:SER:HB3  | 2.32                     | 0.64              |
| 1:A:83:TYR:CE1   | 1:A:159:ILE:HD11 | 2.34                     | 0.63              |
| 1:A:445:THR:OG1  | 1:A:448:GLU:HB2  | 1.98                     | 0.63              |
| 1:A:26:VAL:HG21  | 1:A:297:TYR:CB   | 2.28                     | 0.63              |
| 3:C:800:FAD:C1'  | 3:C:800:FAD:C3'  | 2.74                     | 0.63              |
| 1:C:231:ASP:HB3  | 1:C:245:ARG:HG3  | 1.78                     | 0.63              |
| 1:D:145:ARG:HH11 | 1:D:268:GLY:H    | 1.44                     | 0.63              |
| 1:D:154:LEU:HD13 | 1:D:277:VAL:CG2  | 2.28                     | 0.63              |
| 1:B:362:GLN:NE2  | 1:B:544:ARG:HH21 | 1.97                     | 0.63              |
| 1:A:514:LYS:HE3  | 1:A:516:GLU:CD   | 2.24                     | 0.63              |
| 1:A:127:ASP:HB2  | 1:A:150:LYS:O    | 1.96                     | 0.63              |
| 1:B:173:ALA:HA   | 1:B:215:SER:HB2  | 1.81                     | 0.63              |
| 1:B:228:ASP:HB3  | 1:B:247:THR:OG1  | 1.98                     | 0.63              |
| 1:B:449:LEU:HD22 | 1:B:495:ALA:HB2  | 1.81                     | 0.63              |
| 1:A:514:LYS:HE3  | 1:A:516:GLU:OE1  | 1.99                     | 0.63              |
| 3:A:600:FAD:C2'  | 3:A:600:FAD:N10  | 2.58                     | 0.63              |
| 1:A:387:VAL:O    | 1:A:416:ALA:HB1  | 1.98                     | 0.62              |
| 1:B:35:ASN:HD21  | 1:B:71:THR:H     | 1.46                     | 0.62              |
| 1:B:509:LEU:H    | 1:B:536:THR:HA   | 1.64                     | 0.62              |
| 1:A:106:PRO:HG2  | 1:A:109:ALA:HB2  | 1.81                     | 0.62              |
| 3:B:700:FAD:C2'  | 3:B:700:FAD:N10  | 2.58                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:431:ILE:O    | 1:C:435:VAL:HG23 | 1.99                     | 0.62              |
| 1:A:392:ASN:HA   | 1:A:463:THR:HG21 | 1.79                     | 0.62              |
| 1:B:71:THR:HA    | 1:B:74:HIS:O     | 1.99                     | 0.62              |
| 1:D:20:VAL:HG22  | 1:D:33:HIS:CG    | 2.34                     | 0.62              |
| 1:B:337:HIS:HB2  | 1:B:338:PRO:HD2  | 1.82                     | 0.62              |
| 1:A:246:PRO:HD2  | 1:A:250:ALA:O    | 2.00                     | 0.62              |
| 1:D:52:ALA:CA    | 1:D:52:ALA:O     | 2.47                     | 0.62              |
| 1:B:450:ALA:HA   | 1:B:455:VAL:HG22 | 1.81                     | 0.62              |
| 1:C:388:ASN:ND2  | 1:C:390:GLU:HB2  | 2.15                     | 0.62              |
| 1:D:553:ILE:HG13 | 1:D:554:VAL:N    | 2.13                     | 0.62              |
| 1:C:87:CYS:SG    | 2:C:601:HEC:C3C  | 2.87                     | 0.61              |
| 1:D:52:ALA:CA    | 1:D:53:PRO:CD    | 2.79                     | 0.61              |
| 1:C:409:LEU:HA   | 1:C:414:GLU:HB3  | 1.82                     | 0.61              |
| 1:B:73:CYS:CB    | 2:B:602:HEC:HAC  | 2.31                     | 0.61              |
| 1:B:325:TYR:O    | 2:D:604:HEC:HMD3 | 2.00                     | 0.61              |
| 1:B:154:LEU:HD22 | 1:B:293:VAL:HG11 | 1.82                     | 0.61              |
| 1:C:445:THR:OG1  | 1:C:448:GLU:HB2  | 2.01                     | 0.61              |
| 1:D:431:ILE:HA   | 1:D:434:TYR:CD2  | 2.36                     | 0.61              |
| 1:A:453:ILE:O    | 1:A:454:ASP:HB2  | 2.00                     | 0.61              |
| 1:B:435:VAL:HG22 | 1:B:440:VAL:HG21 | 1.82                     | 0.60              |
| 1:C:374:MET:HE1  | 3:C:800:FAD:H6   | 1.81                     | 0.60              |
| 1:D:405:SER:O    | 1:D:409:LEU:HD12 | 2.01                     | 0.60              |
| 1:B:259:VAL:O    | 1:B:263:ASN:ND2  | 2.35                     | 0.60              |
| 3:C:800:FAD:C1'  | 3:C:800:FAD:O2'  | 2.47                     | 0.60              |
| 1:A:283:ASP:OD2  | 1:A:284:ALA:N    | 2.34                     | 0.60              |
| 1:B:332:PHE:HZ   | 1:B:409:LEU:HD11 | 1.66                     | 0.60              |
| 1:C:155:GLU:OE1  | 3:C:800:FAD:H1B  | 2.01                     | 0.60              |
| 1:C:231:ASP:OD2  | 1:C:245:ARG:HD2  | 2.00                     | 0.60              |
| 1:D:228:ASP:O    | 1:D:229:MET:HE2  | 2.02                     | 0.60              |
| 1:A:35:ASN:ND2   | 1:A:70:CYS:HB2   | 2.15                     | 0.60              |
| 1:A:142:VAL:HG21 | 1:A:225:MET:CE   | 2.30                     | 0.60              |
| 1:A:153:LEU:HD22 | 1:A:271:ILE:HG23 | 1.84                     | 0.60              |
| 3:D:900:FAD:C1'  | 3:D:900:FAD:O2'  | 2.47                     | 0.60              |
| 1:C:409:LEU:HD21 | 1:C:500:PRO:HG3  | 1.84                     | 0.59              |
| 1:C:558:ARG:HH11 | 1:C:558:ARG:HG2  | 1.66                     | 0.59              |
| 1:D:394:PHE:CE1  | 1:D:395:MET:HE3  | 2.36                     | 0.59              |
| 1:B:467:TYR:HA   | 1:B:470:PHE:CD2  | 2.36                     | 0.59              |
| 1:C:389:ARG:HD2  | 1:C:412:LYS:CB   | 2.31                     | 0.59              |
| 1:C:467:TYR:HA   | 1:C:470:PHE:CD2  | 2.37                     | 0.59              |
| 1:D:73:CYS:SG    | 2:D:602:HEC:C3C  | 2.89                     | 0.59              |
| 1:C:131:ILE:HG12 | 1:C:277:VAL:HG21 | 1.83                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:388:ASN:HB3  | 1:C:411:GLN:HE21 | 1.67                     | 0.59              |
| 1:C:514:LYS:O    | 1:C:515:ALA:HB3  | 2.03                     | 0.59              |
| 1:C:68:ILE:HG13  | 1:C:68:ILE:O     | 2.02                     | 0.59              |
| 1:A:294:LYS:HB2  | 1:A:300:TYR:CE2  | 2.38                     | 0.59              |
| 1:B:527:THR:HG22 | 1:B:567:PHE:CZ   | 2.37                     | 0.59              |
| 1:D:234:ARG:HB2  | 1:D:241:ASN:OD1  | 2.02                     | 0.59              |
| 1:C:166:LEU:HD13 | 2:C:601:HEC:HMD1 | 1.84                     | 0.59              |
| 1:D:49:ALA:HB1   | 1:D:61:LYS:HB3   | 1.84                     | 0.59              |
| 1:D:218:SER:HB3  | 1:D:554:VAL:HG12 | 1.85                     | 0.59              |
| 1:B:68:ILE:HG13  | 1:B:68:ILE:O     | 2.03                     | 0.58              |
| 1:B:375:ILE:HG21 | 1:B:418:LEU:HD11 | 1.84                     | 0.58              |
| 1:B:421:ASP:HB3  | 1:B:424:ILE:HG12 | 1.85                     | 0.58              |
| 1:B:375:ILE:HG12 | 1:B:496:LEU:HD22 | 1.85                     | 0.58              |
| 1:D:78:GLU:O     | 1:D:79:LYS:C     | 2.45                     | 0.58              |
| 1:A:145:ARG:NH1  | 1:A:268:GLY:H    | 1.99                     | 0.58              |
| 1:A:163:ASN:HD21 | 1:A:336:ASN:ND2  | 2.01                     | 0.58              |
| 3:B:700:FAD:C1'  | 3:B:700:FAD:C3'  | 2.76                     | 0.58              |
| 1:A:170:GLY:HA2  | 1:A:252:VAL:HG21 | 1.85                     | 0.58              |
| 1:C:87:CYS:O     | 1:C:372:GLY:HA3  | 2.03                     | 0.58              |
| 1:B:375:ILE:HG21 | 1:B:418:LEU:CD1  | 2.33                     | 0.58              |
| 1:D:470:PHE:CG   | 1:D:476:ASP:HA   | 2.39                     | 0.58              |
| 1:C:375:ILE:HG13 | 1:C:496:LEU:HD22 | 1.86                     | 0.58              |
| 1:D:35:ASN:ND2   | 1:D:70:CYS:H     | 2.01                     | 0.58              |
| 1:A:171:MET:HE3  | 1:A:551:SER:HA   | 1.85                     | 0.58              |
| 1:C:558:ARG:HH11 | 1:C:558:ARG:CG   | 2.15                     | 0.58              |
| 1:D:159:ILE:HG13 | 5:D:930:HOH:O    | 2.04                     | 0.58              |
| 1:D:235:MET:HE3  | 1:D:547:GLY:N    | 2.19                     | 0.58              |
| 1:D:453:ILE:HD11 | 1:D:495:ALA:CB   | 2.34                     | 0.57              |
| 3:D:900:FAD:C1'  | 3:D:900:FAD:C3'  | 2.74                     | 0.57              |
| 1:C:343:ASP:HB3  | 3:C:800:FAD:H61A | 1.69                     | 0.57              |
| 1:D:28:ASN:C     | 1:D:28:ASN:HD22  | 2.12                     | 0.57              |
| 1:A:452:GLN:HA   | 1:A:452:GLN:NE2  | 2.11                     | 0.57              |
| 1:B:196:MET:CE   | 1:B:203:ASN:HB2  | 2.33                     | 0.57              |
| 1:C:294:LYS:O    | 1:C:294:LYS:HG3  | 2.04                     | 0.57              |
| 1:B:66:GLY:H     | 1:B:258:GLN:NE2  | 1.97                     | 0.57              |
| 1:D:326:ASP:OD2  | 1:D:328:LYS:HG3  | 2.04                     | 0.57              |
| 1:C:118:ILE:CD1  | 1:C:279:ARG:NH1  | 2.67                     | 0.57              |
| 3:C:800:FAD:C2'  | 3:C:800:FAD:N10  | 2.63                     | 0.57              |
| 1:D:83:TYR:CE1   | 1:D:159:ILE:HD13 | 2.39                     | 0.57              |
| 1:C:429:LYS:O    | 1:C:430:ALA:C    | 2.47                     | 0.57              |
| 1:A:470:PHE:CG   | 1:A:476:ASP:HA   | 2.40                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:517:VAL:HG21 | 1:A:529:LEU:HD22 | 1.87                     | 0.57              |
| 1:B:455:VAL:HB   | 1:B:456:PRO:HD2  | 1.87                     | 0.57              |
| 1:A:293:VAL:HG21 | 1:A:303:ILE:HD12 | 1.86                     | 0.56              |
| 1:A:71:THR:HA    | 1:A:74:HIS:O     | 2.05                     | 0.56              |
| 1:B:228:ASP:OD1  | 1:B:247:THR:HG21 | 2.06                     | 0.56              |
| 1:D:470:PHE:HA   | 1:D:475:LYS:O    | 2.05                     | 0.56              |
| 1:B:114:GLN:HE21 | 1:B:279:ARG:HH21 | 1.54                     | 0.56              |
| 1:D:516:GLU:HG2  | 1:D:525:PRO:HB3  | 1.87                     | 0.56              |
| 1:D:192:ILE:HG23 | 1:D:208:VAL:HG12 | 1.88                     | 0.56              |
| 1:B:283:ASP:CG   | 1:B:284:ALA:H    | 2.13                     | 0.56              |
| 1:C:409:LEU:CD2  | 1:C:414:GLU:HB3  | 2.36                     | 0.56              |
| 1:C:235:MET:HE2  | 1:C:243:SER:OG   | 2.05                     | 0.56              |
| 1:C:388:ASN:HD22 | 1:C:390:GLU:H    | 1.53                     | 0.56              |
| 1:A:28:ASN:HD21  | 1:A:32:THR:H     | 1.53                     | 0.56              |
| 1:A:68:ILE:C     | 1:A:68:ILE:HD12  | 2.30                     | 0.56              |
| 1:A:388:ASN:HD21 | 1:A:392:ASN:HB2  | 1.71                     | 0.56              |
| 1:B:230:THR:OG1  | 1:B:247:THR:HG23 | 2.06                     | 0.56              |
| 1:C:453:ILE:CG2  | 1:C:455:VAL:HG13 | 2.36                     | 0.56              |
| 1:D:319:ASN:ND2  | 1:D:331:GLY:H    | 2.04                     | 0.56              |
| 1:A:470:PHE:HB3  | 1:A:476:ASP:HA   | 1.87                     | 0.55              |
| 1:B:102:ARG:NH2  | 1:B:157:GLU:OE1  | 2.39                     | 0.55              |
| 1:B:403:LYS:O    | 1:B:406:ALA:HB3  | 2.06                     | 0.55              |
| 1:C:421:ASP:HB3  | 1:C:424:ILE:CG1  | 2.36                     | 0.55              |
| 1:D:41:CYS:SG    | 2:D:604:HEC:C3C  | 2.92                     | 0.55              |
| 1:D:393:ARG:HD3  | 1:D:478:GLN:NE2  | 2.20                     | 0.55              |
| 1:B:234:ARG:HB2  | 1:B:241:ASN:OD1  | 2.07                     | 0.55              |
| 1:D:403:LYS:O    | 1:D:406:ALA:HB3  | 2.07                     | 0.55              |
| 1:B:122:VAL:HG22 | 1:B:302:VAL:HG11 | 1.89                     | 0.55              |
| 1:C:380:ARG:HA   | 1:C:384:ALA:HB3  | 1.88                     | 0.55              |
| 1:C:420:PHE:CE2  | 1:C:431:ILE:HG21 | 2.42                     | 0.55              |
| 1:D:384:ALA:HB2  | 1:D:420:PHE:HB3  | 1.89                     | 0.55              |
| 1:B:366:THR:HA   | 1:B:498:ILE:HB   | 1.89                     | 0.55              |
| 1:C:376:THR:HG23 | 1:C:379:VAL:H    | 1.71                     | 0.55              |
| 1:A:135:GLY:O    | 1:A:136:ALA:C    | 2.49                     | 0.55              |
| 1:D:70:CYS:SG    | 2:D:602:HEC:C3B  | 2.93                     | 0.55              |
| 1:C:240:VAL:HG12 | 1:C:241:ASN:N    | 2.21                     | 0.55              |
| 1:C:281:LEU:N    | 1:C:290:GLY:O    | 2.26                     | 0.55              |
| 1:D:52:ALA:CA    | 1:D:53:PRO:HD3   | 2.37                     | 0.55              |
| 1:C:376:THR:HG22 | 1:C:379:VAL:HG23 | 1.89                     | 0.54              |
| 1:C:452:GLN:HA   | 1:C:452:GLN:NE2  | 2.21                     | 0.54              |
| 1:C:471:VAL:CG1  | 1:C:487:GLU:HG3  | 2.37                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:19:HIS:ND1   | 1:D:34:GLU:OE2   | 2.40                     | 0.54              |
| 1:A:461:ALA:O    | 1:A:465:THR:HG23 | 2.07                     | 0.54              |
| 1:D:468:ASN:OD1  | 1:D:487:GLU:HB3  | 2.06                     | 0.54              |
| 1:C:28:ASN:C     | 1:C:28:ASN:HD22  | 2.16                     | 0.54              |
| 1:C:453:ILE:O    | 1:C:454:ASP:HB2  | 2.07                     | 0.54              |
| 1:D:225:MET:CE   | 1:D:260:LEU:HD23 | 2.38                     | 0.54              |
| 1:A:367:TYR:HB3  | 1:A:499:ALA:O    | 2.07                     | 0.54              |
| 1:C:375:ILE:HG21 | 1:C:418:LEU:CD1  | 2.37                     | 0.54              |
| 1:A:393:ARG:HH11 | 1:A:478:GLN:HE22 | 1.53                     | 0.54              |
| 1:B:540:HIS:ND1  | 1:B:544:ARG:HG3  | 2.23                     | 0.54              |
| 1:D:175:GLU:OE2  | 1:D:188:LYS:HG3  | 2.07                     | 0.54              |
| 1:D:198:GLY:HA3  | 1:D:545:LEU:HD21 | 1.89                     | 0.54              |
| 1:B:80:SER:HB3   | 1:B:94:MET:HE3   | 1.90                     | 0.54              |
| 1:D:421:ASP:OD2  | 1:D:424:ILE:HG12 | 2.08                     | 0.54              |
| 1:A:79:LYS:HG2   | 1:A:96:PHE:O     | 2.08                     | 0.54              |
| 1:D:322:VAL:HG22 | 1:D:361:ILE:HD13 | 1.89                     | 0.54              |
| 1:A:343:ASP:HB2  | 5:A:609:HOH:O    | 2.08                     | 0.54              |
| 1:A:459:GLU:O    | 1:A:463:THR:HG23 | 2.07                     | 0.54              |
| 1:A:172:ASN:OD1  | 1:A:548:ASN:ND2  | 2.41                     | 0.53              |
| 1:A:231:ASP:HB3  | 1:A:245:ARG:HG2  | 1.89                     | 0.53              |
| 1:B:393:ARG:HD3  | 1:B:478:GLN:NE2  | 2.23                     | 0.53              |
| 1:C:385:ILE:HG12 | 1:C:488:LEU:HD21 | 1.89                     | 0.53              |
| 1:A:367:TYR:O    | 1:A:369:PRO:HD3  | 2.08                     | 0.53              |
| 1:A:504:HIS:CD2  | 1:A:544:ARG:HE   | 2.27                     | 0.53              |
| 3:A:600:FAD:C1'  | 3:A:600:FAD:O2'  | 2.51                     | 0.53              |
| 1:B:319:ASN:HD21 | 1:B:330:LYS:HA   | 1.74                     | 0.53              |
| 1:D:145:ARG:HG2  | 1:D:151:VAL:CG2  | 2.39                     | 0.53              |
| 1:D:145:ARG:NH1  | 1:D:268:GLY:H    | 2.06                     | 0.53              |
| 1:B:527:THR:HG22 | 1:B:567:PHE:HZ   | 1.72                     | 0.53              |
| 1:A:394:PHE:CE1  | 1:A:395:MET:HE3  | 2.44                     | 0.53              |
| 1:C:8:PHE:HE2    | 2:C:604:HEC:HHA  | 1.74                     | 0.53              |
| 1:C:187:LYS:HB2  | 1:C:190:ILE:CD1  | 2.38                     | 0.53              |
| 1:C:420:PHE:CE2  | 1:C:431:ILE:HD13 | 2.43                     | 0.53              |
| 1:C:453:ILE:HG21 | 1:C:455:VAL:HG13 | 1.90                     | 0.53              |
| 1:C:461:ALA:O    | 1:C:465:THR:HG22 | 2.09                     | 0.53              |
| 1:A:245:ARG:HD3  | 1:A:249:GLY:HA2  | 1.90                     | 0.53              |
| 1:A:422:ASP:OD1  | 1:A:494:TYR:OH   | 2.22                     | 0.53              |
| 1:B:58:SER:HB3   | 1:B:61:LYS:HE3   | 1.91                     | 0.53              |
| 1:B:446:ILE:CD1  | 1:B:464:VAL:HG11 | 2.38                     | 0.53              |
| 1:A:317:LYS:HB3  | 1:A:340:ALA:O    | 2.09                     | 0.53              |
| 1:C:187:LYS:HB2  | 1:C:190:ILE:HD12 | 1.90                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:550:ILE:HA   | 1:A:553:ILE:HG12 | 1.90                     | 0.53              |
| 1:B:393:ARG:HD3  | 1:B:478:GLN:HE22 | 1.73                     | 0.53              |
| 1:B:455:VAL:HB   | 1:B:456:PRO:CD   | 2.39                     | 0.53              |
| 1:C:172:ASN:O    | 1:C:551:SER:OG   | 2.26                     | 0.53              |
| 1:D:389:ARG:HG3  | 1:D:389:ARG:HH11 | 1.73                     | 0.53              |
| 1:A:167:ALA:HA   | 3:A:600:FAD:N5   | 2.24                     | 0.52              |
| 1:A:176:THR:HB   | 1:A:178:PRO:HD2  | 1.89                     | 0.52              |
| 1:D:179:GLN:NE2  | 1:D:242:ARG:HB3  | 2.23                     | 0.52              |
| 1:A:206:GLU:HA   | 1:A:209:LYS:HD2  | 1.90                     | 0.52              |
| 1:B:450:ALA:HA   | 1:B:455:VAL:CG2  | 2.40                     | 0.52              |
| 1:B:544:ARG:HD2  | 1:B:549:ALA:HB2  | 1.91                     | 0.52              |
| 1:C:173:ALA:HA   | 1:C:215:SER:HB2  | 1.91                     | 0.52              |
| 1:C:315:PHE:CD1  | 1:C:321:ARG:HG2  | 2.45                     | 0.52              |
| 1:A:458:ALA:O    | 1:A:462:LYS:HB2  | 2.09                     | 0.52              |
| 1:B:376:THR:HG22 | 1:B:434:TYR:OH   | 2.10                     | 0.52              |
| 1:B:288:VAL:CG2  | 1:B:526:ILE:HD11 | 2.39                     | 0.52              |
| 1:A:35:ASN:HD22  | 1:A:70:CYS:HB2   | 1.75                     | 0.52              |
| 1:D:377:GLU:OE1  | 1:D:401:ARG:HD3  | 2.10                     | 0.52              |
| 1:D:463:THR:O    | 1:D:464:VAL:C    | 2.52                     | 0.52              |
| 1:D:467:TYR:O    | 1:D:470:PHE:HB2  | 2.09                     | 0.52              |
| 1:B:428:LEU:O    | 1:B:429:LYS:C    | 2.53                     | 0.52              |
| 1:D:446:ILE:HD13 | 1:D:464:VAL:HG11 | 1.92                     | 0.52              |
| 1:C:225:MET:HE3  | 1:C:260:LEU:HD23 | 1.92                     | 0.52              |
| 1:D:233:GLY:HA3  | 1:D:245:ARG:NH2  | 2.24                     | 0.52              |
| 1:D:376:THR:OG1  | 1:D:377:GLU:N    | 2.41                     | 0.51              |
| 1:A:550:ILE:O    | 1:A:554:VAL:HG23 | 2.09                     | 0.51              |
| 1:D:225:MET:HE3  | 1:D:263:ASN:HB2  | 1.91                     | 0.51              |
| 1:D:68:ILE:HD12  | 1:D:68:ILE:C     | 2.34                     | 0.51              |
| 1:D:192:ILE:HD13 | 1:D:209:LYS:HG2  | 1.92                     | 0.51              |
| 1:C:146:ASP:CG   | 1:C:267:ARG:HH11 | 2.18                     | 0.51              |
| 1:C:450:ALA:HA   | 1:C:455:VAL:CG2  | 2.40                     | 0.51              |
| 3:B:700:FAD:C1'  | 3:B:700:FAD:O2'  | 2.52                     | 0.51              |
| 1:A:142:VAL:O    | 1:A:143:SER:C    | 2.54                     | 0.51              |
| 1:B:28:ASN:C     | 1:B:28:ASN:ND2   | 2.69                     | 0.51              |
| 1:B:44:ASP:OD2   | 1:B:44:ASP:C     | 2.53                     | 0.51              |
| 1:B:187:LYS:HB2  | 1:B:190:ILE:HD12 | 1.91                     | 0.51              |
| 1:C:387:VAL:HG12 | 1:C:388:ASN:O    | 2.10                     | 0.51              |
| 1:C:394:PHE:O    | 1:C:395:MET:HB3  | 2.09                     | 0.51              |
| 1:D:441:LYS:O    | 1:D:494:TYR:HA   | 2.11                     | 0.51              |
| 1:D:498:ILE:HD12 | 1:D:498:ILE:O    | 2.10                     | 0.51              |
| 1:A:526:ILE:HG12 | 1:A:529:LEU:HB2  | 1.93                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:175:GLU:HG2  | 1:B:186:ASP:O    | 2.10                     | 0.51              |
| 1:B:362:GLN:NE2  | 1:B:544:ARG:NH2  | 2.58                     | 0.51              |
| 1:B:446:ILE:HD11 | 1:B:464:VAL:HG11 | 1.92                     | 0.51              |
| 1:C:37:GLN:O     | 1:C:40:SER:HB2   | 2.11                     | 0.51              |
| 1:D:62:SER:HB3   | 2:D:601:HEC:HBB3 | 1.93                     | 0.51              |
| 1:D:80:SER:O     | 1:D:97:GLY:HA2   | 2.11                     | 0.51              |
| 1:B:362:GLN:HE22 | 1:B:544:ARG:NH2  | 2.09                     | 0.51              |
| 1:C:450:ALA:HA   | 1:C:455:VAL:HG22 | 1.93                     | 0.51              |
| 1:C:455:VAL:HB   | 1:C:456:PRO:HD2  | 1.91                     | 0.51              |
| 1:D:368:SER:HB2  | 1:D:375:ILE:HD13 | 1.92                     | 0.51              |
| 1:D:428:LEU:HB3  | 1:D:431:ILE:HG13 | 1.91                     | 0.51              |
| 1:A:366:THR:HA   | 1:A:498:ILE:HB   | 1.92                     | 0.51              |
| 1:A:322:VAL:HG13 | 1:A:361:ILE:HG21 | 1.93                     | 0.50              |
| 1:C:270:ASP:OD1  | 1:C:272:ARG:NH2  | 2.43                     | 0.50              |
| 1:D:453:ILE:CG2  | 1:D:455:VAL:HG13 | 2.41                     | 0.50              |
| 1:A:35:ASN:ND2   | 1:A:71:THR:H     | 1.99                     | 0.50              |
| 1:A:166:LEU:HD11 | 2:A:601:HEC:HBC2 | 1.93                     | 0.50              |
| 1:B:48:LEU:HD11  | 2:B:602:HEC:HMB2 | 1.93                     | 0.50              |
| 1:B:394:PHE:O    | 1:B:395:MET:HB3  | 2.11                     | 0.50              |
| 1:B:540:HIS:CG   | 1:B:544:ARG:HG3  | 2.47                     | 0.50              |
| 1:D:155:GLU:HB3  | 1:D:273:LEU:CD2  | 2.42                     | 0.50              |
| 1:D:280:ILE:HG23 | 1:D:288:VAL:HG13 | 1.93                     | 0.50              |
| 1:D:4:VAL:O      | 1:D:5:LEU:C      | 2.52                     | 0.50              |
| 1:A:80:SER:O     | 1:A:97:GLY:HA2   | 2.11                     | 0.50              |
| 1:B:441:LYS:HB2  | 1:B:495:ALA:HB3  | 1.93                     | 0.50              |
| 1:C:556:TYR:O    | 1:C:557:GLY:C    | 2.54                     | 0.50              |
| 1:D:251:GLY:O    | 1:D:252:VAL:C    | 2.54                     | 0.50              |
| 1:A:181:LYS:HE3  | 1:A:181:LYS:H    | 1.77                     | 0.50              |
| 1:A:236:GLY:N    | 1:A:377:GLU:OE2  | 2.27                     | 0.50              |
| 1:B:153:LEU:HD22 | 1:B:271:ILE:HG23 | 1.93                     | 0.50              |
| 1:A:388:ASN:ND2  | 1:A:392:ASN:H    | 2.09                     | 0.50              |
| 1:B:388:ASN:OD1  | 1:B:411:GLN:NE2  | 2.44                     | 0.50              |
| 1:C:277:VAL:HG13 | 1:C:291:VAL:CG2  | 2.42                     | 0.50              |
| 1:D:453:ILE:HD11 | 1:D:495:ALA:HB3  | 1.94                     | 0.50              |
| 1:B:68:ILE:HD12  | 1:B:68:ILE:C     | 2.37                     | 0.50              |
| 1:B:335:THR:HG22 | 1:B:367:TYR:CD2  | 2.46                     | 0.50              |
| 1:C:526:ILE:HG12 | 1:C:529:LEU:HB2  | 1.92                     | 0.50              |
| 1:D:383:GLY:HA3  | 1:D:424:ILE:HD12 | 1.94                     | 0.50              |
| 1:C:153:LEU:HD23 | 1:C:153:LEU:C    | 2.36                     | 0.50              |
| 1:C:376:THR:CG2  | 1:C:378:ALA:HB3  | 2.41                     | 0.50              |
| 1:D:385:ILE:HD13 | 1:D:488:LEU:HD13 | 1.94                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:446:ILE:HD11 | 1:A:493:PHE:CZ   | 2.47                     | 0.49              |
| 1:B:394:PHE:HD1  | 1:B:407:ALA:HB1  | 1.76                     | 0.49              |
| 1:C:399:THR:CG2  | 1:C:404:ALA:HB2  | 2.43                     | 0.49              |
| 1:D:31:LEU:HD21  | 2:D:603:HEC:CAD  | 2.39                     | 0.49              |
| 1:D:380:ARG:HH11 | 1:D:380:ARG:HB2  | 1.77                     | 0.49              |
| 1:A:187:LYS:HB2  | 1:A:190:ILE:HG13 | 1.94                     | 0.49              |
| 1:B:194:ASP:OD2  | 1:B:242:ARG:NH2  | 2.45                     | 0.49              |
| 2:C:604:HEC:HBC2 | 2:C:604:HEC:HHD  | 1.94                     | 0.49              |
| 1:A:246:PRO:HG3  | 1:A:255:HIS:CD2  | 2.47                     | 0.49              |
| 1:D:468:ASN:OD1  | 1:D:487:GLU:OE1  | 2.30                     | 0.49              |
| 1:A:234:ARG:HG3  | 1:A:235:MET:N    | 2.27                     | 0.49              |
| 1:B:228:ASP:O    | 1:B:246:PRO:HA   | 2.12                     | 0.49              |
| 1:C:203:ASN:O    | 1:C:205:PRO:HD3  | 2.12                     | 0.49              |
| 1:C:386:VAL:HG22 | 1:C:418:LEU:HD23 | 1.95                     | 0.49              |
| 1:A:171:MET:HB2  | 1:A:550:ILE:HB   | 1.93                     | 0.49              |
| 1:A:177:LYS:HE3  | 1:A:220:ASP:OD2  | 2.11                     | 0.49              |
| 1:B:196:MET:HE1  | 1:B:203:ASN:HB2  | 1.94                     | 0.49              |
| 1:D:207:LEU:O    | 1:D:211:LEU:HB2  | 2.13                     | 0.49              |
| 1:A:39:VAL:HG13  | 1:A:44:ASP:HB3   | 1.95                     | 0.49              |
| 1:A:566:LYS:O    | 1:A:567:PHE:C    | 2.55                     | 0.49              |
| 1:B:263:ASN:O    | 1:B:267:ARG:HG2  | 2.13                     | 0.49              |
| 1:B:368:SER:OG   | 1:B:371:GLY:N    | 2.38                     | 0.49              |
| 1:A:368:SER:HB2  | 1:A:375:ILE:HD13 | 1.93                     | 0.49              |
| 1:B:5:LEU:HD22   | 1:B:9:HIS:CE1    | 2.48                     | 0.49              |
| 2:B:603:HEC:HBA2 | 2:B:603:HEC:HHA  | 1.95                     | 0.49              |
| 3:C:800:FAD:O2'  | 3:C:800:FAD:C9A  | 2.61                     | 0.49              |
| 1:D:349:LEU:HD21 | 1:D:355:THR:CG2  | 2.43                     | 0.49              |
| 1:D:549:ALA:HB3  | 3:D:900:FAD:N1   | 2.27                     | 0.49              |
| 1:A:154:LEU:HD23 | 1:A:272:ARG:HB2  | 1.95                     | 0.48              |
| 1:A:506:MET:HE3  | 1:A:542:ALA:C    | 2.38                     | 0.48              |
| 1:C:346:ASP:O    | 1:C:350:GLN:HG2  | 2.12                     | 0.48              |
| 1:A:127:ASP:O    | 1:A:305:ALA:HB1  | 2.13                     | 0.48              |
| 1:B:5:LEU:HD23   | 1:B:96:PHE:CE1   | 2.49                     | 0.48              |
| 1:B:389:ARG:HH21 | 1:B:413:GLY:HA3  | 1.79                     | 0.48              |
| 1:B:453:ILE:HD11 | 1:B:495:ALA:HB2  | 1.94                     | 0.48              |
| 1:A:293:VAL:CG2  | 1:A:303:ILE:HD12 | 2.43                     | 0.48              |
| 1:C:240:VAL:CG1  | 1:C:241:ASN:N    | 2.76                     | 0.48              |
| 1:C:367:TYR:HB3  | 1:C:499:ALA:O    | 2.14                     | 0.48              |
| 1:D:73:CYS:SG    | 2:D:602:HEC:CBC  | 2.89                     | 0.48              |
| 1:D:128:VAL:HG22 | 1:D:307:ALA:HB3  | 1.94                     | 0.48              |
| 1:D:459:GLU:OE1  | 1:D:459:GLU:HA   | 2.13                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:52:ALA:HB1   | 1:A:53:PRO:HD2   | 1.94                     | 0.48              |
| 1:A:175:GLU:OE2  | 1:A:188:LYS:HG3  | 2.13                     | 0.48              |
| 1:A:360:TYR:CD2  | 1:A:542:ALA:HB1  | 2.49                     | 0.48              |
| 1:B:505:THR:HB   | 5:B:732:HOH:O    | 2.13                     | 0.48              |
| 1:C:291:VAL:HG12 | 1:C:303:ILE:HB   | 1.95                     | 0.48              |
| 1:C:394:PHE:CE1  | 1:C:395:MET:HE3  | 2.48                     | 0.48              |
| 1:A:109:ALA:O    | 1:A:110:ASP:CB   | 2.61                     | 0.48              |
| 1:A:326:ASP:OD2  | 1:A:328:LYS:HG3  | 2.14                     | 0.48              |
| 1:B:320:GLU:O    | 1:B:324:LYS:HG3  | 2.13                     | 0.48              |
| 1:B:533:GLY:CA   | 1:B:553:ILE:HG22 | 2.38                     | 0.48              |
| 1:C:512:ASP:OD1  | 1:C:512:ASP:C    | 2.56                     | 0.48              |
| 1:D:205:PRO:O    | 1:D:209:LYS:HG3  | 2.13                     | 0.48              |
| 1:D:249:GLY:O    | 1:D:250:ALA:CB   | 2.62                     | 0.48              |
| 1:D:267:ARG:HG3  | 1:D:267:ARG:HH21 | 1.78                     | 0.48              |
| 1:B:337:HIS:CE1  | 1:B:339:GLY:H    | 2.32                     | 0.48              |
| 1:C:459:GLU:HA   | 1:C:459:GLU:OE1  | 2.14                     | 0.48              |
| 1:D:102:ARG:NH2  | 1:D:157:GLU:OE1  | 2.47                     | 0.48              |
| 1:D:196:MET:CE   | 1:D:203:ASN:HB2  | 2.44                     | 0.48              |
| 1:B:468:ASN:O    | 1:B:471:VAL:HB   | 2.14                     | 0.48              |
| 1:C:533:GLY:HA2  | 1:C:553:ILE:HG22 | 1.96                     | 0.48              |
| 1:D:114:GLN:O    | 1:D:118:ILE:HG13 | 2.13                     | 0.48              |
| 1:A:72:SER:HB2   | 1:A:158:PRO:HB2  | 1.95                     | 0.48              |
| 1:A:394:PHE:HE1  | 1:A:395:MET:HE3  | 1.79                     | 0.48              |
| 2:A:601:HEC:HBA1 | 2:A:601:HEC:CHA  | 2.44                     | 0.48              |
| 1:C:421:ASP:HB3  | 1:C:424:ILE:CD1  | 2.44                     | 0.48              |
| 1:D:82:ALA:O     | 1:D:83:TYR:C     | 2.54                     | 0.48              |
| 1:A:310:ILE:CD1  | 1:A:529:LEU:HD21 | 2.43                     | 0.47              |
| 1:B:115:ASP:HA   | 1:B:118:ILE:HD12 | 1.96                     | 0.47              |
| 1:C:376:THR:HG21 | 1:C:428:LEU:HD21 | 1.95                     | 0.47              |
| 1:D:418:LEU:O    | 1:D:495:ALA:HA   | 2.14                     | 0.47              |
| 1:D:421:ASP:HB2  | 1:D:490:VAL:O    | 2.13                     | 0.47              |
| 1:A:283:ASP:CG   | 1:A:284:ALA:N    | 2.72                     | 0.47              |
| 3:B:700:FAD:H9   | 3:B:700:FAD:H1'1 | 1.60                     | 0.47              |
| 1:B:429:LYS:O    | 1:B:432:GLU:HB2  | 2.14                     | 0.47              |
| 1:C:375:ILE:HG21 | 1:C:418:LEU:HD11 | 1.94                     | 0.47              |
| 1:C:413:GLY:O    | 1:C:414:GLU:C    | 2.56                     | 0.47              |
| 1:C:446:ILE:CD1  | 1:C:464:VAL:HG11 | 2.43                     | 0.47              |
| 1:B:433:GLY:CA   | 2:B:601:HEC:HBA2 | 2.44                     | 0.47              |
| 1:C:10:GLY:HA2   | 1:C:14:GLY:HA2   | 1.95                     | 0.47              |
| 1:C:225:MET:HG2  | 1:C:263:ASN:CG   | 2.39                     | 0.47              |
| 1:A:56:LYS:HB3   | 1:A:57:VAL:HG23  | 1.96                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:167:ALA:HA   | 3:A:600:FAD:C6   | 2.43                     | 0.47              |
| 1:C:249:GLY:O    | 1:C:250:ALA:HB3  | 2.15                     | 0.47              |
| 1:C:87:CYS:SG    | 2:C:601:HEC:CBC  | 2.90                     | 0.47              |
| 1:D:156:LYS:HD3  | 3:D:900:FAD:C4A  | 2.44                     | 0.47              |
| 1:D:249:GLY:O    | 1:D:250:ALA:HB3  | 2.15                     | 0.47              |
| 1:D:293:VAL:O    | 1:D:300:TYR:HA   | 2.15                     | 0.47              |
| 1:D:506:MET:HG3  | 1:D:540:HIS:HB2  | 1.96                     | 0.47              |
| 1:D:510:VAL:HG12 | 1:D:518:LYS:HG3  | 1.96                     | 0.47              |
| 1:A:174:ALA:O    | 1:A:175:GLU:HB2  | 2.15                     | 0.47              |
| 1:C:68:ILE:HA    | 5:C:824:HOH:O    | 2.15                     | 0.47              |
| 1:C:154:LEU:HD22 | 1:C:293:VAL:HG11 | 1.96                     | 0.47              |
| 1:C:180:ALA:O    | 1:C:181:LYS:C    | 2.58                     | 0.47              |
| 1:C:192:ILE:HD13 | 1:C:209:LYS:HG2  | 1.96                     | 0.47              |
| 1:D:28:ASN:ND2   | 1:D:31:LEU:H     | 2.11                     | 0.47              |
| 1:D:319:ASN:HD21 | 1:D:331:GLY:H    | 1.61                     | 0.47              |
| 1:A:133:SER:HB3  | 1:A:155:GLU:HB2  | 1.96                     | 0.47              |
| 1:C:59:PRO:HG3   | 2:C:602:HEC:CMD  | 2.45                     | 0.47              |
| 1:C:358:LEU:HA   | 1:C:507:GLY:HA3  | 1.96                     | 0.47              |
| 1:C:549:ALA:CB   | 3:C:800:FAD:H1'2 | 2.45                     | 0.47              |
| 1:D:145:ARG:HG2  | 1:D:151:VAL:HG21 | 1.95                     | 0.47              |
| 1:D:173:ALA:HA   | 1:D:215:SER:HB2  | 1.96                     | 0.47              |
| 1:A:5:LEU:HD23   | 1:A:96:PHE:CE1   | 2.50                     | 0.47              |
| 1:B:279:ARG:HB3  | 1:B:292:LEU:HB3  | 1.97                     | 0.47              |
| 1:B:431:ILE:HG22 | 1:B:431:ILE:O    | 2.15                     | 0.47              |
| 1:C:245:ARG:HA   | 1:C:252:VAL:HG13 | 1.97                     | 0.47              |
| 1:C:421:ASP:OD1  | 1:C:490:VAL:O    | 2.33                     | 0.47              |
| 1:D:210:VAL:O    | 1:D:211:LEU:C    | 2.57                     | 0.47              |
| 1:B:20:VAL:HG22  | 1:B:33:HIS:CD2   | 2.50                     | 0.47              |
| 1:B:534:GLU:OE2  | 3:B:700:FAD:O3'  | 2.30                     | 0.47              |
| 1:C:395:MET:HG2  | 1:C:396:ASN:N    | 2.28                     | 0.47              |
| 1:C:498:ILE:HD12 | 1:C:498:ILE:O    | 2.15                     | 0.47              |
| 1:D:364:HIS:O    | 1:D:500:PRO:HA   | 2.15                     | 0.47              |
| 1:A:170:GLY:HA2  | 1:A:252:VAL:CG2  | 2.45                     | 0.46              |
| 1:B:35:ASN:ND2   | 1:B:70:CYS:H     | 2.14                     | 0.46              |
| 1:B:356:ARG:NH1  | 1:B:357:ASP:OD2  | 2.44                     | 0.46              |
| 1:B:361:ILE:HG22 | 1:B:361:ILE:O    | 2.15                     | 0.46              |
| 1:A:198:GLY:O    | 1:A:543:ASN:HB3  | 2.15                     | 0.46              |
| 1:A:356:ARG:NE   | 1:A:357:ASP:OD2  | 2.43                     | 0.46              |
| 1:B:231:ASP:HB3  | 1:B:245:ARG:HG3  | 1.97                     | 0.46              |
| 1:B:240:VAL:HG13 | 1:B:241:ASN:N    | 2.29                     | 0.46              |
| 1:C:422:ASP:OD1  | 1:C:492:PRO:HD2  | 2.15                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:26:VAL:HG21  | 1:D:297:TYR:HB3  | 1.97                     | 0.46              |
| 1:C:421:ASP:OD1  | 1:C:422:ASP:N    | 2.47                     | 0.46              |
| 1:D:424:ILE:HD11 | 1:D:486:ARG:HB2  | 1.97                     | 0.46              |
| 1:A:235:MET:SD   | 1:A:377:GLU:HB3  | 2.56                     | 0.46              |
| 1:A:504:HIS:CG   | 1:A:544:ARG:HE   | 2.33                     | 0.46              |
| 1:B:32:THR:O     | 1:B:33:HIS:C     | 2.58                     | 0.46              |
| 1:B:158:PRO:O    | 1:B:273:LEU:HD13 | 2.16                     | 0.46              |
| 1:B:402:ASP:OD1  | 1:B:403:LYS:N    | 2.44                     | 0.46              |
| 1:C:26:VAL:HG21  | 1:C:297:TYR:HB3  | 1.96                     | 0.46              |
| 1:D:28:ASN:C     | 1:D:28:ASN:ND2   | 2.74                     | 0.46              |
| 1:D:52:ALA:O     | 1:D:52:ALA:HB3   | 2.16                     | 0.46              |
| 1:D:367:TYR:O    | 1:D:369:PRO:HD3  | 2.15                     | 0.46              |
| 1:D:498:ILE:HD12 | 1:D:498:ILE:C    | 2.40                     | 0.46              |
| 3:D:900:FAD:H1'1 | 5:D:922:HOH:O    | 2.14                     | 0.46              |
| 1:A:517:VAL:CG2  | 1:A:529:LEU:HD22 | 2.45                     | 0.46              |
| 1:A:177:LYS:HG3  | 5:A:650:HOH:O    | 2.15                     | 0.46              |
| 1:C:74:HIS:HB3   | 2:C:604:HEC:HMB2 | 1.97                     | 0.46              |
| 1:C:393:ARG:NH1  | 1:C:467:TYR:HD2  | 2.14                     | 0.46              |
| 1:A:246:PRO:O    | 1:A:247:THR:C    | 2.56                     | 0.46              |
| 3:A:600:FAD:C1'  | 3:A:600:FAD:O3'  | 2.64                     | 0.46              |
| 1:B:222:LEU:HD13 | 1:B:256:VAL:HG22 | 1.97                     | 0.46              |
| 1:B:424:ILE:O    | 1:B:425:ARG:C    | 2.58                     | 0.46              |
| 1:B:481:ARG:HA   | 1:B:482:PRO:HD3  | 1.79                     | 0.46              |
| 1:C:164:THR:O    | 1:C:253:GLY:HA3  | 2.15                     | 0.46              |
| 1:C:409:LEU:HD21 | 1:C:500:PRO:CG   | 2.46                     | 0.46              |
| 1:C:420:PHE:HE2  | 1:C:431:ILE:HG21 | 1.80                     | 0.46              |
| 1:C:505:THR:O    | 1:C:506:MET:C    | 2.57                     | 0.46              |
| 1:A:118:ILE:HD13 | 1:A:281:LEU:CD2  | 2.46                     | 0.46              |
| 1:A:375:ILE:HG12 | 1:A:496:LEU:HD22 | 1.98                     | 0.46              |
| 1:B:8:PHE:HE2    | 2:B:604:HEC:HHA  | 1.81                     | 0.46              |
| 1:D:376:THR:HG22 | 1:D:434:TYR:OH   | 2.15                     | 0.46              |
| 1:A:282:GLU:O    | 1:A:283:ASP:HB3  | 2.15                     | 0.46              |
| 1:C:177:LYS:O    | 1:C:181:LYS:HG2  | 2.15                     | 0.46              |
| 1:C:184:ILE:HD13 | 1:C:241:ASN:CB   | 2.46                     | 0.46              |
| 1:C:422:ASP:HB2  | 1:C:492:PRO:HD2  | 1.97                     | 0.46              |
| 1:D:477:ALA:O    | 1:D:478:GLN:C    | 2.59                     | 0.46              |
| 1:A:266:LYS:O    | 1:A:266:LYS:HG2  | 2.15                     | 0.46              |
| 1:A:368:SER:HB2  | 1:A:375:ILE:CD1  | 2.46                     | 0.46              |
| 1:C:163:ASN:ND2  | 1:C:336:ASN:ND2  | 2.62                     | 0.46              |
| 1:C:506:MET:HE3  | 1:C:542:ALA:O    | 2.16                     | 0.46              |
| 1:D:5:LEU:HD23   | 1:D:96:PHE:CD1   | 2.50                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:291:VAL:HG12 | 1:D:303:ILE:HB   | 1.97                     | 0.46              |
| 1:A:48:LEU:HD13  | 1:A:60:HIS:CE1   | 2.51                     | 0.45              |
| 1:A:170:GLY:CA   | 1:A:252:VAL:HG21 | 2.45                     | 0.45              |
| 1:A:222:LEU:O    | 1:A:223:THR:C    | 2.59                     | 0.45              |
| 1:A:346:ASP:O    | 1:A:347:VAL:C    | 2.59                     | 0.45              |
| 1:A:422:ASP:O    | 1:A:426:LYS:HG3  | 2.15                     | 0.45              |
| 1:C:393:ARG:O    | 1:C:394:PHE:HB3  | 2.16                     | 0.45              |
| 1:C:471:VAL:HG11 | 1:C:487:GLU:HG3  | 1.96                     | 0.45              |
| 1:D:394:PHE:HE1  | 1:D:395:MET:HE3  | 1.79                     | 0.45              |
| 1:A:186:ASP:CB   | 1:A:240:VAL:HG11 | 2.43                     | 0.45              |
| 1:B:145:ARG:HH11 | 1:B:268:GLY:H    | 1.64                     | 0.45              |
| 1:B:366:THR:HG21 | 1:B:380:ARG:HE   | 1.81                     | 0.45              |
| 1:C:68:ILE:HD11  | 2:C:602:HEC:HMC2 | 1.97                     | 0.45              |
| 1:C:407:ALA:O    | 1:C:411:GLN:HG2  | 2.16                     | 0.45              |
| 1:B:512:ASP:OD2  | 1:B:516:GLU:OE2  | 2.34                     | 0.45              |
| 1:C:330:LYS:HB2  | 1:C:330:LYS:NZ   | 2.31                     | 0.45              |
| 1:D:195:THR:HG22 | 1:D:203:ASN:ND2  | 2.31                     | 0.45              |
| 1:D:240:VAL:O    | 1:D:242:ARG:HG2  | 2.16                     | 0.45              |
| 1:D:471:VAL:HG11 | 1:D:487:GLU:HG2  | 1.97                     | 0.45              |
| 1:C:109:ALA:O    | 1:C:110:ASP:CB   | 2.63                     | 0.45              |
| 1:C:402:ASP:OD1  | 1:C:402:ASP:N    | 2.44                     | 0.45              |
| 1:C:429:LYS:O    | 1:C:431:ILE:N    | 2.50                     | 0.45              |
| 1:B:135:GLY:HA3  | 1:B:553:ILE:HD12 | 1.99                     | 0.45              |
| 1:C:512:ASP:OD1  | 1:C:514:LYS:N    | 2.39                     | 0.45              |
| 1:D:378:ALA:O    | 1:D:382:ASN:HB2  | 2.17                     | 0.45              |
| 1:D:514:LYS:O    | 1:D:515:ALA:CB   | 2.64                     | 0.45              |
| 1:A:94:MET:HE2   | 2:A:602:HEC:HMD2 | 1.97                     | 0.45              |
| 1:A:145:ARG:HG2  | 1:A:151:VAL:CG2  | 2.46                     | 0.45              |
| 1:A:544:ARG:HD2  | 1:A:549:ALA:HB2  | 1.97                     | 0.45              |
| 1:B:326:ASP:OD2  | 1:B:328:LYS:HG3  | 2.16                     | 0.45              |
| 1:C:28:ASN:HD21  | 1:C:32:THR:H     | 1.65                     | 0.45              |
| 1:D:118:ILE:HD12 | 1:D:279:ARG:NH1  | 2.31                     | 0.45              |
| 1:B:267:ARG:HG2  | 1:B:267:ARG:H    | 1.63                     | 0.45              |
| 1:B:510:VAL:HA   | 5:B:734:HOH:O    | 2.16                     | 0.45              |
| 1:D:232:VAL:HA   | 1:D:243:SER:O    | 2.17                     | 0.45              |
| 2:D:601:HEC:CBD  | 2:D:601:HEC:HHA  | 2.47                     | 0.45              |
| 1:B:26:VAL:HG21  | 1:B:297:TYR:HB2  | 1.98                     | 0.45              |
| 1:B:276:ARG:NH2  | 1:B:343:ASP:OD1  | 2.38                     | 0.45              |
| 1:B:396:ASN:OD1  | 1:B:481:ARG:HA   | 2.16                     | 0.45              |
| 1:C:26:VAL:HG21  | 1:C:297:TYR:CB   | 2.46                     | 0.45              |
| 1:D:326:ASP:OD2  | 1:D:326:ASP:C    | 2.58                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:90:PHE:O     | 1:A:91:GLY:C     | 2.59                     | 0.45              |
| 1:A:480:GLU:CD   | 1:A:480:GLU:H    | 2.25                     | 0.45              |
| 1:B:410:GLN:HE21 | 1:B:410:GLN:HB2  | 1.38                     | 0.45              |
| 1:D:268:GLY:O    | 1:D:269:THR:C    | 2.59                     | 0.45              |
| 1:B:395:MET:HE2  | 1:B:404:ALA:HB1  | 1.98                     | 0.44              |
| 1:C:418:LEU:O    | 1:C:495:ALA:HA   | 2.17                     | 0.44              |
| 1:A:146:ASP:O    | 1:A:147:ALA:HB2  | 2.17                     | 0.44              |
| 1:A:366:THR:HG21 | 1:A:380:ARG:HE   | 1.82                     | 0.44              |
| 1:A:379:VAL:HG12 | 1:A:384:ALA:HB2  | 1.98                     | 0.44              |
| 1:A:413:GLY:O    | 1:A:414:GLU:C    | 2.60                     | 0.44              |
| 1:A:453:ILE:O    | 1:A:454:ASP:CB   | 2.66                     | 0.44              |
| 1:C:424:ILE:HD13 | 1:C:424:ILE:N    | 2.32                     | 0.44              |
| 1:C:459:GLU:O    | 1:C:460:LEU:C    | 2.60                     | 0.44              |
| 1:D:87:CYS:O     | 1:D:372:GLY:HA3  | 2.16                     | 0.44              |
| 1:D:371:GLY:CA   | 1:D:439:ILE:HG21 | 2.46                     | 0.44              |
| 1:A:417:TYR:CZ   | 1:A:453:ILE:HG23 | 2.52                     | 0.44              |
| 1:B:263:ASN:O    | 1:B:264:ALA:C    | 2.59                     | 0.44              |
| 1:B:282:GLU:HA   | 1:B:287:LYS:O    | 2.17                     | 0.44              |
| 1:D:192:ILE:O    | 1:D:193:ASP:C    | 2.61                     | 0.44              |
| 1:D:288:VAL:CG2  | 1:D:526:ILE:HD11 | 2.45                     | 0.44              |
| 1:D:336:ASN:HD22 | 1:D:340:ALA:CB   | 2.30                     | 0.44              |
| 1:D:375:ILE:HG21 | 1:D:418:LEU:HD11 | 1.99                     | 0.44              |
| 1:C:199:GLY:O    | 1:C:202:ILE:HG23 | 2.18                     | 0.44              |
| 1:C:200:ARG:O    | 1:C:202:ILE:HG22 | 2.18                     | 0.44              |
| 1:D:326:ASP:OD1  | 1:D:328:LYS:HD2  | 2.17                     | 0.44              |
| 1:B:85:ASP:O     | 1:B:86:ALA:C     | 2.56                     | 0.44              |
| 1:B:449:LEU:HD22 | 1:B:495:ALA:CB   | 2.46                     | 0.44              |
| 1:A:62:SER:CB    | 2:A:601:HEC:HBB3 | 2.44                     | 0.44              |
| 1:A:167:ALA:HA   | 3:A:600:FAD:C5X  | 2.48                     | 0.44              |
| 1:C:7:ASP:O      | 1:C:8:PHE:C      | 2.58                     | 0.44              |
| 1:D:52:ALA:O     | 1:D:52:ALA:CB    | 2.66                     | 0.44              |
| 1:D:431:ILE:HA   | 1:D:434:TYR:HD2  | 1.83                     | 0.44              |
| 1:A:12:MET:HE1   | 2:A:604:HEC:CAD  | 2.47                     | 0.44              |
| 1:A:46:LYS:O     | 1:A:49:ALA:HB3   | 2.18                     | 0.44              |
| 1:A:280:ILE:HA   | 1:A:291:VAL:HG23 | 1.99                     | 0.44              |
| 1:A:425:ARG:HH21 | 1:A:435:VAL:HG21 | 1.83                     | 0.44              |
| 1:B:422:ASP:OD1  | 1:B:494:TYR:OH   | 2.36                     | 0.44              |
| 1:C:321:ARG:NH2  | 1:C:342:GLY:HA3  | 2.32                     | 0.44              |
| 1:C:511:ILE:HA   | 1:C:516:GLU:O    | 2.17                     | 0.44              |
| 1:D:66:GLY:H     | 1:D:258:GLN:NE2  | 2.10                     | 0.44              |
| 1:D:187:LYS:HB2  | 1:D:190:ILE:HG13 | 1.99                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:470:PHE:CD1  | 1:D:476:ASP:HA   | 2.52                     | 0.44              |
| 1:A:177:LYS:O    | 1:A:181:LYS:HE3  | 2.18                     | 0.44              |
| 1:B:394:PHE:CD1  | 1:B:407:ALA:HB1  | 2.52                     | 0.44              |
| 1:C:35:ASN:ND2   | 1:C:69:ALA:HB1   | 2.33                     | 0.44              |
| 1:C:428:LEU:HD23 | 1:C:431:ILE:HG13 | 1.99                     | 0.44              |
| 1:D:225:MET:HE3  | 1:D:263:ASN:HB3  | 1.99                     | 0.44              |
| 1:A:82:ALA:O     | 1:A:85:ASP:HB2   | 2.18                     | 0.43              |
| 1:A:294:LYS:HB2  | 1:A:300:TYR:CD2  | 2.53                     | 0.43              |
| 1:A:410:GLN:HE21 | 1:A:410:GLN:HB2  | 1.38                     | 0.43              |
| 1:B:283:ASP:OD2  | 1:B:284:ALA:N    | 2.51                     | 0.43              |
| 1:D:280:ILE:HD12 | 1:D:347:VAL:HG13 | 2.00                     | 0.43              |
| 1:A:141:ALA:O    | 1:A:142:VAL:O    | 2.36                     | 0.43              |
| 1:A:478:GLN:HB3  | 1:A:479:PHE:CD1  | 2.53                     | 0.43              |
| 1:B:467:TYR:O    | 1:B:471:VAL:HG23 | 2.18                     | 0.43              |
| 1:B:26:VAL:HG21  | 1:B:297:TYR:CB   | 2.49                     | 0.43              |
| 1:B:516:GLU:HG2  | 5:B:741:HOH:O    | 2.18                     | 0.43              |
| 1:B:87:CYS:O     | 1:B:372:GLY:HA3  | 2.19                     | 0.43              |
| 1:B:514:LYS:O    | 1:B:515:ALA:HB3  | 2.18                     | 0.43              |
| 1:B:557:GLY:O    | 1:B:558:ARG:C    | 2.59                     | 0.43              |
| 1:C:28:ASN:C     | 1:C:28:ASN:ND2   | 2.76                     | 0.43              |
| 1:C:366:THR:HG23 | 1:C:380:ARG:HH21 | 1.83                     | 0.43              |
| 1:D:471:VAL:CG1  | 1:D:487:GLU:HG2  | 2.48                     | 0.43              |
| 1:A:130:ILE:O    | 1:A:153:LEU:HA   | 2.18                     | 0.43              |
| 1:B:246:PRO:HD3  | 1:B:252:VAL:HG13 | 2.00                     | 0.43              |
| 1:B:448:GLU:HA   | 1:B:451:LYS:HD2  | 2.00                     | 0.43              |
| 1:C:514:LYS:O    | 1:C:515:ALA:CB   | 2.66                     | 0.43              |
| 1:A:145:ARG:HG2  | 1:A:151:VAL:HG21 | 2.00                     | 0.43              |
| 1:A:206:GLU:OE2  | 1:A:209:LYS:NZ   | 2.48                     | 0.43              |
| 1:D:155:GLU:HB3  | 1:D:273:LEU:HD22 | 1.99                     | 0.43              |
| 1:D:196:MET:HE1  | 1:D:203:ASN:HB2  | 1.99                     | 0.43              |
| 1:D:383:GLY:HA3  | 1:D:424:ILE:CD1  | 2.49                     | 0.43              |
| 1:A:225:MET:HG2  | 1:A:263:ASN:OD1  | 2.18                     | 0.43              |
| 1:A:470:PHE:CB   | 1:A:476:ASP:HA   | 2.49                     | 0.43              |
| 1:B:33:HIS:O     | 1:B:34:GLU:C     | 2.60                     | 0.43              |
| 1:C:163:ASN:HD21 | 1:C:336:ASN:CG   | 2.27                     | 0.43              |
| 1:C:175:GLU:CD   | 1:C:188:LYS:HG3  | 2.44                     | 0.43              |
| 1:C:397:GLU:HB2  | 1:C:481:ARG:NH1  | 2.34                     | 0.43              |
| 1:D:44:ASP:H     | 1:D:47:GLU:HB2   | 1.83                     | 0.43              |
| 1:D:179:GLN:HE22 | 1:D:242:ARG:HB3  | 1.84                     | 0.43              |
| 1:D:400:THR:O    | 1:D:403:LYS:N    | 2.47                     | 0.43              |
| 1:A:132:GLY:CA   | 3:A:600:FAD:H4B  | 2.49                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:171:MET:O    | 1:B:244:HIS:HB2  | 2.19                     | 0.43              |
| 1:B:195:THR:HG21 | 1:B:208:VAL:HG13 | 2.01                     | 0.43              |
| 1:B:317:LYS:HG3  | 1:B:317:LYS:O    | 2.19                     | 0.43              |
| 1:B:349:LEU:HD21 | 1:B:355:THR:HG23 | 2.01                     | 0.43              |
| 1:B:433:GLY:HA2  | 2:B:601:HEC:HBA2 | 2.01                     | 0.43              |
| 1:C:127:ASP:HB2  | 1:C:150:LYS:O    | 2.19                     | 0.43              |
| 1:D:53:PRO:O     | 1:D:54:LYS:C     | 2.61                     | 0.43              |
| 1:D:198:GLY:O    | 1:D:543:ASN:HB3  | 2.18                     | 0.43              |
| 1:D:422:ASP:HB3  | 1:D:490:VAL:HG12 | 2.00                     | 0.43              |
| 1:B:234:ARG:HB2  | 1:B:234:ARG:HE   | 1.74                     | 0.43              |
| 1:B:435:VAL:CG2  | 1:B:440:VAL:HG21 | 2.49                     | 0.43              |
| 1:D:172:ASN:OD1  | 1:D:548:ASN:ND2  | 2.52                     | 0.43              |
| 1:A:225:MET:HE2  | 1:A:263:ASN:HB2  | 2.00                     | 0.42              |
| 1:B:240:VAL:HG22 | 1:B:241:ASN:H    | 1.84                     | 0.42              |
| 1:B:278:VAL:HG23 | 1:B:292:LEU:HD12 | 2.01                     | 0.42              |
| 1:C:170:GLY:HA2  | 1:C:252:VAL:HG21 | 2.01                     | 0.42              |
| 1:D:65:ILE:HB    | 1:D:258:GLN:NE2  | 2.33                     | 0.42              |
| 1:D:177:LYS:HB2  | 1:D:178:PRO:HD3  | 2.00                     | 0.42              |
| 1:D:375:ILE:HG21 | 1:D:418:LEU:CD1  | 2.49                     | 0.42              |
| 1:A:428:LEU:HB3  | 1:A:431:ILE:HD12 | 2.02                     | 0.42              |
| 1:B:164:THR:O    | 1:B:253:GLY:HA3  | 2.19                     | 0.42              |
| 1:D:204:ASP:O    | 1:D:208:VAL:HG23 | 2.19                     | 0.42              |
| 1:D:266:LYS:C    | 1:D:267:ARG:O    | 2.61                     | 0.42              |
| 1:D:488:LEU:HD23 | 1:D:488:LEU:O    | 2.19                     | 0.42              |
| 1:B:127:ASP:HB2  | 1:B:150:LYS:H    | 1.84                     | 0.42              |
| 1:B:456:PRO:HB2  | 1:B:459:GLU:HB2  | 2.00                     | 0.42              |
| 1:D:42:HIS:CE1   | 2:D:604:HEC:ND   | 2.87                     | 0.42              |
| 1:D:455:VAL:HB   | 1:D:456:PRO:CD   | 2.46                     | 0.42              |
| 1:A:153:LEU:HD23 | 1:A:153:LEU:C    | 2.44                     | 0.42              |
| 1:A:326:ASP:OD2  | 1:A:328:LYS:HB2  | 2.18                     | 0.42              |
| 1:A:334:ALA:HA   | 1:A:502:VAL:O    | 2.19                     | 0.42              |
| 1:A:453:ILE:CG2  | 1:A:455:VAL:HG13 | 2.49                     | 0.42              |
| 1:C:145:ARG:NH1  | 1:C:267:ARG:O    | 2.52                     | 0.42              |
| 1:C:184:ILE:HD13 | 1:C:241:ASN:HB3  | 2.02                     | 0.42              |
| 1:C:367:TYR:O    | 1:C:369:PRO:HD3  | 2.19                     | 0.42              |
| 1:C:394:PHE:O    | 1:C:395:MET:CB   | 2.67                     | 0.42              |
| 1:D:376:THR:O    | 1:D:379:VAL:HG23 | 2.20                     | 0.42              |
| 1:A:74:HIS:CE1   | 2:A:602:HEC:ND   | 2.87                     | 0.42              |
| 1:B:394:PHE:CE1  | 1:B:395:MET:SD   | 3.13                     | 0.42              |
| 1:D:119:ALA:O    | 1:D:121:GLY:N    | 2.38                     | 0.42              |
| 1:D:192:ILE:HG23 | 1:D:208:VAL:CG1  | 2.49                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:65:ILE:H     | 1:A:65:ILE:HG13  | 1.71                     | 0.42              |
| 1:A:272:ARG:O    | 1:A:275:SER:HB2  | 2.20                     | 0.42              |
| 1:B:204:ASP:OD1  | 1:B:206:GLU:N    | 2.53                     | 0.42              |
| 1:C:234:ARG:HE   | 1:C:234:ARG:HB2  | 1.43                     | 0.42              |
| 1:D:68:ILE:HG13  | 1:D:68:ILE:O     | 2.20                     | 0.42              |
| 1:D:450:ALA:HA   | 1:D:455:VAL:HG22 | 2.02                     | 0.42              |
| 1:A:506:MET:HE3  | 1:A:542:ALA:O    | 2.20                     | 0.42              |
| 1:B:171:MET:HG3  | 1:B:550:ILE:HG22 | 2.01                     | 0.42              |
| 1:B:401:ARG:NH2  | 4:B:714:SO4:O1   | 2.38                     | 0.42              |
| 1:B:409:LEU:HD23 | 1:B:409:LEU:HA   | 1.89                     | 0.42              |
| 1:C:471:VAL:HG21 | 1:C:487:GLU:HA   | 2.01                     | 0.42              |
| 1:D:136:ALA:HB2  | 1:D:553:ILE:HB   | 2.01                     | 0.42              |
| 1:D:188:LYS:O    | 1:D:192:ILE:HG13 | 2.19                     | 0.42              |
| 1:A:26:VAL:CG2   | 1:A:297:TYR:HB3  | 2.49                     | 0.42              |
| 1:B:196:MET:HE3  | 1:B:196:MET:HA   | 2.02                     | 0.42              |
| 1:B:396:ASN:O    | 1:B:397:GLU:C    | 2.62                     | 0.42              |
| 1:C:154:LEU:HD13 | 1:C:293:VAL:HG22 | 2.01                     | 0.42              |
| 1:C:279:ARG:HB3  | 1:C:292:LEU:HB2  | 2.01                     | 0.42              |
| 1:C:374:MET:CE   | 3:C:800:FAD:H6   | 2.48                     | 0.42              |
| 1:D:460:LEU:HD23 | 1:D:460:LEU:HA   | 1.91                     | 0.42              |
| 1:A:181:LYS:HE3  | 1:A:181:LYS:N    | 2.34                     | 0.42              |
| 1:B:445:THR:O    | 1:B:446:ILE:C    | 2.63                     | 0.42              |
| 1:C:146:ASP:OD2  | 1:C:267:ARG:NH1  | 2.51                     | 0.42              |
| 1:C:364:HIS:O    | 1:C:500:PRO:HA   | 2.20                     | 0.42              |
| 1:C:484:LEU:HA   | 1:C:485:PRO:HD2  | 1.89                     | 0.42              |
| 3:C:800:FAD:H8A  | 3:C:800:FAD:H2B  | 1.90                     | 0.42              |
| 1:D:39:VAL:HA    | 1:D:43:GLY:O     | 2.20                     | 0.42              |
| 3:D:900:FAD:N10  | 3:D:900:FAD:O2'  | 2.52                     | 0.42              |
| 1:A:433:GLY:HA3  | 2:A:601:HEC:HBA2 | 2.02                     | 0.42              |
| 1:C:60:HIS:CD2   | 2:C:602:HEC:NC   | 2.87                     | 0.42              |
| 1:C:80:SER:O     | 1:C:97:GLY:HA2   | 2.20                     | 0.42              |
| 1:C:233:GLY:HA3  | 1:C:245:ARG:HH22 | 1.78                     | 0.42              |
| 1:D:181:LYS:HE2  | 1:D:181:LYS:HA   | 2.02                     | 0.42              |
| 1:D:26:VAL:HG11  | 1:D:31:LEU:HD11  | 2.02                     | 0.41              |
| 1:D:319:ASN:HD21 | 1:D:331:GLY:N    | 2.17                     | 0.41              |
| 1:D:485:PRO:HB2  | 1:D:486:ARG:H    | 1.58                     | 0.41              |
| 1:D:83:TYR:O     | 1:D:84:CYS:C     | 2.62                     | 0.41              |
| 1:A:68:ILE:O     | 1:A:68:ILE:HG13  | 2.20                     | 0.41              |
| 1:B:199:GLY:HA3  | 1:B:203:ASN:OD1  | 2.19                     | 0.41              |
| 1:B:210:VAL:HG13 | 1:B:214:ASN:ND2  | 2.36                     | 0.41              |
| 1:B:316:ALA:HB3  | 1:B:336:ASN:ND2  | 2.35                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:37:GLN:O     | 1:D:40:SER:HB2   | 2.21                     | 0.41              |
| 1:D:376:THR:HG23 | 1:D:379:VAL:HG23 | 2.03                     | 0.41              |
| 1:D:430:ALA:O    | 1:D:433:GLY:N    | 2.47                     | 0.41              |
| 1:D:458:ALA:O    | 1:D:462:LYS:HB2  | 2.20                     | 0.41              |
| 1:A:310:ILE:HD12 | 1:A:529:LEU:HD21 | 2.02                     | 0.41              |
| 1:A:449:LEU:HD11 | 1:A:495:ALA:HB2  | 2.00                     | 0.41              |
| 1:B:220:ASP:O    | 1:B:224:SER:HB3  | 2.20                     | 0.41              |
| 1:D:37:GLN:HA    | 1:D:40:SER:HB2   | 2.03                     | 0.41              |
| 1:D:105:VAL:HA   | 1:D:106:PRO:HD2  | 1.90                     | 0.41              |
| 1:D:114:GLN:HG2  | 1:D:300:TYR:CE2  | 2.55                     | 0.41              |
| 1:D:329:LEU:HD13 | 1:D:502:VAL:HG22 | 2.02                     | 0.41              |
| 1:D:446:ILE:HG21 | 1:D:464:VAL:HG21 | 2.02                     | 0.41              |
| 1:D:499:ALA:HA   | 1:D:500:PRO:HD3  | 1.96                     | 0.41              |
| 3:D:900:FAD:H1'1 | 3:D:900:FAD:H9   | 1.82                     | 0.41              |
| 1:A:26:VAL:HG21  | 1:A:297:TYR:HB2  | 2.01                     | 0.41              |
| 1:A:433:GLY:O    | 1:A:437:LEU:HG   | 2.20                     | 0.41              |
| 1:C:63:HIS:CD2   | 2:C:601:HEC:NA   | 2.89                     | 0.41              |
| 1:C:409:LEU:CD2  | 1:C:500:PRO:HG3  | 2.50                     | 0.41              |
| 1:A:409:LEU:HD23 | 1:A:409:LEU:HA   | 1.92                     | 0.41              |
| 1:A:453:ILE:HG21 | 1:A:455:VAL:HG13 | 2.01                     | 0.41              |
| 2:A:602:HEC:HBA2 | 1:C:360:TYR:OH   | 2.21                     | 0.41              |
| 1:C:376:THR:HG23 | 1:C:378:ALA:HB3  | 2.03                     | 0.41              |
| 1:C:376:THR:HG21 | 1:C:378:ALA:HB3  | 2.02                     | 0.41              |
| 1:D:62:SER:CB    | 2:D:601:HEC:HBB3 | 2.51                     | 0.41              |
| 1:B:79:LYS:NZ    | 1:B:97:GLY:O     | 2.46                     | 0.41              |
| 1:C:471:VAL:HB   | 1:C:487:GLU:HG3  | 2.03                     | 0.41              |
| 1:D:110:ASP:O    | 1:D:114:GLN:HG3  | 2.21                     | 0.41              |
| 1:D:270:ASP:OD2  | 1:D:270:ASP:C    | 2.64                     | 0.41              |
| 1:D:371:GLY:HA2  | 1:D:439:ILE:HG21 | 2.01                     | 0.41              |
| 1:A:204:ASP:HB3  | 1:A:207:LEU:HD12 | 2.02                     | 0.41              |
| 1:A:286:GLY:O    | 1:A:526:ILE:HD12 | 2.20                     | 0.41              |
| 1:A:471:VAL:HG22 | 1:A:484:LEU:HB3  | 2.03                     | 0.41              |
| 1:B:87:CYS:SG    | 2:B:601:HEC:CBC  | 2.94                     | 0.41              |
| 1:B:186:ASP:OD2  | 1:B:242:ARG:HD3  | 2.21                     | 0.41              |
| 1:B:499:ALA:HA   | 1:B:500:PRO:HD3  | 1.83                     | 0.41              |
| 1:C:425:ARG:HD2  | 1:C:432:GLU:OE1  | 2.21                     | 0.41              |
| 1:D:153:LEU:C    | 1:D:153:LEU:HD23 | 2.46                     | 0.41              |
| 1:D:428:LEU:HD23 | 1:D:431:ILE:HG13 | 2.03                     | 0.41              |
| 1:A:44:ASP:O     | 1:A:45:LEU:C     | 2.64                     | 0.41              |
| 1:C:483:ASP:OD2  | 1:C:485:PRO:HD3  | 2.21                     | 0.41              |
| 1:D:75:LYS:HB2   | 1:D:78:GLU:O     | 2.21                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:166:LEU:HD21 | 2:D:601:HEC:HBC2 | 2.02                     | 0.41              |
| 1:C:342:GLY:O    | 1:C:343:ASP:C    | 2.62                     | 0.40              |
| 1:C:540:HIS:O    | 1:C:541:GLY:C    | 2.63                     | 0.40              |
| 1:D:94:MET:HB2   | 2:D:602:HEC:HMD2 | 2.01                     | 0.40              |
| 1:A:554:VAL:O    | 1:A:555:THR:C    | 2.64                     | 0.40              |
| 1:C:15:CYS:HB3   | 1:C:22:ASP:HA    | 2.03                     | 0.40              |
| 1:C:116:LYS:O    | 1:C:120:ALA:HB2  | 2.22                     | 0.40              |
| 1:B:280:ILE:HG13 | 1:B:347:VAL:CG1  | 2.51                     | 0.40              |
| 1:B:400:THR:O    | 1:B:401:ARG:C    | 2.64                     | 0.40              |
| 1:C:8:PHE:HE2    | 2:C:604:HEC:CHA  | 2.34                     | 0.40              |
| 1:C:109:ALA:O    | 1:C:110:ASP:HB2  | 2.21                     | 0.40              |
| 1:C:409:LEU:HD22 | 1:C:414:GLU:CB   | 2.49                     | 0.40              |
| 1:C:455:VAL:HB   | 1:C:456:PRO:CD   | 2.51                     | 0.40              |
| 1:C:263:ASN:O    | 1:C:264:ALA:C    | 2.64                     | 0.40              |
| 1:C:398:ILE:CD1  | 1:C:482:PRO:HD2  | 2.51                     | 0.40              |
| 1:D:190:ILE:O    | 1:D:194:ASP:HB2  | 2.22                     | 0.40              |
| 1:D:380:ARG:O    | 1:D:481:ARG:NH2  | 2.55                     | 0.40              |
| 1:A:316:ALA:HB1  | 1:A:502:VAL:HG12 | 2.03                     | 0.40              |
| 1:B:82:ALA:O     | 1:B:83:TYR:C     | 2.64                     | 0.40              |
| 1:C:39:VAL:O     | 1:C:40:SER:C     | 2.65                     | 0.40              |
| 1:C:332:PHE:HE1  | 1:C:500:PRO:HB2  | 1.87                     | 0.40              |

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:A:125:THR:OG1 | 1:C:247:THR:OG1[4_555] | 2.12                     | 0.08              |
| 1:C:125:THR:OG1 | 1:D:247:THR:OG1[4_456] | 2.15                     | 0.05              |

## 5.3 Torsion angles [i](#)

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

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

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



| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|-----------|----------|-------------|----|
| 1   | A     | 568/572 (99%)   | 504 (89%)  | 51 (9%)   | 13 (2%)  | 5           | 19 |
| 1   | B     | 562/572 (98%)   | 495 (88%)  | 52 (9%)   | 15 (3%)  | 4           | 16 |
| 1   | C     | 566/572 (99%)   | 482 (85%)  | 64 (11%)  | 20 (4%)  | 3           | 12 |
| 1   | D     | 566/572 (99%)   | 488 (86%)  | 61 (11%)  | 17 (3%)  | 3           | 14 |
| All | All   | 2262/2288 (99%) | 1969 (87%) | 228 (10%) | 65 (3%)  | 3           | 15 |

All (65) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 57  | VAL  |
| 1   | A     | 142 | VAL  |
| 1   | A     | 147 | ALA  |
| 1   | A     | 454 | ASP  |
| 1   | B     | 250 | ALA  |
| 1   | B     | 357 | ASP  |
| 1   | B     | 388 | ASN  |
| 1   | B     | 454 | ASP  |
| 1   | C     | 250 | ALA  |
| 1   | C     | 284 | ALA  |
| 1   | C     | 394 | PHE  |
| 1   | C     | 401 | ARG  |
| 1   | C     | 454 | ASP  |
| 1   | D     | 120 | ALA  |
| 1   | D     | 250 | ALA  |
| 1   | D     | 357 | ASP  |
| 1   | D     | 454 | ASP  |
| 1   | D     | 485 | PRO  |
| 1   | A     | 143 | SER  |
| 1   | A     | 283 | ASP  |
| 1   | A     | 513 | THR  |
| 1   | B     | 240 | VAL  |
| 1   | B     | 247 | THR  |
| 1   | B     | 251 | GLY  |
| 1   | B     | 412 | LYS  |
| 1   | B     | 478 | GLN  |
| 1   | C     | 120 | ALA  |
| 1   | C     | 414 | GLU  |
| 1   | C     | 415 | SER  |
| 1   | C     | 451 | LYS  |
| 1   | C     | 485 | PRO  |
| 1   | D     | 267 | ARG  |
| 1   | D     | 401 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 478 | GLN  |
| 1   | A     | 110 | ASP  |
| 1   | A     | 120 | ALA  |
| 1   | A     | 343 | ASP  |
| 1   | B     | 148 | GLY  |
| 1   | B     | 201 | ASN  |
| 1   | B     | 489 | VAL  |
| 1   | C     | 180 | ALA  |
| 1   | C     | 343 | ASP  |
| 1   | C     | 410 | GLN  |
| 1   | D     | 11  | GLU  |
| 1   | D     | 17  | SER  |
| 1   | D     | 148 | GLY  |
| 1   | B     | 215 | SER  |
| 1   | B     | 284 | ALA  |
| 1   | C     | 56  | LYS  |
| 1   | C     | 201 | ASN  |
| 1   | C     | 492 | PRO  |
| 1   | D     | 329 | LEU  |
| 1   | A     | 55  | ASP  |
| 1   | C     | 430 | ALA  |
| 1   | D     | 464 | VAL  |
| 1   | B     | 13  | GLY  |
| 1   | C     | 412 | LYS  |
| 1   | D     | 13  | GLY  |
| 1   | D     | 283 | ASP  |
| 1   | A     | 4   | VAL  |
| 1   | A     | 162 | GLY  |
| 1   | D     | 369 | PRO  |
| 1   | C     | 286 | GLY  |
| 1   | C     | 398 | ILE  |
| 1   | D     | 482 | PRO  |

### 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     | 409/429 (95%)   | 343 (84%)  | 66 (16%)  | 2           | 8 |
| 1   | B     | 406/429 (95%)   | 339 (84%)  | 67 (16%)  | 2           | 8 |
| 1   | C     | 405/429 (94%)   | 328 (81%)  | 77 (19%)  | 1           | 5 |
| 1   | D     | 407/429 (95%)   | 339 (83%)  | 68 (17%)  | 2           | 7 |
| All | All   | 1627/1716 (95%) | 1349 (83%) | 278 (17%) | 2           | 7 |

All (278) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 11  | GLU  |
| 1   | A     | 16  | ASP  |
| 1   | A     | 17  | SER  |
| 1   | A     | 20  | VAL  |
| 1   | A     | 28  | ASN  |
| 1   | A     | 31  | LEU  |
| 1   | A     | 32  | THR  |
| 1   | A     | 55  | ASP  |
| 1   | A     | 67  | GLU  |
| 1   | A     | 68  | ILE  |
| 1   | A     | 79  | LYS  |
| 1   | A     | 80  | SER  |
| 1   | A     | 102 | ARG  |
| 1   | A     | 105 | VAL  |
| 1   | A     | 150 | LYS  |
| 1   | A     | 156 | LYS  |
| 1   | A     | 181 | LYS  |
| 1   | A     | 192 | ILE  |
| 1   | A     | 211 | LEU  |
| 1   | A     | 239 | SER  |
| 1   | A     | 245 | ARG  |
| 1   | A     | 252 | VAL  |
| 1   | A     | 259 | VAL  |
| 1   | A     | 273 | LEU  |
| 1   | A     | 282 | GLU  |
| 1   | A     | 283 | ASP  |
| 1   | A     | 291 | VAL  |
| 1   | A     | 292 | LEU  |
| 1   | A     | 296 | GLU  |
| 1   | A     | 328 | LYS  |
| 1   | A     | 330 | LYS  |
| 1   | A     | 345 | LEU  |
| 1   | A     | 350 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 359 | GLU  |
| 1   | A     | 375 | ILE  |
| 1   | A     | 385 | ILE  |
| 1   | A     | 387 | VAL  |
| 1   | A     | 388 | ASN  |
| 1   | A     | 390 | GLU  |
| 1   | A     | 395 | MET  |
| 1   | A     | 401 | ARG  |
| 1   | A     | 402 | ASP  |
| 1   | A     | 414 | GLU  |
| 1   | A     | 423 | SER  |
| 1   | A     | 426 | LYS  |
| 1   | A     | 432 | GLU  |
| 1   | A     | 442 | GLU  |
| 1   | A     | 444 | LYS  |
| 1   | A     | 446 | ILE  |
| 1   | A     | 448 | GLU  |
| 1   | A     | 449 | LEU  |
| 1   | A     | 452 | GLN  |
| 1   | A     | 459 | GLU  |
| 1   | A     | 460 | LEU  |
| 1   | A     | 463 | THR  |
| 1   | A     | 465 | THR  |
| 1   | A     | 480 | GLU  |
| 1   | A     | 487 | GLU  |
| 1   | A     | 488 | LEU  |
| 1   | A     | 489 | VAL  |
| 1   | A     | 496 | LEU  |
| 1   | A     | 518 | LYS  |
| 1   | A     | 520 | GLU  |
| 1   | A     | 526 | ILE  |
| 1   | A     | 529 | LEU  |
| 1   | A     | 534 | GLU  |
| 1   | B     | 5   | LEU  |
| 1   | B     | 16  | ASP  |
| 1   | B     | 26  | VAL  |
| 1   | B     | 28  | ASN  |
| 1   | B     | 31  | LEU  |
| 1   | B     | 54  | LYS  |
| 1   | B     | 61  | LYS  |
| 1   | B     | 68  | ILE  |
| 1   | B     | 78  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 79  | LYS  |
| 1   | B     | 81  | VAL  |
| 1   | B     | 89  | SER  |
| 1   | B     | 93  | ASP  |
| 1   | B     | 102 | ARG  |
| 1   | B     | 105 | VAL  |
| 1   | B     | 165 | LYS  |
| 1   | B     | 184 | ILE  |
| 1   | B     | 201 | ASN  |
| 1   | B     | 206 | GLU  |
| 1   | B     | 211 | LEU  |
| 1   | B     | 219 | ILE  |
| 1   | B     | 224 | SER  |
| 1   | B     | 232 | VAL  |
| 1   | B     | 234 | ARG  |
| 1   | B     | 240 | VAL  |
| 1   | B     | 247 | THR  |
| 1   | B     | 252 | VAL  |
| 1   | B     | 259 | VAL  |
| 1   | B     | 267 | ARG  |
| 1   | B     | 282 | GLU  |
| 1   | B     | 287 | LYS  |
| 1   | B     | 291 | VAL  |
| 1   | B     | 294 | LYS  |
| 1   | B     | 322 | VAL  |
| 1   | B     | 345 | LEU  |
| 1   | B     | 347 | VAL  |
| 1   | B     | 350 | GLN  |
| 1   | B     | 374 | MET  |
| 1   | B     | 375 | ILE  |
| 1   | B     | 376 | THR  |
| 1   | B     | 377 | GLU  |
| 1   | B     | 386 | VAL  |
| 1   | B     | 387 | VAL  |
| 1   | B     | 392 | ASN  |
| 1   | B     | 395 | MET  |
| 1   | B     | 405 | SER  |
| 1   | B     | 410 | GLN  |
| 1   | B     | 415 | SER  |
| 1   | B     | 423 | SER  |
| 1   | B     | 429 | LYS  |
| 1   | B     | 432 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 444 | LYS  |
| 1   | B     | 445 | THR  |
| 1   | B     | 447 | GLU  |
| 1   | B     | 452 | GLN  |
| 1   | B     | 460 | LEU  |
| 1   | B     | 463 | THR  |
| 1   | B     | 478 | GLN  |
| 1   | B     | 480 | GLU  |
| 1   | B     | 488 | LEU  |
| 1   | B     | 489 | VAL  |
| 1   | B     | 496 | LEU  |
| 1   | B     | 506 | MET  |
| 1   | B     | 518 | LYS  |
| 1   | B     | 522 | THR  |
| 1   | B     | 526 | ILE  |
| 1   | B     | 529 | LEU  |
| 1   | C     | 15  | CYS  |
| 1   | C     | 16  | ASP  |
| 1   | C     | 17  | SER  |
| 1   | C     | 21  | SER  |
| 1   | C     | 26  | VAL  |
| 1   | C     | 27  | THR  |
| 1   | C     | 28  | ASN  |
| 1   | C     | 31  | LEU  |
| 1   | C     | 40  | SER  |
| 1   | C     | 61  | LYS  |
| 1   | C     | 68  | ILE  |
| 1   | C     | 75  | LYS  |
| 1   | C     | 79  | LYS  |
| 1   | C     | 102 | ARG  |
| 1   | C     | 106 | PRO  |
| 1   | C     | 124 | GLU  |
| 1   | C     | 129 | VAL  |
| 1   | C     | 143 | SER  |
| 1   | C     | 145 | ARG  |
| 1   | C     | 201 | ASN  |
| 1   | C     | 202 | ILE  |
| 1   | C     | 203 | ASN  |
| 1   | C     | 205 | PRO  |
| 1   | C     | 211 | LEU  |
| 1   | C     | 223 | THR  |
| 1   | C     | 224 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 225 | MET  |
| 1   | C     | 234 | ARG  |
| 1   | C     | 242 | ARG  |
| 1   | C     | 243 | SER  |
| 1   | C     | 245 | ARG  |
| 1   | C     | 252 | VAL  |
| 1   | C     | 259 | VAL  |
| 1   | C     | 280 | ILE  |
| 1   | C     | 288 | VAL  |
| 1   | C     | 292 | LEU  |
| 1   | C     | 294 | LYS  |
| 1   | C     | 320 | GLU  |
| 1   | C     | 321 | ARG  |
| 1   | C     | 322 | VAL  |
| 1   | C     | 324 | LYS  |
| 1   | C     | 330 | LYS  |
| 1   | C     | 347 | VAL  |
| 1   | C     | 368 | SER  |
| 1   | C     | 373 | VAL  |
| 1   | C     | 374 | MET  |
| 1   | C     | 376 | THR  |
| 1   | C     | 387 | VAL  |
| 1   | C     | 388 | ASN  |
| 1   | C     | 395 | MET  |
| 1   | C     | 398 | ILE  |
| 1   | C     | 400 | THR  |
| 1   | C     | 402 | ASP  |
| 1   | C     | 409 | LEU  |
| 1   | C     | 410 | GLN  |
| 1   | C     | 424 | ILE  |
| 1   | C     | 426 | LYS  |
| 1   | C     | 435 | VAL  |
| 1   | C     | 444 | LYS  |
| 1   | C     | 448 | GLU  |
| 1   | C     | 452 | GLN  |
| 1   | C     | 459 | GLU  |
| 1   | C     | 460 | LEU  |
| 1   | C     | 462 | LYS  |
| 1   | C     | 463 | THR  |
| 1   | C     | 465 | THR  |
| 1   | C     | 480 | GLU  |
| 1   | C     | 484 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 487 | GLU  |
| 1   | C     | 489 | VAL  |
| 1   | C     | 496 | LEU  |
| 1   | C     | 520 | GLU  |
| 1   | C     | 526 | ILE  |
| 1   | C     | 529 | LEU  |
| 1   | C     | 551 | SER  |
| 1   | C     | 558 | ARG  |
| 1   | C     | 570 | ASP  |
| 1   | D     | 5   | LEU  |
| 1   | D     | 11  | GLU  |
| 1   | D     | 17  | SER  |
| 1   | D     | 20  | VAL  |
| 1   | D     | 28  | ASN  |
| 1   | D     | 31  | LEU  |
| 1   | D     | 32  | THR  |
| 1   | D     | 40  | SER  |
| 1   | D     | 45  | LEU  |
| 1   | D     | 68  | ILE  |
| 1   | D     | 72  | SER  |
| 1   | D     | 75  | LYS  |
| 1   | D     | 78  | GLU  |
| 1   | D     | 81  | VAL  |
| 1   | D     | 89  | SER  |
| 1   | D     | 126 | THR  |
| 1   | D     | 130 | ILE  |
| 1   | D     | 145 | ARG  |
| 1   | D     | 159 | ILE  |
| 1   | D     | 175 | GLU  |
| 1   | D     | 210 | VAL  |
| 1   | D     | 211 | LEU  |
| 1   | D     | 230 | THR  |
| 1   | D     | 235 | MET  |
| 1   | D     | 243 | SER  |
| 1   | D     | 247 | THR  |
| 1   | D     | 252 | VAL  |
| 1   | D     | 259 | VAL  |
| 1   | D     | 273 | LEU  |
| 1   | D     | 282 | GLU  |
| 1   | D     | 283 | ASP  |
| 1   | D     | 291 | VAL  |
| 1   | D     | 292 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 303 | ILE  |
| 1   | D     | 328 | LYS  |
| 1   | D     | 330 | LYS  |
| 1   | D     | 345 | LEU  |
| 1   | D     | 347 | VAL  |
| 1   | D     | 350 | GLN  |
| 1   | D     | 368 | SER  |
| 1   | D     | 376 | THR  |
| 1   | D     | 382 | ASN  |
| 1   | D     | 385 | ILE  |
| 1   | D     | 387 | VAL  |
| 1   | D     | 388 | ASN  |
| 1   | D     | 392 | ASN  |
| 1   | D     | 395 | MET  |
| 1   | D     | 396 | ASN  |
| 1   | D     | 401 | ARG  |
| 1   | D     | 415 | SER  |
| 1   | D     | 440 | VAL  |
| 1   | D     | 444 | LYS  |
| 1   | D     | 447 | GLU  |
| 1   | D     | 449 | LEU  |
| 1   | D     | 452 | GLN  |
| 1   | D     | 459 | GLU  |
| 1   | D     | 460 | LEU  |
| 1   | D     | 462 | LYS  |
| 1   | D     | 463 | THR  |
| 1   | D     | 473 | SER  |
| 1   | D     | 480 | GLU  |
| 1   | D     | 488 | LEU  |
| 1   | D     | 496 | LEU  |
| 1   | D     | 526 | ILE  |
| 1   | D     | 529 | LEU  |
| 1   | D     | 555 | THR  |
| 1   | D     | 558 | ARG  |
| 1   | D     | 570 | ASP  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 28  | ASN  |
| 1   | A     | 33  | HIS  |
| 1   | A     | 35  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 114 | GLN  |
| 1   | A     | 172 | ASN  |
| 1   | A     | 258 | GLN  |
| 1   | A     | 319 | ASN  |
| 1   | A     | 336 | ASN  |
| 1   | A     | 362 | GLN  |
| 1   | A     | 382 | ASN  |
| 1   | A     | 388 | ASN  |
| 1   | A     | 396 | ASN  |
| 1   | A     | 410 | GLN  |
| 1   | A     | 411 | GLN  |
| 1   | A     | 452 | GLN  |
| 1   | A     | 468 | ASN  |
| 1   | A     | 478 | GLN  |
| 1   | A     | 548 | ASN  |
| 1   | B     | 28  | ASN  |
| 1   | B     | 35  | ASN  |
| 1   | B     | 114 | GLN  |
| 1   | B     | 172 | ASN  |
| 1   | B     | 258 | GLN  |
| 1   | B     | 319 | ASN  |
| 1   | B     | 336 | ASN  |
| 1   | B     | 362 | GLN  |
| 1   | B     | 388 | ASN  |
| 1   | B     | 392 | ASN  |
| 1   | B     | 410 | GLN  |
| 1   | B     | 411 | GLN  |
| 1   | B     | 452 | GLN  |
| 1   | B     | 478 | GLN  |
| 1   | B     | 548 | ASN  |
| 1   | C     | 28  | ASN  |
| 1   | C     | 35  | ASN  |
| 1   | C     | 37  | GLN  |
| 1   | C     | 114 | GLN  |
| 1   | C     | 172 | ASN  |
| 1   | C     | 213 | ASN  |
| 1   | C     | 214 | ASN  |
| 1   | C     | 319 | ASN  |
| 1   | C     | 336 | ASN  |
| 1   | C     | 350 | GLN  |
| 1   | C     | 362 | GLN  |
| 1   | C     | 364 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 388 | ASN  |
| 1   | C     | 411 | GLN  |
| 1   | C     | 452 | GLN  |
| 1   | C     | 548 | ASN  |
| 1   | D     | 28  | ASN  |
| 1   | D     | 35  | ASN  |
| 1   | D     | 37  | GLN  |
| 1   | D     | 114 | GLN  |
| 1   | D     | 172 | ASN  |
| 1   | D     | 258 | GLN  |
| 1   | D     | 319 | ASN  |
| 1   | D     | 336 | ASN  |
| 1   | D     | 350 | GLN  |
| 1   | D     | 382 | ASN  |
| 1   | D     | 411 | GLN  |
| 1   | D     | 452 | GLN  |
| 1   | D     | 468 | ASN  |
| 1   | D     | 478 | GLN  |
| 1   | D     | 548 | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

23 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 | $\# Z  > 2$ |
| 2   | HEC  | A     | 602 | 1    | 46,50,50     | 2.01 | 9 (19%)     | 58,82,82    | 1.51 | 9 (15%)     |
| 2   | HEC  | A     | 603 | 1    | 46,50,50     | 1.94 | 7 (15%)     | 58,82,82    | 1.49 | 8 (13%)     |
| 3   | FAD  | A     | 600 | -    | 58,58,58     | 2.90 | 11 (18%)    | 85,89,89    | 2.82 | 31 (36%)    |
| 4   | SO4  | C     | 814 | -    | 4,4,4        | 0.65 | 0           | 6,6,6       | 0.65 | 0           |
| 2   | HEC  | D     | 604 | 1    | 46,50,50     | 1.91 | 6 (13%)     | 58,82,82    | 2.19 | 9 (15%)     |
| 3   | FAD  | C     | 800 | -    | 58,58,58     | 2.92 | 10 (17%)    | 85,89,89    | 3.42 | 27 (31%)    |
| 3   | FAD  | B     | 700 | -    | 58,58,58     | 2.89 | 9 (15%)     | 85,89,89    | 2.77 | 34 (40%)    |
| 2   | HEC  | C     | 604 | 1    | 46,50,50     | 2.01 | 6 (13%)     | 58,82,82    | 2.43 | 16 (27%)    |
| 4   | SO4  | D     | 914 | -    | 4,4,4        | 0.57 | 0           | 6,6,6       | 0.68 | 0           |
| 2   | HEC  | D     | 602 | 1    | 46,50,50     | 1.93 | 9 (19%)     | 58,82,82    | 1.71 | 6 (10%)     |
| 2   | HEC  | B     | 603 | 1    | 46,50,50     | 1.94 | 6 (13%)     | 58,82,82    | 1.43 | 7 (12%)     |
| 2   | HEC  | C     | 602 | 1    | 46,50,50     | 1.94 | 10 (21%)    | 58,82,82    | 1.96 | 11 (18%)    |
| 2   | HEC  | B     | 601 | 1    | 46,50,50     | 1.96 | 7 (15%)     | 58,82,82    | 2.11 | 11 (18%)    |
| 2   | HEC  | C     | 601 | 1    | 46,50,50     | 1.85 | 7 (15%)     | 58,82,82    | 1.87 | 9 (15%)     |
| 2   | HEC  | A     | 604 | 1    | 46,50,50     | 1.94 | 9 (19%)     | 58,82,82    | 1.80 | 12 (20%)    |
| 2   | HEC  | D     | 603 | 1    | 46,50,50     | 1.91 | 7 (15%)     | 58,82,82    | 1.29 | 5 (8%)      |
| 2   | HEC  | B     | 602 | 1    | 46,50,50     | 1.94 | 5 (10%)     | 58,82,82    | 1.39 | 5 (8%)      |
| 3   | FAD  | D     | 900 | -    | 58,58,58     | 2.87 | 10 (17%)    | 85,89,89    | 2.93 | 22 (25%)    |
| 2   | HEC  | C     | 603 | 1    | 46,50,50     | 1.91 | 5 (10%)     | 58,82,82    | 1.40 | 7 (12%)     |
| 2   | HEC  | B     | 604 | 1    | 46,50,50     | 1.90 | 8 (17%)     | 58,82,82    | 2.09 | 15 (25%)    |
| 2   | HEC  | A     | 601 | 1    | 46,50,50     | 1.98 | 10 (21%)    | 58,82,82    | 2.25 | 18 (31%)    |
| 4   | SO4  | B     | 714 | -    | 4,4,4        | 0.58 | 0           | 6,6,6       | 0.45 | 0           |
| 2   | HEC  | D     | 601 | 1    | 46,50,50     | 2.01 | 9 (19%)     | 58,82,82    | 2.03 | 12 (20%)    |

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   |
|-----|------|-------|-----|------|---------|-------------|---------|
| 2   | HEC  | A     | 602 | 1    | -       | 11/14/54/54 | -       |
| 2   | HEC  | A     | 603 | 1    | -       | 7/14/54/54  | -       |
| 3   | FAD  | A     | 600 | -    | 2/2/9/9 | 14/34/50/50 | 0/6/6/6 |
| 2   | HEC  | D     | 604 | 1    | -       | 7/14/54/54  | -       |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions    | Rings   |
|-----|------|-------|-----|------|---------|-------------|---------|
| 3   | FAD  | C     | 800 | -    | 3/3/9/9 | 15/34/50/50 | 0/5/6/6 |
| 3   | FAD  | B     | 700 | -    | 2/2/9/9 | 13/34/50/50 | 0/6/6/6 |
| 2   | HEC  | C     | 604 | 1    | -       | 10/14/54/54 | -       |
| 2   | HEC  | D     | 602 | 1    | -       | 9/14/54/54  | -       |
| 2   | HEC  | B     | 603 | 1    | -       | 4/14/54/54  | -       |
| 2   | HEC  | C     | 602 | 1    | -       | 9/14/54/54  | -       |
| 2   | HEC  | B     | 601 | 1    | -       | 10/14/54/54 | -       |
| 2   | HEC  | C     | 601 | 1    | -       | 9/14/54/54  | -       |
| 2   | HEC  | A     | 604 | 1    | -       | 6/14/54/54  | -       |
| 2   | HEC  | D     | 603 | 1    | -       | 6/14/54/54  | -       |
| 2   | HEC  | B     | 602 | 1    | -       | 9/14/54/54  | -       |
| 3   | FAD  | D     | 900 | -    | 2/2/9/9 | 16/34/50/50 | 0/6/6/6 |
| 2   | HEC  | C     | 603 | 1    | -       | 9/14/54/54  | -       |
| 2   | HEC  | B     | 604 | 1    | -       | 7/14/54/54  | -       |
| 2   | HEC  | A     | 601 | 1    | -       | 10/14/54/54 | -       |
| 2   | HEC  | D     | 601 | 1    | -       | 10/14/54/54 | -       |

All (160) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | C     | 800 | FAD  | C1'-C2' | 18.79 | 1.78        | 1.52     |
| 3   | D     | 900 | FAD  | C1'-C2' | 18.35 | 1.78        | 1.52     |
| 3   | A     | 600 | FAD  | C1'-C2' | 18.22 | 1.78        | 1.52     |
| 3   | B     | 700 | FAD  | C1'-C2' | 17.72 | 1.77        | 1.52     |
| 2   | D     | 601 | HEC  | CAC-C3C | 7.31  | 1.58        | 1.35     |
| 2   | A     | 602 | HEC  | CAC-C3C | 7.19  | 1.58        | 1.35     |
| 2   | B     | 601 | HEC  | CAB-C3B | 7.14  | 1.58        | 1.35     |
| 2   | A     | 604 | HEC  | CAB-C3B | 7.13  | 1.58        | 1.35     |
| 2   | C     | 602 | HEC  | CAB-C3B | 7.01  | 1.57        | 1.35     |
| 2   | B     | 601 | HEC  | CAC-C3C | 6.99  | 1.57        | 1.35     |
| 2   | A     | 602 | HEC  | CAB-C3B | 6.98  | 1.57        | 1.35     |
| 2   | A     | 603 | HEC  | CAB-C3B | 6.94  | 1.57        | 1.35     |
| 2   | D     | 604 | HEC  | CAB-C3B | 6.90  | 1.57        | 1.35     |
| 2   | C     | 604 | HEC  | CAC-C3C | 6.89  | 1.57        | 1.35     |
| 2   | D     | 602 | HEC  | CAC-C3C | 6.87  | 1.57        | 1.35     |
| 2   | C     | 604 | HEC  | CAB-C3B | 6.86  | 1.57        | 1.35     |
| 2   | D     | 603 | HEC  | CAB-C3B | 6.85  | 1.57        | 1.35     |
| 3   | A     | 600 | FAD  | C5B-C4B | 6.83  | 1.72        | 1.51     |
| 2   | A     | 603 | HEC  | CAC-C3C | 6.79  | 1.57        | 1.35     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | B     | 603 | HEC  | CAB-C3B | 6.77  | 1.57        | 1.35     |
| 2   | D     | 604 | HEC  | CAC-C3C | 6.76  | 1.57        | 1.35     |
| 2   | B     | 604 | HEC  | CAC-C3C | 6.75  | 1.56        | 1.35     |
| 3   | D     | 900 | FAD  | C5B-C4B | 6.73  | 1.71        | 1.51     |
| 2   | C     | 603 | HEC  | CAB-C3B | 6.69  | 1.56        | 1.35     |
| 2   | A     | 601 | HEC  | CAC-C3C | 6.65  | 1.56        | 1.35     |
| 2   | B     | 604 | HEC  | CAB-C3B | 6.65  | 1.56        | 1.35     |
| 2   | C     | 602 | HEC  | CAC-C3C | 6.61  | 1.56        | 1.35     |
| 3   | B     | 700 | FAD  | C5B-C4B | 6.61  | 1.71        | 1.51     |
| 2   | C     | 601 | HEC  | CAC-C3C | 6.61  | 1.56        | 1.35     |
| 2   | B     | 603 | HEC  | CAC-C3C | 6.56  | 1.56        | 1.35     |
| 2   | D     | 602 | HEC  | CAB-C3B | 6.55  | 1.56        | 1.35     |
| 2   | C     | 601 | HEC  | CAB-C3B | 6.54  | 1.56        | 1.35     |
| 2   | C     | 603 | HEC  | CAC-C3C | 6.52  | 1.56        | 1.35     |
| 2   | A     | 604 | HEC  | CAC-C3C | 6.48  | 1.56        | 1.35     |
| 2   | D     | 603 | HEC  | CAC-C3C | 6.46  | 1.56        | 1.35     |
| 2   | B     | 602 | HEC  | CAC-C3C | 6.44  | 1.55        | 1.35     |
| 2   | B     | 602 | HEC  | CAB-C3B | 6.39  | 1.55        | 1.35     |
| 2   | D     | 601 | HEC  | CAB-C3B | 6.25  | 1.55        | 1.35     |
| 2   | A     | 601 | HEC  | CAB-C3B | 6.15  | 1.55        | 1.35     |
| 3   | C     | 800 | FAD  | P-O3P   | -5.42 | 1.53        | 1.59     |
| 3   | C     | 800 | FAD  | C5B-C4B | 5.41  | 1.67        | 1.51     |
| 3   | B     | 700 | FAD  | P-O3P   | -5.39 | 1.53        | 1.59     |
| 2   | C     | 604 | HEC  | CBC-CAC | -4.29 | 1.33        | 1.49     |
| 2   | D     | 601 | HEC  | CBB-CAB | -4.28 | 1.33        | 1.49     |
| 3   | D     | 900 | FAD  | P-O3P   | -4.26 | 1.54        | 1.59     |
| 2   | B     | 604 | HEC  | CBC-CAC | -4.17 | 1.34        | 1.49     |
| 2   | B     | 603 | HEC  | CBC-CAC | -4.15 | 1.34        | 1.49     |
| 2   | B     | 602 | HEC  | CBC-CAC | -4.05 | 1.34        | 1.49     |
| 2   | D     | 604 | HEC  | CBC-CAC | -4.05 | 1.34        | 1.49     |
| 2   | D     | 603 | HEC  | CBC-CAC | -3.94 | 1.34        | 1.49     |
| 2   | C     | 603 | HEC  | CBC-CAC | -3.90 | 1.35        | 1.49     |
| 2   | B     | 603 | HEC  | CBB-CAB | -3.90 | 1.35        | 1.49     |
| 2   | C     | 601 | HEC  | CBC-CAC | -3.87 | 1.35        | 1.49     |
| 2   | D     | 603 | HEC  | CBB-CAB | -3.81 | 1.35        | 1.49     |
| 2   | A     | 601 | HEC  | CBC-CAC | -3.80 | 1.35        | 1.49     |
| 2   | C     | 601 | HEC  | CBB-CAB | -3.80 | 1.35        | 1.49     |
| 2   | D     | 601 | HEC  | CBC-CAC | -3.67 | 1.35        | 1.49     |
| 2   | B     | 602 | HEC  | CBB-CAB | -3.66 | 1.36        | 1.49     |
| 2   | B     | 601 | HEC  | CBB-CAB | -3.64 | 1.36        | 1.49     |
| 3   | A     | 600 | FAD  | P-O3P   | -3.62 | 1.55        | 1.59     |
| 2   | A     | 603 | HEC  | CBB-CAB | -3.61 | 1.36        | 1.49     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | C     | 603 | HEC  | CBB-CAB | -3.52 | 1.36        | 1.49     |
| 2   | A     | 603 | HEC  | CBC-CAC | -3.49 | 1.36        | 1.49     |
| 2   | A     | 601 | HEC  | CBB-CAB | -3.47 | 1.36        | 1.49     |
| 2   | A     | 602 | HEC  | CBC-CAC | -3.41 | 1.36        | 1.49     |
| 3   | A     | 600 | FAD  | C5'-C4' | -3.40 | 1.47        | 1.51     |
| 2   | A     | 602 | HEC  | CBB-CAB | -3.39 | 1.37        | 1.49     |
| 2   | A     | 604 | HEC  | CBC-CAC | -3.30 | 1.37        | 1.49     |
| 2   | D     | 602 | HEC  | CBC-CAC | -3.22 | 1.37        | 1.49     |
| 2   | A     | 604 | HEC  | CBB-CAB | -3.21 | 1.37        | 1.49     |
| 2   | D     | 602 | HEC  | CBB-CAB | -3.18 | 1.37        | 1.49     |
| 2   | C     | 604 | HEC  | CBB-CAB | -3.18 | 1.37        | 1.49     |
| 2   | B     | 601 | HEC  | CBC-CAC | -3.17 | 1.37        | 1.49     |
| 2   | B     | 604 | HEC  | CBB-CAB | -3.12 | 1.38        | 1.49     |
| 2   | C     | 602 | HEC  | CBC-CAC | -3.10 | 1.38        | 1.49     |
| 3   | B     | 700 | FAD  | C6-C7   | 3.08  | 1.43        | 1.39     |
| 3   | C     | 800 | FAD  | C8-C7   | 3.06  | 1.48        | 1.40     |
| 2   | C     | 602 | HEC  | CBB-CAB | -3.05 | 1.38        | 1.49     |
| 3   | D     | 900 | FAD  | C5X-N5  | -3.03 | 1.33        | 1.39     |
| 2   | D     | 604 | HEC  | CBB-CAB | -3.02 | 1.38        | 1.49     |
| 2   | A     | 601 | HEC  | C3B-C2B | -3.01 | 1.31        | 1.41     |
| 3   | A     | 600 | FAD  | PA-O3P  | 2.98  | 1.62        | 1.59     |
| 2   | B     | 602 | HEC  | CMB-C2B | 2.97  | 1.56        | 1.50     |
| 2   | A     | 604 | HEC  | CMD-C2D | 2.91  | 1.56        | 1.50     |
| 3   | B     | 700 | FAD  | C5X-N5  | -2.87 | 1.34        | 1.39     |
| 3   | C     | 800 | FAD  | C5'-C4' | -2.84 | 1.47        | 1.51     |
| 2   | A     | 602 | HEC  | O1A-CGA | 2.82  | 1.31        | 1.22     |
| 3   | C     | 800 | FAD  | P-O1P   | -2.79 | 1.41        | 1.50     |
| 2   | C     | 604 | HEC  | CMC-C2C | 2.76  | 1.56        | 1.50     |
| 3   | B     | 700 | FAD  | PA-O3P  | -2.72 | 1.56        | 1.59     |
| 3   | D     | 900 | FAD  | C5A-C4A | 2.67  | 1.43        | 1.39     |
| 3   | A     | 600 | FAD  | PA-O2A  | -2.65 | 1.43        | 1.55     |
| 3   | A     | 600 | FAD  | C6-C7   | 2.61  | 1.43        | 1.39     |
| 3   | A     | 600 | FAD  | P-O2P   | -2.61 | 1.43        | 1.55     |
| 2   | D     | 602 | HEC  | C3B-C2B | -2.56 | 1.32        | 1.41     |
| 2   | C     | 602 | HEC  | C3C-C2C | -2.53 | 1.32        | 1.41     |
| 3   | B     | 700 | FAD  | C5A-C4A | 2.53  | 1.43        | 1.39     |
| 3   | C     | 800 | FAD  | C6-C7   | 2.50  | 1.43        | 1.39     |
| 3   | D     | 900 | FAD  | P-O2P   | -2.50 | 1.43        | 1.55     |
| 2   | C     | 602 | HEC  | C3B-C2B | -2.49 | 1.32        | 1.41     |
| 2   | C     | 602 | HEC  | CMB-C2B | 2.49  | 1.55        | 1.50     |
| 2   | A     | 603 | HEC  | C3C-C2C | -2.49 | 1.32        | 1.41     |
| 2   | B     | 604 | HEC  | C3B-C2B | -2.47 | 1.32        | 1.41     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | D     | 602 | HEC  | CMB-C2B | 2.46  | 1.55        | 1.50     |
| 2   | C     | 602 | HEC  | C3B-C4B | -2.46 | 1.41        | 1.46     |
| 2   | C     | 603 | HEC  | C3C-C2C | -2.42 | 1.33        | 1.41     |
| 2   | A     | 603 | HEC  | C3B-C2B | -2.42 | 1.33        | 1.41     |
| 3   | B     | 700 | FAD  | C8-C7   | 2.39  | 1.46        | 1.40     |
| 3   | A     | 600 | FAD  | P-O1P   | -2.39 | 1.42        | 1.50     |
| 2   | A     | 601 | HEC  | O2D-CGD | -2.36 | 1.23        | 1.30     |
| 2   | B     | 601 | HEC  | C3C-C2C | -2.36 | 1.33        | 1.41     |
| 3   | A     | 600 | FAD  | O4'-C4' | -2.35 | 1.38        | 1.43     |
| 2   | D     | 601 | HEC  | C3B-C2B | -2.35 | 1.33        | 1.41     |
| 2   | B     | 604 | HEC  | CMB-C2B | 2.35  | 1.55        | 1.50     |
| 2   | C     | 604 | HEC  | C3B-C2B | -2.33 | 1.33        | 1.41     |
| 2   | A     | 604 | HEC  | C3C-C2C | -2.32 | 1.33        | 1.41     |
| 2   | A     | 602 | HEC  | C3C-C2C | -2.31 | 1.33        | 1.41     |
| 2   | D     | 603 | HEC  | C3C-C2C | -2.30 | 1.33        | 1.41     |
| 2   | D     | 601 | HEC  | CMC-C2C | 2.30  | 1.55        | 1.50     |
| 2   | A     | 601 | HEC  | CMC-C2C | 2.28  | 1.55        | 1.50     |
| 2   | B     | 603 | HEC  | C3D-C2D | -2.28 | 1.33        | 1.38     |
| 3   | D     | 900 | FAD  | C6-C7   | 2.27  | 1.42        | 1.39     |
| 3   | C     | 800 | FAD  | C5X-N5  | -2.27 | 1.35        | 1.39     |
| 3   | B     | 700 | FAD  | PA-O2A  | -2.27 | 1.44        | 1.55     |
| 2   | D     | 602 | HEC  | O1D-CGD | 2.26  | 1.29        | 1.22     |
| 2   | A     | 602 | HEC  | O1D-CGD | 2.25  | 1.29        | 1.22     |
| 2   | D     | 602 | HEC  | CMC-C2C | 2.24  | 1.55        | 1.50     |
| 2   | A     | 602 | HEC  | C3D-C2D | -2.23 | 1.33        | 1.38     |
| 2   | D     | 603 | HEC  | C3B-C2B | -2.23 | 1.33        | 1.41     |
| 2   | C     | 601 | HEC  | C3B-C2B | -2.22 | 1.33        | 1.41     |
| 2   | D     | 601 | HEC  | C2A-C3A | -2.21 | 1.32        | 1.36     |
| 2   | B     | 601 | HEC  | C3B-C2B | -2.21 | 1.33        | 1.41     |
| 2   | D     | 604 | HEC  | C3C-C2C | -2.18 | 1.33        | 1.41     |
| 2   | A     | 604 | HEC  | C3D-C2D | -2.17 | 1.33        | 1.38     |
| 2   | C     | 601 | HEC  | C3C-C2C | -2.15 | 1.33        | 1.41     |
| 3   | A     | 600 | FAD  | P-O5'   | -2.15 | 1.51        | 1.59     |
| 2   | C     | 602 | HEC  | CMA-C3A | 2.15  | 1.55        | 1.50     |
| 3   | C     | 800 | FAD  | O4B-C4B | -2.15 | 1.40        | 1.45     |
| 2   | D     | 604 | HEC  | CMB-C2B | 2.14  | 1.55        | 1.50     |
| 2   | A     | 604 | HEC  | CMB-C2B | 2.13  | 1.55        | 1.50     |
| 2   | D     | 603 | HEC  | C3D-C2D | -2.13 | 1.33        | 1.38     |
| 2   | A     | 602 | HEC  | CMB-C2B | 2.12  | 1.55        | 1.50     |
| 2   | A     | 603 | HEC  | O1A-CGA | 2.11  | 1.29        | 1.22     |
| 2   | A     | 604 | HEC  | CMC-C2C | 2.11  | 1.55        | 1.50     |
| 2   | A     | 601 | HEC  | C3D-C2D | -2.11 | 1.33        | 1.38     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | D     | 601 | HEC  | C3C-C2C | -2.10 | 1.34        | 1.41     |
| 2   | B     | 601 | HEC  | CMA-C3A | 2.10  | 1.55        | 1.50     |
| 2   | B     | 604 | HEC  | C3D-C2D | -2.09 | 1.33        | 1.38     |
| 2   | C     | 601 | HEC  | CMB-C2B | 2.09  | 1.55        | 1.50     |
| 3   | D     | 900 | FAD  | C2'-C3' | -2.08 | 1.49        | 1.53     |
| 2   | B     | 603 | HEC  | C3C-C2C | -2.08 | 1.34        | 1.41     |
| 3   | D     | 900 | FAD  | PA-O3P  | -2.07 | 1.57        | 1.59     |
| 3   | D     | 900 | FAD  | PA-O2A  | -2.06 | 1.45        | 1.55     |
| 2   | A     | 601 | HEC  | C3C-C2C | -2.06 | 1.34        | 1.41     |
| 2   | D     | 601 | HEC  | C3D-C2D | -2.06 | 1.33        | 1.38     |
| 2   | D     | 602 | HEC  | C3C-C2C | -2.05 | 1.34        | 1.41     |
| 2   | A     | 601 | HEC  | CBD-CAD | 2.03  | 1.59        | 1.51     |
| 2   | B     | 604 | HEC  | C3C-C2C | -2.03 | 1.34        | 1.41     |
| 2   | C     | 602 | HEC  | O1D-CGD | 2.03  | 1.28        | 1.22     |
| 3   | C     | 800 | FAD  | PA-O2A  | -2.01 | 1.46        | 1.55     |

All (274) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 3   | C     | 800 | FAD  | O4B-C4B-C5B | 16.97  | 163.68      | 109.33   |
| 3   | C     | 800 | FAD  | O5B-C5B-C4B | 16.46  | 165.03      | 108.99   |
| 3   | D     | 900 | FAD  | O5B-C5B-C4B | 11.62  | 148.57      | 108.99   |
| 3   | D     | 900 | FAD  | C5B-C4B-C3B | -11.44 | 74.02       | 115.21   |
| 3   | A     | 600 | FAD  | C5B-C4B-C3B | -11.29 | 74.55       | 115.21   |
| 3   | C     | 800 | FAD  | C5B-C4B-C3B | -11.26 | 74.68       | 115.21   |
| 3   | B     | 700 | FAD  | C5B-C4B-C3B | -11.19 | 74.91       | 115.21   |
| 3   | A     | 600 | FAD  | O5B-C5B-C4B | 10.61  | 145.13      | 108.99   |
| 3   | D     | 900 | FAD  | O4B-C4B-C5B | 9.88   | 140.99      | 109.33   |
| 2   | C     | 604 | HEC  | CBD-CAD-C3D | 9.87   | 139.81      | 112.53   |
| 2   | D     | 604 | HEC  | CBB-CAB-C3B | -9.65  | 108.16      | 127.43   |
| 3   | B     | 700 | FAD  | O5B-C5B-C4B | 9.58   | 141.62      | 108.99   |
| 3   | B     | 700 | FAD  | O4B-C4B-C5B | 8.90   | 137.85      | 109.33   |
| 3   | A     | 600 | FAD  | O4B-C1B-N9A | -8.71  | 91.36       | 108.09   |
| 2   | C     | 602 | HEC  | CBB-CAB-C3B | -8.48  | 110.48      | 127.43   |
| 2   | D     | 602 | HEC  | CBB-CAB-C3B | -8.27  | 110.90      | 127.43   |
| 2   | B     | 604 | HEC  | CBB-CAB-C3B | -8.19  | 111.06      | 127.43   |
| 2   | B     | 601 | HEC  | CBB-CAB-C3B | -8.09  | 111.27      | 127.43   |
| 2   | D     | 601 | HEC  | O2D-CGD-O1D | 7.13   | 141.68      | 123.33   |
| 2   | C     | 601 | HEC  | CBB-CAB-C3B | -6.94  | 113.56      | 127.43   |
| 3   | A     | 600 | FAD  | O4B-C4B-C5B | 6.89   | 131.40      | 109.33   |
| 2   | B     | 601 | HEC  | CBC-CAC-C3C | -6.85  | 113.74      | 127.43   |
| 2   | D     | 601 | HEC  | CBB-CAB-C3B | -6.77  | 113.90      | 127.43   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | A     | 601 | HEC  | CBB-CAB-C3B | -6.62 | 114.21      | 127.43   |
| 2   | C     | 604 | HEC  | CBB-CAB-C3B | -6.56 | 114.32      | 127.43   |
| 2   | D     | 604 | HEC  | O2D-CGD-O1D | 6.38  | 139.75      | 123.33   |
| 2   | A     | 604 | HEC  | CBB-CAB-C3B | -6.35 | 114.75      | 127.43   |
| 3   | D     | 900 | FAD  | O3'-C3'-C4' | 6.27  | 123.17      | 108.93   |
| 2   | B     | 604 | HEC  | CBC-CAC-C3C | -6.21 | 115.01      | 127.43   |
| 2   | A     | 602 | HEC  | CAA-CBA-CGA | 6.11  | 129.87      | 113.67   |
| 2   | B     | 602 | HEC  | CBB-CAB-C3B | -5.98 | 115.49      | 127.43   |
| 2   | B     | 603 | HEC  | CAA-CBA-CGA | 5.83  | 129.12      | 113.67   |
| 3   | B     | 700 | FAD  | N3A-C2A-N1A | 5.80  | 137.35      | 128.58   |
| 2   | A     | 601 | HEC  | CBD-CAD-C3D | -5.69 | 96.80       | 112.53   |
| 2   | C     | 602 | HEC  | CBC-CAC-C3C | -5.67 | 116.09      | 127.43   |
| 2   | D     | 603 | HEC  | CBB-CAB-C3B | -5.66 | 116.12      | 127.43   |
| 2   | C     | 604 | HEC  | CHB-C4A-NA  | 5.61  | 130.57      | 124.45   |
| 3   | D     | 900 | FAD  | N3A-C2A-N1A | 5.58  | 137.03      | 128.58   |
| 2   | A     | 603 | HEC  | CBB-CAB-C3B | -5.55 | 116.33      | 127.43   |
| 3   | B     | 700 | FAD  | C4-N3-C2    | -5.54 | 115.80      | 125.64   |
| 3   | C     | 800 | FAD  | N6A-C6A-N1A | 5.52  | 130.66      | 118.38   |
| 3   | D     | 900 | FAD  | C4-N3-C2    | -5.46 | 115.94      | 125.64   |
| 3   | D     | 900 | FAD  | C4'-C3'-C2' | 5.37  | 122.50      | 113.57   |
| 3   | D     | 900 | FAD  | C9A-C5X-N5  | -5.35 | 116.77      | 122.45   |
| 2   | C     | 604 | HEC  | CBA-CAA-C2A | 5.35  | 127.32      | 112.53   |
| 2   | A     | 601 | HEC  | O1D-CGD-CBD | -5.30 | 106.29      | 123.09   |
| 2   | A     | 603 | HEC  | CBC-CAC-C3C | -5.19 | 117.05      | 127.43   |
| 2   | D     | 604 | HEC  | CAD-CBD-CGD | -5.19 | 99.91       | 113.67   |
| 3   | C     | 800 | FAD  | O5'-C5'-C4' | 5.18  | 123.19      | 109.36   |
| 2   | D     | 604 | HEC  | CBC-CAC-C3C | -5.06 | 117.33      | 127.43   |
| 2   | C     | 604 | HEC  | CBC-CAC-C3C | -5.05 | 117.34      | 127.43   |
| 2   | B     | 601 | HEC  | CBD-CAD-C3D | 4.97  | 126.27      | 112.53   |
| 2   | C     | 602 | HEC  | CBA-CAA-C2A | 4.96  | 126.25      | 112.53   |
| 2   | C     | 603 | HEC  | CBB-CAB-C3B | -4.87 | 117.70      | 127.43   |
| 2   | A     | 601 | HEC  | O1A-CGA-CBA | -4.86 | 107.67      | 123.09   |
| 3   | B     | 700 | FAD  | O4'-C4'-C5' | -4.81 | 99.39       | 109.99   |
| 3   | B     | 700 | FAD  | C1'-N10-C9A | -4.78 | 111.34      | 120.63   |
| 3   | A     | 600 | FAD  | C2A-N1A-C6A | 4.65  | 126.38      | 118.73   |
| 3   | C     | 800 | FAD  | O4-C4-C4X   | -4.62 | 114.34      | 126.53   |
| 2   | C     | 601 | HEC  | O2D-CGD-O1D | 4.52  | 134.96      | 123.33   |
| 2   | A     | 604 | HEC  | CBC-CAC-C3C | -4.50 | 118.43      | 127.43   |
| 2   | A     | 604 | HEC  | O2D-CGD-O1D | 4.38  | 134.60      | 123.33   |
| 3   | D     | 900 | FAD  | O4'-C4'-C5' | -4.35 | 100.39      | 109.99   |
| 3   | C     | 800 | FAD  | O4B-C1B-N9A | -4.32 | 99.79       | 108.09   |
| 2   | A     | 601 | HEC  | O2D-CGD-O1D | 4.30  | 134.38      | 123.33   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | B     | 601 | HEC  | O2D-CGD-O1D | 4.29  | 134.37      | 123.33   |
| 3   | A     | 600 | FAD  | O4B-C1B-C2B | -4.28 | 97.45       | 106.62   |
| 3   | A     | 600 | FAD  | N6A-C6A-N1A | 4.28  | 127.91      | 118.38   |
| 2   | C     | 601 | HEC  | CBD-CAD-C3D | 4.27  | 124.35      | 112.53   |
| 2   | D     | 601 | HEC  | CAA-CBA-CGA | -4.24 | 102.42      | 113.67   |
| 3   | A     | 600 | FAD  | O2-C2-N1    | -4.22 | 114.79      | 121.80   |
| 2   | D     | 601 | HEC  | CAD-CBD-CGD | -4.18 | 102.57      | 113.67   |
| 3   | C     | 800 | FAD  | O4-C4-N3    | 4.14  | 127.90      | 120.11   |
| 2   | C     | 601 | HEC  | CBC-CAC-C3C | -4.14 | 119.16      | 127.43   |
| 2   | A     | 601 | HEC  | C3D-C4D-ND  | -4.08 | 105.63      | 110.15   |
| 2   | A     | 601 | HEC  | O2A-CGA-O1A | 4.06  | 133.78      | 123.33   |
| 3   | A     | 600 | FAD  | C4B-O4B-C1B | -4.05 | 100.52      | 109.47   |
| 2   | B     | 604 | HEC  | CBD-CAD-C3D | 3.97  | 123.52      | 112.53   |
| 3   | A     | 600 | FAD  | C4A-N9A-C8A | 3.89  | 109.82      | 105.74   |
| 2   | C     | 601 | HEC  | O2A-CGA-O1A | 3.85  | 133.23      | 123.33   |
| 2   | D     | 604 | HEC  | O1D-CGD-CBD | -3.79 | 111.06      | 123.09   |
| 2   | B     | 601 | HEC  | CAD-CBD-CGD | -3.77 | 103.67      | 113.67   |
| 2   | B     | 603 | HEC  | CBC-CAC-C3C | -3.69 | 120.05      | 127.43   |
| 3   | A     | 600 | FAD  | C4X-C10-N10 | 3.69  | 121.76      | 116.48   |
| 3   | D     | 900 | FAD  | C7M-C7-C6   | 3.65  | 126.00      | 119.57   |
| 3   | B     | 700 | FAD  | C5X-C9A-N10 | -3.59 | 114.72      | 117.97   |
| 2   | C     | 601 | HEC  | O1A-CGA-CBA | -3.58 | 111.73      | 123.09   |
| 2   | D     | 604 | HEC  | CBA-CAA-C2A | 3.56  | 122.37      | 112.53   |
| 3   | B     | 700 | FAD  | C4A-C5A-N7A | -3.53 | 106.55      | 110.58   |
| 2   | A     | 602 | HEC  | CBB-CAB-C3B | -3.52 | 120.39      | 127.43   |
| 3   | C     | 800 | FAD  | C4-N3-C2    | -3.52 | 119.40      | 125.64   |
| 2   | C     | 603 | HEC  | CBC-CAC-C3C | -3.51 | 120.41      | 127.43   |
| 3   | A     | 600 | FAD  | C4-C4X-N5   | 3.49  | 123.03      | 118.21   |
| 2   | D     | 601 | HEC  | CBC-CAC-C3C | -3.44 | 120.56      | 127.43   |
| 2   | D     | 602 | HEC  | O1A-CGA-CBA | -3.39 | 112.33      | 123.09   |
| 2   | D     | 601 | HEC  | O1A-CGA-CBA | -3.36 | 112.42      | 123.09   |
| 2   | B     | 602 | HEC  | CBC-CAC-C3C | -3.35 | 120.73      | 127.43   |
| 2   | D     | 602 | HEC  | CAA-CBA-CGA | 3.35  | 122.54      | 113.67   |
| 3   | A     | 600 | FAD  | O2A-PA-O1A  | 3.33  | 127.95      | 112.44   |
| 3   | A     | 600 | FAD  | C10-C4X-N5  | -3.30 | 118.07      | 124.81   |
| 2   | D     | 603 | HEC  | CBC-CAC-C3C | -3.29 | 120.85      | 127.43   |
| 3   | D     | 900 | FAD  | O2-C2-N3    | -3.29 | 112.28      | 118.58   |
| 2   | A     | 604 | HEC  | CMA-C3A-C4A | -3.28 | 118.96      | 124.73   |
| 2   | C     | 604 | HEC  | CHC-C1C-NC  | 3.28  | 129.80      | 123.86   |
| 3   | A     | 600 | FAD  | C4'-C3'-C2' | -3.26 | 108.15      | 113.57   |
| 2   | B     | 604 | HEC  | CAD-CBD-CGD | -3.23 | 105.10      | 113.67   |
| 2   | B     | 602 | HEC  | CAA-CBA-CGA | 3.23  | 122.23      | 113.67   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | D     | 900 | FAD  | O2'-C2'-C3' | 3.23  | 116.80      | 109.25   |
| 3   | B     | 700 | FAD  | O3'-C3'-C4' | 3.22  | 116.26      | 108.93   |
| 3   | A     | 600 | FAD  | O4'-C4'-C3' | -3.21 | 101.72      | 109.25   |
| 2   | C     | 602 | HEC  | CAD-CBD-CGD | -3.21 | 105.15      | 113.67   |
| 3   | C     | 800 | FAD  | O2-C2-N1    | -3.18 | 116.52      | 121.80   |
| 2   | B     | 603 | HEC  | CBB-CAB-C3B | -3.17 | 121.10      | 127.43   |
| 2   | C     | 601 | HEC  | CAD-CBD-CGD | -3.13 | 105.36      | 113.67   |
| 3   | B     | 700 | FAD  | C4'-C3'-C2' | -3.12 | 108.37      | 113.57   |
| 2   | A     | 604 | HEC  | CBA-CAA-C2A | 3.11  | 121.13      | 112.53   |
| 3   | C     | 800 | FAD  | C4A-N9A-C8A | 3.11  | 109.00      | 105.74   |
| 2   | A     | 602 | HEC  | CBA-CAA-C2A | 3.08  | 121.06      | 112.53   |
| 2   | B     | 604 | HEC  | O1A-CGA-CBA | -3.08 | 113.33      | 123.09   |
| 3   | B     | 700 | FAD  | O4'-C4'-C3' | -3.04 | 102.14      | 109.25   |
| 2   | D     | 601 | HEC  | O2D-CGD-CBD | -3.02 | 104.45      | 114.00   |
| 2   | B     | 602 | HEC  | CBA-CAA-C2A | 2.99  | 120.79      | 112.53   |
| 2   | D     | 601 | HEC  | O1D-CGD-CBD | -2.98 | 113.63      | 123.09   |
| 2   | B     | 601 | HEC  | CBA-CAA-C2A | 2.98  | 120.77      | 112.53   |
| 2   | B     | 604 | HEC  | C2A-C1A-NA  | -2.98 | 107.45      | 110.32   |
| 2   | C     | 604 | HEC  | C2A-C1A-NA  | -2.96 | 107.47      | 110.32   |
| 3   | C     | 800 | FAD  | O2B-C2B-C3B | -2.95 | 102.36      | 111.82   |
| 2   | D     | 602 | HEC  | O2D-CGD-O1D | 2.94  | 130.89      | 123.33   |
| 2   | B     | 604 | HEC  | O2D-CGD-O1D | 2.93  | 130.87      | 123.33   |
| 2   | C     | 601 | HEC  | O1D-CGD-CBD | -2.93 | 113.80      | 123.09   |
| 3   | B     | 700 | FAD  | C10-C4X-N5  | -2.90 | 118.89      | 124.81   |
| 2   | D     | 601 | HEC  | CAA-C2A-C1A | -2.90 | 118.96      | 124.85   |
| 2   | A     | 603 | HEC  | O2A-CGA-O1A | 2.89  | 130.75      | 123.33   |
| 2   | A     | 601 | HEC  | CHB-C4A-NA  | 2.87  | 127.58      | 124.45   |
| 3   | B     | 700 | FAD  | C4X-C10-N1  | -2.86 | 117.58      | 124.59   |
| 2   | C     | 603 | HEC  | CAD-C3D-C2D | 2.86  | 133.48      | 127.07   |
| 3   | D     | 900 | FAD  | C2A-N1A-C6A | -2.82 | 114.09      | 118.73   |
| 3   | B     | 700 | FAD  | C2A-N3A-C4A | -2.82 | 104.95      | 111.83   |
| 3   | C     | 800 | FAD  | O2A-PA-O3P  | 2.81  | 114.87      | 107.27   |
| 2   | B     | 601 | HEC  | O1D-CGD-CBD | -2.80 | 114.20      | 123.09   |
| 2   | C     | 603 | HEC  | CAA-CBA-CGA | 2.80  | 121.09      | 113.67   |
| 3   | D     | 900 | FAD  | C4A-C5A-N7A | -2.80 | 107.39      | 110.58   |
| 2   | A     | 602 | HEC  | O2A-CGA-O1A | 2.78  | 130.48      | 123.33   |
| 2   | B     | 604 | HEC  | CMB-C2B-C1B | -2.76 | 121.22      | 125.42   |
| 3   | A     | 600 | FAD  | O2A-PA-O3P  | 2.75  | 114.71      | 107.27   |
| 2   | C     | 602 | HEC  | O2A-CGA-O1A | 2.74  | 130.38      | 123.33   |
| 2   | A     | 602 | HEC  | CAD-CBD-CGD | -2.74 | 106.40      | 113.67   |
| 2   | A     | 601 | HEC  | CAD-CBD-CGD | -2.72 | 106.44      | 113.67   |
| 2   | D     | 604 | HEC  | C3D-C4D-ND  | -2.72 | 107.14      | 110.15   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | B     | 700 | FAD  | C9-C8-C7    | 2.71  | 123.66      | 119.69   |
| 2   | A     | 602 | HEC  | O1A-CGA-CBA | -2.71 | 114.51      | 123.09   |
| 3   | C     | 800 | FAD  | C2A-N3A-C4A | -2.70 | 105.25      | 111.83   |
| 3   | C     | 800 | FAD  | C6-C5X-N5   | -2.69 | 113.98      | 118.44   |
| 2   | A     | 601 | HEC  | CHC-C4B-C3B | 2.68  | 129.74      | 125.21   |
| 3   | D     | 900 | FAD  | C5X-N5-C4X  | 2.68  | 122.42      | 118.09   |
| 3   | B     | 700 | FAD  | C5'-C4'-C3' | 2.67  | 117.26      | 112.22   |
| 2   | A     | 604 | HEC  | CMA-C3A-C2A | 2.67  | 133.36      | 126.15   |
| 2   | A     | 603 | HEC  | O1A-CGA-CBA | -2.66 | 114.67      | 123.09   |
| 2   | A     | 601 | HEC  | C4D-C3D-C2D | 2.65  | 110.97      | 106.87   |
| 2   | C     | 602 | HEC  | CHA-C4D-ND  | 2.64  | 128.65      | 123.86   |
| 2   | B     | 601 | HEC  | O1A-CGA-CBA | -2.64 | 114.73      | 123.09   |
| 2   | A     | 602 | HEC  | CHA-C1A-NA  | -2.63 | 121.59      | 124.45   |
| 3   | A     | 600 | FAD  | C4-N3-C2    | -2.61 | 121.01      | 125.64   |
| 3   | B     | 700 | FAD  | C10-N1-C2   | 2.60  | 122.49      | 116.85   |
| 3   | C     | 800 | FAD  | N3A-C2A-N1A | 2.60  | 132.52      | 128.58   |
| 2   | B     | 603 | HEC  | CHB-C4A-NA  | 2.59  | 127.28      | 124.45   |
| 2   | A     | 601 | HEC  | CAD-C3D-C4D | -2.59 | 119.89      | 124.94   |
| 3   | C     | 800 | FAD  | C5A-C6A-N6A | -2.58 | 116.90      | 123.29   |
| 3   | B     | 700 | FAD  | C5X-N5-C4X  | 2.57  | 122.25      | 118.09   |
| 3   | B     | 700 | FAD  | O4B-C1B-N9A | -2.57 | 103.16      | 108.09   |
| 3   | B     | 700 | FAD  | O3P-PA-O1A  | 2.56  | 118.41      | 110.70   |
| 3   | D     | 900 | FAD  | C4X-C4-N3   | 2.55  | 119.75      | 113.25   |
| 2   | D     | 603 | HEC  | O1A-CGA-CBA | -2.55 | 115.00      | 123.09   |
| 2   | C     | 602 | HEC  | CHD-C4C-NC  | -2.55 | 121.67      | 124.45   |
| 2   | C     | 604 | HEC  | O2D-CGD-O1D | 2.54  | 129.86      | 123.33   |
| 2   | A     | 604 | HEC  | CMC-C2C-C1C | -2.53 | 121.57      | 125.42   |
| 3   | D     | 900 | FAD  | N3-C2-N1    | 2.52  | 124.85      | 119.50   |
| 3   | A     | 600 | FAD  | O5'-C5'-C4' | 2.51  | 116.06      | 109.36   |
| 2   | B     | 604 | HEC  | O1D-CGD-CBD | -2.50 | 115.15      | 123.09   |
| 3   | A     | 600 | FAD  | O5B-PA-O1A  | -2.50 | 99.02       | 108.94   |
| 2   | C     | 604 | HEC  | O2A-CGA-O1A | 2.50  | 129.76      | 123.33   |
| 2   | B     | 604 | HEC  | CAA-C2A-C1A | -2.50 | 119.77      | 124.85   |
| 2   | D     | 604 | HEC  | CHA-C1A-C2A | 2.49  | 128.80      | 124.86   |
| 3   | B     | 700 | FAD  | C9A-C5X-N5  | -2.49 | 119.81      | 122.45   |
| 2   | C     | 603 | HEC  | CAD-C3D-C4D | -2.49 | 120.08      | 124.94   |
| 3   | B     | 700 | FAD  | N3-C2-N1    | 2.48  | 124.76      | 119.50   |
| 3   | A     | 600 | FAD  | C9A-C5X-N5  | -2.46 | 119.84      | 122.45   |
| 3   | C     | 800 | FAD  | C6-C5X-C9A  | 2.46  | 122.43      | 119.05   |
| 3   | A     | 600 | FAD  | C2A-N3A-C4A | -2.46 | 105.83      | 111.83   |
| 2   | A     | 601 | HEC  | CMB-C2B-C1B | -2.45 | 121.68      | 125.42   |
| 3   | A     | 600 | FAD  | N9A-C8A-N7A | -2.45 | 110.46      | 113.94   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | B     | 700 | FAD  | C9A-C9-C8   | -2.44 | 114.31      | 119.22   |
| 3   | B     | 700 | FAD  | C4X-C4-N3   | 2.43  | 119.43      | 113.25   |
| 2   | A     | 601 | HEC  | CMD-C2D-C3D | 2.42  | 130.77      | 125.62   |
| 3   | C     | 800 | FAD  | C5'-C4'-C3' | -2.42 | 107.65      | 112.22   |
| 2   | B     | 601 | HEC  | CAD-C3D-C4D | -2.42 | 120.21      | 124.94   |
| 2   | A     | 602 | HEC  | CBD-CAD-C3D | 2.42  | 119.22      | 112.53   |
| 2   | A     | 601 | HEC  | CBC-CAC-C3C | -2.42 | 122.60      | 127.43   |
| 2   | A     | 603 | HEC  | CMA-C3A-C4A | -2.42 | 120.47      | 124.73   |
| 2   | B     | 603 | HEC  | CMA-C3A-C4A | -2.40 | 120.50      | 124.73   |
| 2   | B     | 601 | HEC  | CHB-C4A-NA  | -2.39 | 121.85      | 124.45   |
| 2   | A     | 604 | HEC  | O1D-CGD-CBD | -2.38 | 115.53      | 123.09   |
| 2   | A     | 602 | HEC  | O1D-CGD-CBD | -2.36 | 115.60      | 123.09   |
| 3   | A     | 600 | FAD  | C7M-C7-C6   | 2.35  | 123.72      | 119.57   |
| 2   | B     | 604 | HEC  | CHC-C4B-C3B | 2.35  | 129.16      | 125.21   |
| 2   | C     | 604 | HEC  | CAA-CBA-CGA | -2.35 | 107.44      | 113.67   |
| 3   | B     | 700 | FAD  | O3B-C3B-C4B | 2.34  | 117.81      | 111.08   |
| 3   | C     | 800 | FAD  | C6A-C5A-C4A | 2.34  | 120.38      | 117.18   |
| 3   | A     | 600 | FAD  | C5'-C4'-C3' | -2.34 | 107.80      | 112.22   |
| 2   | C     | 604 | HEC  | CMD-C2D-C1D | -2.34 | 121.86      | 125.42   |
| 2   | D     | 601 | HEC  | CAA-C2A-C3A | 2.28  | 132.14      | 127.87   |
| 3   | B     | 700 | FAD  | C9-C9A-C5X  | 2.28  | 124.05      | 120.03   |
| 2   | B     | 602 | HEC  | O1A-CGA-CBA | -2.28 | 115.87      | 123.09   |
| 3   | A     | 600 | FAD  | C7M-C7-C8   | -2.27 | 116.12      | 120.76   |
| 2   | C     | 602 | HEC  | CHA-C1A-NA  | 2.27  | 126.92      | 124.45   |
| 2   | B     | 604 | HEC  | CAA-CBA-CGA | -2.26 | 107.67      | 113.67   |
| 2   | C     | 603 | HEC  | CHA-C4D-ND  | 2.25  | 127.94      | 123.86   |
| 3   | A     | 600 | FAD  | C5A-C6A-N1A | -2.24 | 111.83      | 117.51   |
| 3   | C     | 800 | FAD  | C5X-C9A-N10 | -2.23 | 115.95      | 117.97   |
| 3   | C     | 800 | FAD  | C2A-N1A-C6A | 2.21  | 122.36      | 118.73   |
| 2   | D     | 601 | HEC  | O2A-CGA-O1A | 2.21  | 129.01      | 123.33   |
| 2   | B     | 604 | HEC  | C3D-C4D-ND  | -2.21 | 107.70      | 110.15   |
| 2   | C     | 602 | HEC  | C3D-C4D-ND  | -2.19 | 107.72      | 110.15   |
| 2   | C     | 602 | HEC  | O2A-CGA-CBA | -2.19 | 107.07      | 114.00   |
| 2   | A     | 603 | HEC  | CMA-C3A-C2A | 2.18  | 132.06      | 126.15   |
| 3   | D     | 900 | FAD  | C7M-C7-C8   | -2.18 | 116.30      | 120.76   |
| 2   | C     | 602 | HEC  | CHD-C4C-C3C | 2.18  | 128.89      | 125.21   |
| 2   | D     | 602 | HEC  | CHD-C4C-NC  | -2.18 | 122.08      | 124.45   |
| 3   | B     | 700 | FAD  | C5A-N7A-C8A | 2.17  | 106.86      | 103.45   |
| 3   | B     | 700 | FAD  | C8M-C8-C7   | -2.17 | 116.33      | 120.76   |
| 3   | B     | 700 | FAD  | C4-C4X-N5   | 2.16  | 121.19      | 118.21   |
| 2   | C     | 604 | HEC  | CHA-C1A-C2A | 2.15  | 128.26      | 124.86   |
| 2   | B     | 603 | HEC  | CMA-C3A-C2A | 2.15  | 131.96      | 126.15   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | A     | 603 | HEC  | CMD-C2D-C3D | 2.15  | 130.18      | 125.62   |
| 2   | A     | 604 | HEC  | CHC-C1C-NC  | 2.14  | 127.74      | 123.86   |
| 2   | C     | 601 | HEC  | CAA-C2A-C1A | -2.13 | 120.52      | 124.85   |
| 3   | D     | 900 | FAD  | O2'-C2'-C1' | -2.13 | 101.46      | 110.20   |
| 2   | A     | 604 | HEC  | CHB-C4A-NA  | 2.12  | 126.77      | 124.45   |
| 3   | C     | 800 | FAD  | O2'-C2'-C1' | -2.12 | 101.49      | 110.20   |
| 3   | D     | 900 | FAD  | O4B-C1B-C2B | -2.11 | 102.09      | 106.62   |
| 3   | B     | 700 | FAD  | O5B-PA-O1A  | -2.11 | 100.56      | 108.94   |
| 3   | B     | 700 | FAD  | N10-C10-N1  | 2.11  | 124.71      | 118.51   |
| 2   | C     | 604 | HEC  | CMD-C2D-C3D | 2.10  | 130.08      | 125.62   |
| 3   | A     | 600 | FAD  | C8M-C8-C9   | 2.10  | 123.27      | 119.57   |
| 2   | A     | 601 | HEC  | C2A-C1A-NA  | -2.10 | 108.30      | 110.32   |
| 2   | C     | 604 | HEC  | CHC-C1C-C2C | -2.10 | 121.34      | 127.43   |
| 3   | C     | 800 | FAD  | O2A-PA-O1A  | 2.10  | 122.20      | 112.44   |
| 2   | A     | 604 | HEC  | CHA-C1A-C2A | 2.09  | 128.17      | 124.86   |
| 2   | D     | 602 | HEC  | C3D-C4D-ND  | -2.09 | 107.83      | 110.15   |
| 2   | A     | 604 | HEC  | CMD-C2D-C3D | 2.08  | 130.04      | 125.62   |
| 2   | A     | 601 | HEC  | CMC-C2C-C1C | -2.07 | 122.26      | 125.42   |
| 2   | D     | 603 | HEC  | CAD-C3D-C4D | -2.07 | 120.89      | 124.94   |
| 2   | D     | 604 | HEC  | C2A-C1A-NA  | -2.06 | 108.33      | 110.32   |
| 3   | D     | 900 | FAD  | C6-C5X-N5   | 2.06  | 121.86      | 118.44   |
| 2   | C     | 603 | HEC  | O1A-CGA-CBA | -2.05 | 116.59      | 123.09   |
| 3   | C     | 800 | FAD  | O3B-C3B-C2B | -2.05 | 105.26      | 111.82   |
| 2   | B     | 604 | HEC  | CHA-C1A-NA  | 2.04  | 126.67      | 124.45   |
| 3   | A     | 600 | FAD  | C5A-C4A-N3A | 2.04  | 129.52      | 126.72   |
| 2   | A     | 603 | HEC  | CHC-C1C-NC  | 2.04  | 127.55      | 123.86   |
| 3   | C     | 800 | FAD  | C5A-C6A-N1A | -2.03 | 112.35      | 117.51   |
| 2   | C     | 604 | HEC  | CHB-C4A-C3A | -2.03 | 121.26      | 125.49   |
| 3   | A     | 600 | FAD  | C5A-N7A-C8A | 2.03  | 106.64      | 103.45   |
| 3   | D     | 900 | FAD  | C5A-N7A-C8A | 2.03  | 106.64      | 103.45   |
| 3   | B     | 700 | FAD  | C2B-C3B-C4B | 2.03  | 106.53      | 102.61   |
| 3   | A     | 600 | FAD  | C5A-C4A-N9A | -2.02 | 103.61      | 105.81   |
| 2   | B     | 603 | HEC  | CBA-CAA-C2A | -2.02 | 106.95      | 112.53   |
| 2   | A     | 601 | HEC  | CAA-CBA-CGA | -2.02 | 108.31      | 113.67   |
| 2   | D     | 603 | HEC  | O1D-CGD-CBD | -2.02 | 116.69      | 123.09   |
| 2   | B     | 604 | HEC  | CBA-CAA-C2A | 2.02  | 118.11      | 112.53   |
| 2   | D     | 601 | HEC  | CHD-C1D-ND  | 2.01  | 127.51      | 123.86   |
| 2   | C     | 604 | HEC  | CAA-C2A-C3A | -2.01 | 124.10      | 127.87   |
| 3   | C     | 800 | FAD  | C9A-N10-C10 | -2.01 | 117.69      | 120.75   |
| 3   | B     | 700 | FAD  | O4-C4-N3    | -2.01 | 116.34      | 120.11   |
| 2   | B     | 601 | HEC  | C3D-C4D-ND  | -2.00 | 107.93      | 110.15   |

All (9) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 3   | A     | 600 | FAD  | C3'  |
| 3   | A     | 600 | FAD  | C4'  |
| 3   | B     | 700 | FAD  | C3'  |
| 3   | B     | 700 | FAD  | C4'  |
| 3   | C     | 800 | FAD  | C4B  |
| 3   | C     | 800 | FAD  | C3'  |
| 3   | C     | 800 | FAD  | C4'  |
| 3   | D     | 900 | FAD  | C3'  |
| 3   | D     | 900 | FAD  | C4'  |

All (191) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | A     | 601 | HEC  | C2C-C3C-CAC-CBC |
| 2   | A     | 601 | HEC  | C4C-C3C-CAC-CBC |
| 2   | A     | 601 | HEC  | C3D-CAD-CBD-CGD |
| 2   | A     | 602 | HEC  | C2C-C3C-CAC-CBC |
| 2   | A     | 602 | HEC  | C4C-C3C-CAC-CBC |
| 2   | A     | 603 | HEC  | C2B-C3B-CAB-CBB |
| 2   | A     | 603 | HEC  | C4B-C3B-CAB-CBB |
| 2   | A     | 604 | HEC  | C2C-C3C-CAC-CBC |
| 2   | A     | 604 | HEC  | C4C-C3C-CAC-CBC |
| 2   | B     | 601 | HEC  | C2B-C3B-CAB-CBB |
| 2   | B     | 601 | HEC  | C2C-C3C-CAC-CBC |
| 2   | B     | 601 | HEC  | C4C-C3C-CAC-CBC |
| 2   | B     | 602 | HEC  | C2A-CAA-CBA-CGA |
| 2   | B     | 602 | HEC  | C2B-C3B-CAB-CBB |
| 2   | B     | 602 | HEC  | C4B-C3B-CAB-CBB |
| 2   | B     | 604 | HEC  | C2B-C3B-CAB-CBB |
| 2   | B     | 604 | HEC  | C4D-C3D-CAD-CBD |
| 2   | C     | 601 | HEC  | C2B-C3B-CAB-CBB |
| 2   | C     | 601 | HEC  | C2C-C3C-CAC-CBC |
| 2   | C     | 601 | HEC  | C4C-C3C-CAC-CBC |
| 2   | C     | 602 | HEC  | C2A-CAA-CBA-CGA |
| 2   | C     | 602 | HEC  | C2B-C3B-CAB-CBB |
| 2   | C     | 602 | HEC  | C4B-C3B-CAB-CBB |
| 2   | C     | 602 | HEC  | C2C-C3C-CAC-CBC |
| 2   | C     | 602 | HEC  | C4C-C3C-CAC-CBC |
| 2   | C     | 603 | HEC  | C2B-C3B-CAB-CBB |
| 2   | C     | 603 | HEC  | C4B-C3B-CAB-CBB |
| 2   | C     | 603 | HEC  | C4C-C3C-CAC-CBC |
| 2   | C     | 604 | HEC  | C2B-C3B-CAB-CBB |
| 2   | C     | 604 | HEC  | C4B-C3B-CAB-CBB |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | C     | 604 | HEC  | C2C-C3C-CAC-CBC |
| 2   | C     | 604 | HEC  | C4C-C3C-CAC-CBC |
| 2   | C     | 604 | HEC  | C4D-C3D-CAD-CBD |
| 2   | D     | 601 | HEC  | C2C-C3C-CAC-CBC |
| 2   | D     | 601 | HEC  | C4C-C3C-CAC-CBC |
| 2   | D     | 601 | HEC  | C4D-C3D-CAD-CBD |
| 2   | D     | 602 | HEC  | C2B-C3B-CAB-CBB |
| 2   | D     | 602 | HEC  | C2C-C3C-CAC-CBC |
| 2   | D     | 602 | HEC  | C4C-C3C-CAC-CBC |
| 3   | A     | 600 | FAD  | C5B-O5B-PA-O1A  |
| 3   | A     | 600 | FAD  | C3B-C4B-C5B-O5B |
| 3   | A     | 600 | FAD  | C1'-C2'-C3'-O3' |
| 3   | A     | 600 | FAD  | C1'-C2'-C3'-C4' |
| 3   | A     | 600 | FAD  | C3'-C4'-C5'-O5' |
| 3   | A     | 600 | FAD  | O4'-C4'-C5'-O5' |
| 3   | B     | 700 | FAD  | C3B-C4B-C5B-O5B |
| 3   | B     | 700 | FAD  | C1'-C2'-C3'-O3' |
| 3   | B     | 700 | FAD  | C1'-C2'-C3'-C4' |
| 3   | B     | 700 | FAD  | O2'-C2'-C3'-O3' |
| 3   | B     | 700 | FAD  | O2'-C2'-C3'-C4' |
| 3   | B     | 700 | FAD  | C3'-C4'-C5'-O5' |
| 3   | B     | 700 | FAD  | O4'-C4'-C5'-O5' |
| 3   | C     | 800 | FAD  | C1'-C2'-C3'-O3' |
| 3   | C     | 800 | FAD  | C1'-C2'-C3'-C4' |
| 3   | C     | 800 | FAD  | C3'-C4'-C5'-O5' |
| 3   | C     | 800 | FAD  | O4'-C4'-C5'-O5' |
| 3   | D     | 900 | FAD  | C1'-C2'-C3'-C4' |
| 3   | D     | 900 | FAD  | O2'-C2'-C3'-C4' |
| 3   | D     | 900 | FAD  | C3'-C4'-C5'-O5' |
| 3   | D     | 900 | FAD  | O4'-C4'-C5'-O5' |
| 2   | C     | 604 | HEC  | C1A-C2A-CAA-CBA |
| 3   | C     | 800 | FAD  | O2'-C2'-C3'-O3' |
| 3   | D     | 900 | FAD  | O3'-C3'-C4'-O4' |
| 3   | A     | 600 | FAD  | O2'-C2'-C3'-C4' |
| 3   | C     | 800 | FAD  | O2'-C2'-C3'-C4' |
| 3   | C     | 800 | FAD  | C3B-C4B-C5B-O5B |
| 3   | D     | 900 | FAD  | O4B-C4B-C5B-O5B |
| 3   | D     | 900 | FAD  | C3B-C4B-C5B-O5B |
| 2   | B     | 601 | HEC  | C3D-CAD-CBD-CGD |
| 2   | C     | 603 | HEC  | C3D-CAD-CBD-CGD |
| 2   | D     | 603 | HEC  | C3D-CAD-CBD-CGD |
| 2   | C     | 604 | HEC  | C2D-C3D-CAD-CBD |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 3   | D     | 900 | FAD  | O2'-C2'-C3'-O3' |
| 3   | A     | 600 | FAD  | O4B-C4B-C5B-O5B |
| 2   | A     | 602 | HEC  | C2A-CAA-CBA-CGA |
| 2   | B     | 601 | HEC  | C2A-CAA-CBA-CGA |
| 2   | C     | 601 | HEC  | C3D-CAD-CBD-CGD |
| 2   | D     | 601 | HEC  | C3D-CAD-CBD-CGD |
| 2   | D     | 602 | HEC  | C2A-CAA-CBA-CGA |
| 2   | C     | 604 | HEC  | C3A-C2A-CAA-CBA |
| 3   | B     | 700 | FAD  | O4B-C4B-C5B-O5B |
| 3   | C     | 800 | FAD  | O4B-C4B-C5B-O5B |
| 2   | D     | 601 | HEC  | C2D-C3D-CAD-CBD |
| 3   | A     | 600 | FAD  | O2'-C2'-C3'-O3' |
| 2   | A     | 601 | HEC  | C1A-C2A-CAA-CBA |
| 2   | B     | 604 | HEC  | C2D-C3D-CAD-CBD |
| 3   | D     | 900 | FAD  | P-O3P-PA-O1A    |
| 2   | A     | 601 | HEC  | C3A-C2A-CAA-CBA |
| 3   | D     | 900 | FAD  | O3'-C3'-C4'-C5' |
| 2   | A     | 603 | HEC  | C3D-CAD-CBD-CGD |
| 3   | A     | 600 | FAD  | PA-O3P-P-O5'    |
| 3   | B     | 700 | FAD  | PA-O3P-P-O5'    |
| 3   | C     | 800 | FAD  | PA-O3P-P-O5'    |
| 3   | D     | 900 | FAD  | PA-O3P-P-O5'    |
| 3   | C     | 800 | FAD  | C2B-C1B-N9A-C8A |
| 3   | D     | 900 | FAD  | C1'-C2'-C3'-O3' |
| 3   | A     | 600 | FAD  | P-O3P-PA-O2A    |
| 3   | D     | 900 | FAD  | P-O3P-PA-O2A    |
| 2   | A     | 603 | HEC  | C4C-C3C-CAC-CBC |
| 2   | B     | 601 | HEC  | C4B-C3B-CAB-CBB |
| 2   | B     | 602 | HEC  | C4C-C3C-CAC-CBC |
| 2   | B     | 603 | HEC  | C4B-C3B-CAB-CBB |
| 2   | B     | 603 | HEC  | C4C-C3C-CAC-CBC |
| 2   | B     | 604 | HEC  | C4B-C3B-CAB-CBB |
| 2   | C     | 601 | HEC  | C4B-C3B-CAB-CBB |
| 2   | D     | 602 | HEC  | C4B-C3B-CAB-CBB |
| 2   | D     | 603 | HEC  | C4B-C3B-CAB-CBB |
| 2   | D     | 604 | HEC  | C4C-C3C-CAC-CBC |
| 2   | A     | 602 | HEC  | C3A-C2A-CAA-CBA |
| 2   | A     | 602 | HEC  | C2B-C3B-CAB-CBB |
| 2   | A     | 603 | HEC  | C2C-C3C-CAC-CBC |
| 2   | A     | 604 | HEC  | C2B-C3B-CAB-CBB |
| 2   | B     | 602 | HEC  | C2C-C3C-CAC-CBC |
| 2   | C     | 603 | HEC  | C2C-C3C-CAC-CBC |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | D     | 603 | HEC  | C2B-C3B-CAB-CBB |
| 2   | D     | 604 | HEC  | C2C-C3C-CAC-CBC |
| 3   | A     | 600 | FAD  | C5B-O5B-PA-O2A  |
| 3   | A     | 600 | FAD  | C5B-O5B-PA-O3P  |
| 3   | D     | 900 | FAD  | C5B-O5B-PA-O2A  |
| 3   | D     | 900 | FAD  | C5B-O5B-PA-O3P  |
| 3   | B     | 700 | FAD  | PA-O3P-P-O1P    |
| 3   | C     | 800 | FAD  | P-O3P-PA-O2A    |
| 2   | D     | 604 | HEC  | C3D-CAD-CBD-CGD |
| 2   | D     | 601 | HEC  | CAA-CBA-CGA-O1A |
| 2   | D     | 603 | HEC  | CAD-CBD-CGD-O1D |
| 2   | C     | 602 | HEC  | CAA-CBA-CGA-O1A |
| 2   | D     | 604 | HEC  | CAD-CBD-CGD-O1D |
| 2   | D     | 604 | HEC  | CAD-CBD-CGD-O2D |
| 2   | D     | 602 | HEC  | CAA-CBA-CGA-O1A |
| 2   | D     | 603 | HEC  | CAD-CBD-CGD-O2D |
| 2   | C     | 602 | HEC  | CAD-CBD-CGD-O2D |
| 2   | A     | 602 | HEC  | C1A-C2A-CAA-CBA |
| 2   | A     | 602 | HEC  | CAD-CBD-CGD-O2D |
| 2   | C     | 602 | HEC  | CAA-CBA-CGA-O2A |
| 2   | B     | 601 | HEC  | CAD-CBD-CGD-O1D |
| 2   | C     | 602 | HEC  | CAD-CBD-CGD-O1D |
| 2   | B     | 603 | HEC  | CAD-CBD-CGD-O1D |
| 2   | C     | 601 | HEC  | CAD-CBD-CGD-O2D |
| 2   | C     | 603 | HEC  | CAA-CBA-CGA-O1A |
| 2   | A     | 602 | HEC  | CAD-CBD-CGD-O1D |
| 2   | A     | 603 | HEC  | CAD-CBD-CGD-O1D |
| 2   | C     | 603 | HEC  | CAD-CBD-CGD-O1D |
| 2   | D     | 601 | HEC  | CAD-CBD-CGD-O2D |
| 2   | D     | 602 | HEC  | CAD-CBD-CGD-O2D |
| 2   | A     | 602 | HEC  | CAA-CBA-CGA-O2A |
| 2   | C     | 603 | HEC  | CAA-CBA-CGA-O2A |
| 2   | D     | 601 | HEC  | CAA-CBA-CGA-O2A |
| 2   | B     | 601 | HEC  | CAD-CBD-CGD-O2D |
| 2   | B     | 602 | HEC  | CAA-CBA-CGA-O1A |
| 3   | B     | 700 | FAD  | P-O3P-PA-O2A    |
| 3   | C     | 800 | FAD  | P-O3P-PA-O1A    |
| 3   | C     | 800 | FAD  | PA-O3P-P-O1P    |
| 2   | C     | 601 | HEC  | CAD-CBD-CGD-O1D |
| 2   | D     | 601 | HEC  | CAD-CBD-CGD-O1D |
| 2   | D     | 602 | HEC  | CAA-CBA-CGA-O2A |
| 2   | D     | 602 | HEC  | CAD-CBD-CGD-O1D |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 3   | C     | 800 | FAD  | O4B-C1B-N9A-C8A |
| 2   | A     | 602 | HEC  | CAA-CBA-CGA-O1A |
| 2   | B     | 601 | HEC  | CAA-CBA-CGA-O2A |
| 3   | A     | 600 | FAD  | O3'-C3'-C4'-C5' |
| 2   | A     | 603 | HEC  | CAD-CBD-CGD-O2D |
| 2   | B     | 602 | HEC  | CAA-CBA-CGA-O2A |
| 2   | C     | 601 | HEC  | CAA-CBA-CGA-O2A |
| 2   | C     | 603 | HEC  | CAD-CBD-CGD-O2D |
| 2   | A     | 604 | HEC  | CAD-CBD-CGD-O1D |
| 2   | B     | 603 | HEC  | CAD-CBD-CGD-O2D |
| 2   | A     | 604 | HEC  | CAD-CBD-CGD-O2D |
| 2   | C     | 601 | HEC  | CAA-CBA-CGA-O1A |
| 2   | B     | 602 | HEC  | CAD-CBD-CGD-O2D |
| 2   | A     | 601 | HEC  | CAD-CBD-CGD-O2D |
| 2   | B     | 601 | HEC  | CAA-CBA-CGA-O1A |
| 2   | B     | 602 | HEC  | CAD-CBD-CGD-O1D |
| 2   | A     | 601 | HEC  | CAD-CBD-CGD-O1D |
| 2   | B     | 604 | HEC  | CAD-CBD-CGD-O1D |
| 2   | C     | 604 | HEC  | CAA-CBA-CGA-O2A |
| 3   | B     | 700 | FAD  | C2B-C1B-N9A-C8A |
| 3   | D     | 900 | FAD  | C2B-C1B-N9A-C8A |
| 2   | A     | 601 | HEC  | CAA-CBA-CGA-O2A |
| 2   | D     | 604 | HEC  | C4D-C3D-CAD-CBD |
| 2   | B     | 604 | HEC  | CAD-CBD-CGD-O2D |
| 2   | A     | 601 | HEC  | C4B-C3B-CAB-CBB |
| 2   | A     | 602 | HEC  | C4B-C3B-CAB-CBB |
| 2   | A     | 604 | HEC  | C4B-C3B-CAB-CBB |
| 2   | B     | 604 | HEC  | C4C-C3C-CAC-CBC |
| 2   | D     | 601 | HEC  | C4B-C3B-CAB-CBB |
| 2   | D     | 603 | HEC  | C4C-C3C-CAC-CBC |
| 2   | D     | 604 | HEC  | C4B-C3B-CAB-CBB |
| 2   | C     | 604 | HEC  | CAA-CBA-CGA-O1A |
| 3   | C     | 800 | FAD  | C2'-C3'-C4'-O4' |
| 3   | B     | 700 | FAD  | P-O3P-PA-O1A    |
| 2   | A     | 601 | HEC  | CAA-CBA-CGA-O1A |

There are no ring outliers.

19 monomers are involved in 95 short contacts:

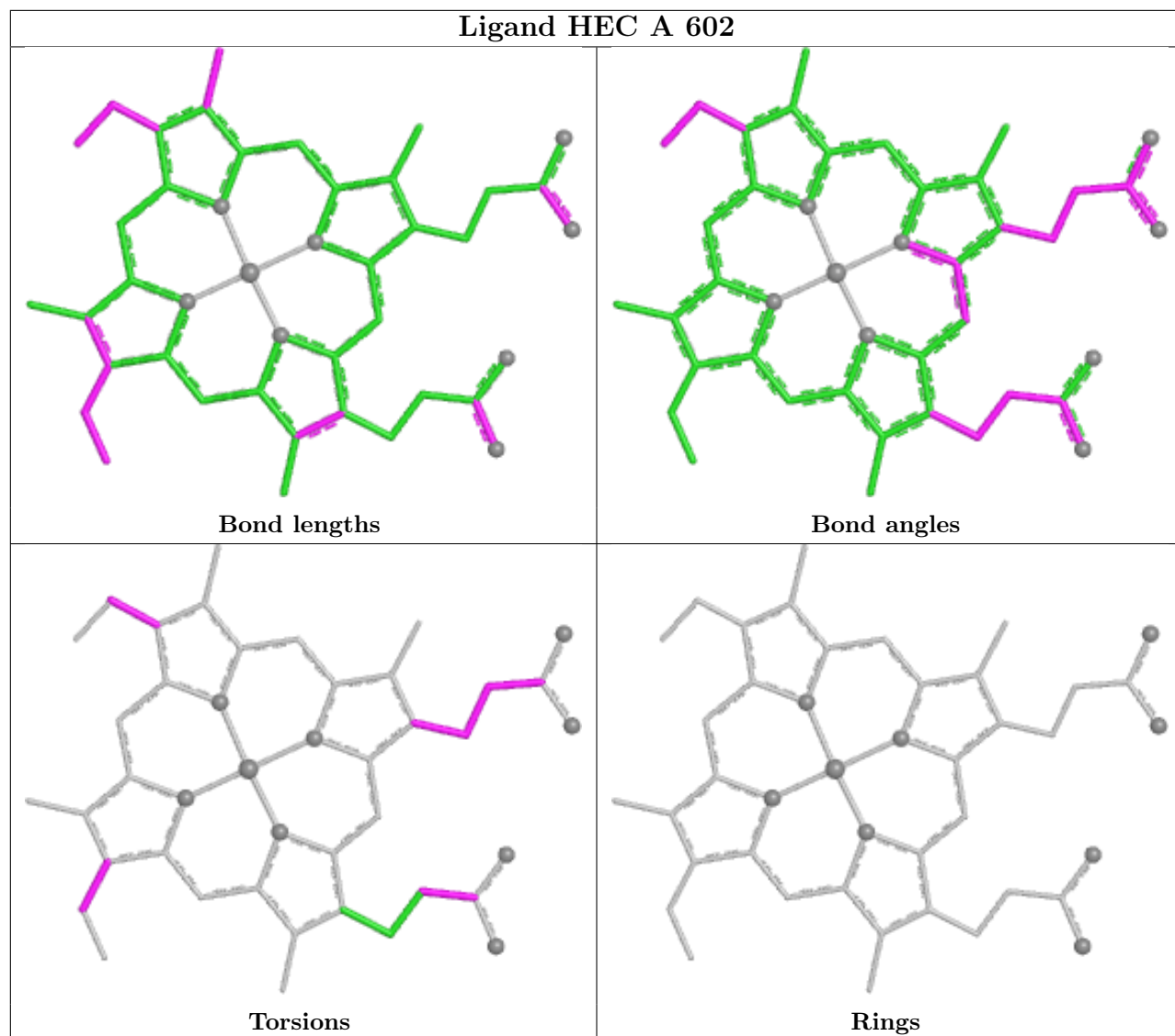
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2   | A     | 602 | HEC  | 5       | 0            |
| 3   | A     | 600 | FAD  | 9       | 0            |

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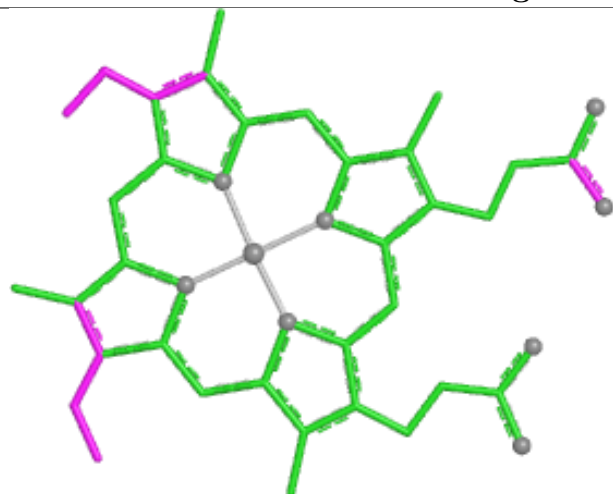
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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2   | D     | 604 | HEC  | 3       | 0            |
| 3   | C     | 800 | FAD  | 12      | 0            |
| 3   | B     | 700 | FAD  | 8       | 0            |
| 2   | C     | 604 | HEC  | 4       | 0            |
| 2   | D     | 602 | HEC  | 7       | 0            |
| 2   | B     | 603 | HEC  | 1       | 0            |
| 2   | C     | 602 | HEC  | 4       | 0            |
| 2   | B     | 601 | HEC  | 4       | 0            |
| 2   | C     | 601 | HEC  | 4       | 0            |
| 2   | A     | 604 | HEC  | 3       | 0            |
| 2   | D     | 603 | HEC  | 4       | 0            |
| 2   | B     | 602 | HEC  | 6       | 0            |
| 3   | D     | 900 | FAD  | 9       | 0            |
| 2   | B     | 604 | HEC  | 1       | 0            |
| 2   | A     | 601 | HEC  | 6       | 0            |
| 4   | B     | 714 | SO4  | 1       | 0            |
| 2   | D     | 601 | HEC  | 4       | 0            |

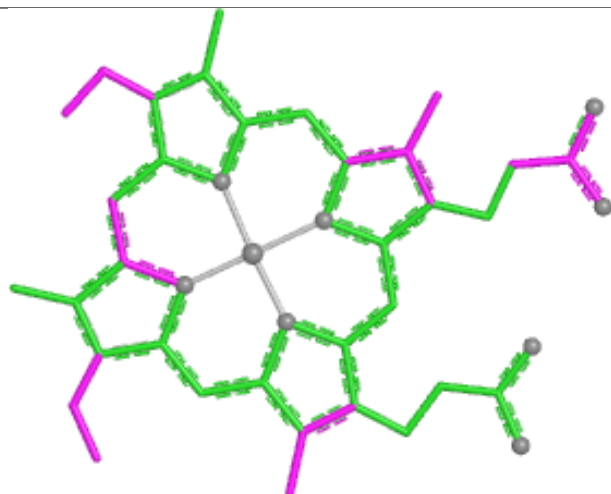
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



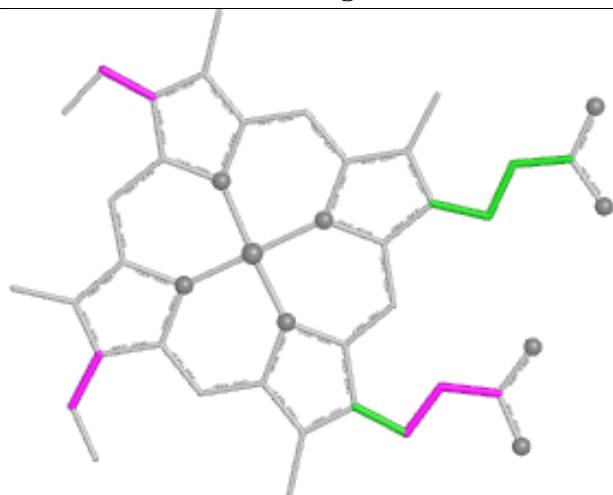
## Ligand HEC A 603



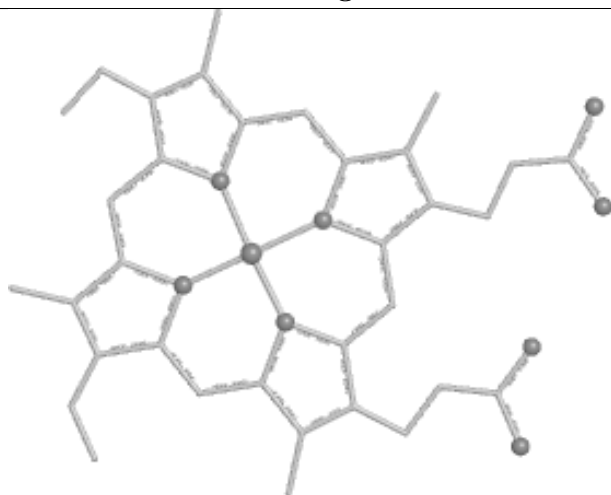
Bond lengths



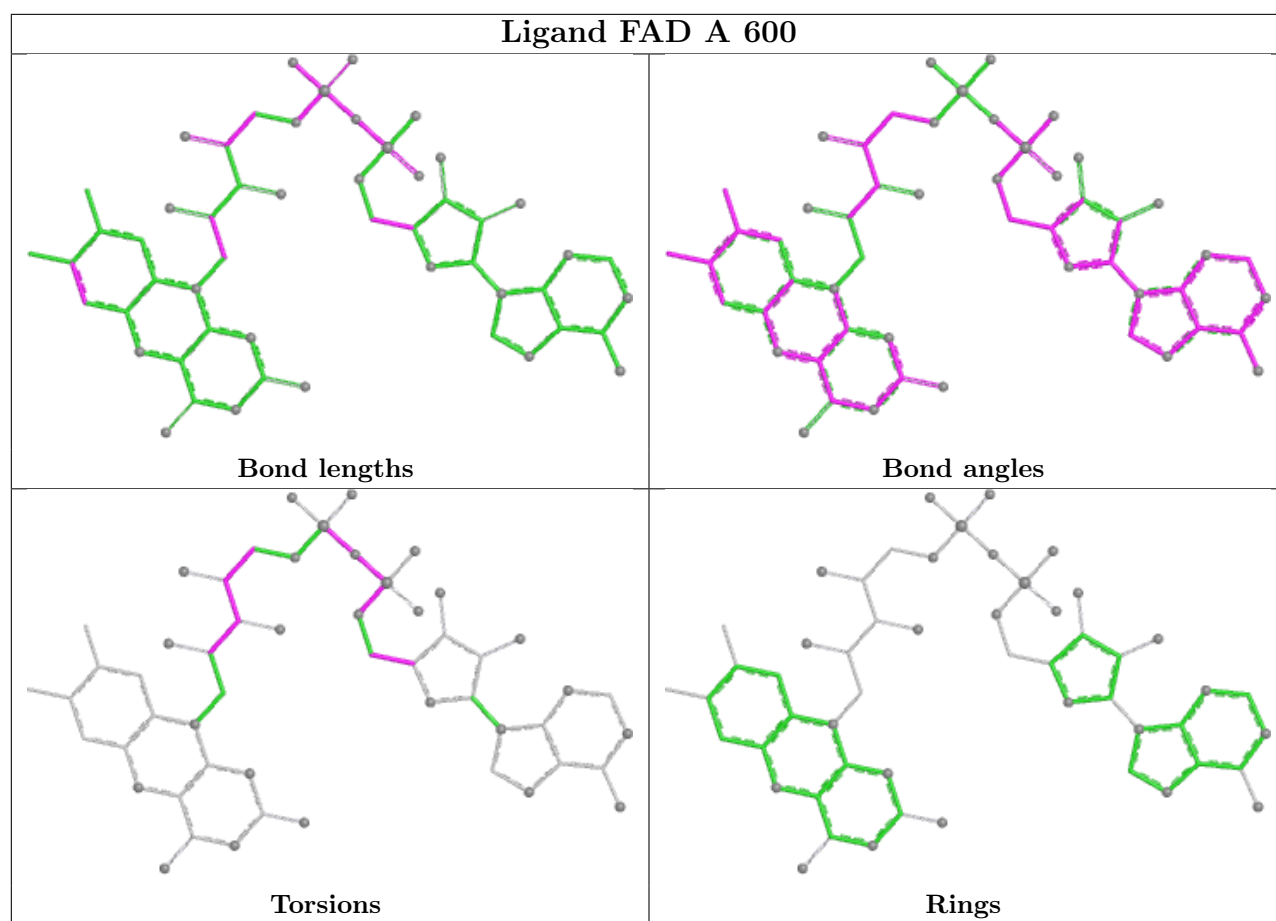
Bond angles

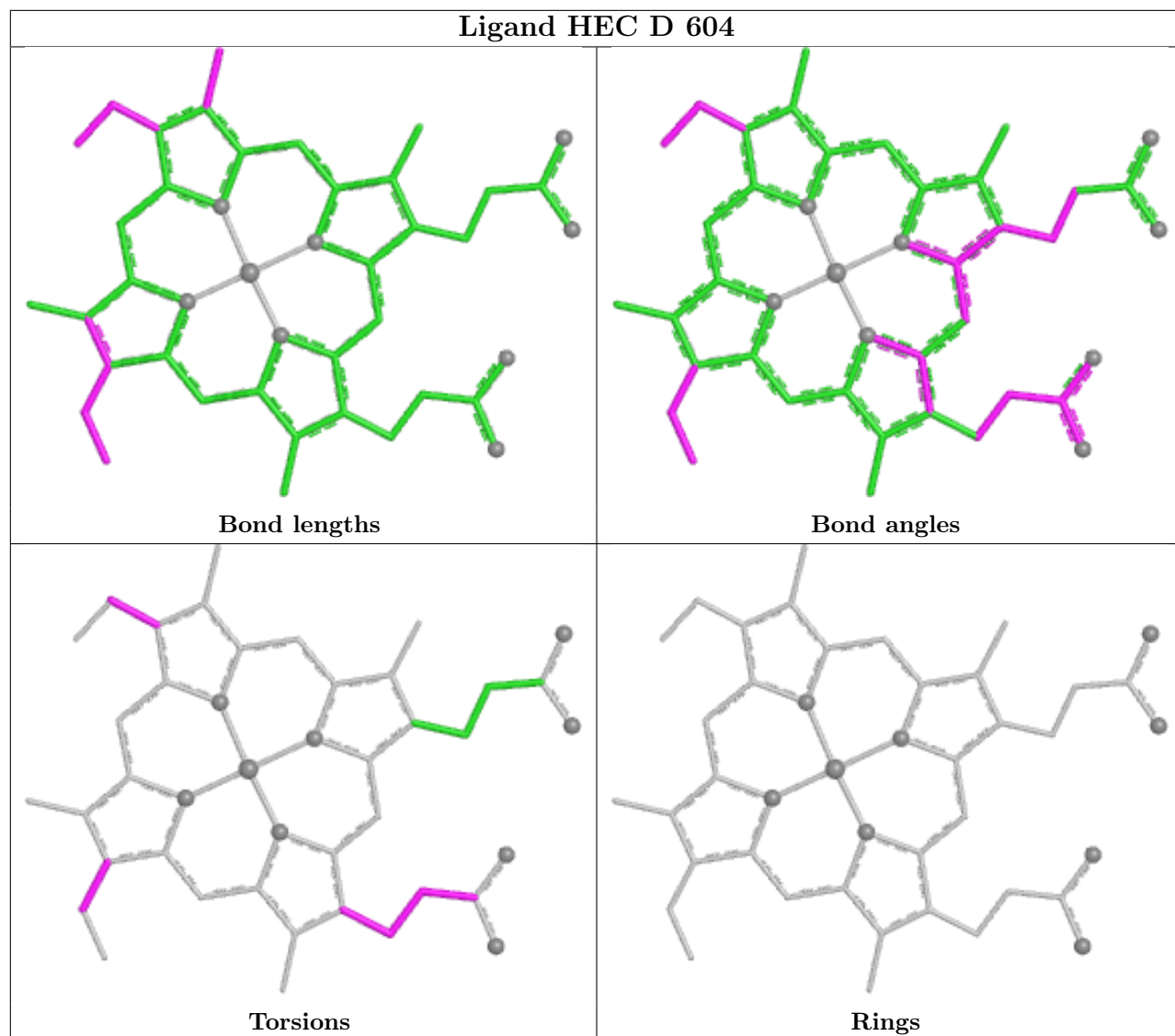


Torsions

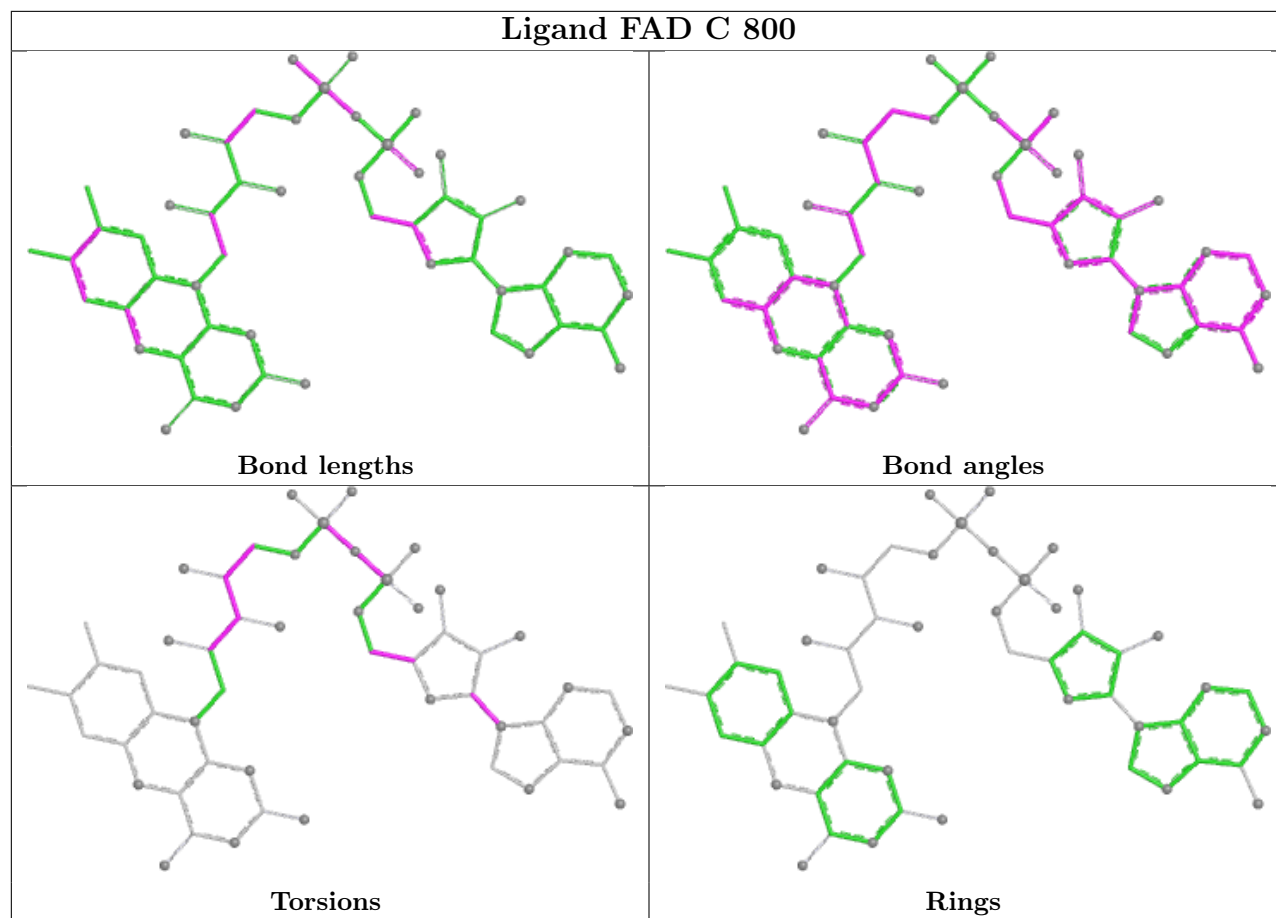


Rings

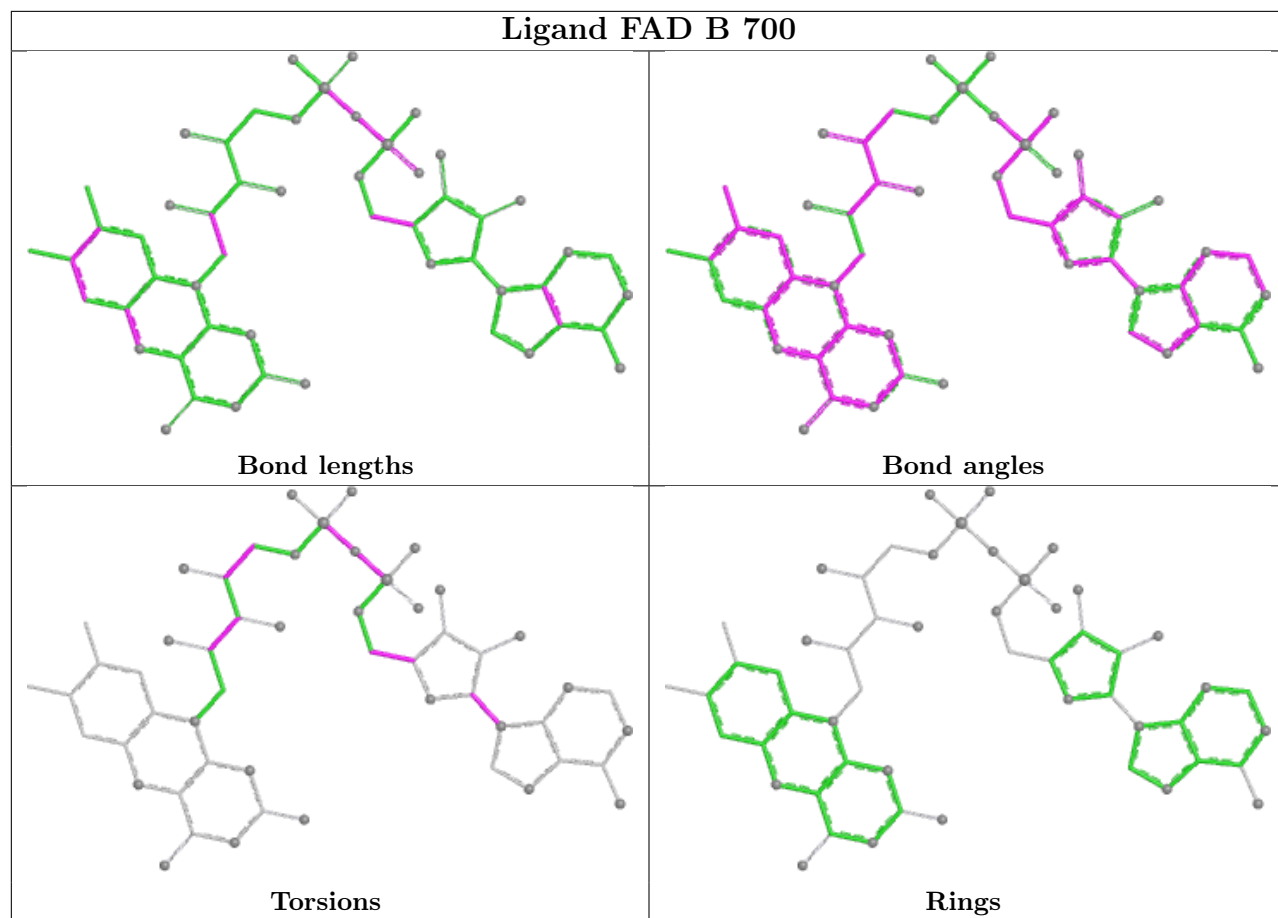




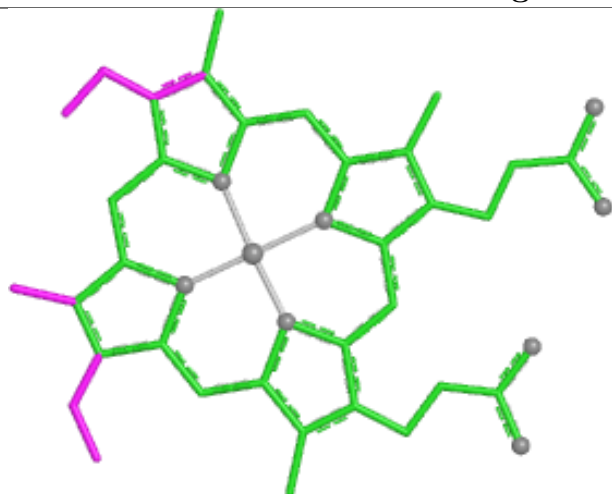




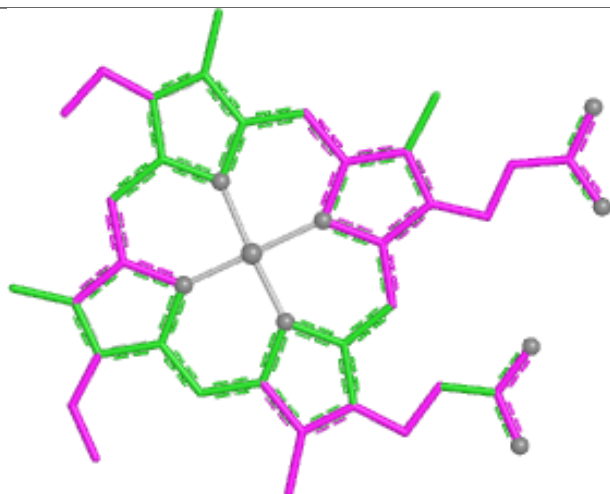
## Ligand FAD B 700



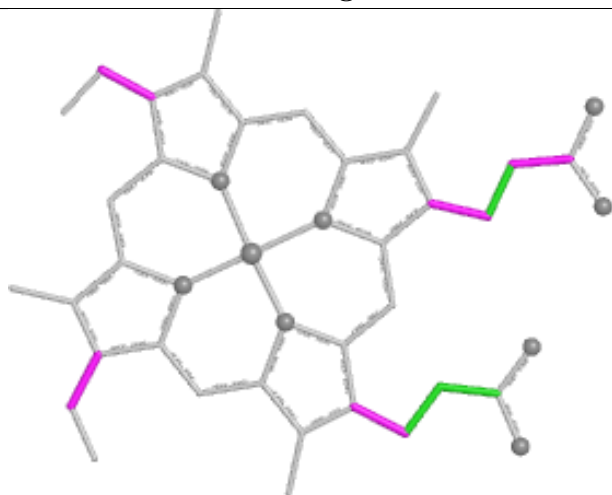
## Ligand HEC C 604



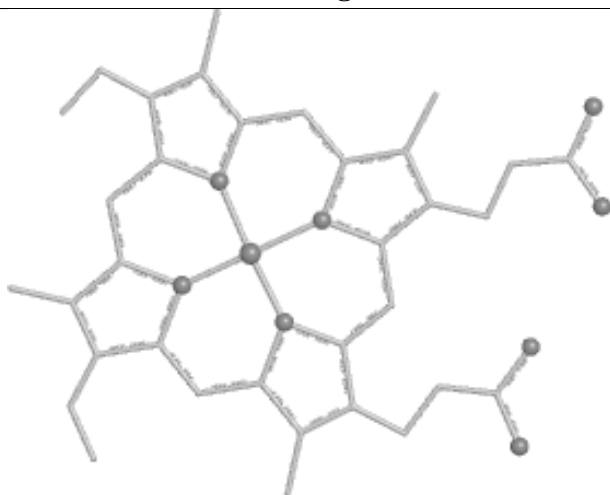
Bond lengths



Bond angles

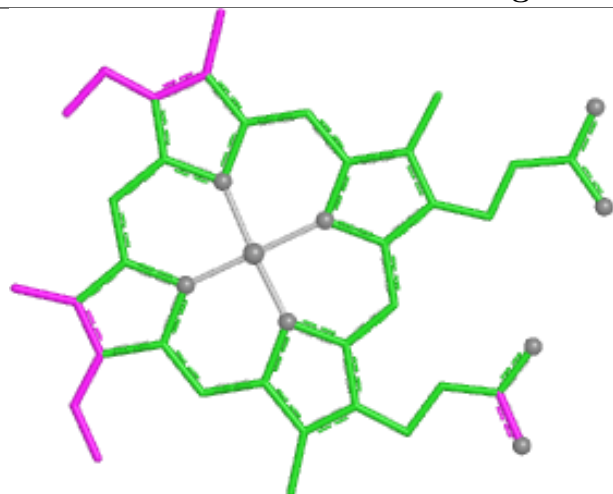


Torsions

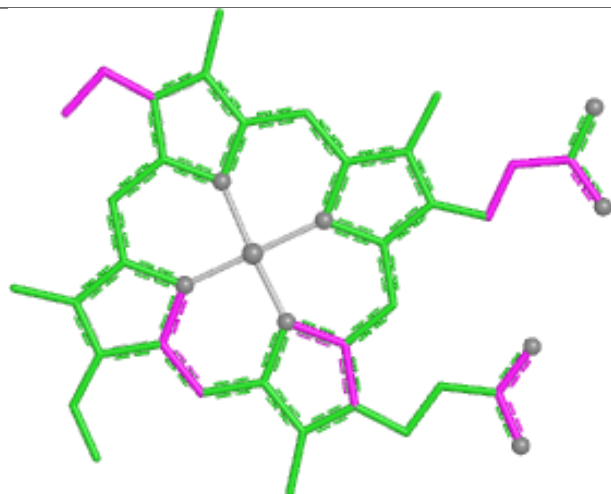


Rings

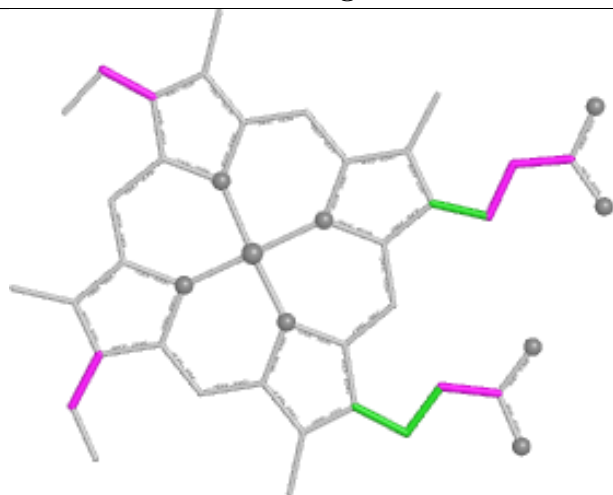
## Ligand HEC D 602



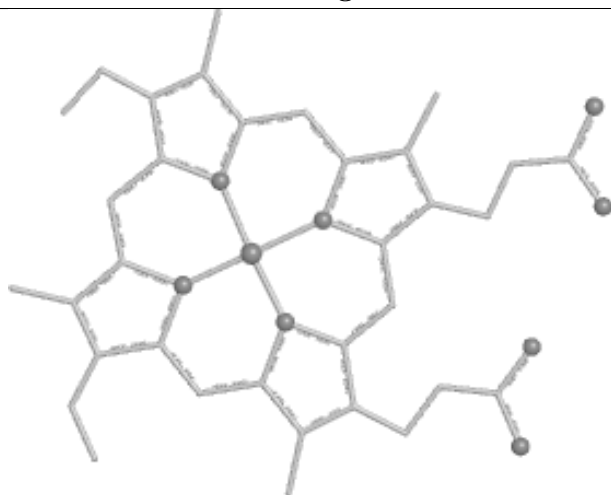
Bond lengths



Bond angles

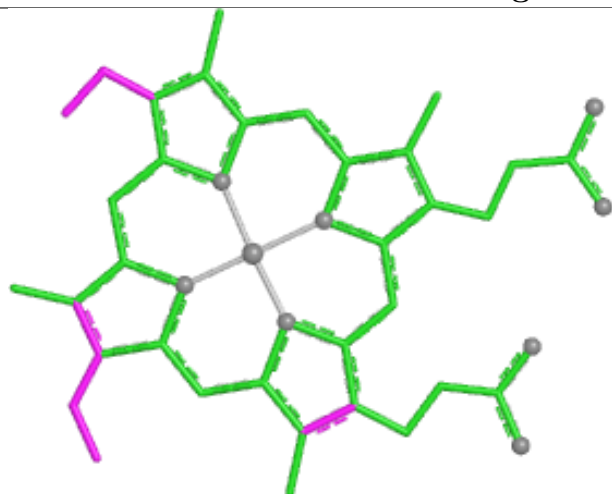


Torsions

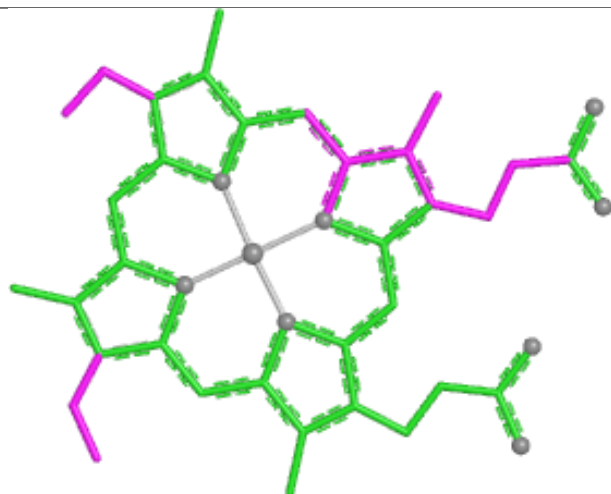


Rings

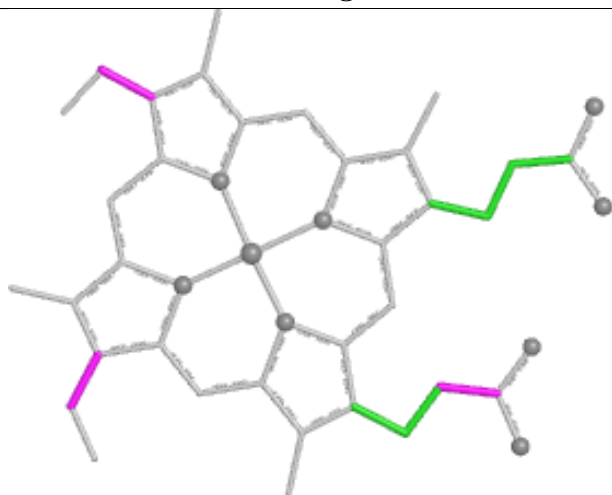
## Ligand HEC B 603



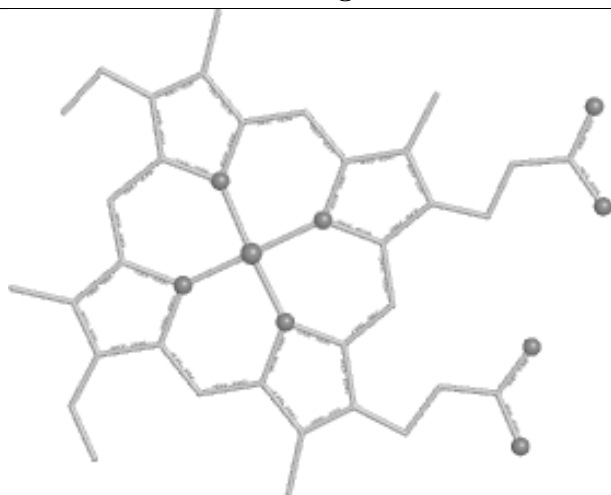
Bond lengths



Bond angles

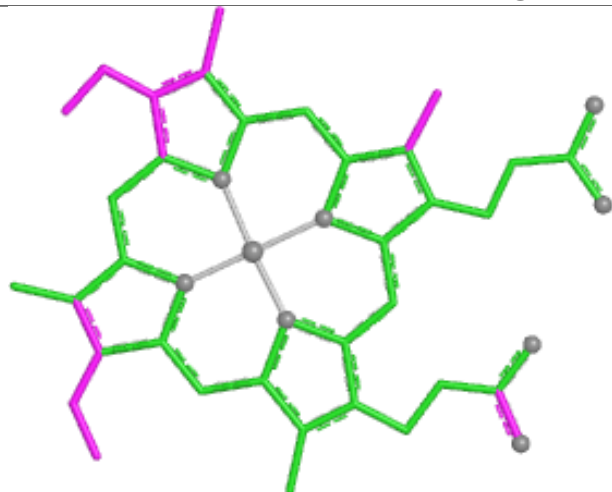


Torsions

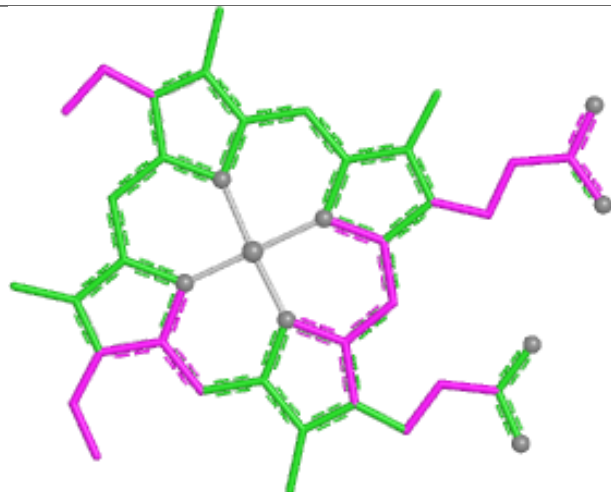


Rings

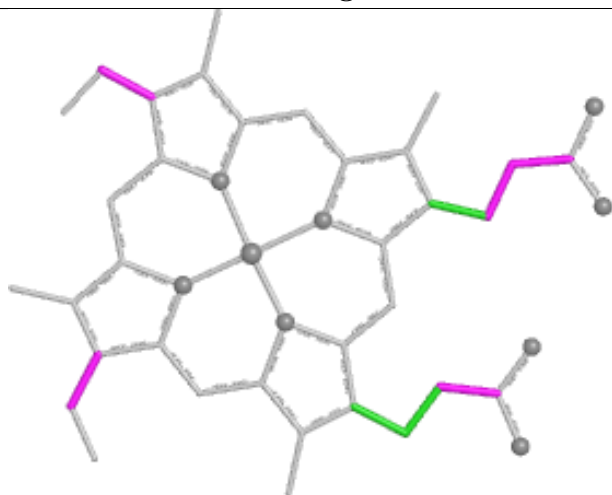
## Ligand HEC C 602



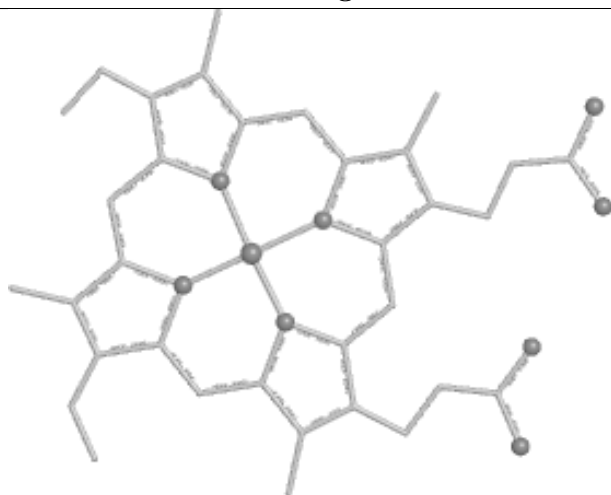
Bond lengths



Bond angles

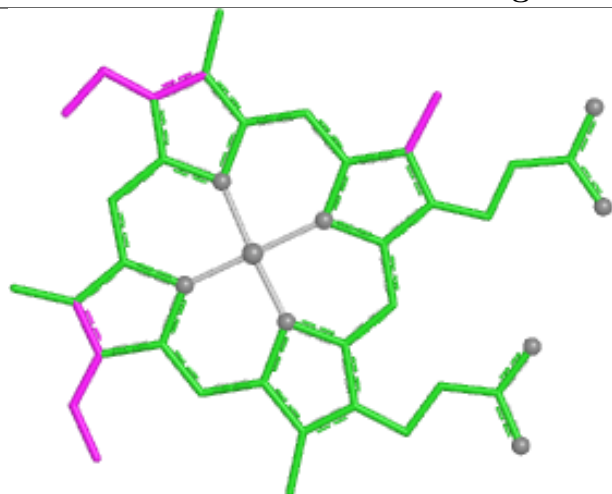


Torsions

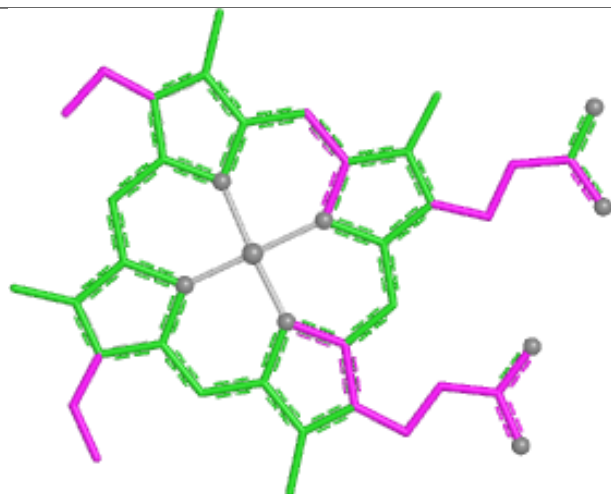


Rings

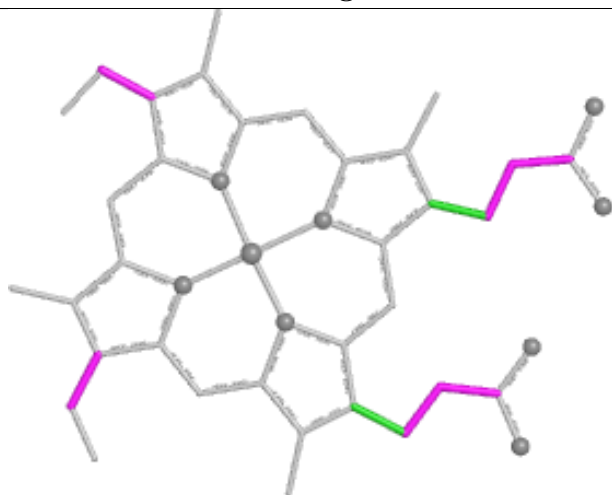
## Ligand HEC B 601



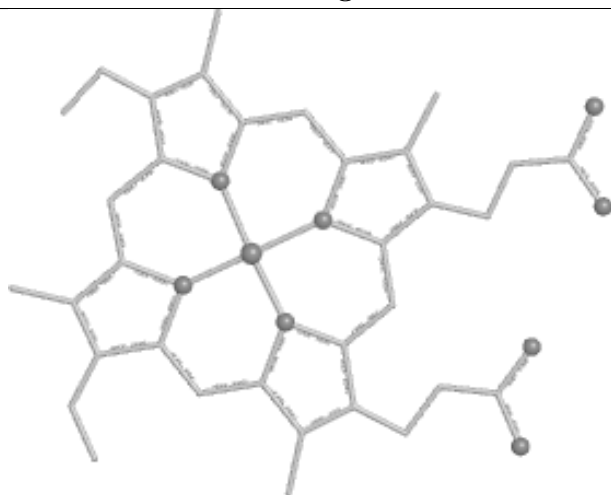
Bond lengths



Bond angles

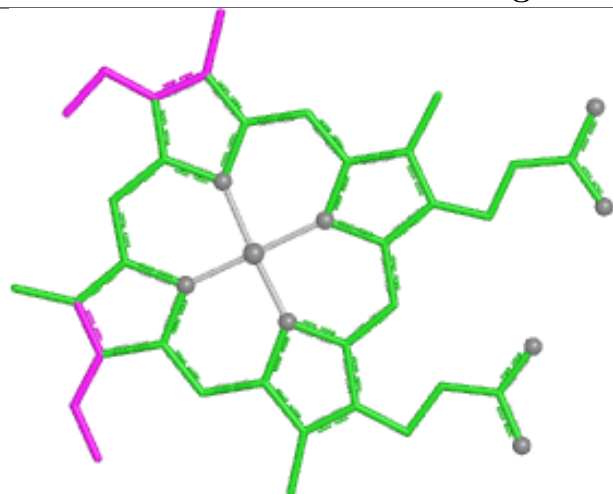


Torsions

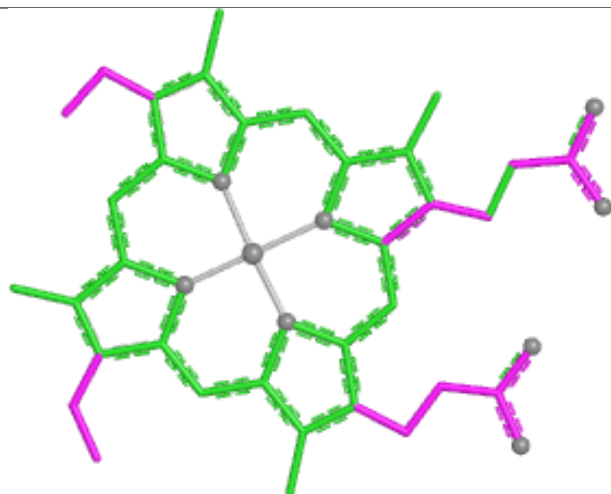


Rings

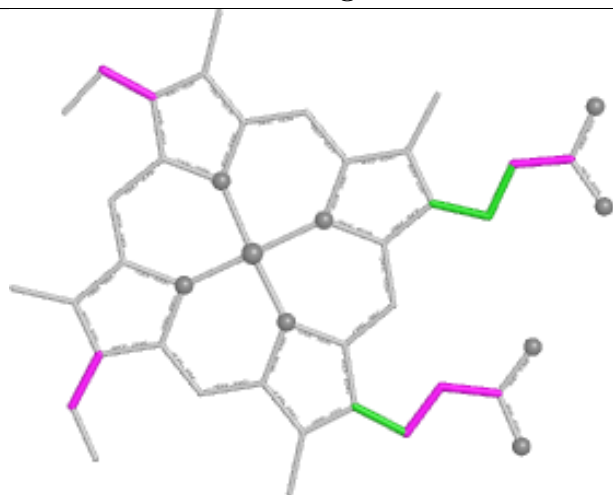
## Ligand HEC C 601



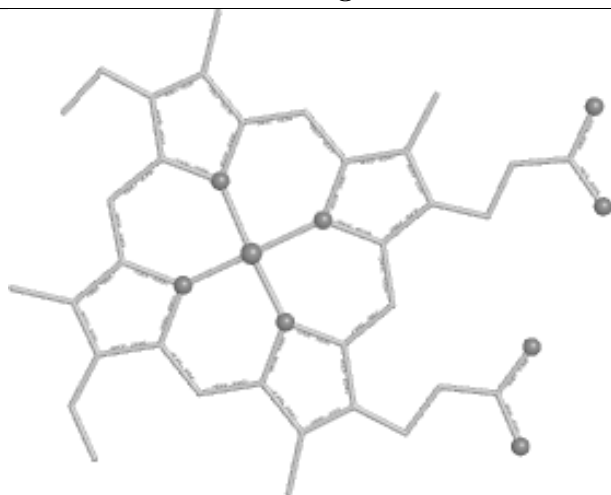
Bond lengths



Bond angles

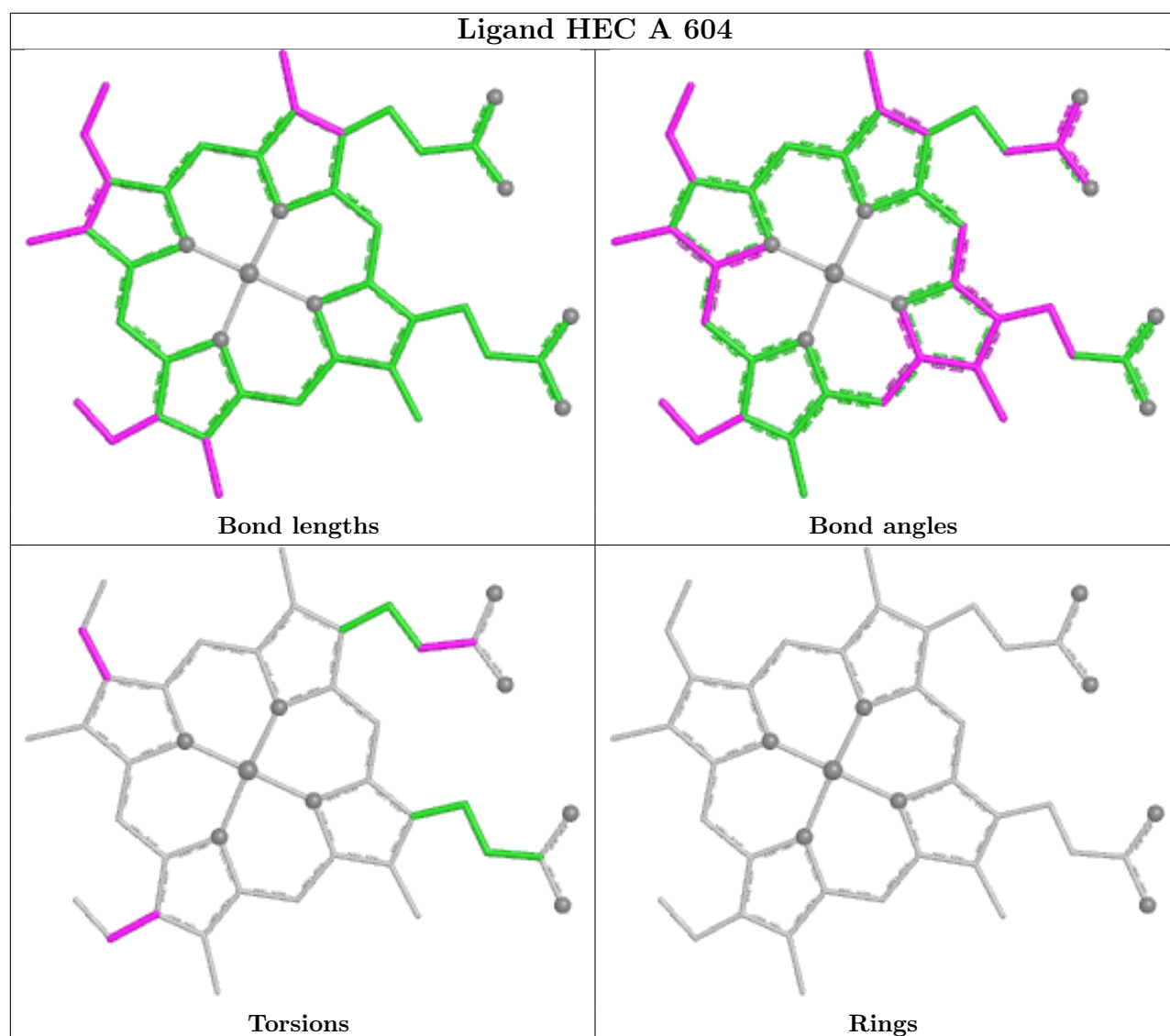


Torsions

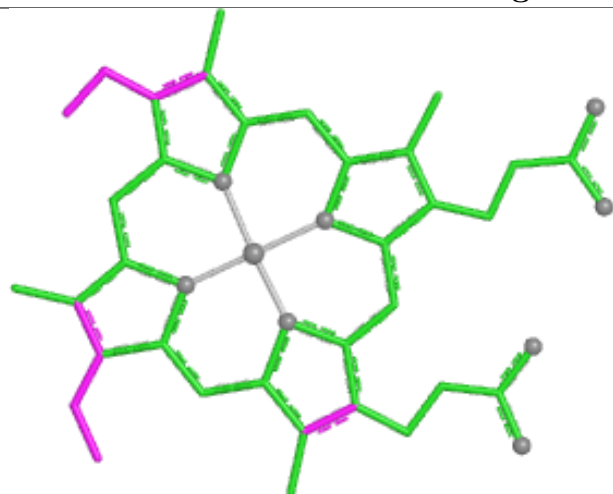


Rings

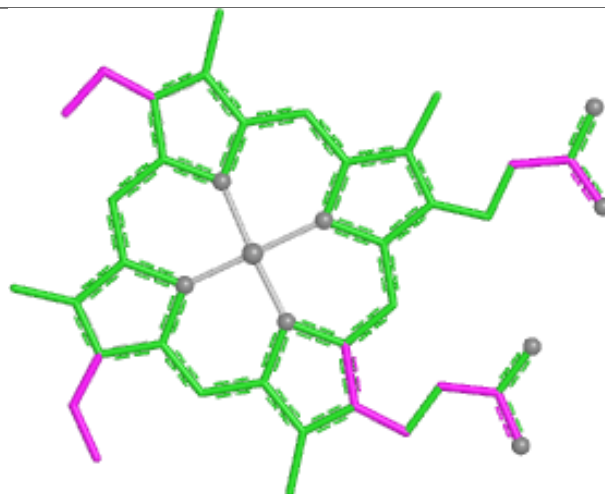




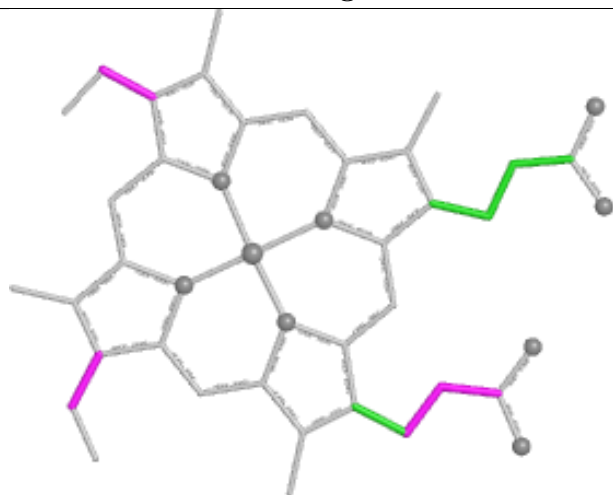
## Ligand HEC D 603



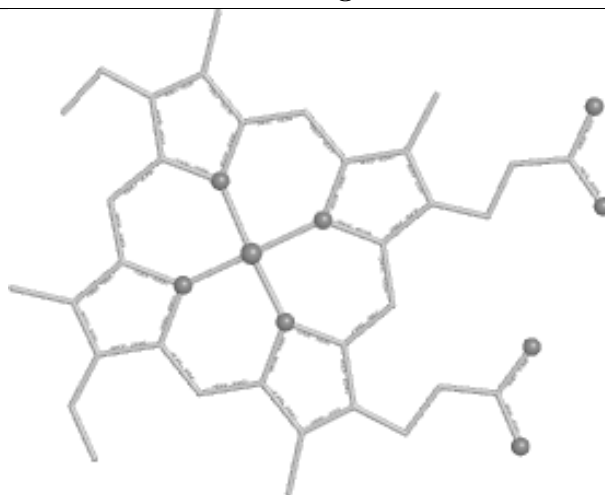
Bond lengths



Bond angles

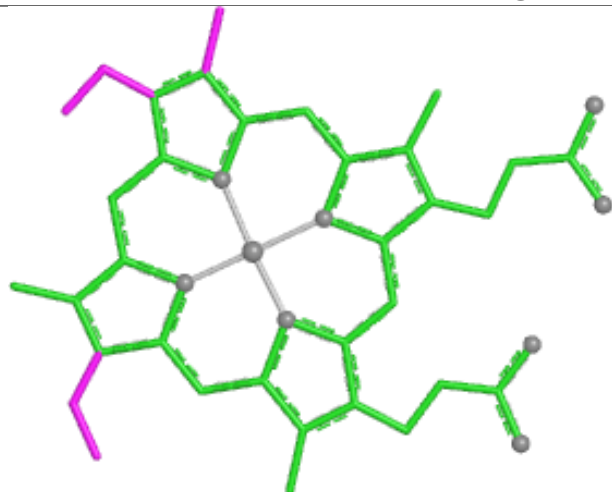


Torsions

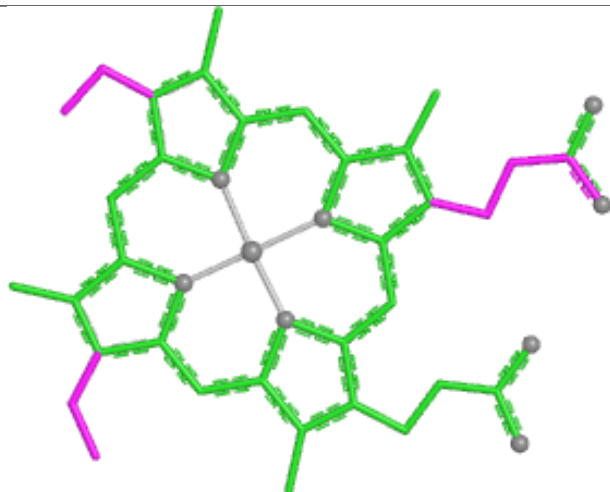


Rings

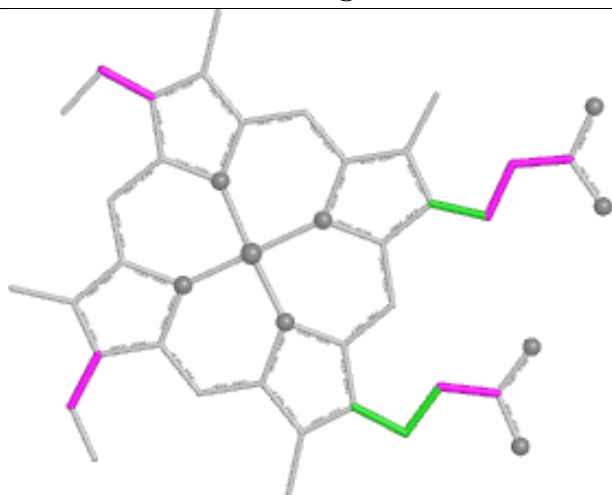
## Ligand HEC B 602



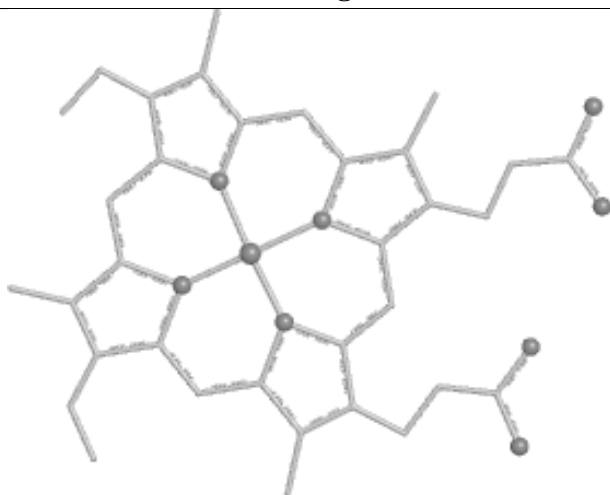
Bond lengths



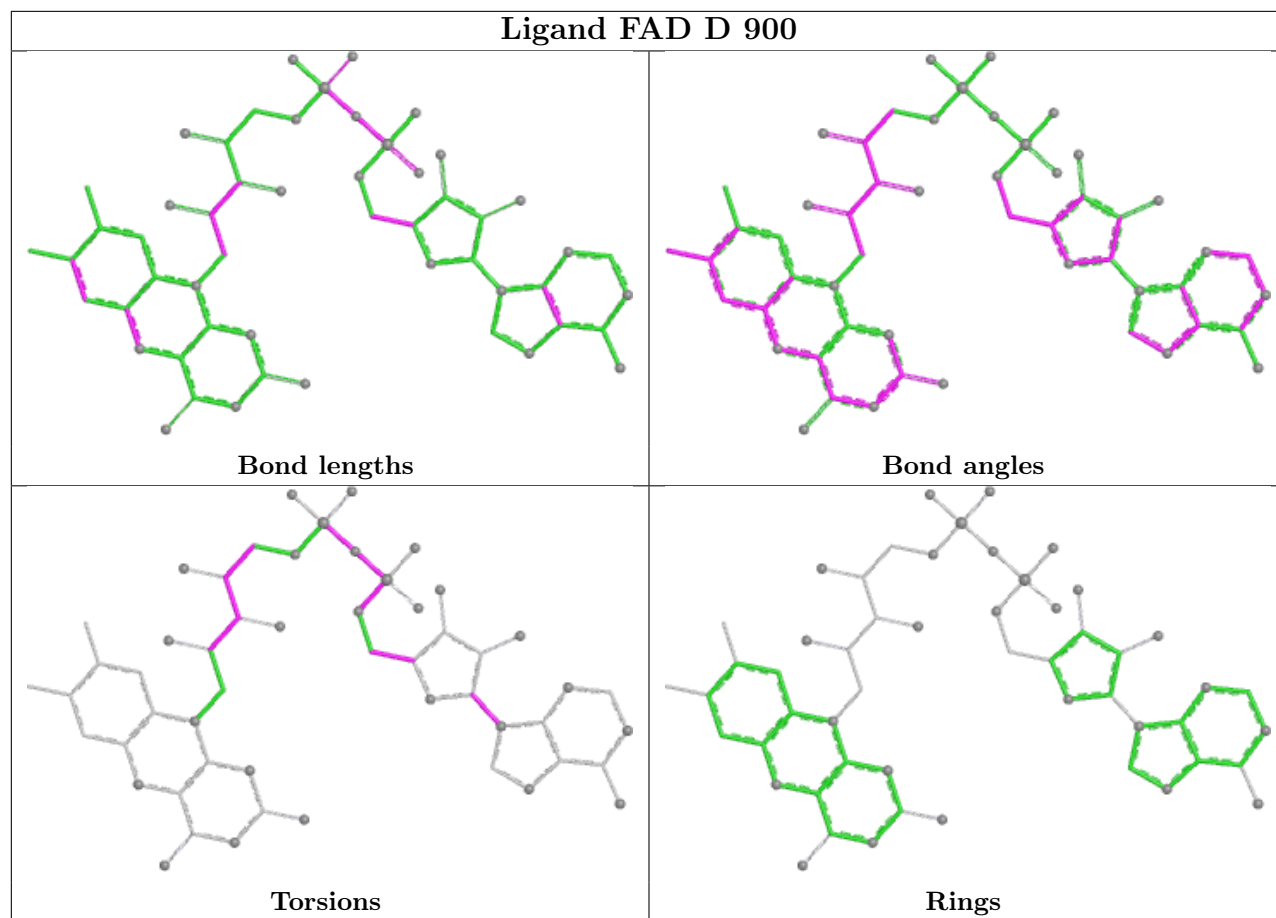
Bond angles



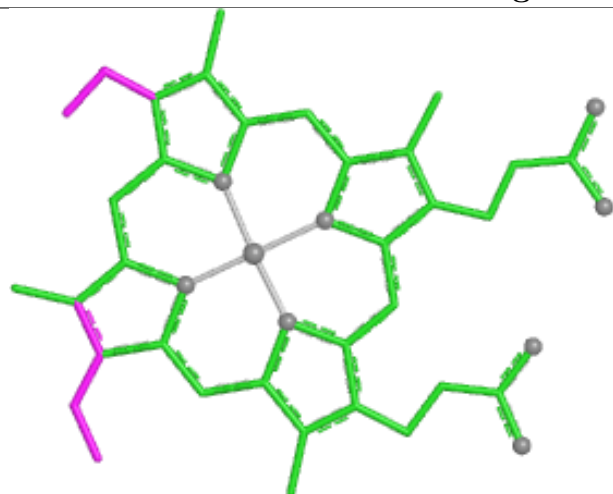
Torsions



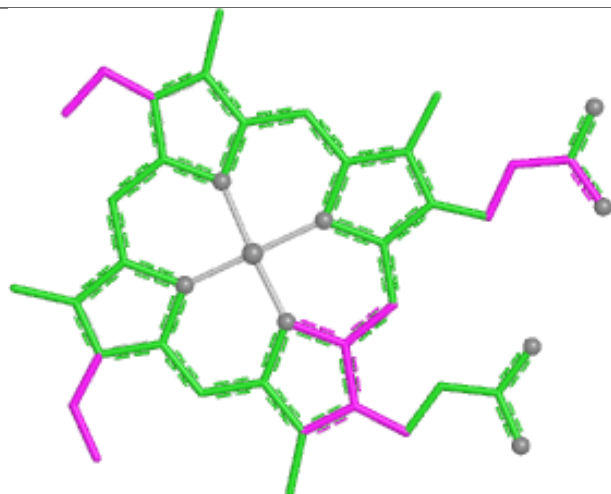
Rings



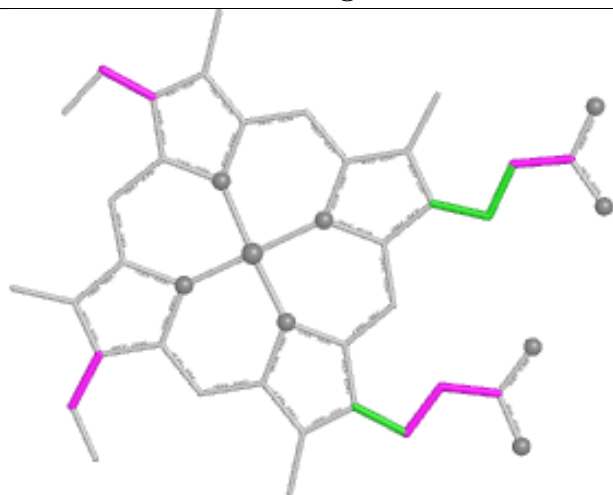
## Ligand HEC C 603



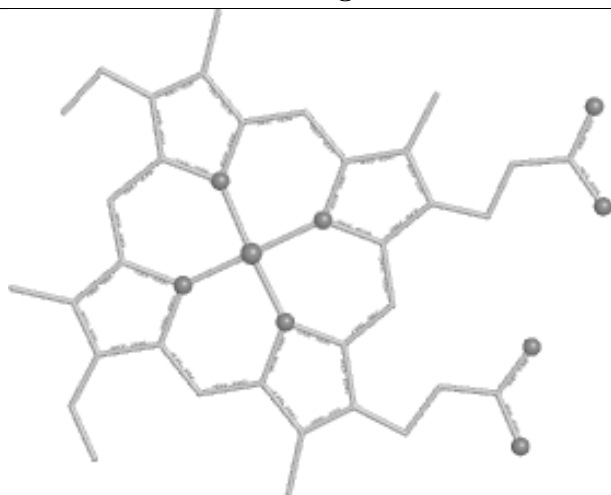
Bond lengths



Bond angles

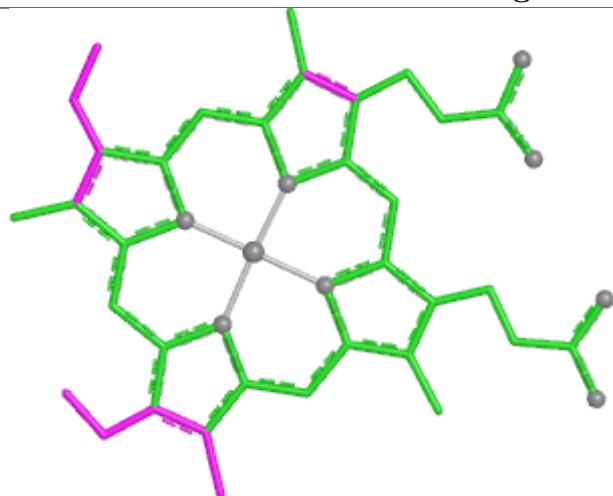


Torsions

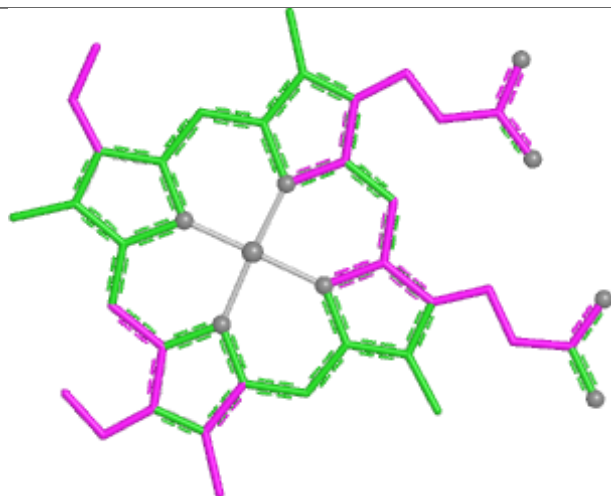


Rings

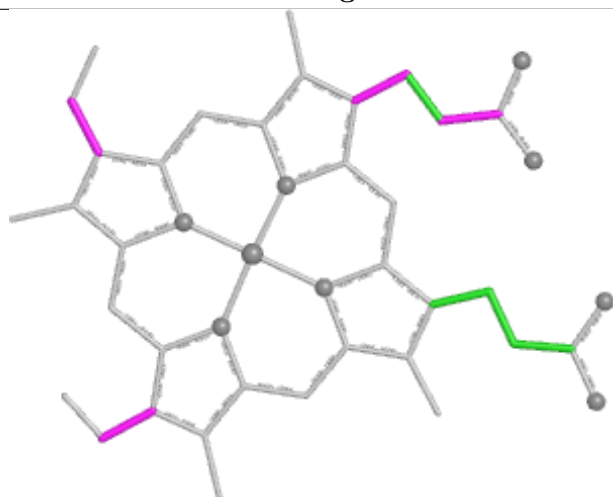
## Ligand HEC B 604



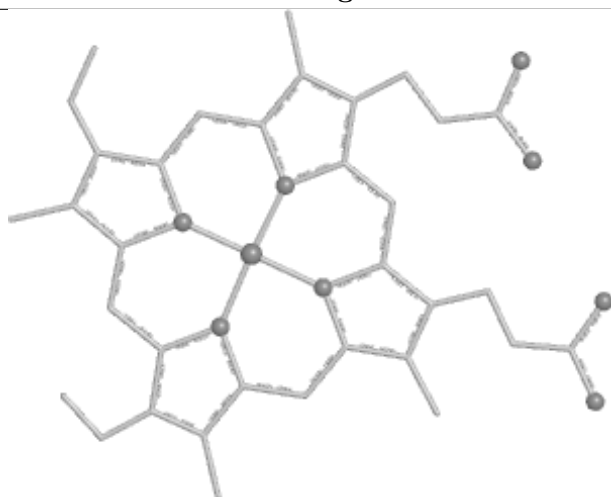
Bond lengths



Bond angles

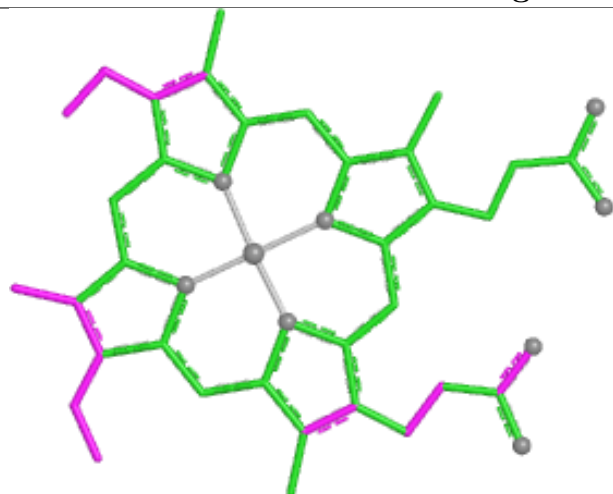


Torsions

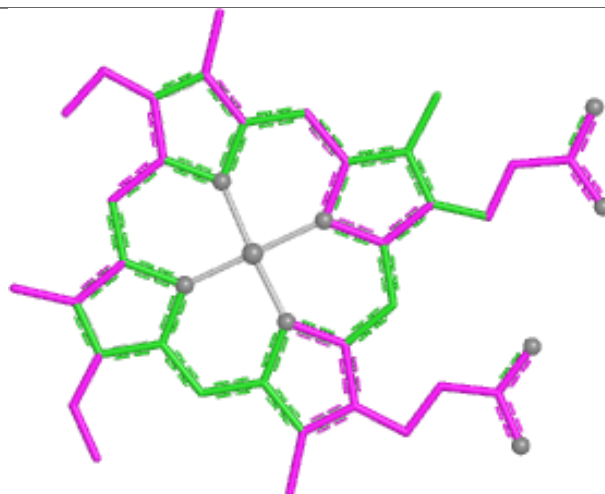


Rings

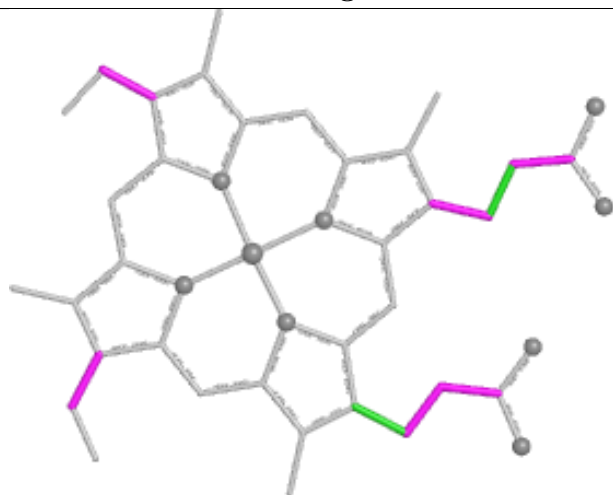
## Ligand HEC A 601



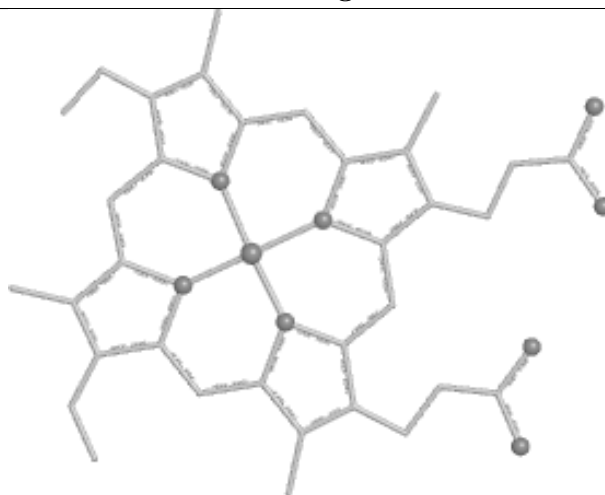
Bond lengths



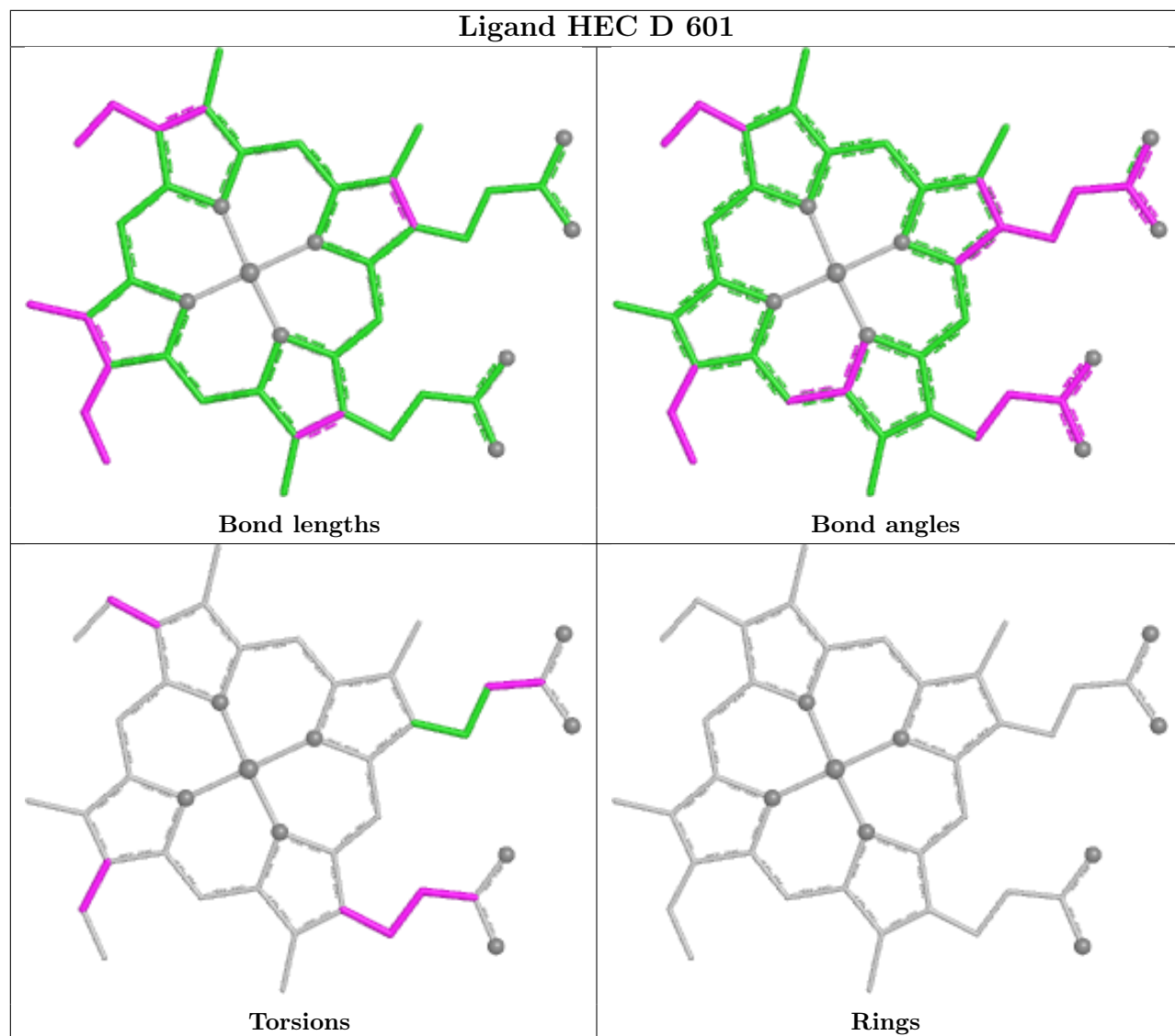
Bond angles



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

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.