



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 11:45 AM EDT

PDB ID : 2E76 / pdb\_00002e76  
Title : Crystal Structure of the Cytochrome b6f Complex with tridecyl-stigmatellin (TDS) from *M.laminosus*  
Authors : Cramer, W.A.; Yamashita, E.; Zhang, H.  
Deposited on : 2007-01-05  
Resolution : 3.41 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

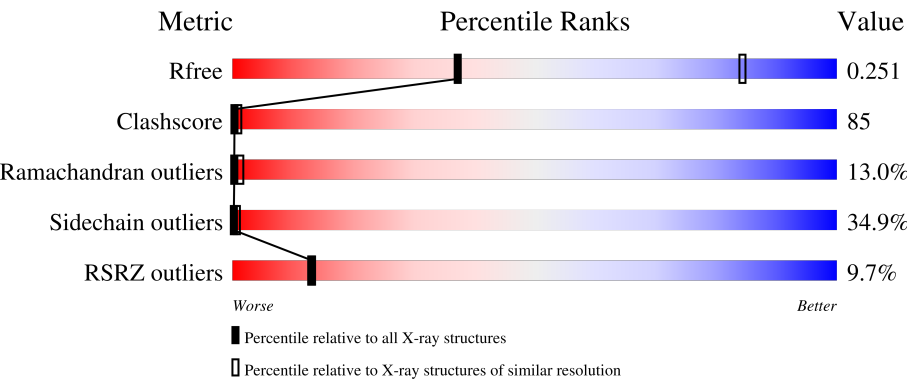
|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                     |
| Xtriage (Phenix)               | : | 2.0                                                              |
| EDS                            | : | 3.0                                                              |
| Buster-report                  | : | wwPDB partial adaption of 1.1.7 (2018)                           |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| CCP4                           | : | 9.0.015 (Gargrove)                                               |
| Density-Fitness                | : | 1.0.12                                                           |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.50                                                             |

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.41 Å.

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



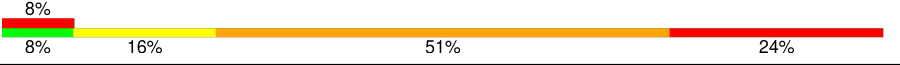
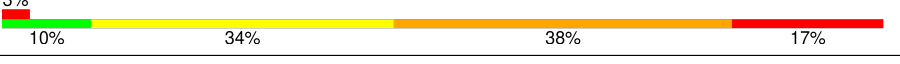
| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| R <sub>free</sub>     | 180053                      | 1210 (3.48-3.36)                                      |
| Clashscore            | 190562                      | 1234 (3.48-3.36)                                      |
| Ramachandran outliers | 187476                      | 1222 (3.48-3.36)                                      |
| Sidechain outliers    | 187428                      | 1222 (3.48-3.36)                                      |
| RSRZ outliers         | 180081                      | 1210 (3.48-3.36)                                      |

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

| Mol | Chain | Length | Quality of chain                        |
|-----|-------|--------|-----------------------------------------|
| 1   | A     | 215    | <div><div>16%37%34%13%</div></div>      |
| 2   | B     | 160    | <div><div>11%32%39%18%</div></div>      |
| 3   | C     | 289    | <div><div>11%14%39%32%15%</div></div>   |
| 4   | D     | 179    | <div><div>25%13%37%30%13%6%</div></div> |
| 5   | E     | 32     | <div><div>6%9%34%34%22%</div></div>     |

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| Mol | Chain | Length | Quality of chain                                                                   |
|-----|-------|--------|------------------------------------------------------------------------------------|
| 6   | F     | 35     |  |
| 7   | G     | 37     |  |
| 8   | H     | 29     |  |

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

| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 10  | HEM  | A     | 302  | -         | -        | X       | -                |
| 11  | HEC  | A     | 303  | X         | -        | X       | -                |
| 11  | HEC  | C     | 301  | X         | -        | X       | -                |
| 12  | OPC  | B     | 1001 | -         | X        | -       | -                |
| 13  | UMQ  | A     | 1101 | X         | -        | -       | -                |
| 13  | UMQ  | A     | 1102 | X         | -        | -       | -                |
| 13  | UMQ  | A     | 1103 | X         | -        | -       | -                |
| 13  | UMQ  | A     | 1104 | X         | -        | -       | -                |
| 14  | CLA  | B     | 201  | X         | -        | -       | -                |
| 15  | TDS  | B     | 1201 | -         | X        | -       | -                |
| 15  | TDS  | B     | 1202 | -         | X        | -       | -                |
| 17  | SQD  | D     | 201  | X         | X        | -       | -                |

## 2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 8112 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 Cytochrome b6.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 215      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1711  | 1140 | 272 | 288 | 11 |         |         |       |

- Molecule 2 is a protein called Cytochrome b6-f complex subunit 4.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2   | B     | 160      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1249  | 841 | 193 | 209 | 6 |         |         |       |

- Molecule 3 is a protein called Apocytochrome f.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3   | C     | 288      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2216  | 1415 | 369 | 424 | 8 |         |         |       |

- Molecule 4 is a protein called Cytochrome b6-f complex iron-sulfur subunit.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 4   | D     | 168      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1288  | 823 | 221 | 237 | 7 |         |         |       |

- Molecule 5 is a protein called Cytochrome b6-f complex subunit 6.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 5   | E     | 32       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 248   | 179 | 34 | 34 | 1 |         |         |       |

- Molecule 6 is a protein called Cytochrome b6-f complex subunit 7.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 6   | F     | 32       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 242   | 165 | 35 | 40 | 2 |         |         |       |

- Molecule 7 is a protein called Cytochrome b6-f complex subunit 5.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 7   | G     | 37       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 283   | 188 | 44 | 50 | 1 |         |         |       |

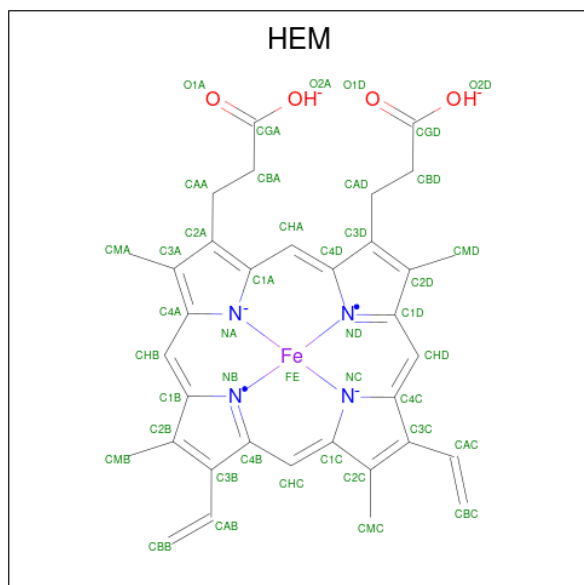
- Molecule 8 is a protein called Cytochrome b6-f complex subunit 8.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 8   | H     | 29       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 230   | 156 | 36 | 36 | 2 |         |         |       |

- Molecule 9 is CADMIUM ION (CCD ID: CD) (formula: Cd).

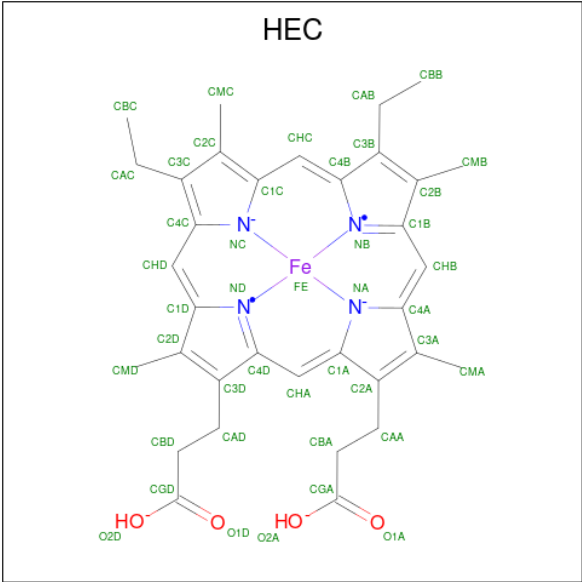
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 9   | A     | 1        | Total | Cd | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 10 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>).



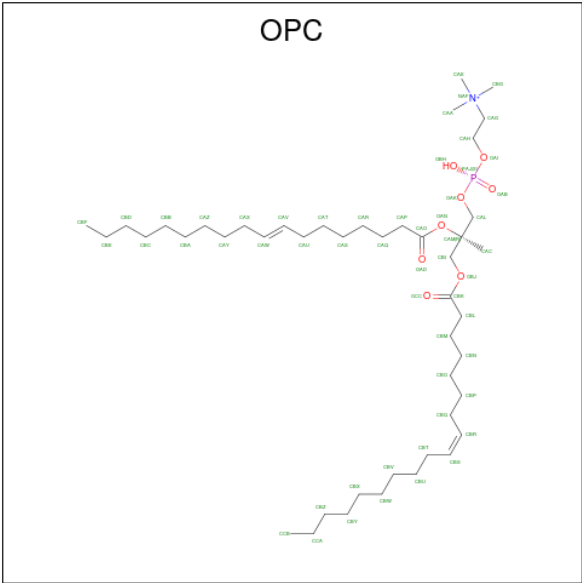
| Mol | Chain | Residues | Atoms |    |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 10  | A     | 1        | Total | C  | Fe | N | O | 0       | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |         |
| 10  | A     | 1        | Total | C  | Fe | N | O | 0       | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |         |

- Molecule 11 is HEME C (CCD ID: HEC) (formula: C<sub>34</sub>H<sub>36</sub>FeN<sub>4</sub>O<sub>4</sub>).



| Mol | Chain | Residues | Atoms |    |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 11  | A     | 1        | Total | C  | Fe | N | O | 0       | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |         |
| 11  | C     | 1        | Total | C  | Fe | N | O | 0       | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |         |

- Molecule 12 is (7R,17E)-4-HYDROXY-N,N,N,7-TETRAMETHYL-7-[(8E)-OCTADEC-8-ENOYLOXY]-10-OXO-3,5,9-TRIOXA-4-PHOSPHAHEPTACOS-17-EN-1-AMINIUM 4-OXIDE (CCD ID: OPC) (formula: C<sub>45</sub>H<sub>87</sub>NO<sub>8</sub>P).



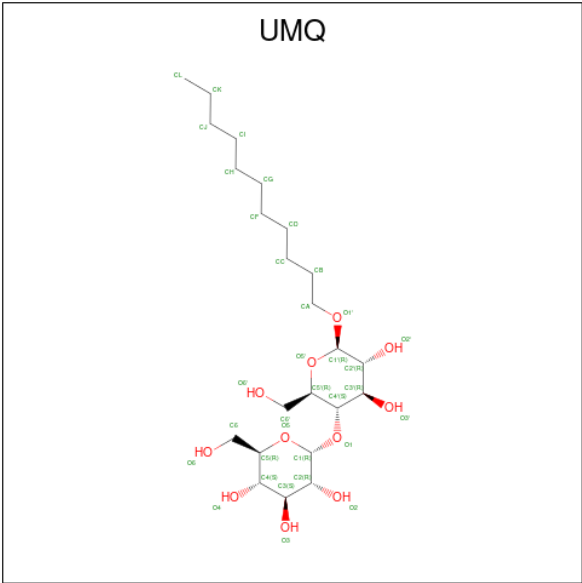
| Mol | Chain | Residues | Atoms |    |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|---------|
| 12  | A     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 54    | 44 | 1 | 8 | 1 |         |         |

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| Mol | Chain | Residues | Atoms |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 12  | B     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 54    | 44 | 1 | 8 |         |         |

- Molecule 13 is UNDECYL-MALTOSIDE (CCD ID: UMQ) (formula: C<sub>23</sub>H<sub>44</sub>O<sub>11</sub>).



| Mol | Chain | Residues | Atoms |    |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 13  | A     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 34    | 23 | 11 |         |         |
| 13  | A     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 34    | 23 | 11 |         |         |
| 13  | A     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 34    | 23 | 11 |         |         |
| 13  | A     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 34    | 23 | 11 |         |         |

- Molecule 14 is CHLOROPHYLL A (CCD ID: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).

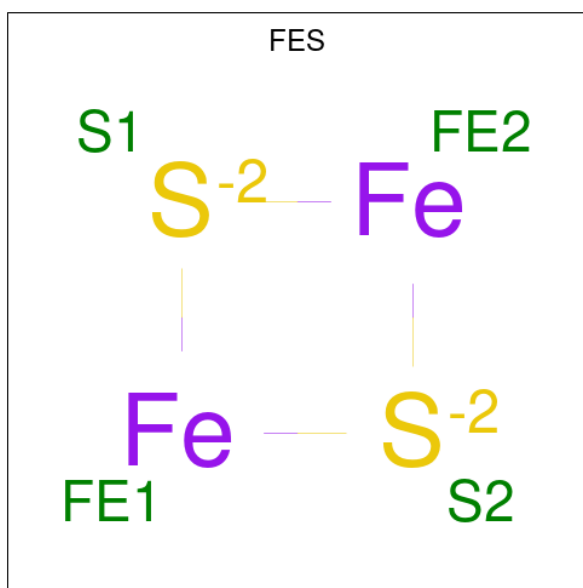


- Molecule 15 is 8-HYDROXY-5,7-DIMETHOXY-3-METHYL-2-TRIDECYL-4H-CHROME N-4-ONE (CCD ID: TDS) (formula:  $C_{25}H_{38}O_5$ ).



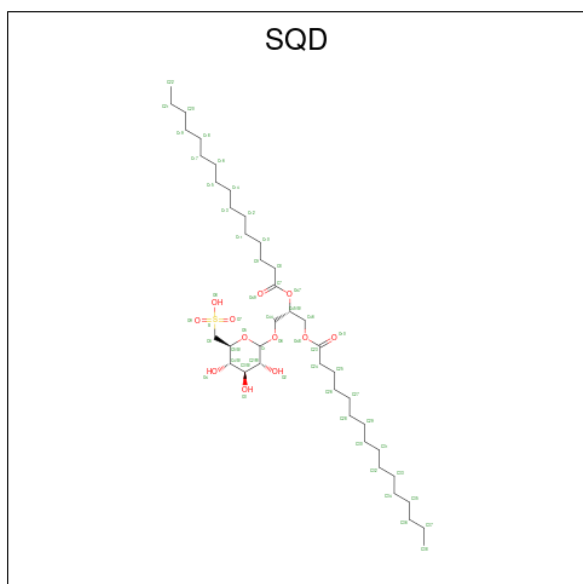


- Molecule 16 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula:  $\text{Fe}_2\text{S}_2$ ).



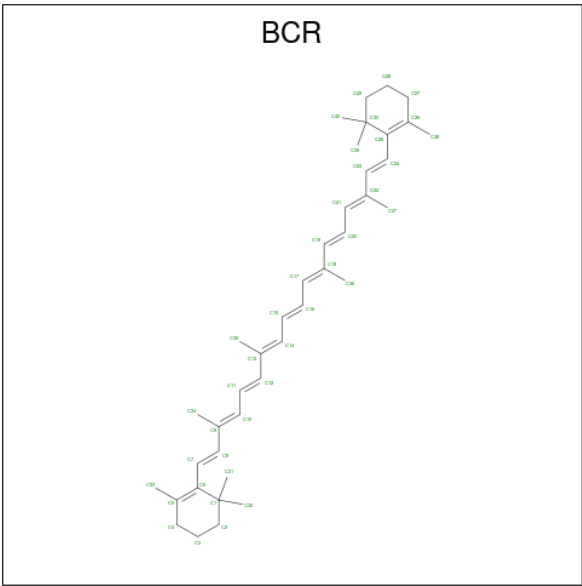
| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 16  | D     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 4     | 2  | 2 |         |         |

- Molecule 17 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula:  $\text{C}_{41}\text{H}_{78}\text{O}_{12}\text{S}$ ).



| Mol | Chain | Residues | Atoms |    |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 17  | D     | 1        | Total | C  | O  | S | 0       | 0       |
|     |       |          | 54    | 41 | 12 | 1 |         |         |

- Molecule 18 is BETA-CAROTENE (CCD ID: BCR) (formula: C<sub>40</sub>H<sub>56</sub>).



| Mol | Chain | Residues | Atoms            | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 18  | G     | 1        | Total C<br>40 40 | 0       | 0       |

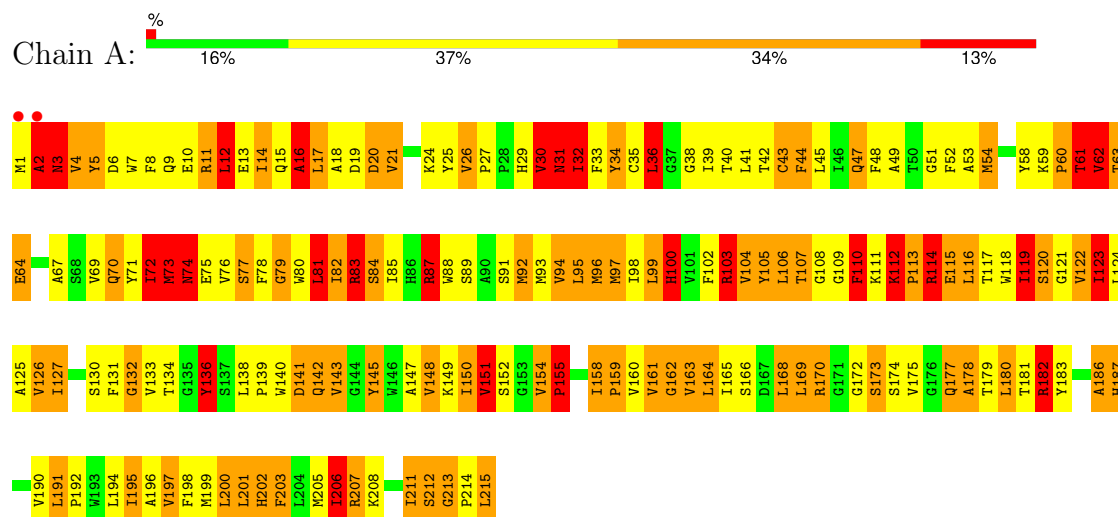
- Molecule 19 is water.

| Mol | Chain | Residues | Atoms          | ZeroOcc | AltConf |
|-----|-------|----------|----------------|---------|---------|
| 19  | A     | 2        | Total O<br>2 2 | 0       | 0       |
| 19  | B     | 2        | Total O<br>2 2 | 0       | 0       |
| 19  | C     | 1        | Total O<br>1 1 | 0       | 0       |

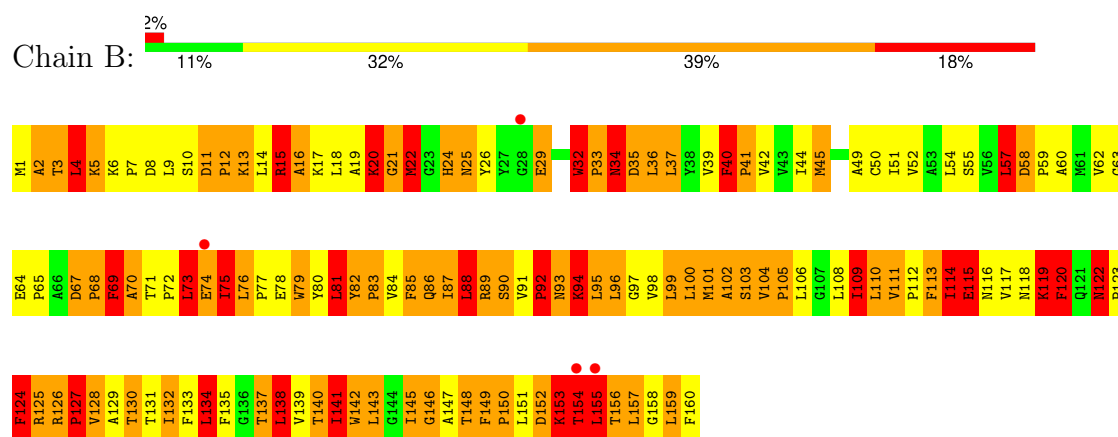
### 3 Residue-property plots

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

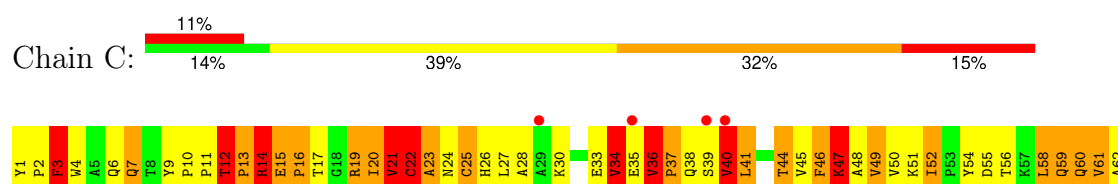
#### • Molecule 1: Cytochrome b6

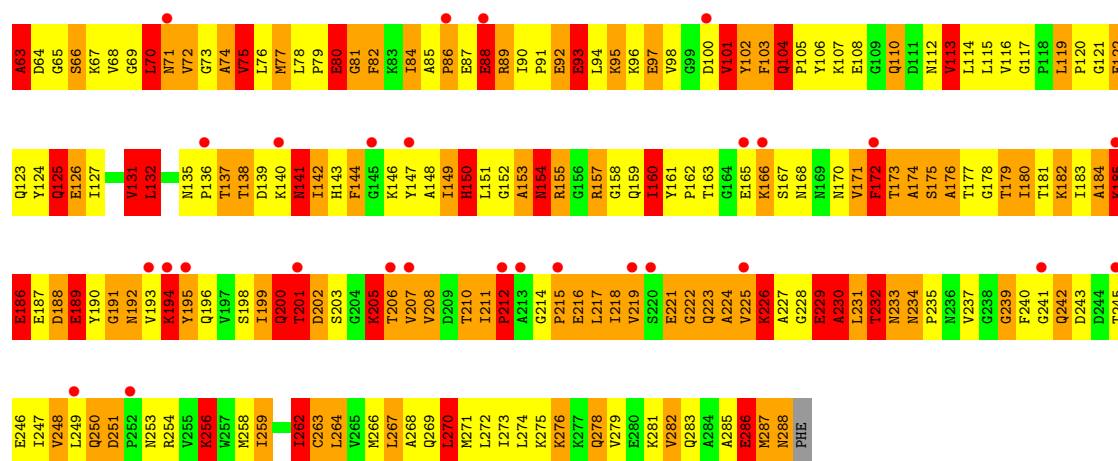


#### • Molecule 2: Cytochrome b6-f complex subunit 4

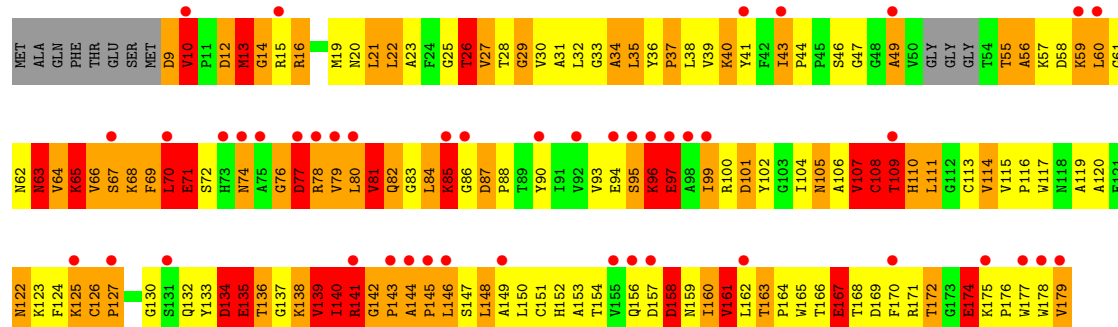


#### • Molecule 3: Apocytochrome f





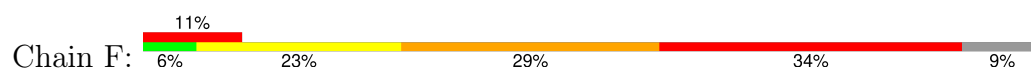
• Molecule 4: Cytochrome b6-f complex iron-sulfur subunit



• Molecule 5: Cytochrome b6-f complex subunit 6



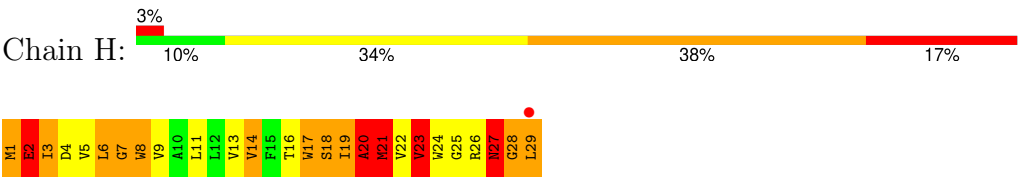
• Molecule 6: Cytochrome b6-f complex subunit 7



• Molecule 7: Cytochrome b6-f complex subunit 5



● Molecule 8: Cytochrome b6-f complex subunit 8



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 61 2 2                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 157.23Å 157.23Å 363.30Å<br>90.00° 90.00° 120.00°            | Depositor        |
| Resolution (Å)                                                          | 41.27 – 3.41<br>41.27 – 3.41                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.7 (41.27-3.41)<br>99.7 (41.27-3.41)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.12                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 4.84 (at 3.40Å)                                             | Xtriage          |
| Refinement program                                                      | REFMAC 5.2.0019                                             | Depositor        |
| R, $R_{free}$                                                           | 0.185 , 0.256<br>0.182 , 0.251                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 1852 reflections (4.99%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 92.6                                                        | Xtriage          |
| Anisotropy                                                              | 0.186                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.29 , 95.2                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.91                                                        | EDS              |
| Total number of atoms                                                   | 8112                                                        | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 62.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.12% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TDS, SQD, OPC, HEC, FES, CLA, CD, BCR, HEM, UMQ

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     | 2.17         | 63/1763 (3.6%)  | 2.44        | 123/2405 (5.1%)  |
| 2   | B     | 2.20         | 39/1288 (3.0%)  | 2.58        | 110/1765 (6.2%)  |
| 3   | C     | 1.81         | 45/2264 (2.0%)  | 2.10        | 111/3082 (3.6%)  |
| 4   | D     | 1.72         | 18/1320 (1.4%)  | 2.06        | 58/1798 (3.2%)   |
| 5   | E     | 2.21         | 10/253 (4.0%)   | 2.58        | 19/340 (5.6%)    |
| 6   | F     | 2.39         | 15/246 (6.1%)   | 2.33        | 13/331 (3.9%)    |
| 7   | G     | 2.38         | 16/289 (5.5%)   | 2.32        | 17/391 (4.3%)    |
| 8   | H     | 2.23         | 12/236 (5.1%)   | 2.13        | 8/323 (2.5%)     |
| All | All   | 2.02         | 218/7659 (2.8%) | 2.30        | 459/10435 (4.4%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 4                   |
| 2   | B     | 0                   | 3                   |
| 3   | C     | 0                   | 7                   |
| 4   | D     | 0                   | 5                   |
| 5   | E     | 0                   | 1                   |
| 6   | F     | 0                   | 3                   |
| 7   | G     | 0                   | 2                   |
| 8   | H     | 0                   | 2                   |
| All | All   | 0                   | 27                  |

All (218) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 1   | A     | 63  | THR  | CA-CB | -13.55 | 1.31        | 1.53     |
| 1   | A     | 67  | ALA  | CA-CB | -13.26 | 1.31        | 1.53     |

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| Mol | Chain | Res | Type | Atoms  | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 4   | D     | 44  | PRO  | CA-C   | -11.17 | 1.45        | 1.51     |
| 2   | B     | 141 | ILE  | CA-CB  | -10.98 | 1.39        | 1.54     |
| 1   | A     | 186 | ALA  | CA-CB  | -10.94 | 1.36        | 1.53     |
| 3   | C     | 40  | VAL  | CA-CB  | -10.13 | 1.40        | 1.54     |
| 4   | D     | 107 | VAL  | CA-CB  | -10.05 | 1.41        | 1.54     |
| 1   | A     | 165 | ILE  | CA-CB  | -9.76  | 1.43        | 1.54     |
| 7   | G     | 3   | GLU  | CG-CD  | 9.71   | 1.76        | 1.52     |
| 1   | A     | 85  | ILE  | CA-CB  | -9.34  | 1.44        | 1.54     |
| 3   | C     | 256 | LYS  | CG-CD  | 9.20   | 1.80        | 1.52     |
| 1   | A     | 62  | VAL  | CA-CB  | -9.11  | 1.41        | 1.54     |
| 6   | F     | 2   | THR  | CA-CB  | 9.09   | 1.68        | 1.53     |
| 6   | F     | 29  | ILE  | CA-CB  | 9.03   | 1.66        | 1.54     |
| 2   | B     | 117 | VAL  | CA-CB  | 9.00   | 1.66        | 1.54     |
| 3   | C     | 148 | ALA  | CA-CB  | -8.97  | 1.38        | 1.53     |
| 3   | C     | 207 | VAL  | CA-CB  | 8.96   | 1.63        | 1.54     |
| 4   | D     | 10  | VAL  | CA-CB  | 8.88   | 1.63        | 1.53     |
| 1   | A     | 62  | VAL  | CA-C   | -8.55  | 1.40        | 1.52     |
| 2   | B     | 49  | ALA  | CA-CB  | -8.53  | 1.39        | 1.53     |
| 2   | B     | 15  | ARG  | CZ-NH1 | 8.49   | 1.44        | 1.32     |
| 3   | C     | 49  | VAL  | CA-CB  | -8.47  | 1.44        | 1.53     |
| 3   | C     | 256 | LYS  | CE-NZ  | 8.27   | 1.74        | 1.49     |
| 1   | A     | 72  | ILE  | CA-CB  | -8.26  | 1.45        | 1.54     |
| 2   | B     | 119 | LYS  | N-CA   | -8.24  | 1.37        | 1.46     |
| 4   | D     | 141 | ARG  | N-CA   | 8.17   | 1.57        | 1.45     |
| 2   | B     | 150 | PRO  | CA-C   | -8.16  | 1.44        | 1.52     |
| 1   | A     | 160 | VAL  | CA-CB  | 8.06   | 1.64        | 1.54     |
| 3   | C     | 16  | PRO  | C-O    | 8.05   | 1.34        | 1.24     |
| 4   | D     | 27  | VAL  | CA-CB  | -8.04  | 1.44        | 1.54     |
| 3   | C     | 84  | ILE  | CA-CB  | -7.93  | 1.45        | 1.54     |
| 6   | F     | 2   | THR  | N-CA   | 7.92   | 1.55        | 1.46     |
| 1   | A     | 175 | VAL  | CA-CB  | -7.85  | 1.46        | 1.54     |
| 6   | F     | 25  | LEU  | CG-CD1 | 7.52   | 1.77        | 1.52     |
| 7   | G     | 3   | GLU  | CA-CB  | 7.46   | 1.63        | 1.53     |
| 7   | G     | 24  | ALA  | CA-CB  | 7.43   | 1.65        | 1.53     |
| 1   | A     | 113 | PRO  | N-CA   | 7.38   | 1.56        | 1.47     |
| 1   | A     | 114 | ARG  | CA-C   | 7.37   | 1.62        | 1.52     |
| 3   | C     | 286 | GLU  | N-CA   | 7.33   | 1.55        | 1.46     |
| 2   | B     | 120 | PHE  | CA-C   | -7.32  | 1.43        | 1.52     |
| 8   | H     | 26  | ARG  | CZ-NH1 | 7.26   | 1.43        | 1.32     |
| 6   | F     | 20  | TRP  | C-O    | 7.26   | 1.33        | 1.24     |
| 3   | C     | 246 | GLU  | CD-OE2 | 7.21   | 1.39        | 1.25     |
| 3   | C     | 131 | VAL  | CA-C   | -7.14  | 1.44        | 1.52     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 3   | C     | 246 | GLU  | CG-CD  | 7.13  | 1.69        | 1.52     |
| 1   | A     | 120 | SER  | C-O    | 7.12  | 1.32        | 1.24     |
| 3   | C     | 147 | TYR  | C-O    | 7.09  | 1.32        | 1.23     |
| 1   | A     | 178 | ALA  | CA-CB  | -7.08 | 1.41        | 1.53     |
| 1   | A     | 30  | VAL  | CA-CB  | 7.05  | 1.61        | 1.53     |
| 2   | B     | 149 | PHE  | N-CA   | 7.00  | 1.54        | 1.45     |
| 6   | F     | 3   | GLU  | CB-CG  | 6.97  | 1.73        | 1.52     |
| 2   | B     | 134 | LEU  | N-CA   | 6.95  | 1.55        | 1.46     |
| 7   | G     | 1   | MET  | SD-CE  | 6.94  | 1.97        | 1.79     |
| 2   | B     | 114 | ILE  | C-O    | -6.83 | 1.16        | 1.24     |
| 1   | A     | 140 | TRP  | CA-CB  | -6.82 | 1.42        | 1.53     |
| 1   | A     | 59  | LYS  | C-O    | -6.79 | 1.16        | 1.24     |
| 2   | B     | 20  | LYS  | C-O    | 6.73  | 1.32        | 1.24     |
| 3   | C     | 40  | VAL  | CA-C   | -6.68 | 1.44        | 1.52     |
| 2   | B     | 138 | LEU  | CG-CD1 | 6.66  | 1.74        | 1.52     |
| 1   | A     | 34  | TYR  | CA-C   | 6.64  | 1.61        | 1.52     |
| 2   | B     | 115 | GLU  | CG-CD  | 6.63  | 1.68        | 1.52     |
| 7   | G     | 2   | VAL  | N-CA   | 6.55  | 1.54        | 1.46     |
| 3   | C     | 22  | CYS  | CA-C   | 6.51  | 1.61        | 1.52     |
| 5   | E     | 4   | GLY  | C-O    | 6.49  | 1.32        | 1.23     |
| 1   | A     | 120 | SER  | CA-C   | 6.48  | 1.61        | 1.52     |
| 2   | B     | 40  | PHE  | CE2-CZ | 6.47  | 1.58        | 1.38     |
| 3   | C     | 81  | GLY  | N-CA   | 6.45  | 1.54        | 1.45     |
| 2   | B     | 73  | LEU  | N-CA   | 6.45  | 1.54        | 1.45     |
| 5   | E     | 26  | ILE  | CA-CB  | 6.45  | 1.63        | 1.54     |
| 1   | A     | 190 | VAL  | CA-CB  | -6.44 | 1.47        | 1.54     |
| 2   | B     | 143 | LEU  | C-O    | 6.39  | 1.32        | 1.24     |
| 1   | A     | 13  | GLU  | CB-CG  | 6.37  | 1.71        | 1.52     |
| 2   | B     | 140 | THR  | CA-CB  | 6.36  | 1.64        | 1.53     |
| 3   | C     | 48  | ALA  | CA-CB  | -6.35 | 1.44        | 1.53     |
| 7   | G     | 1   | MET  | N-CA   | 6.32  | 1.58        | 1.46     |
| 2   | B     | 72  | PRO  | CA-C   | -6.29 | 1.46        | 1.52     |
| 1   | A     | 154 | VAL  | N-CA   | -6.29 | 1.38        | 1.46     |
| 1   | A     | 73  | MET  | C-O    | 6.27  | 1.31        | 1.24     |
| 5   | E     | 2   | ILE  | C-O    | 6.26  | 1.31        | 1.24     |
| 3   | C     | 142 | ILE  | C-O    | 6.26  | 1.30        | 1.24     |
| 6   | F     | 14  | GLY  | C-O    | 6.25  | 1.31        | 1.23     |
| 7   | G     | 26  | TYR  | N-CA   | -6.24 | 1.40        | 1.46     |
| 5   | E     | 13  | ALA  | CA-CB  | -6.21 | 1.43        | 1.53     |
| 1   | A     | 136 | TYR  | CA-C   | -6.16 | 1.44        | 1.52     |
| 3   | C     | 248 | VAL  | CA-CB  | -6.16 | 1.47        | 1.54     |
| 6   | F     | 8   | ALA  | CA-CB  | -6.15 | 1.45        | 1.53     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | A     | 119 | ILE  | CA-C   | 6.14  | 1.60        | 1.52     |
| 5   | E     | 12  | ILE  | C-O    | 6.06  | 1.30        | 1.24     |
| 3   | C     | 201 | THR  | N-CA   | 6.06  | 1.54        | 1.46     |
| 8   | H     | 17  | TRP  | C-O    | 6.06  | 1.31        | 1.24     |
| 7   | G     | 3   | GLU  | CB-CG  | 6.05  | 1.70        | 1.52     |
| 2   | B     | 64  | GLU  | C-O    | -6.03 | 1.15        | 1.23     |
| 7   | G     | 27  | GLN  | CA-C   | 6.02  | 1.60        | 1.52     |
| 1   | A     | 32  | ILE  | N-CA   | 6.01  | 1.53        | 1.46     |
| 2   | B     | 71  | THR  | CA-C   | 6.00  | 1.59        | 1.52     |
| 2   | B     | 98  | VAL  | CA-CB  | -5.99 | 1.47        | 1.54     |
| 8   | H     | 23  | VAL  | CA-CB  | -5.99 | 1.46        | 1.54     |
| 2   | B     | 12  | PRO  | CA-C   | -5.98 | 1.44        | 1.52     |
| 4   | D     | 60  | LEU  | CA-C   | 5.97  | 1.61        | 1.52     |
| 3   | C     | 176 | ALA  | N-CA   | 5.95  | 1.50        | 1.46     |
| 1   | A     | 16  | ALA  | CA-CB  | -5.93 | 1.43        | 1.53     |
| 1   | A     | 186 | ALA  | CA-C   | -5.89 | 1.45        | 1.52     |
| 1   | A     | 119 | ILE  | CA-CB  | -5.83 | 1.46        | 1.54     |
| 8   | H     | 23  | VAL  | CA-C   | 5.83  | 1.60        | 1.52     |
| 1   | A     | 61  | THR  | CA-C   | -5.82 | 1.45        | 1.52     |
| 1   | A     | 114 | ARG  | N-CA   | 5.80  | 1.53        | 1.46     |
| 1   | A     | 213 | GLY  | C-O    | 5.79  | 1.31        | 1.24     |
| 3   | C     | 13  | PRO  | CA-C   | 5.78  | 1.60        | 1.52     |
| 1   | A     | 141 | ASP  | N-CA   | -5.77 | 1.38        | 1.45     |
| 3   | C     | 144 | PHE  | CA-CB  | -5.77 | 1.43        | 1.53     |
| 2   | B     | 83  | PRO  | CA-C   | -5.77 | 1.44        | 1.52     |
| 1   | A     | 174 | SER  | CA-C   | 5.77  | 1.59        | 1.52     |
| 3   | C     | 262 | ILE  | CA-CB  | -5.75 | 1.47        | 1.54     |
| 1   | A     | 112 | LYS  | CG-CD  | 5.75  | 1.69        | 1.52     |
| 2   | B     | 114 | ILE  | CA-C   | 5.74  | 1.60        | 1.52     |
| 2   | B     | 148 | THR  | CB-CG2 | 5.74  | 1.71        | 1.52     |
| 2   | B     | 16  | ALA  | CA-CB  | -5.74 | 1.43        | 1.53     |
| 5   | E     | 19  | ALA  | CA-CB  | -5.73 | 1.43        | 1.53     |
| 1   | A     | 87  | ARG  | CG-CD  | 5.72  | 1.69        | 1.52     |
| 4   | D     | 97  | GLU  | N-CA   | 5.72  | 1.53        | 1.46     |
| 1   | A     | 169 | LEU  | CG-CD2 | 5.72  | 1.71        | 1.52     |
| 2   | B     | 75  | ILE  | C-O    | -5.68 | 1.18        | 1.24     |
| 8   | H     | 28  | GLY  | N-CA   | 5.67  | 1.52        | 1.45     |
| 4   | D     | 140 | ILE  | CA-C   | 5.66  | 1.60        | 1.52     |
| 5   | E     | 9   | ILE  | CA-CB  | -5.66 | 1.47        | 1.54     |
| 2   | B     | 142 | TRP  | N-CA   | -5.66 | 1.39        | 1.46     |
| 6   | F     | 3   | GLU  | CG-CD  | 5.65  | 1.66        | 1.52     |
| 3   | C     | 256 | LYS  | CB-CG  | 5.63  | 1.69        | 1.52     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | A     | 134 | THR  | CB-CG2 | -5.63 | 1.33        | 1.52     |
| 1   | A     | 213 | GLY  | C-N    | 5.62  | 1.40        | 1.33     |
| 1   | A     | 123 | ILE  | C-O    | 5.61  | 1.31        | 1.24     |
| 1   | A     | 179 | THR  | C-O    | 5.60  | 1.30        | 1.24     |
| 3   | C     | 246 | GLU  | CB-CG  | 5.60  | 1.69        | 1.52     |
| 1   | A     | 75  | GLU  | N-CA   | 5.59  | 1.53        | 1.46     |
| 6   | F     | 27  | LEU  | CA-C   | -5.59 | 1.46        | 1.53     |
| 4   | D     | 174 | GLU  | CA-C   | 5.58  | 1.60        | 1.52     |
| 2   | B     | 70  | ALA  | CA-CB  | -5.58 | 1.43        | 1.53     |
| 7   | G     | 22  | PHE  | N-CA   | 5.58  | 1.53        | 1.46     |
| 1   | A     | 13  | GLU  | N-CA   | 5.57  | 1.53        | 1.46     |
| 3   | C     | 15  | GLU  | N-CA   | 5.55  | 1.52        | 1.46     |
| 2   | B     | 15  | ARG  | CG-CD  | 5.55  | 1.69        | 1.52     |
| 1   | A     | 113 | PRO  | CB-CG  | 5.54  | 1.77        | 1.49     |
| 2   | B     | 34  | ASN  | N-CA   | -5.52 | 1.39        | 1.46     |
| 4   | D     | 74  | ASN  | CA-C   | 5.51  | 1.56        | 1.53     |
| 5   | E     | 27  | LYS  | CE-NZ  | 5.51  | 1.65        | 1.49     |
| 3   | C     | 263 | CYS  | CA-C   | -5.51 | 1.45        | 1.52     |
| 3   | C     | 143 | HIS  | CA-C   | -5.49 | 1.46        | 1.52     |
| 2   | B     | 111 | VAL  | C-O    | -5.49 | 1.17        | 1.24     |
| 4   | D     | 134 | ASP  | N-CA   | 5.48  | 1.52        | 1.45     |
| 1   | A     | 127 | ILE  | CA-CB  | -5.46 | 1.47        | 1.54     |
| 3   | C     | 176 | ALA  | CA-C   | 5.46  | 1.56        | 1.53     |
| 7   | G     | 1   | MET  | CG-SD  | 5.45  | 1.94        | 1.80     |
| 1   | A     | 60  | PRO  | CA-C   | -5.45 | 1.44        | 1.52     |
| 1   | A     | 105 | TYR  | C-O    | -5.44 | 1.17        | 1.24     |
| 2   | B     | 68  | PRO  | N-CA   | -5.42 | 1.40        | 1.47     |
| 7   | G     | 1   | MET  | CB-CG  | 5.42  | 1.68        | 1.52     |
| 1   | A     | 70  | GLN  | C-O    | 5.41  | 1.30        | 1.24     |
| 1   | A     | 45  | LEU  | CA-C   | 5.40  | 1.60        | 1.52     |
| 1   | A     | 206 | ILE  | CA-CB  | -5.39 | 1.47        | 1.54     |
| 1   | A     | 13  | GLU  | CG-CD  | 5.37  | 1.65        | 1.52     |
| 3   | C     | 154 | ASN  | CA-C   | -5.37 | 1.46        | 1.52     |
| 1   | A     | 2   | ALA  | N-CA   | 5.36  | 1.53        | 1.46     |
| 3   | C     | 36  | VAL  | C-O    | -5.36 | 1.17        | 1.24     |
| 3   | C     | 226 | LYS  | N-CA   | 5.35  | 1.53        | 1.46     |
| 4   | D     | 40  | LYS  | N-CA   | -5.35 | 1.39        | 1.46     |
| 7   | G     | 21  | LEU  | C-O    | 5.34  | 1.30        | 1.24     |
| 3   | C     | 153 | ALA  | N-CA   | 5.33  | 1.52        | 1.45     |
| 8   | H     | 20  | ALA  | CA-CB  | -5.33 | 1.44        | 1.53     |
| 8   | H     | 1   | MET  | N-CA   | 5.31  | 1.56        | 1.46     |
| 8   | H     | 29  | LEU  | CB-CG  | 5.30  | 1.64        | 1.53     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 6   | F     | 1   | MET  | CA-C    | 5.29  | 1.64        | 1.52     |
| 1   | A     | 73  | MET  | CA-C    | 5.29  | 1.59        | 1.52     |
| 5   | E     | 29  | ILE  | CG1-CD1 | 5.28  | 1.72        | 1.51     |
| 2   | B     | 85  | PHE  | C-O     | 5.27  | 1.30        | 1.24     |
| 6   | F     | 22  | LEU  | CA-C    | 5.27  | 1.59        | 1.52     |
| 1   | A     | 70  | GLN  | CA-CB   | -5.25 | 1.45        | 1.53     |
| 1   | A     | 61  | THR  | N-CA    | -5.24 | 1.39        | 1.46     |
| 1   | A     | 3   | ASN  | N-CA    | 5.23  | 1.52        | 1.46     |
| 1   | A     | 103 | ARG  | N-CA    | 5.23  | 1.52        | 1.46     |
| 4   | D     | 99  | ILE  | CA-CB   | 5.23  | 1.61        | 1.54     |
| 1   | A     | 30  | VAL  | C-O     | 5.23  | 1.30        | 1.23     |
| 8   | H     | 1   | MET  | CG-SD   | 5.22  | 1.93        | 1.80     |
| 8   | H     | 8   | TRP  | CB-CG   | -5.21 | 1.34        | 1.50     |
| 7   | G     | 17  | THR  | CA-C    | 5.21  | 1.57        | 1.52     |
| 3   | C     | 89  | ARG  | CB-CG   | -5.20 | 1.36        | 1.52     |
| 6   | F     | 30  | GLN  | CA-C    | -5.17 | 1.45        | 1.52     |
| 3   | C     | 148 | ALA  | N-CA    | 5.17  | 1.52        | 1.45     |
| 4   | D     | 158 | ASP  | CA-C    | 5.17  | 1.60        | 1.52     |
| 3   | C     | 25  | CYS  | CA-C    | -5.17 | 1.45        | 1.52     |
| 4   | D     | 136 | THR  | CA-C    | 5.16  | 1.58        | 1.52     |
| 7   | G     | 1   | MET  | CA-CB   | 5.15  | 1.63        | 1.53     |
| 4   | D     | 135 | GLU  | CA-C    | 5.14  | 1.59        | 1.52     |
| 1   | A     | 26  | VAL  | CA-C    | 5.12  | 1.57        | 1.53     |
| 3   | C     | 185 | LYS  | N-CA    | 5.12  | 1.53        | 1.46     |
| 2   | B     | 145 | ILE  | CA-CB   | -5.12 | 1.47        | 1.54     |
| 1   | A     | 112 | LYS  | CB-CG   | 5.12  | 1.67        | 1.52     |
| 3   | C     | 40  | VAL  | N-CA    | -5.12 | 1.40        | 1.46     |
| 3   | C     | 166 | LYS  | N-CA    | 5.09  | 1.52        | 1.45     |
| 4   | D     | 34  | ALA  | CA-CB   | -5.09 | 1.45        | 1.53     |
| 6   | F     | 13  | PHE  | CA-C    | 5.08  | 1.59        | 1.52     |
| 3   | C     | 142 | ILE  | CA-CB   | -5.07 | 1.47        | 1.54     |
| 3   | C     | 153 | ALA  | CA-C    | -5.07 | 1.46        | 1.52     |
| 1   | A     | 48  | PHE  | CA-CB   | -5.07 | 1.45        | 1.53     |
| 5   | E     | 2   | ILE  | CA-CB   | 5.07  | 1.60        | 1.54     |
| 2   | B     | 127 | PRO  | CA-C    | -5.06 | 1.45        | 1.52     |
| 7   | G     | 10  | VAL  | CA-CB   | -5.06 | 1.47        | 1.54     |
| 3   | C     | 226 | LYS  | CA-C    | 5.06  | 1.59        | 1.52     |
| 4   | D     | 166 | THR  | CA-CB   | 5.05  | 1.61        | 1.53     |
| 2   | B     | 114 | ILE  | CA-CB   | -5.04 | 1.47        | 1.54     |
| 3   | C     | 80  | GLU  | CA-C    | 5.04  | 1.59        | 1.52     |
| 1   | A     | 145 | TYR  | CA-CB   | -5.03 | 1.44        | 1.53     |
| 3   | C     | 208 | VAL  | CA-C    | 5.03  | 1.58        | 1.52     |

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| Mol | Chain | Res | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 8   | H     | 1   | MET  | CB-CG  | 5.03 | 1.67        | 1.52     |
| 2   | B     | 93  | ASN  | CA-C   | 5.02 | 1.59        | 1.52     |
| 2   | B     | 60  | ALA  | N-CA   | 5.02 | 1.52        | 1.46     |
| 8   | H     | 29  | LEU  | CG-CD2 | 5.02 | 1.69        | 1.52     |
| 1   | A     | 168 | LEU  | C-O    | 5.01 | 1.29        | 1.24     |
| 6   | F     | 9   | ALA  | CA-C   | 5.00 | 1.59        | 1.52     |

All (459) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 5   | E     | 23  | ILE  | CB-CA-C | -17.53 | 89.90       | 111.81   |
| 2   | B     | 70  | ALA  | CA-C-N  | -15.15 | 100.36      | 120.67   |
| 2   | B     | 70  | ALA  | C-N-CA  | -15.15 | 100.36      | 120.67   |
| 1   | A     | 26  | VAL  | N-CA-C  | 14.30  | 122.90      | 107.60   |
| 5   | E     | 23  | ILE  | N-CA-CB | 14.04  | 125.93      | 110.62   |
| 3   | C     | 239 | GLY  | N-CA-C  | 13.24  | 125.45      | 112.08   |
| 4   | D     | 74  | ASN  | N-CA-C  | 12.60  | 120.85      | 108.75   |
| 2   | B     | 153 | LYS  | N-CA-C  | -12.52 | 98.91       | 112.93   |
| 1   | A     | 112 | LYS  | CA-C-N  | -12.52 | 104.19      | 119.84   |
| 1   | A     | 112 | LYS  | C-N-CA  | -12.52 | 104.19      | 119.84   |
| 1   | A     | 158 | ILE  | CA-C-N  | 12.34  | 131.80      | 118.97   |
| 1   | A     | 158 | ILE  | C-N-CA  | 12.34  | 131.80      | 118.97   |
| 2   | B     | 111 | VAL  | CA-C-N  | -12.14 | 106.32      | 119.19   |
| 2   | B     | 111 | VAL  | C-N-CA  | -12.14 | 106.32      | 119.19   |
| 3   | C     | 205 | LYS  | N-CA-C  | 11.45  | 125.33      | 111.02   |
| 4   | D     | 109 | THR  | N-CA-C  | -11.45 | 96.44       | 113.61   |
| 4   | D     | 87  | ASP  | CA-C-N  | -11.35 | 107.99      | 119.90   |
| 4   | D     | 87  | ASP  | C-N-CA  | -11.35 | 107.99      | 119.90   |
| 1   | A     | 74  | ASN  | N-CA-C  | 11.34  | 134.96      | 110.80   |
| 4   | D     | 163 | THR  | CA-C-N  | -10.93 | 108.75      | 119.90   |
| 4   | D     | 163 | THR  | C-N-CA  | -10.93 | 108.75      | 119.90   |
| 2   | B     | 11  | ASP  | CA-C-N  | 10.91  | 133.48      | 119.84   |
| 2   | B     | 11  | ASP  | C-N-CA  | 10.91  | 133.48      | 119.84   |
| 1   | A     | 59  | LYS  | CA-C-N  | -10.82 | 106.32      | 119.84   |
| 1   | A     | 59  | LYS  | C-N-CA  | -10.82 | 106.32      | 119.84   |
| 2   | B     | 63  | GLY  | N-CA-C  | -10.67 | 99.99       | 112.79   |
| 6   | F     | 4   | GLU  | N-CA-C  | -10.58 | 99.05       | 112.90   |
| 2   | B     | 82  | TYR  | CA-C-N  | 10.52  | 132.99      | 119.84   |
| 2   | B     | 82  | TYR  | C-N-CA  | 10.52  | 132.99      | 119.84   |
| 1   | A     | 191 | LEU  | CA-C-N  | -10.24 | 108.01      | 119.28   |
| 1   | A     | 191 | LEU  | C-N-CA  | -10.24 | 108.01      | 119.28   |
| 1   | A     | 159 | PRO  | CA-C-N  | -10.22 | 110.29      | 122.35   |

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| Mol | Chain | Res | Type | Atoms    | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|--------|-------------|----------|
| 1   | A     | 159 | PRO  | C-N-CA   | -10.22 | 110.29      | 122.35   |
| 2   | B     | 67  | ASP  | CA-C-N   | 10.20  | 131.30      | 119.47   |
| 2   | B     | 67  | ASP  | C-N-CA   | 10.20  | 131.30      | 119.47   |
| 2   | B     | 154 | THR  | N-CA-C   | 10.18  | 122.07      | 110.97   |
| 2   | B     | 149 | PHE  | N-CA-C   | 10.15  | 122.49      | 110.31   |
| 2   | B     | 71  | THR  | CA-C-N   | -10.10 | 107.81      | 120.23   |
| 2   | B     | 71  | THR  | C-N-CA   | -10.10 | 107.81      | 120.23   |
| 4   | D     | 44  | PRO  | CA-C-N   | 10.04  | 130.67      | 119.83   |
| 4   | D     | 44  | PRO  | C-N-CA   | 10.04  | 130.67      | 119.83   |
| 7   | G     | 3   | GLU  | CA-C-N   | 9.81   | 132.10      | 119.84   |
| 7   | G     | 3   | GLU  | C-N-CA   | 9.81   | 132.10      | 119.84   |
| 1   | A     | 62  | VAL  | CB-CA-C  | -9.64  | 96.65       | 112.26   |
| 3   | C     | 70  | LEU  | N-CA-C   | 9.59   | 121.97      | 108.74   |
| 2   | B     | 4   | LEU  | N-CA-C   | 9.56   | 123.68      | 109.24   |
| 4   | D     | 107 | VAL  | CB-CA-C  | -9.42  | 98.91       | 111.15   |
| 1   | A     | 187 | HIS  | N-CA-C   | -9.40  | 100.91      | 111.82   |
| 1   | A     | 3   | ASN  | N-CA-C   | 9.39   | 130.81      | 110.80   |
| 3   | C     | 90  | ILE  | CA-C-N   | -9.29  | 108.23      | 119.84   |
| 3   | C     | 90  | ILE  | C-N-CA   | -9.29  | 108.23      | 119.84   |
| 3   | C     | 10  | PRO  | N-CA-C   | 9.26   | 121.99      | 110.70   |
| 3   | C     | 176 | ALA  | N-CA-C   | 9.20   | 116.32      | 108.78   |
| 3   | C     | 41  | LEU  | CA-C-N   | -9.20  | 111.42      | 120.52   |
| 3   | C     | 41  | LEU  | C-N-CA   | -9.20  | 111.42      | 120.52   |
| 2   | B     | 22  | MET  | N-CA-C   | 9.11   | 130.19      | 110.80   |
| 2   | B     | 104 | VAL  | CA-C-N   | 9.07   | 131.18      | 119.84   |
| 2   | B     | 104 | VAL  | C-N-CA   | 9.07   | 131.18      | 119.84   |
| 2   | B     | 72  | PRO  | CB-CA-C  | -9.06  | 101.69      | 111.56   |
| 2   | B     | 24  | HIS  | N-CA-C   | 9.06   | 123.43      | 112.38   |
| 1   | A     | 114 | ARG  | N-CA-C   | 9.00   | 129.98      | 110.80   |
| 3   | C     | 101 | VAL  | CA-C-N   | -8.84  | 109.36      | 123.23   |
| 3   | C     | 101 | VAL  | C-N-CA   | -8.84  | 109.36      | 123.23   |
| 4   | D     | 126 | CYS  | CA-C-N   | 8.80   | 129.54      | 120.04   |
| 4   | D     | 126 | CYS  | C-N-CA   | 8.80   | 129.54      | 120.04   |
| 3   | C     | 102 | TYR  | CA-C-N   | -8.75  | 108.26      | 122.26   |
| 3   | C     | 102 | TYR  | C-N-CA   | -8.75  | 108.26      | 122.26   |
| 7   | G     | 28  | GLN  | N-CA-C   | -8.62  | 101.71      | 113.18   |
| 1   | A     | 63  | THR  | CB-CA-C  | -8.49  | 97.48       | 110.90   |
| 2   | B     | 62  | VAL  | CA-C-N   | -8.46  | 112.61      | 122.85   |
| 2   | B     | 62  | VAL  | C-N-CA   | -8.46  | 112.61      | 122.85   |
| 3   | C     | 229 | GLU  | N-CA-C   | 8.46   | 121.75      | 109.14   |
| 7   | G     | 9   | LEU  | CA-CB-CG | -8.42  | 86.84       | 116.30   |
| 1   | A     | 109 | GLY  | N-CA-C   | -8.39  | 104.01      | 114.16   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | B     | 89  | ARG  | N-CA-C  | 8.39  | 123.74      | 113.17   |
| 7   | G     | 2   | VAL  | CA-C-N  | -8.37 | 112.86      | 123.16   |
| 7   | G     | 2   | VAL  | C-N-CA  | -8.37 | 112.86      | 123.16   |
| 3   | C     | 12  | THR  | N-CA-C  | 8.35  | 118.88      | 108.11   |
| 2   | B     | 15  | ARG  | N-CA-C  | -8.26 | 102.23      | 111.07   |
| 2   | B     | 58  | ASP  | CA-C-N  | 8.23  | 129.33      | 120.11   |
| 2   | B     | 58  | ASP  | C-N-CA  | 8.23  | 129.33      | 120.11   |
| 2   | B     | 69  | PHE  | CA-C-N  | -8.18 | 110.78      | 123.13   |
| 2   | B     | 69  | PHE  | C-N-CA  | -8.18 | 110.78      | 123.13   |
| 2   | B     | 41  | PRO  | N-CA-C  | -8.17 | 102.17      | 113.53   |
| 3   | C     | 167 | SER  | N-CA-C  | -8.15 | 97.48       | 109.63   |
| 2   | B     | 82  | TYR  | N-CA-CB | 8.10  | 118.08      | 110.39   |
| 5   | E     | 11  | PHE  | N-CA-C  | -8.06 | 102.57      | 111.36   |
| 2   | B     | 40  | PHE  | CA-C-N  | 8.06  | 128.00      | 119.05   |
| 2   | B     | 40  | PHE  | C-N-CA  | 8.06  | 128.00      | 119.05   |
| 4   | D     | 85  | LYS  | N-CA-C  | -8.04 | 103.97      | 113.38   |
| 7   | G     | 2   | VAL  | CB-CA-C | -8.01 | 99.31       | 111.08   |
| 3   | C     | 39  | SER  | CA-C-N  | -8.00 | 110.68      | 122.68   |
| 3   | C     | 39  | SER  | C-N-CA  | -8.00 | 110.68      | 122.68   |
| 3   | C     | 104 | GLN  | CA-C-N  | 8.00  | 128.29      | 119.90   |
| 3   | C     | 104 | GLN  | C-N-CA  | 8.00  | 128.29      | 119.90   |
| 1   | A     | 110 | PHE  | CB-CA-C | -7.99 | 98.95       | 111.17   |
| 2   | B     | 126 | ARG  | CA-C-N  | 7.93  | 129.76      | 119.84   |
| 2   | B     | 126 | ARG  | C-N-CA  | 7.93  | 129.76      | 119.84   |
| 8   | H     | 18  | SER  | N-CA-C  | -7.93 | 101.01      | 111.24   |
| 4   | D     | 44  | PRO  | O-C-N   | 7.92  | 124.95      | 121.31   |
| 5   | E     | 7   | PHE  | N-CA-C  | -7.89 | 102.68      | 111.28   |
| 4   | D     | 79  | VAL  | N-CA-C  | 7.82  | 119.06      | 108.11   |
| 3   | C     | 185 | LYS  | N-CA-C  | 7.81  | 119.63      | 110.41   |
| 4   | D     | 144 | ALA  | CA-C-N  | 7.77  | 129.56      | 119.84   |
| 4   | D     | 144 | ALA  | C-N-CA  | 7.77  | 129.56      | 119.84   |
| 3   | C     | 148 | ALA  | N-CA-C  | 7.75  | 121.01      | 110.55   |
| 1   | A     | 151 | VAL  | CA-C-N  | -7.74 | 108.03      | 121.66   |
| 1   | A     | 151 | VAL  | C-N-CA  | -7.74 | 108.03      | 121.66   |
| 3   | C     | 226 | LYS  | N-CA-C  | 7.70  | 127.21      | 110.80   |
| 4   | D     | 97  | GLU  | N-CA-C  | 7.69  | 127.18      | 110.80   |
| 2   | B     | 82  | TYR  | O-C-N   | 7.66  | 125.55      | 120.27   |
| 8   | H     | 3   | ILE  | N-CA-C  | -7.65 | 102.82      | 110.62   |
| 4   | D     | 95  | SER  | N-CA-C  | 7.64  | 122.00      | 113.21   |
| 1   | A     | 26  | VAL  | CA-C-N  | 7.63  | 128.24      | 120.38   |
| 1   | A     | 26  | VAL  | C-N-CA  | 7.63  | 128.24      | 120.38   |
| 2   | B     | 72  | PRO  | CA-C-O  | -7.63 | 112.00      | 120.92   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 3   | C     | 160 | ILE  | N-CA-C    | 7.62  | 119.73      | 108.45   |
| 2   | B     | 81  | LEU  | N-CA-C    | 7.60  | 122.40      | 113.20   |
| 3   | C     | 286 | GLU  | N-CA-C    | 7.59  | 122.73      | 113.17   |
| 1   | A     | 136 | TYR  | CA-C-N    | -7.58 | 110.78      | 122.60   |
| 1   | A     | 136 | TYR  | C-N-CA    | -7.58 | 110.78      | 122.60   |
| 3   | C     | 51  | LYS  | N-CA-C    | 7.52  | 121.50      | 109.24   |
| 4   | D     | 140 | ILE  | CB-CA-C   | 7.51  | 121.76      | 111.92   |
| 1   | A     | 165 | ILE  | CB-CA-C   | -7.49 | 102.30      | 111.88   |
| 1   | A     | 175 | VAL  | CB-CA-C   | -7.49 | 99.16       | 111.51   |
| 5   | E     | 10  | VAL  | CB-CA-C   | -7.48 | 100.14      | 112.26   |
| 2   | B     | 59  | PRO  | CA-C-N    | 7.46  | 131.34      | 120.82   |
| 2   | B     | 59  | PRO  | C-N-CA    | 7.46  | 131.34      | 120.82   |
| 1   | A     | 44  | PHE  | N-CA-C    | 7.41  | 119.00      | 111.07   |
| 1   | A     | 64  | GLU  | N-CA-C    | 7.38  | 122.28      | 113.28   |
| 4   | D     | 108 | CYS  | N-CA-CB   | 7.37  | 120.55      | 110.38   |
| 6   | F     | 15  | LEU  | N-CA-C    | -7.37 | 103.75      | 112.89   |
| 5   | E     | 23  | ILE  | N-CA-C    | -7.37 | 103.16      | 110.30   |
| 3   | C     | 39  | SER  | N-CA-C    | 7.34  | 121.36      | 109.40   |
| 1   | A     | 172 | GLY  | N-CA-C    | -7.33 | 99.64       | 111.59   |
| 5   | E     | 31  | LEU  | N-CA-C    | -7.33 | 103.44      | 113.18   |
| 3   | C     | 49  | VAL  | N-CA-C    | 7.28  | 119.09      | 107.73   |
| 1   | A     | 63  | THR  | CA-CB-CG2 | -7.25 | 98.18       | 110.50   |
| 3   | C     | 80  | GLU  | N-CA-C    | 7.24  | 126.23      | 110.80   |
| 3   | C     | 92  | GLU  | N-CA-C    | 7.23  | 120.57      | 111.24   |
| 1   | A     | 177 | GLN  | CA-C-N    | -7.23 | 109.83      | 120.38   |
| 1   | A     | 177 | GLN  | C-N-CA    | -7.23 | 109.83      | 120.38   |
| 7   | G     | 1   | MET  | CG-SD-CE  | 7.22  | 116.77      | 100.90   |
| 4   | D     | 125 | LYS  | N-CA-C    | 7.21  | 120.17      | 108.34   |
| 1   | A     | 72  | ILE  | CB-CA-C   | -7.20 | 102.67      | 111.88   |
| 3   | C     | 3   | PHE  | CB-CA-C   | 7.19  | 122.32      | 110.81   |
| 8   | H     | 21  | MET  | CB-CG-SD  | -7.17 | 91.20       | 112.70   |
| 8   | H     | 1   | MET  | CB-CG-SD  | 7.12  | 134.06      | 112.70   |
| 1   | A     | 4   | VAL  | N-CA-C    | 7.11  | 117.62      | 110.23   |
| 3   | C     | 123 | GLN  | N-CA-C    | -7.11 | 104.48      | 113.72   |
| 1   | A     | 25  | TYR  | CA-C-N    | -7.09 | 110.22      | 123.34   |
| 1   | A     | 25  | TYR  | C-N-CA    | -7.09 | 110.22      | 123.34   |
| 3   | C     | 88  | GLU  | CA-C-N    | -7.08 | 111.25      | 122.08   |
| 3   | C     | 88  | GLU  | C-N-CA    | -7.08 | 111.25      | 122.08   |
| 2   | B     | 110 | LEU  | CA-CB-CG  | -7.06 | 91.60       | 116.30   |
| 2   | B     | 62  | VAL  | O-C-N     | -7.05 | 115.56      | 123.10   |
| 4   | D     | 71  | GLU  | N-CA-C    | 7.04  | 125.79      | 110.80   |
| 5   | E     | 12  | ILE  | O-C-N     | 6.93  | 129.36      | 121.94   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2   | B     | 146 | GLY  | CA-C-N    | -6.92 | 109.48      | 121.66   |
| 2   | B     | 146 | GLY  | C-N-CA    | -6.92 | 109.48      | 121.66   |
| 3   | C     | 200 | GLN  | N-CA-C    | 6.90  | 125.50      | 110.80   |
| 1   | A     | 32  | ILE  | N-CA-C    | 6.88  | 123.64      | 109.34   |
| 1   | A     | 202 | HIS  | CA-C-N    | -6.87 | 110.53      | 120.29   |
| 1   | A     | 202 | HIS  | C-N-CA    | -6.87 | 110.53      | 120.29   |
| 4   | D     | 12  | ASP  | N-CA-C    | 6.87  | 119.32      | 108.67   |
| 3   | C     | 202 | ASP  | N-CA-C    | 6.86  | 125.41      | 110.80   |
| 1   | A     | 105 | TYR  | CA-C-N    | -6.85 | 111.49      | 122.66   |
| 1   | A     | 105 | TYR  | C-N-CA    | -6.85 | 111.49      | 122.66   |
| 1   | A     | 190 | VAL  | N-CA-C    | 6.84  | 116.94      | 110.30   |
| 1   | A     | 43  | CYS  | CA-C-N    | -6.83 | 111.56      | 120.44   |
| 1   | A     | 43  | CYS  | C-N-CA    | -6.83 | 111.56      | 120.44   |
| 5   | E     | 29  | ILE  | N-CA-C    | -6.82 | 95.15       | 109.34   |
| 1   | A     | 126 | VAL  | N-CA-C    | 6.82  | 117.58      | 110.62   |
| 2   | B     | 155 | LEU  | N-CA-C    | -6.82 | 102.22      | 112.04   |
| 3   | C     | 125 | GLN  | N-CA-C    | -6.81 | 103.31      | 111.69   |
| 1   | A     | 79  | GLY  | N-CA-C    | -6.78 | 104.59      | 112.73   |
| 2   | B     | 15  | ARG  | CB-CG-CD  | 6.73  | 126.78      | 111.30   |
| 4   | D     | 13  | MET  | CB-CG-SD  | -6.73 | 92.52       | 112.70   |
| 3   | C     | 93  | GLU  | N-CA-C    | -6.73 | 105.04      | 113.18   |
| 4   | D     | 81  | VAL  | CB-CA-C   | -6.72 | 100.27      | 111.29   |
| 4   | D     | 29  | GLY  | CA-C-N    | -6.71 | 111.26      | 120.46   |
| 4   | D     | 29  | GLY  | C-N-CA    | -6.71 | 111.26      | 120.46   |
| 5   | E     | 26  | ILE  | CB-CA-C   | 6.71  | 121.23      | 112.24   |
| 3   | C     | 15  | GLU  | N-CA-CB   | 6.67  | 117.03      | 109.49   |
| 5   | E     | 12  | ILE  | N-CA-CB   | 6.67  | 118.19      | 110.65   |
| 4   | D     | 139 | VAL  | CB-CA-C   | -6.67 | 100.36      | 111.29   |
| 1   | A     | 63  | THR  | N-CA-C    | 6.66  | 118.33      | 111.14   |
| 2   | B     | 149 | PHE  | CB-CA-C   | -6.65 | 99.98       | 109.96   |
| 3   | C     | 127 | ILE  | CB-CA-C   | -6.61 | 100.68      | 110.33   |
| 2   | B     | 26  | TYR  | N-CA-C    | -6.59 | 105.78      | 113.88   |
| 2   | B     | 15  | ARG  | NE-CZ-NH2 | -6.58 | 113.27      | 119.20   |
| 1   | A     | 49  | ALA  | N-CA-C    | 6.58  | 118.14      | 110.97   |
| 1   | A     | 212 | SER  | N-CA-C    | -6.57 | 96.81       | 110.80   |
| 2   | B     | 142 | TRP  | N-CA-C    | -6.56 | 103.33      | 112.45   |
| 3   | C     | 246 | GLU  | N-CA-C    | -6.55 | 99.62       | 110.17   |
| 1   | A     | 170 | ARG  | CA-C-O    | 6.53  | 126.19      | 118.69   |
| 2   | B     | 76  | LEU  | CA-C-N    | -6.52 | 111.69      | 119.84   |
| 2   | B     | 76  | LEU  | C-N-CA    | -6.52 | 111.69      | 119.84   |
| 1   | A     | 100 | HIS  | CB-CA-C   | 6.52  | 121.11      | 110.88   |
| 5   | E     | 6   | VAL  | N-CA-C    | 6.50  | 116.61      | 110.30   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4   | D     | 134 | ASP  | N-CA-C     | 6.50  | 118.91      | 110.53   |
| 3   | C     | 44  | THR  | CA-C-N     | -6.48 | 111.99      | 121.71   |
| 3   | C     | 44  | THR  | C-N-CA     | -6.48 | 111.99      | 121.71   |
| 6   | F     | 23  | GLY  | N-CA-C     | 6.47  | 120.33      | 112.49   |
| 3   | C     | 46  | PHE  | CA-C-N     | -6.47 | 112.51      | 122.09   |
| 3   | C     | 46  | PHE  | C-N-CA     | -6.47 | 112.51      | 122.09   |
| 1   | A     | 197 | VAL  | N-CA-C     | -6.47 | 103.57      | 110.36   |
| 3   | C     | 157 | ARG  | N-CA-C     | 6.46  | 119.61      | 110.50   |
| 3   | C     | 262 | ILE  | N-CA-C     | 6.46  | 117.98      | 110.62   |
| 2   | B     | 117 | VAL  | CA-C-N     | -6.46 | 109.21      | 121.54   |
| 2   | B     | 117 | VAL  | C-N-CA     | -6.46 | 109.21      | 121.54   |
| 2   | B     | 104 | VAL  | CA-C-O     | 6.45  | 123.01      | 118.69   |
| 2   | B     | 52  | VAL  | N-CA-C     | -6.43 | 104.37      | 110.42   |
| 1   | A     | 160 | VAL  | N-CA-CB    | 6.43  | 122.11      | 110.86   |
| 3   | C     | 172 | PHE  | N-CA-C     | 6.43  | 119.98      | 109.76   |
| 1   | A     | 119 | ILE  | CB-CA-C    | -6.41 | 100.78      | 111.29   |
| 4   | D     | 113 | CYS  | CA-CB-SG   | -6.41 | 99.66       | 114.40   |
| 2   | B     | 70  | ALA  | N-CA-C     | 6.38  | 120.52      | 107.69   |
| 4   | D     | 35  | LEU  | N-CA-C     | 6.38  | 119.05      | 111.33   |
| 1   | A     | 69  | VAL  | CB-CA-C    | -6.35 | 103.72      | 112.04   |
| 3   | C     | 36  | VAL  | N-CA-C     | -6.35 | 95.17       | 108.88   |
| 5   | E     | 14  | LEU  | CD1-CG-CD2 | 6.34  | 124.75      | 110.80   |
| 5   | E     | 9   | ILE  | N-CA-C     | 6.34  | 117.84      | 110.62   |
| 3   | C     | 10  | PRO  | CA-C-N     | -6.33 | 113.69      | 120.47   |
| 3   | C     | 10  | PRO  | C-N-CA     | -6.33 | 113.69      | 120.47   |
| 2   | B     | 119 | LYS  | CA-C-N     | -6.33 | 111.88      | 122.64   |
| 2   | B     | 119 | LYS  | C-N-CA     | -6.33 | 111.88      | 122.64   |
| 7   | G     | 33  | ASN  | N-CA-C     | 6.33  | 124.28      | 110.80   |
| 6   | F     | 3   | GLU  | N-CA-C     | -6.31 | 104.04      | 112.94   |
| 1   | A     | 92  | MET  | CA-CB-CG   | -6.29 | 101.52      | 114.10   |
| 4   | D     | 107 | VAL  | N-CA-C     | 6.29  | 117.19      | 108.89   |
| 3   | C     | 192 | ASN  | N-CA-C     | 6.29  | 124.19      | 110.80   |
| 2   | B     | 120 | PHE  | N-CA-CB    | 6.27  | 120.85      | 110.63   |
| 1   | A     | 58  | TYR  | O-C-N      | -6.26 | 115.86      | 123.19   |
| 2   | B     | 32  | TRP  | CA-C-N     | 6.25  | 127.66      | 119.84   |
| 2   | B     | 32  | TRP  | C-N-CA     | 6.25  | 127.66      | 119.84   |
| 1   | A     | 113 | PRO  | CA-C-N     | 6.18  | 133.35      | 121.54   |
| 1   | A     | 113 | PRO  | C-N-CA     | 6.18  | 133.35      | 121.54   |
| 6   | F     | 22  | LEU  | CB-CA-C    | 6.18  | 120.70      | 110.81   |
| 3   | C     | 262 | ILE  | CB-CA-C    | -6.17 | 103.96      | 112.04   |
| 5   | E     | 26  | ILE  | N-CA-C     | -6.16 | 104.28      | 111.00   |
| 4   | D     | 39  | VAL  | N-CA-C     | -6.10 | 105.78      | 111.45   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 7   | G     | 7   | ASP  | CB-CA-C    | 6.09  | 120.91      | 110.79   |
| 3   | C     | 113 | VAL  | CB-CA-C    | -6.09 | 103.08      | 110.99   |
| 1   | A     | 203 | PHE  | N-CA-C     | 6.08  | 117.99      | 111.36   |
| 3   | C     | 113 | VAL  | N-CA-CB    | -6.08 | 104.23      | 111.90   |
| 7   | G     | 34  | GLU  | N-CA-C     | 6.08  | 123.76      | 110.80   |
| 1   | A     | 91  | SER  | CA-CB-OG   | -6.08 | 98.94       | 111.10   |
| 7   | G     | 26  | TYR  | N-CA-C     | -6.06 | 102.31      | 111.34   |
| 3   | C     | 34  | VAL  | CB-CA-C    | -6.06 | 101.35      | 111.29   |
| 2   | B     | 122 | ASN  | N-CA-C     | 6.05  | 123.19      | 109.81   |
| 1   | A     | 64  | GLU  | CA-CB-CG   | -6.05 | 101.99      | 114.10   |
| 1   | A     | 160 | VAL  | CB-CA-C    | -6.05 | 104.59      | 111.55   |
| 3   | C     | 103 | PHE  | N-CA-C     | 6.03  | 119.02      | 108.52   |
| 1   | A     | 62  | VAL  | CG1-CB-CG2 | 6.03  | 124.07      | 110.80   |
| 1   | A     | 197 | VAL  | CA-C-N     | -6.03 | 110.44      | 120.68   |
| 1   | A     | 197 | VAL  | C-N-CA     | -6.03 | 110.44      | 120.68   |
| 4   | D     | 175 | LYS  | N-CA-C     | 6.02  | 117.29      | 109.64   |
| 1   | A     | 186 | ALA  | CB-CA-C    | -6.02 | 101.69      | 110.96   |
| 4   | D     | 70  | LEU  | N-CA-C     | -6.02 | 97.98       | 110.80   |
| 3   | C     | 37  | PRO  | CB-CA-C    | -6.01 | 102.15      | 111.22   |
| 1   | A     | 149 | LYS  | N-CA-C     | 5.97  | 117.48      | 110.97   |
| 1   | A     | 169 | LEU  | CB-CG-CD1  | -5.97 | 92.78       | 110.70   |
| 1   | A     | 58  | TYR  | CA-C-N     | -5.96 | 111.72      | 122.28   |
| 1   | A     | 58  | TYR  | C-N-CA     | -5.96 | 111.72      | 122.28   |
| 3   | C     | 201 | THR  | N-CA-C     | 5.96  | 123.50      | 110.80   |
| 1   | A     | 132 | GLY  | N-CA-C     | 5.96  | 127.31      | 113.18   |
| 1   | A     | 180 | LEU  | N-CA-C     | -5.96 | 104.79      | 111.28   |
| 3   | C     | 263 | CYS  | N-CA-C     | -5.96 | 104.72      | 112.23   |
| 3   | C     | 137 | THR  | CB-CA-C    | -5.93 | 98.77       | 110.27   |
| 2   | B     | 21  | GLY  | CA-C-N     | -5.92 | 110.24      | 121.54   |
| 2   | B     | 21  | GLY  | C-N-CA     | -5.92 | 110.24      | 121.54   |
| 1   | A     | 83  | ARG  | CG-CD-NE   | -5.91 | 99.00       | 112.00   |
| 5   | E     | 12  | ILE  | CB-CA-C    | -5.91 | 104.25      | 111.87   |
| 4   | D     | 46  | SER  | CA-C-N     | 5.90  | 126.49      | 120.00   |
| 4   | D     | 46  | SER  | C-N-CA     | 5.90  | 126.49      | 120.00   |
| 1   | A     | 123 | ILE  | N-CA-C     | -5.90 | 103.54      | 111.44   |
| 1   | A     | 114 | ARG  | CA-C-N     | -5.89 | 111.17      | 120.60   |
| 1   | A     | 114 | ARG  | C-N-CA     | -5.89 | 111.17      | 120.60   |
| 2   | B     | 141 | ILE  | N-CA-C     | 5.88  | 121.58      | 109.34   |
| 1   | A     | 141 | ASP  | N-CA-CB    | -5.88 | 101.04      | 110.51   |
| 2   | B     | 20  | LYS  | CA-C-O     | 5.88  | 125.60      | 119.14   |
| 4   | D     | 139 | VAL  | N-CA-C     | 5.87  | 121.55      | 109.34   |
| 7   | G     | 5   | LEU  | CA-CB-CG   | -5.87 | 95.77       | 116.30   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | B     | 125 | ARG  | N-CA-C     | 5.86  | 123.28      | 110.80   |
| 2   | B     | 130 | THR  | CB-CA-C    | 5.85  | 122.06      | 110.42   |
| 7   | G     | 2   | VAL  | O-C-N      | -5.84 | 116.60      | 122.62   |
| 3   | C     | 217 | LEU  | N-CA-C     | -5.83 | 100.39      | 109.72   |
| 1   | A     | 63  | THR  | OG1-CB-CG2 | 5.82  | 120.94      | 109.30   |
| 6   | F     | 10  | LEU  | CA-C-N     | -5.82 | 110.81      | 121.52   |
| 6   | F     | 10  | LEU  | C-N-CA     | -5.82 | 110.81      | 121.52   |
| 1   | A     | 134 | THR  | N-CA-C     | 5.81  | 118.09      | 111.11   |
| 1   | A     | 136 | TYR  | CB-CA-C    | -5.81 | 98.86       | 110.42   |
| 1   | A     | 186 | ALA  | O-C-N      | 5.80  | 128.06      | 122.03   |
| 6   | F     | 3   | GLU  | CB-CG-CD   | 5.79  | 122.44      | 112.60   |
| 3   | C     | 138 | THR  | CA-C-N     | -5.77 | 115.34      | 122.84   |
| 3   | C     | 138 | THR  | C-N-CA     | -5.77 | 115.34      | 122.84   |
| 3   | C     | 149 | ILE  | CB-CA-C    | -5.77 | 101.62      | 110.50   |
| 3   | C     | 102 | TYR  | N-CA-C     | 5.75  | 119.03      | 107.41   |
| 3   | C     | 182 | LYS  | N-CA-C     | 5.75  | 118.03      | 108.13   |
| 3   | C     | 194 | LYS  | N-CA-C     | 5.75  | 123.04      | 110.80   |
| 2   | B     | 57  | LEU  | CA-C-N     | -5.74 | 116.66      | 122.74   |
| 2   | B     | 57  | LEU  | C-N-CA     | -5.74 | 116.66      | 122.74   |
| 1   | A     | 12  | LEU  | N-CA-C     | 5.73  | 120.41      | 113.41   |
| 1   | A     | 177 | GLN  | N-CA-CB    | 5.73  | 118.55      | 110.12   |
| 2   | B     | 34  | ASN  | N-CA-C     | 5.73  | 123.00      | 110.80   |
| 2   | B     | 22  | MET  | CA-C-N     | -5.72 | 110.19      | 121.41   |
| 2   | B     | 22  | MET  | C-N-CA     | -5.72 | 110.19      | 121.41   |
| 8   | H     | 21  | MET  | N-CA-C     | 5.72  | 119.07      | 111.75   |
| 4   | D     | 26  | THR  | N-CA-CB    | 5.71  | 120.03      | 110.32   |
| 3   | C     | 246 | GLU  | CB-CA-C    | 5.70  | 119.13      | 109.50   |
| 3   | C     | 256 | LYS  | CB-CG-CD   | 5.70  | 124.40      | 111.30   |
| 2   | B     | 152 | ASP  | CA-C-N     | -5.69 | 113.20      | 122.65   |
| 2   | B     | 152 | ASP  | C-N-CA     | -5.69 | 113.20      | 122.65   |
| 4   | D     | 37  | PRO  | N-CA-C     | -5.68 | 106.13      | 113.57   |
| 5   | E     | 14  | LEU  | N-CA-CB    | -5.66 | 101.51      | 109.94   |
| 3   | C     | 89  | ARG  | NE-CZ-NH1  | -5.66 | 115.84      | 121.50   |
| 3   | C     | 14  | ARG  | CA-C-N     | -5.62 | 113.37      | 122.48   |
| 3   | C     | 14  | ARG  | C-N-CA     | -5.62 | 113.37      | 122.48   |
| 2   | B     | 99  | LEU  | CA-CB-CG   | -5.62 | 96.63       | 116.30   |
| 1   | A     | 62  | VAL  | N-CA-CB    | 5.62  | 120.94      | 110.77   |
| 1   | A     | 85  | ILE  | CB-CA-C    | -5.61 | 104.70      | 111.88   |
| 1   | A     | 31  | ASN  | N-CA-C     | -5.60 | 101.91      | 110.14   |
| 3   | C     | 47  | LYS  | CA-C-N     | -5.60 | 115.10      | 123.00   |
| 3   | C     | 47  | LYS  | C-N-CA     | -5.60 | 115.10      | 123.00   |
| 1   | A     | 134 | THR  | CB-CA-C    | -5.59 | 101.86      | 110.81   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 3   | C     | 141 | ASN  | CA-C-N     | 5.58  | 131.24      | 122.70   |
| 3   | C     | 141 | ASN  | C-N-CA     | 5.58  | 131.24      | 122.70   |
| 3   | C     | 256 | LYS  | N-CA-CB    | 5.58  | 118.05      | 109.91   |
| 4   | D     | 63  | ASN  | N-CA-C     | 5.57  | 122.67      | 110.80   |
| 3   | C     | 132 | LEU  | CB-CG-CD2  | -5.57 | 93.98       | 110.70   |
| 1   | A     | 191 | LEU  | CA-CB-CG   | -5.57 | 96.81       | 116.30   |
| 4   | D     | 27  | VAL  | CB-CA-C    | 5.56  | 119.31      | 112.02   |
| 3   | C     | 150 | HIS  | CB-CA-C    | -5.56 | 99.64       | 109.70   |
| 4   | D     | 136 | THR  | CB-CA-C    | -5.56 | 101.89      | 109.28   |
| 4   | D     | 43  | ILE  | CA-C-N     | 5.56  | 123.72      | 119.66   |
| 4   | D     | 43  | ILE  | C-N-CA     | 5.56  | 123.72      | 119.66   |
| 2   | B     | 138 | LEU  | CD1-CG-CD2 | 5.54  | 123.00      | 110.80   |
| 4   | D     | 158 | ASP  | N-CA-C     | 5.54  | 119.99      | 113.23   |
| 2   | B     | 11  | ASP  | CB-CA-C    | 5.52  | 116.30      | 110.17   |
| 2   | B     | 29  | GLU  | CB-CA-C    | 5.52  | 117.37      | 109.26   |
| 3   | C     | 63  | ALA  | CA-C-N     | 5.52  | 128.23      | 120.28   |
| 3   | C     | 63  | ALA  | C-N-CA     | 5.52  | 128.23      | 120.28   |
| 6   | F     | 5   | MET  | CA-CB-CG   | -5.52 | 103.06      | 114.10   |
| 2   | B     | 141 | ILE  | CB-CA-C    | -5.51 | 102.25      | 111.29   |
| 2   | B     | 62  | VAL  | N-CA-C     | -5.50 | 100.26      | 108.46   |
| 2   | B     | 41  | PRO  | CA-C-N     | -5.50 | 113.56      | 120.77   |
| 2   | B     | 41  | PRO  | C-N-CA     | -5.50 | 113.56      | 120.77   |
| 2   | B     | 50  | CYS  | N-CA-C     | 5.49  | 118.03      | 111.71   |
| 3   | C     | 21  | VAL  | CB-CA-C    | -5.49 | 104.64      | 112.22   |
| 7   | G     | 2   | VAL  | N-CA-C     | 5.49  | 118.46      | 109.78   |
| 1   | A     | 62  | VAL  | CA-CB-CG1  | -5.49 | 101.07      | 110.40   |
| 3   | C     | 86  | PRO  | N-CA-C     | -5.49 | 102.51      | 111.68   |
| 2   | B     | 65  | PRO  | N-CD-CG    | -5.49 | 94.97       | 103.20   |
| 1   | A     | 169 | LEU  | CD1-CG-CD2 | 5.48  | 122.86      | 110.80   |
| 1   | A     | 133 | VAL  | CB-CA-C    | -5.48 | 104.87      | 111.88   |
| 1   | A     | 126 | VAL  | CA-CB-CG2  | -5.48 | 101.09      | 110.40   |
| 3   | C     | 147 | TYR  | CA-C-N     | -5.47 | 109.83      | 121.32   |
| 3   | C     | 147 | TYR  | C-N-CA     | -5.47 | 109.83      | 121.32   |
| 1   | A     | 173 | SER  | CA-CB-OG   | -5.47 | 100.16      | 111.10   |
| 3   | C     | 75  | VAL  | CB-CA-C    | -5.45 | 103.43      | 110.84   |
| 3   | C     | 246 | GLU  | CB-CG-CD   | 5.43  | 121.84      | 112.60   |
| 3   | C     | 52  | ILE  | CB-CA-C    | -5.43 | 101.48      | 111.36   |
| 1   | A     | 187 | HIS  | CA-C-N     | -5.42 | 113.64      | 122.26   |
| 1   | A     | 187 | HIS  | C-N-CA     | -5.42 | 113.64      | 122.26   |
| 1   | A     | 26  | VAL  | CB-CA-C    | 5.41  | 117.40      | 111.18   |
| 4   | D     | 142 | GLY  | N-CA-C     | -5.41 | 101.31      | 112.34   |
| 3   | C     | 71  | ASN  | N-CA-C     | 5.41  | 117.90      | 108.76   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 6   | F     | 27  | LEU  | O-C-N     | 5.40  | 128.53      | 122.32   |
| 3   | C     | 11  | PRO  | CA-C-N    | -5.39 | 112.21      | 122.08   |
| 3   | C     | 11  | PRO  | C-N-CA    | -5.39 | 112.21      | 122.08   |
| 2   | B     | 69  | PHE  | N-CA-C    | 5.38  | 119.47      | 113.02   |
| 2   | B     | 128 | VAL  | N-CA-C    | 5.37  | 116.15      | 110.72   |
| 4   | D     | 130 | GLY  | N-CA-C    | 5.37  | 125.91      | 113.18   |
| 1   | A     | 10  | GLU  | CA-C-N    | 5.37  | 131.79      | 121.54   |
| 1   | A     | 10  | GLU  | C-N-CA    | 5.37  | 131.79      | 121.54   |
| 3   | C     | 97  | GLU  | N-CA-C    | -5.37 | 106.73      | 113.28   |
| 1   | A     | 105 | TYR  | CB-CA-C   | -5.36 | 101.84      | 110.74   |
| 2   | B     | 120 | PHE  | O-C-N     | 5.35  | 129.25      | 123.10   |
| 4   | D     | 135 | GLU  | N-CA-C    | 5.32  | 122.13      | 110.80   |
| 2   | B     | 153 | LYS  | CB-CG-CD  | 5.32  | 123.52      | 111.30   |
| 1   | A     | 83  | ARG  | CA-CB-CG  | -5.31 | 103.48      | 114.10   |
| 3   | C     | 38  | GLN  | CA-C-N    | -5.31 | 114.97      | 122.94   |
| 3   | C     | 38  | GLN  | C-N-CA    | -5.31 | 114.97      | 122.94   |
| 2   | B     | 71  | THR  | N-CA-C    | 5.30  | 117.30      | 109.50   |
| 2   | B     | 117 | VAL  | N-CA-CB   | 5.30  | 119.98      | 111.23   |
| 4   | D     | 62  | ASN  | N-CA-C    | 5.30  | 118.46      | 109.76   |
| 3   | C     | 253 | ASN  | N-CA-C    | 5.30  | 116.74      | 111.07   |
| 8   | H     | 14  | VAL  | CB-CA-C   | -5.29 | 104.91      | 112.22   |
| 2   | B     | 92  | PRO  | CA-C-N    | -5.29 | 113.60      | 122.17   |
| 2   | B     | 92  | PRO  | C-N-CA    | -5.29 | 113.60      | 122.17   |
| 1   | A     | 54  | MET  | CA-C-N    | -5.28 | 110.72      | 121.18   |
| 1   | A     | 54  | MET  | C-N-CA    | -5.28 | 110.72      | 121.18   |
| 3   | C     | 234 | ASN  | N-CA-C    | 5.28  | 121.49      | 109.81   |
| 4   | D     | 55  | THR  | N-CA-C    | 5.27  | 117.34      | 109.59   |
| 3   | C     | 25  | CYS  | CA-C-N    | -5.27 | 115.41      | 122.42   |
| 3   | C     | 25  | CYS  | C-N-CA    | -5.27 | 115.41      | 122.42   |
| 4   | D     | 27  | VAL  | N-CA-C    | 5.27  | 115.48      | 110.53   |
| 4   | D     | 76  | GLY  | N-CA-C    | -5.26 | 107.74      | 114.37   |
| 8   | H     | 14  | VAL  | N-CA-CB   | 5.26  | 118.47      | 110.58   |
| 3   | C     | 93  | GLU  | N-CA-CB   | 5.26  | 119.25      | 110.41   |
| 7   | G     | 24  | ALA  | N-CA-CB   | 5.25  | 118.39      | 110.30   |
| 2   | B     | 122 | ASN  | CA-C-N    | -5.22 | 113.31      | 119.84   |
| 2   | B     | 122 | ASN  | C-N-CA    | -5.22 | 113.31      | 119.84   |
| 3   | C     | 90  | ILE  | N-CA-C    | -5.22 | 97.60       | 108.88   |
| 1   | A     | 122 | VAL  | CA-C-N    | -5.22 | 111.31      | 120.29   |
| 1   | A     | 122 | VAL  | C-N-CA    | -5.22 | 111.31      | 120.29   |
| 2   | B     | 59  | PRO  | O-C-N     | 5.22  | 128.97      | 122.71   |
| 3   | C     | 250 | GLN  | CB-CG-CD  | -5.22 | 103.73      | 112.60   |
| 2   | B     | 81  | LEU  | CB-CG-CD2 | -5.21 | 95.06       | 110.70   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4   | D     | 106 | ALA  | N-CA-C     | 5.21  | 119.49      | 113.18   |
| 8   | H     | 8   | TRP  | N-CA-C     | 5.21  | 117.36      | 111.11   |
| 2   | B     | 45  | MET  | N-CA-C     | 5.21  | 117.64      | 111.33   |
| 1   | A     | 63  | THR  | CA-C-N     | -5.20 | 112.39      | 122.06   |
| 1   | A     | 63  | THR  | C-N-CA     | -5.20 | 112.39      | 122.06   |
| 2   | B     | 74  | GLU  | CA-C-N     | -5.19 | 116.17      | 123.13   |
| 2   | B     | 74  | GLU  | C-N-CA     | -5.19 | 116.17      | 123.13   |
| 3   | C     | 127 | ILE  | CA-C-N     | -5.19 | 115.49      | 122.91   |
| 3   | C     | 127 | ILE  | C-N-CA     | -5.19 | 115.49      | 122.91   |
| 4   | D     | 161 | VAL  | N-CA-C     | 5.18  | 114.96      | 106.72   |
| 1   | A     | 20  | ASP  | CA-C-N     | -5.18 | 112.26      | 120.55   |
| 1   | A     | 20  | ASP  | C-N-CA     | -5.18 | 112.26      | 120.55   |
| 2   | B     | 125 | ARG  | CA-C-O     | -5.17 | 113.12      | 120.51   |
| 3   | C     | 248 | VAL  | CB-CA-C    | -5.17 | 103.81      | 110.84   |
| 1   | A     | 119 | ILE  | CB-CG1-CD1 | -5.17 | 102.95      | 113.80   |
| 2   | B     | 111 | VAL  | N-CA-C     | 5.16  | 120.03      | 108.88   |
| 1   | A     | 102 | PHE  | CA-C-N     | -5.16 | 113.37      | 120.28   |
| 1   | A     | 102 | PHE  | C-N-CA     | -5.16 | 113.37      | 120.28   |
| 3   | C     | 270 | LEU  | N-CA-C     | -5.16 | 105.57      | 111.14   |
| 5   | E     | 14  | LEU  | N-CA-C     | 5.15  | 117.29      | 111.11   |
| 1   | A     | 67  | ALA  | N-CA-CB    | -5.14 | 102.30      | 110.22   |
| 3   | C     | 126 | GLU  | N-CA-C     | -5.14 | 101.50      | 109.72   |
| 1   | A     | 24  | LYS  | N-CA-C     | -5.13 | 101.51      | 109.72   |
| 1   | A     | 94  | VAL  | N-CA-CB    | 5.12  | 116.88      | 110.47   |
| 2   | B     | 127 | PRO  | CA-CB-CG   | -5.12 | 94.77       | 104.50   |
| 4   | D     | 127 | PRO  | N-CA-C     | -5.12 | 107.36      | 114.27   |
| 2   | B     | 29  | GLU  | CA-C-N     | -5.10 | 114.66      | 119.76   |
| 2   | B     | 29  | GLU  | C-N-CA     | -5.10 | 114.66      | 119.76   |
| 6   | F     | 26  | LEU  | O-C-N      | 5.10  | 128.01      | 122.20   |
| 1   | A     | 113 | PRO  | CA-N-CD    | 5.10  | 119.14      | 112.00   |
| 5   | E     | 29  | ILE  | N-CA-CB    | 5.10  | 119.64      | 111.23   |
| 3   | C     | 14  | ARG  | N-CA-C     | 5.10  | 117.27      | 109.07   |
| 3   | C     | 82  | PHE  | N-CA-C     | -5.09 | 102.95      | 110.48   |
| 1   | A     | 182 | ARG  | NE-CZ-NH1  | -5.08 | 116.42      | 121.50   |
| 6   | F     | 25  | LEU  | CB-CG-CD2  | -5.08 | 95.45       | 110.70   |
| 1   | A     | 81  | LEU  | CB-CG-CD2  | -5.08 | 95.47       | 110.70   |
| 1   | A     | 105 | TYR  | N-CA-C     | 5.06  | 119.72      | 111.37   |
| 1   | A     | 103 | ARG  | N-CA-CB    | 5.05  | 117.54      | 110.12   |
| 4   | D     | 80  | LEU  | N-CA-C     | 5.05  | 117.04      | 110.43   |
| 6   | F     | 18  | VAL  | CB-CA-C    | -5.05 | 105.42      | 111.88   |
| 2   | B     | 127 | PRO  | CA-C-N     | -5.03 | 113.27      | 120.42   |
| 2   | B     | 127 | PRO  | C-N-CA     | -5.03 | 113.27      | 120.42   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 7   | G     | 7   | ASP  | CB-CG-OD1 | 5.03  | 129.97      | 118.40   |
| 1   | A     | 162 | GLY  | N-CA-C    | 5.03  | 125.09      | 113.18   |
| 2   | B     | 109 | ILE  | CB-CA-C   | -5.03 | 103.05      | 111.29   |
| 3   | C     | 142 | ILE  | N-CA-CB   | -5.03 | 104.55      | 111.99   |
| 4   | D     | 35  | LEU  | CA-CB-CG  | -5.02 | 98.73       | 116.30   |
| 3   | C     | 232 | THR  | N-CA-C    | 5.02  | 117.52      | 111.40   |
| 1   | A     | 87  | ARG  | CB-CG-CD  | 5.00  | 122.80      | 111.30   |

There are no chirality outliers.

All (27) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | A     | 112 | LYS  | Peptide |
| 1   | A     | 161 | VAL  | Peptide |
| 1   | A     | 2   | ALA  | Peptide |
| 1   | A     | 73  | MET  | Peptide |
| 2   | B     | 124 | PHE  | Peptide |
| 2   | B     | 2   | ALA  | Peptide |
| 2   | B     | 32  | TRP  | Peptide |
| 3   | C     | 191 | GLY  | Peptide |
| 3   | C     | 200 | GLN  | Peptide |
| 3   | C     | 216 | GLU  | Peptide |
| 3   | C     | 222 | GLY  | Peptide |
| 3   | C     | 225 | VAL  | Peptide |
| 3   | C     | 230 | ALA  | Peptide |
| 3   | C     | 81  | GLY  | Peptide |
| 4   | D     | 108 | CYS  | Peptide |
| 4   | D     | 158 | ASP  | Peptide |
| 4   | D     | 65  | LYS  | Peptide |
| 4   | D     | 96  | LYS  | Peptide |
| 4   | D     | 97  | GLU  | Peptide |
| 5   | E     | 28  | SER  | Peptide |
| 6   | F     | 26  | LEU  | Peptide |
| 6   | F     | 27  | LEU  | Peptide |
| 6   | F     | 9   | ALA  | Peptide |
| 7   | G     | 27  | GLN  | Peptide |
| 7   | G     | 31  | ARG  | Peptide |
| 8   | H     | 2   | GLU  | Peptide |
| 8   | H     | 27  | ASN  | 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     | 1711  | 0        | 1736     | 315     | 0            |
| 2   | B     | 1249  | 0        | 1308     | 265     | 0            |
| 3   | C     | 2216  | 0        | 2233     | 418     | 1            |
| 4   | D     | 1288  | 0        | 1273     | 236     | 0            |
| 5   | E     | 248   | 0        | 284      | 41      | 0            |
| 6   | F     | 242   | 0        | 260      | 63      | 0            |
| 7   | G     | 283   | 0        | 289      | 76      | 1            |
| 8   | H     | 230   | 0        | 239      | 52      | 0            |
| 9   | A     | 1     | 0        | 0        | 0       | 0            |
| 10  | A     | 86    | 0        | 60       | 41      | 0            |
| 11  | A     | 43    | 0        | 31       | 24      | 0            |
| 11  | C     | 43    | 0        | 32       | 30      | 0            |
| 12  | A     | 54    | 0        | 79       | 17      | 0            |
| 12  | B     | 54    | 0        | 83       | 2       | 0            |
| 13  | A     | 136   | 0        | 165      | 6       | 0            |
| 14  | B     | 65    | 0        | 72       | 6       | 0            |
| 15  | B     | 60    | 0        | 70       | 39      | 0            |
| 16  | D     | 4     | 0        | 0        | 1       | 0            |
| 17  | D     | 54    | 0        | 53       | 9       | 0            |
| 18  | G     | 40    | 0        | 52       | 9       | 0            |
| 19  | A     | 2     | 0        | 0        | 0       | 0            |
| 19  | B     | 2     | 0        | 0        | 0       | 0            |
| 19  | C     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 8112  | 0        | 8319     | 1394    | 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 85.

All (1394) 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) |
|----------------|-----------------|--------------------------|-------------------|
| 6:F:25:LEU:CD1 | 6:F:25:LEU:CG   | 1.77                     | 1.62              |
| 3:C:256:LYS:CG | 3:C:256:LYS:CD  | 1.80                     | 1.59              |
| 2:B:138:LEU:CG | 2:B:138:LEU:CD1 | 1.74                     | 1.59              |
| 7:G:3:GLU:CD   | 7:G:3:GLU:CG    | 1.76                     | 1.58              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 3:C:256:LYS:CE    | 3:C:256:LYS:NZ     | 1.74                     | 1.50              |
| 1:A:92:MET:CE     | 12:A:1002:OPC:HCB2 | 1.37                     | 1.48              |
| 1:A:113:PRO:CG    | 1:A:113:PRO:CB     | 1.77                     | 1.46              |
| 7:G:29:TYR:O      | 7:G:29:TYR:CD2     | 1.69                     | 1.44              |
| 1:A:92:MET:HE3    | 12:A:1002:OPC:CCB  | 1.45                     | 1.43              |
| 10:A:301:HEM:HBB2 | 10:A:301:HEM:CMB   | 1.35                     | 1.37              |
| 3:C:22:CYS:HB2    | 11:C:301:HEC:CAB   | 1.55                     | 1.35              |
| 6:F:29:ILE:O      | 6:F:29:ILE:CD1     | 1.75                     | 1.35              |
| 6:F:29:ILE:O      | 6:F:29:ILE:HD12    | 1.20                     | 1.33              |
| 4:D:85:LYS:NZ     | 4:D:85:LYS:HB2     | 1.17                     | 1.31              |
| 2:B:93:ASN:OD1    | 2:B:96:LEU:HB2     | 1.25                     | 1.28              |
| 6:F:7:TYR:O       | 6:F:11:LEU:CD1     | 1.83                     | 1.27              |
| 4:D:122:ASN:HB3   | 4:D:135:GLU:OE2    | 1.33                     | 1.26              |
| 3:C:65:GLY:O      | 3:C:66:SER:O       | 1.52                     | 1.26              |
| 2:B:9:LEU:O       | 2:B:15:ARG:HD2     | 1.31                     | 1.24              |
| 3:C:200:GLN:HG3   | 3:C:205:LYS:O      | 1.37                     | 1.24              |
| 4:D:111:LEU:N     | 4:D:111:LEU:CD1    | 2.04                     | 1.19              |
| 3:C:15:GLU:HB3    | 3:C:16:PRO:HD2     | 1.23                     | 1.19              |
| 13:A:1104:UMQ:H31 | 13:A:1104:UMQ:H6'2 | 1.20                     | 1.15              |
| 2:B:142:TRP:CH2   | 2:B:155:LEU:O      | 1.99                     | 1.15              |
| 4:D:85:LYS:NZ     | 4:D:85:LYS:CB      | 2.11                     | 1.14              |
| 3:C:157:ARG:HB2   | 11:C:301:HEC:HAD2  | 1.25                     | 1.14              |
| 4:D:111:LEU:N     | 4:D:111:LEU:HD13   | 1.51                     | 1.14              |
| 10:A:301:HEM:CBB  | 10:A:301:HEM:HMB2  | 1.77                     | 1.13              |
| 1:A:54:MET:CE     | 10:A:301:HEM:HBD1  | 1.78                     | 1.13              |
| 4:D:139:VAL:HG22  | 4:D:147:SER:CA     | 1.77                     | 1.13              |
| 2:B:34:ASN:ND2    | 3:C:283:GLN:HE22   | 1.47                     | 1.12              |
| 3:C:25:CYS:SG     | 11:C:301:HEC:CAC   | 2.38                     | 1.11              |
| 3:C:93:GLU:N      | 3:C:93:GLU:OE1     | 1.83                     | 1.11              |
| 3:C:188:ASP:O     | 3:C:190:TYR:N      | 1.81                     | 1.11              |
| 6:F:11:LEU:HB3    | 6:F:15:LEU:HD12    | 1.32                     | 1.11              |
| 4:D:109:THR:CG2   | 4:D:144:ALA:HB1    | 1.80                     | 1.11              |
| 4:D:146:LEU:HD12  | 4:D:177:TRP:CD2    | 1.84                     | 1.11              |
| 2:B:95:LEU:O      | 2:B:95:LEU:HD23    | 1.49                     | 1.11              |
| 3:C:19:ARG:O      | 3:C:20:ILE:HB      | 1.46                     | 1.11              |
| 3:C:211:ILE:O     | 3:C:211:ILE:HG13   | 1.38                     | 1.10              |
| 2:B:152:ASP:HA    | 2:B:154:THR:HG22   | 1.12                     | 1.10              |
| 6:F:7:TYR:O       | 6:F:11:LEU:HD12    | 0.92                     | 1.10              |
| 1:A:39:ILE:HD11   | 18:G:101:BCR:H312  | 1.17                     | 1.09              |
| 4:D:109:THR:HG22  | 4:D:144:ALA:CB     | 1.82                     | 1.09              |
| 2:B:96:LEU:HD13   | 2:B:100:LEU:CD1    | 1.81                     | 1.09              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:A:1002:OPC:HBV1 | 7:G:9:LEU:HD21     | 1.34                     | 1.09              |
| 15:B:1202:TDS:HAA3 | 15:B:1202:TDS:OAC  | 1.51                     | 1.08              |
| 1:A:163:VAL:HG12   | 1:A:164:LEU:N      | 1.58                     | 1.08              |
| 3:C:171:VAL:HG12   | 3:C:235:PRO:HD2    | 1.11                     | 1.08              |
| 3:C:171:VAL:HG12   | 3:C:235:PRO:CD     | 1.84                     | 1.08              |
| 2:B:91:VAL:HG12    | 2:B:91:VAL:O       | 1.29                     | 1.07              |
| 7:G:2:VAL:CG1      | 7:G:4:PRO:HD3      | 1.84                     | 1.07              |
| 3:C:22:CYS:CB      | 11:C:301:HEC:HAB   | 1.83                     | 1.07              |
| 7:G:26:TYR:O       | 7:G:28:GLN:N       | 1.86                     | 1.07              |
| 1:A:97:MET:HE1     | 1:A:125:ALA:HA     | 1.10                     | 1.06              |
| 1:A:97:MET:CE      | 1:A:125:ALA:HA     | 1.83                     | 1.06              |
| 2:B:124:PHE:HE1    | 7:G:26:TYR:HB2     | 1.20                     | 1.06              |
| 3:C:171:VAL:CG1    | 3:C:235:PRO:HD2    | 1.85                     | 1.06              |
| 1:A:54:MET:HE3     | 10:A:301:HEM:HBD1  | 1.22                     | 1.06              |
| 4:D:137:GLY:HA3    | 4:D:171:ARG:NH1    | 1.71                     | 1.06              |
| 1:A:92:MET:HB3     | 12:A:1002:OPC:HCB1 | 1.38                     | 1.05              |
| 3:C:70:LEU:N       | 3:C:70:LEU:HD23    | 1.69                     | 1.05              |
| 3:C:144:PHE:CZ     | 3:C:251:ASP:HB2    | 1.91                     | 1.05              |
| 1:A:7:TRP:CE2      | 1:A:11:ARG:NH2     | 2.24                     | 1.04              |
| 4:D:139:VAL:H      | 4:D:147:SER:HB3    | 1.16                     | 1.04              |
| 2:B:132:ILE:HD12   | 2:B:132:ILE:H      | 1.22                     | 1.03              |
| 1:A:36:LEU:HB3     | 1:A:100:HIS:HB2    | 1.38                     | 1.03              |
| 10:A:302:HEM:HBC2  | 10:A:302:HEM:HMC2  | 1.40                     | 1.03              |
| 1:A:106:LEU:HD21   | 2:B:133:PHE:CE1    | 1.93                     | 1.02              |
| 1:A:207:ARG:HG3    | 1:A:207:ARG:HH11   | 1.24                     | 1.02              |
| 4:D:122:ASN:CB     | 4:D:135:GLU:OE2    | 2.07                     | 1.02              |
| 7:G:29:TYR:O       | 7:G:29:TYR:CG      | 2.10                     | 1.02              |
| 6:F:11:LEU:HB3     | 6:F:15:LEU:CD1     | 1.89                     | 1.02              |
| 10:A:301:HEM:CMB   | 10:A:301:HEM:CBB   | 2.30                     | 1.01              |
| 3:C:70:LEU:HD23    | 3:C:70:LEU:H       | 1.18                     | 1.01              |
| 3:C:84:ILE:HD11    | 3:C:114:LEU:HD13   | 1.42                     | 1.01              |
| 6:F:13:PHE:CE2     | 6:F:17:PHE:HE1     | 1.79                     | 1.01              |
| 1:A:47:GLN:HE21    | 1:A:47:GLN:CA      | 1.74                     | 1.01              |
| 2:B:96:LEU:HD13    | 2:B:100:LEU:HD11   | 1.39                     | 1.00              |
| 4:D:139:VAL:CG2    | 4:D:147:SER:HB3    | 1.90                     | 1.00              |
| 1:A:113:PRO:HG3    | 2:B:21:GLY:HA3     | 1.39                     | 1.00              |
| 3:C:70:LEU:N       | 3:C:70:LEU:CD2     | 2.25                     | 0.99              |
| 4:D:133:TYR:CE2    | 4:D:148:LEU:HD23   | 1.96                     | 0.99              |
| 1:A:61:THR:HA      | 1:A:177:GLN:HE22   | 1.25                     | 0.99              |
| 1:A:103:ARG:HD2    | 1:A:103:ARG:C      | 1.86                     | 0.98              |
| 3:C:171:VAL:CG1    | 3:C:234:ASN:HD22   | 1.75                     | 0.98              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:A:41:LEU:HD23   | 11:A:303:HEC:CBC   | 1.93                     | 0.98              |
| 1:A:32:ILE:HG22   | 1:A:33:PHE:CD2     | 1.99                     | 0.97              |
| 5:E:22:ILE:O      | 5:E:26:ILE:HB      | 1.63                     | 0.97              |
| 2:B:128:VAL:O     | 2:B:132:ILE:CD1    | 2.12                     | 0.97              |
| 3:C:28:ALA:HB3    | 3:C:239:GLY:HA3    | 1.45                     | 0.97              |
| 3:C:15:GLU:CB     | 3:C:16:PRO:HD2     | 1.95                     | 0.97              |
| 1:A:110:PHE:HD1   | 2:B:112:PRO:HB3    | 1.26                     | 0.97              |
| 1:A:150:ILE:HD13  | 15:B:1201:TDS:CAA  | 1.95                     | 0.96              |
| 5:E:18:ILE:O      | 5:E:22:ILE:HG22    | 1.63                     | 0.96              |
| 3:C:176:ALA:HB1   | 3:C:205:LYS:NZ     | 1.80                     | 0.96              |
| 1:A:26:VAL:HG21   | 1:A:30:VAL:HG11    | 1.47                     | 0.96              |
| 1:A:110:PHE:H     | 1:A:110:PHE:HD2    | 1.09                     | 0.96              |
| 2:B:91:VAL:O      | 2:B:91:VAL:CG1     | 2.07                     | 0.96              |
| 3:C:189:GLU:O     | 3:C:190:TYR:CD2    | 2.18                     | 0.96              |
| 3:C:273:ILE:HG13  | 8:H:21:MET:HG3     | 1.44                     | 0.96              |
| 2:B:82:TYR:N      | 2:B:83:PRO:HD2     | 1.78                     | 0.96              |
| 2:B:142:TRP:HH2   | 2:B:155:LEU:O      | 1.45                     | 0.96              |
| 3:C:120:PRO:HD2   | 3:C:124:TYR:HD1    | 1.30                     | 0.96              |
| 11:A:303:HEC:HBB2 | 11:A:303:HEC:HMB3  | 1.46                     | 0.95              |
| 6:F:20:TRP:O      | 6:F:24:VAL:HG23    | 1.65                     | 0.95              |
| 2:B:128:VAL:O     | 2:B:132:ILE:HD12   | 1.65                     | 0.95              |
| 1:A:150:ILE:HD13  | 15:B:1201:TDS:HAA3 | 1.48                     | 0.95              |
| 10:A:301:HEM:O2D  | 10:A:301:HEM:HBA2  | 1.66                     | 0.95              |
| 3:C:15:GLU:HB3    | 3:C:16:PRO:CD      | 1.96                     | 0.95              |
| 4:D:84:LEU:HD12   | 4:D:84:LEU:H       | 1.31                     | 0.95              |
| 2:B:34:ASN:HD21   | 3:C:283:GLN:NE2    | 1.65                     | 0.95              |
| 3:C:141:ASN:N     | 3:C:141:ASN:HD22   | 1.59                     | 0.95              |
| 1:A:163:VAL:CG1   | 1:A:164:LEU:N      | 2.30                     | 0.95              |
| 2:B:40:PHE:CB     | 2:B:41:PRO:HD3     | 1.95                     | 0.95              |
| 7:G:2:VAL:HG13    | 7:G:4:PRO:HD3      | 1.46                     | 0.94              |
| 1:A:39:ILE:HD11   | 18:G:101:BCR:C31   | 1.97                     | 0.94              |
| 2:B:25:ASN:HD22   | 2:B:25:ASN:H       | 1.15                     | 0.94              |
| 3:C:170:ASN:O     | 3:C:235:PRO:HG3    | 1.67                     | 0.94              |
| 4:D:146:LEU:CD1   | 4:D:177:TRP:CG     | 2.50                     | 0.94              |
| 1:A:31:ASN:C      | 1:A:31:ASN:HD22    | 1.74                     | 0.94              |
| 1:A:147:ALA:HB2   | 15:B:1201:TDS:HAJ3 | 1.46                     | 0.94              |
| 10:A:301:HEM:HBB2 | 10:A:301:HEM:HMB2  | 0.95                     | 0.94              |
| 2:B:152:ASP:CA    | 2:B:154:THR:HG22   | 1.97                     | 0.94              |
| 2:B:93:ASN:OD1    | 2:B:96:LEU:CB      | 2.17                     | 0.93              |
| 6:F:29:ILE:O      | 6:F:29:ILE:HD13    | 1.67                     | 0.93              |
| 1:A:70:GLN:O      | 1:A:74:ASN:HB2     | 1.69                     | 0.93              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 4:D:66:VAL:HG23  | 4:D:158:ASP:O      | 1.69                     | 0.93              |
| 3:C:285:ALA:C    | 3:C:286:GLU:OE1    | 2.11                     | 0.93              |
| 4:D:109:THR:HG22 | 4:D:144:ALA:HB1    | 0.94                     | 0.93              |
| 2:B:109:ILE:O    | 2:B:112:PRO:HD2    | 1.69                     | 0.93              |
| 3:C:288:ASN:C    | 3:C:288:ASN:HD22   | 1.76                     | 0.93              |
| 3:C:200:GLN:CG   | 3:C:205:LYS:O      | 2.16                     | 0.93              |
| 3:C:193:VAL:O    | 3:C:194:LYS:HG2    | 1.69                     | 0.92              |
| 3:C:178:GLY:O    | 3:C:224:ALA:HA     | 1.69                     | 0.92              |
| 2:B:79:TRP:CD1   | 2:B:80:TYR:N       | 2.38                     | 0.92              |
| 11:A:303:HEC:CGA | 15:B:1202:TDS:HAA2 | 2.00                     | 0.92              |
| 3:C:170:ASN:O    | 3:C:235:PRO:CG     | 2.17                     | 0.92              |
| 6:F:29:ILE:HD12  | 6:F:29:ILE:C       | 1.96                     | 0.91              |
| 3:C:180:ILE:HD11 | 3:C:183:ILE:CD1    | 2.00                     | 0.91              |
| 3:C:141:ASN:HD22 | 3:C:141:ASN:H      | 1.12                     | 0.91              |
| 1:A:103:ARG:NH1  | 1:A:104:VAL:HG23   | 1.86                     | 0.91              |
| 3:C:144:PHE:CE2  | 3:C:251:ASP:HB2    | 2.05                     | 0.91              |
| 1:A:39:ILE:CD1   | 18:G:101:BCR:H312  | 2.01                     | 0.90              |
| 2:B:96:LEU:CD1   | 2:B:100:LEU:HD11   | 2.01                     | 0.90              |
| 1:A:47:GLN:HE21  | 1:A:47:GLN:HA      | 1.31                     | 0.90              |
| 1:A:112:LYS:O    | 1:A:113:PRO:C      | 2.12                     | 0.90              |
| 4:D:94:GLU:OE2   | 4:D:100:ARG:HG2    | 1.70                     | 0.90              |
| 3:C:200:GLN:O    | 3:C:205:LYS:HG2    | 1.70                     | 0.90              |
| 7:G:11:LEU:N     | 7:G:11:LEU:HD23    | 1.85                     | 0.90              |
| 2:B:115:GLU:OE2  | 2:B:126:ARG:NH1    | 2.04                     | 0.90              |
| 4:D:146:LEU:HD12 | 4:D:177:TRP:CG     | 2.06                     | 0.90              |
| 1:A:26:VAL:CG2   | 1:A:30:VAL:HG11    | 2.02                     | 0.90              |
| 11:A:303:HEC:O2A | 15:B:1202:TDS:HAA2 | 1.71                     | 0.90              |
| 2:B:57:LEU:HD12  | 8:H:8:TRP:CE3      | 2.06                     | 0.90              |
| 2:B:138:LEU:CD1  | 2:B:138:LEU:HG     | 2.01                     | 0.90              |
| 4:D:139:VAL:HG22 | 4:D:147:SER:CB     | 2.01                     | 0.90              |
| 3:C:211:ILE:O    | 3:C:212:PRO:O      | 1.91                     | 0.89              |
| 3:C:119:LEU:CD2  | 3:C:124:TYR:CD1    | 2.55                     | 0.89              |
| 2:B:88:LEU:HD13  | 15:B:1201:TDS:CAI  | 2.03                     | 0.89              |
| 2:B:124:PHE:CE1  | 7:G:26:TYR:HB2     | 2.07                     | 0.89              |
| 1:A:30:VAL:HG22  | 1:A:34:TYR:CG      | 2.08                     | 0.89              |
| 1:A:47:GLN:HA    | 1:A:47:GLN:NE2     | 1.87                     | 0.89              |
| 4:D:139:VAL:HG23 | 4:D:147:SER:HB3    | 1.54                     | 0.89              |
| 3:C:40:VAL:HG12  | 8:H:1:MET:HE1      | 1.56                     | 0.89              |
| 3:C:60:GLN:HE22  | 3:C:157:ARG:HG2    | 1.36                     | 0.89              |
| 1:A:108:GLY:HA2  | 1:A:110:PHE:CE2    | 2.07                     | 0.88              |
| 4:D:85:LYS:HB2   | 4:D:85:LYS:HZ3     | 1.06                     | 0.88              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 7:G:10:VAL:HG12  | 7:G:11:LEU:HD23   | 1.55                     | 0.88              |
| 2:B:152:ASP:HA   | 2:B:154:THR:CG2   | 2.03                     | 0.88              |
| 6:F:6:LEU:O      | 6:F:10:LEU:HB2    | 1.74                     | 0.88              |
| 7:G:29:TYR:O     | 7:G:29:TYR:HD2    | 1.55                     | 0.88              |
| 4:D:139:VAL:HG22 | 4:D:147:SER:HA    | 1.54                     | 0.88              |
| 3:C:171:VAL:HG11 | 3:C:234:ASN:HD22  | 1.36                     | 0.88              |
| 1:A:103:ARG:HH12 | 1:A:104:VAL:HG23  | 1.38                     | 0.87              |
| 3:C:22:CYS:HB2   | 11:C:301:HEC:HAB  | 0.89                     | 0.87              |
| 3:C:71:ASN:HB2   | 11:C:301:HEC:O2A  | 1.74                     | 0.87              |
| 2:B:118:ASN:HD22 | 2:B:120:PHE:H     | 1.22                     | 0.87              |
| 1:A:100:HIS:HE1  | 10:A:302:HEM:C1A  | 1.93                     | 0.87              |
| 3:C:119:LEU:HD23 | 3:C:124:TYR:CD1   | 2.10                     | 0.87              |
| 4:D:110:HIS:HB3  | 16:D:200:FES:S2   | 2.14                     | 0.87              |
| 2:B:4:LEU:H      | 3:C:287:MET:CE    | 1.87                     | 0.86              |
| 2:B:79:TRP:CG    | 2:B:80:TYR:N      | 2.43                     | 0.86              |
| 3:C:52:ILE:O     | 3:C:52:ILE:HG22   | 1.75                     | 0.86              |
| 1:A:163:VAL:HG12 | 1:A:164:LEU:H     | 1.40                     | 0.86              |
| 4:D:109:THR:HG21 | 4:D:146:LEU:O     | 1.74                     | 0.86              |
| 6:F:22:LEU:HD13  | 6:F:22:LEU:C      | 1.99                     | 0.86              |
| 4:D:85:LYS:CB    | 4:D:85:LYS:HZ3    | 1.83                     | 0.86              |
| 4:D:134:ASP:OD1  | 4:D:134:ASP:C     | 2.18                     | 0.86              |
| 1:A:61:THR:HG22  | 1:A:64:GLU:H      | 1.41                     | 0.86              |
| 3:C:22:CYS:CB    | 11:C:301:HEC:CAB  | 2.50                     | 0.86              |
| 3:C:211:ILE:O    | 3:C:211:ILE:CG1   | 2.22                     | 0.86              |
| 3:C:219:VAL:HG12 | 3:C:219:VAL:O     | 1.73                     | 0.86              |
| 6:F:25:LEU:CD1   | 6:F:25:LEU:HG     | 2.05                     | 0.86              |
| 3:C:223:GLN:HG3  | 3:C:224:ALA:H     | 1.41                     | 0.85              |
| 4:D:21:LEU:HD11  | 17:D:201:SQD:H301 | 1.58                     | 0.85              |
| 4:D:102:TYR:HA   | 4:D:151:CYS:O     | 1.76                     | 0.85              |
| 4:D:69:PHE:HD2   | 4:D:69:PHE:C      | 1.83                     | 0.85              |
| 1:A:26:VAL:CG2   | 1:A:30:VAL:CG1    | 2.54                     | 0.85              |
| 1:A:39:ILE:HG22  | 1:A:96:MET:HG3    | 1.56                     | 0.85              |
| 3:C:226:LYS:HB3  | 3:C:226:LYS:HZ3   | 1.40                     | 0.85              |
| 6:F:13:PHE:CE2   | 6:F:17:PHE:CE1    | 2.64                     | 0.85              |
| 3:C:60:GLN:NE2   | 3:C:157:ARG:HG2   | 1.90                     | 0.85              |
| 3:C:71:ASN:N     | 11:C:301:HEC:O2A  | 2.10                     | 0.85              |
| 3:C:28:ALA:HB3   | 3:C:239:GLY:CA    | 2.07                     | 0.85              |
| 2:B:77:PRO:HB3   | 15:B:1201:TDS:CAM | 2.07                     | 0.85              |
| 4:D:68:LYS:HA    | 4:D:71:GLU:HB2    | 1.59                     | 0.85              |
| 2:B:95:LEU:HD23  | 2:B:95:LEU:C      | 2.02                     | 0.84              |
| 3:C:259:ILE:HD12 | 8:H:6:LEU:HD13    | 1.57                     | 0.84              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 4:D:110:HIS:C     | 4:D:111:LEU:CD1    | 2.50                     | 0.84              |
| 2:B:114:ILE:HG22  | 2:B:115:GLU:N      | 1.90                     | 0.84              |
| 6:F:5:MET:HG2     | 6:F:6:LEU:N        | 1.92                     | 0.84              |
| 14:B:201:CLA:HBB1 | 14:B:201:CLA:HMB1  | 1.57                     | 0.84              |
| 3:C:46:PHE:CE2    | 3:C:131:VAL:HG22   | 2.13                     | 0.83              |
| 1:A:142:GLN:OE1   | 1:A:142:GLN:HA     | 1.78                     | 0.83              |
| 11:C:301:HEC:HMC1 | 11:C:301:HEC:HBC3  | 1.60                     | 0.83              |
| 11:A:303:HEC:HBB2 | 11:A:303:HEC:CMB   | 2.09                     | 0.83              |
| 2:B:34:ASN:HD21   | 3:C:283:GLN:HE22   | 0.88                     | 0.83              |
| 2:B:79:TRP:CD1    | 2:B:79:TRP:C       | 2.57                     | 0.83              |
| 2:B:82:TYR:HB2    | 2:B:83:PRO:HD3     | 1.59                     | 0.83              |
| 1:A:103:ARG:HD2   | 1:A:103:ARG:O      | 1.79                     | 0.83              |
| 4:D:143:PRO:O     | 4:D:145:PRO:HD3    | 1.79                     | 0.82              |
| 1:A:92:MET:CB     | 12:A:1002:OPC:HCB1 | 2.08                     | 0.82              |
| 5:E:5:ALA:O       | 5:E:9:ILE:HG13     | 1.80                     | 0.82              |
| 2:B:159:LEU:O     | 2:B:160:PHE:CD2    | 2.33                     | 0.82              |
| 1:A:215:LEU:HD13  | 2:B:122:ASN:HA     | 1.61                     | 0.82              |
| 2:B:70:ALA:HB1    | 3:C:17:THR:HG22    | 1.61                     | 0.82              |
| 4:D:111:LEU:N     | 4:D:111:LEU:HD12   | 1.90                     | 0.82              |
| 4:D:139:VAL:H     | 4:D:147:SER:CB     | 1.92                     | 0.82              |
| 4:D:133:TYR:CD2   | 4:D:148:LEU:HD23   | 2.15                     | 0.81              |
| 4:D:21:LEU:CD1    | 17:D:201:SQD:H301  | 2.10                     | 0.81              |
| 1:A:26:VAL:HG21   | 1:A:30:VAL:CG1     | 2.10                     | 0.81              |
| 4:D:102:TYR:OH    | 4:D:136:THR:HG22   | 1.80                     | 0.81              |
| 1:A:108:GLY:HA2   | 1:A:110:PHE:HE2    | 1.45                     | 0.81              |
| 3:C:229:GLU:HA    | 3:C:229:GLU:OE1    | 1.78                     | 0.81              |
| 3:C:13:PRO:O      | 3:C:21:VAL:HG22    | 1.81                     | 0.81              |
| 2:B:130:THR:CG2   | 7:G:22:PHE:HE2     | 1.93                     | 0.81              |
| 2:B:82:TYR:N      | 2:B:83:PRO:CD      | 2.44                     | 0.81              |
| 3:C:139:ASP:OD1   | 3:C:139:ASP:C      | 2.19                     | 0.81              |
| 3:C:119:LEU:CD2   | 3:C:124:TYR:CE1    | 2.64                     | 0.81              |
| 4:D:80:LEU:C      | 4:D:81:VAL:HG23    | 2.05                     | 0.81              |
| 1:A:155:PRO:HD3   | 15:B:1201:TDS:HAX2 | 1.63                     | 0.80              |
| 3:C:171:VAL:CG1   | 3:C:234:ASN:HA     | 2.11                     | 0.80              |
| 5:E:10:VAL:O      | 5:E:14:LEU:HB2     | 1.81                     | 0.80              |
| 10:A:302:HEM:HMC2 | 10:A:302:HEM:CBC   | 2.11                     | 0.80              |
| 4:D:12:ASP:O      | 4:D:13:MET:C       | 2.23                     | 0.80              |
| 4:D:137:GLY:HA3   | 4:D:171:ARG:HH11   | 1.46                     | 0.80              |
| 2:B:57:LEU:HD12   | 8:H:8:TRP:CD2      | 2.17                     | 0.80              |
| 3:C:250:GLN:HG3   | 3:C:251:ASP:N      | 1.97                     | 0.80              |
| 2:B:118:ASN:ND2   | 2:B:120:PHE:H      | 1.78                     | 0.80              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 2:B:90:SER:O     | 2:B:91:VAL:HG23    | 1.81                     | 0.80              |
| 2:B:57:LEU:CD1   | 8:H:8:TRP:CD2      | 2.64                     | 0.80              |
| 4:D:139:VAL:HG22 | 4:D:147:SER:HB3    | 1.60                     | 0.80              |
| 4:D:139:VAL:HG22 | 4:D:147:SER:N      | 1.97                     | 0.80              |
| 2:B:91:VAL:O     | 2:B:93:ASN:N       | 2.15                     | 0.79              |
| 3:C:107:LYS:HE3  | 3:C:110:GLN:HE22   | 1.45                     | 0.79              |
| 3:C:177:THR:HG21 | 3:C:226:LYS:HD2    | 1.62                     | 0.79              |
| 5:E:8:TYR:CZ     | 5:E:12:ILE:HD11    | 2.17                     | 0.79              |
| 6:F:24:VAL:O     | 6:F:27:LEU:HB2     | 1.81                     | 0.79              |
| 1:A:7:TRP:NE1    | 1:A:11:ARG:NH2     | 2.29                     | 0.79              |
| 3:C:84:ILE:HD11  | 3:C:114:LEU:CD1    | 2.12                     | 0.79              |
| 1:A:110:PHE:CD1  | 2:B:112:PRO:HB3    | 2.15                     | 0.79              |
| 3:C:226:LYS:HB3  | 3:C:226:LYS:NZ     | 1.96                     | 0.79              |
| 4:D:105:ASN:HB3  | 4:D:149:ALA:HB3    | 1.63                     | 0.79              |
| 7:G:26:TYR:C     | 7:G:28:GLN:H       | 1.91                     | 0.79              |
| 2:B:104:VAL:O    | 2:B:108:LEU:HB2    | 1.81                     | 0.79              |
| 4:D:85:LYS:HB2   | 4:D:85:LYS:HZ2     | 0.97                     | 0.79              |
| 1:A:207:ARG:NH1  | 15:B:1202:TDS:HAI2 | 1.98                     | 0.79              |
| 3:C:206:THR:CG2  | 3:C:206:THR:O      | 2.30                     | 0.78              |
| 1:A:36:LEU:HD21  | 1:A:99:LEU:HB3     | 1.65                     | 0.78              |
| 3:C:107:LYS:HE3  | 3:C:110:GLN:NE2    | 1.97                     | 0.78              |
| 3:C:141:ASN:N    | 3:C:141:ASN:ND2    | 2.31                     | 0.78              |
| 4:D:69:PHE:C     | 4:D:69:PHE:CD2     | 2.61                     | 0.78              |
| 4:D:85:LYS:CB    | 4:D:85:LYS:HZ2     | 1.83                     | 0.78              |
| 4:D:105:ASN:HD21 | 4:D:107:VAL:HG23   | 1.46                     | 0.78              |
| 3:C:46:PHE:CZ    | 3:C:131:VAL:HG22   | 2.19                     | 0.78              |
| 10:A:302:HEM:HHA | 10:A:302:HEM:HBA1  | 1.66                     | 0.78              |
| 1:A:83:ARG:HD2   | 10:A:301:HEM:O1D   | 1.84                     | 0.78              |
| 3:C:171:VAL:CG1  | 3:C:234:ASN:ND2    | 2.46                     | 0.78              |
| 3:C:199:ILE:O    | 3:C:200:GLN:HB2    | 1.82                     | 0.78              |
| 3:C:120:PRO:HD2  | 3:C:124:TYR:CD1    | 2.18                     | 0.77              |
| 3:C:107:LYS:CE   | 3:C:110:GLN:HE22   | 1.96                     | 0.77              |
| 3:C:219:VAL:O    | 3:C:219:VAL:CG1    | 2.32                     | 0.77              |
| 3:C:286:GLU:OE1  | 3:C:286:GLU:N      | 2.17                     | 0.77              |
| 4:D:21:LEU:HD12  | 17:D:201:SQD:H282  | 1.66                     | 0.77              |
| 2:B:40:PHE:HB2   | 2:B:41:PRO:HD3     | 1.64                     | 0.77              |
| 6:F:29:ILE:CD1   | 6:F:29:ILE:C       | 2.57                     | 0.77              |
| 3:C:176:ALA:HB1  | 3:C:205:LYS:HZ1    | 1.49                     | 0.77              |
| 3:C:19:ARG:O     | 3:C:20:ILE:CB      | 2.20                     | 0.77              |
| 3:C:180:ILE:HD11 | 3:C:183:ILE:HD12   | 1.67                     | 0.77              |
| 1:A:103:ARG:HA   | 7:G:21:LEU:HD21    | 1.67                     | 0.77              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 10:A:301:HEM:HBB2 | 10:A:301:HEM:HMB3  | 1.63                     | 0.77              |
| 3:C:119:LEU:HD23  | 3:C:124:TYR:CE1    | 2.19                     | 0.77              |
| 3:C:270:LEU:HA    | 8:H:21:MET:CE      | 2.15                     | 0.77              |
| 4:D:80:LEU:C      | 4:D:81:VAL:CG2     | 2.56                     | 0.77              |
| 5:E:29:ILE:HG22   | 5:E:29:ILE:O       | 1.85                     | 0.77              |
| 3:C:171:VAL:HG11  | 3:C:234:ASN:HA     | 1.64                     | 0.77              |
| 4:D:110:HIS:C     | 4:D:111:LEU:HD12   | 2.08                     | 0.77              |
| 4:D:139:VAL:CG2   | 4:D:147:SER:N      | 2.48                     | 0.77              |
| 1:A:207:ARG:HH11  | 1:A:207:ARG:CG     | 1.97                     | 0.77              |
| 2:B:16:ALA:O      | 2:B:19:ALA:HB3     | 1.85                     | 0.77              |
| 3:C:178:GLY:O     | 3:C:224:ALA:CA     | 2.32                     | 0.77              |
| 3:C:178:GLY:O     | 3:C:224:ALA:CB     | 2.33                     | 0.76              |
| 12:A:1002:OPC:CBV | 7:G:9:LEU:HD21     | 2.13                     | 0.76              |
| 4:D:161:VAL:HG12  | 4:D:161:VAL:O      | 1.83                     | 0.76              |
| 4:D:12:ASP:O      | 4:D:14:GLY:N       | 2.18                     | 0.76              |
| 1:A:150:ILE:CD1   | 15:B:1201:TDS:CAA  | 2.64                     | 0.76              |
| 2:B:10:SER:O      | 2:B:12:PRO:HD3     | 1.86                     | 0.76              |
| 3:C:14:ARG:CZ     | 3:C:150:HIS:CD2    | 2.69                     | 0.76              |
| 3:C:200:GLN:NE2   | 3:C:206:THR:OG1    | 2.19                     | 0.76              |
| 6:F:13:PHE:HE2    | 6:F:17:PHE:CE1     | 2.02                     | 0.76              |
| 4:D:69:PHE:O      | 4:D:70:LEU:O       | 2.03                     | 0.76              |
| 4:D:108:CYS:HB2   | 4:D:133:TYR:OH     | 1.86                     | 0.76              |
| 3:C:71:ASN:OD1    | 3:C:120:PRO:HA     | 1.86                     | 0.75              |
| 3:C:270:LEU:HB2   | 8:H:21:MET:CE      | 2.16                     | 0.75              |
| 4:D:139:VAL:CG2   | 4:D:147:SER:CB     | 2.60                     | 0.75              |
| 4:D:150:LEU:HD21  | 4:D:171:ARG:NH1    | 2.01                     | 0.75              |
| 2:B:152:ASP:C     | 2:B:154:THR:H      | 1.94                     | 0.75              |
| 3:C:172:PHE:CD1   | 3:C:172:PHE:N      | 2.54                     | 0.75              |
| 4:D:111:LEU:HD13  | 4:D:111:LEU:H      | 1.45                     | 0.75              |
| 2:B:81:LEU:CD1    | 15:B:1201:TDS:HAR1 | 2.16                     | 0.75              |
| 4:D:15:ARG:HB3    | 5:E:31:LEU:CD2     | 2.15                     | 0.75              |
| 3:C:171:VAL:HG13  | 3:C:234:ASN:HD22   | 1.50                     | 0.75              |
| 3:C:225:VAL:HG12  | 3:C:229:GLU:CG     | 2.17                     | 0.75              |
| 4:D:64:VAL:HG13   | 4:D:69:PHE:HD1     | 1.51                     | 0.75              |
| 11:C:301:HEC:CMB  | 11:C:301:HEC:HBB3  | 2.17                     | 0.75              |
| 3:C:180:ILE:HD11  | 3:C:183:ILE:HD11   | 1.68                     | 0.75              |
| 3:C:171:VAL:HG13  | 3:C:234:ASN:ND2    | 2.03                     | 0.74              |
| 1:A:147:ALA:HB2   | 15:B:1201:TDS:CAJ  | 2.16                     | 0.74              |
| 2:B:123:PRO:HA    | 2:B:126:ARG:HG3    | 1.69                     | 0.74              |
| 3:C:270:LEU:HB2   | 8:H:21:MET:HE2     | 1.70                     | 0.74              |
| 4:D:146:LEU:HD13  | 4:D:177:TRP:CG     | 2.23                     | 0.74              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 4:D:66:VAL:HG23   | 4:D:158:ASP:C      | 2.13                     | 0.74              |
| 1:A:202:HIS:O     | 1:A:206:ILE:HG13   | 1.87                     | 0.74              |
| 1:A:150:ILE:CD1   | 15:B:1201:TDS:HAA3 | 2.18                     | 0.74              |
| 2:B:25:ASN:H      | 2:B:25:ASN:ND2     | 1.86                     | 0.74              |
| 11:A:303:HEC:O2A  | 15:B:1202:TDS:CAA  | 2.35                     | 0.74              |
| 3:C:270:LEU:HA    | 8:H:21:MET:HE2     | 1.70                     | 0.74              |
| 3:C:285:ALA:HB2   | 4:D:10:VAL:HG21    | 1.68                     | 0.74              |
| 4:D:146:LEU:CD1   | 4:D:177:TRP:CD2    | 2.66                     | 0.74              |
| 8:H:19:ILE:HG22   | 8:H:20:ALA:N       | 2.03                     | 0.74              |
| 13:A:1101:UMQ:H51 | 13:A:1101:UMQ:H6'1 | 1.69                     | 0.73              |
| 3:C:119:LEU:HD22  | 3:C:124:TYR:CD1    | 2.21                     | 0.73              |
| 2:B:45:MET:HE1    | 4:D:27:VAL:HG22    | 1.70                     | 0.73              |
| 3:C:4:TRP:CD2     | 3:C:162:PRO:HG3    | 2.23                     | 0.73              |
| 3:C:221:GLU:OE1   | 3:C:222:GLY:N      | 2.22                     | 0.73              |
| 3:C:229:GLU:CD    | 3:C:230:ALA:H      | 1.96                     | 0.73              |
| 1:A:127:ILE:CG2   | 1:A:195:ILE:HG13   | 2.18                     | 0.73              |
| 1:A:47:GLN:HE21   | 1:A:47:GLN:N       | 1.87                     | 0.73              |
| 4:D:117:TRP:CH2   | 4:D:122:ASN:C      | 2.67                     | 0.73              |
| 3:C:94:LEU:O      | 3:C:94:LEU:HD23    | 1.89                     | 0.73              |
| 1:A:112:LYS:O     | 1:A:114:ARG:N      | 2.21                     | 0.73              |
| 2:B:82:TYR:H      | 2:B:83:PRO:HD2     | 1.53                     | 0.73              |
| 2:B:9:LEU:O       | 2:B:15:ARG:CD      | 2.25                     | 0.73              |
| 7:G:2:VAL:HG12    | 7:G:2:VAL:O        | 1.87                     | 0.73              |
| 3:C:226:LYS:NZ    | 3:C:226:LYS:CB     | 2.52                     | 0.72              |
| 8:H:1:MET:O       | 8:H:2:GLU:HB3      | 1.87                     | 0.72              |
| 1:A:7:TRP:NE1     | 1:A:11:ARG:HH21    | 1.83                     | 0.72              |
| 2:B:124:PHE:HE1   | 7:G:26:TYR:CB      | 1.99                     | 0.72              |
| 3:C:65:GLY:C      | 3:C:66:SER:O       | 2.32                     | 0.72              |
| 1:A:33:PHE:CD1    | 7:G:21:LEU:HD13    | 2.24                     | 0.72              |
| 2:B:88:LEU:HD13   | 15:B:1201:TDS:HAI3 | 1.72                     | 0.72              |
| 3:C:23:ALA:HB2    | 3:C:240:PHE:CE2    | 2.24                     | 0.72              |
| 3:C:189:GLU:O     | 3:C:190:TYR:HD2    | 1.70                     | 0.72              |
| 1:A:100:HIS:CE1   | 10:A:302:HEM:C1A   | 2.76                     | 0.72              |
| 1:A:111:LYS:O     | 1:A:113:PRO:HD2    | 1.90                     | 0.72              |
| 2:B:14:LEU:HD11   | 2:B:18:LEU:HD11    | 1.71                     | 0.72              |
| 5:E:10:VAL:HG12   | 5:E:14:LEU:HD12    | 1.69                     | 0.72              |
| 8:H:23:VAL:HA     | 8:H:28:GLY:HA3     | 1.72                     | 0.72              |
| 1:A:166:SER:HB3   | 1:A:170:ARG:NH2    | 2.04                     | 0.72              |
| 3:C:15:GLU:CB     | 3:C:16:PRO:CD      | 2.60                     | 0.72              |
| 6:F:27:LEU:O      | 6:F:30:GLN:HG3     | 1.89                     | 0.72              |
| 11:A:303:HEC:CHB  | 15:B:1202:TDS:OAK  | 2.37                     | 0.72              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:B:126:ARG:N     | 2:B:127:PRO:HD3    | 2.04                     | 0.72              |
| 3:C:54:TYR:HE1    | 3:C:70:LEU:HD21    | 1.54                     | 0.72              |
| 2:B:132:ILE:HD12  | 2:B:132:ILE:N      | 2.00                     | 0.72              |
| 3:C:237:VAL:HG22  | 3:C:237:VAL:O      | 1.88                     | 0.72              |
| 2:B:149:PHE:HB3   | 2:B:150:PRO:CD     | 2.19                     | 0.72              |
| 3:C:19:ARG:O      | 3:C:242:GLN:OE1    | 2.08                     | 0.72              |
| 1:A:31:ASN:C      | 1:A:31:ASN:ND2     | 2.45                     | 0.71              |
| 5:E:6:VAL:O       | 5:E:10:VAL:HG23    | 1.89                     | 0.71              |
| 7:G:24:ALA:O      | 7:G:28:GLN:HB2     | 1.90                     | 0.71              |
| 13:A:1104:UMQ:H31 | 13:A:1104:UMQ:C6'  | 2.10                     | 0.71              |
| 1:A:36:LEU:HB3    | 1:A:100:HIS:CB     | 2.20                     | 0.71              |
| 1:A:36:LEU:CD2    | 1:A:99:LEU:HB3     | 2.20                     | 0.71              |
| 11:A:303:HEC:CBA  | 15:B:1202:TDS:HAA2 | 2.21                     | 0.71              |
| 2:B:118:ASN:ND2   | 2:B:120:PHE:CD1    | 2.59                     | 0.71              |
| 3:C:223:GLN:HG3   | 3:C:224:ALA:N      | 2.05                     | 0.71              |
| 1:A:20:ASP:O      | 1:A:20:ASP:OD2     | 2.08                     | 0.71              |
| 1:A:83:ARG:NH1    | 10:A:301:HEM:O2A   | 2.23                     | 0.71              |
| 4:D:170:PHE:CE2   | 4:D:171:ARG:HG3    | 2.26                     | 0.71              |
| 3:C:174:ALA:HB2   | 3:C:231:LEU:HD23   | 1.73                     | 0.71              |
| 5:E:9:ILE:O       | 5:E:13:ALA:HB2     | 1.91                     | 0.71              |
| 1:A:111:LYS:HE2   | 2:B:115:GLU:O      | 1.91                     | 0.71              |
| 2:B:77:PRO:HA     | 15:B:1201:TDS:HAJ2 | 1.73                     | 0.71              |
| 3:C:94:LEU:HD23   | 3:C:94:LEU:C       | 2.15                     | 0.70              |
| 3:C:259:ILE:CD1   | 8:H:6:LEU:HD13     | 2.21                     | 0.70              |
| 3:C:9:TYR:CG      | 3:C:21:VAL:HG11    | 2.26                     | 0.70              |
| 6:F:16:ILE:HG22   | 6:F:17:PHE:N       | 2.05                     | 0.70              |
| 1:A:32:ILE:CG2    | 1:A:33:PHE:N       | 2.54                     | 0.70              |
| 3:C:275:LYS:HE2   | 4:D:20:ASN:OD1     | 1.90                     | 0.70              |
| 1:A:54:MET:HE1    | 10:A:301:HEM:HBD1  | 1.70                     | 0.70              |
| 1:A:54:MET:CE     | 10:A:301:HEM:CBD   | 2.66                     | 0.70              |
| 2:B:79:TRP:CG     | 2:B:80:TYR:H       | 2.10                     | 0.70              |
| 3:C:264:LEU:O     | 3:C:264:LEU:HD22   | 1.91                     | 0.70              |
| 7:G:26:TYR:O      | 7:G:27:GLN:C       | 2.32                     | 0.70              |
| 1:A:110:PHE:N     | 1:A:110:PHE:CD2    | 2.56                     | 0.70              |
| 1:A:92:MET:CE     | 12:A:1002:OPC:CCB  | 2.27                     | 0.70              |
| 13:A:1104:UMQ:O3' | 13:A:1104:UMQ:H11  | 1.92                     | 0.70              |
| 3:C:22:CYS:O      | 3:C:24:ASN:N       | 2.24                     | 0.70              |
| 7:G:26:TYR:C      | 7:G:28:GLN:N       | 2.48                     | 0.70              |
| 11:C:301:HEC:HBB3 | 11:C:301:HEC:HMB1  | 1.72                     | 0.70              |
| 2:B:123:PRO:HD3   | 7:G:25:ALA:HB1     | 1.73                     | 0.70              |
| 4:D:55:THR:HG23   | 4:D:159:ASN:HB3    | 1.74                     | 0.70              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:F:11:LEU:O      | 6:F:15:LEU:HB2    | 1.91                     | 0.70              |
| 6:F:13:PHE:C      | 6:F:13:PHE:CD2    | 2.70                     | 0.70              |
| 2:B:40:PHE:CB     | 2:B:41:PRO:CD     | 2.70                     | 0.69              |
| 1:A:127:ILE:HG22  | 1:A:195:ILE:HG13  | 1.74                     | 0.69              |
| 2:B:147:ALA:C     | 2:B:149:PHE:N     | 2.48                     | 0.69              |
| 3:C:270:LEU:CA    | 8:H:21:MET:HE2    | 2.21                     | 0.69              |
| 4:D:63:ASN:O      | 4:D:64:VAL:C      | 2.34                     | 0.69              |
| 4:D:146:LEU:HD13  | 4:D:177:TRP:CB    | 2.23                     | 0.69              |
| 1:A:39:ILE:CG2    | 1:A:96:MET:HG3    | 2.22                     | 0.69              |
| 1:A:61:THR:HA     | 1:A:177:GLN:NE2   | 2.03                     | 0.69              |
| 3:C:60:GLN:OE1    | 3:C:70:LEU:HB3    | 1.91                     | 0.69              |
| 4:D:9:ASP:HA      | 5:E:30:LYS:NZ     | 2.07                     | 0.69              |
| 14:B:201:CLA:HBB1 | 14:B:201:CLA:CMB  | 2.22                     | 0.69              |
| 4:D:55:THR:HG21   | 4:D:63:ASN:OD1    | 1.92                     | 0.69              |
| 5:E:26:ILE:CG2    | 5:E:32:ILE:HG13   | 2.22                     | 0.69              |
| 2:B:57:LEU:HD11   | 8:H:8:TRP:HA      | 1.75                     | 0.69              |
| 3:C:270:LEU:C     | 3:C:270:LEU:HD13  | 2.17                     | 0.69              |
| 3:C:270:LEU:HD13  | 3:C:271:MET:N     | 2.08                     | 0.69              |
| 4:D:178:TRP:CD1   | 4:D:179:VAL:HB    | 2.27                     | 0.69              |
| 1:A:72:ILE:O      | 1:A:79:GLY:HA3    | 1.93                     | 0.69              |
| 3:C:259:ILE:HD12  | 8:H:6:LEU:CD1     | 2.22                     | 0.69              |
| 3:C:172:PHE:HD1   | 3:C:172:PHE:H     | 1.41                     | 0.68              |
| 3:C:25:CYS:SG     | 11:C:301:HEC:CBC  | 2.81                     | 0.68              |
| 3:C:180:ILE:CD1   | 3:C:183:ILE:HD11  | 2.23                     | 0.68              |
| 3:C:176:ALA:HB1   | 3:C:205:LYS:HZ2   | 1.57                     | 0.68              |
| 3:C:221:GLU:OE1   | 3:C:221:GLU:HA    | 1.93                     | 0.68              |
| 5:E:14:LEU:O      | 5:E:18:ILE:HG12   | 1.92                     | 0.68              |
| 2:B:4:LEU:H       | 3:C:287:MET:HE1   | 1.56                     | 0.68              |
| 2:B:40:PHE:HZ     | 15:B:1202:TDS:HBD | 1.41                     | 0.68              |
| 2:B:42:VAL:HG13   | 3:C:269:GLN:HB3   | 1.75                     | 0.68              |
| 3:C:188:ASP:C     | 3:C:190:TYR:H     | 1.99                     | 0.68              |
| 6:F:11:LEU:CB     | 6:F:15:LEU:HD12   | 2.19                     | 0.68              |
| 2:B:95:LEU:HD21   | 2:B:99:LEU:HD11   | 1.74                     | 0.68              |
| 2:B:122:ASN:HD21  | 7:G:29:TYR:HB2    | 1.59                     | 0.68              |
| 1:A:26:VAL:HG22   | 1:A:30:VAL:HG12   | 1.75                     | 0.68              |
| 1:A:127:ILE:HG21  | 1:A:195:ILE:CG1   | 2.22                     | 0.68              |
| 3:C:34:VAL:HG21   | 3:C:151:LEU:CB    | 2.24                     | 0.68              |
| 15:B:1202:TDS:OAC | 15:B:1202:TDS:CAA | 2.38                     | 0.67              |
| 4:D:104:ILE:HG22  | 4:D:148:LEU:HD12  | 1.77                     | 0.67              |
| 11:C:301:HEC:HMC1 | 11:C:301:HEC:CBC  | 2.25                     | 0.67              |
| 1:A:88:TRP:CZ3    | 2:B:54:LEU:HD13   | 2.29                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:23:ALA:HB2    | 3:C:240:PHE:CD2   | 2.29                     | 0.67              |
| 4:D:32:LEU:O      | 4:D:33:GLY:C      | 2.36                     | 0.67              |
| 4:D:110:HIS:C     | 4:D:111:LEU:HD13  | 2.15                     | 0.67              |
| 3:C:14:ARG:NH2    | 3:C:150:HIS:CD2   | 2.63                     | 0.67              |
| 4:D:65:LYS:CB     | 4:D:68:LYS:HZ1    | 2.08                     | 0.67              |
| 4:D:117:TRP:CZ2   | 4:D:122:ASN:HA    | 2.28                     | 0.67              |
| 4:D:100:ARG:NH1   | 4:D:102:TYR:OH    | 2.28                     | 0.67              |
| 2:B:128:VAL:O     | 2:B:132:ILE:HD11  | 1.93                     | 0.67              |
| 3:C:101:VAL:HG11  | 3:C:103:PHE:CE2   | 2.29                     | 0.67              |
| 7:G:29:TYR:CD2    | 7:G:29:TYR:C      | 2.66                     | 0.67              |
| 8:H:23:VAL:O      | 8:H:24:TRP:C      | 2.33                     | 0.66              |
| 1:A:41:LEU:HD23   | 11:A:303:HEC:HBC1 | 1.76                     | 0.66              |
| 2:B:21:GLY:O      | 2:B:22:MET:HB3    | 1.93                     | 0.66              |
| 7:G:20:GLY:N      | 18:G:101:BCR:H363 | 2.10                     | 0.66              |
| 1:A:82:ILE:HG12   | 4:D:41:TYR:CD1    | 2.31                     | 0.66              |
| 3:C:288:ASN:C     | 3:C:288:ASN:ND2   | 2.48                     | 0.66              |
| 3:C:41:LEU:HB2    | 8:H:1:MET:SD      | 2.36                     | 0.66              |
| 3:C:215:PRO:HB3   | 3:C:232:THR:HG22  | 1.76                     | 0.66              |
| 3:C:229:GLU:O     | 3:C:231:LEU:N     | 2.29                     | 0.66              |
| 3:C:262:ILE:HG22  | 3:C:263:CYS:N     | 2.11                     | 0.66              |
| 4:D:90:TYR:OH     | 4:D:116:PRO:HA    | 1.96                     | 0.66              |
| 3:C:36:VAL:HG11   | 3:C:149:ILE:CD1   | 2.25                     | 0.65              |
| 3:C:87:GLU:C      | 3:C:89:ARG:H      | 2.04                     | 0.65              |
| 2:B:17:LYS:O      | 2:B:20:LYS:N      | 2.17                     | 0.65              |
| 3:C:136:PRO:HB3   | 3:C:142:ILE:O     | 1.97                     | 0.65              |
| 4:D:117:TRP:CH2   | 4:D:123:LYS:N     | 2.65                     | 0.65              |
| 6:F:28:LYS:O      | 6:F:30:GLN:N      | 2.29                     | 0.65              |
| 18:G:101:BCR:C8   | 18:G:101:BCR:H321 | 2.09                     | 0.65              |
| 3:C:278:GLN:O     | 3:C:278:GLN:HG2   | 1.97                     | 0.65              |
| 6:F:25:LEU:C      | 6:F:27:LEU:H      | 2.03                     | 0.65              |
| 3:C:158:GLY:H     | 11:C:301:HEC:C3D  | 2.09                     | 0.65              |
| 3:C:195:TYR:CD1   | 3:C:195:TYR:N     | 2.59                     | 0.65              |
| 15:B:1202:TDS:CAS | 15:B:1202:TDS:OAO | 2.44                     | 0.65              |
| 3:C:200:GLN:HG3   | 3:C:205:LYS:HB3   | 1.77                     | 0.65              |
| 1:A:80:TRP:O      | 1:A:84:SER:HB2    | 1.97                     | 0.65              |
| 1:A:195:ILE:CD1   | 1:A:199:MET:HE2   | 2.26                     | 0.65              |
| 3:C:14:ARG:CZ     | 3:C:150:HIS:HD2   | 2.10                     | 0.65              |
| 3:C:285:ALA:CB    | 4:D:10:VAL:HG21   | 2.26                     | 0.65              |
| 4:D:65:LYS:HB3    | 4:D:68:LYS:NZ     | 2.12                     | 0.64              |
| 4:D:161:VAL:O     | 4:D:161:VAL:CG1   | 2.44                     | 0.64              |
| 4:D:139:VAL:N     | 4:D:147:SER:HB3   | 2.01                     | 0.64              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 2:B:104:VAL:N    | 2:B:105:PRO:HD2    | 2.12                     | 0.64              |
| 3:C:71:ASN:CB    | 11:C:301:HEC:O2A   | 2.45                     | 0.64              |
| 3:C:206:THR:O    | 3:C:206:THR:HG22   | 1.97                     | 0.64              |
| 4:D:150:LEU:HD21 | 4:D:171:ARG:CZ     | 2.28                     | 0.64              |
| 1:A:95:LEU:O     | 1:A:96:MET:C       | 2.40                     | 0.64              |
| 1:A:150:ILE:CD1  | 15:B:1201:TDS:HAA2 | 2.27                     | 0.64              |
| 2:B:106:LEU:O    | 2:B:109:ILE:HB     | 1.96                     | 0.64              |
| 4:D:69:PHE:HD2   | 4:D:69:PHE:O       | 1.78                     | 0.64              |
| 1:A:207:ARG:NH1  | 15:B:1202:TDS:CAI  | 2.60                     | 0.64              |
| 4:D:9:ASP:HA     | 5:E:30:LYS:HZ3     | 1.63                     | 0.64              |
| 6:F:13:PHE:C     | 6:F:13:PHE:HD2     | 2.05                     | 0.64              |
| 1:A:136:TYR:HE2  | 15:B:1201:TDS:CAJ  | 2.11                     | 0.64              |
| 3:C:60:GLN:OE1   | 3:C:70:LEU:CB      | 2.46                     | 0.64              |
| 3:C:279:VAL:C    | 3:C:281:LYS:H      | 2.05                     | 0.64              |
| 4:D:25:GLY:HA3   | 17:D:201:SQD:H341  | 1.78                     | 0.64              |
| 1:A:26:VAL:CG2   | 1:A:30:VAL:HG12    | 2.26                     | 0.63              |
| 3:C:232:THR:O    | 3:C:233:ASN:HB3    | 1.97                     | 0.63              |
| 4:D:108:CYS:HB3  | 4:D:115:VAL:CG2    | 2.28                     | 0.63              |
| 6:F:14:GLY:O     | 6:F:17:PHE:HB2     | 1.97                     | 0.63              |
| 7:G:13:LEU:O     | 7:G:14:VAL:C       | 2.41                     | 0.63              |
| 1:A:41:LEU:HD23  | 11:A:303:HEC:HBC2  | 1.78                     | 0.63              |
| 2:B:22:MET:HA    | 2:B:24:HIS:HD2     | 1.63                     | 0.63              |
| 4:D:146:LEU:CD1  | 4:D:177:TRP:CB     | 2.76                     | 0.63              |
| 11:A:303:HEC:FE  | 15:B:1202:TDS:OBD  | 1.49                     | 0.63              |
| 7:G:24:ALA:C     | 7:G:26:TYR:H       | 2.06                     | 0.63              |
| 3:C:2:PRO:HD3    | 11:C:301:HEC:CHB   | 2.28                     | 0.63              |
| 3:C:71:ASN:HB2   | 11:C:301:HEC:CGA   | 2.29                     | 0.63              |
| 3:C:94:LEU:O     | 3:C:98:VAL:HG23    | 1.99                     | 0.63              |
| 2:B:118:ASN:HD22 | 2:B:120:PHE:N      | 1.94                     | 0.63              |
| 2:B:58:ASP:OD2   | 2:B:58:ASP:C       | 2.42                     | 0.63              |
| 3:C:25:CYS:SG    | 11:C:301:HEC:C3C   | 2.86                     | 0.63              |
| 3:C:26:HIS:HD1   | 3:C:154:ASN:ND2    | 1.97                     | 0.63              |
| 1:A:95:LEU:HD22  | 1:A:96:MET:HE2     | 1.80                     | 0.62              |
| 2:B:45:MET:CE    | 4:D:27:VAL:HG13    | 2.28                     | 0.62              |
| 1:A:8:PHE:HB3    | 1:A:14:ILE:HG12    | 1.81                     | 0.62              |
| 1:A:63:THR:O     | 1:A:63:THR:HG22    | 1.91                     | 0.62              |
| 1:A:211:ILE:C    | 1:A:212:SER:O      | 2.35                     | 0.62              |
| 4:D:55:THR:CG2   | 4:D:63:ASN:OD1     | 2.47                     | 0.62              |
| 7:G:2:VAL:HG13   | 7:G:3:GLU:N        | 2.09                     | 0.62              |
| 1:A:29:HIS:CD2   | 1:A:213:GLY:O      | 2.52                     | 0.62              |
| 3:C:180:ILE:HG12 | 3:C:181:THR:N      | 2.12                     | 0.62              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:D:65:LYS:CB    | 4:D:68:LYS:NZ     | 2.62                     | 0.62              |
| 7:G:17:THR:O     | 7:G:21:LEU:HB2    | 1.99                     | 0.62              |
| 1:A:105:TYR:HD2  | 1:A:106:LEU:HD23  | 1.64                     | 0.62              |
| 3:C:19:ARG:HG2   | 3:C:19:ARG:HH11   | 1.64                     | 0.62              |
| 4:D:63:ASN:O     | 4:D:64:VAL:O      | 2.17                     | 0.62              |
| 4:D:137:GLY:HA3  | 4:D:171:ARG:HH12  | 1.63                     | 0.62              |
| 4:D:150:LEU:O    | 4:D:151:CYS:HB3   | 2.00                     | 0.62              |
| 1:A:30:VAL:CG2   | 1:A:34:TYR:CG     | 2.80                     | 0.62              |
| 2:B:95:LEU:CD2   | 2:B:99:LEU:CD1    | 2.77                     | 0.62              |
| 3:C:161:TYR:C    | 3:C:163:THR:H     | 2.07                     | 0.62              |
| 3:C:225:VAL:HG12 | 3:C:229:GLU:HG2   | 1.81                     | 0.62              |
| 3:C:74:ALA:H     | 11:C:301:HEC:HMB2 | 1.65                     | 0.62              |
| 3:C:179:THR:HA   | 3:C:223:GLN:O     | 2.00                     | 0.62              |
| 3:C:200:GLN:HE21 | 3:C:206:THR:HA    | 1.64                     | 0.62              |
| 2:B:95:LEU:O     | 2:B:99:LEU:HD12   | 1.99                     | 0.62              |
| 2:B:126:ARG:N    | 2:B:127:PRO:CD    | 2.63                     | 0.62              |
| 3:C:62:ALA:HB2   | 3:C:68:VAL:HG12   | 1.81                     | 0.62              |
| 3:C:119:LEU:HD22 | 3:C:124:TYR:CG    | 2.35                     | 0.62              |
| 4:D:64:VAL:CG1   | 4:D:69:PHE:HD1    | 2.12                     | 0.62              |
| 2:B:69:PHE:N     | 2:B:69:PHE:CD2    | 2.68                     | 0.61              |
| 2:B:32:TRP:CD1   | 2:B:33:PRO:CD     | 2.84                     | 0.61              |
| 3:C:180:ILE:HG22 | 3:C:223:GLN:HB3   | 1.83                     | 0.61              |
| 6:F:17:PHE:O     | 6:F:20:TRP:HB3    | 2.00                     | 0.61              |
| 2:B:57:LEU:CD1   | 8:H:8:TRP:CE3     | 2.81                     | 0.61              |
| 3:C:282:VAL:HG11 | 4:D:16:ARG:HE     | 1.65                     | 0.61              |
| 1:A:44:PHE:C     | 1:A:44:PHE:CD2    | 2.79                     | 0.61              |
| 1:A:103:ARG:O    | 1:A:107:THR:HB    | 2.00                     | 0.61              |
| 2:B:6:LYS:O      | 2:B:7:PRO:C       | 2.43                     | 0.61              |
| 2:B:158:GLY:C    | 2:B:159:LEU:HD23  | 2.25                     | 0.61              |
| 1:A:111:LYS:NZ   | 2:B:120:PHE:O     | 2.31                     | 0.61              |
| 1:A:215:LEU:HD13 | 2:B:122:ASN:CA    | 2.29                     | 0.61              |
| 1:A:215:LEU:HB3  | 2:B:122:ASN:HB2   | 1.81                     | 0.61              |
| 4:D:90:TYR:HE1   | 4:D:115:VAL:O     | 1.84                     | 0.61              |
| 4:D:170:PHE:CE2  | 4:D:171:ARG:CG    | 2.83                     | 0.61              |
| 7:G:10:VAL:HG12  | 7:G:11:LEU:N      | 2.15                     | 0.61              |
| 1:A:12:LEU:CB    | 1:A:14:ILE:CD1    | 2.79                     | 0.61              |
| 3:C:34:VAL:HG21  | 3:C:151:LEU:HB2   | 1.82                     | 0.61              |
| 3:C:186:GLU:HB2  | 3:C:194:LYS:HB2   | 1.83                     | 0.61              |
| 5:E:29:ILE:O     | 5:E:29:ILE:CG2    | 2.49                     | 0.61              |
| 1:A:32:ILE:HG23  | 1:A:33:PHE:N      | 2.14                     | 0.61              |
| 3:C:1:TYR:HA     | 11:C:301:HEC:C4A  | 2.30                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:D:168:THR:HA    | 4:D:176:PRO:HD3   | 1.83                     | 0.61              |
| 2:B:134:LEU:HD13  | 2:B:134:LEU:N     | 2.14                     | 0.61              |
| 6:F:10:LEU:CD1    | 6:F:10:LEU:C      | 2.74                     | 0.61              |
| 1:A:111:LYS:CE    | 2:B:115:GLU:O     | 2.48                     | 0.60              |
| 2:B:151:LEU:O     | 2:B:154:THR:CG2   | 2.48                     | 0.60              |
| 3:C:93:GLU:O      | 3:C:97:GLU:HG3    | 2.01                     | 0.60              |
| 1:A:15:GLN:O      | 1:A:16:ALA:C      | 2.43                     | 0.60              |
| 3:C:28:ALA:CB     | 3:C:239:GLY:HA3   | 2.25                     | 0.60              |
| 3:C:54:TYR:HE1    | 3:C:70:LEU:CD2    | 2.13                     | 0.60              |
| 4:D:65:LYS:HB3    | 4:D:68:LYS:HZ1    | 1.67                     | 0.60              |
| 5:E:27:LYS:O      | 5:E:30:LYS:HA     | 2.02                     | 0.60              |
| 2:B:75:ILE:HG23   | 2:B:75:ILE:O      | 2.01                     | 0.60              |
| 3:C:62:ALA:HB2    | 3:C:68:VAL:CG1    | 2.31                     | 0.60              |
| 3:C:173:THR:O     | 3:C:231:LEU:CD2   | 2.50                     | 0.60              |
| 3:C:176:ALA:CB    | 3:C:205:LYS:HZ2   | 2.15                     | 0.60              |
| 5:E:24:PHE:CE1    | 6:F:29:ILE:HD11   | 2.37                     | 0.60              |
| 1:A:12:LEU:HB3    | 1:A:14:ILE:CD1    | 2.32                     | 0.60              |
| 1:A:96:MET:HE2    | 1:A:96:MET:HA     | 1.84                     | 0.60              |
| 4:D:132:GLN:OE1   | 4:D:141:ARG:HG2   | 2.02                     | 0.60              |
| 3:C:54:TYR:CE1    | 3:C:70:LEU:HD21   | 2.35                     | 0.60              |
| 3:C:173:THR:HB    | 3:C:228:GLY:C     | 2.26                     | 0.60              |
| 3:C:286:GLU:OE1   | 3:C:286:GLU:CA    | 2.50                     | 0.60              |
| 4:D:105:ASN:ND2   | 4:D:107:VAL:HG23  | 2.16                     | 0.60              |
| 1:A:105:TYR:CD2   | 1:A:106:LEU:HD23  | 2.37                     | 0.60              |
| 10:A:302:HEM:CMB  | 10:A:302:HEM:HBB2 | 2.31                     | 0.60              |
| 3:C:271:MET:HE2   | 4:D:22:LEU:HD12   | 1.84                     | 0.60              |
| 1:A:195:ILE:O     | 1:A:199:MET:HG3   | 2.02                     | 0.59              |
| 3:C:19:ARG:HG2    | 3:C:19:ARG:NH1    | 2.17                     | 0.59              |
| 1:A:211:ILE:CD1   | 1:A:212:SER:H     | 2.15                     | 0.59              |
| 3:C:172:PHE:N     | 3:C:172:PHE:HD1   | 1.96                     | 0.59              |
| 2:B:104:VAL:HB    | 2:B:105:PRO:CD    | 2.32                     | 0.59              |
| 4:D:152:HIS:O     | 4:D:162:LEU:HA    | 2.01                     | 0.59              |
| 6:F:23:GLY:O      | 6:F:26:LEU:HB2    | 2.02                     | 0.59              |
| 1:A:32:ILE:CG2    | 1:A:33:PHE:CD2    | 2.82                     | 0.59              |
| 1:A:87:ARG:HH11   | 1:A:87:ARG:HG2    | 1.67                     | 0.59              |
| 3:C:158:GLY:C     | 3:C:159:GLN:NE2   | 2.60                     | 0.59              |
| 4:D:64:VAL:HG13   | 4:D:69:PHE:CD1    | 2.35                     | 0.59              |
| 1:A:211:ILE:HG23  | 1:A:212:SER:O     | 2.02                     | 0.59              |
| 3:C:80:GLU:OE2    | 3:C:80:GLU:HA     | 2.02                     | 0.59              |
| 1:A:200:LEU:C     | 1:A:200:LEU:HD22  | 2.28                     | 0.59              |
| 13:A:1101:UMQ:HK2 | 4:D:34:ALA:HA     | 1.85                     | 0.59              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 4:D:84:LEU:C      | 4:D:86:GLY:H       | 2.11                     | 0.59              |
| 1:A:187:HIS:HE1   | 10:A:301:HEM:C1B   | 2.21                     | 0.59              |
| 13:A:1102:UMQ:O3' | 13:A:1102:UMQ:H11  | 2.02                     | 0.59              |
| 1:A:112:LYS:HA    | 1:A:115:GLU:OE2    | 2.02                     | 0.59              |
| 2:B:91:VAL:C      | 2:B:93:ASN:N       | 2.58                     | 0.59              |
| 4:D:78:ARG:HD2    | 4:D:117:TRP:CD1    | 2.37                     | 0.59              |
| 4:D:156:GLN:O     | 4:D:157:ASP:HB2    | 2.03                     | 0.59              |
| 1:A:120:SER:O     | 1:A:123:ILE:N      | 2.35                     | 0.59              |
| 3:C:171:VAL:HG23  | 3:C:171:VAL:O      | 2.01                     | 0.59              |
| 4:D:170:PHE:CD2   | 4:D:171:ARG:HG3    | 2.38                     | 0.59              |
| 3:C:61:VAL:HG21   | 3:C:214:GLY:O      | 2.03                     | 0.59              |
| 1:A:92:MET:HE2    | 12:A:1002:OPC:HCB2 | 1.70                     | 0.58              |
| 2:B:25:ASN:HD22   | 2:B:25:ASN:N       | 1.87                     | 0.58              |
| 2:B:95:LEU:HD23   | 2:B:99:LEU:HD12    | 1.84                     | 0.58              |
| 3:C:155:ARG:O     | 3:C:155:ARG:HG2    | 2.01                     | 0.58              |
| 11:A:303:HEC:HBC2 | 11:A:303:HEC:HHD   | 1.85                     | 0.58              |
| 2:B:134:LEU:HD21  | 7:G:22:PHE:CZ      | 2.38                     | 0.58              |
| 5:E:4:GLY:O       | 5:E:8:TYR:N        | 2.26                     | 0.58              |
| 1:A:32:ILE:HG22   | 1:A:33:PHE:CE2     | 2.38                     | 0.58              |
| 1:A:141:ASP:C     | 1:A:141:ASP:OD2    | 2.45                     | 0.58              |
| 1:A:207:ARG:NH1   | 1:A:207:ARG:CG     | 2.61                     | 0.58              |
| 10:A:302:HEM:HBA1 | 10:A:302:HEM:CHA   | 2.27                     | 0.58              |
| 3:C:237:VAL:O     | 3:C:237:VAL:CG2    | 2.50                     | 0.58              |
| 3:C:270:LEU:CB    | 8:H:21:MET:HE2     | 2.32                     | 0.58              |
| 4:D:64:VAL:CG1    | 4:D:69:PHE:CD1     | 2.87                     | 0.58              |
| 3:C:264:LEU:HD22  | 3:C:264:LEU:C      | 2.21                     | 0.58              |
| 4:D:122:ASN:HB3   | 4:D:135:GLU:CD     | 2.24                     | 0.58              |
| 4:D:165:TRP:CD1   | 4:D:165:TRP:C      | 2.82                     | 0.58              |
| 1:A:36:LEU:HD23   | 1:A:99:LEU:C       | 2.28                     | 0.58              |
| 6:F:23:GLY:HA2    | 6:F:26:LEU:HD23    | 1.84                     | 0.58              |
| 3:C:171:VAL:O     | 3:C:171:VAL:CG2    | 2.51                     | 0.58              |
| 4:D:22:LEU:N      | 4:D:22:LEU:HD23    | 2.17                     | 0.58              |
| 4:D:105:ASN:ND2   | 4:D:105:ASN:C      | 2.62                     | 0.58              |
| 4:D:105:ASN:O     | 4:D:148:LEU:HD13   | 2.03                     | 0.58              |
| 4:D:117:TRP:NE1   | 4:D:119:ALA:HA     | 2.19                     | 0.58              |
| 3:C:34:VAL:CG2    | 3:C:151:LEU:CB     | 2.81                     | 0.58              |
| 1:A:95:LEU:C      | 1:A:95:LEU:HD23    | 2.28                     | 0.58              |
| 3:C:26:HIS:CE1    | 11:C:301:HEC:NA    | 2.72                     | 0.58              |
| 3:C:34:VAL:HG21   | 3:C:151:LEU:HB3    | 1.84                     | 0.58              |
| 3:C:78:LEU:HB2    | 3:C:112:ASN:O      | 2.04                     | 0.58              |
| 4:D:59:LYS:H      | 4:D:59:LYS:HD3     | 1.69                     | 0.58              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 3:C:154:ASN:CG   | 3:C:155:ARG:N      | 2.62                     | 0.57              |
| 6:F:27:LEU:HD11  | 8:H:27:ASN:HA      | 1.84                     | 0.57              |
| 1:A:95:LEU:O     | 1:A:97:MET:N       | 2.36                     | 0.57              |
| 2:B:81:LEU:HD11  | 15:B:1201:TDS:HAR1 | 1.85                     | 0.57              |
| 2:B:104:VAL:HB   | 2:B:105:PRO:HD3    | 1.85                     | 0.57              |
| 3:C:60:GLN:HE22  | 3:C:157:ARG:H      | 1.52                     | 0.57              |
| 3:C:87:GLU:C     | 3:C:89:ARG:N       | 2.59                     | 0.57              |
| 2:B:149:PHE:CB   | 2:B:150:PRO:CD     | 2.82                     | 0.57              |
| 3:C:94:LEU:C     | 3:C:94:LEU:CD2     | 2.77                     | 0.57              |
| 4:D:133:TYR:CE2  | 4:D:148:LEU:CD2    | 2.80                     | 0.57              |
| 6:F:27:LEU:O     | 6:F:30:GLN:CG      | 2.51                     | 0.57              |
| 1:A:39:ILE:CD1   | 18:G:101:BCR:C31   | 2.74                     | 0.57              |
| 1:A:87:ARG:CG    | 1:A:87:ARG:NH1     | 2.68                     | 0.57              |
| 1:A:195:ILE:HD13 | 1:A:199:MET:HE2    | 1.86                     | 0.57              |
| 3:C:221:GLU:OE1  | 3:C:221:GLU:CA     | 2.52                     | 0.57              |
| 3:C:285:ALA:O    | 3:C:286:GLU:OE1    | 2.23                     | 0.57              |
| 4:D:28:THR:O     | 4:D:29:GLY:C       | 2.45                     | 0.57              |
| 1:A:47:GLN:HE22  | 1:A:89:SER:HB3     | 1.69                     | 0.57              |
| 1:A:103:ARG:HH21 | 1:A:211:ILE:HD11   | 1.69                     | 0.57              |
| 3:C:79:PRO:HG2   | 3:C:82:PHE:CD1     | 2.39                     | 0.57              |
| 3:C:183:ILE:HG22 | 3:C:183:ILE:O      | 2.05                     | 0.57              |
| 4:D:133:TYR:HB3  | 4:D:137:GLY:O      | 2.04                     | 0.57              |
| 1:A:127:ILE:CG2  | 1:A:195:ILE:CG1    | 2.81                     | 0.57              |
| 1:A:177:GLN:O    | 1:A:178:ALA:C      | 2.39                     | 0.57              |
| 4:D:102:TYR:H    | 4:D:102:TYR:HD2    | 1.52                     | 0.57              |
| 2:B:85:PHE:HD2   | 15:B:1201:TDS:OAC  | 1.87                     | 0.57              |
| 3:C:225:VAL:HG12 | 3:C:229:GLU:HG3    | 1.87                     | 0.57              |
| 7:G:7:ASP:OD2    | 7:G:7:ASP:N        | 2.32                     | 0.57              |
| 2:B:150:PRO:O    | 2:B:152:ASP:N      | 2.38                     | 0.57              |
| 5:E:26:ILE:HG23  | 5:E:32:ILE:HG13    | 1.85                     | 0.57              |
| 2:B:84:VAL:HG11  | 2:B:101:MET:HG3    | 1.86                     | 0.57              |
| 3:C:171:VAL:CG1  | 3:C:233:ASN:O      | 2.52                     | 0.57              |
| 3:C:172:PHE:N    | 3:C:232:THR:OG1    | 2.38                     | 0.57              |
| 7:G:34:GLU:N     | 7:G:34:GLU:OE2     | 2.38                     | 0.57              |
| 8:H:9:VAL:O      | 8:H:13:VAL:HG23    | 2.05                     | 0.57              |
| 1:A:207:ARG:HH12 | 15:B:1202:TDS:CAI  | 2.18                     | 0.56              |
| 1:A:27:PRO:HB2   | 1:A:29:HIS:CE1     | 2.40                     | 0.56              |
| 1:A:96:MET:HE2   | 1:A:96:MET:CA      | 2.34                     | 0.56              |
| 1:A:105:TYR:CZ   | 14:B:201:CLA:CBB   | 2.88                     | 0.56              |
| 11:A:303:HEC:CMB | 11:A:303:HEC:CBB   | 2.76                     | 0.56              |
| 3:C:171:VAL:HG12 | 3:C:234:ASN:HA     | 1.87                     | 0.56              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 3:C:200:GLN:NE2  | 3:C:205:LYS:O      | 2.39                     | 0.56              |
| 4:D:78:ARG:CD    | 4:D:117:TRP:CG     | 2.88                     | 0.56              |
| 5:E:2:ILE:O      | 5:E:6:VAL:HG23     | 2.05                     | 0.56              |
| 5:E:15:PHE:HA    | 5:E:18:ILE:HG13    | 1.87                     | 0.56              |
| 6:F:25:LEU:C     | 6:F:27:LEU:N       | 2.62                     | 0.56              |
| 1:A:168:LEU:O    | 1:A:182:ARG:HD3    | 2.05                     | 0.56              |
| 3:C:271:MET:HE2  | 4:D:22:LEU:CD1     | 2.35                     | 0.56              |
| 8:H:23:VAL:HG13  | 8:H:28:GLY:H       | 1.70                     | 0.56              |
| 2:B:122:ASN:ND2  | 7:G:29:TYR:HB2     | 2.21                     | 0.56              |
| 1:A:33:PHE:CD2   | 1:A:33:PHE:N       | 2.73                     | 0.56              |
| 2:B:97:GLY:HA2   | 2:B:100:LEU:HB2    | 1.88                     | 0.56              |
| 2:B:123:PRO:CD   | 7:G:25:ALA:HB1     | 2.35                     | 0.56              |
| 3:C:193:VAL:HG12 | 3:C:194:LYS:N      | 2.21                     | 0.56              |
| 3:C:210:THR:C    | 3:C:211:ILE:CG2    | 2.79                     | 0.56              |
| 4:D:21:LEU:HD11  | 17:D:201:SQD:C30   | 2.32                     | 0.56              |
| 7:G:34:GLU:C     | 7:G:35:LEU:HD23    | 2.31                     | 0.56              |
| 1:A:92:MET:CG    | 12:A:1002:OPC:HCB1 | 2.35                     | 0.56              |
| 1:A:96:MET:HE2   | 1:A:96:MET:N       | 2.20                     | 0.56              |
| 3:C:34:VAL:HG23  | 3:C:151:LEU:CD2    | 2.36                     | 0.56              |
| 4:D:110:HIS:O    | 4:D:111:LEU:HD12   | 2.05                     | 0.56              |
| 1:A:33:PHE:H     | 1:A:33:PHE:HD2     | 1.51                     | 0.56              |
| 1:A:87:ARG:HH11  | 1:A:87:ARG:CG      | 2.19                     | 0.56              |
| 2:B:57:LEU:HD12  | 8:H:8:TRP:CZ3      | 2.41                     | 0.56              |
| 3:C:54:TYR:HD2   | 3:C:125:GLN:HE22   | 1.53                     | 0.56              |
| 3:C:223:GLN:O    | 3:C:224:ALA:HB2    | 2.04                     | 0.56              |
| 4:D:139:VAL:CG2  | 4:D:147:SER:CA     | 2.66                     | 0.56              |
| 4:D:165:TRP:HD1  | 4:D:165:TRP:O      | 1.89                     | 0.56              |
| 8:H:23:VAL:HG12  | 8:H:24:TRP:N       | 2.13                     | 0.56              |
| 3:C:181:THR:O    | 3:C:182:LYS:HG3    | 2.06                     | 0.56              |
| 4:D:96:LYS:HB2   | 4:D:96:LYS:HZ3     | 1.70                     | 0.56              |
| 5:E:26:ILE:O     | 5:E:31:LEU:HB2     | 2.06                     | 0.56              |
| 7:G:2:VAL:HG12   | 7:G:4:PRO:HD3      | 1.83                     | 0.56              |
| 1:A:100:HIS:HE1  | 10:A:302:HEM:CHA   | 2.19                     | 0.55              |
| 3:C:270:LEU:HA   | 8:H:21:MET:HE3     | 1.87                     | 0.55              |
| 7:G:30:LYS:C     | 7:G:32:PRO:HD3     | 2.31                     | 0.55              |
| 1:A:94:VAL:HG11  | 2:B:80:TYR:CG      | 2.41                     | 0.55              |
| 4:D:21:LEU:HD11  | 17:D:201:SQD:H312  | 1.88                     | 0.55              |
| 8:H:8:TRP:O      | 8:H:9:VAL:C        | 2.45                     | 0.55              |
| 1:A:83:ARG:O     | 1:A:83:ARG:HG3     | 2.05                     | 0.55              |
| 1:A:205:MET:O    | 1:A:206:ILE:C      | 2.47                     | 0.55              |
| 2:B:91:VAL:C     | 2:B:93:ASN:H       | 2.15                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:161:TYR:C     | 3:C:163:THR:N     | 2.64                     | 0.55              |
| 3:C:206:THR:O     | 3:C:206:THR:HG23  | 2.05                     | 0.55              |
| 1:A:30:VAL:HG22   | 1:A:34:TYR:CD2    | 2.41                     | 0.55              |
| 11:C:301:HEC:CBC  | 11:C:301:HEC:CMC  | 2.83                     | 0.55              |
| 4:D:69:PHE:O      | 4:D:70:LEU:C      | 2.48                     | 0.55              |
| 1:A:82:ILE:HD13   | 1:A:82:ILE:N      | 2.21                     | 0.55              |
| 10:A:302:HEM:HMB1 | 10:A:302:HEM:CBB  | 2.37                     | 0.55              |
| 3:C:14:ARG:NE     | 3:C:150:HIS:HD2   | 2.05                     | 0.55              |
| 3:C:170:ASN:O     | 3:C:235:PRO:CD    | 2.54                     | 0.55              |
| 8:H:5:VAL:O       | 8:H:6:LEU:C       | 2.49                     | 0.55              |
| 1:A:93:MET:O      | 1:A:94:VAL:C      | 2.47                     | 0.55              |
| 1:A:155:PRO:HB2   | 1:A:166:SER:OG    | 2.06                     | 0.55              |
| 1:A:211:ILE:HD12  | 1:A:212:SER:H     | 1.72                     | 0.55              |
| 3:C:34:VAL:CG2    | 3:C:151:LEU:HB2   | 2.37                     | 0.55              |
| 3:C:217:LEU:N     | 3:C:217:LEU:HD12  | 2.21                     | 0.55              |
| 3:C:271:MET:HE2   | 4:D:22:LEU:HB3    | 1.87                     | 0.55              |
| 1:A:80:TRP:H      | 1:A:80:TRP:CD1    | 2.25                     | 0.55              |
| 2:B:87:ILE:HG22   | 2:B:88:LEU:N      | 2.22                     | 0.55              |
| 2:B:96:LEU:O      | 2:B:99:LEU:HB2    | 2.07                     | 0.55              |
| 4:D:66:VAL:CG2    | 4:D:158:ASP:C     | 2.79                     | 0.55              |
| 7:G:15:PHE:O      | 7:G:17:THR:N      | 2.40                     | 0.55              |
| 1:A:44:PHE:HB2    | 1:A:93:MET:SD     | 2.46                     | 0.55              |
| 2:B:22:MET:HA     | 2:B:24:HIS:CD2    | 2.41                     | 0.55              |
| 2:B:123:PRO:HD2   | 2:B:124:PHE:H     | 1.72                     | 0.55              |
| 3:C:171:VAL:HB    | 3:C:232:THR:HB    | 1.87                     | 0.55              |
| 3:C:270:LEU:CD1   | 3:C:271:MET:N     | 2.70                     | 0.55              |
| 1:A:54:MET:HE1    | 10:A:301:HEM:CBD  | 2.33                     | 0.55              |
| 1:A:143:VAL:HG13  | 1:A:143:VAL:O     | 2.07                     | 0.55              |
| 2:B:4:LEU:H       | 3:C:287:MET:HE3   | 1.70                     | 0.55              |
| 2:B:129:ALA:O     | 2:B:130:THR:C     | 2.49                     | 0.55              |
| 2:B:130:THR:CG2   | 7:G:22:PHE:CE2    | 2.83                     | 0.55              |
| 4:D:78:ARG:HD2    | 4:D:117:TRP:CG    | 2.42                     | 0.55              |
| 6:F:10:LEU:C      | 6:F:10:LEU:HD13   | 2.30                     | 0.55              |
| 1:A:35:CYS:SG     | 11:A:303:HEC:HMB3 | 2.47                     | 0.55              |
| 1:A:72:ILE:HA     | 1:A:76:VAL:CG2    | 2.36                     | 0.55              |
| 2:B:138:LEU:CD1   | 2:B:138:LEU:CB    | 2.76                     | 0.55              |
| 4:D:47:GLY:C      | 4:D:49:ALA:H      | 2.14                     | 0.55              |
| 1:A:6:ASP:O       | 1:A:9:GLN:N       | 2.40                     | 0.54              |
| 2:B:147:ALA:C     | 2:B:149:PHE:H     | 2.15                     | 0.54              |
| 11:A:303:HEC:HBD1 | 11:A:303:HEC:HHA  | 1.89                     | 0.54              |
| 2:B:96:LEU:C      | 2:B:100:LEU:HD12  | 2.32                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:124:PHE:CE1  | 7:G:26:TYR:CB    | 2.83                     | 0.54              |
| 2:B:151:LEU:O    | 2:B:154:THR:HG21 | 2.06                     | 0.54              |
| 3:C:176:ALA:CB   | 3:C:205:LYS:NZ   | 2.63                     | 0.54              |
| 3:C:266:MET:CE   | 5:E:15:PHE:CD1   | 2.90                     | 0.54              |
| 1:A:97:MET:SD    | 10:A:302:HEM:HAB | 2.47                     | 0.54              |
| 1:A:108:GLY:HA2  | 1:A:110:PHE:CD2  | 2.43                     | 0.54              |
| 2:B:11:ASP:OD1   | 2:B:13:LYS:HB2   | 2.08                     | 0.54              |
| 2:B:151:LEU:HD13 | 2:B:151:LEU:C    | 2.32                     | 0.54              |
| 3:C:54:TYR:CE1   | 3:C:70:LEU:HG    | 2.43                     | 0.54              |
| 3:C:181:THR:HG22 | 3:C:182:LYS:HG3  | 1.88                     | 0.54              |
| 2:B:151:LEU:O    | 2:B:151:LEU:HD13 | 2.08                     | 0.54              |
| 2:B:114:ILE:O    | 2:B:116:ASN:N    | 2.41                     | 0.54              |
| 3:C:47:LYS:HD2   | 3:C:49:VAL:CG2   | 2.38                     | 0.54              |
| 6:F:22:LEU:HD12  | 8:H:20:ALA:CB    | 2.37                     | 0.54              |
| 1:A:7:TRP:CD2    | 1:A:11:ARG:NH2   | 2.68                     | 0.54              |
| 4:D:34:ALA:O     | 4:D:37:PRO:HD2   | 2.08                     | 0.54              |
| 4:D:80:LEU:O     | 4:D:81:VAL:HG22  | 2.07                     | 0.54              |
| 1:A:110:PHE:CE1  | 2:B:111:VAL:HG12 | 2.43                     | 0.54              |
| 1:A:111:LYS:O    | 1:A:112:LYS:C    | 2.50                     | 0.54              |
| 2:B:159:LEU:O    | 2:B:160:PHE:CG   | 2.61                     | 0.54              |
| 3:C:9:TYR:CE1    | 3:C:21:VAL:HB    | 2.43                     | 0.54              |
| 3:C:180:ILE:CG2  | 3:C:222:GLY:O    | 2.56                     | 0.54              |
| 1:A:103:ARG:NH1  | 1:A:104:VAL:CG2  | 2.65                     | 0.54              |
| 1:A:145:TYR:O    | 1:A:145:TYR:CD1  | 2.61                     | 0.54              |
| 1:A:145:TYR:O    | 1:A:145:TYR:CG   | 2.59                     | 0.53              |
| 2:B:79:TRP:O     | 2:B:82:TYR:N     | 2.40                     | 0.53              |
| 2:B:96:LEU:HD13  | 2:B:100:LEU:HD12 | 1.80                     | 0.53              |
| 2:B:114:ILE:HG22 | 2:B:115:GLU:H    | 1.73                     | 0.53              |
| 1:A:54:MET:HE1   | 10:A:301:HEM:CGD | 2.38                     | 0.53              |
| 3:C:15:GLU:N     | 3:C:15:GLU:OE1   | 2.39                     | 0.53              |
| 3:C:279:VAL:C    | 3:C:281:LYS:N    | 2.66                     | 0.53              |
| 4:D:90:TYR:CE1   | 4:D:115:VAL:O    | 2.61                     | 0.53              |
| 4:D:152:HIS:CE1  | 4:D:165:TRP:CE3  | 2.96                     | 0.53              |
| 6:F:28:LYS:C     | 6:F:30:GLN:H     | 2.17                     | 0.53              |
| 1:A:29:HIS:NE2   | 1:A:213:GLY:C    | 2.67                     | 0.53              |
| 1:A:98:ILE:HD11  | 14:B:201:CLA:CED | 2.38                     | 0.53              |
| 2:B:81:LEU:HD23  | 2:B:81:LEU:N     | 2.14                     | 0.53              |
| 3:C:40:VAL:HG12  | 8:H:1:MET:CE     | 2.35                     | 0.53              |
| 3:C:54:TYR:HE1   | 3:C:70:LEU:CG    | 2.21                     | 0.53              |
| 3:C:194:LYS:O    | 3:C:195:TYR:C    | 2.51                     | 0.53              |
| 4:D:119:ALA:O    | 4:D:122:ASN:OD1  | 2.26                     | 0.53              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 4:D:167:GLU:CD     | 4:D:167:GLU:H     | 2.15                     | 0.53              |
| 1:A:31:ASN:ND2     | 1:A:33:PHE:H      | 2.06                     | 0.53              |
| 3:C:158:GLY:H      | 11:C:301:HEC:CAD  | 2.21                     | 0.53              |
| 1:A:7:TRP:CD1      | 1:A:11:ARG:NH2    | 2.76                     | 0.53              |
| 3:C:200:GLN:CD     | 3:C:205:LYS:O     | 2.51                     | 0.53              |
| 4:D:114:VAL:O      | 4:D:114:VAL:CG1   | 2.55                     | 0.53              |
| 4:D:146:LEU:HD12   | 4:D:177:TRP:CE3   | 2.40                     | 0.53              |
| 1:A:145:TYR:CD1    | 1:A:145:TYR:C     | 2.84                     | 0.53              |
| 7:G:23:TYR:C       | 7:G:23:TYR:CD2    | 2.87                     | 0.53              |
| 8:H:3:ILE:O        | 8:H:7:GLY:N       | 2.38                     | 0.53              |
| 1:A:119:ILE:O      | 1:A:123:ILE:HD12  | 2.09                     | 0.53              |
| 2:B:45:MET:HE2     | 4:D:30:VAL:HB     | 1.91                     | 0.53              |
| 2:B:113:PHE:O      | 2:B:114:ILE:C     | 2.51                     | 0.53              |
| 3:C:273:ILE:HG13   | 8:H:21:MET:CG     | 2.29                     | 0.53              |
| 4:D:169:ASP:O      | 4:D:170:PHE:C     | 2.51                     | 0.53              |
| 5:E:8:TYR:OH       | 5:E:12:ILE:HD11   | 2.09                     | 0.53              |
| 12:A:1002:OPC:HBP2 | 6:F:8:ALA:HA      | 1.90                     | 0.53              |
| 2:B:69:PHE:N       | 2:B:69:PHE:HD2    | 2.05                     | 0.53              |
| 3:C:1:TYR:HB3      | 3:C:2:PRO:HD2     | 1.90                     | 0.53              |
| 3:C:180:ILE:HG22   | 3:C:222:GLY:O     | 2.08                     | 0.53              |
| 3:C:188:ASP:O      | 3:C:190:TYR:O     | 2.25                     | 0.53              |
| 3:C:226:LYS:CB     | 3:C:226:LYS:HZ2   | 2.22                     | 0.53              |
| 1:A:31:ASN:ND2     | 1:A:33:PHE:HD2    | 2.07                     | 0.52              |
| 1:A:80:TRP:CD2     | 3:C:254:ARG:NH2   | 2.77                     | 0.52              |
| 1:A:147:ALA:O      | 1:A:148:VAL:C     | 2.49                     | 0.52              |
| 3:C:22:CYS:C       | 3:C:24:ASN:H      | 2.16                     | 0.52              |
| 3:C:75:VAL:HG13    | 3:C:75:VAL:O      | 2.08                     | 0.52              |
| 1:A:95:LEU:C       | 1:A:97:MET:N      | 2.67                     | 0.52              |
| 3:C:159:GLN:C      | 3:C:160:ILE:HG13  | 2.34                     | 0.52              |
| 1:A:72:ILE:HA      | 1:A:76:VAL:HG23   | 1.90                     | 0.52              |
| 1:A:92:MET:CG      | 12:A:1002:OPC:CCB | 2.87                     | 0.52              |
| 2:B:119:LYS:O      | 2:B:119:LYS:HG2   | 2.10                     | 0.52              |
| 2:B:134:LEU:HD13   | 2:B:134:LEU:H     | 1.74                     | 0.52              |
| 3:C:171:VAL:HG11   | 3:C:234:ASN:ND2   | 2.15                     | 0.52              |
| 8:H:2:GLU:HB2      | 8:H:5:VAL:CG2     | 2.39                     | 0.52              |
| 2:B:118:ASN:ND2    | 2:B:120:PHE:HD1   | 2.06                     | 0.52              |
| 1:A:12:LEU:HB2     | 1:A:14:ILE:CD1    | 2.39                     | 0.52              |
| 2:B:134:LEU:CD2    | 7:G:22:PHE:CZ     | 2.93                     | 0.52              |
| 4:D:165:TRP:CD1    | 4:D:165:TRP:O     | 2.62                     | 0.52              |
| 3:C:25:CYS:SG      | 11:C:301:HEC:HBC3 | 2.49                     | 0.52              |
| 3:C:55:ASP:C       | 3:C:55:ASP:OD1    | 2.52                     | 0.52              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 3:C:200:GLN:CG    | 3:C:205:LYS:HB3    | 2.39                     | 0.52              |
| 4:D:84:LEU:C      | 4:D:86:GLY:N       | 2.65                     | 0.52              |
| 6:F:21:GLY:O      | 6:F:22:LEU:C       | 2.52                     | 0.52              |
| 1:A:29:HIS:CD2    | 1:A:214:PRO:HA     | 2.45                     | 0.52              |
| 1:A:38:GLY:HA3    | 11:A:303:HEC:C1C   | 2.40                     | 0.52              |
| 2:B:40:PHE:HZ     | 15:B:1202:TDS:OBD  | 1.93                     | 0.52              |
| 3:C:59:GLN:HB2    | 3:C:67:LYS:HE3     | 1.92                     | 0.52              |
| 3:C:272:LEU:O     | 3:C:275:LYS:HB3    | 2.10                     | 0.52              |
| 4:D:38:LEU:O      | 4:D:38:LEU:HG      | 2.09                     | 0.52              |
| 2:B:154:THR:HG23  | 2:B:155:LEU:H      | 1.75                     | 0.52              |
| 3:C:64:ASP:OD2    | 3:C:65:GLY:N       | 2.43                     | 0.52              |
| 3:C:1:TYR:HA      | 11:C:301:HEC:NA    | 2.25                     | 0.52              |
| 3:C:250:GLN:HE21  | 3:C:251:ASP:H      | 1.58                     | 0.52              |
| 1:A:92:MET:HG3    | 12:A:1002:OPC:CCB  | 2.40                     | 0.51              |
| 15:B:1202:TDS:OAO | 15:B:1202:TDS:HAS1 | 2.09                     | 0.51              |
| 3:C:160:ILE:O     | 11:C:301:HEC:HAC   | 2.10                     | 0.51              |
| 1:A:18:ALA:O      | 1:A:21:VAL:N       | 2.39                     | 0.51              |
| 3:C:200:GLN:HG2   | 3:C:201:THR:N      | 2.24                     | 0.51              |
| 4:D:69:PHE:CD2    | 4:D:69:PHE:O       | 2.61                     | 0.51              |
| 5:E:9:ILE:O       | 5:E:13:ALA:CB      | 2.57                     | 0.51              |
| 1:A:103:ARG:CA    | 7:G:21:LEU:HD21    | 2.38                     | 0.51              |
| 1:A:191:LEU:O     | 1:A:192:PRO:C      | 2.50                     | 0.51              |
| 2:B:57:LEU:HD13   | 8:H:8:TRP:CD2      | 2.45                     | 0.51              |
| 3:C:266:MET:SD    | 8:H:13:VAL:HG12    | 2.51                     | 0.51              |
| 4:D:13:MET:O      | 4:D:15:ARG:N       | 2.43                     | 0.51              |
| 1:A:105:TYR:CZ    | 14:B:201:CLA:HBB2  | 2.45                     | 0.51              |
| 10:A:302:HEM:CMB  | 10:A:302:HEM:CBB   | 2.87                     | 0.51              |
| 2:B:84:VAL:HG11   | 2:B:101:MET:SD     | 2.50                     | 0.51              |
| 1:A:53:ALA:HB1    | 4:D:41:TYR:CE2     | 2.45                     | 0.51              |
| 3:C:45:VAL:HG13   | 3:C:85:ALA:HB2     | 1.93                     | 0.51              |
| 1:A:111:LYS:O     | 1:A:113:PRO:CD     | 2.57                     | 0.51              |
| 2:B:32:TRP:CD1    | 2:B:33:PRO:HD3     | 2.45                     | 0.51              |
| 2:B:155:LEU:C     | 2:B:157:LEU:H      | 2.18                     | 0.51              |
| 7:G:10:VAL:HG12   | 7:G:11:LEU:CD2     | 2.34                     | 0.51              |
| 1:A:163:VAL:O     | 1:A:164:LEU:C      | 2.53                     | 0.51              |
| 4:D:132:GLN:OE1   | 4:D:141:ARG:NH1    | 2.44                     | 0.51              |
| 6:F:15:LEU:HD23   | 8:H:16:THR:OG1     | 2.10                     | 0.51              |
| 1:A:88:TRP:CE3    | 2:B:54:LEU:HD13    | 2.46                     | 0.51              |
| 1:A:103:ARG:NH2   | 1:A:211:ILE:HD11   | 2.25                     | 0.51              |
| 2:B:84:VAL:CG1    | 2:B:101:MET:SD     | 2.99                     | 0.51              |
| 6:F:24:VAL:O      | 6:F:27:LEU:CB      | 2.55                     | 0.51              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 2:B:45:MET:HE1   | 4:D:27:VAL:HG13    | 1.91                     | 0.51              |
| 3:C:102:TYR:O    | 3:C:104:GLN:N      | 2.44                     | 0.51              |
| 4:D:74:ASN:O     | 4:D:93:VAL:HG11    | 2.10                     | 0.51              |
| 1:A:39:ILE:O     | 1:A:42:THR:N       | 2.43                     | 0.50              |
| 2:B:34:ASN:O     | 3:C:276:LYS:HE3    | 2.10                     | 0.50              |
| 3:C:144:PHE:CE1  | 3:C:251:ASP:HB2    | 2.41                     | 0.50              |
| 3:C:180:ILE:CD1  | 3:C:183:ILE:CD1    | 2.79                     | 0.50              |
| 3:C:232:THR:O    | 3:C:233:ASN:CB     | 2.59                     | 0.50              |
| 1:A:15:GLN:O     | 1:A:18:ALA:N       | 2.45                     | 0.50              |
| 1:A:15:GLN:O     | 1:A:17:LEU:N       | 2.44                     | 0.50              |
| 1:A:80:TRP:CZ3   | 1:A:81:LEU:HG      | 2.45                     | 0.50              |
| 1:A:207:ARG:HG3  | 1:A:207:ARG:NH1    | 2.05                     | 0.50              |
| 3:C:87:GLU:O     | 3:C:89:ARG:N       | 2.44                     | 0.50              |
| 4:D:167:GLU:O    | 4:D:176:PRO:HG3    | 2.11                     | 0.50              |
| 6:F:4:GLU:HG2    | 7:G:5:LEU:HD12     | 1.94                     | 0.50              |
| 7:G:24:ALA:C     | 7:G:26:TYR:N       | 2.68                     | 0.50              |
| 3:C:34:VAL:CG2   | 3:C:151:LEU:HD22   | 2.42                     | 0.50              |
| 3:C:117:GLY:HA2  | 3:C:119:LEU:HD12   | 1.93                     | 0.50              |
| 4:D:80:LEU:O     | 4:D:81:VAL:CG2     | 2.59                     | 0.50              |
| 2:B:130:THR:HG21 | 7:G:22:PHE:HE2     | 1.75                     | 0.50              |
| 1:A:212:SER:HB3  | 10:A:302:HEM:O2D   | 2.12                     | 0.50              |
| 3:C:159:GLN:CD   | 3:C:159:GLN:N      | 2.70                     | 0.50              |
| 3:C:214:GLY:C    | 3:C:215:PRO:O      | 2.50                     | 0.50              |
| 3:C:229:GLU:OE1  | 3:C:229:GLU:CA     | 2.51                     | 0.50              |
| 6:F:22:LEU:HD12  | 8:H:20:ALA:HB1     | 1.94                     | 0.50              |
| 2:B:147:ALA:O    | 2:B:148:THR:C      | 2.55                     | 0.50              |
| 3:C:173:THR:O    | 3:C:231:LEU:HD23   | 2.12                     | 0.50              |
| 3:C:184:ALA:HB3  | 3:C:196:GLN:HB2    | 1.94                     | 0.50              |
| 4:D:13:MET:HA    | 4:D:16:ARG:HD3     | 1.94                     | 0.50              |
| 8:H:5:VAL:C      | 8:H:7:GLY:N        | 2.68                     | 0.50              |
| 1:A:106:LEU:HD12 | 7:G:21:LEU:HD23    | 1.94                     | 0.50              |
| 3:C:186:GLU:OE2  | 3:C:196:GLN:HG3    | 2.12                     | 0.50              |
| 5:E:26:ILE:HG22  | 5:E:32:ILE:HG13    | 1.91                     | 0.50              |
| 1:A:103:ARG:HH12 | 1:A:104:VAL:CG2    | 2.18                     | 0.50              |
| 1:A:71:TYR:O     | 1:A:72:ILE:C       | 2.50                     | 0.49              |
| 1:A:147:ALA:CB   | 15:B:1201:TDS:HAJ3 | 2.32                     | 0.49              |
| 3:C:268:ALA:HA   | 4:D:26:THR:OG1     | 2.12                     | 0.49              |
| 1:A:124:LEU:HD21 | 1:A:199:MET:N      | 2.27                     | 0.49              |
| 1:A:138:LEU:N    | 1:A:139:PRO:HD3    | 2.28                     | 0.49              |
| 3:C:196:GLN:NE2  | 3:C:210:THR:HG23   | 2.28                     | 0.49              |
| 4:D:146:LEU:CD1  | 4:D:177:TRP:HB2    | 2.42                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:E:20:VAL:HG12    | 5:E:21:GLY:N       | 2.26                     | 0.49              |
| 3:C:80:GLU:OE2     | 3:C:80:GLU:CA      | 2.60                     | 0.49              |
| 4:D:117:TRP:CZ2    | 4:D:122:ASN:CA     | 2.95                     | 0.49              |
| 4:D:138:LYS:HA     | 4:D:147:SER:CB     | 2.43                     | 0.49              |
| 1:A:29:HIS:CD2     | 1:A:213:GLY:C      | 2.90                     | 0.49              |
| 2:B:16:ALA:C       | 2:B:19:ALA:HB3     | 2.38                     | 0.49              |
| 2:B:118:ASN:HD22   | 2:B:119:LYS:N      | 2.11                     | 0.49              |
| 2:B:118:ASN:OD1    | 12:B:1001:OPC:HAH2 | 2.13                     | 0.49              |
| 2:B:151:LEU:HD13   | 2:B:152:ASP:HB3    | 1.93                     | 0.49              |
| 15:B:1202:TDS:HAA3 | 15:B:1202:TDS:CAG  | 2.38                     | 0.49              |
| 3:C:54:TYR:OH      | 3:C:121:GLY:HA3    | 2.12                     | 0.49              |
| 2:B:155:LEU:C      | 2:B:157:LEU:N      | 2.68                     | 0.49              |
| 3:C:86:PRO:O       | 3:C:86:PRO:HG2     | 2.11                     | 0.49              |
| 4:D:25:GLY:CA      | 17:D:201:SQD:H341  | 2.43                     | 0.49              |
| 4:D:172:THR:HG23   | 4:D:174:GLU:OE2    | 2.12                     | 0.49              |
| 1:A:95:LEU:HD22    | 1:A:96:MET:CE      | 2.43                     | 0.49              |
| 3:C:9:TYR:CD1      | 3:C:21:VAL:HB      | 2.47                     | 0.49              |
| 3:C:101:VAL:CG1    | 3:C:103:PHE:CE2    | 2.95                     | 0.49              |
| 4:D:163:THR:O      | 4:D:164:PRO:C      | 2.54                     | 0.49              |
| 7:G:26:TYR:C       | 7:G:26:TYR:CD2     | 2.91                     | 0.49              |
| 1:A:51:GLY:HA3     | 10:A:301:HEM:C3C   | 2.48                     | 0.49              |
| 1:A:151:VAL:HG23   | 1:A:151:VAL:O      | 2.13                     | 0.49              |
| 1:A:215:LEU:HD22   | 2:B:122:ASN:H      | 1.78                     | 0.49              |
| 4:D:133:TYR:CD2    | 4:D:148:LEU:CD2    | 2.93                     | 0.49              |
| 6:F:22:LEU:C       | 6:F:22:LEU:CD1     | 2.81                     | 0.49              |
| 7:G:20:GLY:H       | 18:G:101:BCR:H363  | 1.77                     | 0.49              |
| 1:A:122:VAL:O      | 1:A:125:ALA:HB3    | 2.13                     | 0.49              |
| 2:B:159:LEU:O      | 2:B:160:PHE:CB     | 2.60                     | 0.49              |
| 5:E:23:ILE:O       | 5:E:27:LYS:N       | 2.43                     | 0.49              |
| 1:A:12:LEU:CB      | 1:A:14:ILE:HD11    | 2.43                     | 0.49              |
| 2:B:95:LEU:C       | 2:B:95:LEU:CD2     | 2.78                     | 0.49              |
| 7:G:6:LEU:O        | 7:G:9:LEU:HB2      | 2.12                     | 0.49              |
| 2:B:45:MET:HE3     | 4:D:27:VAL:HG13    | 1.95                     | 0.48              |
| 3:C:77:MET:HB3     | 3:C:113:VAL:HG13   | 1.94                     | 0.48              |
| 4:D:101:ASP:OD1    | 4:D:101:ASP:N      | 2.44                     | 0.48              |
| 3:C:34:VAL:CG2     | 3:C:151:LEU:HB3    | 2.43                     | 0.48              |
| 3:C:54:TYR:CE2     | 3:C:125:GLN:NE2    | 2.81                     | 0.48              |
| 2:B:151:LEU:CD1    | 2:B:152:ASP:HB3    | 2.44                     | 0.48              |
| 3:C:94:LEU:O       | 3:C:95:LYS:C       | 2.57                     | 0.48              |
| 3:C:185:LYS:HB2    | 3:C:185:LYS:NZ     | 2.28                     | 0.48              |
| 4:D:47:GLY:C       | 4:D:49:ALA:N       | 2.71                     | 0.48              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:B:122:ASN:OD1   | 2:B:124:PHE:HB2  | 2.13                     | 0.48              |
| 3:C:200:GLN:HG3   | 3:C:205:LYS:C    | 2.25                     | 0.48              |
| 1:A:81:LEU:O      | 1:A:82:ILE:C     | 2.57                     | 0.48              |
| 3:C:151:LEU:HG    | 3:C:152:GLY:N    | 2.23                     | 0.48              |
| 4:D:83:GLY:HA2    | 4:D:162:LEU:CD1  | 2.43                     | 0.48              |
| 1:A:12:LEU:CB     | 1:A:14:ILE:HD13  | 2.43                     | 0.48              |
| 1:A:95:LEU:CD2    | 1:A:99:LEU:HG    | 2.43                     | 0.48              |
| 2:B:40:PHE:N      | 2:B:41:PRO:CD    | 2.77                     | 0.48              |
| 1:A:3:ASN:O       | 1:A:6:ASP:HB2    | 2.12                     | 0.48              |
| 2:B:99:LEU:O      | 2:B:103:SER:OG   | 2.32                     | 0.48              |
| 14:B:201:CLA:HMB1 | 14:B:201:CLA:CBB | 2.38                     | 0.48              |
| 7:G:35:LEU:HD23   | 7:G:35:LEU:N     | 2.29                     | 0.48              |
| 1:A:196:ALA:O     | 1:A:197:VAL:C    | 2.56                     | 0.48              |
| 2:B:113:PHE:O     | 2:B:116:ASN:HB2  | 2.13                     | 0.48              |
| 4:D:28:THR:O      | 4:D:31:ALA:N     | 2.47                     | 0.48              |
| 8:H:17:TRP:O      | 8:H:21:MET:HB2   | 2.14                     | 0.48              |
| 1:A:4:VAL:O       | 1:A:5:TYR:C      | 2.57                     | 0.48              |
| 1:A:119:ILE:HD13  | 2:B:109:ILE:HD13 | 1.95                     | 0.48              |
| 3:C:13:PRO:O      | 3:C:20:ILE:HA    | 2.14                     | 0.48              |
| 3:C:70:LEU:N      | 3:C:70:LEU:HD22  | 2.23                     | 0.48              |
| 6:F:30:GLN:HG3    | 6:F:31:GLY:N     | 2.28                     | 0.48              |
| 2:B:104:VAL:CB    | 2:B:105:PRO:CD   | 2.92                     | 0.48              |
| 3:C:9:TYR:CD1     | 3:C:21:VAL:HG11  | 2.48                     | 0.48              |
| 3:C:15:GLU:OE1    | 3:C:19:ARG:HB3   | 2.14                     | 0.48              |
| 3:C:115:LEU:N     | 3:C:115:LEU:HD23 | 2.24                     | 0.47              |
| 5:E:14:LEU:C      | 5:E:14:LEU:HD23  | 2.39                     | 0.47              |
| 7:G:27:GLN:OE1    | 8:H:29:LEU:HD21  | 2.14                     | 0.47              |
| 1:A:34:TYR:CE1    | 1:A:103:ARG:NE   | 2.75                     | 0.47              |
| 1:A:80:TRP:CG     | 3:C:254:ARG:NH2  | 2.83                     | 0.47              |
| 4:D:56:ALA:O      | 4:D:57:LYS:HG3   | 2.14                     | 0.47              |
| 4:D:120:ALA:C     | 4:D:122:ASN:H    | 2.22                     | 0.47              |
| 4:D:142:GLY:HA2   | 4:D:144:ALA:N    | 2.29                     | 0.47              |
| 7:G:11:LEU:O      | 7:G:12:GLY:C     | 2.57                     | 0.47              |
| 3:C:270:LEU:C     | 3:C:270:LEU:CD1  | 2.87                     | 0.47              |
| 4:D:115:VAL:HG12  | 4:D:124:PHE:HB3  | 1.96                     | 0.47              |
| 7:G:4:PRO:O       | 7:G:5:LEU:C      | 2.56                     | 0.47              |
| 3:C:61:VAL:CG1    | 3:C:168:ASN:HD21 | 2.28                     | 0.47              |
| 4:D:101:ASP:O     | 4:D:153:ALA:HB3  | 2.13                     | 0.47              |
| 6:F:24:VAL:C      | 6:F:27:LEU:HB2   | 2.40                     | 0.47              |
| 1:A:95:LEU:C      | 1:A:95:LEU:CD2   | 2.87                     | 0.47              |
| 1:A:127:ILE:HG21  | 1:A:195:ILE:HG12 | 1.94                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:B:87:ILE:O       | 2:B:88:LEU:C       | 2.57                     | 0.47              |
| 3:C:34:VAL:HG23    | 3:C:151:LEU:HD23   | 1.96                     | 0.47              |
| 3:C:73:GLY:O       | 3:C:74:ALA:HB2     | 2.15                     | 0.47              |
| 3:C:139:ASP:OD1    | 3:C:140:LYS:N      | 2.46                     | 0.47              |
| 3:C:263:CYS:O      | 3:C:267:LEU:HB2    | 2.15                     | 0.47              |
| 4:D:142:GLY:HA2    | 4:D:144:ALA:H      | 1.79                     | 0.47              |
| 1:A:62:VAL:HG23    | 1:A:63:THR:N       | 2.29                     | 0.47              |
| 2:B:124:PHE:CE1    | 7:G:26:TYR:HD1     | 2.31                     | 0.47              |
| 3:C:34:VAL:O       | 3:C:34:VAL:HG12    | 2.14                     | 0.47              |
| 6:F:21:GLY:O       | 6:F:24:VAL:HB      | 2.15                     | 0.47              |
| 6:F:22:LEU:HD13    | 6:F:23:GLY:N       | 2.30                     | 0.47              |
| 1:A:12:LEU:HB2     | 1:A:14:ILE:HD11    | 1.96                     | 0.47              |
| 2:B:12:PRO:HB2     | 2:B:13:LYS:HD3     | 1.97                     | 0.47              |
| 3:C:14:ARG:NE      | 3:C:150:HIS:CD2    | 2.82                     | 0.47              |
| 3:C:77:MET:HG3     | 3:C:150:HIS:HB2    | 1.97                     | 0.47              |
| 4:D:134:ASP:OD1    | 4:D:134:ASP:O      | 2.31                     | 0.47              |
| 3:C:23:ALA:HB2     | 3:C:240:PHE:HE2    | 1.78                     | 0.47              |
| 3:C:107:LYS:HE2    | 3:C:110:GLN:HE22   | 1.77                     | 0.47              |
| 4:D:29:GLY:O       | 4:D:30:VAL:C       | 2.53                     | 0.47              |
| 6:F:20:TRP:CD1     | 6:F:24:VAL:CG2     | 2.98                     | 0.47              |
| 8:H:19:ILE:O       | 8:H:20:ALA:C       | 2.58                     | 0.47              |
| 1:A:183:TYR:O      | 1:A:186:ALA:HB3    | 2.15                     | 0.46              |
| 12:A:1002:OPC:HBX1 | 12:A:1002:OPC:HBU2 | 1.44                     | 0.46              |
| 2:B:41:PRO:O       | 2:B:42:VAL:C       | 2.56                     | 0.46              |
| 3:C:44:THR:O       | 3:C:132:LEU:HA     | 2.15                     | 0.46              |
| 3:C:62:ALA:O       | 3:C:63:ALA:C       | 2.57                     | 0.46              |
| 3:C:136:PRO:HG3    | 3:C:142:ILE:HG22   | 1.97                     | 0.46              |
| 4:D:16:ARG:O       | 4:D:20:ASN:N       | 2.45                     | 0.46              |
| 4:D:144:ALA:HA     | 4:D:145:PRO:HD2    | 1.75                     | 0.46              |
| 1:A:7:TRP:O        | 1:A:11:ARG:CG      | 2.62                     | 0.46              |
| 5:E:10:VAL:O       | 5:E:10:VAL:HG12    | 2.14                     | 0.46              |
| 8:H:2:GLU:C        | 8:H:2:GLU:OE1      | 2.59                     | 0.46              |
| 1:A:33:PHE:C       | 1:A:35:CYS:H       | 2.22                     | 0.46              |
| 2:B:157:LEU:O      | 2:B:159:LEU:HD23   | 2.14                     | 0.46              |
| 3:C:171:VAL:HG12   | 3:C:233:ASN:O      | 2.14                     | 0.46              |
| 3:C:251:ASP:OD2    | 3:C:251:ASP:C      | 2.57                     | 0.46              |
| 2:B:57:LEU:CD2     | 3:C:258:MET:HE2    | 2.44                     | 0.46              |
| 2:B:82:TYR:O       | 2:B:85:PHE:N       | 2.49                     | 0.46              |
| 1:A:110:PHE:HD1    | 2:B:112:PRO:CB     | 2.13                     | 0.46              |
| 2:B:11:ASP:HA      | 2:B:12:PRO:HD2     | 1.44                     | 0.46              |
| 2:B:134:LEU:O      | 2:B:135:PHE:C      | 2.57                     | 0.46              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 3:C:12:THR:OG1   | 3:C:13:PRO:CD      | 2.63                     | 0.46              |
| 4:D:21:LEU:O     | 4:D:21:LEU:HG      | 2.13                     | 0.46              |
| 1:A:121:GLY:HA3  | 10:A:302:HEM:C3C   | 2.51                     | 0.46              |
| 2:B:156:THR:C    | 2:B:158:GLY:N      | 2.72                     | 0.46              |
| 3:C:270:LEU:CB   | 8:H:21:MET:CE      | 2.91                     | 0.46              |
| 4:D:115:VAL:HG13 | 4:D:116:PRO:HD2    | 1.98                     | 0.46              |
| 4:D:126:CYS:HA   | 4:D:127:PRO:HD3    | 1.54                     | 0.46              |
| 4:D:139:VAL:HG21 | 4:D:147:SER:N      | 2.29                     | 0.46              |
| 2:B:109:ILE:O    | 2:B:112:PRO:CD     | 2.52                     | 0.46              |
| 3:C:172:PHE:O    | 3:C:231:LEU:HG     | 2.16                     | 0.46              |
| 3:C:219:VAL:HB   | 3:C:231:LEU:HA     | 1.98                     | 0.46              |
| 4:D:102:TYR:HH   | 4:D:136:THR:HG22   | 1.79                     | 0.46              |
| 6:F:28:LYS:C     | 6:F:30:GLN:N       | 2.73                     | 0.46              |
| 1:A:14:ILE:CD1   | 1:A:14:ILE:N       | 2.78                     | 0.46              |
| 1:A:150:ILE:HD13 | 15:B:1201:TDS:HAA2 | 1.80                     | 0.46              |
| 1:A:195:ILE:HD13 | 1:A:199:MET:CE     | 2.45                     | 0.46              |
| 1:A:202:HIS:HE1  | 10:A:302:HEM:C4C   | 2.33                     | 0.46              |
| 2:B:84:VAL:O     | 2:B:87:ILE:HB      | 2.16                     | 0.46              |
| 2:B:152:ASP:C    | 2:B:154:THR:N      | 2.60                     | 0.46              |
| 3:C:274:LEU:HB3  | 4:D:19:MET:HE1     | 1.98                     | 0.46              |
| 4:D:177:TRP:NE1  | 4:D:178:TRP:HE3    | 2.13                     | 0.46              |
| 1:A:141:ASP:OD2  | 1:A:141:ASP:O      | 2.34                     | 0.46              |
| 1:A:195:ILE:HG23 | 1:A:199:MET:HE3    | 1.97                     | 0.46              |
| 1:A:206:ILE:HG21 | 11:A:303:HEC:HBD1  | 1.97                     | 0.46              |
| 2:B:124:PHE:CZ   | 7:G:26:TYR:HD1     | 2.34                     | 0.46              |
| 2:B:130:THR:HG23 | 7:G:22:PHE:HE2     | 1.76                     | 0.46              |
| 2:B:153:LYS:NZ   | 2:B:153:LYS:HB3    | 2.30                     | 0.46              |
| 3:C:4:TRP:HA     | 3:C:7:GLN:CB       | 2.45                     | 0.46              |
| 3:C:153:ALA:O    | 3:C:240:PHE:CD1    | 2.69                     | 0.46              |
| 2:B:110:LEU:HA   | 2:B:110:LEU:HD23   | 1.16                     | 0.46              |
| 3:C:14:ARG:NH2   | 3:C:150:HIS:HD2    | 2.11                     | 0.46              |
| 3:C:149:ILE:HB   | 3:C:245:THR:HG23   | 1.97                     | 0.46              |
| 4:D:150:LEU:HD11 | 4:D:171:ARG:NE     | 2.31                     | 0.46              |
| 5:E:27:LYS:O     | 5:E:30:LYS:N       | 2.47                     | 0.46              |
| 1:A:29:HIS:CG    | 1:A:214:PRO:HA     | 2.51                     | 0.45              |
| 1:A:30:VAL:CG2   | 1:A:34:TYR:CD1     | 2.98                     | 0.45              |
| 1:A:92:MET:HE3   | 12:A:1002:OPC:HCB2 | 0.54                     | 0.45              |
| 3:C:104:GLN:HA   | 3:C:105:PRO:HD3    | 1.69                     | 0.45              |
| 1:A:35:CYS:O     | 1:A:36:LEU:C       | 2.58                     | 0.45              |
| 1:A:103:ARG:C    | 1:A:103:ARG:CD     | 2.70                     | 0.45              |
| 2:B:4:LEU:HG     | 2:B:5:LYS:H        | 1.81                     | 0.45              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B:122:ASN:OD1  | 2:B:122:ASN:C     | 2.59                     | 0.45              |
| 8:H:11:LEU:C     | 8:H:11:LEU:HD12   | 2.37                     | 0.45              |
| 1:A:83:ARG:CD    | 10:A:301:HEM:O1D  | 2.60                     | 0.45              |
| 2:B:33:PRO:O     | 2:B:34:ASN:C      | 2.57                     | 0.45              |
| 2:B:137:THR:O    | 2:B:141:ILE:HG13  | 2.16                     | 0.45              |
| 3:C:273:ILE:HD12 | 8:H:25:GLY:HA3    | 1.98                     | 0.45              |
| 4:D:21:LEU:CD1   | 17:D:201:SQD:C30  | 2.89                     | 0.45              |
| 4:D:134:ASP:HB3  | 4:D:140:ILE:HD12  | 1.97                     | 0.45              |
| 7:G:3:GLU:HA     | 7:G:4:PRO:HD2     | 1.72                     | 0.45              |
| 3:C:65:GLY:O     | 3:C:66:SER:C      | 2.46                     | 0.45              |
| 3:C:241:GLY:O    | 3:C:242:GLN:HG2   | 2.16                     | 0.45              |
| 5:E:8:TYR:CD2    | 5:E:8:TYR:C       | 2.93                     | 0.45              |
| 1:A:94:VAL:HG11  | 2:B:80:TYR:CD2    | 2.52                     | 0.45              |
| 3:C:101:VAL:HG11 | 3:C:103:PHE:CZ    | 2.51                     | 0.45              |
| 3:C:171:VAL:HA   | 3:C:232:THR:HG21  | 1.98                     | 0.45              |
| 2:B:108:LEU:HD12 | 2:B:108:LEU:HA    | 1.74                     | 0.45              |
| 2:B:156:THR:C    | 2:B:158:GLY:H     | 2.25                     | 0.45              |
| 4:D:76:GLY:C     | 4:D:77:ASP:O      | 2.60                     | 0.45              |
| 6:F:1:MET:HE3    | 6:F:1:MET:HB2     | 1.53                     | 0.45              |
| 7:G:21:LEU:HD12  | 7:G:21:LEU:HA     | 1.73                     | 0.45              |
| 2:B:18:LEU:HD23  | 2:B:18:LEU:HA     | 1.56                     | 0.45              |
| 2:B:95:LEU:HD23  | 2:B:99:LEU:CD1    | 2.44                     | 0.45              |
| 2:B:32:TRP:CD1   | 2:B:33:PRO:HD2    | 2.50                     | 0.45              |
| 2:B:32:TRP:CG    | 2:B:33:PRO:CD     | 3.00                     | 0.45              |
| 2:B:34:ASN:ND2   | 3:C:283:GLN:NE2   | 2.32                     | 0.45              |
| 2:B:36:LEU:O     | 2:B:37:LEU:C      | 2.59                     | 0.45              |
| 3:C:36:VAL:HG23  | 3:C:37:PRO:O      | 2.16                     | 0.45              |
| 3:C:200:GLN:O    | 3:C:205:LYS:CG    | 2.53                     | 0.45              |
| 2:B:85:PHE:CD2   | 15:B:1201:TDS:OAC | 2.69                     | 0.45              |
| 3:C:4:TRP:CG     | 3:C:162:PRO:HG3   | 2.52                     | 0.45              |
| 4:D:141:ARG:CG   | 4:D:141:ARG:HH11  | 2.30                     | 0.45              |
| 10:A:302:HEM:CBC | 10:A:302:HEM:CMC  | 2.83                     | 0.45              |
| 2:B:93:ASN:O     | 2:B:94:LYS:C      | 2.60                     | 0.45              |
| 2:B:102:ALA:O    | 2:B:106:LEU:HG    | 2.16                     | 0.45              |
| 3:C:1:TYR:O      | 3:C:2:PRO:C       | 2.60                     | 0.45              |
| 3:C:271:MET:CE   | 4:D:22:LEU:HD12   | 2.47                     | 0.45              |
| 4:D:59:LYS:HD3   | 4:D:59:LYS:N      | 2.32                     | 0.45              |
| 5:E:11:PHE:HE2   | 5:E:15:PHE:CE1    | 2.35                     | 0.45              |
| 5:E:24:PHE:O     | 5:E:25:ALA:C      | 2.61                     | 0.45              |
| 1:A:5:TYR:O      | 1:A:6:ASP:C       | 2.59                     | 0.44              |
| 1:A:80:TRP:CG    | 1:A:81:LEU:H      | 2.36                     | 0.44              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:A:112:LYS:HB3   | 1:A:113:PRO:HD3    | 1.99                     | 0.44              |
| 3:C:94:LEU:CD2    | 3:C:98:VAL:CG2     | 2.95                     | 0.44              |
| 3:C:286:GLU:OE1   | 3:C:286:GLU:HA     | 2.17                     | 0.44              |
| 4:D:117:TRP:HE1   | 4:D:119:ALA:HA     | 1.82                     | 0.44              |
| 4:D:143:PRO:O     | 4:D:145:PRO:CD     | 2.58                     | 0.44              |
| 6:F:20:TRP:CD1    | 6:F:24:VAL:HG21    | 2.52                     | 0.44              |
| 1:A:80:TRP:CG     | 1:A:81:LEU:N       | 2.85                     | 0.44              |
| 1:A:211:ILE:CD1   | 10:A:302:HEM:O2D   | 2.65                     | 0.44              |
| 3:C:36:VAL:HG11   | 3:C:149:ILE:HD12   | 1.97                     | 0.44              |
| 4:D:160:ILE:HG23  | 4:D:160:ILE:HD13   | 1.66                     | 0.44              |
| 6:F:11:LEU:HD23   | 6:F:15:LEU:HD11    | 2.00                     | 0.44              |
| 7:G:19:GLY:O      | 7:G:21:LEU:N       | 2.49                     | 0.44              |
| 2:B:33:PRO:O      | 2:B:35:ASP:N       | 2.50                     | 0.44              |
| 2:B:73:LEU:H      | 2:B:73:LEU:HG      | 1.46                     | 0.44              |
| 15:B:1202:TDS:OAO | 15:B:1202:TDS:HAS2 | 2.17                     | 0.44              |
| 3:C:242:GLN:HE21  | 3:C:242:GLN:HB3    | 1.49                     | 0.44              |
| 3:C:271:MET:O     | 4:D:23:ALA:HB2     | 2.17                     | 0.44              |
| 2:B:84:VAL:HG11   | 2:B:101:MET:CG     | 2.46                     | 0.44              |
| 2:B:131:THR:C     | 2:B:133:PHE:N      | 2.73                     | 0.44              |
| 3:C:266:MET:HE2   | 5:E:15:PHE:CE1     | 2.53                     | 0.44              |
| 4:D:74:ASN:O      | 4:D:93:VAL:CG1     | 2.66                     | 0.44              |
| 1:A:114:ARG:CZ    | 1:A:212:SER:HA     | 2.47                     | 0.44              |
| 2:B:40:PHE:HB3    | 2:B:41:PRO:HD3     | 1.92                     | 0.44              |
| 2:B:134:LEU:N     | 2:B:134:LEU:CD1    | 2.70                     | 0.44              |
| 2:B:150:PRO:O     | 2:B:151:LEU:C      | 2.61                     | 0.44              |
| 3:C:36:VAL:HG11   | 3:C:149:ILE:HD13   | 1.99                     | 0.44              |
| 3:C:210:THR:C     | 3:C:211:ILE:HG22   | 2.43                     | 0.44              |
| 7:G:11:LEU:N      | 7:G:11:LEU:CD2     | 2.58                     | 0.44              |
| 1:A:122:VAL:HG22  | 10:A:302:HEM:CBC   | 2.48                     | 0.44              |
| 2:B:118:ASN:ND2   | 2:B:119:LYS:N      | 2.65                     | 0.44              |
| 3:C:171:VAL:HB    | 3:C:233:ASN:O      | 2.18                     | 0.44              |
| 3:C:193:VAL:CG1   | 3:C:194:LYS:N      | 2.80                     | 0.44              |
| 4:D:65:LYS:HB2    | 4:D:68:LYS:NZ      | 2.31                     | 0.44              |
| 1:A:104:VAL:HG21  | 10:A:302:HEM:C2D   | 2.53                     | 0.44              |
| 2:B:151:LEU:O     | 2:B:151:LEU:HD22   | 2.16                     | 0.44              |
| 2:B:159:LEU:O     | 2:B:160:PHE:HD2    | 1.95                     | 0.44              |
| 18:G:101:BCR:H20C | 18:G:101:BCR:H361  | 1.34                     | 0.44              |
| 1:A:47:GLN:CA     | 1:A:47:GLN:NE2     | 2.45                     | 0.44              |
| 1:A:117:THR:O     | 1:A:118:TRP:C      | 2.61                     | 0.44              |
| 3:C:135:ASN:ND2   | 3:C:138:THR:HG23   | 2.33                     | 0.44              |
| 4:D:81:VAL:O      | 4:D:83:GLY:N       | 2.51                     | 0.44              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 5:E:27:LYS:O       | 5:E:30:LYS:CA     | 2.66                     | 0.44              |
| 1:A:26:VAL:N       | 2:B:29:GLU:O      | 2.31                     | 0.43              |
| 12:A:1002:OPC:CBN  | 7:G:5:LEU:HD11    | 2.48                     | 0.43              |
| 2:B:124:PHE:CE1    | 7:G:26:TYR:CD1    | 3.06                     | 0.43              |
| 3:C:73:GLY:O       | 3:C:74:ALA:CB     | 2.66                     | 0.43              |
| 3:C:264:LEU:HD23   | 3:C:264:LEU:HA    | 1.46                     | 0.43              |
| 4:D:63:ASN:HD22    | 4:D:63:ASN:H      | 1.66                     | 0.43              |
| 1:A:18:ALA:O       | 1:A:19:ASP:C      | 2.57                     | 0.43              |
| 1:A:31:ASN:HD22    | 1:A:32:ILE:N      | 2.15                     | 0.43              |
| 1:A:40:THR:HG22    | 10:A:302:HEM:HMB1 | 1.98                     | 0.43              |
| 12:A:1002:OPC:HBN1 | 7:G:5:LEU:HD11    | 1.99                     | 0.43              |
| 2:B:131:THR:O      | 2:B:133:PHE:N     | 2.51                     | 0.43              |
| 3:C:278:GLN:HG3    | 5:E:31:LEU:O      | 2.18                     | 0.43              |
| 1:A:103:ARG:HG3    | 1:A:103:ARG:HH11  | 1.83                     | 0.43              |
| 1:A:154:VAL:HB     | 1:A:155:PRO:CD    | 2.48                     | 0.43              |
| 1:A:118:TRP:O      | 1:A:119:ILE:C     | 2.56                     | 0.43              |
| 2:B:106:LEU:HG     | 2:B:106:LEU:H     | 1.64                     | 0.43              |
| 3:C:60:GLN:HG2     | 3:C:70:LEU:HB3    | 1.99                     | 0.43              |
| 6:F:30:GLN:HE21    | 6:F:30:GLN:HB2    | 1.68                     | 0.43              |
| 1:A:112:LYS:HB3    | 1:A:113:PRO:CD    | 2.49                     | 0.43              |
| 11:A:303:HEC:C3C   | 2:B:40:PHE:CE2    | 3.01                     | 0.43              |
| 2:B:120:PHE:CD1    | 2:B:120:PHE:N     | 2.85                     | 0.43              |
| 3:C:34:VAL:CG2     | 3:C:151:LEU:CD2   | 2.96                     | 0.43              |
| 11:C:301:HEC:CMB   | 11:C:301:HEC:CBB  | 2.94                     | 0.43              |
| 4:D:178:TRP:O      | 4:D:179:VAL:HG23  | 2.19                     | 0.43              |
| 1:A:11:ARG:H       | 1:A:11:ARG:HG2    | 1.19                     | 0.43              |
| 1:A:77:SER:O       | 1:A:78:PHE:HB2    | 2.18                     | 0.43              |
| 1:A:114:ARG:NH1    | 10:A:302:HEM:O1D  | 2.51                     | 0.43              |
| 3:C:4:TRP:HA       | 3:C:7:GLN:HB2     | 1.99                     | 0.43              |
| 3:C:76:LEU:HG      | 3:C:77:MET:N      | 2.34                     | 0.43              |
| 3:C:258:MET:HE3    | 3:C:258:MET:HB3   | 1.93                     | 0.43              |
| 4:D:122:ASN:HB2    | 4:D:135:GLU:OE2   | 2.08                     | 0.43              |
| 1:A:30:VAL:HG22    | 1:A:34:TYR:CB     | 2.49                     | 0.43              |
| 1:A:163:VAL:O      | 1:A:166:SER:N     | 2.51                     | 0.43              |
| 11:A:303:HEC:C1C   | 2:B:40:PHE:CZ     | 3.02                     | 0.43              |
| 2:B:33:PRO:HB2     | 2:B:34:ASN:H      | 1.13                     | 0.43              |
| 3:C:46:PHE:CZ      | 3:C:131:VAL:CG2   | 2.95                     | 0.43              |
| 3:C:171:VAL:HG11   | 3:C:234:ASN:CA    | 2.41                     | 0.43              |
| 4:D:139:VAL:CG2    | 4:D:146:LEU:C     | 2.91                     | 0.43              |
| 1:A:32:ILE:HG22    | 1:A:33:PHE:N      | 2.32                     | 0.43              |
| 1:A:138:LEU:N      | 1:A:139:PRO:CD    | 2.82                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:142:GLN:HE22 | 2:B:67:ASP:HB3    | 1.84                     | 0.43              |
| 2:B:80:TYR:CD1   | 2:B:80:TYR:C      | 2.96                     | 0.43              |
| 2:B:115:GLU:HG3  | 12:B:1001:OPC:OCC | 2.19                     | 0.43              |
| 3:C:171:VAL:HG12 | 3:C:235:PRO:HD3   | 1.87                     | 0.43              |
| 4:D:65:LYS:O     | 4:D:67:SER:N      | 2.52                     | 0.43              |
| 1:A:7:TRP:O      | 1:A:11:ARG:HG3    | 2.19                     | 0.43              |
| 2:B:11:ASP:C     | 2:B:13:LYS:N      | 2.72                     | 0.43              |
| 2:B:88:LEU:HD12  | 2:B:101:MET:SD    | 2.59                     | 0.43              |
| 3:C:3:PHE:O      | 3:C:6:GLN:HB3     | 2.18                     | 0.43              |
| 3:C:4:TRP:CE2    | 3:C:162:PRO:HG3   | 2.53                     | 0.43              |
| 4:D:107:VAL:HG23 | 4:D:107:VAL:H     | 1.37                     | 0.43              |
| 2:B:41:PRO:O     | 2:B:45:MET:HB2    | 2.19                     | 0.42              |
| 2:B:96:LEU:HD11  | 2:B:100:LEU:HD11  | 1.97                     | 0.42              |
| 3:C:21:VAL:O     | 3:C:22:CYS:C      | 2.62                     | 0.42              |
| 3:C:52:ILE:O     | 3:C:52:ILE:CG2    | 2.41                     | 0.42              |
| 3:C:193:VAL:HG12 | 3:C:194:LYS:H     | 1.82                     | 0.42              |
| 11:C:301:HEC:HHA | 11:C:301:HEC:HAA2 | 1.74                     | 0.42              |
| 8:H:6:LEU:HD23   | 8:H:6:LEU:HA      | 1.51                     | 0.42              |
| 2:B:91:VAL:O     | 2:B:92:PRO:C      | 2.62                     | 0.42              |
| 3:C:34:VAL:HG23  | 3:C:151:LEU:HD22  | 2.01                     | 0.42              |
| 3:C:64:ASP:CG    | 3:C:65:GLY:N      | 2.77                     | 0.42              |
| 4:D:21:LEU:HD11  | 17:D:201:SQD:C31  | 2.49                     | 0.42              |
| 4:D:78:ARG:HD3   | 4:D:117:TRP:CG    | 2.54                     | 0.42              |
| 1:A:103:ARG:HB2  | 7:G:21:LEU:HD11   | 2.00                     | 0.42              |
| 3:C:158:GLY:H    | 11:C:301:HEC:HAD2 | 1.83                     | 0.42              |
| 4:D:81:VAL:O     | 4:D:82:GLN:C      | 2.62                     | 0.42              |
| 6:F:10:LEU:HD13  | 6:F:10:LEU:HA     | 1.61                     | 0.42              |
| 7:G:14:VAL:HG12  | 7:G:15:PHE:N      | 2.34                     | 0.42              |
| 1:A:180:LEU:O    | 1:A:181:THR:C     | 2.62                     | 0.42              |
| 1:A:206:ILE:CG2  | 11:A:303:HEC:HBD1 | 2.50                     | 0.42              |
| 3:C:61:VAL:CG1   | 3:C:168:ASN:ND2   | 2.82                     | 0.42              |
| 3:C:267:LEU:HD22 | 3:C:267:LEU:HA    | 1.85                     | 0.42              |
| 4:D:65:LYS:HD3   | 4:D:158:ASP:O     | 2.18                     | 0.42              |
| 1:A:38:GLY:HA3   | 11:A:303:HEC:NC   | 2.35                     | 0.42              |
| 1:A:82:ILE:HD13  | 1:A:82:ILE:H      | 1.84                     | 0.42              |
| 1:A:88:TRP:O     | 1:A:92:MET:HG2    | 2.20                     | 0.42              |
| 3:C:27:LEU:HA    | 3:C:27:LEU:HD23   | 1.82                     | 0.42              |
| 3:C:36:VAL:HG23  | 3:C:37:PRO:N      | 2.34                     | 0.42              |
| 3:C:155:ARG:HD2  | 3:C:239:GLY:O     | 2.19                     | 0.42              |
| 7:G:15:PHE:O     | 7:G:16:ALA:C      | 2.62                     | 0.42              |
| 8:H:3:ILE:HD12   | 8:H:3:ILE:HA      | 1.92                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:A:30:VAL:CG2    | 1:A:34:TYR:CD2     | 3.02                     | 0.42              |
| 1:A:36:LEU:HD12   | 1:A:36:LEU:HA      | 1.63                     | 0.42              |
| 1:A:96:MET:HA     | 1:A:96:MET:CE      | 2.50                     | 0.42              |
| 1:A:203:PHE:CD1   | 1:A:203:PHE:N      | 2.83                     | 0.42              |
| 3:C:102:TYR:CD2   | 3:C:102:TYR:C      | 2.97                     | 0.42              |
| 4:D:13:MET:O      | 4:D:16:ARG:N       | 2.52                     | 0.42              |
| 1:A:104:VAL:HG12  | 1:A:118:TRP:HZ3    | 1.83                     | 0.42              |
| 1:A:116:LEU:HD23  | 1:A:116:LEU:HA     | 1.39                     | 0.42              |
| 2:B:3:THR:HG21    | 3:C:283:GLN:OE1    | 2.20                     | 0.42              |
| 3:C:122:GLU:H     | 3:C:122:GLU:HG2    | 1.18                     | 0.42              |
| 4:D:12:ASP:O      | 4:D:15:ARG:N       | 2.50                     | 0.42              |
| 4:D:36:TYR:OH     | 4:D:40:LYS:HE3     | 2.19                     | 0.42              |
| 6:F:16:ILE:HG22   | 6:F:17:PHE:H       | 1.82                     | 0.42              |
| 1:A:15:GLN:C      | 1:A:17:LEU:N       | 2.77                     | 0.42              |
| 1:A:44:PHE:CE1    | 1:A:195:ILE:HG21   | 2.54                     | 0.42              |
| 1:A:127:ILE:CD1   | 1:A:194:LEU:HB3    | 2.49                     | 0.42              |
| 1:A:150:ILE:HD11  | 15:B:1201:TDS:HAA2 | 2.00                     | 0.42              |
| 10:A:301:HEM:HBA2 | 10:A:301:HEM:CGD   | 2.46                     | 0.42              |
| 2:B:93:ASN:OD1    | 2:B:96:LEU:N       | 2.52                     | 0.42              |
| 3:C:58:LEU:CD1    | 3:C:58:LEU:C       | 2.93                     | 0.42              |
| 4:D:15:ARG:HB3    | 5:E:31:LEU:HD23    | 1.96                     | 0.42              |
| 1:A:139:PRO:HG3   | 10:A:301:HEM:O2D   | 2.20                     | 0.42              |
| 2:B:129:ALA:O     | 2:B:131:THR:N      | 2.53                     | 0.42              |
| 2:B:138:LEU:O     | 2:B:139:VAL:C      | 2.61                     | 0.42              |
| 4:D:146:LEU:HD12  | 4:D:177:TRP:CE2    | 2.48                     | 0.42              |
| 1:A:182:ARG:O     | 1:A:183:TYR:C      | 2.63                     | 0.42              |
| 2:B:130:THR:HG23  | 7:G:22:PHE:CE2     | 2.54                     | 0.42              |
| 4:D:58:ASP:O      | 4:D:61:GLY:N       | 2.53                     | 0.42              |
| 4:D:172:THR:O     | 4:D:174:GLU:OE2    | 2.37                     | 0.42              |
| 1:A:20:ASP:OD2    | 1:A:20:ASP:C       | 2.63                     | 0.41              |
| 2:B:87:ILE:O      | 2:B:89:ARG:N       | 2.53                     | 0.41              |
| 4:D:22:LEU:HD22   | 4:D:22:LEU:HA      | 1.62                     | 0.41              |
| 4:D:170:PHE:CZ    | 4:D:171:ARG:HG2    | 2.54                     | 0.41              |
| 6:F:22:LEU:CD1    | 8:H:20:ALA:HB1     | 2.50                     | 0.41              |
| 1:A:106:LEU:CD2   | 2:B:133:PHE:CE1    | 2.83                     | 0.41              |
| 3:C:54:TYR:CE1    | 3:C:70:LEU:CG      | 3.01                     | 0.41              |
| 3:C:93:GLU:OE1    | 3:C:93:GLU:CA      | 2.66                     | 0.41              |
| 3:C:223:GLN:O     | 3:C:224:ALA:CB     | 2.68                     | 0.41              |
| 4:D:36:TYR:N      | 4:D:37:PRO:HD2     | 2.36                     | 0.41              |
| 4:D:139:VAL:HG21  | 4:D:146:LEU:C      | 2.45                     | 0.41              |
| 3:C:94:LEU:CD2    | 3:C:98:VAL:HG23    | 2.50                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:C:157:ARG:N    | 11:C:301:HEC:HBA1 | 2.35                     | 0.41              |
| 6:F:20:TRP:O     | 6:F:24:VAL:CG2    | 2.52                     | 0.41              |
| 7:G:34:GLU:O     | 7:G:35:LEU:HG     | 2.21                     | 0.41              |
| 1:A:214:PRO:HD3  | 2:B:24:HIS:CE1    | 2.55                     | 0.41              |
| 2:B:14:LEU:HD11  | 2:B:18:LEU:CD1    | 2.47                     | 0.41              |
| 3:C:215:PRO:HB3  | 3:C:232:THR:CG2   | 2.49                     | 0.41              |
| 5:E:31:LEU:HD23  | 5:E:31:LEU:HA     | 1.50                     | 0.41              |
| 7:G:31:ARG:O     | 7:G:32:PRO:O      | 2.38                     | 0.41              |
| 1:A:158:ILE:HA   | 1:A:159:PRO:HD3   | 1.46                     | 0.41              |
| 1:A:194:LEU:HD23 | 1:A:194:LEU:HA    | 1.74                     | 0.41              |
| 2:B:68:PRO:C     | 2:B:69:PHE:HD2    | 2.29                     | 0.41              |
| 2:B:131:THR:O    | 2:B:132:ILE:C     | 2.59                     | 0.41              |
| 3:C:94:LEU:C     | 3:C:96:LYS:N      | 2.74                     | 0.41              |
| 3:C:189:GLU:N    | 3:C:189:GLU:OE1   | 2.54                     | 0.41              |
| 3:C:279:VAL:O    | 3:C:281:LYS:N     | 2.54                     | 0.41              |
| 3:C:72:VAL:H     | 3:C:72:VAL:HG13   | 1.46                     | 0.41              |
| 4:D:169:ASP:O    | 4:D:171:ARG:N     | 2.54                     | 0.41              |
| 1:A:38:GLY:HA3   | 11:A:303:HEC:C4C  | 2.51                     | 0.41              |
| 2:B:152:ASP:CA   | 2:B:154:THR:H     | 2.32                     | 0.41              |
| 3:C:94:LEU:HD23  | 3:C:98:VAL:HG23   | 2.02                     | 0.41              |
| 3:C:189:GLU:OE1  | 3:C:189:GLU:CA    | 2.68                     | 0.41              |
| 3:C:200:GLN:HG2  | 3:C:201:THR:HA    | 2.03                     | 0.41              |
| 5:E:24:PHE:CZ    | 6:F:29:ILE:HD11   | 2.55                     | 0.41              |
| 3:C:33:GLU:HA    | 3:C:243:ASP:OD2   | 2.21                     | 0.41              |
| 3:C:174:ALA:HB3  | 3:C:229:GLU:H     | 1.86                     | 0.41              |
| 3:C:229:GLU:CD   | 3:C:230:ALA:N     | 2.72                     | 0.41              |
| 5:E:24:PHE:CZ    | 6:F:29:ILE:CD1    | 3.04                     | 0.41              |
| 1:A:39:ILE:HD13  | 1:A:39:ILE:HG21   | 1.72                     | 0.41              |
| 1:A:43:CYS:HB3   | 1:A:93:MET:HB2    | 2.02                     | 0.41              |
| 1:A:105:TYR:OH   | 2:B:129:ALA:HB1   | 2.21                     | 0.41              |
| 1:A:198:PHE:HA   | 1:A:201:LEU:HD12  | 2.03                     | 0.41              |
| 11:A:303:HEC:CGA | 15:B:1202:TDS:CAA | 2.85                     | 0.41              |
| 2:B:134:LEU:HA   | 2:B:134:LEU:HD12  | 1.12                     | 0.41              |
| 3:C:214:GLY:N    | 3:C:215:PRO:CD    | 2.84                     | 0.41              |
| 3:C:247:ILE:HD13 | 3:C:247:ILE:HG21  | 1.82                     | 0.41              |
| 3:C:270:LEU:HB2  | 8:H:21:MET:HE1    | 1.98                     | 0.41              |
| 4:D:87:ASP:HB3   | 4:D:105:ASN:OD1   | 2.21                     | 0.41              |
| 4:D:105:ASN:HD21 | 4:D:107:VAL:CG2   | 2.23                     | 0.41              |
| 4:D:114:VAL:O    | 4:D:114:VAL:HG12  | 2.19                     | 0.41              |
| 7:G:18:LEU:O     | 7:G:22:PHE:HD1    | 2.03                     | 0.41              |
| 3:C:151:LEU:CG   | 3:C:152:GLY:N     | 2.80                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:C:173:THR:O      | 3:C:231:LEU:HG     | 2.21                     | 0.41              |
| 3:C:229:GLU:C      | 3:C:231:LEU:H      | 2.28                     | 0.41              |
| 3:C:230:ALA:O      | 3:C:232:THR:N      | 2.53                     | 0.41              |
| 1:A:126:VAL:H      | 1:A:126:VAL:HG23   | 1.75                     | 0.40              |
| 12:A:1002:OPC:HBZ2 | 18:G:101:BCR:H333  | 2.03                     | 0.40              |
| 2:B:83:PRO:O       | 2:B:84:VAL:C       | 2.63                     | 0.40              |
| 3:C:13:PRO:HB3     | 3:C:106:TYR:CE1    | 2.56                     | 0.40              |
| 4:D:64:VAL:HG11    | 4:D:69:PHE:CD1     | 2.56                     | 0.40              |
| 1:A:17:LEU:HA      | 1:A:17:LEU:HD13    | 1.67                     | 0.40              |
| 1:A:117:THR:HG22   | 10:A:302:HEM:C2D   | 2.57                     | 0.40              |
| 1:A:142:GLN:NE2    | 2:B:67:ASP:HB3     | 2.36                     | 0.40              |
| 2:B:97:GLY:HA2     | 2:B:100:LEU:CD1    | 2.51                     | 0.40              |
| 3:C:149:ILE:HB     | 3:C:245:THR:CG2    | 2.52                     | 0.40              |
| 3:C:218:ILE:HD12   | 3:C:218:ILE:H      | 1.86                     | 0.40              |
| 3:C:226:LYS:O      | 3:C:228:GLY:N      | 2.54                     | 0.40              |
| 6:F:22:LEU:HD12    | 8:H:20:ALA:HB2     | 2.02                     | 0.40              |
| 1:A:9:GLN:HA       | 1:A:9:GLN:OE1      | 2.21                     | 0.40              |
| 1:A:80:TRP:CD2     | 1:A:81:LEU:N       | 2.89                     | 0.40              |
| 3:C:72:VAL:O       | 3:C:72:VAL:HG22    | 2.20                     | 0.40              |
| 3:C:79:PRO:HD3     | 3:C:149:ILE:HG12   | 2.03                     | 0.40              |
| 3:C:178:GLY:O      | 3:C:224:ALA:HB1    | 2.20                     | 0.40              |
| 3:C:285:ALA:HB2    | 4:D:10:VAL:CG2     | 2.46                     | 0.40              |
| 4:D:87:ASP:O       | 4:D:88:PRO:C       | 2.62                     | 0.40              |
| 1:A:26:VAL:HA      | 1:A:27:PRO:HD2     | 1.56                     | 0.40              |
| 1:A:211:ILE:O      | 1:A:212:SER:O      | 2.40                     | 0.40              |
| 10:A:302:HEM:HBB2  | 10:A:302:HEM:HMB1  | 2.00                     | 0.40              |
| 11:A:303:HEC:HBA2  | 15:B:1202:TDS:HAA2 | 2.02                     | 0.40              |
| 2:B:1:MET:HE2      | 2:B:1:MET:HB2      | 1.95                     | 0.40              |
| 2:B:94:LYS:O       | 2:B:95:LEU:C       | 2.65                     | 0.40              |
| 2:B:149:PHE:CB     | 2:B:150:PRO:HD3    | 2.50                     | 0.40              |
| 3:C:274:LEU:HA     | 3:C:274:LEU:HD23   | 1.58                     | 0.40              |
| 1:A:215:LEU:HB2    | 7:G:28:GLN:OE1     | 2.21                     | 0.40              |
| 2:B:85:PHE:HE1     | 2:B:147:ALA:CB     | 2.34                     | 0.40              |
| 2:B:159:LEU:HD23   | 2:B:159:LEU:N      | 2.35                     | 0.40              |
| 3:C:115:LEU:HD23   | 3:C:115:LEU:HA     | 1.59                     | 0.40              |
| 3:C:146:LYS:HG3    | 3:C:248:VAL:HG23   | 2.02                     | 0.40              |
| 7:G:27:GLN:OE1     | 8:H:29:LEU:CD2     | 2.70                     | 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) |
|-----------------|----------------------|--------------------------|-------------------|
| 3:C:108:GLU:OE2 | 7:G:33:ASN:CB[8_565] | 2.09                     | 0.11              |

## 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     | 213/215 (99%) | 154 (72%) | 41 (19%)  | 18 (8%)   | 0           | 4 |
| 2   | B     | 158/160 (99%) | 89 (56%)  | 43 (27%)  | 26 (16%)  | 0           | 0 |
| 3   | C     | 286/289 (99%) | 204 (71%) | 51 (18%)  | 31 (11%)  | 0           | 3 |
| 4   | D     | 164/179 (92%) | 114 (70%) | 28 (17%)  | 22 (13%)  | 0           | 1 |
| 5   | E     | 30/32 (94%)   | 15 (50%)  | 11 (37%)  | 4 (13%)   | 0           | 1 |
| 6   | F     | 30/35 (86%)   | 15 (50%)  | 8 (27%)   | 7 (23%)   | 0           | 0 |
| 7   | G     | 35/37 (95%)   | 11 (31%)  | 15 (43%)  | 9 (26%)   | 0           | 0 |
| 8   | H     | 27/29 (93%)   | 15 (56%)  | 6 (22%)   | 6 (22%)   | 0           | 0 |
| All | All   | 943/976 (97%) | 617 (65%) | 203 (22%) | 123 (13%) | 0           | 1 |

All (123) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 16  | ALA  |
| 1   | A     | 36  | LEU  |
| 1   | A     | 73  | MET  |
| 1   | A     | 74  | ASN  |
| 1   | A     | 112 | LYS  |
| 1   | A     | 162 | GLY  |
| 2   | B     | 22  | MET  |
| 2   | B     | 33  | PRO  |
| 2   | B     | 34  | ASN  |
| 2   | B     | 37  | LEU  |
| 2   | B     | 87  | ILE  |
| 2   | B     | 88  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 113 | PHE  |
| 2   | B     | 114 | ILE  |
| 2   | B     | 115 | GLU  |
| 2   | B     | 125 | ARG  |
| 3   | C     | 23  | ALA  |
| 3   | C     | 63  | ALA  |
| 3   | C     | 66  | SER  |
| 3   | C     | 74  | ALA  |
| 3   | C     | 173 | THR  |
| 3   | C     | 186 | GLU  |
| 3   | C     | 189 | GLU  |
| 3   | C     | 192 | ASN  |
| 3   | C     | 200 | GLN  |
| 3   | C     | 201 | THR  |
| 3   | C     | 202 | ASP  |
| 3   | C     | 212 | PRO  |
| 3   | C     | 224 | ALA  |
| 3   | C     | 226 | LYS  |
| 3   | C     | 227 | ALA  |
| 3   | C     | 230 | ALA  |
| 4   | D     | 13  | MET  |
| 4   | D     | 14  | GLY  |
| 4   | D     | 49  | ALA  |
| 4   | D     | 63  | ASN  |
| 4   | D     | 64  | VAL  |
| 4   | D     | 70  | LEU  |
| 4   | D     | 71  | GLU  |
| 4   | D     | 77  | ASP  |
| 4   | D     | 135 | GLU  |
| 4   | D     | 139 | VAL  |
| 4   | D     | 145 | PRO  |
| 4   | D     | 167 | GLU  |
| 6   | F     | 9   | ALA  |
| 6   | F     | 10  | LEU  |
| 6   | F     | 29  | ILE  |
| 7   | G     | 16  | ALA  |
| 7   | G     | 20  | GLY  |
| 7   | G     | 27  | GLN  |
| 7   | G     | 32  | PRO  |
| 7   | G     | 34  | GLU  |
| 8   | H     | 2   | GLU  |
| 8   | H     | 4   | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 2   | ALA  |
| 1   | A     | 3   | ASN  |
| 1   | A     | 114 | ARG  |
| 1   | A     | 132 | GLY  |
| 1   | A     | 136 | TYR  |
| 1   | A     | 150 | ILE  |
| 2   | B     | 146 | GLY  |
| 3   | C     | 34  | VAL  |
| 3   | C     | 174 | ALA  |
| 3   | C     | 191 | GLY  |
| 3   | C     | 278 | GLN  |
| 4   | D     | 21  | LEU  |
| 4   | D     | 56  | ALA  |
| 4   | D     | 81  | VAL  |
| 4   | D     | 97  | GLU  |
| 4   | D     | 110 | HIS  |
| 6   | F     | 24  | VAL  |
| 7   | G     | 19  | GLY  |
| 1   | A     | 32  | ILE  |
| 1   | A     | 131 | PHE  |
| 2   | B     | 94  | LYS  |
| 2   | B     | 95  | LEU  |
| 3   | C     | 20  | ILE  |
| 3   | C     | 91  | PRO  |
| 3   | C     | 184 | ALA  |
| 3   | C     | 195 | TYR  |
| 4   | D     | 82  | GLN  |
| 4   | D     | 138 | LYS  |
| 4   | D     | 174 | GLU  |
| 5   | E     | 13  | ALA  |
| 6   | F     | 17  | PHE  |
| 7   | G     | 4   | PRO  |
| 7   | G     | 14  | VAL  |
| 1   | A     | 96  | MET  |
| 2   | B     | 78  | GLU  |
| 2   | B     | 134 | LEU  |
| 2   | B     | 145 | ILE  |
| 3   | C     | 175 | SER  |
| 3   | C     | 187 | GLU  |
| 3   | C     | 231 | LEU  |
| 4   | D     | 122 | ASN  |
| 8   | H     | 7   | GLY  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | H     | 20  | ALA  |
| 1   | A     | 60  | PRO  |
| 1   | A     | 155 | PRO  |
| 2   | B     | 2   | ALA  |
| 2   | B     | 36  | LEU  |
| 2   | B     | 86  | GLN  |
| 2   | B     | 102 | ALA  |
| 2   | B     | 124 | PHE  |
| 2   | B     | 137 | THR  |
| 2   | B     | 141 | ILE  |
| 3   | C     | 194 | LYS  |
| 5   | E     | 17  | GLY  |
| 5   | E     | 19  | ALA  |
| 6   | F     | 6   | LEU  |
| 7   | G     | 31  | ARG  |
| 2   | B     | 92  | PRO  |
| 2   | B     | 105 | PRO  |
| 2   | B     | 122 | ASN  |
| 3   | C     | 88  | GLU  |
| 3   | C     | 215 | PRO  |
| 1   | A     | 206 | ILE  |
| 5   | E     | 18  | ILE  |
| 6   | F     | 16  | ILE  |
| 8   | H     | 19  | ILE  |
| 8   | H     | 23  | VAL  |
| 3   | C     | 69  | GLY  |
| 4   | D     | 143 | PRO  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |   |
|-----|-------|----------------|-----------|----------|-------------|---|
| 1   | A     | 184/184 (100%) | 126 (68%) | 58 (32%) | 0           | 1 |
| 2   | B     | 137/137 (100%) | 90 (66%)  | 47 (34%) | 0           | 1 |
| 3   | C     | 242/243 (100%) | 153 (63%) | 89 (37%) | 0           | 0 |

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| Mol | Chain | Analysed      | Rotameric | Outliers  | Percentiles |   |
|-----|-------|---------------|-----------|-----------|-------------|---|
| 4   | D     | 139/146 (95%) | 94 (68%)  | 45 (32%)  | 0           | 1 |
| 5   | E     | 25/25 (100%)  | 17 (68%)  | 8 (32%)   | 0           | 1 |
| 6   | F     | 24/27 (89%)   | 11 (46%)  | 13 (54%)  | 0           | 0 |
| 7   | G     | 28/28 (100%)  | 15 (54%)  | 13 (46%)  | 0           | 0 |
| 8   | H     | 24/24 (100%)  | 17 (71%)  | 7 (29%)   | 0           | 1 |
| All | All   | 803/814 (99%) | 523 (65%) | 280 (35%) | 0           | 1 |

All (280) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 1   | MET  |
| 1   | A     | 5   | TYR  |
| 1   | A     | 11  | ARG  |
| 1   | A     | 12  | LEU  |
| 1   | A     | 14  | ILE  |
| 1   | A     | 17  | LEU  |
| 1   | A     | 21  | VAL  |
| 1   | A     | 30  | VAL  |
| 1   | A     | 31  | ASN  |
| 1   | A     | 32  | ILE  |
| 1   | A     | 36  | LEU  |
| 1   | A     | 47  | GLN  |
| 1   | A     | 52  | PHE  |
| 1   | A     | 61  | THR  |
| 1   | A     | 62  | VAL  |
| 1   | A     | 72  | ILE  |
| 1   | A     | 77  | SER  |
| 1   | A     | 81  | LEU  |
| 1   | A     | 82  | ILE  |
| 1   | A     | 83  | ARG  |
| 1   | A     | 84  | SER  |
| 1   | A     | 87  | ARG  |
| 1   | A     | 95  | LEU  |
| 1   | A     | 97  | MET  |
| 1   | A     | 99  | LEU  |
| 1   | A     | 100 | HIS  |
| 1   | A     | 103 | ARG  |
| 1   | A     | 104 | VAL  |
| 1   | A     | 106 | LEU  |
| 1   | A     | 107 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 110 | PHE  |
| 1   | A     | 112 | LYS  |
| 1   | A     | 114 | ARG  |
| 1   | A     | 115 | GLU  |
| 1   | A     | 116 | LEU  |
| 1   | A     | 119 | ILE  |
| 1   | A     | 123 | ILE  |
| 1   | A     | 130 | SER  |
| 1   | A     | 142 | GLN  |
| 1   | A     | 143 | VAL  |
| 1   | A     | 148 | VAL  |
| 1   | A     | 151 | VAL  |
| 1   | A     | 152 | SER  |
| 1   | A     | 155 | PRO  |
| 1   | A     | 161 | VAL  |
| 1   | A     | 163 | VAL  |
| 1   | A     | 164 | LEU  |
| 1   | A     | 169 | LEU  |
| 1   | A     | 173 | SER  |
| 1   | A     | 182 | ARG  |
| 1   | A     | 195 | ILE  |
| 1   | A     | 200 | LEU  |
| 1   | A     | 201 | LEU  |
| 1   | A     | 206 | ILE  |
| 1   | A     | 207 | ARG  |
| 1   | A     | 208 | LYS  |
| 1   | A     | 211 | ILE  |
| 1   | A     | 215 | LEU  |
| 2   | B     | 3   | THR  |
| 2   | B     | 4   | LEU  |
| 2   | B     | 5   | LYS  |
| 2   | B     | 8   | ASP  |
| 2   | B     | 13  | LYS  |
| 2   | B     | 15  | ARG  |
| 2   | B     | 20  | LYS  |
| 2   | B     | 25  | ASN  |
| 2   | B     | 35  | ASP  |
| 2   | B     | 39  | VAL  |
| 2   | B     | 40  | PHE  |
| 2   | B     | 44  | ILE  |
| 2   | B     | 51  | ILE  |
| 2   | B     | 55  | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 57  | LEU  |
| 2   | B     | 69  | PHE  |
| 2   | B     | 73  | LEU  |
| 2   | B     | 74  | GLU  |
| 2   | B     | 75  | ILE  |
| 2   | B     | 76  | LEU  |
| 2   | B     | 79  | TRP  |
| 2   | B     | 81  | LEU  |
| 2   | B     | 86  | GLN  |
| 2   | B     | 88  | LEU  |
| 2   | B     | 90  | SER  |
| 2   | B     | 94  | LYS  |
| 2   | B     | 96  | LEU  |
| 2   | B     | 100 | LEU  |
| 2   | B     | 101 | MET  |
| 2   | B     | 103 | SER  |
| 2   | B     | 109 | ILE  |
| 2   | B     | 115 | GLU  |
| 2   | B     | 119 | LYS  |
| 2   | B     | 120 | PHE  |
| 2   | B     | 127 | PRO  |
| 2   | B     | 132 | ILE  |
| 2   | B     | 134 | LEU  |
| 2   | B     | 138 | LEU  |
| 2   | B     | 140 | THR  |
| 2   | B     | 141 | ILE  |
| 2   | B     | 143 | LEU  |
| 2   | B     | 153 | LYS  |
| 2   | B     | 154 | THR  |
| 2   | B     | 155 | LEU  |
| 2   | B     | 156 | THR  |
| 2   | B     | 157 | LEU  |
| 2   | B     | 159 | LEU  |
| 3   | C     | 3   | PHE  |
| 3   | C     | 7   | GLN  |
| 3   | C     | 12  | THR  |
| 3   | C     | 14  | ARG  |
| 3   | C     | 19  | ARG  |
| 3   | C     | 21  | VAL  |
| 3   | C     | 22  | CYS  |
| 3   | C     | 30  | LYS  |
| 3   | C     | 35  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 36  | VAL  |
| 3   | C     | 40  | VAL  |
| 3   | C     | 47  | LYS  |
| 3   | C     | 50  | VAL  |
| 3   | C     | 56  | THR  |
| 3   | C     | 58  | LEU  |
| 3   | C     | 59  | GLN  |
| 3   | C     | 60  | GLN  |
| 3   | C     | 61  | VAL  |
| 3   | C     | 70  | LEU  |
| 3   | C     | 72  | VAL  |
| 3   | C     | 75  | VAL  |
| 3   | C     | 77  | MET  |
| 3   | C     | 80  | GLU  |
| 3   | C     | 88  | GLU  |
| 3   | C     | 92  | GLU  |
| 3   | C     | 93  | GLU  |
| 3   | C     | 95  | LYS  |
| 3   | C     | 100 | ASP  |
| 3   | C     | 101 | VAL  |
| 3   | C     | 104 | GLN  |
| 3   | C     | 110 | GLN  |
| 3   | C     | 113 | VAL  |
| 3   | C     | 116 | VAL  |
| 3   | C     | 119 | LEU  |
| 3   | C     | 122 | GLU  |
| 3   | C     | 125 | GLN  |
| 3   | C     | 126 | GLU  |
| 3   | C     | 131 | VAL  |
| 3   | C     | 132 | LEU  |
| 3   | C     | 137 | THR  |
| 3   | C     | 141 | ASN  |
| 3   | C     | 150 | HIS  |
| 3   | C     | 154 | ASN  |
| 3   | C     | 155 | ARG  |
| 3   | C     | 160 | ILE  |
| 3   | C     | 165 | GLU  |
| 3   | C     | 166 | LYS  |
| 3   | C     | 171 | VAL  |
| 3   | C     | 172 | PHE  |
| 3   | C     | 175 | SER  |
| 3   | C     | 179 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 180 | ILE  |
| 3   | C     | 185 | LYS  |
| 3   | C     | 186 | GLU  |
| 3   | C     | 188 | ASP  |
| 3   | C     | 189 | GLU  |
| 3   | C     | 198 | SER  |
| 3   | C     | 199 | ILE  |
| 3   | C     | 203 | SER  |
| 3   | C     | 205 | LYS  |
| 3   | C     | 206 | THR  |
| 3   | C     | 207 | VAL  |
| 3   | C     | 208 | VAL  |
| 3   | C     | 210 | THR  |
| 3   | C     | 211 | ILE  |
| 3   | C     | 212 | PRO  |
| 3   | C     | 216 | GLU  |
| 3   | C     | 218 | ILE  |
| 3   | C     | 219 | VAL  |
| 3   | C     | 221 | GLU  |
| 3   | C     | 223 | GLN  |
| 3   | C     | 226 | LYS  |
| 3   | C     | 229 | GLU  |
| 3   | C     | 232 | THR  |
| 3   | C     | 233 | ASN  |
| 3   | C     | 242 | GLN  |
| 3   | C     | 249 | LEU  |
| 3   | C     | 251 | ASP  |
| 3   | C     | 256 | LYS  |
| 3   | C     | 259 | ILE  |
| 3   | C     | 262 | ILE  |
| 3   | C     | 264 | LEU  |
| 3   | C     | 267 | LEU  |
| 3   | C     | 270 | LEU  |
| 3   | C     | 276 | LYS  |
| 3   | C     | 282 | VAL  |
| 3   | C     | 286 | GLU  |
| 3   | C     | 287 | MET  |
| 3   | C     | 288 | ASN  |
| 4   | D     | 9   | ASP  |
| 4   | D     | 10  | VAL  |
| 4   | D     | 13  | MET  |
| 4   | D     | 16  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | D     | 22  | LEU  |
| 4   | D     | 26  | THR  |
| 4   | D     | 35  | LEU  |
| 4   | D     | 43  | ILE  |
| 4   | D     | 59  | LYS  |
| 4   | D     | 60  | LEU  |
| 4   | D     | 65  | LYS  |
| 4   | D     | 66  | VAL  |
| 4   | D     | 67  | SER  |
| 4   | D     | 68  | LYS  |
| 4   | D     | 69  | PHE  |
| 4   | D     | 72  | SER  |
| 4   | D     | 77  | ASP  |
| 4   | D     | 78  | ARG  |
| 4   | D     | 79  | VAL  |
| 4   | D     | 84  | LEU  |
| 4   | D     | 85  | LYS  |
| 4   | D     | 95  | SER  |
| 4   | D     | 96  | LYS  |
| 4   | D     | 97  | GLU  |
| 4   | D     | 99  | ILE  |
| 4   | D     | 101 | ASP  |
| 4   | D     | 105 | ASN  |
| 4   | D     | 107 | VAL  |
| 4   | D     | 109 | THR  |
| 4   | D     | 111 | LEU  |
| 4   | D     | 114 | VAL  |
| 4   | D     | 125 | LYS  |
| 4   | D     | 134 | ASP  |
| 4   | D     | 139 | VAL  |
| 4   | D     | 140 | ILE  |
| 4   | D     | 141 | ARG  |
| 4   | D     | 146 | LEU  |
| 4   | D     | 148 | LEU  |
| 4   | D     | 154 | THR  |
| 4   | D     | 160 | ILE  |
| 4   | D     | 161 | VAL  |
| 4   | D     | 167 | GLU  |
| 4   | D     | 172 | THR  |
| 4   | D     | 174 | GLU  |
| 4   | D     | 179 | VAL  |
| 5   | E     | 9   | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | E     | 12  | ILE  |
| 5   | E     | 14  | LEU  |
| 5   | E     | 18  | ILE  |
| 5   | E     | 26  | ILE  |
| 5   | E     | 29  | ILE  |
| 5   | E     | 30  | LYS  |
| 5   | E     | 32  | ILE  |
| 6   | F     | 1   | MET  |
| 6   | F     | 6   | LEU  |
| 6   | F     | 10  | LEU  |
| 6   | F     | 11  | LEU  |
| 6   | F     | 12  | SER  |
| 6   | F     | 15  | LEU  |
| 6   | F     | 16  | ILE  |
| 6   | F     | 22  | LEU  |
| 6   | F     | 25  | LEU  |
| 6   | F     | 26  | LEU  |
| 6   | F     | 27  | LEU  |
| 6   | F     | 29  | ILE  |
| 6   | F     | 30  | GLN  |
| 7   | G     | 1   | MET  |
| 7   | G     | 2   | VAL  |
| 7   | G     | 3   | GLU  |
| 7   | G     | 4   | PRO  |
| 7   | G     | 5   | LEU  |
| 7   | G     | 6   | LEU  |
| 7   | G     | 9   | LEU  |
| 7   | G     | 23  | TYR  |
| 7   | G     | 28  | GLN  |
| 7   | G     | 29  | TYR  |
| 7   | G     | 30  | LYS  |
| 7   | G     | 34  | GLU  |
| 7   | G     | 35  | LEU  |
| 8   | H     | 2   | GLU  |
| 8   | H     | 6   | LEU  |
| 8   | H     | 14  | VAL  |
| 8   | H     | 18  | SER  |
| 8   | H     | 21  | MET  |
| 8   | H     | 22  | VAL  |
| 8   | H     | 27  | ASN  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 31  | ASN  |
| 1   | A     | 47  | GLN  |
| 2   | B     | 25  | ASN  |
| 2   | B     | 34  | ASN  |
| 2   | B     | 118 | ASN  |
| 3   | C     | 6   | GLN  |
| 3   | C     | 59  | GLN  |
| 3   | C     | 60  | GLN  |
| 3   | C     | 110 | GLN  |
| 3   | C     | 123 | GLN  |
| 3   | C     | 141 | ASN  |
| 3   | C     | 154 | ASN  |
| 3   | C     | 200 | GLN  |
| 3   | C     | 223 | GLN  |
| 3   | C     | 234 | ASN  |
| 3   | C     | 242 | GLN  |
| 3   | C     | 250 | GLN  |
| 3   | C     | 288 | ASN  |
| 4   | D     | 73  | HIS  |
| 4   | D     | 105 | ASN  |
| 4   | D     | 152 | HIS  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 1 is monoatomic - leaving 16 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 12  | OPC  | B     | 1001 | -    | 53,53,54     | 2.28 | 23 (43%) | 59,61,64    | 2.71 | 25 (42%) |
| 11  | HEC  | A     | 303  | 19,1 | 50,50,50     | 2.40 | 14 (28%) | 68,82,82    | 2.16 | 24 (35%) |
| 12  | OPC  | A     | 1002 | -    | 53,53,54     | 2.05 | 14 (26%) | 59,61,64    | 2.88 | 20 (33%) |
| 17  | SQD  | D     | 201  | -    | 52,54,54     | 2.93 | 25 (48%) | 62,65,65    | 5.06 | 31 (50%) |
| 10  | HEM  | A     | 301  | 1    | 50,50,50     | 2.42 | 15 (30%) | 67,82,82    | 3.40 | 35 (52%) |
| 15  | TDS  | B     | 1201 | -    | 31,31,31     | 4.17 | 15 (48%) | 37,40,40    | 5.20 | 17 (45%) |
| 16  | FES  | D     | 200  | 4    | 0,4,4        | -    | -        | -           | -    | -        |
| 11  | HEC  | C     | 301  | 3    | 50,50,50     | 2.33 | 17 (34%) | 68,82,82    | 1.98 | 20 (29%) |
| 13  | UMQ  | A     | 1103 | -    | 35,35,35     | 1.98 | 5 (14%)  | 46,46,46    | 2.59 | 13 (28%) |
| 14  | CLA  | B     | 201  | 19   | 69,73,73     | 2.10 | 20 (28%) | 82,113,113  | 3.04 | 36 (43%) |
| 18  | BCR  | G     | 101  | -    | 41,41,41     | 3.48 | 23 (56%) | 56,56,56    | 6.82 | 27 (48%) |
| 13  | UMQ  | A     | 1101 | -    | 35,35,35     | 1.75 | 5 (14%)  | 46,46,46    | 3.05 | 24 (52%) |
| 13  | UMQ  | A     | 1102 | -    | 35,35,35     | 2.17 | 9 (25%)  | 46,46,46    | 3.03 | 18 (39%) |
| 10  | HEM  | A     | 302  | 1    | 50,50,50     | 2.16 | 18 (36%) | 67,82,82    | 2.06 | 20 (29%) |
| 13  | UMQ  | A     | 1104 | -    | 35,35,35     | 1.58 | 3 (8%)   | 46,46,46    | 3.04 | 19 (41%) |
| 15  | TDS  | B     | 1202 | -    | 31,31,31     | 4.21 | 13 (41%) | 37,40,40    | 5.50 | 23 (62%) |

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   |
|-----|------|-------|------|------|-----------|-------------|---------|
| 12  | OPC  | B     | 1001 | -    | -         | 23/57/57/60 | -       |
| 11  | HEC  | A     | 303  | 19,1 | 1/1/3/7   | 6/14/54/54  | -       |
| 17  | SQD  | D     | 201  | -    | 3/3/9/9   | 27/49/69/69 | 0/1/1/1 |
| 12  | OPC  | A     | 1002 | -    | -         | 32/57/57/60 | -       |
| 10  | HEM  | A     | 301  | 1    | -         | 5/14/54/54  | -       |
| 15  | TDS  | B     | 1201 | -    | -         | 11/17/17/17 | 0/2/2/2 |
| 16  | FES  | D     | 200  | 4    | -         | -           | 0/1/1/1 |
| 11  | HEC  | C     | 301  | 3    | 1/1/3/7   | 10/14/54/54 | -       |
| 13  | UMQ  | A     | 1103 | -    | 2/2/10/10 | 11/20/60/60 | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|------|------|-----------|---------------|---------|
| 14  | CLA  | B     | 201  | 19   | 1/1/15/20 | 13/39/115/115 | -       |
| 18  | BCR  | G     | 101  | -    | -         | 12/29/63/63   | 0/2/2/2 |
| 13  | UMQ  | A     | 1101 | -    | 2/2/10/10 | 11/20/60/60   | 0/2/2/2 |
| 13  | UMQ  | A     | 1102 | -    | 2/2/10/10 | 12/20/60/60   | 0/2/2/2 |
| 10  | HEM  | A     | 302  | 1    | -         | 6/14/54/54    | -       |
| 13  | UMQ  | A     | 1104 | -    | 2/2/10/10 | 13/20/60/60   | 0/2/2/2 |
| 15  | TDS  | B     | 1202 | -    | -         | 11/17/17/17   | 0/2/2/2 |

All (219) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 15  | B     | 1202 | TDS  | CAD-CAE | -10.82 | 1.20        | 1.38     |
| 18  | G     | 101  | BCR  | C8-C9   | -10.35 | 1.23        | 1.46     |
| 15  | B     | 1202 | TDS  | CAD-CAL | -10.08 | 1.21        | 1.38     |
| 15  | B     | 1201 | TDS  | CAD-CAE | -9.85  | 1.22        | 1.38     |
| 15  | B     | 1202 | TDS  | CAM-CAN | 9.63   | 1.54        | 1.39     |
| 15  | B     | 1201 | TDS  | CAL-CAM | 9.23   | 1.53        | 1.40     |
| 15  | B     | 1201 | TDS  | CAD-CAL | -9.07  | 1.23        | 1.38     |
| 18  | G     | 101  | BCR  | C26-C25 | 7.64   | 1.47        | 1.34     |
| 11  | C     | 301  | HEC  | C3D-C2D | 7.42   | 1.52        | 1.36     |
| 18  | G     | 101  | BCR  | C23-C22 | -7.34  | 1.30        | 1.46     |
| 13  | A     | 1102 | UMQ  | O1'-C1' | 7.32   | 1.52        | 1.40     |
| 13  | A     | 1101 | UMQ  | C1'-C2' | -7.15  | 1.31        | 1.52     |
| 12  | B     | 1001 | OPC  | OBJ-CBK | 7.13   | 1.54        | 1.33     |
| 15  | B     | 1201 | TDS  | CAM-CAN | 7.09   | 1.50        | 1.39     |
| 10  | A     | 301  | HEM  | FE-NB   | -7.06  | 1.73        | 1.94     |
| 11  | A     | 303  | HEC  | C3D-C2D | 7.04   | 1.52        | 1.36     |
| 17  | D     | 201  | SQD  | C4-C3   | 6.70   | 1.69        | 1.52     |
| 15  | B     | 1201 | TDS  | CAR-CAQ | -6.66  | 1.27        | 1.52     |
| 13  | A     | 1103 | UMQ  | O1'-C1' | 6.63   | 1.51        | 1.40     |
| 15  | B     | 1202 | TDS  | CAL-CAM | 6.62   | 1.49        | 1.40     |
| 15  | B     | 1202 | TDS  | CAR-CAQ | -6.45  | 1.28        | 1.52     |
| 17  | D     | 201  | SQD  | O47-C7  | 6.40   | 1.52        | 1.34     |
| 17  | D     | 201  | SQD  | C17-C16 | -6.40  | 1.20        | 1.51     |
| 18  | G     | 101  | BCR  | C30-C25 | 6.33   | 1.61        | 1.53     |
| 15  | B     | 1201 | TDS  | OAB-CAE | 6.16   | 1.47        | 1.37     |
| 10  | A     | 301  | HEM  | C3D-C2D | 6.00   | 1.49        | 1.36     |
| 15  | B     | 1202 | TDS  | CAH-CAG | -5.96  | 1.33        | 1.47     |
| 14  | B     | 201  | CLA  | C3C-C2C | 5.86   | 1.49        | 1.36     |
| 13  | A     | 1103 | UMQ  | C1'-C2' | -5.76  | 1.35        | 1.52     |
| 18  | G     | 101  | BCR  | C38-C26 | 5.68   | 1.60        | 1.50     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 11  | A     | 303  | HEC  | FE-NC   | 5.60  | 2.13        | 1.95     |
| 12  | A     | 1002 | OPC  | OAN-CAO | 5.55  | 1.50        | 1.34     |
| 17  | D     | 201  | SQD  | O6-C1   | 5.49  | 1.49        | 1.40     |
| 10  | A     | 301  | HEM  | CMC-C2C | 5.48  | 1.62        | 1.50     |
| 17  | D     | 201  | SQD  | C12-C11 | -5.44 | 1.24        | 1.51     |
| 11  | A     | 303  | HEC  | FE-ND   | 5.25  | 2.11        | 1.94     |
| 12  | B     | 1001 | OPC  | CAG-CAH | -5.24 | 1.35        | 1.51     |
| 10  | A     | 302  | HEM  | C3D-C2D | 5.19  | 1.48        | 1.36     |
| 13  | A     | 1102 | UMQ  | C1'-C2' | -5.10 | 1.37        | 1.52     |
| 15  | B     | 1201 | TDS  | CAF-CAE | 5.08  | 1.49        | 1.40     |
| 14  | B     | 201  | CLA  | OBD-CAD | 5.02  | 1.31        | 1.22     |
| 11  | A     | 303  | HEC  | CBB-CAB | -4.99 | 1.30        | 1.51     |
| 17  | D     | 201  | SQD  | C16-C15 | -4.92 | 1.27        | 1.51     |
| 14  | B     | 201  | CLA  | O2D-CGD | 4.86  | 1.45        | 1.33     |
| 18  | G     | 101  | BCR  | C7-C6   | -4.85 | 1.28        | 1.45     |
| 17  | D     | 201  | SQD  | O48-C23 | 4.84  | 1.47        | 1.33     |
| 11  | C     | 301  | HEC  | CMB-C2B | 4.83  | 1.60        | 1.50     |
| 18  | G     | 101  | BCR  | C8-C7   | -4.81 | 1.18        | 1.33     |
| 13  | A     | 1104 | UMQ  | O1'-C1' | 4.81  | 1.48        | 1.40     |
| 13  | A     | 1104 | UMQ  | C1'-C2' | -4.76 | 1.38        | 1.52     |
| 17  | D     | 201  | SQD  | C18-C17 | -4.76 | 1.28        | 1.51     |
| 10  | A     | 301  | HEM  | CMB-C2B | 4.71  | 1.60        | 1.50     |
| 12  | A     | 1002 | OPC  | CBP-CBQ | -4.66 | 1.32        | 1.52     |
| 11  | A     | 303  | HEC  | C3B-C2B | -4.64 | 1.26        | 1.36     |
| 15  | B     | 1201 | TDS  | CAR-CAS | -4.64 | 1.28        | 1.51     |
| 15  | B     | 1202 | TDS  | CAR-CAS | -4.62 | 1.28        | 1.51     |
| 15  | B     | 1201 | TDS  | OAK-CAL | 4.59  | 1.44        | 1.37     |
| 13  | A     | 1102 | UMQ  | O5'-C1' | 4.59  | 1.53        | 1.41     |
| 15  | B     | 1202 | TDS  | OAB-CAE | 4.57  | 1.44        | 1.37     |
| 14  | B     | 201  | CLA  | CHC-C1C | 4.55  | 1.47        | 1.38     |
| 17  | D     | 201  | SQD  | C13-C12 | -4.55 | 1.29        | 1.51     |
| 14  | B     | 201  | CLA  | O2A-CGA | 4.41  | 1.46        | 1.33     |
| 12  | B     | 1001 | OPC  | CAV-CAW | 4.33  | 1.56        | 1.31     |
| 10  | A     | 302  | HEM  | C3C-C2C | -4.30 | 1.28        | 1.37     |
| 12  | B     | 1001 | OPC  | CAQ-CAP | -4.30 | 1.36        | 1.52     |
| 10  | A     | 301  | HEM  | FE-NC   | 4.27  | 2.09        | 1.95     |
| 12  | A     | 1002 | OPC  | CAV-CAW | 4.25  | 1.55        | 1.31     |
| 12  | A     | 1002 | OPC  | CAQ-CAP | -4.24 | 1.36        | 1.52     |
| 11  | C     | 301  | HEC  | CBC-CAC | -4.23 | 1.33        | 1.51     |
| 14  | B     | 201  | CLA  | C3D-C4D | -4.22 | 1.34        | 1.44     |
| 15  | B     | 1201 | TDS  | CAH-CAG | -4.22 | 1.37        | 1.47     |
| 17  | D     | 201  | SQD  | C11-C10 | -4.21 | 1.30        | 1.51     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 15  | B     | 1202 | TDS  | CAF-CAE | 4.21  | 1.48        | 1.40     |
| 12  | A     | 1002 | OPC  | CBP-CBO | -4.20 | 1.30        | 1.51     |
| 11  | A     | 303  | HEC  | CBC-CAC | -4.12 | 1.34        | 1.51     |
| 12  | A     | 1002 | OPC  | CAG-CAH | -4.03 | 1.39        | 1.51     |
| 17  | D     | 201  | SQD  | C21-C20 | -4.01 | 1.26        | 1.51     |
| 11  | A     | 303  | HEC  | C3C-C2C | -3.98 | 1.28        | 1.38     |
| 11  | C     | 301  | HEC  | FE-NB   | 3.97  | 2.07        | 1.94     |
| 10  | A     | 301  | HEM  | CAD-C3D | 3.89  | 1.61        | 1.51     |
| 18  | G     | 101  | BCR  | C19-C18 | -3.80 | 1.37        | 1.46     |
| 10  | A     | 302  | HEM  | CHC-C1C | -3.79 | 1.30        | 1.38     |
| 15  | B     | 1201 | TDS  | OBD-CAM | 3.78  | 1.45        | 1.36     |
| 13  | A     | 1101 | UMQ  | O1'-C1' | 3.78  | 1.46        | 1.40     |
| 14  | B     | 201  | CLA  | CHD-C4C | 3.75  | 1.47        | 1.39     |
| 11  | C     | 301  | HEC  | FE-ND   | 3.74  | 2.06        | 1.94     |
| 12  | A     | 1002 | OPC  | OBJ-CBK | 3.71  | 1.44        | 1.33     |
| 10  | A     | 302  | HEM  | C4C-NC  | -3.60 | 1.32        | 1.39     |
| 11  | A     | 303  | HEC  | O1A-CGA | 3.58  | 1.33        | 1.22     |
| 12  | B     | 1001 | OPC  | OAN-CAO | 3.58  | 1.44        | 1.34     |
| 10  | A     | 301  | HEM  | C2A-C3A | -3.57 | 1.29        | 1.38     |
| 18  | G     | 101  | BCR  | C1-C6   | -3.56 | 1.49        | 1.53     |
| 11  | C     | 301  | HEC  | CBB-CAB | -3.55 | 1.36        | 1.51     |
| 10  | A     | 302  | HEM  | C1B-C2B | 3.55  | 1.51        | 1.44     |
| 12  | A     | 1002 | OPC  | CAQ-CAR | -3.53 | 1.34        | 1.51     |
| 18  | G     | 101  | BCR  | C24-C25 | -3.53 | 1.33        | 1.45     |
| 11  | C     | 301  | HEC  | C4A-NA  | -3.46 | 1.33        | 1.39     |
| 12  | A     | 1002 | OPC  | CAR-CAS | -3.45 | 1.34        | 1.51     |
| 17  | D     | 201  | SQD  | C22-C21 | -3.43 | 1.25        | 1.50     |
| 11  | C     | 301  | HEC  | CMA-C3A | 3.43  | 1.57        | 1.50     |
| 14  | B     | 201  | CLA  | CHB-C1B | 3.41  | 1.47        | 1.39     |
| 10  | A     | 302  | HEM  | O1A-CGA | 3.37  | 1.33        | 1.22     |
| 17  | D     | 201  | SQD  | C20-C19 | -3.37 | 1.35        | 1.51     |
| 10  | A     | 301  | HEM  | CHA-C4D | -3.35 | 1.31        | 1.38     |
| 17  | D     | 201  | SQD  | C19-C18 | -3.34 | 1.35        | 1.51     |
| 10  | A     | 302  | HEM  | O1D-CGD | 3.34  | 1.33        | 1.22     |
| 18  | G     | 101  | BCR  | C27-C26 | 3.32  | 1.57        | 1.51     |
| 15  | B     | 1202 | TDS  | OBD-CAM | 3.31  | 1.44        | 1.36     |
| 13  | A     | 1103 | UMQ  | O5'-C1' | 3.29  | 1.50        | 1.41     |
| 18  | G     | 101  | BCR  | C12-C13 | -3.27 | 1.38        | 1.46     |
| 10  | A     | 302  | HEM  | CHD-C1D | -3.27 | 1.31        | 1.39     |
| 18  | G     | 101  | BCR  | C36-C18 | 3.26  | 1.57        | 1.50     |
| 11  | C     | 301  | HEC  | C4C-NC  | -3.24 | 1.33        | 1.39     |
| 10  | A     | 301  | HEM  | CHA-C1A | -3.24 | 1.32        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 15  | B     | 1202 | TDS  | OAK-CAL | 3.23  | 1.42        | 1.37     |
| 14  | B     | 201  | CLA  | CHC-C4B | 3.17  | 1.46        | 1.39     |
| 18  | G     | 101  | BCR  | C24-C23 | -3.17 | 1.23        | 1.33     |
| 13  | A     | 1104 | UMQ  | O2'-C2' | -3.14 | 1.35        | 1.43     |
| 11  | A     | 303  | HEC  | FE-NB   | 3.12  | 2.04        | 1.94     |
| 15  | B     | 1201 | TDS  | CAF-CAG | -3.12 | 1.38        | 1.46     |
| 14  | B     | 201  | CLA  | C1B-C2B | 3.12  | 1.50        | 1.43     |
| 13  | A     | 1101 | UMQ  | O2'-C2' | -3.11 | 1.35        | 1.43     |
| 17  | D     | 201  | SQD  | C36-C35 | -3.08 | 1.36        | 1.51     |
| 12  | B     | 1001 | OPC  | CBL-CBK | 3.07  | 1.59        | 1.50     |
| 12  | A     | 1002 | OPC  | CBC-CBD | -3.06 | 1.36        | 1.51     |
| 10  | A     | 302  | HEM  | C1C-NC  | -3.05 | 1.33        | 1.39     |
| 13  | A     | 1103 | UMQ  | O2'-C2' | -3.05 | 1.35        | 1.43     |
| 12  | B     | 1001 | OPC  | CAG-NAF | -3.05 | 1.42        | 1.51     |
| 12  | A     | 1002 | OPC  | CBT-CBS | -3.04 | 1.33        | 1.50     |
| 12  | A     | 1002 | OPC  | CBQ-CBR | -3.01 | 1.33        | 1.50     |
| 12  | B     | 1001 | OPC  | CAQ-CAR | -2.99 | 1.36        | 1.51     |
| 14  | B     | 201  | CLA  | C4C-C3C | 2.98  | 1.50        | 1.45     |
| 12  | B     | 1001 | OPC  | CAR-CAS | -2.95 | 1.37        | 1.51     |
| 10  | A     | 302  | HEM  | CAC-C3C | 2.95  | 1.55        | 1.47     |
| 17  | D     | 201  | SQD  | C15-C14 | -2.94 | 1.37        | 1.51     |
| 15  | B     | 1201 | TDS  | CAQ-CAP | -2.93 | 1.42        | 1.49     |
| 18  | G     | 101  | BCR  | C39-C30 | 2.92  | 1.59        | 1.53     |
| 12  | B     | 1001 | OPC  | CBC-CBD | -2.92 | 1.37        | 1.51     |
| 10  | A     | 301  | HEM  | CHB-C4A | -2.91 | 1.32        | 1.39     |
| 14  | B     | 201  | CLA  | C3D-C2D | 2.89  | 1.46        | 1.39     |
| 12  | B     | 1001 | OPC  | CBB-CBC | -2.88 | 1.37        | 1.51     |
| 10  | A     | 302  | HEM  | C3B-C2B | -2.88 | 1.31        | 1.37     |
| 10  | A     | 301  | HEM  | CBD-CGD | 2.85  | 1.57        | 1.50     |
| 17  | D     | 201  | SQD  | C14-C13 | -2.85 | 1.37        | 1.51     |
| 15  | B     | 1202 | TDS  | CAF-CAG | -2.84 | 1.39        | 1.46     |
| 10  | A     | 302  | HEM  | CMB-C2B | 2.82  | 1.56        | 1.50     |
| 13  | A     | 1102 | UMQ  | C1-C2   | 2.82  | 1.60        | 1.52     |
| 13  | A     | 1101 | UMQ  | O5'-C1' | 2.80  | 1.49        | 1.41     |
| 12  | A     | 1002 | OPC  | CBB-CBC | -2.79 | 1.37        | 1.51     |
| 10  | A     | 302  | HEM  | CMC-C2C | 2.76  | 1.56        | 1.50     |
| 10  | A     | 302  | HEM  | CHD-C4C | -2.74 | 1.33        | 1.38     |
| 11  | C     | 301  | HEC  | C3C-C2C | -2.73 | 1.31        | 1.38     |
| 10  | A     | 301  | HEM  | CAC-C3C | 2.71  | 1.54        | 1.47     |
| 14  | B     | 201  | CLA  | C1D-ND  | -2.68 | 1.34        | 1.37     |
| 11  | C     | 301  | HEC  | CMD-C2D | 2.68  | 1.56        | 1.50     |
| 17  | D     | 201  | SQD  | C34-C33 | -2.68 | 1.38        | 1.51     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 13  | A     | 1102 | UMQ  | C3'-C4' | 2.67  | 1.59        | 1.52     |
| 10  | A     | 302  | HEM  | CHC-C4B | -2.63 | 1.33        | 1.39     |
| 10  | A     | 302  | HEM  | CHA-C1A | -2.61 | 1.33        | 1.39     |
| 11  | A     | 303  | HEC  | C2A-C3A | -2.61 | 1.31        | 1.36     |
| 12  | A     | 1002 | OPC  | PAJ-OAI | 2.60  | 1.69        | 1.59     |
| 10  | A     | 302  | HEM  | CAB-C3B | 2.59  | 1.54        | 1.47     |
| 11  | C     | 301  | HEC  | CHD-C4C | -2.58 | 1.33        | 1.39     |
| 11  | A     | 303  | HEC  | CAD-C3D | 2.56  | 1.57        | 1.51     |
| 17  | D     | 201  | SQD  | C35-C34 | -2.54 | 1.39        | 1.51     |
| 18  | G     | 101  | BCR  | C20-C19 | 2.53  | 1.41        | 1.34     |
| 11  | C     | 301  | HEC  | C1A-C2A | -2.52 | 1.40        | 1.45     |
| 12  | B     | 1001 | OPC  | CBP-CBQ | -2.51 | 1.41        | 1.52     |
| 17  | D     | 201  | SQD  | C37-C36 | -2.50 | 1.36        | 1.51     |
| 17  | D     | 201  | SQD  | C32-C31 | -2.47 | 1.39        | 1.51     |
| 17  | D     | 201  | SQD  | C1-C2   | 2.47  | 1.59        | 1.52     |
| 14  | B     | 201  | CLA  | MG-NA   | -2.47 | 2.00        | 2.06     |
| 17  | D     | 201  | SQD  | C33-C32 | -2.46 | 1.39        | 1.51     |
| 18  | G     | 101  | BCR  | C17-C18 | 2.45  | 1.41        | 1.35     |
| 18  | G     | 101  | BCR  | C40-C30 | 2.43  | 1.58        | 1.53     |
| 15  | B     | 1202 | TDS  | CAQ-CAP | -2.43 | 1.43        | 1.49     |
| 11  | A     | 303  | HEC  | O1D-CGD | 2.43  | 1.30        | 1.22     |
| 10  | A     | 301  | HEM  | C1A-NA  | -2.43 | 1.35        | 1.39     |
| 18  | G     | 101  | BCR  | C11-C10 | -2.40 | 1.35        | 1.43     |
| 14  | B     | 201  | CLA  | C1C-C2C | 2.40  | 1.49        | 1.44     |
| 12  | B     | 1001 | OPC  | CBZ-CBY | 2.40  | 1.63        | 1.51     |
| 14  | B     | 201  | CLA  | CHD-C1D | 2.40  | 1.43        | 1.38     |
| 17  | D     | 201  | SQD  | C38-C37 | -2.39 | 1.33        | 1.50     |
| 11  | C     | 301  | HEC  | CHB-C4A | -2.39 | 1.33        | 1.38     |
| 14  | B     | 201  | CLA  | C4-C3   | 2.37  | 1.56        | 1.50     |
| 13  | A     | 1101 | UMQ  | C4-C5   | 2.35  | 1.58        | 1.53     |
| 13  | A     | 1102 | UMQ  | O2'-C2' | -2.33 | 1.37        | 1.43     |
| 18  | G     | 101  | BCR  | C21-C22 | 2.32  | 1.41        | 1.35     |
| 12  | B     | 1001 | OPC  | CBP-CBO | -2.32 | 1.40        | 1.51     |
| 14  | B     | 201  | CLA  | CBD-CGD | -2.30 | 1.45        | 1.52     |
| 12  | B     | 1001 | OPC  | CBX-CBW | 2.30  | 1.63        | 1.51     |
| 13  | A     | 1102 | UMQ  | O2-C2   | 2.29  | 1.48        | 1.43     |
| 10  | A     | 301  | HEM  | FE-NA   | -2.28 | 1.87        | 1.95     |
| 12  | B     | 1001 | OPC  | CBG-NAF | -2.28 | 1.43        | 1.50     |
| 11  | C     | 301  | HEC  | FE-NC   | 2.27  | 2.02        | 1.95     |
| 11  | C     | 301  | HEC  | O1A-CGA | 2.26  | 1.29        | 1.22     |
| 11  | A     | 303  | HEC  | C1B-NB  | -2.23 | 1.34        | 1.38     |
| 18  | G     | 101  | BCR  | C16-C17 | -2.21 | 1.36        | 1.43     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 13  | A     | 1103 | UMQ  | O5-C1   | 2.19  | 1.47        | 1.41     |
| 15  | B     | 1201 | TDS  | CAH-CAP | 2.19  | 1.38        | 1.34     |
| 10  | A     | 301  | HEM  | C4D-C3D | 2.19  | 1.48        | 1.45     |
| 18  | G     | 101  | BCR  | C29-C28 | 2.17  | 1.57        | 1.52     |
| 12  | B     | 1001 | OPC  | CBW-CBV | 2.17  | 1.62        | 1.51     |
| 15  | B     | 1201 | TDS  | CBC-CBB | -2.16 | 1.34        | 1.50     |
| 12  | B     | 1001 | OPC  | CBY-CBX | 2.14  | 1.62        | 1.51     |
| 12  | B     | 1001 | OPC  | CBI-CAM | 2.13  | 1.57        | 1.50     |
| 11  | A     | 303  | HEC  | C4B-C3B | -2.13 | 1.41        | 1.45     |
| 14  | B     | 201  | CLA  | C2-C3   | 2.11  | 1.37        | 1.33     |
| 18  | G     | 101  | BCR  | C2-C1   | 2.10  | 1.58        | 1.54     |
| 13  | A     | 1102 | UMQ  | O1-C1   | 2.09  | 1.47        | 1.41     |
| 12  | B     | 1001 | OPC  | CBM-CBL | 2.06  | 1.59        | 1.52     |
| 13  | A     | 1102 | UMQ  | C4'-C5' | 2.06  | 1.58        | 1.52     |
| 12  | B     | 1001 | OPC  | CCA-CBZ | 2.05  | 1.64        | 1.51     |
| 14  | B     | 201  | CLA  | C6-C5   | 2.04  | 1.59        | 1.52     |
| 10  | A     | 302  | HEM  | CBA-CGA | 2.04  | 1.55        | 1.50     |
| 17  | D     | 201  | SQD  | C4-C5   | -2.03 | 1.48        | 1.53     |
| 11  | C     | 301  | HEC  | C1D-ND  | -2.02 | 1.36        | 1.40     |
| 12  | B     | 1001 | OPC  | OCC-CBK | 2.01  | 1.28        | 1.22     |
| 12  | B     | 1001 | OPC  | CBV-CBU | 2.00  | 1.61        | 1.51     |

All (352) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 18  | G     | 101  | BCR  | C24-C23-C22 | 28.08  | 167.78      | 126.23   |
| 18  | G     | 101  | BCR  | C7-C8-C9    | 26.41  | 165.30      | 126.23   |
| 15  | B     | 1202 | TDS  | CAE-CAD-CAL | 19.11  | 155.92      | 118.98   |
| 18  | G     | 101  | BCR  | C8-C7-C6    | 18.66  | 176.84      | 127.00   |
| 15  | B     | 1201 | TDS  | CAE-CAD-CAL | 17.87  | 153.53      | 118.98   |
| 17  | D     | 201  | SQD  | O3-C3-C4    | -16.36 | 71.81       | 110.38   |
| 18  | G     | 101  | BCR  | C23-C24-C25 | 15.79  | 169.18      | 127.00   |
| 17  | D     | 201  | SQD  | O4-C4-C3    | 15.48  | 146.87      | 110.38   |
| 15  | B     | 1202 | TDS  | OAK-CAL-CAM | 13.30  | 128.44      | 114.53   |
| 15  | B     | 1201 | TDS  | CAD-CAL-CAM | -12.30 | 108.90      | 120.59   |
| 17  | D     | 201  | SQD  | C17-C16-C15 | 11.93  | 174.66      | 114.37   |
| 17  | D     | 201  | SQD  | C18-C17-C16 | 11.78  | 173.90      | 114.37   |
| 15  | B     | 1201 | TDS  | OAK-CAL-CAM | 11.74  | 126.82      | 114.53   |
| 17  | D     | 201  | SQD  | C12-C11-C10 | 11.00  | 169.96      | 114.37   |
| 12  | A     | 1002 | OPC  | CAA-NAF-CAE | -10.84 | 80.51       | 108.98   |
| 15  | B     | 1201 | TDS  | CAD-CAE-CAF | -10.76 | 103.06      | 121.79   |
| 15  | B     | 1202 | TDS  | CAD-CAE-CAF | -10.64 | 103.27      | 121.79   |

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| Mol | Chain | Res  | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 15  | B     | 1202 | TDS  | CAD-CAL-CAM | -10.41 | 110.70      | 120.59   |
| 13  | A     | 1104 | UMQ  | O1'-C1'-C2' | 10.19  | 123.75      | 108.27   |
| 18  | G     | 101  | BCR  | C32-C1-C6   | -9.77  | 94.91       | 110.24   |
| 17  | D     | 201  | SQD  | C13-C12-C11 | 9.76   | 163.68      | 114.37   |
| 18  | G     | 101  | BCR  | C33-C5-C6   | -9.58  | 114.03      | 124.48   |
| 17  | D     | 201  | SQD  | C22-C21-C20 | 9.42   | 177.00      | 113.36   |
| 10  | A     | 301  | HEM  | C3B-C2B-C1B | -9.25  | 99.46       | 106.41   |
| 17  | D     | 201  | SQD  | O6-C1-C2    | 8.91   | 121.80      | 108.27   |
| 13  | A     | 1103 | UMQ  | CA-O1'-C1'  | 8.62   | 128.41      | 113.68   |
| 12  | B     | 1001 | OPC  | CAA-NAF-CBG | -8.34  | 87.07       | 108.98   |
| 17  | D     | 201  | SQD  | O47-C7-C8   | 8.26   | 129.35      | 111.48   |
| 15  | B     | 1202 | TDS  | OAB-CAE-CAF | 8.14   | 127.37      | 115.84   |
| 10  | A     | 301  | HEM  | CAD-C3D-C4D | 8.00   | 138.64      | 124.70   |
| 15  | B     | 1202 | TDS  | CAL-CAM-CAN | -7.83  | 107.79      | 118.91   |
| 10  | A     | 301  | HEM  | CHC-C1C-NC  | -7.74  | 116.02      | 124.45   |
| 13  | A     | 1104 | UMQ  | CA-O1'-C1'  | 7.70   | 126.84      | 113.68   |
| 10  | A     | 301  | HEM  | C3C-C2C-C1C | -7.70  | 99.76       | 107.05   |
| 13  | A     | 1101 | UMQ  | O2'-C2'-C3' | 7.65   | 128.42      | 110.38   |
| 10  | A     | 301  | HEM  | C4B-C3B-C2B | 7.54   | 114.21      | 107.28   |
| 13  | A     | 1102 | UMQ  | CA-O1'-C1'  | 7.52   | 126.53      | 113.68   |
| 13  | A     | 1103 | UMQ  | O1'-C1'-C2' | 7.19   | 119.19      | 108.27   |
| 18  | G     | 101  | BCR  | C8-C9-C10   | 7.09   | 130.17      | 119.01   |
| 18  | G     | 101  | BCR  | C20-C21-C22 | 7.06   | 137.18      | 127.28   |
| 14  | B     | 201  | CLA  | C4-C3-C5    | 7.06   | 127.48      | 115.23   |
| 10  | A     | 301  | HEM  | CHC-C4B-NB  | 7.01   | 131.96      | 124.42   |
| 11  | C     | 301  | HEC  | CHA-C1A-NA  | 6.97   | 132.04      | 124.45   |
| 15  | B     | 1201 | TDS  | OAB-CAE-CAF | 6.79   | 125.47      | 115.84   |
| 17  | D     | 201  | SQD  | O5-C5-C4    | 6.79   | 121.94      | 109.70   |
| 13  | A     | 1101 | UMQ  | O5'-C1'-O1' | 6.75   | 125.99      | 110.04   |
| 14  | B     | 201  | CLA  | C4A-NA-C1A  | 6.61   | 109.69      | 106.68   |
| 14  | B     | 201  | CLA  | C1D-ND-C4D  | -6.56  | 101.71      | 106.31   |
| 15  | B     | 1202 | TDS  | OAO-CAP-CAQ | 6.56   | 124.04      | 110.12   |
| 15  | B     | 1201 | TDS  | CAA-OAB-CAE | 6.56   | 127.13      | 117.51   |
| 13  | A     | 1103 | UMQ  | O5'-C1'-O1' | 6.39   | 125.14      | 110.04   |
| 12  | A     | 1002 | OPC  | CAA-NAF-CBG | -6.25  | 92.56       | 108.98   |
| 10  | A     | 301  | HEM  | C4D-C3D-C2D | -6.21  | 97.85       | 106.89   |
| 12  | B     | 1001 | OPC  | CBU-CBT-CBS | 6.16   | 147.12      | 112.60   |
| 15  | B     | 1201 | TDS  | CAL-CAM-CAN | -6.13  | 110.20      | 118.91   |
| 11  | A     | 303  | HEC  | CAD-C3D-C4D | 6.10   | 135.33      | 124.70   |
| 14  | B     | 201  | CLA  | CMD-C2D-C1D | 6.08   | 135.44      | 124.73   |
| 17  | D     | 201  | SQD  | C15-C14-C13 | 5.99   | 144.65      | 114.37   |
| 12  | A     | 1002 | OPC  | CAA-NAF-CAG | -5.95  | 86.24       | 109.91   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 12  | B     | 1001 | OPC  | CAM-OAN-CAO | -5.93 | 103.60      | 117.80   |
| 13  | A     | 1102 | UMQ  | C1'-O5'-C5' | 5.89  | 125.23      | 113.72   |
| 14  | B     | 201  | CLA  | C3C-C4C-NC  | 5.86  | 117.94      | 110.43   |
| 14  | B     | 201  | CLA  | O2D-CGD-CBD | 5.86  | 121.47      | 111.23   |
| 13  | A     | 1104 | UMQ  | O5-C5-C4    | 5.82  | 120.19      | 109.70   |
| 12  | A     | 1002 | OPC  | OAN-CAO-CAP | 5.76  | 123.93      | 111.48   |
| 15  | B     | 1202 | TDS  | CAJ-OAK-CAL | -5.70 | 109.14      | 117.51   |
| 13  | A     | 1101 | UMQ  | O1-C4'-C5'  | 5.67  | 124.35      | 109.48   |
| 11  | A     | 303  | HEC  | CAC-C3C-C4C | 5.63  | 132.66      | 124.91   |
| 12  | A     | 1002 | OPC  | CAH-CAG-NAF | 5.62  | 133.85      | 115.82   |
| 13  | A     | 1102 | UMQ  | O5-C5-C4    | 5.61  | 119.81      | 109.70   |
| 13  | A     | 1103 | UMQ  | O2'-C2'-C3' | 5.59  | 123.55      | 110.38   |
| 10  | A     | 301  | HEM  | C3D-C4D-ND  | 5.58  | 116.29      | 110.17   |
| 13  | A     | 1102 | UMQ  | O5'-C1'-O1' | 5.55  | 123.15      | 110.04   |
| 14  | B     | 201  | CLA  | C2D-C1D-ND  | 5.52  | 115.59      | 110.13   |
| 13  | A     | 1102 | UMQ  | O1'-C1'-C2' | 5.47  | 116.58      | 108.27   |
| 12  | B     | 1001 | OPC  | CBG-NAF-CAG | 5.44  | 131.52      | 109.91   |
| 14  | B     | 201  | CLA  | CMB-C2B-C1B | 5.42  | 133.67      | 125.42   |
| 10  | A     | 302  | HEM  | CMB-C2B-C1B | 5.35  | 133.40      | 125.03   |
| 13  | A     | 1104 | UMQ  | O5'-C1'-C2' | 5.34  | 121.34      | 110.37   |
| 14  | B     | 201  | CLA  | C2C-C1C-NC  | 5.32  | 115.57      | 109.98   |
| 10  | A     | 302  | HEM  | C3B-C4B-NB  | 5.31  | 113.28      | 109.47   |
| 13  | A     | 1101 | UMQ  | CA-O1'-C1'  | 5.29  | 122.72      | 113.68   |
| 12  | A     | 1002 | OPC  | CBI-CAM-CAL | -5.16 | 99.75       | 111.78   |
| 14  | B     | 201  | CLA  | CHD-C4C-C3C | -5.16 | 117.25      | 124.77   |
| 10  | A     | 302  | HEM  | CAD-CBD-CGD | -5.14 | 100.02      | 113.67   |
| 18  | G     | 101  | BCR  | C36-C18-C17 | 5.14  | 131.14      | 122.82   |
| 17  | D     | 201  | SQD  | C14-C13-C12 | 5.13  | 140.32      | 114.37   |
| 12  | B     | 1001 | OPC  | CAR-CAQ-CAP | 5.12  | 131.93      | 113.13   |
| 13  | A     | 1102 | UMQ  | O2'-C2'-C3' | 5.10  | 122.39      | 110.38   |
| 14  | B     | 201  | CLA  | C4C-C3C-C2C | -5.08 | 99.50       | 106.89   |
| 14  | B     | 201  | CLA  | C3B-C2B-C1B | -5.06 | 101.20      | 107.17   |
| 10  | A     | 301  | HEM  | CBB-CAB-C3B | -5.03 | 102.37      | 127.53   |
| 13  | A     | 1102 | UMQ  | C3-C4-C5    | 5.01  | 119.31      | 110.23   |
| 13  | A     | 1104 | UMQ  | O2'-C2'-C1' | 5.00  | 122.00      | 110.08   |
| 13  | A     | 1102 | UMQ  | O1-C1-C2    | 5.00  | 120.38      | 108.09   |
| 12  | A     | 1002 | OPC  | OAI-CAH-CAG | 4.98  | 133.63      | 109.65   |
| 14  | B     | 201  | CLA  | C5-C3-C2    | -4.96 | 110.04      | 121.17   |
| 13  | A     | 1101 | UMQ  | O2'-C2'-C1' | 4.95  | 121.87      | 110.08   |
| 14  | B     | 201  | CLA  | C2B-C1B-NB  | 4.94  | 115.45      | 110.33   |
| 10  | A     | 301  | HEM  | CMB-C2B-C1B | 4.93  | 132.73      | 125.03   |
| 18  | G     | 101  | BCR  | C34-C9-C8   | -4.90 | 110.60      | 118.09   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 13  | A     | 1101 | UMQ  | O5-C5-C4    | 4.88  | 118.50      | 109.70   |
| 14  | B     | 201  | CLA  | C6-C5-C3    | -4.88 | 101.58      | 113.47   |
| 10  | A     | 301  | HEM  | C4C-C3C-C2C | 4.86  | 111.02      | 106.81   |
| 13  | A     | 1102 | UMQ  | O5'-C1'-C2' | 4.82  | 120.28      | 110.37   |
| 15  | B     | 1202 | TDS  | OBD-CAM-CAL | -4.81 | 108.87      | 119.21   |
| 14  | B     | 201  | CLA  | C3D-C2D-C1D | -4.77 | 99.32       | 105.83   |
| 13  | A     | 1102 | UMQ  | O2-C2-C1    | 4.71  | 121.31      | 110.08   |
| 11  | A     | 303  | HEC  | CMB-C2B-C1B | 4.67  | 132.33      | 125.03   |
| 11  | A     | 303  | HEC  | CAC-C3C-C2C | -4.64 | 119.55      | 126.89   |
| 18  | G     | 101  | BCR  | C2-C1-C6    | 4.63  | 117.16      | 110.44   |
| 13  | A     | 1102 | UMQ  | C1'-C2'-C3' | 4.63  | 119.74      | 110.01   |
| 13  | A     | 1104 | UMQ  | C1'-C2'-C3' | 4.62  | 119.74      | 110.01   |
| 13  | A     | 1101 | UMQ  | O1-C1-C2    | 4.54  | 119.27      | 108.09   |
| 17  | D     | 201  | SQD  | C16-C15-C14 | 4.52  | 137.22      | 114.37   |
| 15  | B     | 1201 | TDS  | OAO-CAP-CAQ | 4.50  | 119.66      | 110.12   |
| 13  | A     | 1101 | UMQ  | O5'-C1'-C2' | 4.49  | 119.58      | 110.37   |
| 14  | B     | 201  | CLA  | CHD-C1D-ND  | -4.47 | 118.50      | 124.80   |
| 11  | A     | 303  | HEC  | CBA-CAA-C2A | -4.46 | 100.21      | 112.53   |
| 14  | B     | 201  | CLA  | CED-O2D-CGD | -4.45 | 105.83      | 115.92   |
| 12  | B     | 1001 | OPC  | OAN-CAO-OAD | -4.43 | 113.34      | 123.70   |
| 14  | B     | 201  | CLA  | C3B-C4B-NB  | 4.43  | 114.48      | 110.53   |
| 10  | A     | 301  | HEM  | C2B-C1B-NB  | 4.39  | 114.89      | 109.84   |
| 13  | A     | 1101 | UMQ  | C2'-C3'-C4' | -4.38 | 99.73       | 109.68   |
| 12  | A     | 1002 | OPC  | CAR-CAS-CAT | 4.37  | 136.45      | 114.37   |
| 10  | A     | 301  | HEM  | CHD-C1D-ND  | 4.33  | 129.08      | 124.42   |
| 13  | A     | 1103 | UMQ  | O2'-C2'-C1' | 4.32  | 120.37      | 110.08   |
| 13  | A     | 1101 | UMQ  | O5-C1-C2    | -4.32 | 101.50      | 110.37   |
| 11  | C     | 301  | HEC  | CBD-CAD-C3D | -4.31 | 100.60      | 112.53   |
| 15  | B     | 1201 | TDS  | OAO-CAP-CAH | 4.29  | 125.59      | 121.81   |
| 12  | B     | 1001 | OPC  | CBP-CBO-CBN | 4.24  | 135.80      | 114.37   |
| 14  | B     | 201  | CLA  | O2A-CGA-CBA | 4.21  | 124.67      | 111.83   |
| 10  | A     | 301  | HEM  | O2D-CGD-O1D | -4.15 | 112.67      | 123.33   |
| 18  | G     | 101  | BCR  | C36-C18-C19 | -4.12 | 111.79      | 118.09   |
| 17  | D     | 201  | SQD  | C35-C34-C33 | 4.12  | 135.19      | 114.37   |
| 14  | B     | 201  | CLA  | C3D-C4D-ND  | 4.10  | 116.66      | 109.99   |
| 11  | A     | 303  | HEC  | CHA-C4D-ND  | -4.09 | 120.02      | 124.42   |
| 15  | B     | 1202 | TDS  | OAO-CAN-CAF | -3.99 | 115.16      | 121.19   |
| 13  | A     | 1101 | UMQ  | O1'-C1'-C2' | 3.99  | 114.33      | 108.27   |
| 13  | A     | 1104 | UMQ  | C3'-C4'-C5' | -3.96 | 102.15      | 110.93   |
| 10  | A     | 302  | HEM  | CMC-C2C-C1C | 3.96  | 131.70      | 124.73   |
| 13  | A     | 1102 | UMQ  | C3'-C4'-C5' | 3.95  | 119.69      | 110.93   |
| 13  | A     | 1101 | UMQ  | C1-O1-C4'   | -3.94 | 108.65      | 117.98   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 12  | B     | 1001 | OPC  | OAN-CAO-CAP | 3.91  | 119.94      | 111.48   |
| 12  | A     | 1002 | OPC  | CAQ-CAR-CAS | 3.88  | 134.00      | 114.37   |
| 17  | D     | 201  | SQD  | O4-C4-C5    | -3.88 | 99.77       | 109.32   |
| 15  | B     | 1202 | TDS  | OAC-CAG-CAH | -3.87 | 115.36      | 120.45   |
| 12  | B     | 1001 | OPC  | CBI-OBJ-CBK | 3.86  | 131.21      | 117.12   |
| 17  | D     | 201  | SQD  | O6-C44-C45  | 3.83  | 120.14      | 110.82   |
| 14  | B     | 201  | CLA  | CAA-CBA-CGA | -3.81 | 102.39      | 113.21   |
| 12  | B     | 1001 | OPC  | CAA-NAF-CAG | -3.79 | 94.86       | 109.91   |
| 14  | B     | 201  | CLA  | CHB-C4A-NA  | 3.74  | 129.80      | 124.40   |
| 11  | C     | 301  | HEC  | CAD-CBD-CGD | 3.73  | 123.57      | 113.67   |
| 12  | B     | 1001 | OPC  | CAR-CAS-CAT | 3.72  | 133.19      | 114.37   |
| 18  | G     | 101  | BCR  | C32-C1-C2   | 3.72  | 123.24      | 108.95   |
| 10  | A     | 301  | HEM  | C1D-C2D-C3D | 3.68  | 110.85      | 106.98   |
| 13  | A     | 1102 | UMQ  | C1-O5-C5    | 3.68  | 120.90      | 113.72   |
| 10  | A     | 301  | HEM  | O1A-CGA-CBA | -3.61 | 111.63      | 123.09   |
| 13  | A     | 1104 | UMQ  | O3'-C3'-C2' | 3.61  | 118.88      | 110.38   |
| 18  | G     | 101  | BCR  | C33-C5-C4   | 3.60  | 121.28      | 113.60   |
| 10  | A     | 302  | HEM  | CMB-C2B-C3B | -3.60 | 119.72      | 128.43   |
| 10  | A     | 302  | HEM  | C2D-C1D-ND  | 3.60  | 114.06      | 109.90   |
| 18  | G     | 101  | BCR  | C29-C28-C27 | 3.60  | 119.19      | 111.28   |
| 13  | A     | 1104 | UMQ  | O1-C4'-C5'  | 3.59  | 118.90      | 109.48   |
| 15  | B     | 1201 | TDS  | CAU-CAV-CAW | -3.59 | 96.24       | 114.37   |
| 15  | B     | 1201 | TDS  | CAS-CAT-CAU | -3.57 | 96.32       | 114.37   |
| 11  | C     | 301  | HEC  | CHD-C4C-NC  | 3.56  | 130.31      | 123.86   |
| 15  | B     | 1201 | TDS  | CAE-CAF-CAG | -3.54 | 117.82      | 123.49   |
| 13  | A     | 1104 | UMQ  | C3-C4-C5    | 3.53  | 116.64      | 110.23   |
| 10  | A     | 302  | HEM  | CAA-CBA-CGA | 3.52  | 123.00      | 113.67   |
| 14  | B     | 201  | CLA  | O1D-CGD-CBD | -3.48 | 117.66      | 124.52   |
| 15  | B     | 1201 | TDS  | OAB-CAE-CAD | 3.48  | 130.06      | 124.08   |
| 17  | D     | 201  | SQD  | C32-C31-C30 | 3.47  | 131.92      | 114.37   |
| 10  | A     | 302  | HEM  | CHB-C1B-NB  | -3.46 | 120.08      | 124.37   |
| 18  | G     | 101  | BCR  | C3-C4-C5    | -3.46 | 107.88      | 114.06   |
| 17  | D     | 201  | SQD  | O47-C45-C44 | 3.46  | 120.76      | 108.34   |
| 11  | A     | 303  | HEC  | CMC-C2C-C1C | 3.44  | 130.65      | 125.42   |
| 13  | A     | 1104 | UMQ  | O1-C1-C2    | 3.42  | 116.51      | 108.09   |
| 11  | C     | 301  | HEC  | C1D-ND-C4D  | 3.41  | 109.25      | 105.21   |
| 12  | A     | 1002 | OPC  | CBP-CBQ-CBR | 3.38  | 131.51      | 112.60   |
| 11  | C     | 301  | HEC  | CHA-C1A-C2A | -3.37 | 119.55      | 124.86   |
| 12  | A     | 1002 | OPC  | CAS-CAT-CAU | -3.35 | 97.74       | 113.86   |
| 11  | C     | 301  | HEC  | CMD-C2D-C1D | 3.35  | 130.27      | 125.03   |
| 15  | B     | 1202 | TDS  | CAE-CAF-CAG | -3.35 | 118.13      | 123.49   |
| 13  | A     | 1104 | UMQ  | O2'-C2'-C3' | 3.35  | 118.26      | 110.38   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 10  | A     | 301  | HEM  | O2A-CGA-CBA | 3.33  | 124.51      | 114.00   |
| 11  | C     | 301  | HEC  | C3B-C4B-NB  | -3.31 | 106.54      | 110.17   |
| 13  | A     | 1101 | UMQ  | O2-C2-C3    | 3.29  | 118.12      | 110.38   |
| 15  | B     | 1201 | TDS  | CAT-CAU-CAV | 3.27  | 130.88      | 114.37   |
| 13  | A     | 1102 | UMQ  | O2'-C2'-C1' | 3.26  | 117.85      | 110.08   |
| 10  | A     | 302  | HEM  | CBA-CAA-C2A | -3.26 | 103.52      | 112.53   |
| 10  | A     | 301  | HEM  | CMC-C2C-C1C | 3.25  | 130.45      | 124.73   |
| 15  | B     | 1201 | TDS  | CAV-CAW-CAX | 3.24  | 130.72      | 114.37   |
| 12  | B     | 1001 | OPC  | CBO-CBP-CBQ | 3.23  | 129.39      | 113.86   |
| 18  | G     | 101  | BCR  | C23-C22-C21 | -3.21 | 113.96      | 119.01   |
| 10  | A     | 301  | HEM  | C4A-NA-C1A  | -3.21 | 100.59      | 105.82   |
| 11  | C     | 301  | HEC  | C1C-CHC-C4B | -3.21 | 118.71      | 126.25   |
| 17  | D     | 201  | SQD  | O9-S-C6     | 3.19  | 111.52      | 106.76   |
| 13  | A     | 1104 | UMQ  | C2'-C3'-C4' | -3.17 | 102.49      | 109.68   |
| 13  | A     | 1102 | UMQ  | O5-C1-C2    | 3.16  | 116.86      | 110.37   |
| 12  | A     | 1002 | OPC  | PAJ-OAI-CAH | 3.16  | 136.28      | 121.26   |
| 17  | D     | 201  | SQD  | C36-C35-C34 | 3.14  | 130.23      | 114.37   |
| 12  | A     | 1002 | OPC  | OBJ-CBK-OCC | -3.13 | 115.81      | 123.63   |
| 14  | B     | 201  | CLA  | CAC-C3C-C4C | 3.12  | 128.85      | 124.79   |
| 10  | A     | 301  | HEM  | CHA-C4D-ND  | -3.12 | 120.50      | 124.37   |
| 10  | A     | 301  | HEM  | C2C-C1C-NC  | 3.12  | 115.41      | 109.64   |
| 10  | A     | 301  | HEM  | CMD-C2D-C1D | 3.12  | 129.90      | 125.03   |
| 17  | D     | 201  | SQD  | O2-C2-C1    | 3.11  | 117.50      | 110.08   |
| 18  | G     | 101  | BCR  | C39-C30-C25 | 3.11  | 115.11      | 110.24   |
| 13  | A     | 1104 | UMQ  | O2-C2-C3    | 3.10  | 117.69      | 110.38   |
| 17  | D     | 201  | SQD  | C1-C2-C3    | 3.10  | 116.53      | 110.01   |
| 10  | A     | 301  | HEM  | C4A-CHB-C1B | -3.09 | 118.99      | 126.25   |
| 11  | C     | 301  | HEC  | CHC-C4B-NB  | 3.06  | 128.16      | 124.37   |
| 13  | A     | 1101 | UMQ  | C1-O5-C5    | 3.06  | 119.69      | 113.72   |
| 11  | A     | 303  | HEC  | CAD-C3D-C2D | -3.06 | 122.14      | 127.87   |
| 12  | B     | 1001 | OPC  | CCB-CCA-CBZ | 3.05  | 133.99      | 113.36   |
| 10  | A     | 302  | HEM  | C3C-C2C-C1C | -3.05 | 104.16      | 107.05   |
| 18  | G     | 101  | BCR  | C20-C19-C18 | -3.03 | 118.07      | 126.36   |
| 12  | A     | 1002 | OPC  | CAE-NAF-CAG | 3.02  | 121.93      | 109.91   |
| 17  | D     | 201  | SQD  | O5-C1-O6    | 3.02  | 117.19      | 110.04   |
| 11  | A     | 303  | HEC  | C4D-C3D-C2D | -3.02 | 102.50      | 106.89   |
| 15  | B     | 1202 | TDS  | OAB-CAE-CAD | 3.01  | 129.26      | 124.08   |
| 13  | A     | 1102 | UMQ  | C2'-C3'-C4' | 3.00  | 116.48      | 109.68   |
| 13  | A     | 1101 | UMQ  | O2-C2-C1    | 2.95  | 117.09      | 110.08   |
| 12  | A     | 1002 | OPC  | CBA-CBB-CBC | 2.94  | 129.25      | 114.37   |
| 12  | B     | 1001 | OPC  | OBJ-CBI-CAM | 2.93  | 116.83      | 108.40   |
| 11  | A     | 303  | HEC  | CAA-CBA-CGA | 2.93  | 121.42      | 113.67   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 10  | A     | 302  | HEM  | C1D-C2D-C3D | -2.92 | 103.91      | 106.98   |
| 14  | B     | 201  | CLA  | C6-C7-C8    | 2.92  | 125.66      | 115.97   |
| 17  | D     | 201  | SQD  | C33-C32-C31 | 2.92  | 129.11      | 114.37   |
| 12  | B     | 1001 | OPC  | CBP-CBQ-CBR | 2.89  | 128.81      | 112.60   |
| 13  | A     | 1103 | UMQ  | O1-C1-C2    | 2.88  | 115.18      | 108.09   |
| 13  | A     | 1103 | UMQ  | C1'-C2'-C3' | 2.88  | 116.07      | 110.01   |
| 15  | B     | 1202 | TDS  | CAT-CAU-CAV | 2.84  | 128.71      | 114.37   |
| 10  | A     | 301  | HEM  | C2A-C1A-NA  | 2.84  | 113.30      | 110.15   |
| 10  | A     | 301  | HEM  | CHC-C4B-C3B | -2.82 | 119.44      | 125.07   |
| 13  | A     | 1103 | UMQ  | C1-O5-C5    | 2.81  | 119.20      | 113.72   |
| 14  | B     | 201  | CLA  | O2A-C1-C2   | 2.81  | 118.91      | 108.11   |
| 12  | A     | 1002 | OPC  | CBG-NAF-CAE | 2.79  | 116.31      | 108.98   |
| 11  | A     | 303  | HEC  | C1D-ND-C4D  | 2.79  | 108.51      | 105.21   |
| 13  | A     | 1103 | UMQ  | O3'-C3'-C4' | 2.78  | 117.07      | 109.94   |
| 10  | A     | 302  | HEM  | CHC-C4B-C3B | -2.78 | 119.53      | 125.07   |
| 17  | D     | 201  | SQD  | O49-C7-C8   | -2.78 | 112.92      | 123.78   |
| 11  | C     | 301  | HEC  | CMA-C3A-C4A | 2.77  | 129.61      | 124.73   |
| 10  | A     | 302  | HEM  | C4C-NC-C1C  | -2.77 | 101.31      | 105.82   |
| 13  | A     | 1101 | UMQ  | C1'-O5'-C5' | 2.75  | 119.10      | 113.72   |
| 11  | C     | 301  | HEC  | C1A-CHA-C4D | -2.75 | 120.17      | 126.02   |
| 11  | A     | 303  | HEC  | CHD-C1D-ND  | 2.75  | 127.76      | 124.37   |
| 15  | B     | 1202 | TDS  | CAR-CAQ-CAP | 2.74  | 118.79      | 113.08   |
| 12  | B     | 1001 | OPC  | CBW-CBV-CBU | 2.74  | 128.22      | 114.37   |
| 10  | A     | 302  | HEM  | C2C-C1C-NC  | 2.74  | 114.70      | 109.64   |
| 10  | A     | 302  | HEM  | C4C-CHD-C1D | -2.73 | 120.21      | 126.02   |
| 15  | B     | 1202 | TDS  | OAO-CAP-CAH | 2.71  | 124.20      | 121.81   |
| 10  | A     | 301  | HEM  | CHB-C4A-C3A | -2.70 | 119.60      | 127.43   |
| 12  | A     | 1002 | OPC  | CBG-NAF-CAG | 2.68  | 120.58      | 109.91   |
| 15  | B     | 1202 | TDS  | OAC-CAG-CAF | 2.67  | 126.89      | 122.06   |
| 10  | A     | 302  | HEM  | CBD-CAD-C3D | 2.66  | 119.89      | 112.53   |
| 11  | C     | 301  | HEC  | CBC-CAC-C3C | 2.62  | 119.54      | 112.42   |
| 11  | A     | 303  | HEC  | CAA-C2A-C3A | -2.62 | 122.96      | 127.87   |
| 17  | D     | 201  | SQD  | O47-C7-O49  | -2.58 | 117.67      | 123.70   |
| 13  | A     | 1103 | UMQ  | O5'-C1'-C2' | 2.58  | 115.67      | 110.37   |
| 12  | B     | 1001 | OPC  | CBY-CBX-CBW | 2.57  | 127.36      | 114.37   |
| 13  | A     | 1101 | UMQ  | O3'-C3'-C2' | 2.56  | 116.40      | 110.38   |
| 10  | A     | 301  | HEM  | CMD-C2D-C3D | -2.55 | 119.25      | 126.15   |
| 10  | A     | 302  | HEM  | CHC-C4B-NB  | 2.55  | 127.17      | 124.42   |
| 11  | C     | 301  | HEC  | C4B-NB-C1B  | 2.54  | 108.21      | 105.21   |
| 13  | A     | 1101 | UMQ  | C3'-C4'-C5' | -2.53 | 105.32      | 110.93   |
| 15  | B     | 1201 | TDS  | CAS-CAR-CAQ | -2.52 | 103.85      | 113.13   |
| 11  | A     | 303  | HEC  | C1C-CHC-C4B | -2.52 | 120.32      | 126.25   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 11  | A     | 303  | HEC  | CMA-C3A-C4A | 2.52  | 129.17      | 124.73   |
| 15  | B     | 1202 | TDS  | OAQ-CAN-CAM | 2.52  | 121.27      | 116.28   |
| 10  | A     | 302  | HEM  | CHC-C1C-C2C | -2.51 | 120.26      | 125.49   |
| 17  | D     | 201  | SQD  | C19-C18-C17 | 2.50  | 127.02      | 114.37   |
| 10  | A     | 301  | HEM  | O2D-CGD-CBD | 2.50  | 121.89      | 114.00   |
| 15  | B     | 1202 | TDS  | CBC-CBB-CBA | 2.50  | 130.21      | 113.36   |
| 17  | D     | 201  | SQD  | C46-O48-C23 | 2.49  | 126.22      | 117.12   |
| 12  | A     | 1002 | OPC  | CBY-CBX-CBW | -2.49 | 101.80      | 114.37   |
| 10  | A     | 301  | HEM  | CAA-C2A-C1A | 2.48  | 129.78      | 124.94   |
| 13  | A     | 1101 | UMQ  | O4-C4-C3    | -2.47 | 104.56      | 110.38   |
| 13  | A     | 1102 | UMQ  | O6'-C6'-C5' | 2.46  | 119.71      | 111.33   |
| 17  | D     | 201  | SQD  | C34-C33-C32 | 2.46  | 126.79      | 114.37   |
| 11  | C     | 301  | HEC  | CMC-C2C-C1C | 2.46  | 129.16      | 125.42   |
| 10  | A     | 301  | HEM  | CAB-C3B-C2B | -2.46 | 120.44      | 128.43   |
| 12  | B     | 1001 | OPC  | CBZ-CBY-CBX | 2.45  | 126.78      | 114.37   |
| 12  | B     | 1001 | OPC  | OAI-CAH-CAG | 2.42  | 121.28      | 109.65   |
| 18  | G     | 101  | BCR  | C15-C16-C17 | 2.40  | 128.44      | 123.52   |
| 14  | B     | 201  | CLA  | CHB-C1B-NB  | -2.40 | 120.44      | 124.05   |
| 15  | B     | 1201 | TDS  | CAR-CAS-CAT | 2.40  | 126.49      | 114.37   |
| 18  | G     | 101  | BCR  | C34-C9-C10  | -2.40 | 118.93      | 122.82   |
| 13  | A     | 1103 | UMQ  | O2-C2-C1    | 2.38  | 115.74      | 110.08   |
| 11  | A     | 303  | HEC  | CHA-C4D-C3D | 2.37  | 128.23      | 124.77   |
| 13  | A     | 1104 | UMQ  | O3-C3-C2    | 2.37  | 115.95      | 110.38   |
| 11  | A     | 303  | HEC  | O2A-CGA-O1A | 2.37  | 129.41      | 123.33   |
| 10  | A     | 301  | HEM  | C3A-C4A-NA  | 2.36  | 113.93      | 110.14   |
| 17  | D     | 201  | SQD  | O8-S-C6     | 2.36  | 110.52      | 105.97   |
| 13  | A     | 1104 | UMQ  | C6'-C5'-C4' | 2.35  | 120.00      | 113.38   |
| 12  | A     | 1002 | OPC  | CBU-CBT-CBS | 2.35  | 125.74      | 112.60   |
| 15  | B     | 1202 | TDS  | CAV-CAW-CAX | 2.33  | 126.16      | 114.37   |
| 10  | A     | 301  | HEM  | CAD-C3D-C2D | -2.33 | 123.51      | 127.87   |
| 15  | B     | 1202 | TDS  | CAN-CAF-CAG | 2.32  | 123.96      | 119.99   |
| 11  | A     | 303  | HEC  | O1A-CGA-CBA | -2.31 | 115.75      | 123.09   |
| 13  | A     | 1101 | UMQ  | C4-C3-C2    | -2.31 | 106.78      | 110.83   |
| 11  | A     | 303  | HEC  | CMB-C2B-C3B | -2.31 | 119.91      | 126.15   |
| 11  | C     | 301  | HEC  | CAA-C2A-C1A | -2.31 | 120.17      | 124.85   |
| 11  | C     | 301  | HEC  | C4B-C3B-C2B | 2.30  | 110.24      | 106.89   |
| 11  | A     | 303  | HEC  | C4C-CHD-C1D | 2.29  | 131.63      | 126.25   |
| 13  | A     | 1102 | UMQ  | C4-C3-C2    | 2.29  | 114.85      | 110.83   |
| 14  | B     | 201  | CLA  | C7-C6-C5    | -2.28 | 107.18      | 113.26   |
| 11  | C     | 301  | HEC  | C1D-C2D-C3D | -2.28 | 104.58      | 106.98   |
| 12  | B     | 1001 | OPC  | CBA-CBB-CBC | 2.28  | 125.89      | 114.37   |
| 17  | D     | 201  | SQD  | C45-O47-C7  | -2.27 | 112.36      | 117.80   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 10  | A     | 301  | HEM  | CAC-C3C-C4C | -2.27 | 119.41      | 124.82   |
| 11  | A     | 303  | HEC  | CAB-C3B-C4B | 2.27  | 127.74      | 124.79   |
| 12  | B     | 1001 | OPC  | CBM-CBL-CBK | 2.25  | 121.95      | 113.69   |
| 12  | A     | 1002 | OPC  | CAQ-CAP-CAO | 2.25  | 121.93      | 113.69   |
| 18  | G     | 101  | BCR  | C37-C22-C23 | 2.25  | 121.52      | 118.09   |
| 13  | A     | 1104 | UMQ  | O1-C4'-C3'  | 2.24  | 112.92      | 107.23   |
| 15  | B     | 1202 | TDS  | CAY-CAZ-CBA | 2.24  | 125.69      | 114.37   |
| 12  | B     | 1001 | OPC  | CBT-CBS-CBR | 2.24  | 141.61      | 124.83   |
| 13  | A     | 1101 | UMQ  | C1-C2-C3    | -2.22 | 105.33      | 110.01   |
| 14  | B     | 201  | CLA  | CAC-C3C-C2C | 2.22  | 131.64      | 127.56   |
| 14  | B     | 201  | CLA  | O2A-CGA-O1A | -2.22 | 118.09      | 123.63   |
| 14  | B     | 201  | CLA  | C3A-C2A-C1A | 2.21  | 104.64      | 101.34   |
| 10  | A     | 302  | HEM  | C4A-CHB-C1B | -2.19 | 121.09      | 126.25   |
| 15  | B     | 1202 | TDS  | CAS-CAR-CAQ | 2.19  | 121.17      | 113.13   |
| 10  | A     | 301  | HEM  | CHB-C1B-C2B | -2.19 | 120.74      | 126.95   |
| 14  | B     | 201  | CLA  | CBA-CAA-C2A | -2.18 | 107.29      | 113.79   |
| 13  | A     | 1103 | UMQ  | O5-C5-C6    | 2.17  | 111.81      | 106.44   |
| 13  | A     | 1104 | UMQ  | C1-O5-C5    | 2.16  | 117.94      | 113.72   |
| 13  | A     | 1103 | UMQ  | C3-C4-C5    | 2.16  | 114.15      | 110.23   |
| 13  | A     | 1101 | UMQ  | C3-C4-C5    | 2.14  | 114.12      | 110.23   |
| 12  | B     | 1001 | OPC  | CBO-CBN-CBM | 2.14  | 125.17      | 114.37   |
| 18  | G     | 101  | BCR  | C31-C1-C6   | -2.14 | 106.89      | 110.24   |
| 13  | A     | 1101 | UMQ  | O6-C6-C5    | 2.13  | 118.58      | 111.33   |
| 11  | A     | 303  | HEC  | CBB-CAB-C3B | 2.12  | 118.17      | 112.42   |
| 18  | G     | 101  | BCR  | C30-C25-C26 | 2.12  | 125.53      | 122.64   |
| 14  | B     | 201  | CLA  | CAA-C2A-C3A | -2.11 | 107.29      | 113.00   |
| 18  | G     | 101  | BCR  | C32-C1-C31  | -2.10 | 102.61      | 108.63   |
| 11  | C     | 301  | HEC  | CBB-CAB-C3B | -2.10 | 106.72      | 112.42   |
| 14  | B     | 201  | CLA  | C1C-C2C-C3C | -2.10 | 104.77      | 106.98   |
| 18  | G     | 101  | BCR  | C7-C6-C5    | 2.09  | 126.37      | 121.56   |
| 13  | A     | 1101 | UMQ  | CI-CH-CG    | -2.09 | 103.81      | 114.37   |
| 14  | B     | 201  | CLA  | C2A-C1A-CHA | -2.07 | 120.28      | 123.87   |
| 12  | B     | 1001 | OPC  | CAY-CAZ-CBA | 2.07  | 124.82      | 114.37   |
| 10  | A     | 302  | HEM  | CAC-C3C-C4C | 2.07  | 129.75      | 124.82   |
| 18  | G     | 101  | BCR  | C27-C26-C25 | -2.06 | 119.92      | 122.70   |
| 11  | A     | 303  | HEC  | CHD-C1D-C2D | -2.06 | 121.10      | 126.95   |
| 13  | A     | 1104 | UMQ  | O5'-C1'-O1' | 2.06  | 114.91      | 110.04   |
| 12  | B     | 1001 | OPC  | CBX-CBW-CBV | 2.03  | 124.62      | 114.37   |
| 11  | A     | 303  | HEC  | CAA-C2A-C1A | 2.02  | 128.96      | 124.85   |
| 11  | C     | 301  | HEC  | C1B-C2B-C3B | -2.02 | 104.86      | 106.98   |
| 10  | A     | 301  | HEM  | C1B-NB-C4B  | -2.01 | 102.83      | 105.21   |

All (14) chirality outliers are listed below:



| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 11  | A     | 303  | HEC  | NA   |
| 11  | C     | 301  | HEC  | NA   |
| 13  | A     | 1101 | UMQ  | C1'  |
| 13  | A     | 1101 | UMQ  | C2'  |
| 13  | A     | 1102 | UMQ  | C1'  |
| 13  | A     | 1102 | UMQ  | C2'  |
| 13  | A     | 1103 | UMQ  | C1'  |
| 13  | A     | 1103 | UMQ  | C2'  |
| 13  | A     | 1104 | UMQ  | C1'  |
| 13  | A     | 1104 | UMQ  | C2'  |
| 14  | B     | 201  | CLA  | C8   |
| 17  | D     | 201  | SQD  | C5   |
| 17  | D     | 201  | SQD  | C4   |
| 17  | D     | 201  | SQD  | C3   |

All (203) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 10  | A     | 301  | HEM  | C1A-C2A-CAA-CBA |
| 10  | A     | 302  | HEM  | C1A-C2A-CAA-CBA |
| 10  | A     | 302  | HEM  | C2D-C3D-CAD-CBD |
| 10  | A     | 302  | HEM  | C4D-C3D-CAD-CBD |
| 11  | A     | 303  | HEC  | C2D-C3D-CAD-CBD |
| 11  | A     | 303  | HEC  | C4D-C3D-CAD-CBD |
| 12  | A     | 1002 | OPC  | OAN-CAM-CBI-OBJ |
| 12  | A     | 1002 | OPC  | CAM-CAL-OAK-PAJ |
| 12  | A     | 1002 | OPC  | CAL-OAK-PAJ-OBH |
| 12  | A     | 1002 | OPC  | CAL-OAK-PAJ-OAB |
| 12  | A     | 1002 | OPC  | CAL-OAK-PAJ-OAI |
| 12  | A     | 1002 | OPC  | CAH-OAI-PAJ-OBH |
| 12  | A     | 1002 | OPC  | CAH-OAI-PAJ-OAB |
| 12  | A     | 1002 | OPC  | NAF-CAG-CAH-OAI |
| 12  | A     | 1002 | OPC  | CBO-CBP-CBQ-CBR |
| 12  | B     | 1001 | OPC  | CAH-OAI-PAJ-OAK |
| 12  | B     | 1001 | OPC  | CAH-OAI-PAJ-OBH |
| 12  | B     | 1001 | OPC  | NAF-CAG-CAH-OAI |
| 12  | B     | 1001 | OPC  | CBO-CBP-CBQ-CBR |
| 13  | A     | 1101 | UMQ  | O5'-C1'-O1'-CA  |
| 13  | A     | 1102 | UMQ  | C2'-C1'-O1'-CA  |
| 13  | A     | 1103 | UMQ  | O5'-C1'-O1'-CA  |
| 13  | A     | 1104 | UMQ  | C3'-C4'-O1'-C1  |
| 13  | A     | 1104 | UMQ  | O5'-C1'-O1'-CA  |
| 14  | B     | 201  | CLA  | O2A-C1-C2-C3    |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 15  | B     | 1202 | TDS  | CAP-CAQ-CAR-CAS |
| 17  | D     | 201  | SQD  | O5-C1-O6-C44    |
| 17  | D     | 201  | SQD  | O5-C5-C6-S      |
| 17  | D     | 201  | SQD  | C5-C6-S-O7      |
| 17  | D     | 201  | SQD  | C5-C6-S-O8      |
| 17  | D     | 201  | SQD  | C5-C6-S-O9      |
| 18  | G     | 101  | BCR  | C1-C6-C7-C8     |
| 18  | G     | 101  | BCR  | C5-C6-C7-C8     |
| 18  | G     | 101  | BCR  | C6-C7-C8-C9     |
| 18  | G     | 101  | BCR  | C7-C8-C9-C34    |
| 18  | G     | 101  | BCR  | C23-C24-C25-C26 |
| 15  | B     | 1202 | TDS  | CAF-CAE-OAB-CAA |
| 11  | A     | 303  | HEC  | C4B-C3B-CAB-CBB |
| 13  | A     | 1104 | UMQ  | O5-C1-O1-C4'    |
| 11  | C     | 301  | HEC  | C4B-C3B-CAB-CBB |
| 11  | C     | 301  | HEC  | C2B-C3B-CAB-CBB |
| 11  | C     | 301  | HEC  | C4C-C3C-CAC-CBC |
| 11  | A     | 303  | HEC  | C2B-C3B-CAB-CBB |
| 13  | A     | 1104 | UMQ  | C2-C1-O1-C4'    |
| 15  | B     | 1201 | TDS  | CAD-CAL-OAK-CAJ |
| 13  | A     | 1102 | UMQ  | C3'-C4'-O1-C1   |
| 15  | B     | 1201 | TDS  | CAM-CAL-OAK-CAJ |
| 17  | D     | 201  | SQD  | C24-C23-O48-C46 |
| 14  | B     | 201  | CLA  | CBD-CGD-O2D-CED |
| 17  | D     | 201  | SQD  | C8-C7-O47-C45   |
| 11  | C     | 301  | HEC  | C2C-C3C-CAC-CBC |
| 17  | D     | 201  | SQD  | O10-C23-O48-C46 |
| 12  | A     | 1002 | OPC  | CAQ-CAR-CAS-CAT |
| 17  | D     | 201  | SQD  | C33-C34-C35-C36 |
| 17  | D     | 201  | SQD  | C31-C32-C33-C34 |
| 17  | D     | 201  | SQD  | C12-C13-C14-C15 |
| 13  | A     | 1102 | UMQ  | O5'-C5'-C6'-O6' |
| 17  | D     | 201  | SQD  | C13-C14-C15-C16 |
| 13  | A     | 1103 | UMQ  | O5'-C5'-C6'-O6' |
| 13  | A     | 1104 | UMQ  | O5-C5-C6-O6     |
| 17  | D     | 201  | SQD  | O49-C7-O47-C45  |
| 15  | B     | 1202 | TDS  | CAS-CAT-CAU-CAV |
| 13  | A     | 1103 | UMQ  | C4'-C5'-C6'-O6' |
| 15  | B     | 1201 | TDS  | CAD-CAE-OAB-CAA |
| 15  | B     | 1202 | TDS  | CAD-CAE-OAB-CAA |
| 18  | G     | 101  | BCR  | C37-C22-C23-C24 |
| 18  | G     | 101  | BCR  | C7-C8-C9-C10    |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 18  | G     | 101  | BCR  | C21-C22-C23-C24 |
| 12  | A     | 1002 | OPC  | CBM-CBN-CBO-CBP |
| 12  | B     | 1001 | OPC  | CAZ-CBA-CBB-CBC |
| 11  | A     | 303  | HEC  | C2C-C3C-CAC-CBC |
| 14  | B     | 201  | CLA  | C8-C10-C11-C12  |
| 13  | A     | 1101 | UMQ  | O5'-C5'-C6'-O6' |
| 13  | A     | 1104 | UMQ  | C4-C5-C6-O6     |
| 13  | A     | 1101 | UMQ  | O1'-CA-CB-CC    |
| 15  | B     | 1201 | TDS  | CAF-CAE-OAB-CAA |
| 13  | A     | 1104 | UMQ  | O1'-CA-CB-CC    |
| 14  | B     | 201  | CLA  | C10-C11-C12-C13 |
| 18  | G     | 101  | BCR  | C22-C23-C24-C25 |
| 12  | A     | 1002 | OPC  | CBU-CBV-CBW-CBX |
| 13  | A     | 1101 | UMQ  | C4'-C5'-C6'-O6' |
| 13  | A     | 1102 | UMQ  | C4'-C5'-C6'-O6' |
| 12  | B     | 1001 | OPC  | CAP-CAO-OAN-CAM |
| 17  | D     | 201  | SQD  | C10-C11-C12-C13 |
| 11  | A     | 303  | HEC  | C4C-C3C-CAC-CBC |
| 12  | A     | 1002 | OPC  | CAH-CAG-NAF-CAA |
| 14  | B     | 201  | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 201  | CLA  | C15-C16-C17-C18 |
| 13  | A     | 1102 | UMQ  | C4-C5-C6-O6     |
| 13  | A     | 1102 | UMQ  | O5-C5-C6-O6     |
| 13  | A     | 1104 | UMQ  | CB-CC-CD-CF     |
| 12  | B     | 1001 | OPC  | CAY-CAZ-CBA-CBB |
| 13  | A     | 1102 | UMQ  | C5'-C4'-O1-C1   |
| 12  | A     | 1002 | OPC  | CBL-CBM-CBN-CBO |
| 12  | A     | 1002 | OPC  | CBV-CBW-CBX-CBY |
| 14  | B     | 201  | CLA  | C3A-C2A-CAA-CBA |
| 12  | B     | 1001 | OPC  | CBT-CBU-CBV-CBW |
| 12  | A     | 1002 | OPC  | CBY-CBZ-CCA-CCB |
| 13  | A     | 1103 | UMQ  | CG-CH-CI-CJ     |
| 17  | D     | 201  | SQD  | C29-C30-C31-C32 |
| 12  | A     | 1002 | OPC  | CBT-CBU-CBV-CBW |
| 15  | B     | 1202 | TDS  | CAY-CAZ-CBA-CBB |
| 17  | D     | 201  | SQD  | C15-C16-C17-C18 |
| 12  | B     | 1001 | OPC  | CAH-CAG-NAF-CAE |
| 12  | A     | 1002 | OPC  | CBW-CBX-CBY-CBZ |
| 18  | G     | 101  | BCR  | C23-C24-C25-C30 |
| 13  | A     | 1102 | UMQ  | CI-CJ-CK-CL     |
| 12  | B     | 1001 | OPC  | OAD-CAO-OAN-CAM |
| 10  | A     | 301  | HEM  | C3A-C2A-CAA-CBA |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 17  | D     | 201  | SQD  | C11-C12-C13-C14 |
| 12  | A     | 1002 | OPC  | CAZ-CBA-CBB-CBC |
| 12  | B     | 1001 | OPC  | CBC-CBD-CBE-CBF |
| 13  | A     | 1101 | UMQ  | CF-CG-CH-CI     |
| 17  | D     | 201  | SQD  | C28-C29-C30-C31 |
| 13  | A     | 1103 | UMQ  | CF-CG-CH-CI     |
| 15  | B     | 1201 | TDS  | CAT-CAU-CAV-CAW |
| 12  | B     | 1001 | OPC  | CBU-CBV-CBW-CBX |
| 15  | B     | 1201 | TDS  | CAR-CAS-CAT-CAU |
| 13  | A     | 1103 | UMQ  | C4-C5-C6-O6     |
| 13  | A     | 1101 | UMQ  | CA-CB-CC-CD     |
| 15  | B     | 1201 | TDS  | CAW-CAX-CAY-CAZ |
| 14  | B     | 201  | CLA  | C1A-C2A-CAA-CBA |
| 12  | B     | 1001 | OPC  | CBK-CBL-CBM-CBN |
| 15  | B     | 1202 | TDS  | CAU-CAV-CAW-CAX |
| 13  | A     | 1102 | UMQ  | CC-CD-CF-CG     |
| 12  | A     | 1002 | OPC  | CAW-CAX-CAY-CAZ |
| 14  | B     | 201  | CLA  | C4-C3-C5-C6     |
| 13  | A     | 1104 | UMQ  | CH-CI-CJ-CK     |
| 13  | A     | 1104 | UMQ  | CI-CJ-CK-CL     |
| 12  | A     | 1002 | OPC  | CBC-CBD-CBE-CBF |
| 13  | A     | 1104 | UMQ  | CG-CH-CI-CJ     |
| 15  | B     | 1202 | TDS  | CAR-CAS-CAT-CAU |
| 15  | B     | 1202 | TDS  | CAM-CAL-OAK-CAJ |
| 17  | D     | 201  | SQD  | C27-C28-C29-C30 |
| 17  | D     | 201  | SQD  | C2-C1-O6-C44    |
| 14  | B     | 201  | CLA  | C2-C3-C5-C6     |
| 17  | D     | 201  | SQD  | C25-C26-C27-C28 |
| 13  | A     | 1101 | UMQ  | CC-CD-CF-CG     |
| 17  | D     | 201  | SQD  | C16-C17-C18-C19 |
| 15  | B     | 1201 | TDS  | CAV-CAW-CAX-CAY |
| 12  | B     | 1001 | OPC  | CAS-CAT-CAU-CAV |
| 12  | B     | 1001 | OPC  | CAR-CAS-CAT-CAU |
| 12  | B     | 1001 | OPC  | CBL-CBM-CBN-CBO |
| 12  | A     | 1002 | OPC  | CAS-CAT-CAU-CAV |
| 12  | A     | 1002 | OPC  | CBX-CBY-CBZ-CCA |
| 14  | B     | 201  | CLA  | C11-C10-C8-C9   |
| 12  | B     | 1001 | OPC  | CAH-CAG-NAF-CAA |
| 13  | A     | 1103 | UMQ  | CA-CB-CC-CD     |
| 13  | A     | 1101 | UMQ  | O5-C1-O1-C4'    |
| 13  | A     | 1101 | UMQ  | CB-CC-CD-CF     |
| 13  | A     | 1102 | UMQ  | O1'-CA-CB-CC    |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 13  | A     | 1103 | UMQ  | CD-CF-CG-CH     |
| 15  | B     | 1202 | TDS  | CAX-CAY-CAZ-CBA |
| 12  | A     | 1002 | OPC  | CBP-CBQ-CBR-CBS |
| 12  | A     | 1002 | OPC  | CBK-CBL-CBM-CBN |
| 12  | A     | 1002 | OPC  | CAL-CAM-CBI-OBJ |
| 17  | D     | 201  | SQD  | O6-C44-C45-C46  |
| 12  | A     | 1002 | OPC  | CAH-OAI-PAJ-OAK |
| 12  | B     | 1001 | OPC  | CAH-OAI-PAJ-OAB |
| 12  | B     | 1001 | OPC  | CBP-CBQ-CBR-CBS |
| 17  | D     | 201  | SQD  | O6-C44-C45-O47  |
| 17  | D     | 201  | SQD  | C14-C15-C16-C17 |
| 13  | A     | 1102 | UMQ  | CB-CA-O1'-C1'   |
| 11  | C     | 301  | HEC  | C3A-C2A-CAA-CBA |
| 10  | A     | 301  | HEM  | C2A-CAA-CBA-CGA |
| 15  | B     | 1201 | TDS  | CAX-CAY-CAZ-CBA |
| 11  | C     | 301  | HEC  | C1A-C2A-CAA-CBA |
| 12  | A     | 1002 | OPC  | CAT-CAU-CAV-CAW |
| 10  | A     | 301  | HEM  | CAA-CBA-CGA-O2A |
| 13  | A     | 1104 | UMQ  | CC-CD-CF-CG     |
| 18  | G     | 101  | BCR  | C11-C10-C9-C34  |
| 11  | C     | 301  | HEC  | C3D-CAD-CBD-CGD |
| 13  | A     | 1102 | UMQ  | CF-CG-CH-CI     |
| 12  | B     | 1001 | OPC  | CAL-CAM-CBI-OBJ |
| 12  | B     | 1001 | OPC  | CBS-CBT-CBU-CBV |
| 12  | B     | 1001 | OPC  | CBM-CBN-CBO-CBP |
| 10  | A     | 301  | HEM  | CAA-CBA-CGA-O1A |
| 18  | G     | 101  | BCR  | C11-C10-C9-C8   |
| 15  | B     | 1201 | TDS  | CAU-CAV-CAW-CAX |
| 14  | B     | 201  | CLA  | C12-C13-C15-C16 |
| 10  | A     | 302  | HEM  | C3A-C2A-CAA-CBA |
| 13  | A     | 1103 | UMQ  | CH-CI-CJ-CK     |
| 10  | A     | 302  | HEM  | CAD-CBD-CGD-O2D |
| 13  | A     | 1101 | UMQ  | CG-CH-CI-CJ     |
| 12  | A     | 1002 | OPC  | CAY-CAZ-CBA-CBB |
| 11  | C     | 301  | HEC  | CAD-CBD-CGD-O2D |
| 13  | A     | 1104 | UMQ  | CD-CF-CG-CH     |
| 11  | C     | 301  | HEC  | CAD-CBD-CGD-O1D |
| 10  | A     | 302  | HEM  | CAD-CBD-CGD-O1D |
| 12  | A     | 1002 | OPC  | OAK-CAL-CAM-OAN |
| 12  | A     | 1002 | OPC  | CAH-CAG-NAF-CBG |
| 17  | D     | 201  | SQD  | C44-C45-C46-O48 |
| 13  | A     | 1103 | UMQ  | O5-C5-C6-O6     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 15  | B     | 1202 | TDS  | CAT-CAU-CAV-CAW |
| 15  | B     | 1201 | TDS  | CAS-CAT-CAU-CAV |
| 13  | A     | 1103 | UMQ  | CB-CA-O1'-C1'   |
| 17  | D     | 201  | SQD  | O47-C7-C8-C9    |
| 12  | A     | 1002 | OPC  | OAK-CAL-CAM-CBI |
| 15  | B     | 1202 | TDS  | CAD-CAL-OAK-CAJ |
| 13  | A     | 1101 | UMQ  | C2-C1-O1-C4'    |
| 11  | C     | 301  | HEC  | CAA-CBA-CGA-O2A |
| 14  | B     | 201  | CLA  | C2-C1-O2A-CGA   |
| 12  | B     | 1001 | OPC  | OAD-CAO-CAP-CAQ |

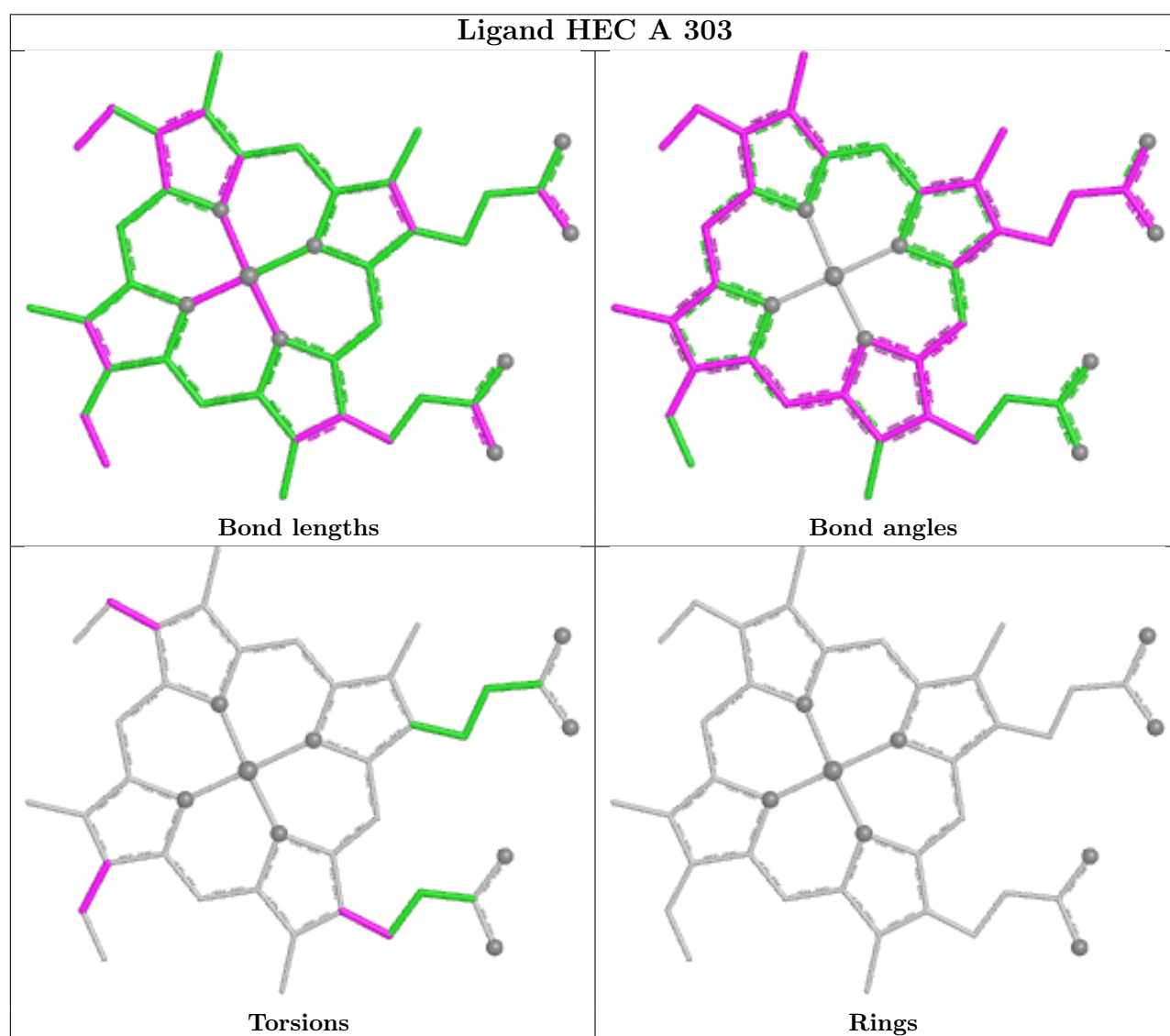
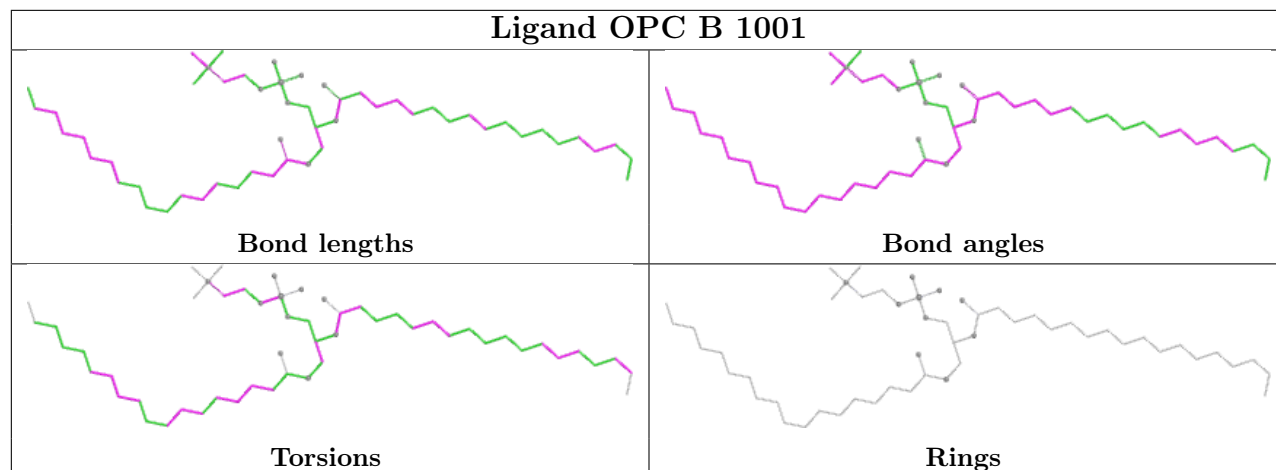
There are no ring outliers.

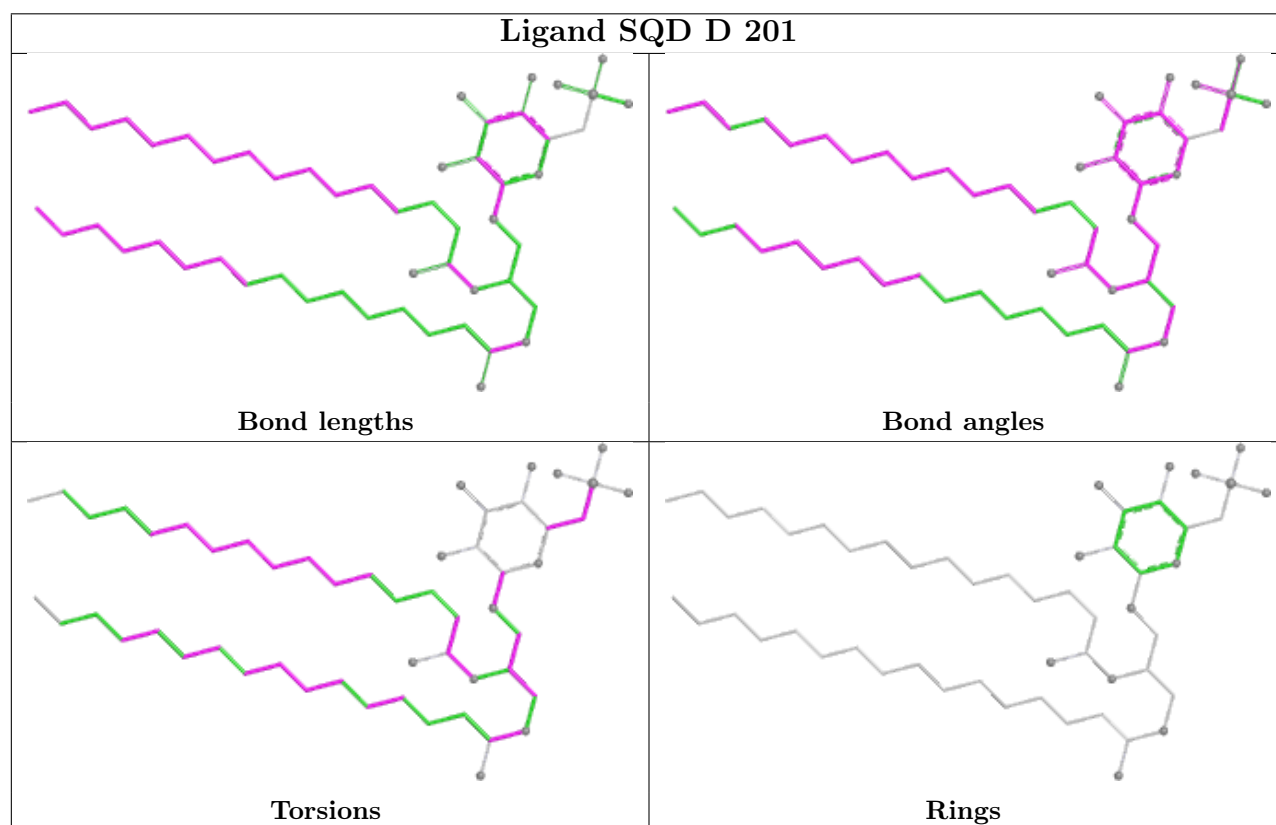
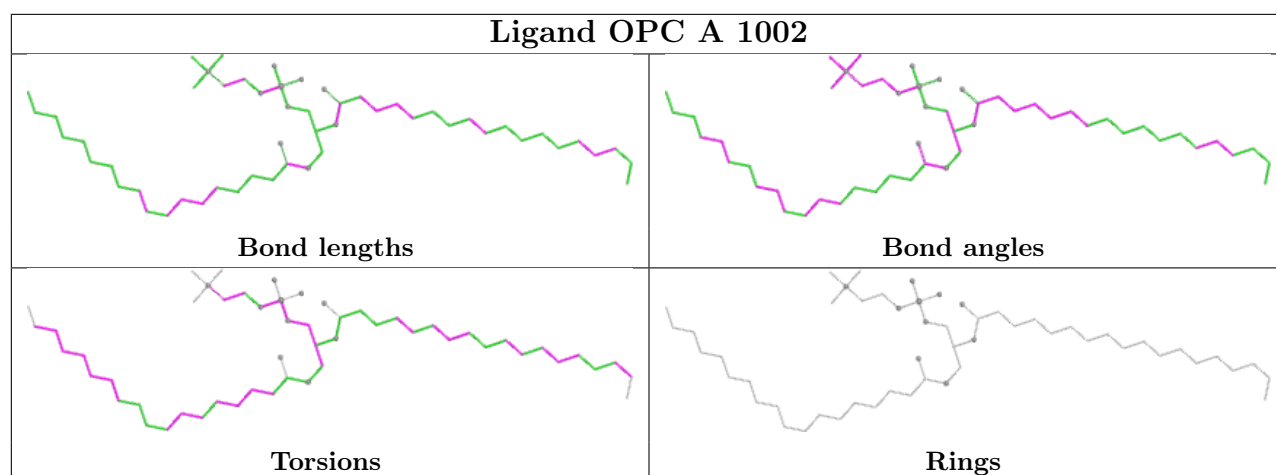
15 monomers are involved in 175 short contacts:

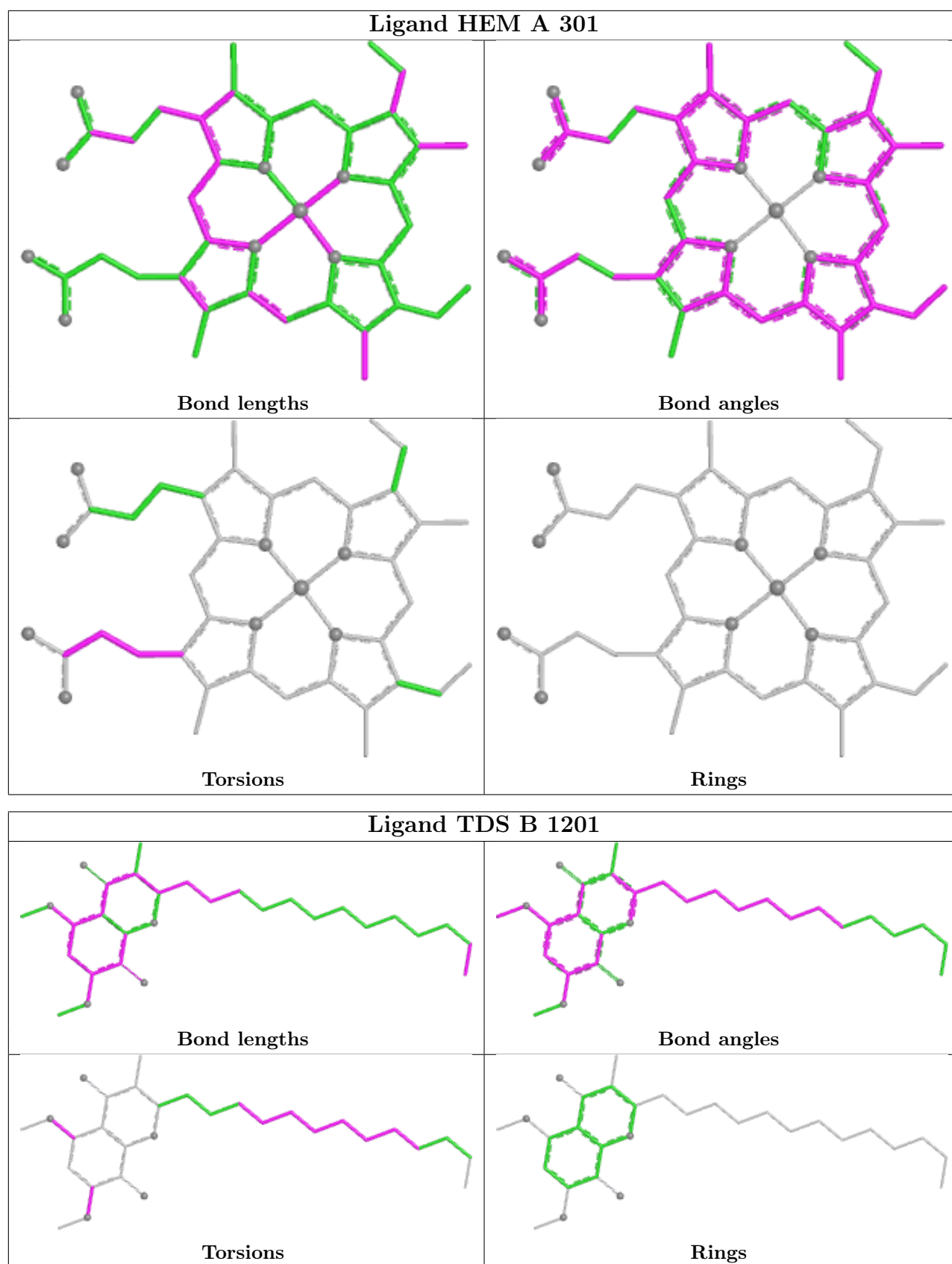
| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 12  | B     | 1001 | OPC  | 2       | 0            |
| 11  | A     | 303  | HEC  | 24      | 0            |
| 12  | A     | 1002 | OPC  | 17      | 0            |
| 17  | D     | 201  | SQD  | 9       | 0            |
| 10  | A     | 301  | HEM  | 19      | 0            |
| 15  | B     | 1201 | TDS  | 20      | 0            |
| 16  | D     | 200  | FES  | 1       | 0            |
| 11  | C     | 301  | HEC  | 30      | 0            |
| 14  | B     | 201  | CLA  | 6       | 0            |
| 18  | G     | 101  | BCR  | 9       | 0            |
| 13  | A     | 1101 | UMQ  | 2       | 0            |
| 13  | A     | 1102 | UMQ  | 1       | 0            |
| 10  | A     | 302  | HEM  | 22      | 0            |
| 13  | A     | 1104 | UMQ  | 3       | 0            |
| 15  | B     | 1202 | TDS  | 19      | 0            |

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

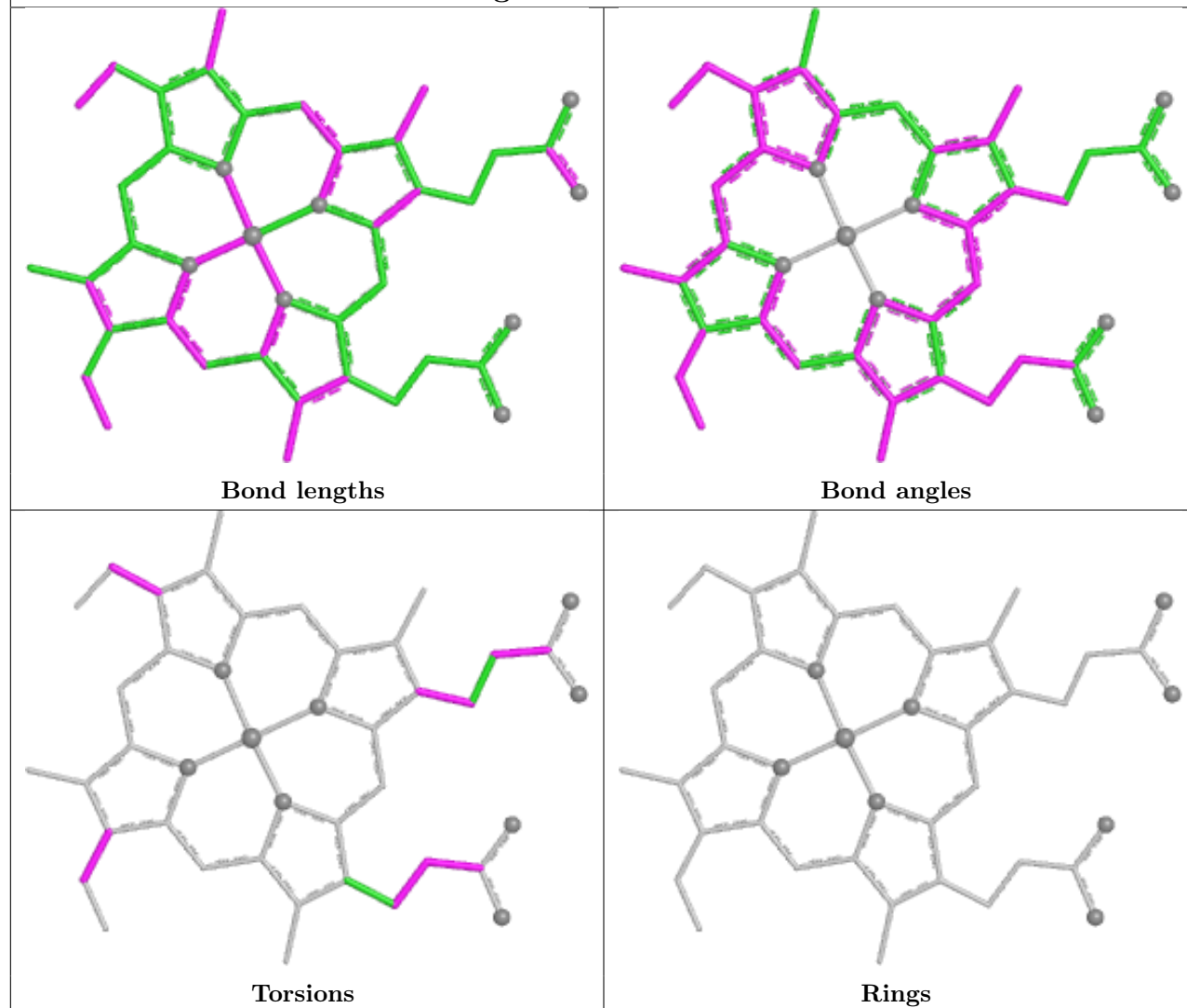
equivalents in the CSD to analyse the geometry.



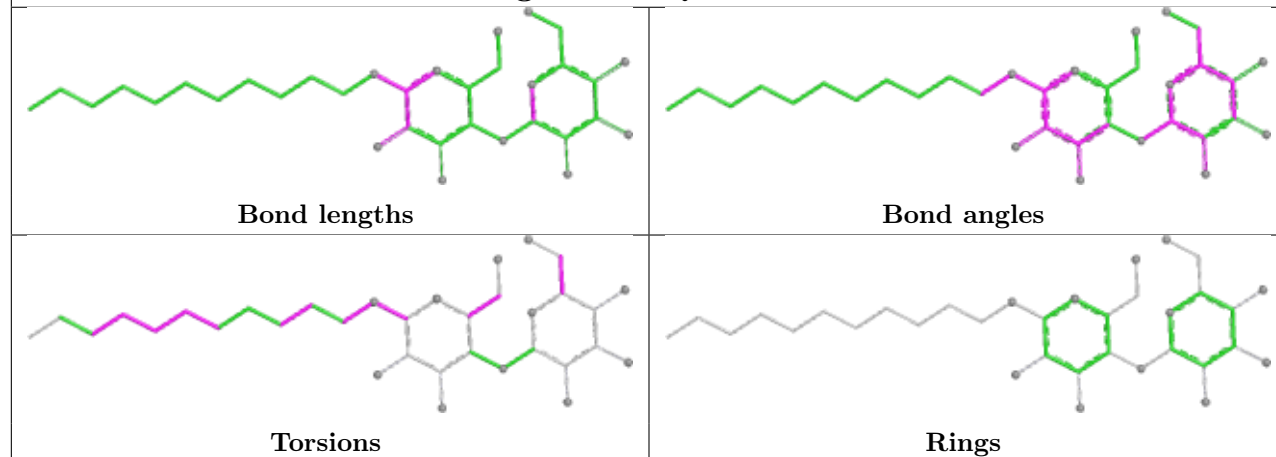




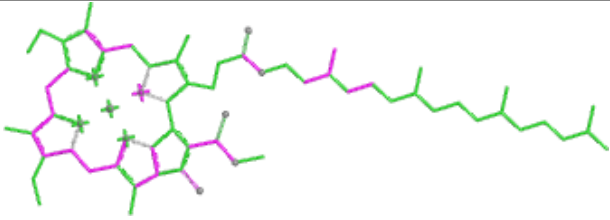
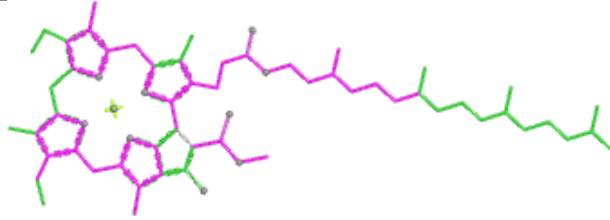
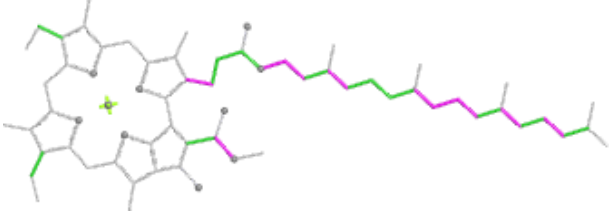
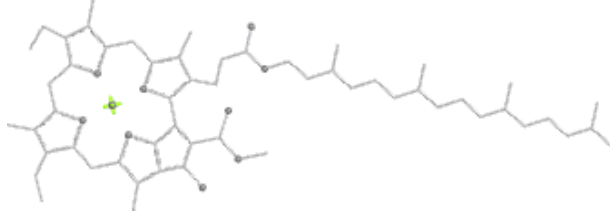
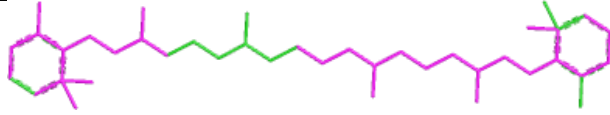
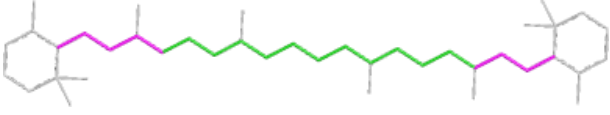
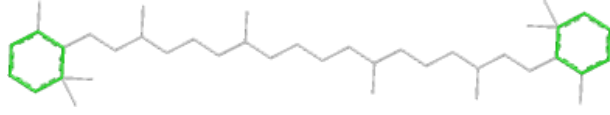
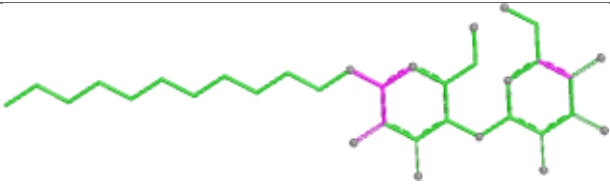
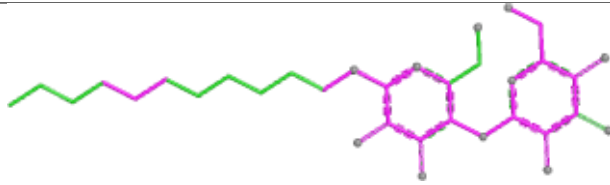
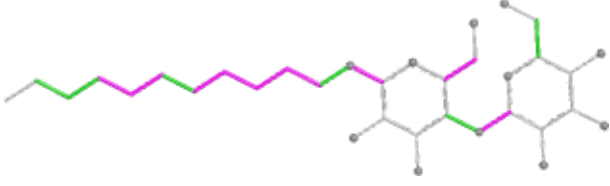
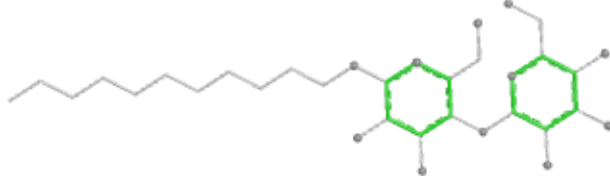
## Ligand HEC C 301



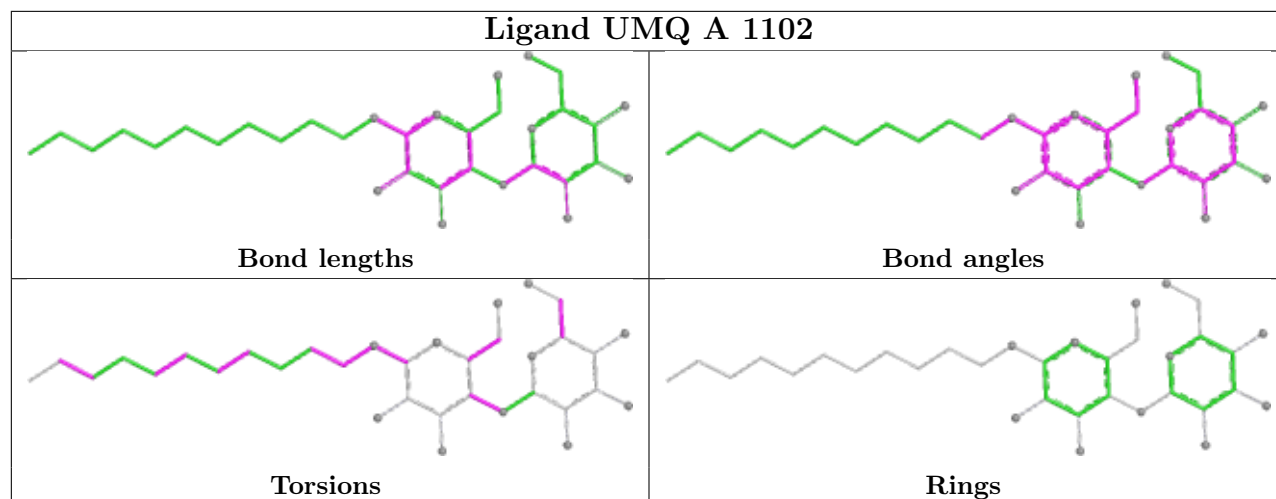
## Ligand UMQ A 1103



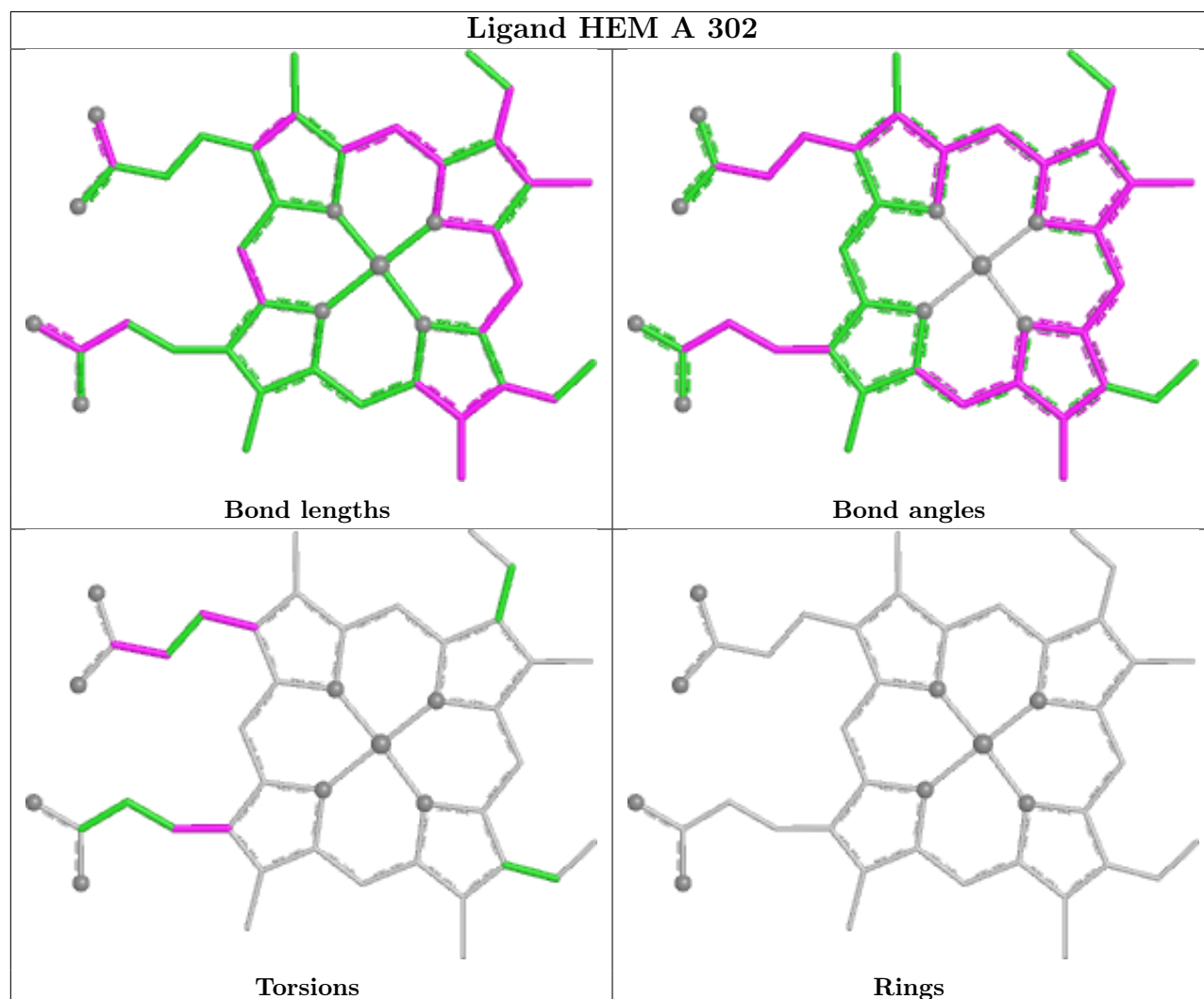


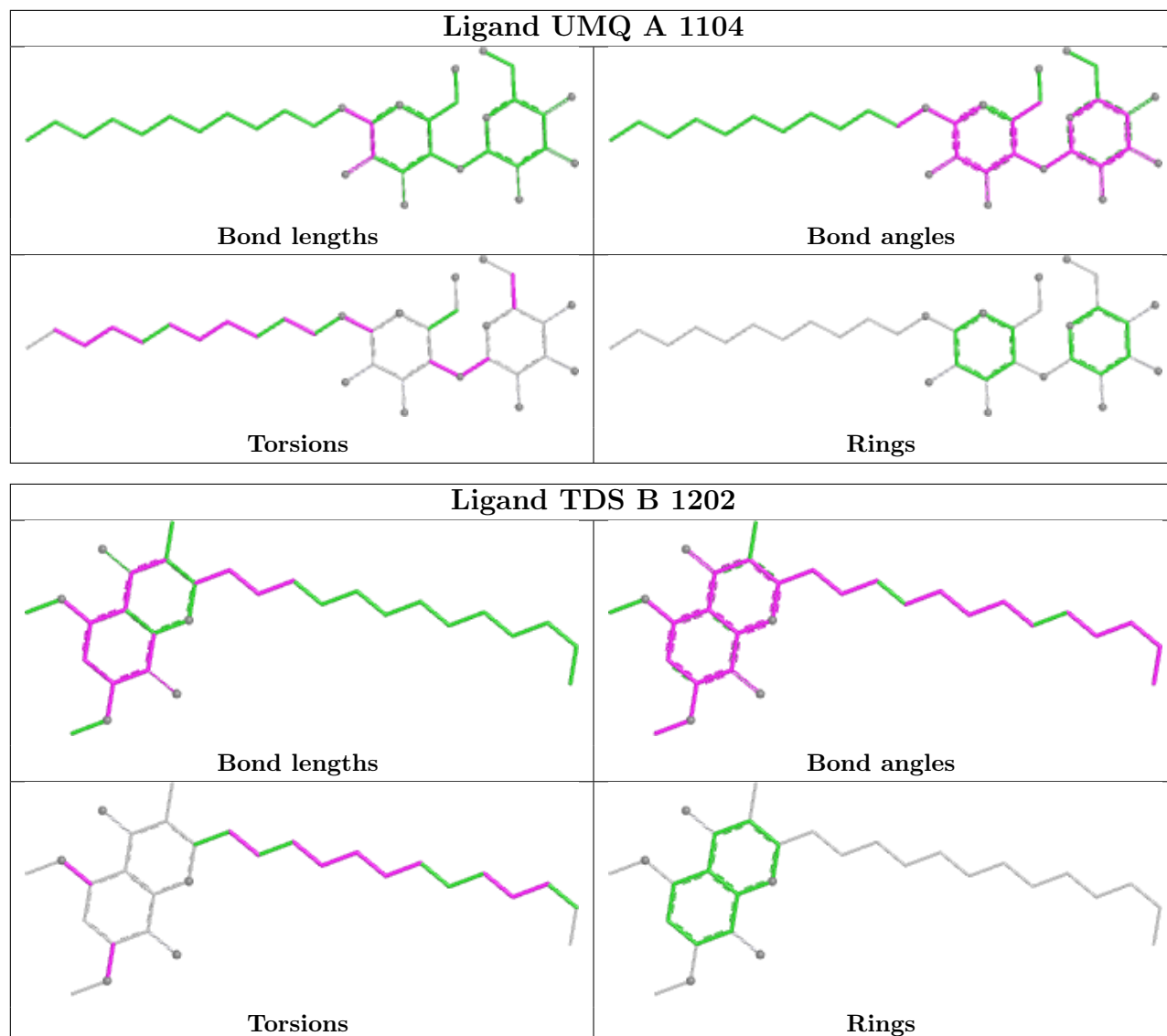
| Ligand CLA B 201                                                                                        |                                                                                                         |
|---------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------|
|  <p>Bond lengths</p>   |  <p>Bond angles</p>   |
|  <p>Torsions</p>       |  <p>Rings</p>         |
| Ligand BCR G 101                                                                                        |                                                                                                         |
|  <p>Bond lengths</p>   |  <p>Bond angles</p>   |
|  <p>Torsions</p>      |  <p>Rings</p>        |
| Ligand UMQ A 1101                                                                                       |                                                                                                         |
|  <p>Bond lengths</p> |  <p>Bond angles</p> |
|  <p>Torsions</p>     |  <p>Rings</p>       |

## Ligand UMQ A 1102



## Ligand HEM A 302





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9  |
|-----|-------|----------------|--------|----------------|-----------------------|--------|
| 1   | A     | 215/215 (100%) | -0.62  | 2 (0%) 81 69   | 5, 31, 72, 170        | 0      |
| 2   | B     | 160/160 (100%) | -0.25  | 4 (2%) 58 43   | 22, 50, 97, 146       | 0      |
| 3   | C     | 288/289 (99%)  | 0.85   | 32 (11%) 10 11 | 4, 55, 142, 159       | 1 (0%) |
| 4   | D     | 168/179 (93%)  | 1.49   | 45 (26%) 1 2   | 24, 90, 140, 156      | 0      |
| 5   | E     | 32/32 (100%)   | 0.02   | 2 (6%) 26 20   | 39, 63, 93, 110       | 0      |
| 6   | F     | 32/35 (91%)    | 0.15   | 4 (12%) 8 9    | 35, 50, 112, 121      | 0      |
| 7   | G     | 37/37 (100%)   | -0.08  | 3 (8%) 18 15   | 29, 44, 119, 138      | 0      |
| 8   | H     | 29/29 (100%)   | -0.42  | 1 (3%) 48 35   | 31, 42, 72, 95        | 0      |
| All | All   | 961/976 (98%)  | 0.33   | 93 (9%) 13 13  | 4, 52, 132, 170       | 1 (0%) |

All (93) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 4   | D     | 96  | LYS  | 9.7  |
| 3   | C     | 40  | VAL  | 7.8  |
| 4   | D     | 95  | SER  | 7.5  |
| 4   | D     | 141 | ARG  | 7.0  |
| 4   | D     | 157 | ASP  | 7.0  |
| 3   | C     | 88  | GLU  | 6.4  |
| 3   | C     | 220 | SER  | 6.0  |
| 4   | D     | 75  | ALA  | 5.2  |
| 3   | C     | 100 | ASP  | 5.2  |
| 3   | C     | 212 | PRO  | 5.2  |
| 4   | D     | 177 | TRP  | 4.9  |
| 4   | D     | 156 | GLN  | 4.8  |
| 3   | C     | 195 | TYR  | 4.2  |
| 4   | D     | 144 | ALA  | 4.0  |
| 4   | D     | 146 | LEU  | 4.0  |
| 3   | C     | 35  | GLU  | 3.9  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | B     | 74  | GLU  | 3.9  |
| 3   | C     | 207 | VAL  | 3.9  |
| 4   | D     | 67  | SER  | 3.8  |
| 3   | C     | 201 | THR  | 3.6  |
| 3   | C     | 165 | GLU  | 3.6  |
| 4   | D     | 79  | VAL  | 3.4  |
| 3   | C     | 71  | ASN  | 3.3  |
| 4   | D     | 77  | ASP  | 3.3  |
| 3   | C     | 145 | GLY  | 3.3  |
| 4   | D     | 78  | ARG  | 3.3  |
| 4   | D     | 85  | LYS  | 3.3  |
| 3   | C     | 225 | VAL  | 3.2  |
| 4   | D     | 97  | GLU  | 3.2  |
| 4   | D     | 90  | TYR  | 3.2  |
| 1   | A     | 1   | MET  | 3.1  |
| 4   | D     | 70  | LEU  | 3.0  |
| 4   | D     | 127 | PRO  | 3.0  |
| 3   | C     | 140 | LYS  | 3.0  |
| 3   | C     | 206 | THR  | 3.0  |
| 4   | D     | 80  | LEU  | 2.9  |
| 3   | C     | 219 | VAL  | 2.9  |
| 3   | C     | 252 | PRO  | 2.9  |
| 4   | D     | 179 | VAL  | 2.9  |
| 2   | B     | 154 | THR  | 2.8  |
| 4   | D     | 145 | PRO  | 2.8  |
| 2   | B     | 155 | LEU  | 2.8  |
| 6   | F     | 3   | GLU  | 2.8  |
| 4   | D     | 41  | TYR  | 2.7  |
| 4   | D     | 125 | LYS  | 2.7  |
| 3   | C     | 249 | LEU  | 2.7  |
| 1   | A     | 2   | ALA  | 2.7  |
| 3   | C     | 213 | ALA  | 2.7  |
| 3   | C     | 29  | ALA  | 2.7  |
| 4   | D     | 170 | PHE  | 2.6  |
| 6   | F     | 4   | GLU  | 2.6  |
| 4   | D     | 10  | VAL  | 2.6  |
| 5   | E     | 1   | MET  | 2.6  |
| 6   | F     | 1   | MET  | 2.6  |
| 3   | C     | 194 | LYS  | 2.6  |
| 3   | C     | 39  | SER  | 2.6  |
| 7   | G     | 37  | GLY  | 2.5  |
| 4   | D     | 99  | ILE  | 2.5  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 4   | D     | 175 | LYS  | 2.5  |
| 4   | D     | 131 | SER  | 2.4  |
| 4   | D     | 149 | ALA  | 2.4  |
| 4   | D     | 74  | ASN  | 2.4  |
| 2   | B     | 28  | GLY  | 2.4  |
| 4   | D     | 49  | ALA  | 2.4  |
| 4   | D     | 94  | GLU  | 2.4  |
| 4   | D     | 155 | VAL  | 2.4  |
| 4   | D     | 60  | LEU  | 2.3  |
| 8   | H     | 29  | LEU  | 2.3  |
| 3   | C     | 215 | PRO  | 2.3  |
| 3   | C     | 185 | LYS  | 2.3  |
| 6   | F     | 31  | GLY  | 2.3  |
| 3   | C     | 86  | PRO  | 2.3  |
| 3   | C     | 136 | PRO  | 2.3  |
| 3   | C     | 172 | PHE  | 2.3  |
| 4   | D     | 178 | TRP  | 2.3  |
| 5   | E     | 2   | ILE  | 2.2  |
| 4   | D     | 143 | PRO  | 2.2  |
| 4   | D     | 162 | LEU  | 2.2  |
| 3   | C     | 241 | GLY  | 2.2  |
| 3   | C     | 245 | THR  | 2.2  |
| 3   | C     | 193 | VAL  | 2.2  |
| 7   | G     | 3   | GLU  | 2.2  |
| 4   | D     | 73  | HIS  | 2.2  |
| 4   | D     | 98  | ALA  | 2.1  |
| 4   | D     | 109 | THR  | 2.1  |
| 7   | G     | 27  | GLN  | 2.1  |
| 4   | D     | 86  | GLY  | 2.1  |
| 3   | C     | 166 | LYS  | 2.1  |
| 4   | D     | 15  | ARG  | 2.1  |
| 3   | C     | 147 | TYR  | 2.0  |
| 4   | D     | 59  | LYS  | 2.0  |
| 4   | D     | 92  | VAL  | 2.0  |
| 4   | D     | 43  | ILE  | 2.0  |

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

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

## 6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 6.4 Ligands ⓘ

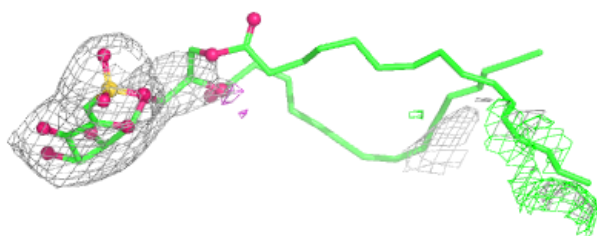
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 17  | SQD  | D     | 201  | 54/54 | 0.79 | 0.27 | 44,147,189,215              | 0     |
| 13  | UMQ  | A     | 1102 | 34/34 | 0.86 | 0.18 | 47,118,166,176              | 0     |
| 12  | OPC  | A     | 1002 | 54/55 | 0.86 | 0.22 | 19,84,180,191               | 0     |
| 13  | UMQ  | A     | 1104 | 34/34 | 0.87 | 0.15 | 61,129,164,178              | 0     |
| 13  | UMQ  | A     | 1103 | 34/34 | 0.88 | 0.14 | 58,109,133,141              | 0     |
| 18  | BCR  | G     | 101  | 40/40 | 0.90 | 0.19 | 24,63,149,159               | 0     |
| 15  | TDS  | B     | 1201 | 30/30 | 0.92 | 0.17 | 46,83,113,127               | 0     |
| 13  | UMQ  | A     | 1101 | 34/34 | 0.93 | 0.13 | 18,110,147,150              | 0     |
| 12  | OPC  | B     | 1001 | 54/55 | 0.95 | 0.14 | 28,80,117,123               | 0     |
| 15  | TDS  | B     | 1202 | 30/30 | 0.96 | 0.11 | 32,78,98,120                | 0     |
| 14  | CLA  | B     | 201  | 65/65 | 0.97 | 0.10 | 23,51,105,119               | 0     |
| 11  | HEC  | A     | 303  | 43/43 | 0.98 | 0.07 | 21,48,67,87                 | 0     |
| 16  | FES  | D     | 200  | 4/4   | 0.98 | 0.08 | 59,69,70,72                 | 0     |
| 10  | HEM  | A     | 301  | 43/43 | 0.99 | 0.06 | 2,21,41,74                  | 0     |
| 10  | HEM  | A     | 302  | 43/43 | 0.99 | 0.07 | 6,26,45,63                  | 0     |
| 9   | CD   | A     | 216  | 1/1   | 0.99 | 0.03 | 63,63,63,63                 | 0     |
| 11  | HEC  | C     | 301  | 43/43 | 0.99 | 0.05 | 3,35,79,104                 | 0     |

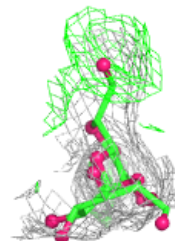
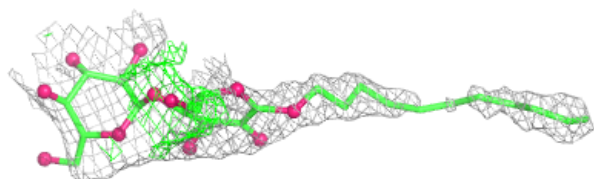
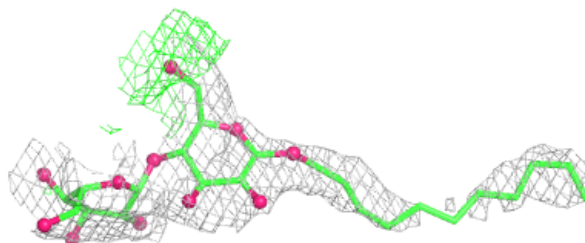
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around SQD D 201:**

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

**Electron density around UMQ A 1102:**

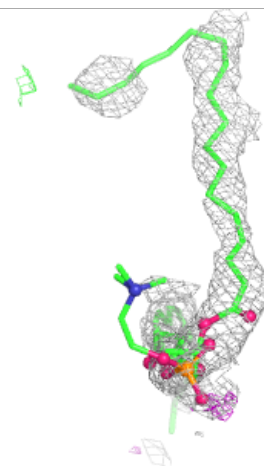
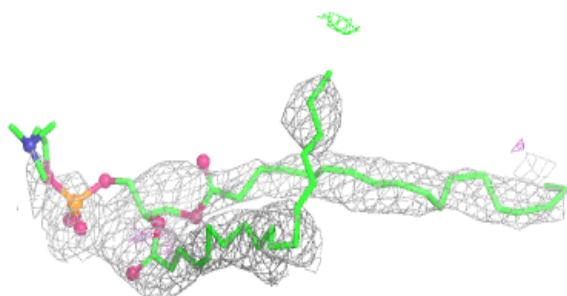
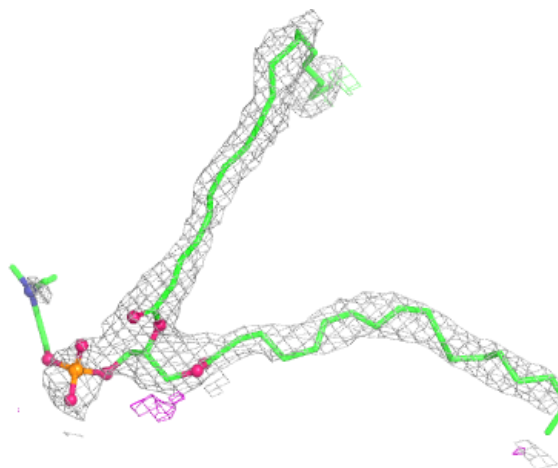
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





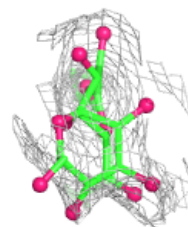
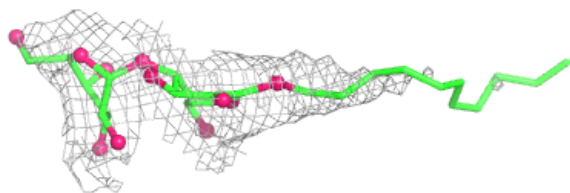
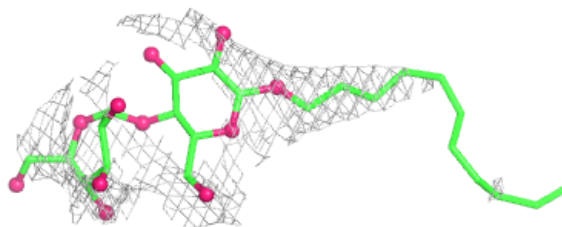
**Electron density around OPC A 1002:**

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

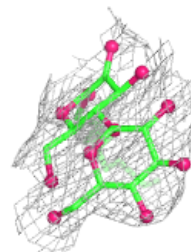
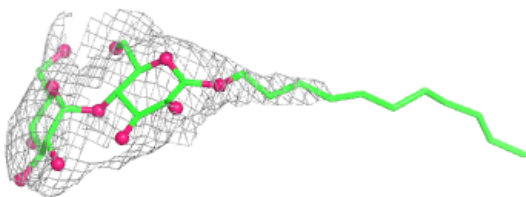
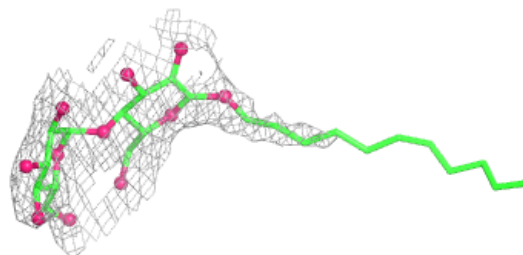


**Electron density around UMQ A 1104:**

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

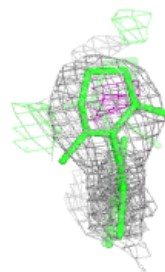
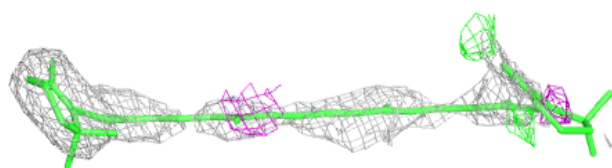
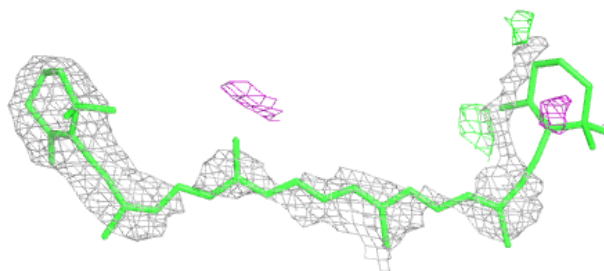
**Electron density around UMQ A 1103:**

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

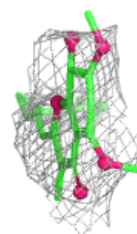
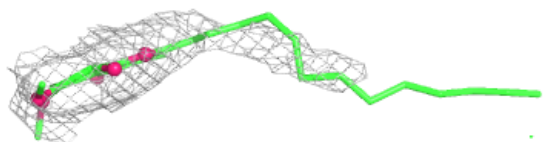
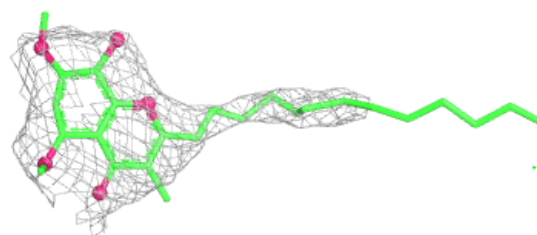


**Electron density around BCR G 101:**

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

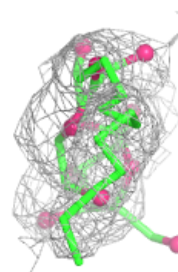
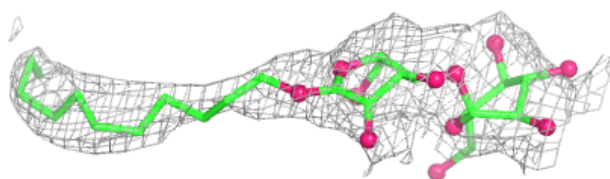
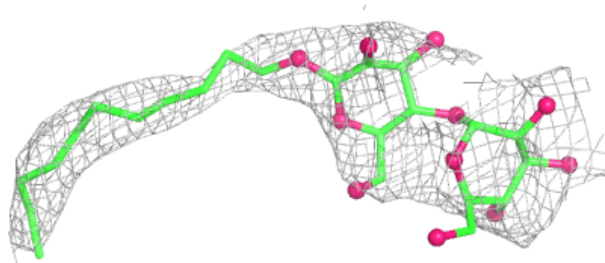
**Electron density around TDS B 1201:**

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

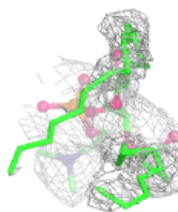
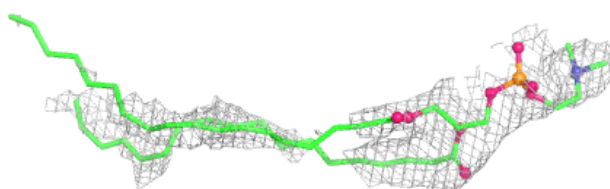
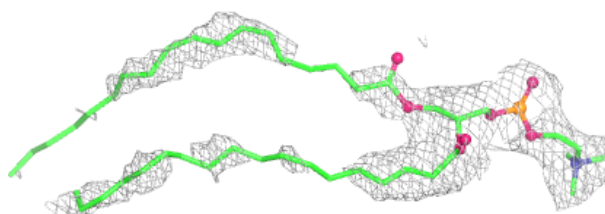


**Electron density around UMQ A 1101:**

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

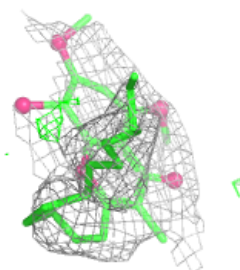
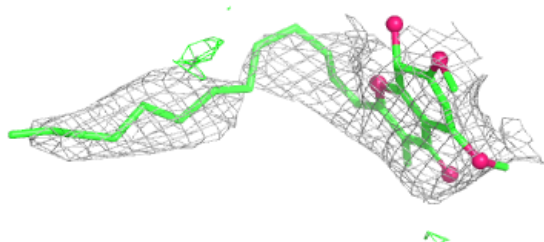
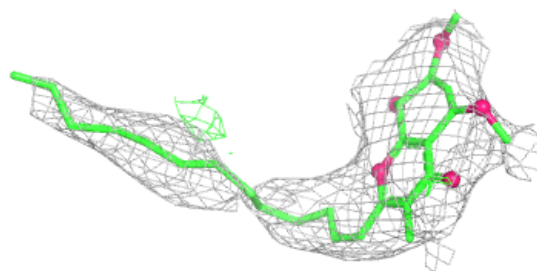
**Electron density around OPC B 1001:**

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

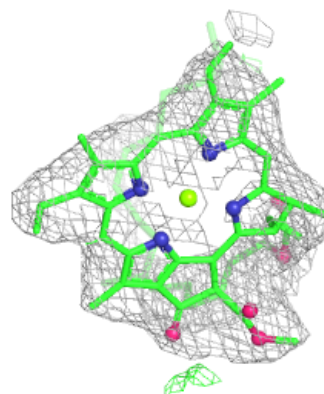
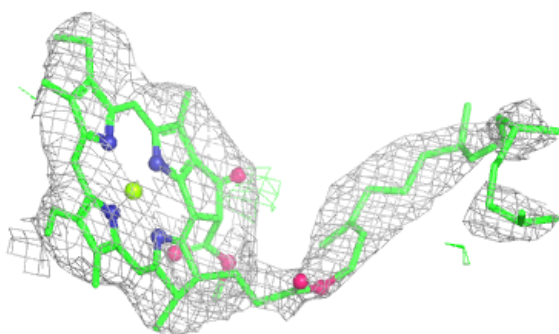
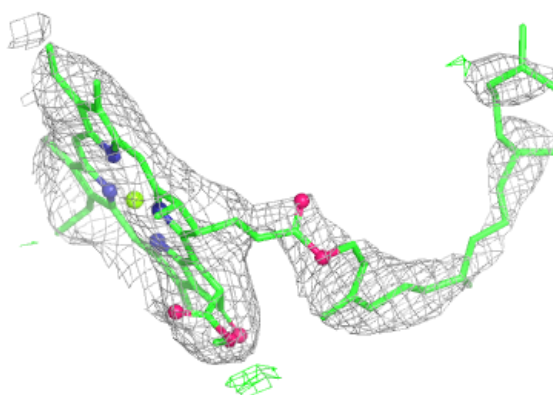


**Electron density around TDS B 1202:**

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

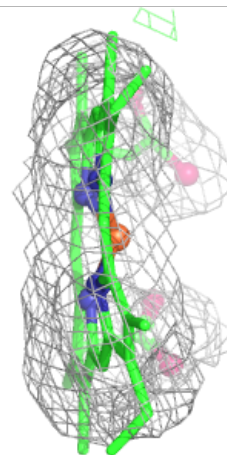
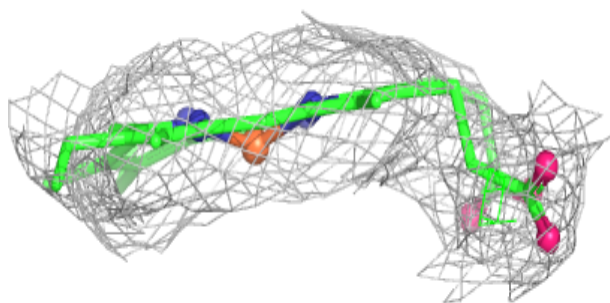
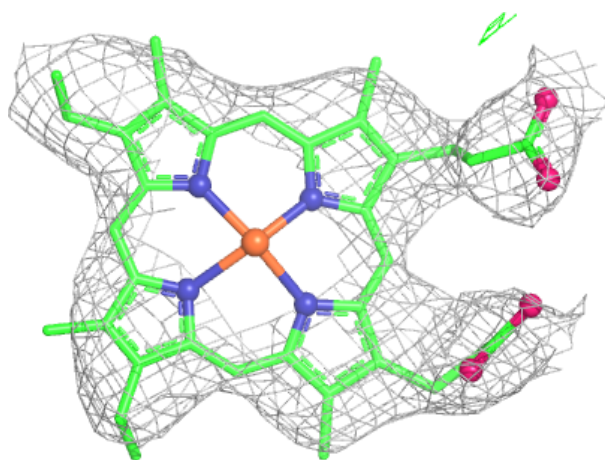
**Electron density around CLA B 201:**

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



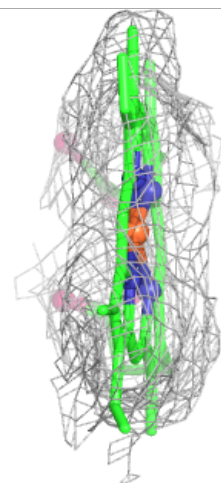
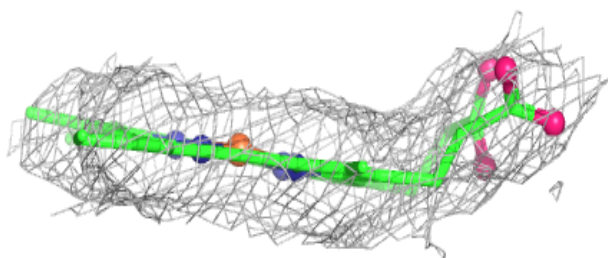
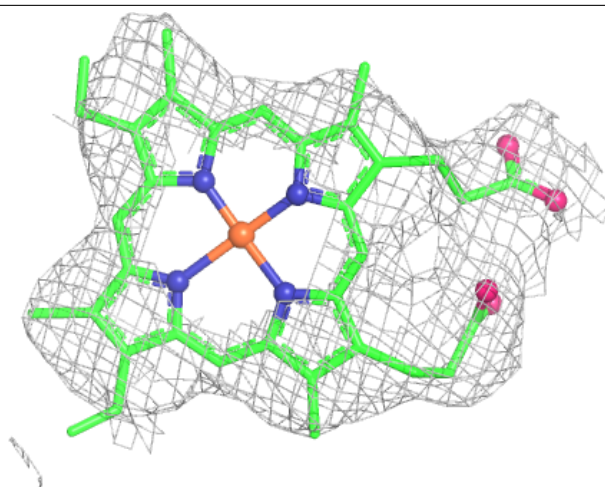
**Electron density around HEC A 303:**

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



**Electron density around HEM A 301:**

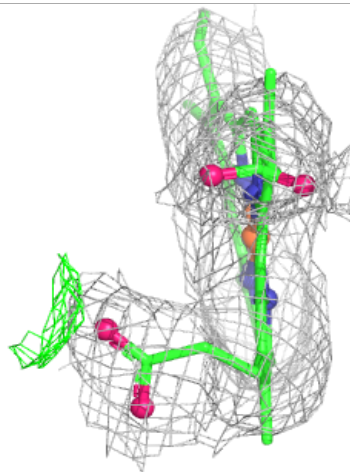
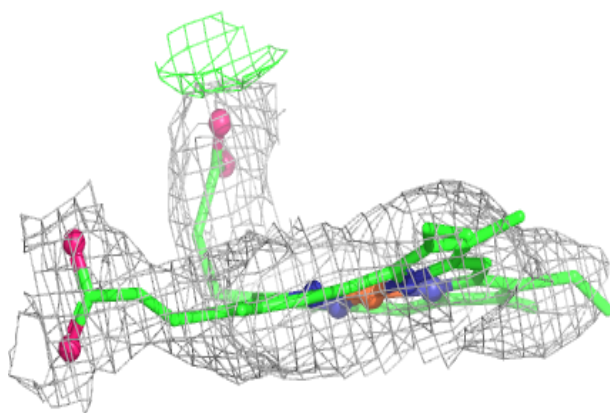
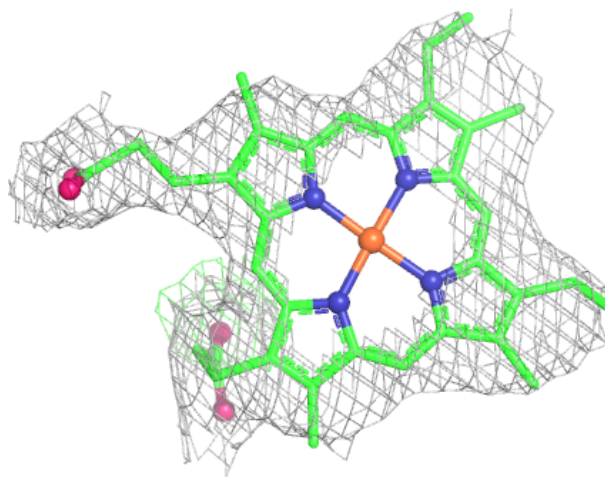
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



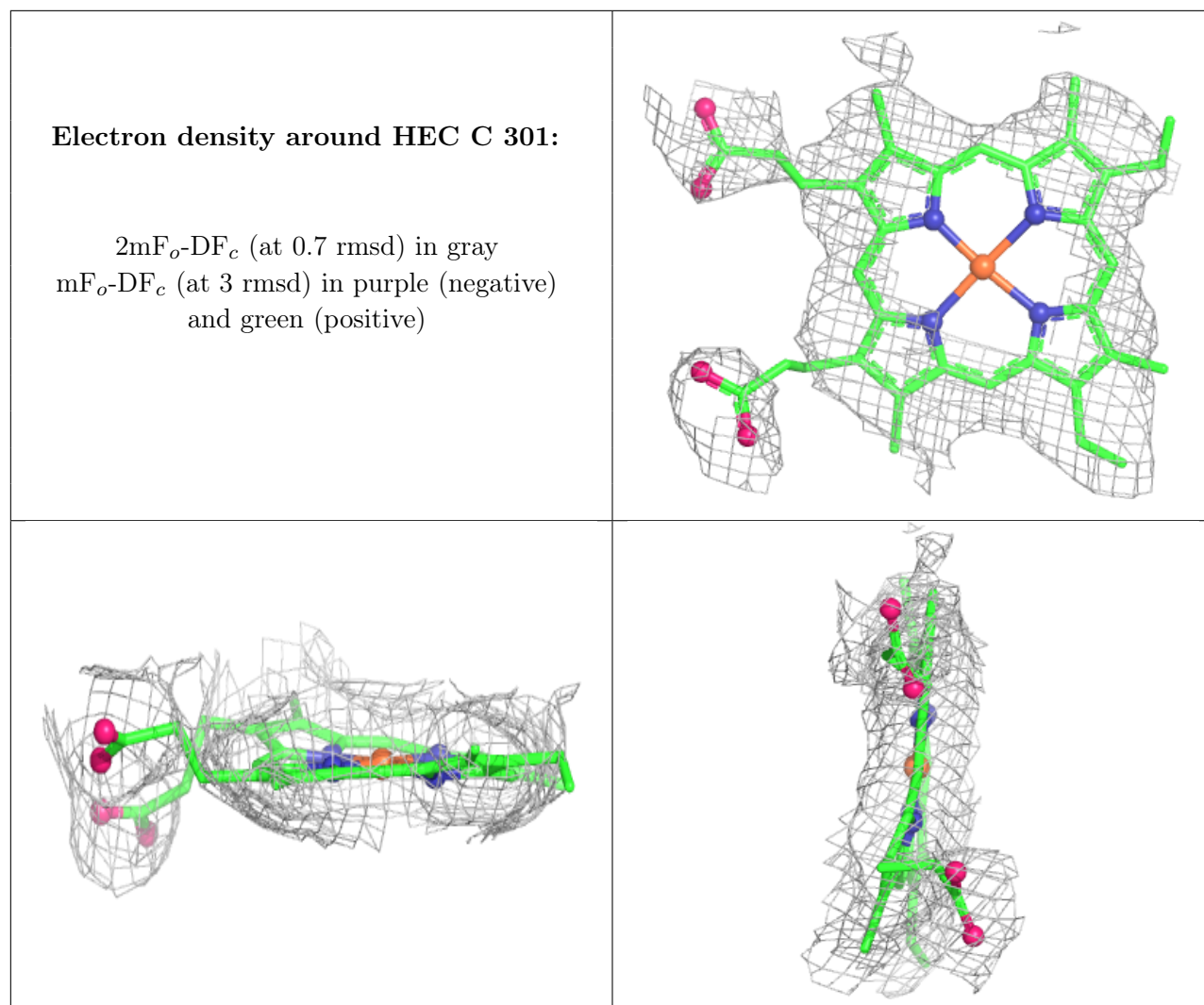


**Electron density around HEM A 302:**

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







## 6.5 Other polymers [i](#)

There are no such residues in this entry.