



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:17 PM UTC

PDB ID : 1QO8 / pdb\_00001qo8  
Title : The structure of the open conformation of a flavocytochrome c3 fumarate reductase  
Authors : Bamford, V.; Dobbin, P.S.; Richardson, D.J.; Hemmings, A.M.  
Deposited on : 1999-11-04  
Resolution : 2.15 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                                                             |

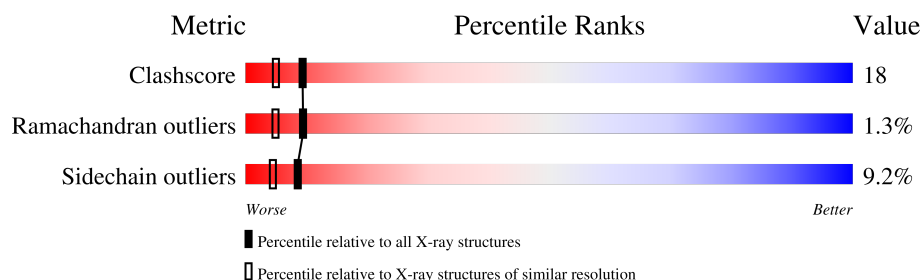
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 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                      | 2159 (2.16-2.16)                                      |
| Ramachandran outliers | 187476                      | 2134 (2.16-2.16)                                      |
| Sidechain outliers    | 187428                      | 2133 (2.16-2.16)                                      |

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     | 566    | <br>58% 32% 7% • |
| 1   | D     | 566    | <br>58% 33% 6% • |

## 2 Entry composition [i](#)

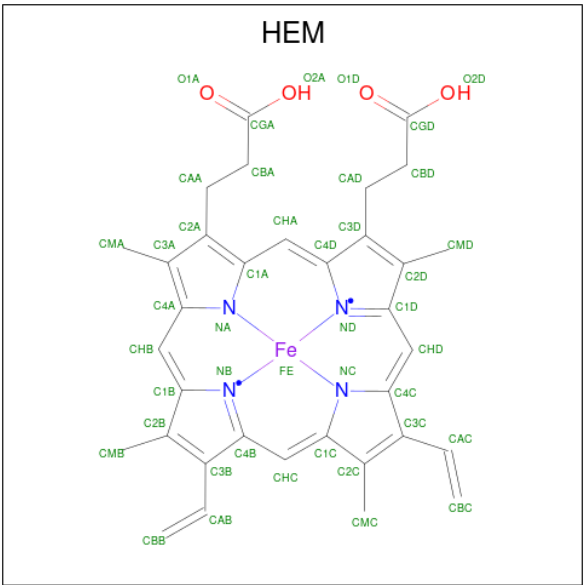
There are 4 unique types of molecules in this entry. The entry contains 9425 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 C3 FUMARATE REDUCTASE.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 564      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4234  | 2627 | 753 | 826 | 28 |         |         |       |
| 1   | D     | 564      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4234  | 2627 | 753 | 826 | 28 |         |         |       |

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



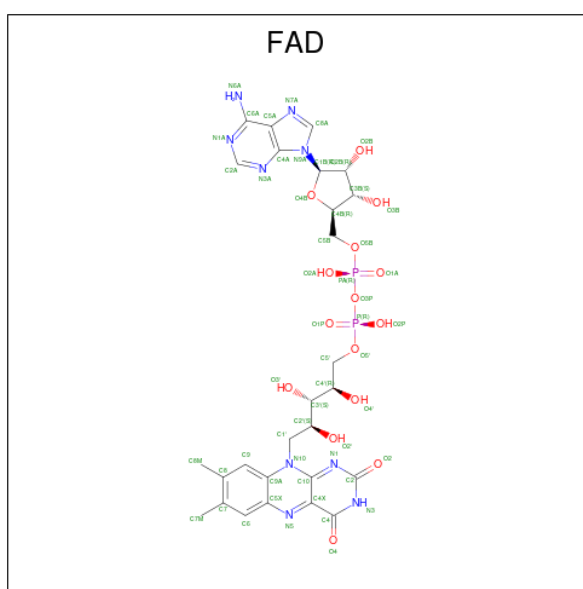
| Mol | Chain | Residues | Atoms |    |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 2   | A     | 1        | Total | C  | Fe | N | O | 0       | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |         |
| 2   | A     | 1        | Total | C  | Fe | N | O | 0       | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |         |
| 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   | 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   | D     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 53    | 27 | 9 | 15 | 2 |         |         |

- Molecule 4 is water.

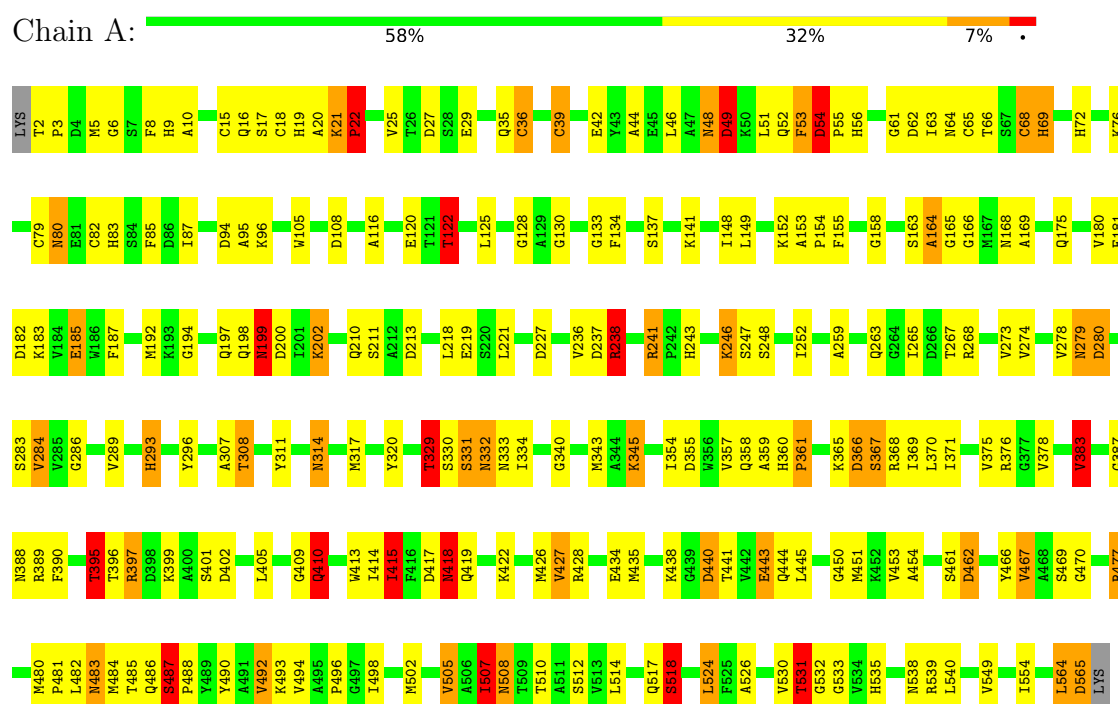
| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 4   | A     | 358      | Total | O   | 0       | 0       |
|     |       |          | 358   | 358 |         |         |
| 4   | D     | 149      | Total | O   | 0       | 0       |
|     |       |          | 149   | 149 |         |         |

### 3 Residue-property plots

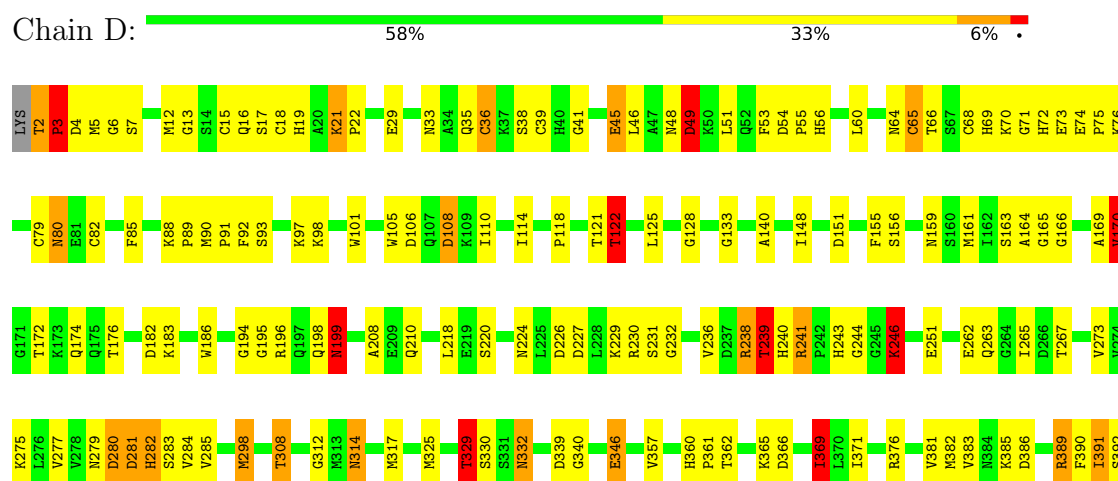
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

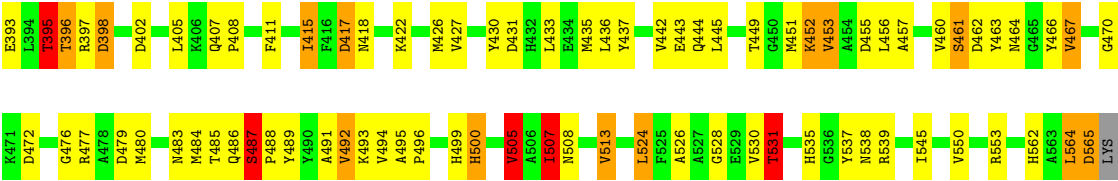
Note EDS was not executed.

#### • Molecule 1: FLAVOCYTOCHROME C3 FUMARATE REDUCTASE



#### • Molecule 1: FLAVOCYTOCHROME C3 FUMARATE REDUCTASE





## 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 21                                     | Depositor |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$ | 71.77Å 109.69Å 227.32Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å)                                           | 20.00 – 2.15                                   | Depositor |
| % Data completeness<br>(in resolution range)             | 93.4 (20.00-2.15)                              | Depositor |
| $R_{merge}$                                              | (Not available)                                | Depositor |
| $R_{sym}$                                                | 0.04                                           | Depositor |
| Refinement program                                       | REFMAC                                         | Depositor |
| R, $R_{free}$                                            | 0.225 , 0.281                                  | Depositor |
| Estimated twinning fraction                              | No twinning to report.                         | Xtriage   |
| Total number of atoms                                    | 9425                                           | wwPDB-VP  |
| Average B, all atoms (Å <sup>2</sup> )                   | 60.0                                           | 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, HEM

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     | 1.23         | 6/4312 (0.1%) | 2.48        | 229/5820 (3.9%)  |
| 1   | D     | 0.80         | 0/4312        | 1.86        | 94/5820 (1.6%)   |
| All | All   | 1.04         | 6/8624 (0.1%) | 2.19        | 323/11640 (2.8%) |

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                   | 10                  |
| 1   | D     | 0                   | 2                   |
| All | All   | 0                   | 12                  |

All (6) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 164 | ALA  | CA-CB   | 7.52  | 1.65        | 1.53     |
| 1   | A     | 83  | HIS  | CE1-NE2 | 6.44  | 1.39        | 1.32     |
| 1   | A     | 61  | GLY  | CA-C    | 5.79  | 1.60        | 1.51     |
| 1   | A     | 164 | ALA  | N-CA    | -5.23 | 1.39        | 1.46     |
| 1   | A     | 10  | ALA  | C-O     | -5.18 | 1.18        | 1.24     |
| 1   | A     | 158 | GLY  | CA-C    | 5.11  | 1.58        | 1.51     |

All (323) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | A     | 21  | LYS  | CA-C-N   | 33.93 | 162.26      | 119.84   |
| 1   | A     | 21  | LYS  | C-N-CA   | 33.93 | 162.26      | 119.84   |
| 1   | D     | 565 | ASP  | CA-CB-CG | 25.22 | 137.82      | 112.60   |

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| Mol | Chain | Res | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 1   | A     | 487 | SER  | CA-C-O     | -22.57 | 102.08      | 119.46   |
| 1   | A     | 418 | ASN  | OD1-CG-ND2 | -20.40 | 102.20      | 122.60   |
| 1   | A     | 415 | ILE  | CA-CB-CG2  | 16.60  | 138.72      | 110.50   |
| 1   | A     | 49  | ASP  | CA-CB-CG   | 15.09  | 127.69      | 112.60   |
| 1   | A     | 22  | PRO  | CA-N-CD    | -15.07 | 90.90       | 112.00   |
| 1   | A     | 376 | ARG  | NE-CZ-NH2  | 14.36  | 132.12      | 119.20   |
| 1   | A     | 565 | ASP  | CA-CB-CG   | 14.30  | 126.90      | 112.60   |
| 1   | A     | 227 | ASP  | CA-CB-CG   | 13.65  | 126.25      | 112.60   |
| 1   | A     | 483 | ASN  | OD1-CG-ND2 | -12.31 | 110.29      | 122.60   |
| 1   | A     | 21  | LYS  | CA-C-O     | -11.54 | 109.66      | 119.36   |
| 1   | A     | 492 | VAL  | CB-CA-C    | -11.48 | 93.51       | 110.62   |
| 1   | A     | 163 | SER  | CA-C-N     | 11.46  | 144.15      | 122.60   |
| 1   | A     | 163 | SER  | C-N-CA     | 11.46  | 144.15      | 122.60   |
| 1   | D     | 196 | ARG  | CD-NE-CZ   | 11.21  | 140.09      | 124.40   |
| 1   | A     | 21  | LYS  | O-C-N      | 11.11  | 131.64      | 121.19   |
| 1   | A     | 483 | ASN  | CA-CB-CG   | -10.87 | 101.73      | 112.60   |
| 1   | A     | 428 | ARG  | CD-NE-CZ   | 10.76  | 139.46      | 124.40   |
| 1   | A     | 428 | ARG  | CA-CB-CG   | 10.56  | 135.22      | 114.10   |
| 1   | A     | 293 | HIS  | CA-CB-CG   | -10.53 | 103.27      | 113.80   |
| 1   | A     | 164 | ALA  | N-CA-CB    | -10.52 | 92.66       | 110.33   |
| 1   | A     | 418 | ASN  | CA-CB-CG   | 10.14  | 122.74      | 112.60   |
| 1   | A     | 410 | GLN  | OE1-CD-NE2 | 10.09  | 132.69      | 122.60   |
| 1   | A     | 505 | VAL  | N-CA-CB    | -10.07 | 97.93       | 110.31   |
| 1   | D     | 199 | ASN  | CA-CB-CG   | 9.76   | 122.36      | 112.60   |
| 1   | A     | 426 | MET  | O-C-N      | -9.57  | 111.97      | 122.12   |
| 1   | D     | 279 | ASN  | OD1-CG-ND2 | -9.53  | 113.07      | 122.60   |
| 1   | A     | 149 | LEU  | CA-C-O     | -9.53  | 110.11      | 120.30   |
| 1   | A     | 488 | PRO  | N-CA-CB    | 9.52   | 113.25      | 103.25   |
| 1   | D     | 156 | SER  | N-CA-C     | 9.48   | 122.85      | 110.43   |
| 1   | A     | 198 | GLN  | OE1-CD-NE2 | -9.21  | 113.39      | 122.60   |
| 1   | D     | 283 | SER  | CA-C-O     | -9.15  | 110.41      | 120.38   |
| 1   | A     | 16  | GLN  | OE1-CD-NE2 | -9.13  | 113.47      | 122.60   |
| 1   | A     | 164 | ALA  | N-CA-C     | 9.05   | 124.72      | 112.68   |
| 1   | A     | 518 | SER  | CB-CA-C    | 8.99   | 123.86      | 111.63   |
| 1   | A     | 21  | LYS  | CB-CA-C    | -8.95  | 101.31      | 110.17   |
| 1   | D     | 280 | ASP  | CA-CB-CG   | -8.93  | 103.67      | 112.60   |
| 1   | A     | 22  | PRO  | N-CD-CG    | 8.65   | 116.17      | 103.20   |
| 1   | A     | 122 | THR  | CA-C-O     | -8.64  | 111.81      | 121.40   |
| 1   | A     | 483 | ASN  | CB-CG-ND2  | 8.47   | 129.10      | 116.40   |
| 1   | A     | 22  | PRO  | N-CA-CB    | 8.46   | 112.13      | 103.25   |
| 1   | D     | 508 | ASN  | OD1-CG-ND2 | -8.41  | 114.19      | 122.60   |
| 1   | A     | 10  | ALA  | CA-C-O     | -8.40  | 111.64      | 120.55   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 532 | GLY  | O-C-N      | -8.35 | 113.83      | 123.09   |
| 1   | A     | 134 | PHE  | CA-CB-CG   | 8.32  | 122.12      | 113.80   |
| 1   | A     | 69  | HIS  | CA-CB-CG   | -8.30 | 105.50      | 113.80   |
| 1   | A     | 428 | ARG  | NE-CZ-NH1  | 8.21  | 129.71      | 121.50   |
| 1   | D     | 499 | HIS  | CA-C-O     | -8.11 | 110.32      | 119.81   |
| 1   | D     | 281 | ASP  | CA-CB-CG   | 8.01  | 120.61      | 112.60   |
| 1   | A     | 54  | ASP  | N-CA-CB    | 8.00  | 124.61      | 110.37   |
| 1   | A     | 401 | SER  | CB-CA-C    | -7.96 | 98.39       | 110.88   |
| 1   | D     | 196 | ARG  | NE-CZ-NH2  | -7.92 | 112.08      | 119.20   |
| 1   | D     | 282 | HIS  | CA-CB-CG   | -7.86 | 105.94      | 113.80   |
| 1   | A     | 487 | SER  | N-CA-C     | 7.85  | 121.03      | 109.42   |
| 1   | D     | 505 | VAL  | N-CA-CB    | -7.79 | 97.04       | 110.13   |
| 1   | A     | 415 | ILE  | CA-CB-CG1  | -7.78 | 97.18       | 110.40   |
| 1   | A     | 122 | THR  | CB-CA-C    | -7.76 | 93.03       | 111.65   |
| 1   | A     | 481 | PRO  | N-CA-CB    | 7.72  | 111.40      | 102.76   |
| 1   | A     | 389 | ARG  | CA-C-O     | -7.69 | 112.95      | 121.87   |
| 1   | A     | 361 | PRO  | O-C-N      | -7.67 | 113.02      | 122.23   |
| 1   | A     | 64  | ASN  | CA-C-O     | -7.61 | 112.24      | 120.92   |
| 1   | A     | 53  | PHE  | CA-CB-CG   | -7.54 | 106.26      | 113.80   |
| 1   | D     | 507 | ILE  | CA-CB-CG2  | 7.53  | 123.30      | 110.50   |
| 1   | A     | 268 | ARG  | CA-CB-CG   | 7.51  | 129.12      | 114.10   |
| 1   | D     | 49  | ASP  | CA-CB-CG   | 7.46  | 120.06      | 112.60   |
| 1   | D     | 170 | VAL  | CB-CA-C    | -7.45 | 100.37      | 110.42   |
| 1   | D     | 56  | HIS  | CA-CB-CG   | -7.44 | 106.36      | 113.80   |
| 1   | A     | 355 | ASP  | CA-CB-CG   | 7.39  | 119.99      | 112.60   |
| 1   | A     | 238 | ARG  | O-C-N      | -7.38 | 114.05      | 122.09   |
| 1   | A     | 389 | ARG  | NE-CZ-NH1  | -7.37 | 114.13      | 121.50   |
| 1   | A     | 470 | GLY  | N-CA-C     | -7.31 | 103.83      | 115.08   |
| 1   | D     | 122 | THR  | CB-CA-C    | -7.19 | 98.70       | 112.43   |
| 1   | A     | 533 | GLY  | O-C-N      | -7.18 | 115.19      | 122.65   |
| 1   | A     | 108 | ASP  | CB-CA-C    | 7.16  | 122.67      | 110.79   |
| 1   | A     | 469 | SER  | CA-C-O     | 7.12  | 126.98      | 119.14   |
| 1   | A     | 390 | PHE  | N-CA-C     | -7.12 | 103.63      | 114.16   |
| 1   | A     | 333 | ASN  | OD1-CG-ND2 | 7.11  | 129.71      | 122.60   |
| 1   | A     | 419 | GLN  | CA-C-O     | 7.09  | 128.01      | 120.70   |
| 1   | A     | 440 | ASP  | CA-CB-CG   | -7.09 | 105.50      | 112.60   |
| 1   | A     | 488 | PRO  | N-CD-CG    | 7.03  | 113.74      | 103.20   |
| 1   | D     | 53  | PHE  | CA-CB-CG   | -7.02 | 106.78      | 113.80   |
| 1   | A     | 21  | LYS  | C-N-CD     | -7.01 | 96.28       | 125.00   |
| 1   | A     | 488 | PRO  | CA-N-CD    | -7.00 | 102.20      | 112.00   |
| 1   | D     | 492 | VAL  | CB-CA-C    | -6.99 | 100.12      | 110.33   |
| 1   | A     | 368 | ARG  | NE-CZ-NH1  | 6.97  | 128.47      | 121.50   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | D     | 564 | LEU  | CA-C-O     | -6.96 | 110.56      | 120.51   |
| 1   | D     | 199 | ASN  | OD1-CG-ND2 | -6.95 | 115.65      | 122.60   |
| 1   | A     | 241 | ARG  | NE-CZ-NH1  | 6.92  | 128.42      | 121.50   |
| 1   | A     | 36  | CYS  | CA-C-O     | -6.90 | 113.19      | 120.92   |
| 1   | A     | 130 | GLY  | N-CA-C     | -6.89 | 102.62      | 112.55   |
| 1   | A     | 80  | ASN  | OD1-CG-ND2 | -6.89 | 115.71      | 122.60   |
| 1   | D     | 513 | VAL  | CA-C-O     | -6.88 | 113.86      | 121.23   |
| 1   | A     | 56  | HIS  | CA-CB-CG   | -6.82 | 106.98      | 113.80   |
| 1   | D     | 108 | ASP  | CA-CB-CG   | 6.78  | 119.38      | 112.60   |
| 1   | A     | 130 | GLY  | CA-C-O     | -6.77 | 114.35      | 121.53   |
| 1   | A     | 415 | ILE  | CA-C-O     | -6.75 | 113.11      | 120.67   |
| 1   | A     | 96  | LYS  | CA-C-O     | 6.72  | 127.20      | 120.88   |
| 1   | A     | 375 | VAL  | N-CA-CB    | 6.72  | 118.42      | 110.55   |
| 1   | A     | 388 | ASN  | OD1-CG-ND2 | -6.71 | 115.89      | 122.60   |
| 1   | D     | 332 | ASN  | OD1-CG-ND2 | -6.70 | 115.90      | 122.60   |
| 1   | A     | 279 | ASN  | OD1-CG-ND2 | -6.67 | 115.93      | 122.60   |
| 1   | A     | 27  | ASP  | CA-CB-CG   | -6.66 | 105.94      | 112.60   |
| 1   | A     | 307 | ALA  | N-CA-C     | -6.65 | 102.30      | 110.61   |
| 1   | A     | 531 | THR  | N-CA-CB    | -6.65 | 99.58       | 110.41   |
| 1   | D     | 369 | ILE  | CA-C-O     | -6.65 | 112.89      | 120.67   |
| 1   | A     | 367 | SER  | CA-CB-OG   | 6.64  | 124.37      | 111.10   |
| 1   | A     | 164 | ALA  | CA-C-O     | 6.60  | 129.38      | 120.13   |
| 1   | D     | 122 | THR  | N-CA-CB    | 6.60  | 121.49      | 110.14   |
| 1   | A     | 383 | VAL  | N-CA-CB    | -6.59 | 99.75       | 111.93   |
| 1   | A     | 443 | GLU  | N-CA-C     | 6.59  | 118.12      | 111.07   |
| 1   | D     | 155 | PHE  | CA-C-N     | 6.58  | 131.99      | 120.87   |
| 1   | D     | 155 | PHE  | C-N-CA     | 6.58  | 131.99      | 120.87   |
| 1   | A     | 199 | ASN  | N-CA-CB    | 6.57  | 119.75      | 109.83   |
| 1   | A     | 155 | PHE  | N-CA-CB    | 6.56  | 122.61      | 111.66   |
| 1   | D     | 452 | LYS  | CA-C-O     | 6.56  | 127.54      | 120.32   |
| 1   | A     | 466 | TYR  | CA-C-N     | -6.56 | 109.01      | 120.29   |
| 1   | A     | 466 | TYR  | C-N-CA     | -6.56 | 109.01      | 120.29   |
| 1   | D     | 346 | GLU  | CB-CG-CD   | 6.55  | 123.73      | 112.60   |
| 1   | D     | 64  | ASN  | OD1-CG-ND2 | -6.54 | 116.06      | 122.60   |
| 1   | D     | 241 | ARG  | NE-CZ-NH1  | -6.54 | 114.95      | 121.50   |
| 1   | A     | 155 | PHE  | N-CA-C     | -6.52 | 99.16       | 109.07   |
| 1   | A     | 238 | ARG  | CA-C-O     | 6.50  | 126.13      | 118.79   |
| 1   | A     | 116 | ALA  | CA-C-O     | -6.50 | 111.22      | 120.51   |
| 1   | A     | 308 | THR  | N-CA-CB    | -6.49 | 101.06      | 110.47   |
| 1   | D     | 553 | ARG  | CA-C-O     | 6.49  | 127.29      | 120.42   |
| 1   | A     | 507 | ILE  | CA-CB-CG2  | 6.45  | 121.47      | 110.50   |
| 1   | D     | 417 | ASP  | CA-CB-CG   | 6.45  | 119.05      | 112.60   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | A     | 153 | ALA  | CA-C-N      | 6.43  | 126.35      | 119.28   |
| 1   | A     | 153 | ALA  | C-N-CA      | 6.43  | 126.35      | 119.28   |
| 1   | A     | 361 | PRO  | N-CA-C      | 6.37  | 122.39      | 113.53   |
| 1   | A     | 477 | ARG  | CA-C-O      | -6.33 | 113.70      | 120.92   |
| 1   | A     | 401 | SER  | CA-CB-OG    | -6.30 | 98.50       | 111.10   |
| 1   | A     | 19  | HIS  | CE1-NE2-CD2 | -6.30 | 102.70      | 109.00   |
| 1   | A     | 48  | ASN  | O-C-N       | -6.30 | 114.21      | 122.59   |
| 1   | A     | 530 | VAL  | CA-C-N      | 6.29  | 132.83      | 122.07   |
| 1   | A     | 530 | VAL  | C-N-CA      | 6.29  | 132.83      | 122.07   |
| 1   | A     | 221 | LEU  | CA-C-O      | -6.29 | 111.67      | 119.28   |
| 1   | A     | 357 | VAL  | CA-C-O      | 6.28  | 126.92      | 120.39   |
| 1   | A     | 83  | HIS  | CE1-NE2-CD2 | -6.27 | 102.73      | 109.00   |
| 1   | D     | 140 | ALA  | CA-C-N      | 6.27  | 129.00      | 120.54   |
| 1   | D     | 140 | ALA  | C-N-CA      | 6.27  | 129.00      | 120.54   |
| 1   | D     | 398 | ASP  | CA-C-O      | -6.26 | 114.19      | 121.07   |
| 1   | A     | 402 | ASP  | CA-C-O      | -6.25 | 113.80      | 120.42   |
| 1   | A     | 163 | SER  | CA-C-O      | 6.24  | 128.14      | 121.16   |
| 1   | D     | 395 | THR  | N-CA-CB     | 6.22  | 118.90      | 110.38   |
| 1   | A     | 274 | VAL  | CA-C-O      | 6.20  | 124.56      | 118.98   |
| 1   | A     | 331 | SER  | CA-CB-OG    | -6.19 | 98.71       | 111.10   |
| 1   | D     | 208 | ALA  | O-C-N       | 6.19  | 128.47      | 122.03   |
| 1   | D     | 530 | VAL  | CA-C-N      | 6.19  | 131.87      | 122.65   |
| 1   | D     | 530 | VAL  | C-N-CA      | 6.19  | 131.87      | 122.65   |
| 1   | D     | 507 | ILE  | CB-CG1-CD1  | -6.18 | 100.82      | 113.80   |
| 1   | D     | 329 | THR  | CB-CA-C     | -6.17 | 99.89       | 114.16   |
| 1   | A     | 211 | SER  | CA-C-O      | -6.17 | 113.88      | 120.42   |
| 1   | A     | 238 | ARG  | N-CA-CB     | -6.17 | 101.38      | 111.01   |
| 1   | A     | 48  | ASN  | OD1-CG-ND2  | 6.17  | 128.76      | 122.60   |
| 1   | D     | 531 | THR  | CA-C-N      | -6.13 | 116.07      | 122.69   |
| 1   | D     | 531 | THR  | C-N-CA      | -6.13 | 116.07      | 122.69   |
| 1   | A     | 331 | SER  | N-CA-CB     | -6.11 | 101.10      | 110.44   |
| 1   | D     | 402 | ASP  | CA-CB-CG    | -6.11 | 106.49      | 112.60   |
| 1   | A     | 418 | ASN  | CB-CG-OD1   | 6.09  | 132.99      | 120.80   |
| 1   | A     | 329 | THR  | OG1-CB-CG2  | 6.08  | 121.47      | 109.30   |
| 1   | A     | 539 | ARG  | CA-C-O      | -6.05 | 113.80      | 120.69   |
| 1   | A     | 83  | HIS  | CG-CD2-NE2  | 6.03  | 113.23      | 107.20   |
| 1   | A     | 55  | PRO  | N-CA-C      | -6.03 | 105.67      | 113.57   |
| 1   | A     | 388 | ASN  | CB-CG-ND2   | 5.99  | 125.39      | 116.40   |
| 1   | A     | 369 | ILE  | N-CA-CB     | -5.99 | 99.52       | 111.91   |
| 1   | A     | 454 | ALA  | CA-C-O      | 5.98  | 126.76      | 120.42   |
| 1   | A     | 410 | GLN  | CB-CA-C     | -5.98 | 102.07      | 111.51   |
| 1   | D     | 500 | HIS  | N-CA-CB     | -5.97 | 100.42      | 111.53   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | A     | 20  | ALA  | CA-C-N      | 5.96  | 132.13      | 121.76   |
| 1   | A     | 20  | ALA  | C-N-CA      | 5.96  | 132.13      | 121.76   |
| 1   | A     | 108 | ASP  | CA-CB-CG    | -5.93 | 106.67      | 112.60   |
| 1   | A     | 518 | SER  | N-CA-CB     | -5.92 | 103.16      | 112.46   |
| 1   | A     | 72  | HIS  | CE1-NE2-CD2 | -5.92 | 103.08      | 109.00   |
| 1   | A     | 369 | ILE  | CA-C-N      | 5.92  | 129.77      | 121.02   |
| 1   | A     | 369 | ILE  | C-N-CA      | 5.92  | 129.77      | 121.02   |
| 1   | A     | 286 | GLY  | N-CA-C      | -5.90 | 102.83      | 110.38   |
| 1   | D     | 531 | THR  | N-CA-CB     | -5.90 | 100.79      | 110.52   |
| 1   | A     | 95  | ALA  | CA-C-N      | 5.86  | 132.11      | 121.97   |
| 1   | A     | 95  | ALA  | C-N-CA      | 5.86  | 132.11      | 121.97   |
| 1   | D     | 431 | ASP  | CA-C-O      | -5.86 | 114.67      | 120.82   |
| 1   | A     | 69  | HIS  | CA-C-O      | -5.86 | 114.08      | 120.81   |
| 1   | A     | 219 | GLU  | CA-C-O      | -5.83 | 114.37      | 120.55   |
| 1   | A     | 498 | ILE  | O-C-N       | -5.82 | 116.46      | 122.63   |
| 1   | A     | 512 | SER  | CA-C-O      | -5.82 | 114.65      | 121.16   |
| 1   | A     | 192 | MET  | CA-C-O      | 5.81  | 126.71      | 120.55   |
| 1   | A     | 345 | LYS  | CA-C-N      | 5.81  | 128.64      | 120.28   |
| 1   | A     | 345 | LYS  | C-N-CA      | 5.81  | 128.64      | 120.28   |
| 1   | D     | 553 | ARG  | CD-NE-CZ    | 5.80  | 132.52      | 124.40   |
| 1   | A     | 10  | ALA  | N-CA-CB     | 5.79  | 118.64      | 110.12   |
| 1   | A     | 17  | SER  | CA-CB-OG    | 5.79  | 122.69      | 111.10   |
| 1   | D     | 426 | MET  | CA-CB-CG    | 5.78  | 125.66      | 114.10   |
| 1   | A     | 376 | ARG  | NH1-CZ-NH2  | -5.78 | 111.79      | 119.30   |
| 1   | A     | 35  | GLN  | CG-CD-NE2   | 5.77  | 125.06      | 116.40   |
| 1   | D     | 366 | ASP  | CA-CB-CG    | -5.76 | 106.83      | 112.60   |
| 1   | D     | 329 | THR  | N-CA-CB     | 5.76  | 118.24      | 109.94   |
| 1   | D     | 29  | GLU  | CA-C-N      | 5.76  | 128.79      | 120.79   |
| 1   | D     | 29  | GLU  | C-N-CA      | 5.76  | 128.79      | 120.79   |
| 1   | A     | 383 | VAL  | CA-CB-CG1   | 5.75  | 120.17      | 110.40   |
| 1   | D     | 98  | LYS  | CA-CB-CG    | 5.75  | 125.59      | 114.10   |
| 1   | A     | 16  | GLN  | CG-CD-NE2   | 5.70  | 124.95      | 116.40   |
| 1   | D     | 312 | GLY  | CA-C-O      | -5.70 | 114.25      | 120.40   |
| 1   | D     | 505 | VAL  | CA-CB-CG1   | 5.69  | 120.07      | 110.40   |
| 1   | D     | 49  | ASP  | N-CA-CB     | 5.69  | 120.10      | 110.49   |
| 1   | A     | 518 | SER  | CA-C-O      | 5.68  | 128.03      | 120.98   |
| 1   | A     | 197 | GLN  | OE1-CD-NE2  | -5.67 | 116.93      | 122.60   |
| 1   | D     | 161 | MET  | CA-C-O      | -5.67 | 111.67      | 119.05   |
| 1   | A     | 246 | LYS  | CA-C-O      | -5.65 | 115.31      | 121.87   |
| 1   | A     | 54  | ASP  | CA-CB-CG    | -5.65 | 106.95      | 112.60   |
| 1   | A     | 482 | LEU  | N-CA-C      | -5.65 | 99.84       | 108.76   |
| 1   | A     | 518 | SER  | O-C-N       | -5.65 | 115.02      | 122.47   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 427 | VAL  | N-CA-CB    | -5.65 | 100.28      | 110.95   |
| 1   | A     | 395 | THR  | CB-CA-C    | -5.64 | 99.19       | 110.42   |
| 1   | A     | 354 | ILE  | CA-C-O     | 5.64  | 126.56      | 120.47   |
| 1   | A     | 164 | ALA  | O-C-N      | -5.64 | 114.81      | 122.19   |
| 1   | A     | 154 | PRO  | CA-C-O     | 5.63  | 128.11      | 119.55   |
| 1   | A     | 247 | SER  | CA-CB-OG   | -5.63 | 99.84       | 111.10   |
| 1   | A     | 168 | ASN  | OD1-CG-ND2 | -5.63 | 116.97      | 122.60   |
| 1   | A     | 539 | ARG  | NE-CZ-NH1  | -5.60 | 115.90      | 121.50   |
| 1   | A     | 530 | VAL  | O-C-N      | -5.60 | 116.25      | 121.90   |
| 1   | A     | 120 | GLU  | CA-C-O     | -5.59 | 114.95      | 121.10   |
| 1   | A     | 418 | ASN  | CB-CG-ND2  | 5.58  | 124.78      | 116.40   |
| 1   | D     | 239 | THR  | CA-C-O     | 5.57  | 126.67      | 120.43   |
| 1   | A     | 94  | ASP  | CA-C-O     | -5.57 | 112.55      | 119.28   |
| 1   | A     | 417 | ASP  | CA-C-N     | 5.56  | 129.49      | 120.60   |
| 1   | A     | 417 | ASP  | C-N-CA     | 5.56  | 129.49      | 120.60   |
| 1   | A     | 498 | ILE  | CA-CB-CG1  | -5.56 | 100.95      | 110.40   |
| 1   | A     | 358 | GLN  | CB-CG-CD   | -5.55 | 103.16      | 112.60   |
| 1   | D     | 163 | SER  | CA-C-N     | 5.52  | 130.68      | 122.17   |
| 1   | D     | 163 | SER  | C-N-CA     | 5.52  | 130.68      | 122.17   |
| 1   | A     | 252 | ILE  | CA-C-N     | 5.50  | 128.23      | 120.42   |
| 1   | A     | 252 | ILE  | C-N-CA     | 5.50  | 128.23      | 120.42   |
| 1   | A     | 76  | LYS  | CA-CB-CG   | -5.50 | 103.11      | 114.10   |
| 1   | A     | 396 | THR  | CA-CB-OG1  | -5.49 | 101.36      | 109.60   |
| 1   | D     | 381 | VAL  | CA-C-O     | -5.49 | 114.51      | 121.48   |
| 1   | A     | 36  | CYS  | N-CA-CB    | 5.49  | 118.72      | 109.78   |
| 1   | A     | 182 | ASP  | CA-CB-CG   | 5.48  | 118.08      | 112.60   |
| 1   | A     | 19  | HIS  | CB-CG-CD2  | 5.48  | 138.32      | 131.20   |
| 1   | A     | 248 | SER  | CA-C-N     | 5.48  | 130.47      | 121.87   |
| 1   | A     | 248 | SER  | C-N-CA     | 5.48  | 130.47      | 121.87   |
| 1   | D     | 329 | THR  | N-CA-C     | -5.47 | 101.54      | 109.31   |
| 1   | A     | 213 | ASP  | CA-C-O     | -5.47 | 114.72      | 120.63   |
| 1   | A     | 376 | ARG  | NE-CZ-NH1  | -5.46 | 116.04      | 121.50   |
| 1   | D     | 273 | VAL  | CA-C-N     | 5.46  | 129.03      | 122.16   |
| 1   | D     | 273 | VAL  | C-N-CA     | 5.46  | 129.03      | 122.16   |
| 1   | A     | 564 | LEU  | CA-C-N     | -5.45 | 111.88      | 121.70   |
| 1   | A     | 564 | LEU  | C-N-CA     | -5.45 | 111.88      | 121.70   |
| 1   | A     | 72  | HIS  | CB-CG-CD2  | 5.44  | 138.28      | 131.20   |
| 1   | A     | 80  | ASN  | CA-CB-CG   | -5.44 | 107.16      | 112.60   |
| 1   | A     | 467 | VAL  | CA-C-O     | -5.43 | 114.39      | 120.25   |
| 1   | A     | 508 | ASN  | CB-CG-OD1  | 5.43  | 131.66      | 120.80   |
| 1   | A     | 246 | LYS  | CA-C-N     | 5.43  | 128.80      | 120.82   |
| 1   | A     | 246 | LYS  | C-N-CA     | 5.43  | 128.80      | 120.82   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 63  | ILE  | CA-C-O     | -5.43 | 116.51      | 121.72   |
| 1   | D     | 122 | THR  | CA-CB-OG1  | 5.39  | 117.68      | 109.60   |
| 1   | D     | 283 | SER  | CA-C-N     | -5.39 | 113.65      | 120.98   |
| 1   | D     | 283 | SER  | C-N-CA     | -5.39 | 113.65      | 120.98   |
| 1   | D     | 208 | ALA  | N-CA-CB    | 5.38  | 117.76      | 109.91   |
| 1   | A     | 175 | GLN  | CA-C-O     | -5.36 | 114.74      | 120.42   |
| 1   | A     | 148 | ILE  | CA-C-O     | -5.36 | 114.61      | 120.72   |
| 1   | D     | 346 | GLU  | CA-CB-CG   | 5.36  | 124.81      | 114.10   |
| 1   | D     | 285 | VAL  | CB-CA-C    | -5.36 | 105.12      | 111.65   |
| 1   | D     | 283 | SER  | O-C-N      | 5.33  | 129.59      | 123.29   |
| 1   | A     | 462 | ASP  | CA-C-N     | -5.33 | 112.72      | 120.29   |
| 1   | A     | 462 | ASP  | C-N-CA     | -5.33 | 112.72      | 120.29   |
| 1   | A     | 428 | ARG  | NH1-CZ-NH2 | -5.31 | 112.39      | 119.30   |
| 1   | A     | 486 | GLN  | CA-C-O     | 5.31  | 125.98      | 120.30   |
| 1   | A     | 505 | VAL  | CB-CA-C    | 5.31  | 119.24      | 111.33   |
| 1   | D     | 151 | ASP  | CA-C-O     | -5.31 | 114.01      | 120.54   |
| 1   | D     | 277 | VAL  | N-CA-CB    | 5.30  | 118.14      | 111.46   |
| 1   | A     | 492 | VAL  | N-CA-CB    | 5.30  | 120.61      | 111.39   |
| 1   | D     | 196 | ARG  | NE-CZ-NH1  | 5.29  | 126.79      | 121.50   |
| 1   | D     | 487 | SER  | O-C-N      | 5.28  | 127.39      | 121.32   |
| 1   | A     | 35  | GLN  | N-CA-C     | 5.27  | 116.83      | 111.14   |
| 1   | A     | 25  | VAL  | O-C-N      | -5.26 | 116.94      | 122.83   |
| 1   | D     | 505 | VAL  | CB-CA-C    | 5.25  | 119.88      | 111.32   |
| 1   | A     | 8   | PHE  | CA-C-O     | -5.24 | 115.29      | 120.90   |
| 1   | A     | 62  | ASP  | CA-CB-CG   | -5.24 | 107.36      | 112.60   |
| 1   | A     | 320 | TYR  | CA-CB-CG   | -5.24 | 104.48      | 113.90   |
| 1   | A     | 39  | CYS  | CA-C-N     | -5.23 | 113.21      | 122.26   |
| 1   | A     | 39  | CYS  | C-N-CA     | -5.23 | 113.21      | 122.26   |
| 1   | A     | 414 | ILE  | O-C-N      | 5.23  | 128.84      | 123.03   |
| 1   | D     | 80  | ASN  | CA-CB-CG   | 5.23  | 117.83      | 112.60   |
| 1   | D     | 436 | LEU  | CA-C-O     | 5.23  | 126.13      | 120.43   |
| 1   | A     | 419 | GLN  | O-C-N      | -5.21 | 116.46      | 122.09   |
| 1   | D     | 339 | ASP  | N-CA-C     | 5.21  | 117.64      | 111.33   |
| 1   | A     | 564 | LEU  | CA-C-O     | -5.20 | 113.07      | 120.51   |
| 1   | A     | 450 | GLY  | O-C-N      | -5.20 | 117.32      | 122.41   |
| 1   | A     | 329 | THR  | CB-CA-C    | -5.17 | 100.13      | 110.42   |
| 1   | A     | 280 | ASP  | CA-CB-CG   | -5.17 | 107.43      | 112.60   |
| 1   | D     | 101 | TRP  | CA-C-O     | 5.17  | 126.03      | 120.55   |
| 1   | A     | 540 | LEU  | O-C-N      | -5.17 | 116.91      | 123.01   |
| 1   | D     | 389 | ARG  | NE-CZ-NH2  | 5.16  | 123.84      | 119.20   |
| 1   | D     | 174 | GLN  | OE1-CD-NE2 | -5.15 | 117.45      | 122.60   |
| 1   | A     | 80  | ASN  | CB-CG-ND2  | 5.14  | 124.12      | 116.40   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 49  | ASP  | N-CA-CB    | 5.14  | 119.17      | 110.49   |
| 1   | A     | 397 | ARG  | CD-NE-CZ   | -5.13 | 117.22      | 124.40   |
| 1   | A     | 19  | HIS  | CA-CB-CG   | 5.13  | 118.93      | 113.80   |
| 1   | D     | 19  | HIS  | CA-CB-CG   | -5.13 | 108.67      | 113.80   |
| 1   | A     | 507 | ILE  | CA-C-O     | -5.12 | 115.85      | 121.28   |
| 1   | D     | 38  | SER  | CA-C-O     | -5.12 | 115.19      | 120.92   |
| 1   | D     | 436 | LEU  | O-C-N      | -5.12 | 117.49      | 123.27   |
| 1   | A     | 419 | GLN  | OE1-CD-NE2 | -5.10 | 117.50      | 122.60   |
| 1   | A     | 44  | ALA  | O-C-N      | -5.08 | 116.74      | 122.12   |
| 1   | A     | 263 | GLN  | OE1-CD-NE2 | 5.08  | 127.67      | 122.60   |
| 1   | D     | 238 | ARG  | CD-NE-CZ   | 5.07  | 131.50      | 124.40   |
| 1   | D     | 64  | ASN  | CA-CB-CG   | 5.07  | 117.67      | 112.60   |
| 1   | D     | 218 | LEU  | N-CA-C     | -5.07 | 105.67      | 111.14   |
| 1   | A     | 42  | GLU  | CA-CB-CG   | 5.06  | 124.21      | 114.10   |
| 1   | A     | 531 | THR  | OG1-CB-CG2 | 5.06  | 119.42      | 109.30   |
| 1   | D     | 492 | VAL  | N-CA-CB    | 5.05  | 118.90      | 111.52   |
| 1   | A     | 137 | SER  | N-CA-C     | 5.05  | 117.17      | 111.11   |
| 1   | A     | 259 | ALA  | CA-C-O     | -5.04 | 114.41      | 120.10   |
| 1   | A     | 330 | SER  | CA-CB-OG   | -5.04 | 101.03      | 111.10   |
| 1   | A     | 502 | MET  | CB-CA-C    | -5.04 | 101.31      | 110.63   |
| 1   | A     | 64  | ASN  | OD1-CG-ND2 | -5.03 | 117.57      | 122.60   |
| 1   | A     | 470 | GLY  | O-C-N      | -5.03 | 116.08      | 122.32   |
| 1   | A     | 164 | ALA  | CB-CA-C    | -5.02 | 101.85      | 110.24   |
| 1   | D     | 411 | PHE  | CA-CB-CG   | 5.02  | 118.82      | 113.80   |
| 1   | A     | 274 | VAL  | O-C-N      | -5.01 | 115.61      | 122.03   |
| 1   | A     | 284 | VAL  | O-C-N      | 5.01  | 128.37      | 122.81   |

There are no chirality outliers.

All (12) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group             |
|-----|-------|-----|------|-------------------|
| 1   | A     | 21  | LYS  | Peptide           |
| 1   | A     | 246 | LYS  | Peptide           |
| 1   | A     | 311 | TYR  | Mainchain         |
| 1   | A     | 331 | SER  | Mainchain         |
| 1   | A     | 334 | ILE  | Mainchain         |
| 1   | A     | 359 | ALA  | Mainchain         |
| 1   | A     | 487 | SER  | Peptide,Mainchain |
| 1   | A     | 5   | MET  | Mainchain         |
| 1   | A     | 68  | CYS  | Mainchain         |
| 1   | D     | 246 | LYS  | Peptide           |
| 1   | D     | 486 | GLN  | Peptide           |



## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 4234  | 0        | 4154     | 139     | 0            |
| 1   | D     | 4234  | 0        | 4154     | 166     | 0            |
| 2   | A     | 172   | 0        | 120      | 40      | 0            |
| 2   | D     | 172   | 0        | 120      | 36      | 0            |
| 3   | A     | 53    | 0        | 30       | 1       | 0            |
| 3   | D     | 53    | 0        | 31       | 0       | 0            |
| 4   | A     | 358   | 0        | 0        | 17      | 1            |
| 4   | D     | 149   | 0        | 0        | 11      | 1            |
| All | All   | 9425  | 0        | 8609     | 316     | 1            |

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 18.

All (316) 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:A:65:CYS:SG    | 2:A:602:HEM:CAB | 2.34                     | 1.15              |
| 1:A:36:CYS:SG    | 2:A:603:HEM:CAB | 2.35                     | 1.13              |
| 1:A:82:CYS:SG    | 2:A:601:HEM:CAC | 2.39                     | 1.11              |
| 1:A:79:CYS:SG    | 2:A:601:HEM:CAB | 2.39                     | 1.10              |
| 1:A:68:CYS:SG    | 2:A:602:HEM:CAC | 2.41                     | 1.07              |
| 1:A:18:CYS:SG    | 2:A:604:HEM:CAC | 2.44                     | 1.06              |
| 1:A:508:ASN:ND2  | 1:A:510:THR:H   | 1.59                     | 0.98              |
| 1:A:308:THR:HG21 | 1:A:340:GLY:HA3 | 1.45                     | 0.98              |
| 1:A:15:CYS:SG    | 2:A:604:HEM:CAB | 2.53                     | 0.97              |
| 1:D:415:ILE:HD11 | 1:D:451:MET:HE1 | 1.43                     | 0.97              |
| 1:A:79:CYS:HG    | 2:A:601:HEM:CAB | 1.78                     | 0.96              |
| 1:A:36:CYS:SG    | 2:A:603:HEM:HAB | 2.01                     | 0.95              |
| 1:A:564:LEU:O    | 1:A:565:ASP:HB3 | 1.65                     | 0.95              |
| 1:A:378:VAL:HB   | 4:A:2247:HOH:O  | 1.67                     | 0.95              |
| 1:A:39:CYS:SG    | 2:A:603:HEM:CAC | 2.56                     | 0.92              |
| 1:D:79:CYS:SG    | 2:D:601:HEM:CAB | 2.58                     | 0.91              |
| 1:D:82:CYS:SG    | 2:D:601:HEM:CAC | 2.58                     | 0.91              |
| 1:D:80:ASN:HD21  | 1:D:85:PHE:H    | 1.19                     | 0.90              |
| 1:A:507:ILE:HD11 | 1:A:526:ALA:HB3 | 1.51                     | 0.90              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:365:LYS:HD3  | 1:D:493:LYS:HD3  | 1.57                     | 0.87              |
| 1:A:2:THR:N      | 1:A:3:PRO:HD3    | 1.89                     | 0.86              |
| 1:A:65:CYS:SG    | 2:A:602:HEM:HAB  | 2.15                     | 0.86              |
| 1:D:21:LYS:HB3   | 1:D:22:PRO:HD3   | 1.58                     | 0.85              |
| 1:A:236:VAL:HG12 | 1:A:237:ASP:H    | 1.41                     | 0.83              |
| 1:A:371:ILE:HD13 | 1:A:494:VAL:HG12 | 1.61                     | 0.83              |
| 1:A:418:ASN:ND2  | 1:A:422:LYS:HG3  | 1.97                     | 0.80              |
| 1:D:472:ASP:HB2  | 1:D:480:MET:HE3  | 1.63                     | 0.79              |
| 1:A:65:CYS:HG    | 2:A:602:HEM:CAB  | 1.92                     | 0.79              |
| 1:A:15:CYS:HG    | 2:A:604:HEM:CAB  | 1.95                     | 0.79              |
| 1:A:308:THR:HG23 | 4:A:2217:HOH:O   | 1.82                     | 0.78              |
| 1:A:15:CYS:SG    | 2:A:604:HEM:HAB  | 2.22                     | 0.78              |
| 1:D:308:THR:HG21 | 1:D:340:GLY:HA3  | 1.64                     | 0.78              |
| 1:A:199:ASN:H    | 1:A:199:ASN:HD22 | 1.32                     | 0.77              |
| 1:D:65:CYS:SG    | 2:D:602:HEM:CAB  | 2.72                     | 0.77              |
| 1:A:508:ASN:HD21 | 1:A:510:THR:H    | 1.30                     | 0.77              |
| 1:D:48:ASN:O     | 1:D:49:ASP:HB3   | 1.84                     | 0.77              |
| 1:A:180:VAL:HG13 | 1:A:236:VAL:HG11 | 1.65                     | 0.77              |
| 1:A:564:LEU:O    | 1:A:565:ASP:CB   | 2.30                     | 0.76              |
| 1:D:82:CYS:HG    | 2:D:601:HEM:CAC  | 1.98                     | 0.76              |
| 1:D:430:TYR:HA   | 1:D:435:MET:HE3  | 1.68                     | 0.75              |
| 1:A:483:ASN:ND2  | 1:A:485:THR:OG1  | 2.18                     | 0.75              |
| 1:A:483:ASN:HD22 | 1:A:485:THR:HG23 | 1.51                     | 0.74              |
| 1:D:437:TYR:HB2  | 1:D:491:ALA:HB3  | 1.70                     | 0.74              |
| 1:D:80:ASN:ND2   | 1:D:85:PHE:H     | 1.86                     | 0.73              |
| 1:A:22:PRO:HD2   | 4:A:2014:HOH:O   | 1.88                     | 0.73              |
| 1:A:308:THR:HG21 | 1:A:340:GLY:CA   | 2.17                     | 0.73              |
| 1:D:5:MET:HE1    | 2:D:603:HEM:HMB3 | 1.68                     | 0.73              |
| 1:D:393:GLU:OE1  | 1:D:477:ARG:HD2  | 1.89                     | 0.73              |
| 1:A:18:CYS:SG    | 2:A:604:HEM:HAC  | 2.30                     | 0.72              |
| 1:A:68:CYS:SG    | 2:A:602:HEM:HAC  | 2.28                     | 0.72              |
| 1:D:36:CYS:SG    | 2:D:603:HEM:CAB  | 2.78                     | 0.71              |
| 1:D:507:ILE:HD11 | 1:D:526:ALA:HB3  | 1.70                     | 0.71              |
| 1:D:68:CYS:SG    | 2:D:602:HEM:CAC  | 2.77                     | 0.71              |
| 1:D:79:CYS:SG    | 2:D:601:HEM:HAB  | 2.30                     | 0.71              |
| 1:D:118:PRO:HA   | 1:D:298:MET:HG2  | 1.71                     | 0.71              |
| 1:D:18:CYS:SG    | 2:D:604:HEM:CAC  | 2.78                     | 0.71              |
| 1:A:82:CYS:SG    | 2:A:601:HEM:HAC  | 2.30                     | 0.70              |
| 1:D:325:MET:HE1  | 1:D:357:VAL:HG11 | 1.73                     | 0.70              |
| 1:D:80:ASN:HD21  | 1:D:85:PHE:N     | 1.88                     | 0.70              |
| 1:A:79:CYS:SG    | 2:A:601:HEM:CBB  | 2.79                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:325:MET:HE1  | 1:D:357:VAL:CG1  | 2.23                     | 0.69              |
| 1:A:483:ASN:HD22 | 1:A:485:THR:CG2  | 2.07                     | 0.67              |
| 1:A:236:VAL:HG12 | 1:A:237:ASP:N    | 2.10                     | 0.67              |
| 1:D:21:LYS:HB3   | 1:D:22:PRO:CD    | 2.24                     | 0.67              |
| 2:D:602:HEM:HAA2 | 2:D:603:HEM:HBA1 | 1.77                     | 0.67              |
| 1:A:267:THR:HG21 | 4:A:2119:HOH:O   | 1.93                     | 0.67              |
| 1:A:507:ILE:HD13 | 1:A:531:THR:OG1  | 1.95                     | 0.67              |
| 1:A:2:THR:N      | 1:A:3:PRO:CD     | 2.57                     | 0.66              |
| 1:D:4:ASP:OD1    | 1:D:72:HIS:HA    | 1.94                     | 0.66              |
| 1:D:122:THR:HG21 | 1:D:148:ILE:HG13 | 1.78                     | 0.65              |
| 1:D:376:ARG:HD3  | 1:D:382:MET:HE2  | 1.78                     | 0.65              |
| 1:A:180:VAL:HG13 | 1:A:236:VAL:CG1  | 2.27                     | 0.65              |
| 1:D:122:THR:CG2  | 1:D:148:ILE:HG13 | 2.27                     | 0.65              |
| 1:D:371:ILE:HD13 | 1:D:494:VAL:HG12 | 1.78                     | 0.65              |
| 1:A:122:THR:HG23 | 4:A:2010:HOH:O   | 1.97                     | 0.65              |
| 1:D:407:GLN:HB3  | 1:D:408:PRO:HD2  | 1.78                     | 0.64              |
| 1:D:199:ASN:HD22 | 1:D:199:ASN:H    | 1.43                     | 0.64              |
| 1:D:531:THR:HG21 | 4:D:2144:HOH:O   | 1.95                     | 0.64              |
| 1:D:360:HIS:CD2  | 1:D:362:THR:H    | 2.15                     | 0.64              |
| 1:D:114:ILE:HD11 | 1:D:275:LYS:HD3  | 1.81                     | 0.62              |
| 1:D:18:CYS:HA    | 1:D:35:GLN:HG3   | 1.81                     | 0.62              |
| 1:D:229:LYS:HG2  | 1:D:230:ARG:H    | 1.65                     | 0.62              |
| 1:A:82:CYS:SG    | 2:A:601:HEM:C3C  | 2.93                     | 0.61              |
| 1:D:231:SER:OG   | 1:D:239:THR:HG21 | 1.99                     | 0.61              |
| 1:D:2:THR:N      | 1:D:3:PRO:CD     | 2.63                     | 0.61              |
| 1:A:418:ASN:HD21 | 1:A:422:LYS:HG3  | 1.65                     | 0.61              |
| 1:A:308:THR:CG2  | 1:A:340:GLY:HA3  | 2.24                     | 0.60              |
| 1:A:415:ILE:HG23 | 1:A:484:MET:HE1  | 1.82                     | 0.60              |
| 1:A:418:ASN:CG   | 4:A:2269:HOH:O   | 2.44                     | 0.60              |
| 1:A:483:ASN:CG   | 4:A:2314:HOH:O   | 2.44                     | 0.59              |
| 1:A:383:VAL:HG13 | 1:A:387:GLY:HA2  | 1.83                     | 0.59              |
| 1:A:29:GLU:OE2   | 1:A:293:HIS:HE1  | 1.85                     | 0.59              |
| 1:D:462:ASP:HB3  | 1:D:466:TYR:CZ   | 2.38                     | 0.58              |
| 1:A:518:SER:HB2  | 4:A:2225:HOH:O   | 2.01                     | 0.58              |
| 1:D:4:ASP:HB3    | 1:D:7:SER:H      | 1.68                     | 0.58              |
| 1:A:80:ASN:HD21  | 1:A:85:PHE:H     | 1.50                     | 0.58              |
| 1:A:371:ILE:HD13 | 1:A:494:VAL:CG1  | 2.33                     | 0.57              |
| 1:A:169:ALA:O    | 1:A:238:ARG:HG2  | 2.04                     | 0.57              |
| 2:D:601:HEM:HBB1 | 2:D:602:HEM:CBC  | 2.34                     | 0.57              |
| 1:A:293:HIS:HD2  | 2:A:604:HEM:O2A  | 1.88                     | 0.57              |
| 1:A:405:LEU:HA   | 1:A:410:GLN:HG3  | 1.86                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:443:GLU:HG3  | 1:A:453:VAL:HG13 | 1.85                     | 0.57              |
| 1:A:361:PRO:HG3  | 1:A:397:ARG:HB3  | 1.86                     | 0.57              |
| 1:D:246:LYS:HD3  | 1:D:251:GLU:HA   | 1.87                     | 0.57              |
| 1:D:487:SER:O    | 1:D:488:PRO:C    | 2.48                     | 0.57              |
| 1:A:441:THR:HG23 | 1:A:444:GLN:NE2  | 2.20                     | 0.56              |
| 1:D:229:LYS:NZ   | 1:D:241:ARG:NH1  | 2.52                     | 0.56              |
| 1:D:418:ASN:ND2  | 1:D:422:LYS:HG3  | 2.20                     | 0.56              |
| 1:A:51:LEU:HD23  | 1:A:54:ASP:HA    | 1.88                     | 0.56              |
| 1:A:367:SER:HB2  | 4:A:2084:HOH:O   | 2.05                     | 0.56              |
| 1:D:74:GLU:OE1   | 1:D:97:LYS:HB3   | 2.06                     | 0.56              |
| 1:D:15:CYS:SG    | 2:D:604:HEM:CAB  | 2.94                     | 0.56              |
| 1:D:390:PHE:O    | 1:D:391:ILE:HB   | 2.06                     | 0.56              |
| 1:D:467:VAL:HG23 | 4:D:2113:HOH:O   | 2.05                     | 0.56              |
| 1:D:60:LEU:HD21  | 2:D:601:HEM:HMC3 | 1.88                     | 0.56              |
| 1:A:218:LEU:HD11 | 1:A:549:VAL:HG21 | 1.87                     | 0.56              |
| 1:D:229:LYS:HZ2  | 1:D:241:ARG:HH11 | 1.52                     | 0.56              |
| 1:A:165:GLY:HA2  | 1:A:241:ARG:HH21 | 1.71                     | 0.56              |
| 1:A:531:THR:HG21 | 4:A:2344:HOH:O   | 2.05                     | 0.56              |
| 1:D:464:ASN:OD1  | 1:D:483:ASN:HB2  | 2.05                     | 0.56              |
| 1:D:389:ARG:NH1  | 1:D:463:TYR:HD2  | 2.04                     | 0.55              |
| 1:A:477:ARG:HD3  | 1:A:480:MET:HG2  | 1.89                     | 0.55              |
| 2:A:602:HEM:HAA2 | 2:A:603:HEM:HBA2 | 1.88                     | 0.55              |
| 1:D:18:CYS:SG    | 2:D:604:HEM:HAC  | 2.46                     | 0.55              |
| 1:D:314:ASN:ND2  | 1:D:317:MET:H    | 2.04                     | 0.55              |
| 1:A:508:ASN:HD21 | 1:A:510:THR:N    | 2.02                     | 0.55              |
| 1:A:141:LYS:HE3  | 1:A:265:ILE:HG12 | 1.89                     | 0.54              |
| 1:A:65:CYS:SG    | 2:A:602:HEM:C3B  | 3.00                     | 0.54              |
| 1:A:508:ASN:ND2  | 1:A:510:THR:N    | 2.43                     | 0.54              |
| 1:A:53:PHE:HE2   | 1:A:434:GLU:OE2  | 1.90                     | 0.54              |
| 1:D:229:LYS:HZ2  | 1:D:241:ARG:NH1  | 2.05                     | 0.54              |
| 1:D:284:VAL:HG21 | 1:D:524:LEU:HG   | 1.90                     | 0.54              |
| 1:D:5:MET:HE1    | 2:D:603:HEM:HBB2 | 1.89                     | 0.54              |
| 1:A:185:GLU:H    | 1:A:185:GLU:CD   | 2.16                     | 0.54              |
| 1:D:170:VAL:HG12 | 1:D:182:ASP:CG   | 2.32                     | 0.54              |
| 1:A:440:ASP:HB2  | 1:A:444:GLN:HE22 | 1.72                     | 0.54              |
| 1:D:456:LEU:HD12 | 1:D:456:LEU:O    | 2.08                     | 0.54              |
| 1:A:415:ILE:HD11 | 1:A:451:MET:HE1  | 1.90                     | 0.53              |
| 1:A:65:CYS:SG    | 2:A:602:HEM:CBB  | 2.95                     | 0.53              |
| 1:D:463:TYR:O    | 1:D:467:VAL:HG12 | 2.08                     | 0.53              |
| 1:D:476:GLY:O    | 1:D:477:ARG:C    | 2.51                     | 0.53              |
| 1:D:443:GLU:HG3  | 1:D:453:VAL:CG1  | 2.39                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:314:ASN:C    | 1:A:314:ASN:HD22 | 2.16                     | 0.53              |
| 1:D:169:ALA:O    | 1:D:238:ARG:HB2  | 2.08                     | 0.53              |
| 1:D:495:ALA:HB1  | 1:D:496:PRO:HD2  | 1.91                     | 0.53              |
| 1:A:9:HIS:HB2    | 2:A:604:HEM:HMC3 | 1.91                     | 0.53              |
| 1:D:365:LYS:HD3  | 1:D:493:LYS:CD   | 2.34                     | 0.52              |
| 1:A:332:ASN:N    | 1:A:332:ASN:HD22 | 2.06                     | 0.52              |
| 1:D:165:GLY:HA2  | 1:D:241:ARG:NE   | 2.25                     | 0.52              |
| 1:D:6:GLY:O      | 2:D:604:HEM:HMC3 | 2.10                     | 0.51              |
| 1:D:443:GLU:HG3  | 1:D:453:VAL:HG11 | 1.91                     | 0.51              |
| 1:D:464:ASN:HA   | 1:D:467:VAL:CG1  | 2.39                     | 0.51              |
| 1:D:66:THR:HA    | 1:D:69:HIS:O     | 2.10                     | 0.51              |
| 1:A:367:SER:HB3  | 1:A:435:MET:HG2  | 1.91                     | 0.51              |
| 1:D:507:ILE:HD13 | 1:D:531:THR:OG1  | 2.11                     | 0.51              |
| 1:A:395:THR:HG22 | 1:A:399:LYS:HD2  | 1.93                     | 0.51              |
| 1:A:128:GLY:O    | 1:A:133:GLY:HA3  | 2.11                     | 0.51              |
| 1:A:210:GLN:HE22 | 1:A:554:ILE:HD11 | 1.74                     | 0.51              |
| 1:D:433:LEU:HB2  | 1:D:435:MET:HE2  | 1.93                     | 0.51              |
| 2:D:602:HEM:HMB1 | 2:D:602:HEM:HBB2 | 1.91                     | 0.51              |
| 1:D:36:CYS:SG    | 2:D:603:HEM:HAB  | 2.50                     | 0.51              |
| 1:D:51:LEU:HD23  | 1:D:55:PRO:HD2   | 1.93                     | 0.51              |
| 1:D:166:GLY:HA3  | 1:D:240:HIS:O    | 2.11                     | 0.51              |
| 1:D:463:TYR:CE2  | 1:D:480:MET:HE2  | 2.46                     | 0.51              |
| 1:D:5:MET:CE     | 2:D:603:HEM:HMB3 | 2.39                     | 0.51              |
| 1:A:79:CYS:SG    | 2:A:601:HEM:HAB  | 2.45                     | 0.51              |
| 1:A:68:CYS:SG    | 2:A:602:HEM:C3C  | 3.03                     | 0.50              |
| 1:D:70:LYS:HB2   | 1:D:73:GLU:O     | 2.12                     | 0.50              |
| 2:A:601:HEM:HBB1 | 2:A:602:HEM:CBC  | 2.41                     | 0.50              |
| 1:A:483:ASN:OD1  | 1:A:483:ASN:N    | 2.35                     | 0.50              |
| 1:D:227:ASP:HB3  | 1:D:241:ARG:HB2  | 1.93                     | 0.50              |
| 1:D:33:ASN:HA    | 1:D:36:CYS:SG    | 2.52                     | 0.50              |
| 1:D:314:ASN:HD22 | 1:D:314:ASN:C    | 2.19                     | 0.50              |
| 1:D:361:PRO:HG3  | 1:D:397:ARG:HA   | 1.93                     | 0.50              |
| 1:D:165:GLY:HA2  | 1:D:241:ARG:HE   | 1.77                     | 0.50              |
| 1:A:18:CYS:HG    | 2:A:604:HEM:CAC  | 2.22                     | 0.50              |
| 1:A:66:THR:HA    | 1:A:69:HIS:O     | 2.12                     | 0.50              |
| 1:A:200:ASP:OD1  | 1:A:202:LYS:HE2  | 2.12                     | 0.49              |
| 1:D:483:ASN:ND2  | 1:D:485:THR:HG23 | 2.28                     | 0.49              |
| 1:A:314:ASN:ND2  | 1:A:317:MET:H    | 2.11                     | 0.49              |
| 1:D:106:ASP:O    | 1:D:110:ILE:HG13 | 2.12                     | 0.49              |
| 1:D:371:ILE:CD1  | 1:D:494:VAL:HG12 | 2.42                     | 0.49              |
| 1:D:396:THR:O    | 1:D:397:ARG:C    | 2.56                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:545:ILE:HG13 | 4:D:2050:HOH:O   | 2.11                     | 0.49              |
| 1:A:36:CYS:SG    | 2:A:603:HEM:CBB  | 2.98                     | 0.49              |
| 1:D:21:LYS:CB    | 1:D:22:PRO:HD3   | 2.38                     | 0.49              |
| 1:D:405:LEU:HG   | 1:D:496:PRO:HG3  | 1.93                     | 0.49              |
| 1:A:273:VAL:HG12 | 1:A:343:MET:SD   | 2.53                     | 0.49              |
| 1:D:433:LEU:HD21 | 2:D:601:HEM:C2A  | 2.47                     | 0.49              |
| 1:A:46:LEU:HD11  | 2:A:602:HEM:CMB  | 2.43                     | 0.48              |
| 1:A:183:LYS:HB3  | 1:A:185:GLU:OE2  | 2.13                     | 0.48              |
| 1:A:418:ASN:ND2  | 1:A:422:LYS:HE2  | 2.28                     | 0.48              |
| 1:A:51:LEU:CD2   | 1:A:54:ASP:HA    | 2.43                     | 0.48              |
| 1:A:79:CYS:SG    | 2:A:601:HEM:C3B  | 2.97                     | 0.48              |
| 1:A:18:CYS:HG    | 2:A:604:HEM:HAC  | 1.76                     | 0.48              |
| 1:D:369:ILE:CD1  | 1:D:433:LEU:HD13 | 2.43                     | 0.48              |
| 1:D:6:GLY:HA2    | 2:D:604:HEM:C2C  | 2.49                     | 0.48              |
| 2:D:601:HEM:HBB1 | 2:D:602:HEM:HBC1 | 1.95                     | 0.48              |
| 1:D:65:CYS:SG    | 2:D:602:HEM:HAB  | 2.54                     | 0.48              |
| 1:A:80:ASN:HD21  | 1:A:85:PHE:N     | 2.12                     | 0.47              |
| 1:A:508:ASN:CG   | 1:A:510:THR:H    | 2.18                     | 0.47              |
| 1:D:72:HIS:N     | 2:D:604:HEM:O2D  | 2.47                     | 0.47              |
| 1:A:82:CYS:SG    | 2:A:601:HEM:CBC  | 2.99                     | 0.47              |
| 1:D:21:LYS:CB    | 1:D:22:PRO:CD    | 2.92                     | 0.47              |
| 1:D:382:MET:O    | 1:D:389:ARG:HG2  | 2.14                     | 0.47              |
| 1:D:564:LEU:O    | 1:D:565:ASP:OD1  | 2.32                     | 0.47              |
| 1:A:199:ASN:H    | 1:A:199:ASN:ND2  | 2.06                     | 0.47              |
| 1:D:68:CYS:HB3   | 1:D:76:LYS:O     | 2.14                     | 0.47              |
| 1:D:243:HIS:HB3  | 4:D:2048:HOH:O   | 2.15                     | 0.47              |
| 2:D:602:HEM:HBC2 | 2:D:602:HEM:HMC2 | 1.97                     | 0.47              |
| 1:A:18:CYS:SG    | 2:A:604:HEM:C3C  | 3.06                     | 0.47              |
| 1:A:39:CYS:SG    | 2:A:603:HEM:C3C  | 3.08                     | 0.47              |
| 1:A:39:CYS:SG    | 2:A:603:HEM:CBC  | 3.03                     | 0.47              |
| 1:A:152:LYS:HE2  | 3:A:605:FAD:C8A  | 2.44                     | 0.47              |
| 1:A:284:VAL:HG21 | 1:A:524:LEU:HG   | 1.95                     | 0.47              |
| 1:A:507:ILE:CD1  | 1:A:526:ALA:HB3  | 2.34                     | 0.47              |
| 1:A:565:ASP:HA   | 4:A:2347:HOH:O   | 2.14                     | 0.47              |
| 1:D:71:GLY:HA3   | 2:D:604:HEM:C2D  | 2.50                     | 0.47              |
| 1:D:39:CYS:SG    | 2:D:603:HEM:CAC  | 3.03                     | 0.46              |
| 1:D:41:GLY:HA3   | 1:D:45:GLU:HG2   | 1.97                     | 0.46              |
| 1:D:195:GLY:HA3  | 1:D:199:ASN:HD21 | 1.81                     | 0.46              |
| 1:D:417:ASP:HB3  | 1:D:484:MET:HG2  | 1.97                     | 0.46              |
| 1:D:82:CYS:SG    | 2:D:601:HEM:C3C  | 3.08                     | 0.46              |
| 1:D:198:GLN:HG3  | 1:D:537:TYR:CE2  | 2.50                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:603:HEM:HMC1 | 2:A:603:HEM:HBC2 | 1.98                     | 0.46              |
| 1:A:535:HIS:HD2  | 4:A:2340:HOH:O   | 1.99                     | 0.46              |
| 1:D:360:HIS:O    | 1:D:496:PRO:HA   | 2.16                     | 0.46              |
| 1:D:418:ASN:HD22 | 1:D:422:LYS:HG3  | 1.80                     | 0.45              |
| 1:A:236:VAL:CG1  | 1:A:237:ASP:H    | 2.21                     | 0.45              |
| 1:D:275:LYS:NZ   | 4:D:2056:HOH:O   | 2.50                     | 0.45              |
| 1:A:164:ALA:HB2  | 4:A:2128:HOH:O   | 2.16                     | 0.45              |
| 1:D:329:THR:HG22 | 1:D:330:SER:H    | 1.81                     | 0.45              |
| 1:A:194:GLY:O    | 1:A:538:ASN:HB3  | 2.16                     | 0.45              |
| 1:D:16:GLN:NE2   | 1:D:21:LYS:O     | 2.50                     | 0.45              |
| 1:D:391:ILE:HD11 | 1:D:395:THR:HG21 | 1.98                     | 0.45              |
| 1:D:5:MET:HG3    | 1:D:92:PHE:CE2   | 2.52                     | 0.45              |
| 1:D:199:ASN:HD22 | 1:D:199:ASN:N    | 2.13                     | 0.45              |
| 1:A:53:PHE:CE2   | 1:A:434:GLU:OE2  | 2.68                     | 0.45              |
| 1:A:68:CYS:SG    | 2:A:602:HEM:CBC  | 3.02                     | 0.45              |
| 1:D:164:ALA:HB2  | 4:D:2035:HOH:O   | 2.16                     | 0.45              |
| 1:A:395:THR:HG23 | 4:A:2112:HOH:O   | 2.17                     | 0.44              |
| 1:D:183:LYS:HE3  | 1:D:186:TRP:CZ2  | 2.51                     | 0.44              |
| 1:D:224:ASN:ND2  | 1:D:226:ASP:OD2  | 2.50                     | 0.44              |
| 1:D:75:PRO:CD    | 1:D:93:SER:HA    | 2.47                     | 0.44              |
| 1:D:243:HIS:C    | 1:D:243:HIS:HD1  | 2.25                     | 0.44              |
| 1:D:308:THR:HG23 | 4:D:2063:HOH:O   | 2.16                     | 0.44              |
| 1:D:449:THR:OG1  | 1:D:451:MET:HG3  | 2.17                     | 0.44              |
| 1:A:267:THR:H    | 1:A:267:THR:HG22 | 1.47                     | 0.44              |
| 1:D:415:ILE:HG23 | 1:D:484:MET:HE1  | 2.00                     | 0.44              |
| 1:D:128:GLY:O    | 1:D:133:GLY:HA3  | 2.17                     | 0.44              |
| 1:D:528:GLY:O    | 1:D:531:THR:HB   | 2.18                     | 0.44              |
| 1:D:71:GLY:HA3   | 2:D:604:HEM:C1D  | 2.52                     | 0.44              |
| 1:A:483:ASN:CB   | 4:A:2314:HOH:O   | 2.66                     | 0.43              |
| 2:D:602:HEM:HBC2 | 2:D:602:HEM:CMC  | 2.48                     | 0.43              |
| 1:A:514:LEU:HB3  | 1:A:518:SER:HA   | 2.00                     | 0.43              |
| 1:D:194:GLY:O    | 1:D:538:ASN:HB3  | 2.18                     | 0.43              |
| 1:D:457:ALA:O    | 1:D:461:SER:OG   | 2.36                     | 0.43              |
| 2:D:602:HEM:HAA2 | 2:D:603:HEM:CBA  | 2.46                     | 0.43              |
| 1:D:386:ASP:CG   | 1:D:452:LYS:HE3  | 2.43                     | 0.43              |
| 1:D:391:ILE:HG23 | 1:D:392:SER:O    | 2.19                     | 0.43              |
| 1:A:6:GLY:HA2    | 2:A:604:HEM:C2C  | 2.54                     | 0.43              |
| 1:D:246:LYS:HD3  | 1:D:251:GLU:CA   | 2.48                     | 0.43              |
| 1:A:18:CYS:SG    | 2:A:604:HEM:CBC  | 3.03                     | 0.43              |
| 1:A:279:ASN:ND2  | 1:A:283:SER:HB2  | 2.33                     | 0.42              |
| 1:D:122:THR:HG23 | 1:D:148:ILE:HG13 | 1.99                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:466:TYR:O    | 1:D:470:GLY:N    | 2.51                     | 0.42              |
| 1:A:48:ASN:OD1   | 1:A:49:ASP:N     | 2.41                     | 0.42              |
| 1:A:51:LEU:HD23  | 1:A:54:ASP:H     | 1.84                     | 0.42              |
| 1:D:452:LYS:NZ   | 1:D:455:ASP:OD2  | 2.52                     | 0.42              |
| 1:A:360:HIS:O    | 1:A:496:PRO:HA   | 2.20                     | 0.42              |
| 1:A:438:LYS:HE2  | 1:A:490:TYR:HE1  | 1.85                     | 0.42              |
| 1:A:278:VAL:HA   | 1:A:283:SER:O    | 2.20                     | 0.42              |
| 1:A:366:ASP:OD1  | 1:A:366:ASP:N    | 2.42                     | 0.42              |
| 1:D:369:ILE:HG21 | 1:D:435:MET:HE1  | 2.00                     | 0.42              |
| 1:D:389:ARG:NH1  | 4:D:2102:HOH:O   | 2.53                     | 0.42              |
| 1:A:289:VAL:O    | 1:A:296:TYR:HA   | 2.20                     | 0.42              |
| 1:A:418:ASN:HD21 | 1:A:422:LYS:CG   | 2.32                     | 0.42              |
| 1:A:409:GLY:O    | 1:A:410:GLN:CB   | 2.66                     | 0.42              |
| 1:D:68:CYS:SG    | 2:D:602:HEM:CBC  | 3.07                     | 0.42              |
| 1:A:418:ASN:CB   | 4:A:2269:HOH:O   | 2.66                     | 0.42              |
| 1:D:75:PRO:HD3   | 1:D:93:SER:HA    | 2.02                     | 0.42              |
| 1:D:90:MET:HB3   | 1:D:91:PRO:HD2   | 2.01                     | 0.42              |
| 1:A:441:THR:H    | 1:A:444:GLN:HE21 | 1.66                     | 0.41              |
| 1:D:90:MET:HG3   | 4:D:2019:HOH:O   | 2.18                     | 0.41              |
| 1:D:487:SER:HB3  | 1:D:488:PRO:HD3  | 2.01                     | 0.41              |
| 1:D:159:ASN:HD21 | 1:D:332:ASN:ND2  | 2.18                     | 0.41              |
| 1:D:265:ILE:HA   | 4:D:2054:HOH:O   | 2.20                     | 0.41              |
| 1:D:308:THR:HG21 | 1:D:340:GLY:CA   | 2.43                     | 0.41              |
| 1:D:82:CYS:SG    | 2:D:601:HEM:CBC  | 3.07                     | 0.41              |
| 1:D:430:TYR:CA   | 1:D:435:MET:HE3  | 2.46                     | 0.41              |
| 1:D:466:TYR:HB2  | 1:D:480:MET:HE1  | 2.01                     | 0.41              |
| 1:A:438:LYS:HE2  | 1:A:490:TYR:CE1  | 2.55                     | 0.41              |
| 1:D:442:VAL:HG23 | 1:D:489:TYR:CE2  | 2.55                     | 0.41              |
| 1:D:88:LYS:O     | 1:D:89:PRO:C     | 2.63                     | 0.41              |
| 1:D:227:ASP:O    | 1:D:240:HIS:HA   | 2.19                     | 0.41              |
| 1:A:141:LYS:HE3  | 1:A:265:ILE:CG1  | 2.49                     | 0.41              |
| 1:D:46:LEU:HD11  | 2:D:602:HEM:CMB  | 2.50                     | 0.41              |
| 1:A:413:TRP:CZ3  | 1:A:493:LYS:HB2  | 2.56                     | 0.41              |
| 1:D:70:LYS:HG3   | 1:D:73:GLU:HG3   | 2.03                     | 0.41              |
| 1:D:464:ASN:HA   | 1:D:467:VAL:HG13 | 2.03                     | 0.41              |
| 1:A:461:SER:O    | 1:A:462:ASP:C    | 2.61                     | 0.41              |
| 1:D:386:ASP:HB3  | 1:D:452:LYS:HE3  | 2.01                     | 0.41              |
| 1:D:4:ASP:H      | 1:D:7:SER:HG     | 1.63                     | 0.41              |
| 1:D:210:GLN:NE2  | 1:D:550:VAL:HG13 | 2.36                     | 0.41              |
| 1:A:187:PHE:CD2  | 1:A:238:ARG:HD3  | 2.56                     | 0.41              |
| 1:D:535:HIS:HB3  | 1:D:539:ARG:HA   | 2.03                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:281:ASP:O    | 1:D:282:HIS:HB2  | 2.21                     | 0.40              |
| 1:D:562:HIS:HE1  | 4:D:2129:HOH:O   | 2.03                     | 0.40              |
| 1:D:5:MET:HE1    | 2:D:603:HEM:CMB  | 2.45                     | 0.40              |
| 1:A:397:ARG:HH11 | 1:A:397:ARG:HD3  | 1.51                     | 0.40              |
| 1:A:517:GLN:HG2  | 4:A:2329:HOH:O   | 2.21                     | 0.40              |
| 1:D:407:GLN:HB3  | 1:D:408:PRO:CD   | 2.48                     | 0.40              |
| 1:D:500:HIS:CG   | 1:D:539:ARG:HD3  | 2.56                     | 0.40              |
| 1:D:460:VAL:HG12 | 1:D:464:ASN:ND2  | 2.36                     | 0.40              |
| 1:D:505:VAL:HG13 | 1:D:513:VAL:HG13 | 2.03                     | 0.40              |
| 2:D:604:HEM:HHA  | 2:D:604:HEM:HAA1 | 1.97                     | 0.40              |

All (1) 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) |
|----------------|-----------------------|--------------------------|-------------------|
| 4:A:2135:HOH:O | 4:D:2105:HOH:O[3_655] | 2.19                     | 0.01              |

## 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     | 562/566 (99%)   | 523 (93%)  | 33 (6%) | 6 (1%)   | 11          | 7 |
| 1   | D     | 562/566 (99%)   | 511 (91%)  | 42 (8%) | 9 (2%)   | 7           | 3 |
| All | All   | 1124/1132 (99%) | 1034 (92%) | 75 (7%) | 15 (1%)  | 9           | 5 |

All (15) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 22  | PRO  |
| 1   | D     | 3   | PRO  |
| 1   | D     | 391 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 487 | SER  |
| 1   | A     | 49  | ASP  |
| 1   | A     | 243 | HIS  |
| 1   | D     | 49  | ASP  |
| 1   | A     | 329 | THR  |
| 1   | D     | 54  | ASP  |
| 1   | D     | 13  | GLY  |
| 1   | D     | 244 | GLY  |
| 1   | A     | 54  | ASP  |
| 1   | A     | 166 | GLY  |
| 1   | D     | 21  | LYS  |
| 1   | D     | 232 | GLY  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |   |
|-----|-------|----------------|-----------|----------|-------------|---|
| 1   | A     | 446/448 (100%) | 413 (93%) | 33 (7%)  | 13          | 8 |
| 1   | D     | 446/448 (100%) | 397 (89%) | 49 (11%) | 6           | 3 |
| All | All   | 892/896 (100%) | 810 (91%) | 82 (9%)  | 8           | 4 |

All (82) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 52  | GLN  |
| 1   | A     | 87  | ILE  |
| 1   | A     | 105 | TRP  |
| 1   | A     | 122 | THR  |
| 1   | A     | 125 | LEU  |
| 1   | A     | 181 | GLU  |
| 1   | A     | 185 | GLU  |
| 1   | A     | 199 | ASN  |
| 1   | A     | 202 | LYS  |
| 1   | A     | 238 | ARG  |
| 1   | A     | 280 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 314 | ASN  |
| 1   | A     | 329 | THR  |
| 1   | A     | 332 | ASN  |
| 1   | A     | 345 | LYS  |
| 1   | A     | 365 | LYS  |
| 1   | A     | 366 | ASP  |
| 1   | A     | 370 | LEU  |
| 1   | A     | 383 | VAL  |
| 1   | A     | 395 | THR  |
| 1   | A     | 410 | GLN  |
| 1   | A     | 415 | ILE  |
| 1   | A     | 418 | ASN  |
| 1   | A     | 427 | VAL  |
| 1   | A     | 445 | LEU  |
| 1   | A     | 467 | VAL  |
| 1   | A     | 487 | SER  |
| 1   | A     | 492 | VAL  |
| 1   | A     | 505 | VAL  |
| 1   | A     | 507 | ILE  |
| 1   | A     | 518 | SER  |
| 1   | A     | 524 | LEU  |
| 1   | A     | 531 | THR  |
| 1   | D     | 2   | THR  |
| 1   | D     | 3   | PRO  |
| 1   | D     | 12  | MET  |
| 1   | D     | 17  | SER  |
| 1   | D     | 36  | CYS  |
| 1   | D     | 45  | GLU  |
| 1   | D     | 49  | ASP  |
| 1   | D     | 65  | CYS  |
| 1   | D     | 105 | TRP  |
| 1   | D     | 108 | ASP  |
| 1   | D     | 121 | THR  |
| 1   | D     | 122 | THR  |
| 1   | D     | 125 | LEU  |
| 1   | D     | 170 | VAL  |
| 1   | D     | 172 | THR  |
| 1   | D     | 176 | THR  |
| 1   | D     | 199 | ASN  |
| 1   | D     | 220 | SER  |
| 1   | D     | 236 | VAL  |
| 1   | D     | 239 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 246 | LYS  |
| 1   | D     | 262 | GLU  |
| 1   | D     | 263 | GLN  |
| 1   | D     | 267 | THR  |
| 1   | D     | 280 | ASP  |
| 1   | D     | 298 | MET  |
| 1   | D     | 308 | THR  |
| 1   | D     | 314 | ASN  |
| 1   | D     | 329 | THR  |
| 1   | D     | 346 | GLU  |
| 1   | D     | 369 | ILE  |
| 1   | D     | 383 | VAL  |
| 1   | D     | 385 | LYS  |
| 1   | D     | 395 | THR  |
| 1   | D     | 396 | THR  |
| 1   | D     | 398 | ASP  |
| 1   | D     | 415 | ILE  |
| 1   | D     | 427 | VAL  |
| 1   | D     | 444 | GLN  |
| 1   | D     | 445 | LEU  |
| 1   | D     | 453 | VAL  |
| 1   | D     | 461 | SER  |
| 1   | D     | 467 | VAL  |
| 1   | D     | 479 | ASP  |
| 1   | D     | 492 | VAL  |
| 1   | D     | 505 | VAL  |
| 1   | D     | 507 | ILE  |
| 1   | D     | 524 | LEU  |
| 1   | D     | 531 | THR  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 80  | ASN  |
| 1   | A     | 199 | ASN  |
| 1   | A     | 210 | GLN  |
| 1   | A     | 293 | HIS  |
| 1   | A     | 314 | ASN  |
| 1   | A     | 418 | ASN  |
| 1   | A     | 419 | GLN  |
| 1   | A     | 444 | GLN  |
| 1   | A     | 483 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 508 | ASN  |
| 1   | D     | 35  | GLN  |
| 1   | D     | 80  | ASN  |
| 1   | D     | 111 | GLN  |
| 1   | D     | 197 | GLN  |
| 1   | D     | 199 | ASN  |
| 1   | D     | 210 | GLN  |
| 1   | D     | 282 | HIS  |
| 1   | D     | 314 | ASN  |
| 1   | D     | 332 | ASN  |
| 1   | D     | 360 | HIS  |
| 1   | D     | 388 | ASN  |
| 1   | D     | 517 | GLN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

10 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   | HEM  | A     | 601 | 1    | 50,50,50     | 1.61 | 11 (22%)    | 67,82,82    | 1.45 | 9 (13%)     |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 2   | HEM  | D     | 604 | 1    | 50,50,50     | 1.47 | 8 (16%)  | 67,82,82    | 2.65 | 12 (17%) |
| 2   | HEM  | A     | 603 | 1    | 50,50,50     | 1.59 | 10 (20%) | 67,82,82    | 1.66 | 15 (22%) |
| 2   | HEM  | D     | 601 | 1    | 50,50,50     | 1.46 | 10 (20%) | 67,82,82    | 1.06 | 3 (4%)   |
| 2   | HEM  | D     | 603 | 1    | 50,50,50     | 1.28 | 6 (12%)  | 67,82,82    | 1.57 | 12 (17%) |
| 3   | FAD  | A     | 605 | -    | 58,58,58     | 2.51 | 16 (27%) | 85,89,89    | 2.01 | 22 (25%) |
| 2   | HEM  | A     | 604 | 1    | 50,50,50     | 1.61 | 12 (24%) | 67,82,82    | 1.85 | 19 (28%) |
| 2   | HEM  | A     | 602 | 1    | 50,50,50     | 1.75 | 16 (32%) | 67,82,82    | 1.71 | 18 (26%) |
| 3   | FAD  | D     | 605 | -    | 58,58,58     | 2.64 | 15 (25%) | 85,89,89    | 1.59 | 14 (16%) |
| 2   | HEM  | D     | 602 | 1    | 50,50,50     | 1.27 | 7 (14%)  | 67,82,82    | 1.37 | 10 (14%) |

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   | HEM  | A     | 601 | 1    | -       | 2/14/54/54 | -       |
| 2   | HEM  | D     | 604 | 1    | -       | 4/14/54/54 | -       |
| 2   | HEM  | A     | 603 | 1    | -       | 4/14/54/54 | -       |
| 2   | HEM  | D     | 601 | 1    | -       | 4/14/54/54 | -       |
| 2   | HEM  | D     | 603 | 1    | -       | 4/14/54/54 | -       |
| 3   | FAD  | A     | 605 | -    | -       | 6/34/50/50 | 0/6/6/6 |
| 2   | HEM  | A     | 604 | 1    | -       | 5/14/54/54 | -       |
| 2   | HEM  | A     | 602 | 1    | -       | 6/14/54/54 | -       |
| 3   | FAD  | D     | 605 | -    | -       | 6/34/50/50 | 0/6/6/6 |
| 2   | HEM  | D     | 602 | 1    | -       | 5/14/54/54 | -       |

All (111) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 3   | D     | 605 | FAD  | P-O3P   | -15.67 | 1.42        | 1.59     |
| 3   | A     | 605 | FAD  | P-O3P   | -13.08 | 1.45        | 1.59     |
| 2   | D     | 604 | HEM  | CBD-CGD | -4.86  | 1.39        | 1.50     |
| 2   | A     | 601 | HEM  | CAB-C3B | 4.48   | 1.59        | 1.47     |
| 3   | D     | 605 | FAD  | PA-O3P  | 4.31   | 1.64        | 1.59     |
| 2   | A     | 604 | HEM  | FE-NB   | 4.29   | 2.08        | 1.94     |
| 3   | D     | 605 | FAD  | PA-O2A  | -4.24  | 1.35        | 1.55     |
| 3   | A     | 605 | FAD  | C5'-C4' | 4.20   | 1.57        | 1.51     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | A     | 605 | FAD  | PA-O2A  | -4.18 | 1.36        | 1.55     |
| 3   | D     | 605 | FAD  | C1'-C2' | 3.91  | 1.58        | 1.52     |
| 2   | A     | 601 | HEM  | CAC-C3C | 3.84  | 1.57        | 1.47     |
| 2   | A     | 603 | HEM  | C3D-C2D | -3.70 | 1.28        | 1.36     |
| 2   | A     | 604 | HEM  | CAC-C3C | 3.56  | 1.56        | 1.47     |
| 2   | D     | 601 | HEM  | CAC-C3C | 3.50  | 1.56        | 1.47     |
| 2   | A     | 604 | HEM  | FE-ND   | 3.49  | 2.05        | 1.94     |
| 2   | A     | 603 | HEM  | CMD-C2D | 3.42  | 1.57        | 1.50     |
| 2   | A     | 602 | HEM  | CMB-C2B | 3.40  | 1.57        | 1.50     |
| 3   | A     | 605 | FAD  | P-O2P   | -3.34 | 1.39        | 1.55     |
| 3   | A     | 605 | FAD  | C5B-C4B | 3.30  | 1.61        | 1.51     |
| 2   | A     | 603 | HEM  | CAC-C3C | 3.29  | 1.56        | 1.47     |
| 2   | A     | 602 | HEM  | C2A-C3A | -3.26 | 1.30        | 1.38     |
| 2   | A     | 604 | HEM  | C3C-C2C | -3.24 | 1.30        | 1.37     |
| 3   | A     | 605 | FAD  | O5'-C5' | 3.21  | 1.56        | 1.44     |
| 2   | A     | 603 | HEM  | CMB-C2B | 3.20  | 1.57        | 1.50     |
| 2   | A     | 602 | HEM  | CMD-C2D | 3.14  | 1.57        | 1.50     |
| 3   | A     | 605 | FAD  | C1'-C2' | 3.14  | 1.57        | 1.52     |
| 2   | A     | 602 | HEM  | CMA-C3A | 3.05  | 1.57        | 1.50     |
| 2   | A     | 601 | HEM  | FE-ND   | 3.05  | 2.04        | 1.94     |
| 3   | A     | 605 | FAD  | O4B-C4B | 2.93  | 1.51        | 1.45     |
| 3   | A     | 605 | FAD  | O4B-C1B | 2.92  | 1.48        | 1.42     |
| 2   | D     | 604 | HEM  | CAC-C3C | 2.89  | 1.55        | 1.47     |
| 2   | D     | 604 | HEM  | CAB-C3B | 2.86  | 1.55        | 1.47     |
| 2   | D     | 601 | HEM  | CMD-C2D | 2.85  | 1.56        | 1.50     |
| 2   | D     | 601 | HEM  | FE-NC   | 2.84  | 2.04        | 1.95     |
| 2   | A     | 602 | HEM  | FE-NA   | 2.80  | 2.04        | 1.95     |
| 3   | A     | 605 | FAD  | O3B-C3B | -2.77 | 1.36        | 1.43     |
| 2   | A     | 602 | HEM  | CAC-C3C | 2.75  | 1.54        | 1.47     |
| 2   | A     | 602 | HEM  | CAD-C3D | 2.74  | 1.58        | 1.51     |
| 3   | D     | 605 | FAD  | O5'-C5' | 2.74  | 1.55        | 1.44     |
| 2   | A     | 604 | HEM  | CMD-C2D | 2.69  | 1.56        | 1.50     |
| 2   | A     | 603 | HEM  | CMA-C3A | 2.68  | 1.56        | 1.50     |
| 2   | D     | 604 | HEM  | CAD-C3D | 2.68  | 1.58        | 1.51     |
| 2   | D     | 603 | HEM  | CAC-C3C | 2.67  | 1.54        | 1.47     |
| 3   | A     | 605 | FAD  | O2-C2   | -2.65 | 1.19        | 1.24     |
| 3   | A     | 605 | FAD  | PA-O3P  | 2.64  | 1.62        | 1.59     |
| 2   | D     | 602 | HEM  | CAC-C3C | 2.64  | 1.54        | 1.47     |
| 2   | A     | 602 | HEM  | C3B-C2B | -2.63 | 1.31        | 1.37     |
| 2   | A     | 602 | HEM  | C1C-NC  | -2.58 | 1.34        | 1.39     |
| 2   | A     | 601 | HEM  | FE-NB   | 2.57  | 2.02        | 1.94     |
| 2   | D     | 601 | HEM  | C3C-C2C | -2.57 | 1.31        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | D     | 601 | HEM  | C2A-C3A | -2.57 | 1.32        | 1.38     |
| 3   | A     | 605 | FAD  | C9A-C5X | 2.56  | 1.45        | 1.41     |
| 2   | D     | 603 | HEM  | CAB-C3B | 2.54  | 1.54        | 1.47     |
| 2   | D     | 601 | HEM  | FE-NB   | 2.51  | 2.02        | 1.94     |
| 2   | D     | 602 | HEM  | FE-NA   | 2.49  | 2.03        | 1.95     |
| 2   | D     | 602 | HEM  | CAD-C3D | 2.49  | 1.57        | 1.51     |
| 2   | D     | 601 | HEM  | FE-NA   | 2.49  | 2.03        | 1.95     |
| 2   | A     | 603 | HEM  | CBC-CAC | 2.47  | 1.42        | 1.30     |
| 3   | D     | 605 | FAD  | C3B-C4B | 2.47  | 1.59        | 1.53     |
| 3   | A     | 605 | FAD  | C2-N1   | -2.46 | 1.31        | 1.36     |
| 2   | A     | 601 | HEM  | FE-NA   | 2.46  | 2.03        | 1.95     |
| 3   | D     | 605 | FAD  | P-O2P   | -2.46 | 1.43        | 1.55     |
| 3   | D     | 605 | FAD  | C2-N1   | -2.44 | 1.31        | 1.36     |
| 2   | D     | 604 | HEM  | FE-NB   | 2.44  | 2.02        | 1.94     |
| 2   | D     | 602 | HEM  | FE-NC   | 2.44  | 2.03        | 1.95     |
| 2   | A     | 601 | HEM  | CAD-C3D | 2.42  | 1.57        | 1.51     |
| 2   | A     | 603 | HEM  | C3B-C2B | -2.40 | 1.32        | 1.37     |
| 3   | D     | 605 | FAD  | O4B-C1B | 2.39  | 1.47        | 1.42     |
| 2   | A     | 604 | HEM  | O1A-CGA | 2.39  | 1.29        | 1.22     |
| 2   | A     | 602 | HEM  | CAB-C3B | 2.39  | 1.53        | 1.47     |
| 3   | D     | 605 | FAD  | C5A-C4A | 2.38  | 1.43        | 1.39     |
| 3   | D     | 605 | FAD  | C2A-N1A | 2.38  | 1.38        | 1.33     |
| 2   | D     | 603 | HEM  | CAD-C3D | 2.36  | 1.57        | 1.51     |
| 2   | A     | 601 | HEM  | C3B-C2B | -2.33 | 1.32        | 1.37     |
| 3   | A     | 605 | FAD  | C2A-N1A | 2.32  | 1.38        | 1.33     |
| 2   | D     | 601 | HEM  | CMB-C2B | 2.32  | 1.55        | 1.50     |
| 2   | A     | 603 | HEM  | CAB-C3B | 2.32  | 1.53        | 1.47     |
| 2   | D     | 602 | HEM  | CAB-C3B | 2.31  | 1.53        | 1.47     |
| 2   | A     | 604 | HEM  | CMC-C2C | 2.29  | 1.55        | 1.50     |
| 2   | A     | 602 | HEM  | C3C-C2C | -2.28 | 1.32        | 1.37     |
| 2   | A     | 601 | HEM  | C2A-C3A | -2.27 | 1.33        | 1.38     |
| 2   | A     | 604 | HEM  | CAB-C3B | 2.26  | 1.53        | 1.47     |
| 2   | A     | 602 | HEM  | C1A-C2A | 2.24  | 1.49        | 1.44     |
| 2   | A     | 602 | HEM  | C1D-ND  | 2.23  | 1.43        | 1.38     |
| 2   | A     | 602 | HEM  | FE-NC   | 2.22  | 2.02        | 1.95     |
| 3   | D     | 605 | FAD  | C5A-C6A | 2.22  | 1.47        | 1.41     |
| 2   | D     | 601 | HEM  | CAB-C3B | 2.19  | 1.53        | 1.47     |
| 2   | D     | 603 | HEM  | CMB-C2B | 2.17  | 1.55        | 1.50     |
| 2   | A     | 601 | HEM  | CMA-C3A | 2.17  | 1.55        | 1.50     |
| 2   | A     | 604 | HEM  | C1B-NB  | -2.17 | 1.36        | 1.40     |
| 2   | D     | 603 | HEM  | CMD-C2D | 2.13  | 1.55        | 1.50     |
| 2   | D     | 604 | HEM  | FE-NA   | 2.12  | 2.02        | 1.95     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | A     | 601 | HEM  | CBD-CGD | 2.12  | 1.55        | 1.50     |
| 2   | A     | 601 | HEM  | CAA-C2A | 2.12  | 1.56        | 1.51     |
| 3   | D     | 605 | FAD  | PA-O5B  | -2.11 | 1.51        | 1.59     |
| 2   | D     | 601 | HEM  | CMC-C2C | 2.11  | 1.55        | 1.50     |
| 2   | A     | 604 | HEM  | CMB-C2B | 2.11  | 1.55        | 1.50     |
| 2   | A     | 603 | HEM  | C4B-NB  | -2.10 | 1.34        | 1.38     |
| 2   | D     | 602 | HEM  | CMC-C2C | 2.10  | 1.55        | 1.50     |
| 2   | A     | 602 | HEM  | C4C-NC  | -2.10 | 1.35        | 1.39     |
| 2   | D     | 604 | HEM  | CMB-C2B | 2.10  | 1.55        | 1.50     |
| 2   | A     | 602 | HEM  | CBC-CAC | 2.09  | 1.40        | 1.30     |
| 2   | D     | 604 | HEM  | CMD-C2D | 2.08  | 1.55        | 1.50     |
| 2   | A     | 604 | HEM  | FE-NA   | 2.07  | 2.02        | 1.95     |
| 3   | A     | 605 | FAD  | C4'-C3' | 2.06  | 1.57        | 1.53     |
| 2   | D     | 602 | HEM  | C2A-C3A | -2.06 | 1.33        | 1.38     |
| 3   | D     | 605 | FAD  | P-O5'   | -2.05 | 1.51        | 1.59     |
| 3   | D     | 605 | FAD  | C8-C7   | 2.05  | 1.45        | 1.40     |
| 2   | D     | 603 | HEM  | FE-NB   | 2.04  | 2.01        | 1.94     |
| 2   | A     | 603 | HEM  | CBD-CAD | 2.02  | 1.58        | 1.51     |
| 2   | A     | 604 | HEM  | C2A-C3A | -2.01 | 1.33        | 1.38     |

All (134) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | D     | 604 | HEM  | CAD-CBD-CGD | 14.96 | 153.35      | 113.67   |
| 2   | D     | 604 | HEM  | CBD-CAD-C3D | -9.13 | 87.30       | 112.53   |
| 2   | D     | 604 | HEM  | CBA-CAA-C2A | 7.08  | 132.10      | 112.53   |
| 2   | D     | 603 | HEM  | CBD-CAD-C3D | -6.29 | 95.14       | 112.53   |
| 3   | D     | 605 | FAD  | C4'-C3'-C2' | -6.00 | 103.58      | 113.57   |
| 3   | A     | 605 | FAD  | C4-N3-C2    | -5.78 | 115.38      | 125.64   |
| 2   | A     | 604 | HEM  | CBA-CAA-C2A | 4.84  | 125.93      | 112.53   |
| 3   | A     | 605 | FAD  | O3'-C3'-C4' | -4.74 | 98.16       | 108.93   |
| 3   | A     | 605 | FAD  | O2-C2-N3    | -4.65 | 109.67      | 118.58   |
| 2   | A     | 604 | HEM  | CAA-CBA-CGA | 4.52  | 125.66      | 113.67   |
| 2   | A     | 603 | HEM  | O2A-CGA-O1A | 4.35  | 134.53      | 123.33   |
| 3   | A     | 605 | FAD  | C10-N1-C2   | 4.29  | 126.14      | 116.85   |
| 3   | A     | 605 | FAD  | C4'-C3'-C2' | -4.29 | 106.43      | 113.57   |
| 2   | A     | 603 | HEM  | C3B-C4B-NB  | -4.24 | 106.42      | 109.47   |
| 2   | A     | 604 | HEM  | CHA-C4D-ND  | 4.22  | 129.58      | 124.37   |
| 2   | D     | 602 | HEM  | CAD-CBD-CGD | 4.01  | 124.29      | 113.67   |
| 3   | D     | 605 | FAD  | O2-C2-N1    | 3.90  | 128.29      | 121.80   |
| 2   | A     | 602 | HEM  | CMA-C3A-C4A | -3.89 | 119.50      | 125.42   |
| 3   | D     | 605 | FAD  | O4B-C1B-N9A | -3.89 | 100.62      | 108.09   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | A     | 602 | HEM  | CHC-C1C-NC  | 3.80  | 128.59      | 124.45   |
| 2   | A     | 603 | HEM  | CHC-C4B-NB  | 3.77  | 128.49      | 124.42   |
| 2   | A     | 603 | HEM  | C1C-CHC-C4B | -3.73 | 118.08      | 126.02   |
| 2   | A     | 602 | HEM  | O1D-CGD-CBD | -3.73 | 111.27      | 123.09   |
| 3   | A     | 605 | FAD  | O2-C2-N1    | 3.71  | 127.96      | 121.80   |
| 2   | A     | 603 | HEM  | O1A-CGA-CBA | -3.63 | 111.58      | 123.09   |
| 2   | D     | 604 | HEM  | C3D-C4D-ND  | -3.61 | 106.21      | 110.17   |
| 3   | D     | 605 | FAD  | C10-N1-C2   | 3.60  | 124.64      | 116.85   |
| 2   | A     | 604 | HEM  | C3D-C4D-ND  | -3.60 | 106.23      | 110.17   |
| 2   | D     | 602 | HEM  | CBD-CAD-C3D | -3.49 | 102.88      | 112.53   |
| 3   | A     | 605 | FAD  | C5'-C4'-C3' | -3.42 | 105.77      | 112.22   |
| 2   | D     | 601 | HEM  | O2D-CGD-O1D | 3.40  | 132.07      | 123.33   |
| 2   | A     | 604 | HEM  | O2A-CGA-CBA | 3.36  | 124.61      | 114.00   |
| 2   | A     | 602 | HEM  | CHD-C4C-NC  | 3.35  | 128.10      | 124.45   |
| 3   | A     | 605 | FAD  | C4X-C10-N1  | -3.34 | 116.39      | 124.59   |
| 2   | D     | 603 | HEM  | C3D-C4D-ND  | -3.33 | 106.52      | 110.17   |
| 2   | A     | 603 | HEM  | CMD-C2D-C1D | -3.27 | 119.93      | 125.03   |
| 2   | D     | 602 | HEM  | O1D-CGD-CBD | -3.22 | 112.88      | 123.09   |
| 3   | D     | 605 | FAD  | N3A-C2A-N1A | -3.21 | 123.72      | 128.58   |
| 2   | A     | 604 | HEM  | C4D-ND-C1D  | 3.20  | 109.00      | 105.21   |
| 2   | D     | 604 | HEM  | O1D-CGD-CBD | -3.16 | 113.06      | 123.09   |
| 2   | A     | 604 | HEM  | C3B-C2B-C1B | 3.11  | 108.75      | 106.41   |
| 2   | D     | 604 | HEM  | C4D-C3D-C2D | 3.10  | 111.40      | 106.89   |
| 3   | A     | 605 | FAD  | O4B-C1B-N9A | -3.09 | 102.16      | 108.09   |
| 2   | D     | 602 | HEM  | C4A-CHB-C1B | -3.08 | 119.01      | 126.25   |
| 2   | A     | 604 | HEM  | O1A-CGA-CBA | -3.02 | 113.50      | 123.09   |
| 3   | A     | 605 | FAD  | C4X-C4-N3   | 3.00  | 120.90      | 113.25   |
| 3   | A     | 605 | FAD  | C2A-N1A-C6A | 2.99  | 123.65      | 118.73   |
| 2   | D     | 603 | HEM  | CHD-C1D-ND  | 2.99  | 127.64      | 124.42   |
| 2   | A     | 603 | HEM  | C1B-NB-C4B  | 2.99  | 108.75      | 105.21   |
| 2   | D     | 603 | HEM  | C4D-ND-C1D  | 2.93  | 108.68      | 105.21   |
| 3   | D     | 605 | FAD  | O2-C2-N3    | -2.91 | 113.00      | 118.58   |
| 2   | A     | 602 | HEM  | O2D-CGD-O1D | 2.91  | 130.81      | 123.33   |
| 3   | A     | 605 | FAD  | O3B-C3B-C4B | 2.90  | 119.41      | 111.08   |
| 2   | A     | 602 | HEM  | CMA-C3A-C2A | 2.86  | 131.69      | 125.62   |
| 2   | A     | 604 | HEM  | C4C-C3C-C2C | 2.86  | 109.29      | 106.81   |
| 3   | D     | 605 | FAD  | O5B-PA-O1A  | -2.83 | 97.71       | 108.94   |
| 2   | A     | 604 | HEM  | CMA-C3A-C4A | -2.82 | 121.13      | 125.42   |
| 2   | A     | 603 | HEM  | CBD-CAD-C3D | -2.81 | 104.77      | 112.53   |
| 2   | A     | 604 | HEM  | CAD-C3D-C4D | -2.79 | 119.83      | 124.70   |
| 3   | A     | 605 | FAD  | O3B-C3B-C2B | 2.78  | 120.72      | 111.82   |
| 2   | A     | 601 | HEM  | C4B-C3B-C2B | 2.78  | 109.83      | 107.28   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | A     | 605 | FAD  | O2A-PA-O3P  | 2.76  | 114.74      | 107.27   |
| 2   | D     | 603 | HEM  | O1A-CGA-CBA | -2.76 | 114.33      | 123.09   |
| 2   | A     | 601 | HEM  | O1A-CGA-CBA | -2.75 | 114.36      | 123.09   |
| 2   | A     | 601 | HEM  | C2A-C1A-NA  | -2.74 | 107.12      | 110.15   |
| 2   | D     | 601 | HEM  | O1D-CGD-CBD | -2.70 | 114.52      | 123.09   |
| 2   | A     | 602 | HEM  | C3B-C2B-C1B | 2.70  | 108.44      | 106.41   |
| 2   | A     | 602 | HEM  | C1A-CHA-C4D | -2.69 | 119.91      | 126.25   |
| 3   | A     | 605 | FAD  | C9-C9A-N10  | 2.69  | 125.47      | 121.85   |
| 2   | A     | 602 | HEM  | C1C-CHC-C4B | -2.68 | 120.32      | 126.02   |
| 2   | A     | 601 | HEM  | CMA-C3A-C2A | 2.67  | 131.28      | 125.62   |
| 2   | A     | 602 | HEM  | O1A-CGA-CBA | -2.66 | 114.64      | 123.09   |
| 2   | A     | 602 | HEM  | CAC-C3C-C4C | -2.64 | 118.52      | 124.82   |
| 2   | A     | 604 | HEM  | C1A-CHA-C4D | -2.63 | 120.06      | 126.25   |
| 2   | A     | 601 | HEM  | C3B-C4B-NB  | -2.62 | 107.58      | 109.47   |
| 3   | A     | 605 | FAD  | O4-C4-C4X   | -2.60 | 119.66      | 126.53   |
| 2   | D     | 604 | HEM  | C1D-C2D-C3D | -2.58 | 104.27      | 106.98   |
| 3   | D     | 605 | FAD  | C2A-N1A-C6A | 2.57  | 122.94      | 118.73   |
| 2   | D     | 603 | HEM  | O2A-CGA-O1A | 2.56  | 129.92      | 123.33   |
| 2   | A     | 603 | HEM  | C1A-CHA-C4D | -2.54 | 120.28      | 126.25   |
| 2   | D     | 601 | HEM  | O1A-CGA-CBA | -2.53 | 115.07      | 123.09   |
| 2   | D     | 602 | HEM  | CMA-C3A-C4A | -2.51 | 121.59      | 125.42   |
| 2   | D     | 603 | HEM  | C3B-C4B-NB  | -2.50 | 107.67      | 109.47   |
| 2   | D     | 604 | HEM  | CMA-C3A-C4A | -2.49 | 121.63      | 125.42   |
| 2   | D     | 602 | HEM  | CHB-C4A-NA  | 2.48  | 128.37      | 123.86   |
| 2   | A     | 604 | HEM  | C1B-NB-C4B  | 2.48  | 108.14      | 105.21   |
| 2   | A     | 604 | HEM  | CAC-C3C-C4C | -2.48 | 118.90      | 124.82   |
| 3   | A     | 605 | FAD  | O5'-C5'-C4' | -2.46 | 102.79      | 109.36   |
| 2   | D     | 604 | HEM  | O2D-CGD-CBD | 2.45  | 121.75      | 114.00   |
| 3   | A     | 605 | FAD  | O4'-C4'-C3' | -2.44 | 103.53      | 109.25   |
| 2   | A     | 604 | HEM  | C4A-C3A-C2A | 2.44  | 109.61      | 106.82   |
| 2   | A     | 602 | HEM  | C4C-C3C-C2C | 2.43  | 108.92      | 106.81   |
| 2   | A     | 604 | HEM  | O2D-CGD-CBD | 2.43  | 121.67      | 114.00   |
| 3   | D     | 605 | FAD  | O2B-C2B-C3B | 2.37  | 119.43      | 111.82   |
| 2   | D     | 602 | HEM  | CMA-C3A-C2A | 2.37  | 130.65      | 125.62   |
| 2   | D     | 603 | HEM  | CHB-C1B-NB  | 2.37  | 127.30      | 124.37   |
| 2   | A     | 602 | HEM  | CMC-C2C-C1C | -2.35 | 120.60      | 124.73   |
| 3   | D     | 605 | FAD  | O4B-C1B-C2B | -2.34 | 101.62      | 106.62   |
| 2   | A     | 602 | HEM  | C4C-NC-C1C  | 2.33  | 109.62      | 105.82   |
| 3   | A     | 605 | FAD  | N10-C10-N1  | 2.32  | 125.35      | 118.51   |
| 3   | D     | 605 | FAD  | O2A-PA-O3P  | 2.31  | 113.52      | 107.27   |
| 2   | D     | 603 | HEM  | C4D-C3D-C2D | 2.28  | 110.21      | 106.89   |
| 2   | D     | 603 | HEM  | C1B-NB-C4B  | 2.26  | 107.88      | 105.21   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | D     | 605 | FAD  | C4-N3-C2    | -2.26 | 121.63      | 125.64   |
| 2   | A     | 601 | HEM  | CMA-C3A-C4A | -2.25 | 121.99      | 125.42   |
| 2   | A     | 601 | HEM  | C4A-CHB-C1B | -2.25 | 120.97      | 126.25   |
| 2   | A     | 604 | HEM  | O1D-CGD-CBD | -2.24 | 115.97      | 123.09   |
| 2   | D     | 602 | HEM  | CHA-C4D-ND  | 2.24  | 127.14      | 124.37   |
| 2   | D     | 604 | HEM  | CHD-C1D-ND  | 2.22  | 126.81      | 124.42   |
| 3   | A     | 605 | FAD  | O2'-C2'-C1' | -2.20 | 101.14      | 110.20   |
| 3   | A     | 605 | FAD  | O2'-C2'-C3' | -2.17 | 104.17      | 109.25   |
| 3   | D     | 605 | FAD  | C3B-C2B-C1B | 2.17  | 105.57      | 101.46   |
| 2   | D     | 603 | HEM  | CHA-C4D-ND  | 2.16  | 127.04      | 124.37   |
| 3   | A     | 605 | FAD  | N3A-C2A-N1A | -2.15 | 125.33      | 128.58   |
| 2   | A     | 603 | HEM  | C4C-C3C-C2C | 2.15  | 108.68      | 106.81   |
| 2   | A     | 603 | HEM  | CBC-CAC-C3C | -2.14 | 116.81      | 127.53   |
| 2   | A     | 601 | HEM  | CMB-C2B-C1B | -2.14 | 121.70      | 125.03   |
| 2   | D     | 603 | HEM  | C4A-CHB-C1B | -2.13 | 121.23      | 126.25   |
| 2   | A     | 601 | HEM  | CMC-C2C-C1C | -2.13 | 120.98      | 124.73   |
| 2   | D     | 604 | HEM  | CHA-C4D-ND  | 2.12  | 126.99      | 124.37   |
| 2   | A     | 602 | HEM  | CMB-C2B-C1B | -2.11 | 121.73      | 125.03   |
| 2   | A     | 603 | HEM  | CHC-C1C-NC  | 2.10  | 126.75      | 124.45   |
| 2   | D     | 602 | HEM  | C3D-C4D-ND  | -2.10 | 107.86      | 110.17   |
| 2   | A     | 603 | HEM  | C4B-C3B-C2B | 2.10  | 109.21      | 107.28   |
| 3   | D     | 605 | FAD  | C4X-C10-N1  | -2.09 | 119.46      | 124.59   |
| 2   | A     | 602 | HEM  | C2A-C1A-NA  | -2.08 | 107.85      | 110.15   |
| 2   | D     | 604 | HEM  | CAA-C2A-C3A | 2.08  | 131.73      | 127.07   |
| 2   | A     | 604 | HEM  | CBD-CAD-C3D | -2.06 | 106.84      | 112.53   |
| 2   | A     | 603 | HEM  | C3D-C4D-ND  | -2.05 | 107.92      | 110.17   |
| 2   | D     | 602 | HEM  | CHB-C1B-NB  | 2.05  | 126.90      | 124.37   |
| 2   | A     | 602 | HEM  | CMC-C2C-C3C | 2.03  | 133.34      | 128.43   |
| 2   | A     | 602 | HEM  | CBD-CAD-C3D | -2.03 | 106.92      | 112.53   |
| 2   | A     | 604 | HEM  | C2B-C1B-NB  | -2.03 | 107.51      | 109.84   |
| 2   | A     | 603 | HEM  | C2A-C1A-NA  | -2.01 | 107.93      | 110.15   |

There are no chirality outliers.

All (46) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 3   | D     | 605 | FAD  | N10-C1'-C2'-C3' |
| 2   | D     | 602 | HEM  | C2A-CAA-CBA-CGA |
| 3   | A     | 605 | FAD  | O2'-C2'-C3'-C4' |
| 3   | A     | 605 | FAD  | PA-O3P-P-O5'    |
| 3   | D     | 605 | FAD  | N10-C1'-C2'-O2' |
| 2   | A     | 602 | HEM  | C3D-CAD-CBD-CGD |

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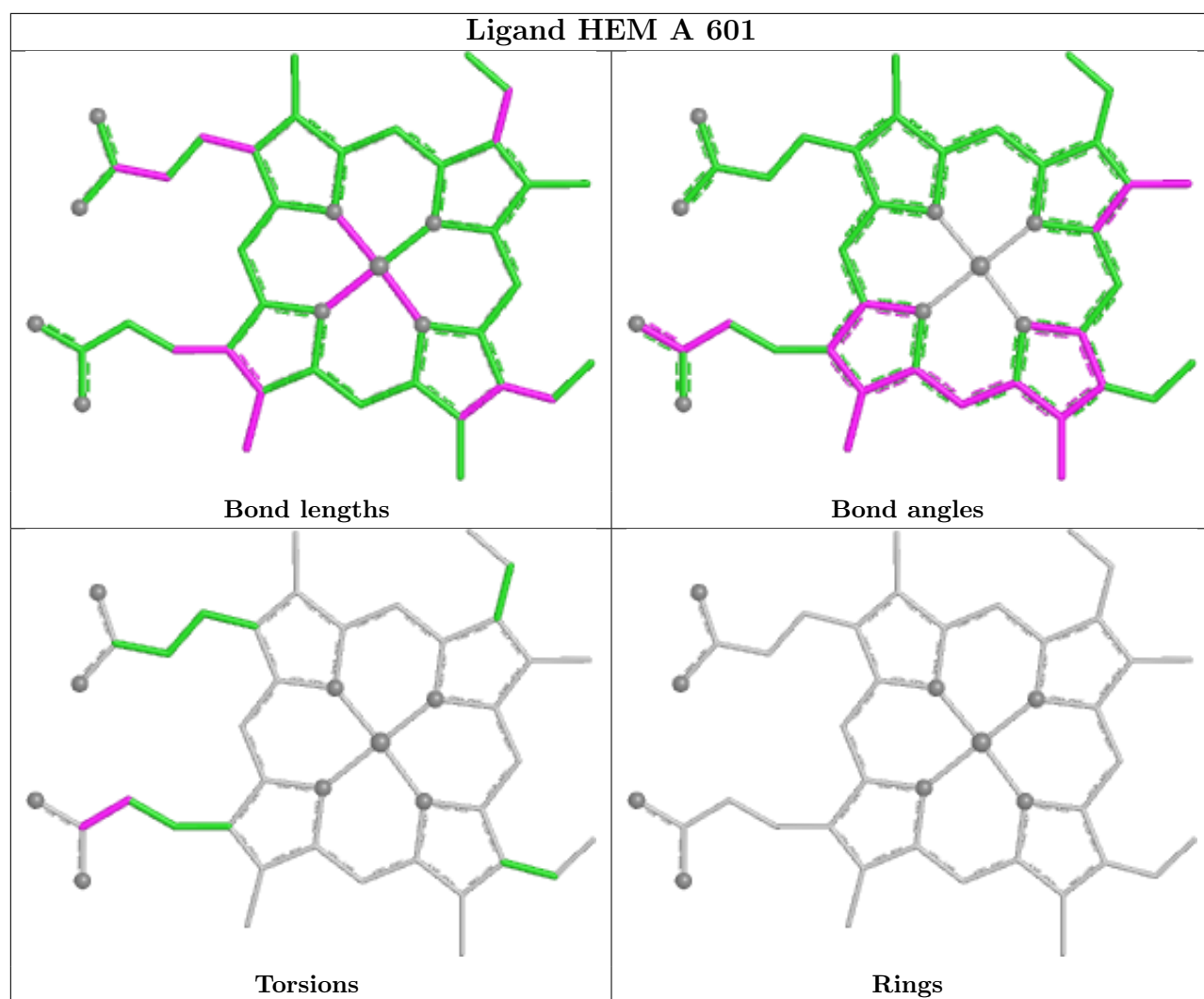
| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 3   | A     | 605 | FAD  | C2'-C1'-N10-C10 |
| 3   | D     | 605 | FAD  | C5'-O5'-P-O3P   |
| 2   | D     | 602 | HEM  | CAD-CBD-CGD-O2D |
| 2   | D     | 602 | HEM  | CAD-CBD-CGD-O1D |
| 2   | A     | 601 | HEM  | CAA-CBA-CGA-O1A |
| 2   | D     | 601 | HEM  | CAA-CBA-CGA-O1A |
| 2   | D     | 603 | HEM  | CAA-CBA-CGA-O2A |
| 2   | A     | 602 | HEM  | CAD-CBD-CGD-O1D |
| 2   | D     | 603 | HEM  | CAA-CBA-CGA-O1A |
| 2   | D     | 601 | HEM  | CAA-CBA-CGA-O2A |
| 2   | D     | 602 | HEM  | CAA-CBA-CGA-O2A |
| 2   | A     | 603 | HEM  | C3D-CAD-CBD-CGD |
| 2   | D     | 604 | HEM  | C3D-CAD-CBD-CGD |
| 2   | A     | 602 | HEM  | CAD-CBD-CGD-O2D |
| 2   | D     | 602 | HEM  | CAA-CBA-CGA-O1A |
| 2   | D     | 604 | HEM  | C3A-C2A-CAA-CBA |
| 2   | D     | 601 | HEM  | CAD-CBD-CGD-O2D |
| 2   | A     | 601 | HEM  | CAA-CBA-CGA-O2A |
| 2   | D     | 603 | HEM  | CAD-CBD-CGD-O2D |
| 2   | D     | 604 | HEM  | C1A-C2A-CAA-CBA |
| 2   | A     | 602 | HEM  | CAA-CBA-CGA-O1A |
| 2   | A     | 602 | HEM  | CAA-CBA-CGA-O2A |
| 2   | A     | 603 | HEM  | CAD-CBD-CGD-O2D |
| 2   | D     | 603 | HEM  | CAD-CBD-CGD-O1D |
| 2   | A     | 603 | HEM  | C4B-C3B-CAB-CBB |
| 2   | D     | 601 | HEM  | CAD-CBD-CGD-O1D |
| 2   | A     | 604 | HEM  | CAA-CBA-CGA-O1A |
| 3   | A     | 605 | FAD  | O4B-C4B-C5B-O5B |
| 2   | A     | 604 | HEM  | CAD-CBD-CGD-O2D |
| 2   | A     | 604 | HEM  | C3D-CAD-CBD-CGD |
| 2   | A     | 604 | HEM  | CAA-CBA-CGA-O2A |
| 2   | A     | 602 | HEM  | C2A-CAA-CBA-CGA |
| 3   | D     | 605 | FAD  | C2B-C1B-N9A-C8A |
| 3   | A     | 605 | FAD  | N10-C1'-C2'-C3' |
| 3   | D     | 605 | FAD  | O4B-C4B-C5B-O5B |
| 2   | A     | 603 | HEM  | CAD-CBD-CGD-O1D |
| 2   | A     | 604 | HEM  | CAD-CBD-CGD-O1D |
| 3   | A     | 605 | FAD  | C2B-C1B-N9A-C8A |
| 2   | D     | 604 | HEM  | CAA-CBA-CGA-O1A |
| 3   | D     | 605 | FAD  | P-O3P-PA-O2A    |

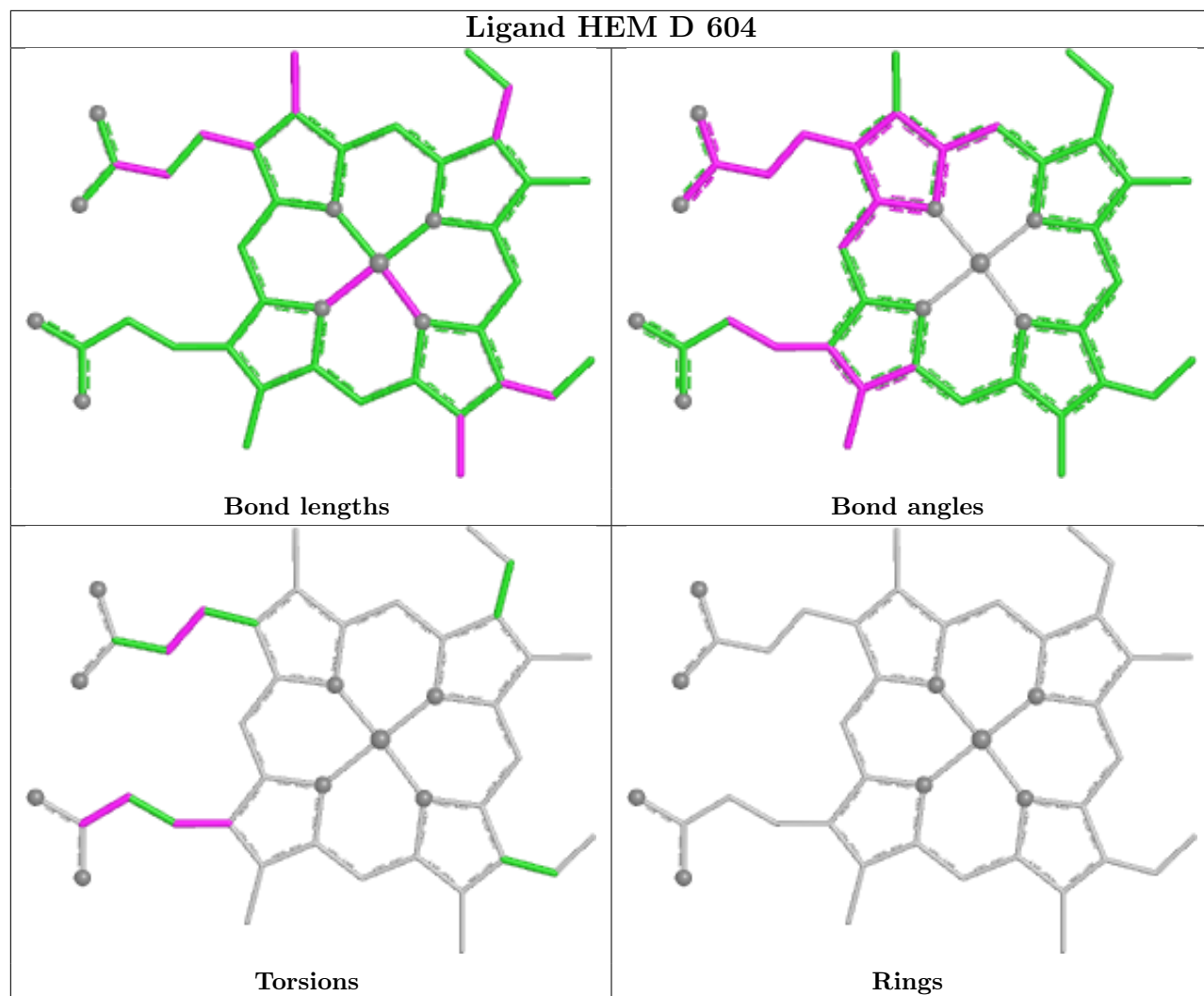
There are no ring outliers.

9 monomers are involved in 77 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2   | A     | 601 | HEM  | 10      | 0            |
| 2   | D     | 604 | HEM  | 9       | 0            |
| 2   | A     | 603 | HEM  | 8       | 0            |
| 2   | D     | 601 | HEM  | 10      | 0            |
| 2   | D     | 603 | HEM  | 9       | 0            |
| 3   | A     | 605 | FAD  | 1       | 0            |
| 2   | A     | 604 | HEM  | 12      | 0            |
| 2   | A     | 602 | HEM  | 12      | 0            |
| 2   | D     | 602 | HEM  | 12      | 0            |

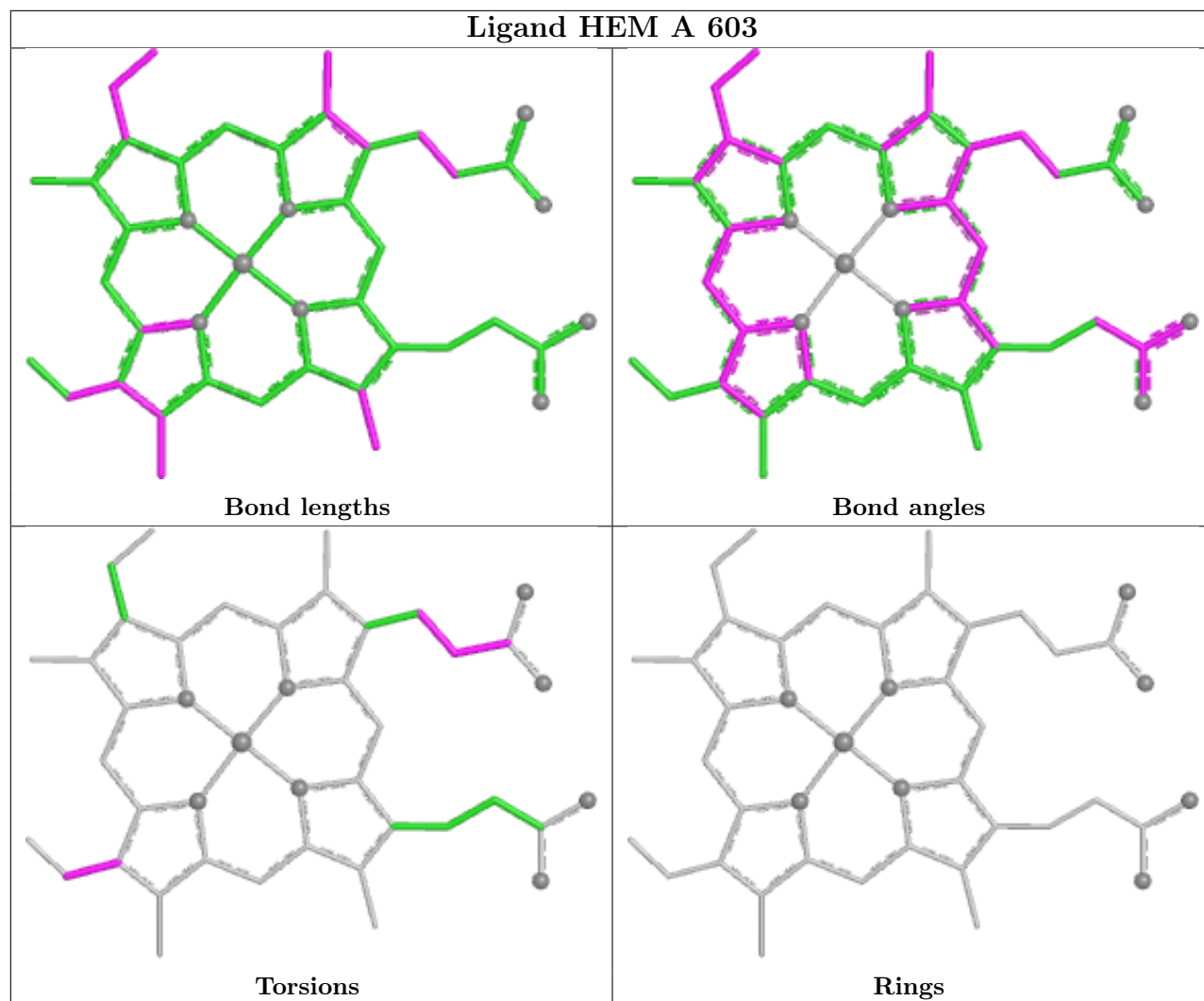
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

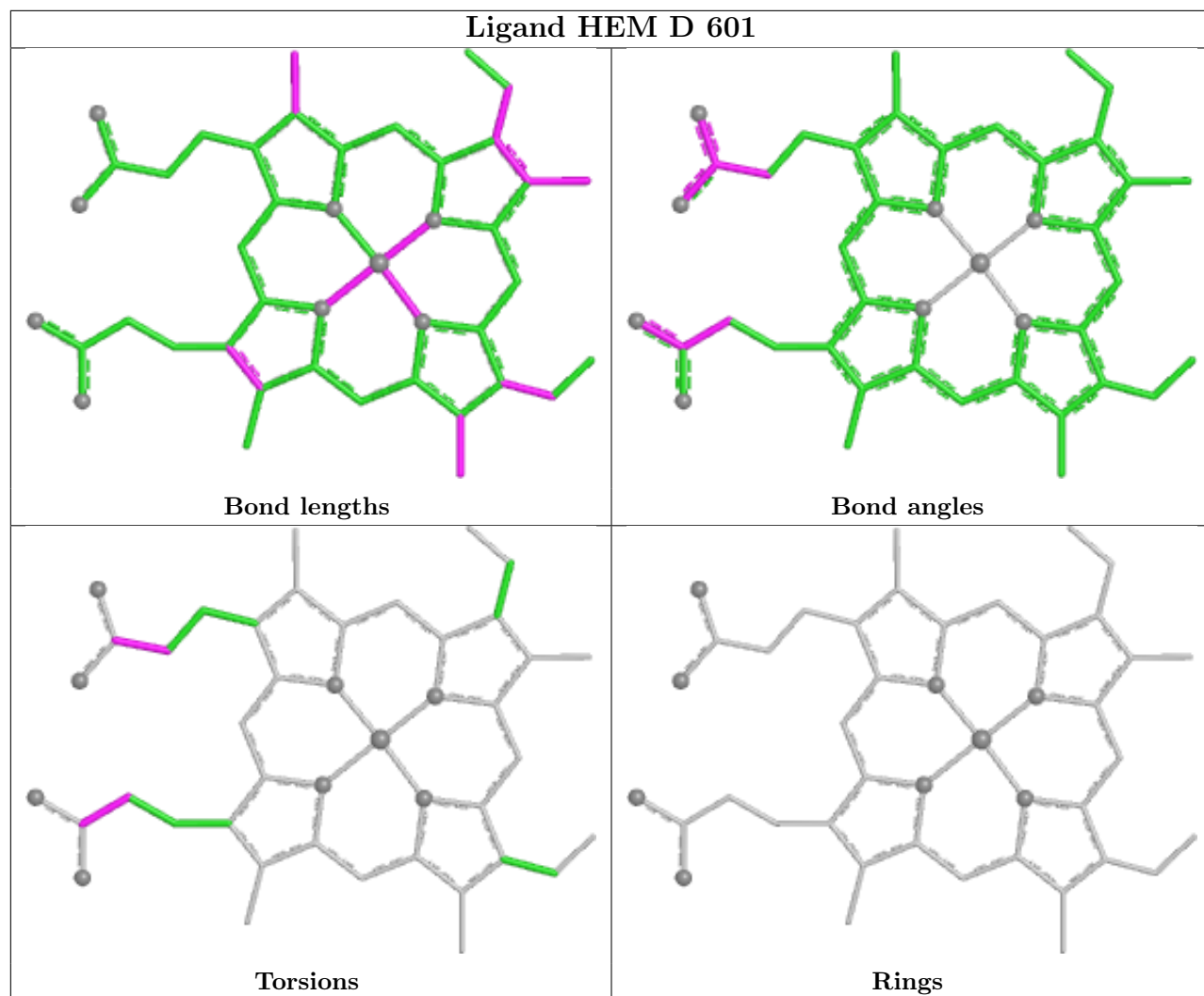


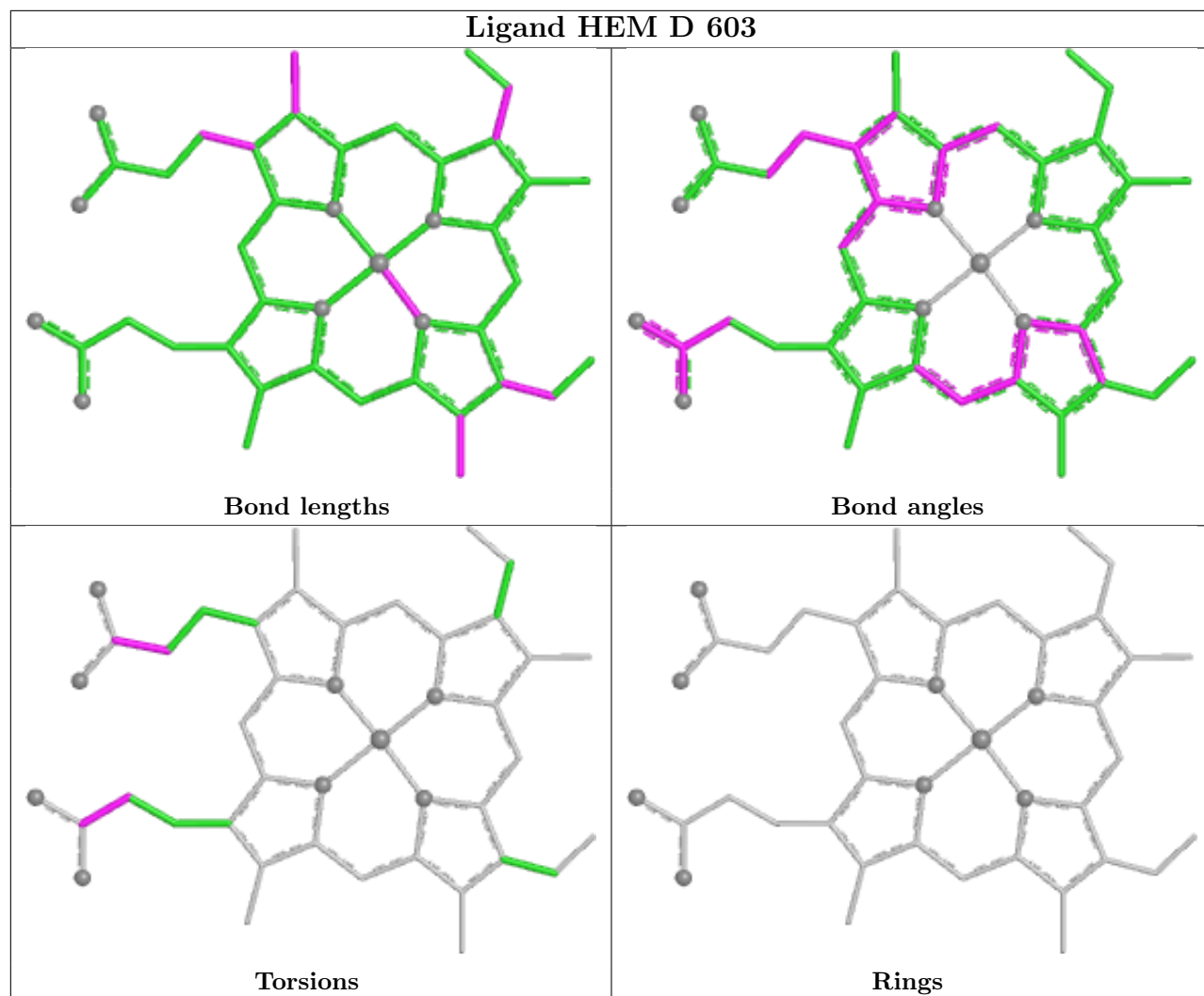


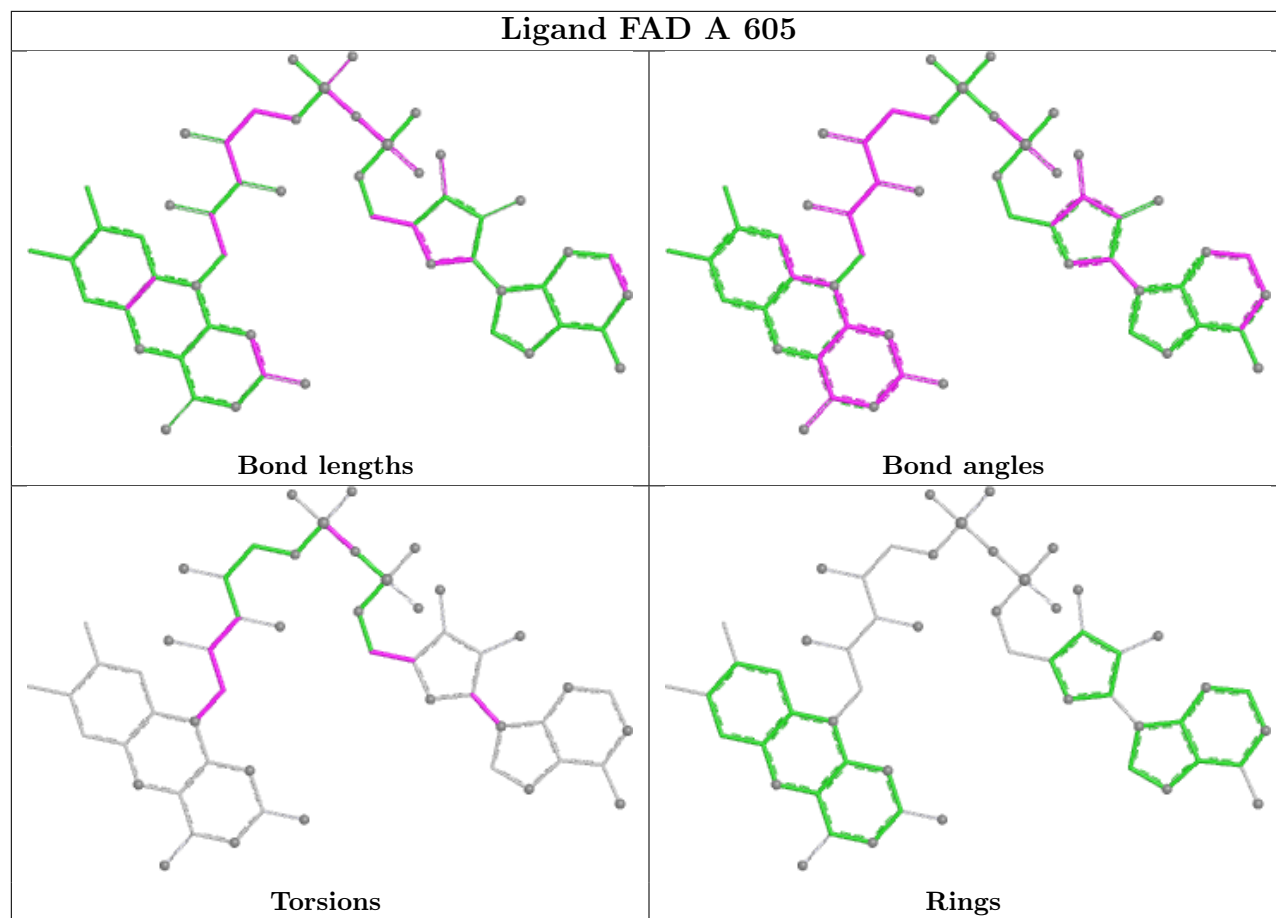


## Ligand HEM A 603

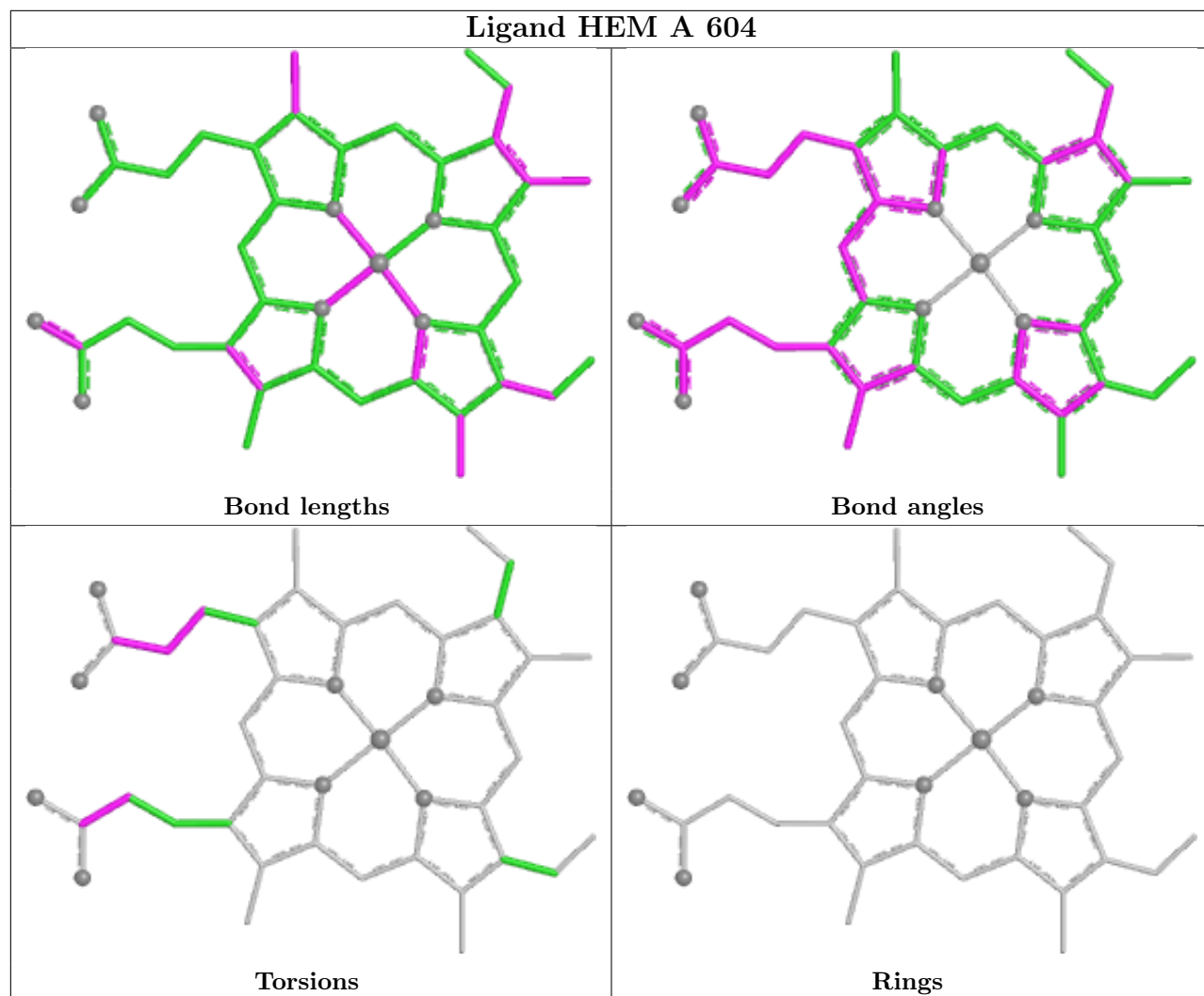


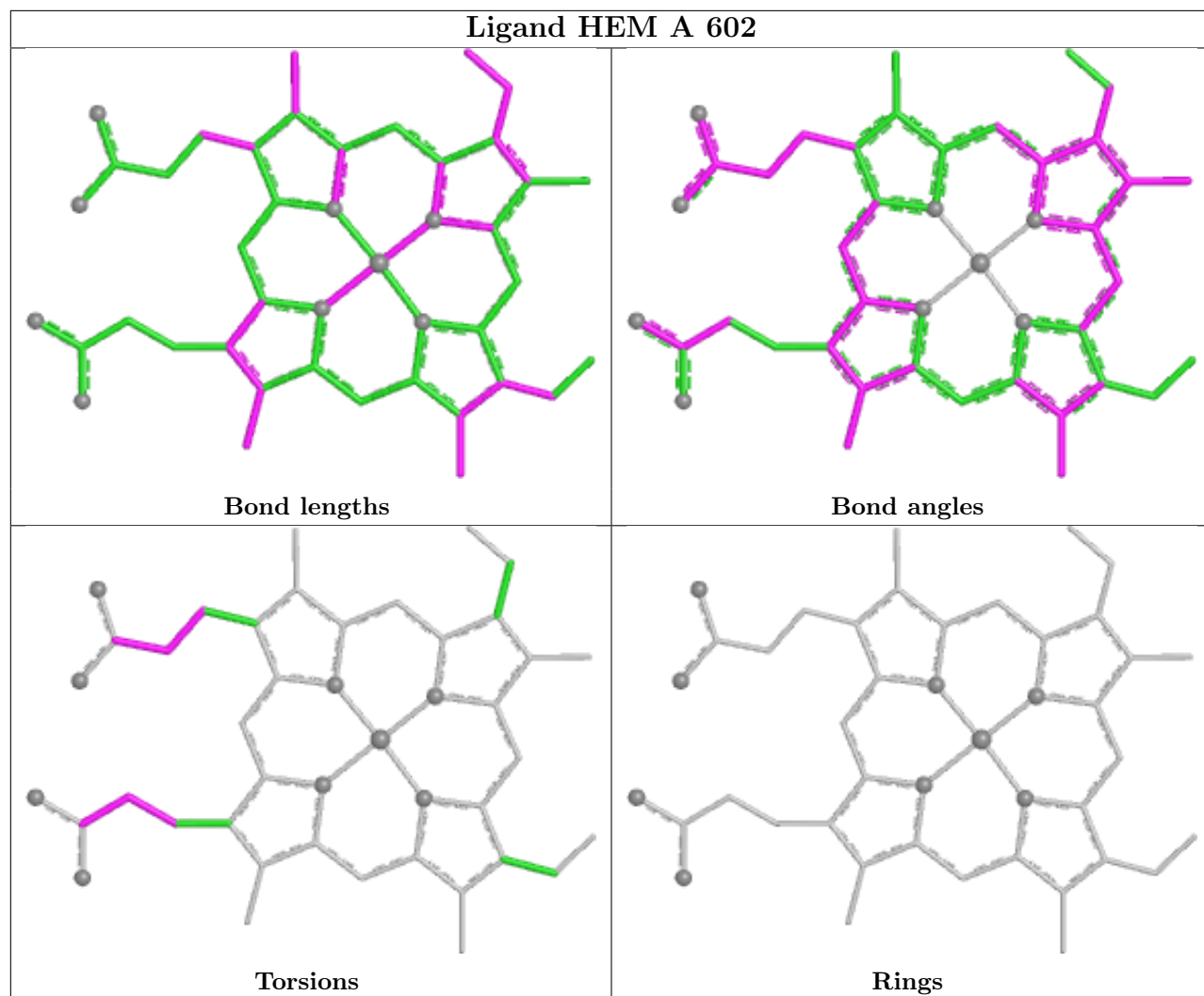


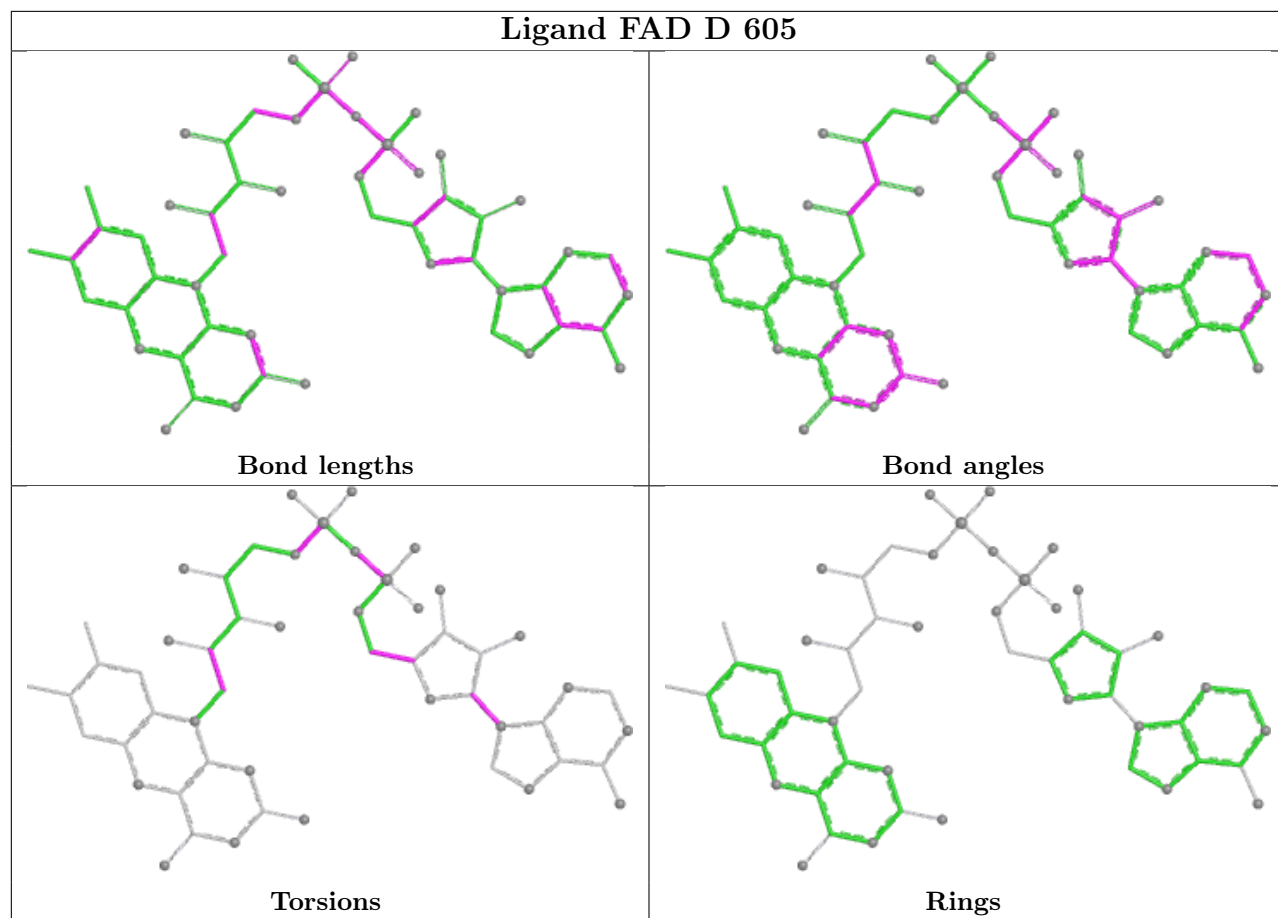


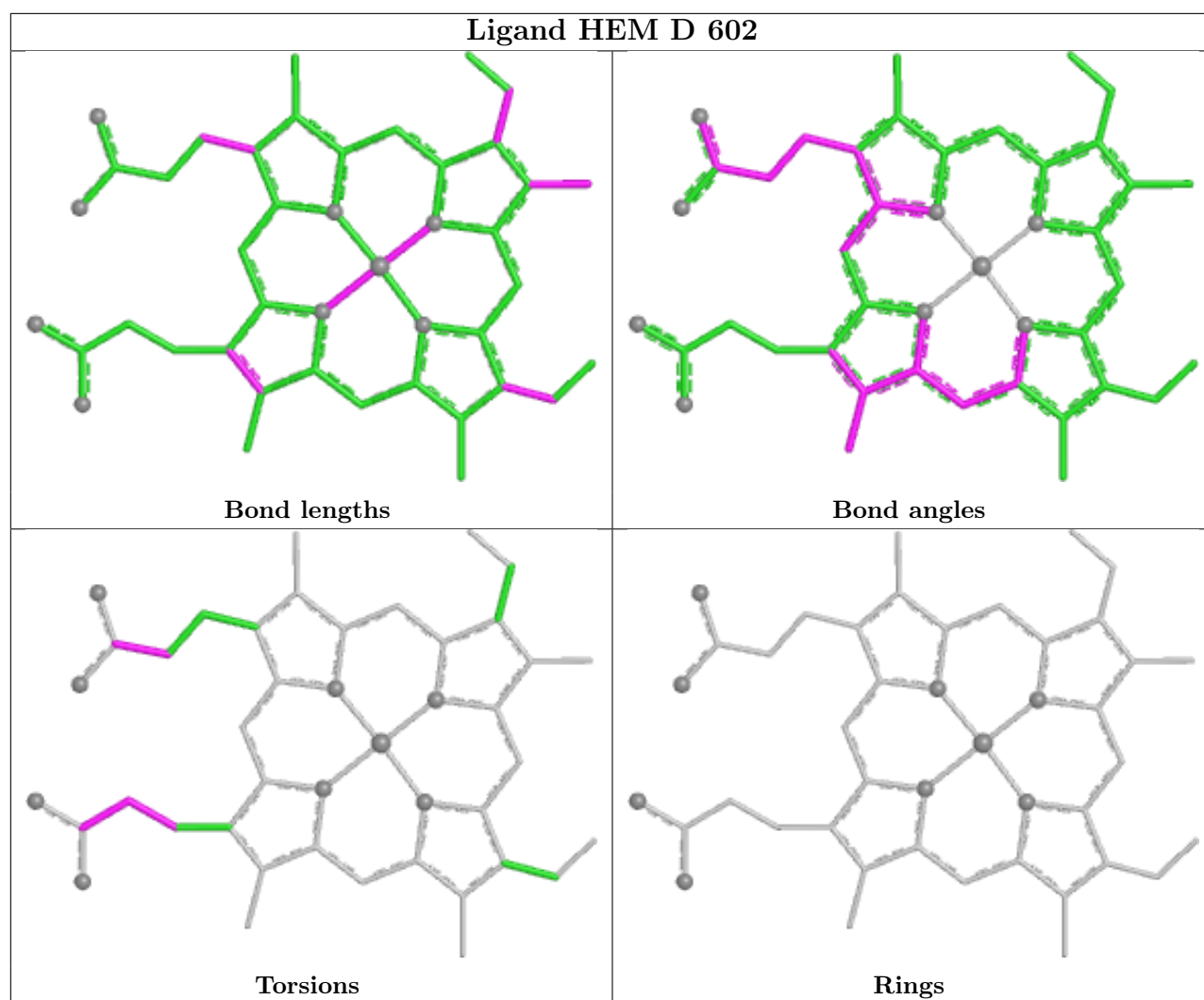


## Ligand HEM A 604









## 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.