



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2023 – 03:19 AM EDT

PDB ID : 2H7S  
Title : L244A mutant of Cytochrome P450cam  
Authors : Verras, A.; Alian, A.; Montellano, P.R.  
Deposited on : 2006-06-02  
Resolution : 2.15 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35

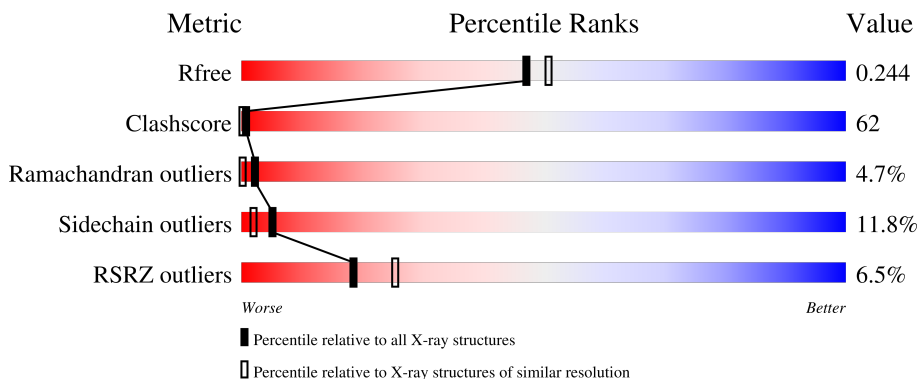
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 130704                      | 1479 (2.16-2.16)                                      |
| Clashscore            | 141614                      | 1585 (2.16-2.16)                                      |
| Ramachandran outliers | 138981                      | 1560 (2.16-2.16)                                      |
| Sidechain outliers    | 138945                      | 1559 (2.16-2.16)                                      |
| RSRZ outliers         | 127900                      | 1456 (2.16-2.16)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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     | 414    |                  |
| 1   | C     | 414    |                  |

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6696 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 P450-cam.

| Mol | Chain | Residues | Atoms         |           |          |          |         | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---------|---------|-------|
|     |       |          | Total         | C         | N        | O        | S       |         |         |       |
| 1   | A     | 405      | Total<br>3201 | C<br>2029 | N<br>560 | O<br>595 | S<br>17 | 0       | 0       | 0     |
| 1   | C     | 405      | Total<br>3199 | C<br>2026 | N<br>559 | O<br>597 | S<br>17 | 0       | 0       | 0     |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| A     | 244     | ALA      | LEU    | engineered mutation | UNP P00183 |
| A     | 334     | ALA      | CYS    | engineered mutation | UNP P00183 |
| C     | 244     | ALA      | LEU    | engineered mutation | UNP P00183 |
| C     | 334     | ALA      | CYS    | engineered mutation | UNP P00183 |

- Molecule 2 is HEME C (three-letter code: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ).



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

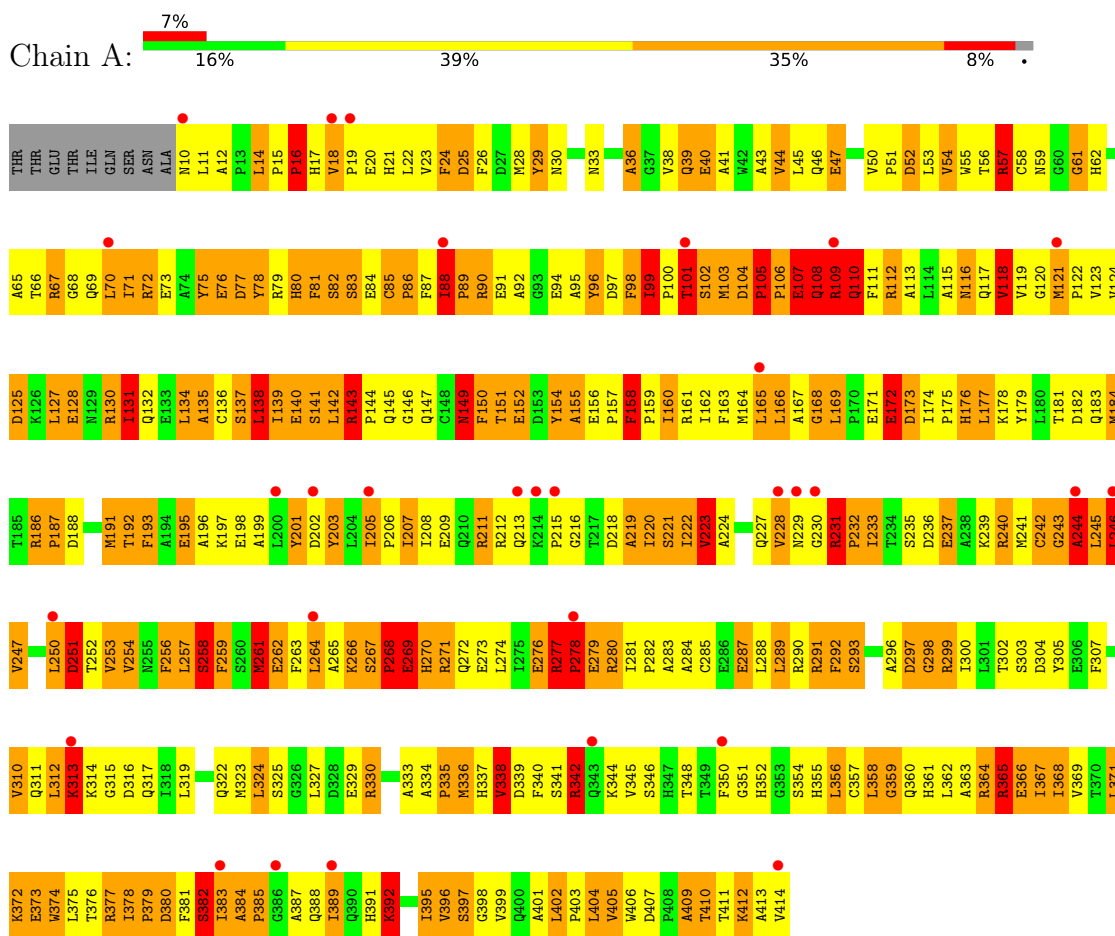
- Molecule 3 is water.

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 3   | A     | 111      | Total | O   | 25      | 0       |
|     |       |          | 111   | 111 |         |         |
| 3   | C     | 99       | Total | O   | 24      | 0       |
|     |       |          | 99    | 99  |         |         |

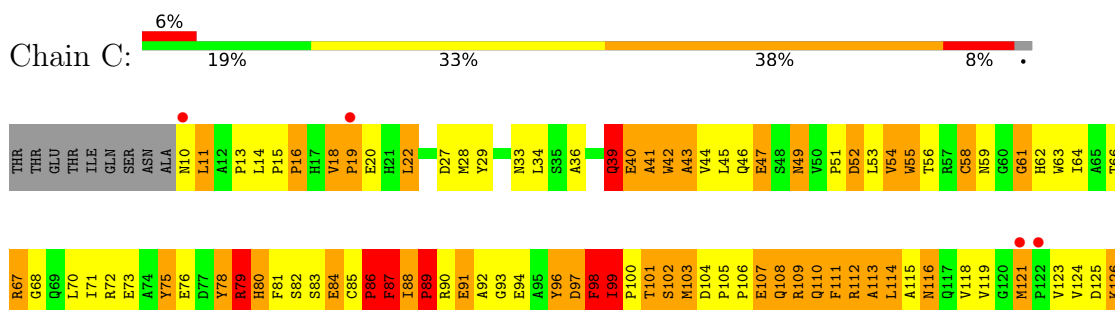
### 3 Residue-property plots i

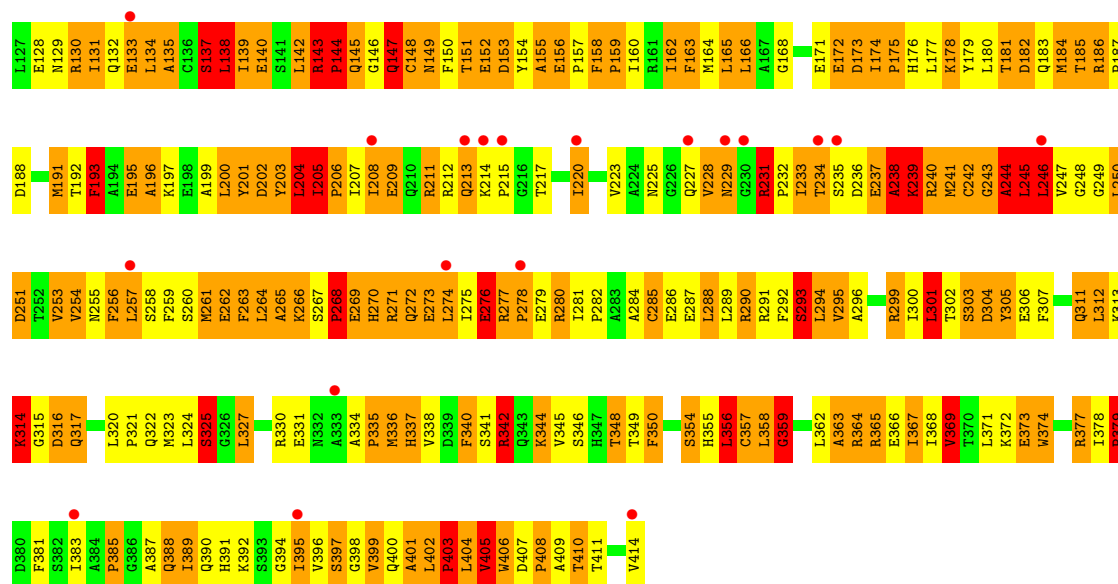
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Cytochrome P450-cam



- Molecule 1: Cytochrome P450-cam





## 4 Data and refinement statistics i

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 1 21 1  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 57.70Å 59.85Å 114.12Å<br>90.00° 104.69° 90.00°              | Depositor        |
| Resolution (Å)  | 50.00 – 2.15<br>45.43 – 2.15                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | (Not available) (50.00-2.15)<br>80.3 (45.43-2.15)           | Depositor<br>EDS |
| $R_{merge}$   | (Not available)   | Depositor        |
| $R_{sym}$   | 0.07  | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 0.77 (at 2.14Å)   | Xtrriage         |
| Refinement program  | CNS 1.1   | Depositor        |
| R, $R_{free}$   | 0.235 , 0.249<br>0.237 , 0.244                              | Depositor<br>DCC |
| $R_{free}$ test set   | 3755 reflections (9.91%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 21.3  | Xtrriage         |
| Anisotropy  | 0.370   | Xtrriage         |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.35 , 14.3   | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$ | Xtrriage         |
| Estimated twinning fraction   | 0.407 for h,-k,-h-l   | Xtrriage         |
| Reported twinning fraction  | 0.391 for h,-k,-h-l   | Depositor        |
| Outliers  | 1 of 37909 reflections (0.003%)                             | Xtrriage         |
| $F_o, F_c$ correlation  | 0.93  | EDS              |
| Total number of atoms   | 6696  | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 24.0  | wwPDB-VP         |

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 52.41 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.8801e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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

## 5 Model quality i

### 5.1 Standard geometry i

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

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     | 2.85         | 278/3280 (8.5%) | 2.29        | 173/4456 (3.9%) |
| 1   | C     | 2.87         | 289/3278 (8.8%) | 2.43        | 180/4454 (4.0%) |
| All | All   | 2.86         | 567/6558 (8.6%) | 2.36        | 353/8910 (4.0%) |

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                   | 8                   |
| 1   | C     | 0                   | 9                   |
| All | All   | 0                   | 17                  |

All (567) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1   | C     | 399 | VAL  | CB-CG2  | 16.70  | 1.88        | 1.52     |
| 1   | A     | 95  | ALA  | CA-CB   | -15.72 | 1.19        | 1.52     |
| 1   | C     | 373 | GLU  | CD-OE1  | 15.07  | 1.42        | 1.25     |
| 1   | C     | 401 | ALA  | C-O     | 13.02  | 1.48        | 1.23     |
| 1   | A     | 40  | GLU  | CD-OE1  | 13.00  | 1.40        | 1.25     |
| 1   | C     | 254 | VAL  | CB-CG1  | 13.00  | 1.80        | 1.52     |
| 1   | C     | 146 | GLY  | N-CA    | 12.60  | 1.65        | 1.46     |
| 1   | C     | 406 | TRP  | CB-CG   | 12.46  | 1.72        | 1.50     |
| 1   | C     | 373 | GLU  | CB-CG   | 12.34  | 1.75        | 1.52     |
| 1   | C     | 130 | ARG  | CZ-NH1  | -12.17 | 1.17        | 1.33     |
| 1   | C     | 103 | MET  | CG-SD   | -12.15 | 1.49        | 1.81     |
| 1   | A     | 367 | ILE  | N-CA    | 12.14  | 1.70        | 1.46     |
| 1   | A     | 96  | TYR  | CD1-CE1 | 12.09  | 1.57        | 1.39     |
| 1   | A     | 231 | ARG  | CZ-NH2  | 11.67  | 1.48        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1   | C     | 113 | ALA  | CA-CB   | -11.54 | 1.28        | 1.52     |
| 1   | C     | 112 | ARG  | CG-CD   | 11.50  | 1.80        | 1.51     |
| 1   | C     | 369 | VAL  | CA-CB   | 11.38  | 1.78        | 1.54     |
| 1   | C     | 237 | GLU  | C-O     | 11.11  | 1.44        | 1.23     |
| 1   | A     | 240 | ARG  | CG-CD   | 11.03  | 1.79        | 1.51     |
| 1   | A     | 409 | ALA  | CA-CB   | 10.95  | 1.75        | 1.52     |
| 1   | C     | 58  | CYS  | CB-SG   | -10.94 | 1.63        | 1.82     |
| 1   | C     | 263 | PHE  | CE2-CZ  | 10.77  | 1.57        | 1.37     |
| 1   | A     | 87  | PHE  | CE1-CZ  | 10.77  | 1.57        | 1.37     |
| 1   | C     | 75  | TYR  | CG-CD2  | 10.76  | 1.53        | 1.39     |
| 1   | A     | 263 | PHE  | CB-CG   | -10.57 | 1.33        | 1.51     |
| 1   | C     | 203 | TYR  | CD2-CE2 | -10.51 | 1.23        | 1.39     |
| 1   | C     | 262 | GLU  | CD-OE1  | 10.35  | 1.37        | 1.25     |
| 1   | C     | 394 | GLY  | N-CA    | 10.35  | 1.61        | 1.46     |
| 1   | A     | 406 | TRP  | CB-CG   | 10.26  | 1.68        | 1.50     |
| 1   | A     | 374 | TRP  | CG-CD1  | 10.25  | 1.51        | 1.36     |
| 1   | C     | 99  | ILE  | CA-CB   | -10.16 | 1.31        | 1.54     |
| 1   | A     | 389 | ILE  | CB-CG2  | 10.12  | 1.84        | 1.52     |
| 1   | C     | 335 | PRO  | CB-CG   | 10.07  | 2.00        | 1.50     |
| 1   | A     | 75  | TYR  | CG-CD2  | -10.07 | 1.26        | 1.39     |
| 1   | A     | 84  | GLU  | CD-OE2  | 10.05  | 1.36        | 1.25     |
| 1   | A     | 310 | VAL  | CB-CG2  | 9.99   | 1.73        | 1.52     |
| 1   | C     | 279 | GLU  | CD-OE2  | 9.77   | 1.36        | 1.25     |
| 1   | C     | 154 | TYR  | CD1-CE1 | 9.59   | 1.53        | 1.39     |
| 1   | C     | 406 | TRP  | CE3-CZ3 | -9.59  | 1.22        | 1.38     |
| 1   | C     | 389 | ILE  | CB-CG2  | 9.59   | 1.82        | 1.52     |
| 1   | A     | 397 | SER  | CA-CB   | 9.58   | 1.67        | 1.52     |
| 1   | A     | 401 | ALA  | C-O     | -9.58  | 1.05        | 1.23     |
| 1   | C     | 291 | ARG  | N-CA    | -9.58  | 1.27        | 1.46     |
| 1   | C     | 75  | TYR  | CE2-CZ  | 9.42   | 1.50        | 1.38     |
| 1   | A     | 134 | LEU  | CG-CD1  | 9.30   | 1.86        | 1.51     |
| 1   | A     | 84  | GLU  | CB-CG   | 9.28   | 1.69        | 1.52     |
| 1   | C     | 185 | THR  | C-O     | -9.20  | 1.05        | 1.23     |
| 1   | C     | 278 | PRO  | CA-C    | -9.19  | 1.34        | 1.52     |
| 1   | A     | 98  | PHE  | CD1-CE1 | -9.18  | 1.20        | 1.39     |
| 1   | A     | 96  | TYR  | CA-C    | 9.11   | 1.76        | 1.52     |
| 1   | A     | 101 | THR  | CB-CG2  | -9.04  | 1.22        | 1.52     |
| 1   | C     | 260 | SER  | CA-CB   | 9.03   | 1.66        | 1.52     |
| 1   | A     | 253 | VAL  | CB-CG1  | 9.02   | 1.71        | 1.52     |
| 1   | A     | 81  | PHE  | CE2-CZ  | 8.87   | 1.54        | 1.37     |
| 1   | A     | 152 | GLU  | CD-OE1  | 8.85   | 1.35        | 1.25     |
| 1   | A     | 259 | PHE  | CG-CD1  | 8.84   | 1.52        | 1.38     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | C     | 111 | PHE  | CD2-CE2 | -8.78 | 1.21        | 1.39     |
| 1   | C     | 112 | ARG  | N-CA    | -8.78 | 1.28        | 1.46     |
| 1   | C     | 346 | SER  | CB-OG   | -8.77 | 1.30        | 1.42     |
| 1   | A     | 205 | ILE  | CB-CG2  | 8.74  | 1.79        | 1.52     |
| 1   | A     | 65  | ALA  | CA-CB   | 8.71  | 1.70        | 1.52     |
| 1   | C     | 90  | ARG  | C-O     | -8.70 | 1.06        | 1.23     |
| 1   | C     | 263 | PHE  | CB-CG   | -8.66 | 1.36        | 1.51     |
| 1   | A     | 172 | GLU  | CG-CD   | 8.66  | 1.65        | 1.51     |
| 1   | C     | 193 | PHE  | CG-CD1  | 8.55  | 1.51        | 1.38     |
| 1   | C     | 154 | TYR  | CD2-CE2 | 8.55  | 1.52        | 1.39     |
| 1   | A     | 264 | LEU  | CG-CD2  | 8.55  | 1.83        | 1.51     |
| 1   | C     | 350 | PHE  | CE2-CZ  | 8.54  | 1.53        | 1.37     |
| 1   | C     | 145 | GLN  | CG-CD   | -8.53 | 1.31        | 1.51     |
| 1   | A     | 257 | LEU  | CA-C    | 8.49  | 1.75        | 1.52     |
| 1   | A     | 102 | SER  | CB-OG   | 8.47  | 1.53        | 1.42     |
| 1   | A     | 231 | ARG  | CZ-NH1  | 8.43  | 1.44        | 1.33     |
| 1   | A     | 262 | GLU  | CB-CG   | 8.43  | 1.68        | 1.52     |
| 1   | C     | 154 | TYR  | CB-CG   | 8.35  | 1.64        | 1.51     |
| 1   | C     | 40  | GLU  | CB-CG   | 8.32  | 1.68        | 1.52     |
| 1   | A     | 242 | CYS  | CB-SG   | -8.31 | 1.68        | 1.82     |
| 1   | A     | 300 | ILE  | C-O     | -8.29 | 1.07        | 1.23     |
| 1   | A     | 80  | HIS  | CA-CB   | -8.29 | 1.35        | 1.53     |
| 1   | A     | 361 | HIS  | C-O     | 8.28  | 1.39        | 1.23     |
| 1   | C     | 79  | ARG  | CB-CG   | -8.27 | 1.30        | 1.52     |
| 1   | C     | 201 | TYR  | C-O     | 8.19  | 1.39        | 1.23     |
| 1   | C     | 228 | VAL  | CB-CG1  | 8.18  | 1.70        | 1.52     |
| 1   | C     | 163 | PHE  | CB-CG   | -8.15 | 1.37        | 1.51     |
| 1   | C     | 20  | GLU  | CG-CD   | -8.13 | 1.39        | 1.51     |
| 1   | C     | 131 | ILE  | CB-CG2  | 8.11  | 1.77        | 1.52     |
| 1   | A     | 345 | VAL  | CB-CG1  | -8.10 | 1.35        | 1.52     |
| 1   | A     | 168 | GLY  | N-CA    | 8.09  | 1.58        | 1.46     |
| 1   | C     | 118 | VAL  | N-CA    | 8.07  | 1.62        | 1.46     |
| 1   | A     | 253 | VAL  | CA-CB   | -8.07 | 1.37        | 1.54     |
| 1   | C     | 240 | ARG  | CB-CG   | 8.06  | 1.74        | 1.52     |
| 1   | A     | 150 | PHE  | CE1-CZ  | 8.05  | 1.52        | 1.37     |
| 1   | C     | 94  | GLU  | CB-CG   | 8.05  | 1.67        | 1.52     |
| 1   | A     | 158 | PHE  | CE2-CZ  | -8.02 | 1.22        | 1.37     |
| 1   | C     | 273 | GLU  | CD-OE1  | 8.02  | 1.34        | 1.25     |
| 1   | C     | 82  | SER  | C-O     | -8.01 | 1.08        | 1.23     |
| 1   | A     | 116 | ASN  | C-O     | 8.00  | 1.38        | 1.23     |
| 1   | C     | 401 | ALA  | CA-CB   | -8.00 | 1.35        | 1.52     |
| 1   | C     | 87  | PHE  | N-CA    | 7.97  | 1.62        | 1.46     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | C     | 265 | ALA  | C-O     | 7.93  | 1.38        | 1.23     |
| 1   | C     | 285 | CYS  | CB-SG   | 7.90  | 1.95        | 1.82     |
| 1   | C     | 403 | PRO  | C-O     | 7.88  | 1.39        | 1.23     |
| 1   | C     | 92  | ALA  | CA-CB   | 7.87  | 1.69        | 1.52     |
| 1   | A     | 228 | VAL  | CA-CB   | 7.87  | 1.71        | 1.54     |
| 1   | C     | 389 | ILE  | N-CA    | -7.86 | 1.30        | 1.46     |
| 1   | C     | 151 | THR  | C-O     | -7.84 | 1.08        | 1.23     |
| 1   | A     | 118 | VAL  | C-O     | -7.79 | 1.08        | 1.23     |
| 1   | A     | 199 | ALA  | CA-CB   | -7.79 | 1.36        | 1.52     |
| 1   | A     | 198 | GLU  | CG-CD   | 7.78  | 1.63        | 1.51     |
| 1   | A     | 94  | GLU  | CD-OE1  | 7.77  | 1.34        | 1.25     |
| 1   | A     | 54  | VAL  | CB-CG1  | 7.77  | 1.69        | 1.52     |
| 1   | A     | 228 | VAL  | C-O     | -7.76 | 1.08        | 1.23     |
| 1   | A     | 227 | GLN  | CG-CD   | -7.71 | 1.33        | 1.51     |
| 1   | A     | 385 | PRO  | CB-CG   | 7.71  | 1.88        | 1.50     |
| 1   | C     | 172 | GLU  | CG-CD   | 7.70  | 1.63        | 1.51     |
| 1   | A     | 254 | VAL  | CB-CG2  | 7.70  | 1.69        | 1.52     |
| 1   | A     | 243 | GLY  | N-CA    | -7.65 | 1.34        | 1.46     |
| 1   | A     | 287 | GLU  | CB-CG   | -7.63 | 1.37        | 1.52     |
| 1   | C     | 377 | ARG  | CG-CD   | 7.56  | 1.70        | 1.51     |
| 1   | A     | 314 | LYS  | CD-CE   | 7.56  | 1.70        | 1.51     |
| 1   | C     | 139 | ILE  | CA-CB   | 7.55  | 1.72        | 1.54     |
| 1   | A     | 346 | SER  | CB-OG   | -7.54 | 1.32        | 1.42     |
| 1   | A     | 110 | GLN  | CB-CG   | 7.51  | 1.72        | 1.52     |
| 1   | A     | 105 | PRO  | CG-CD   | 7.51  | 1.75        | 1.50     |
| 1   | C     | 85  | CYS  | C-O     | -7.50 | 1.09        | 1.23     |
| 1   | C     | 305 | TYR  | CD2-CE2 | -7.50 | 1.28        | 1.39     |
| 1   | A     | 378 | ILE  | N-CA    | 7.48  | 1.61        | 1.46     |
| 1   | A     | 205 | ILE  | N-CA    | 7.48  | 1.61        | 1.46     |
| 1   | C     | 79  | ARG  | CA-C    | -7.48 | 1.33        | 1.52     |
| 1   | C     | 273 | GLU  | CD-OE2  | 7.46  | 1.33        | 1.25     |
| 1   | A     | 139 | ILE  | CB-CG2  | 7.43  | 1.75        | 1.52     |
| 1   | A     | 366 | GLU  | CD-OE2  | -7.41 | 1.17        | 1.25     |
| 1   | A     | 10  | ASN  | CB-CG   | 7.39  | 1.68        | 1.51     |
| 1   | A     | 140 | GLU  | CD-OE1  | 7.38  | 1.33        | 1.25     |
| 1   | C     | 261 | MET  | N-CA    | -7.38 | 1.31        | 1.46     |
| 1   | A     | 284 | ALA  | CA-CB   | -7.38 | 1.36        | 1.52     |
| 1   | A     | 88  | ILE  | CA-C    | 7.36  | 1.72        | 1.52     |
| 1   | C     | 68  | GLY  | C-O     | 7.36  | 1.35        | 1.23     |
| 1   | C     | 265 | ALA  | CA-CB   | -7.35 | 1.37        | 1.52     |
| 1   | C     | 98  | PHE  | CE2-CZ  | 7.34  | 1.51        | 1.37     |
| 1   | A     | 140 | GLU  | CG-CD   | 7.34  | 1.62        | 1.51     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 259 | PHE  | CE1-CZ  | 7.33  | 1.51        | 1.37     |
| 1   | C     | 374 | TRP  | CE3-CZ3 | 7.31  | 1.50        | 1.38     |
| 1   | A     | 237 | GLU  | CD-OE1  | -7.31 | 1.17        | 1.25     |
| 1   | A     | 406 | TRP  | C-O     | 7.31  | 1.37        | 1.23     |
| 1   | C     | 325 | SER  | CB-OG   | 7.29  | 1.51        | 1.42     |
| 1   | A     | 357 | CYS  | CB-SG   | -7.29 | 1.69        | 1.82     |
| 1   | A     | 163 | PHE  | CG-CD2  | 7.27  | 1.49        | 1.38     |
| 1   | A     | 59  | ASN  | C-O     | 7.26  | 1.37        | 1.23     |
| 1   | A     | 77  | ASP  | CG-OD1  | -7.25 | 1.08        | 1.25     |
| 1   | C     | 264 | LEU  | CA-CB   | 7.24  | 1.70        | 1.53     |
| 1   | A     | 40  | GLU  | CG-CD   | -7.23 | 1.41        | 1.51     |
| 1   | C     | 248 | GLY  | N-CA    | -7.22 | 1.35        | 1.46     |
| 1   | C     | 290 | ARG  | CZ-NH2  | 7.19  | 1.42        | 1.33     |
| 1   | A     | 398 | GLY  | N-CA    | 7.15  | 1.56        | 1.46     |
| 1   | C     | 403 | PRO  | CA-C    | 7.15  | 1.67        | 1.52     |
| 1   | A     | 151 | THR  | CB-CG2  | 7.15  | 1.75        | 1.52     |
| 1   | A     | 315 | GLY  | C-O     | -7.15 | 1.12        | 1.23     |
| 1   | C     | 116 | ASN  | CB-CG   | 7.14  | 1.67        | 1.51     |
| 1   | A     | 242 | CYS  | CA-C    | 7.12  | 1.71        | 1.52     |
| 1   | A     | 43  | ALA  | C-O     | -7.10 | 1.09        | 1.23     |
| 1   | C     | 259 | PHE  | C-O     | 7.09  | 1.36        | 1.23     |
| 1   | C     | 315 | GLY  | C-O     | -7.09 | 1.12        | 1.23     |
| 1   | A     | 387 | ALA  | CA-CB   | 7.07  | 1.67        | 1.52     |
| 1   | A     | 292 | PHE  | CG-CD1  | -7.06 | 1.28        | 1.38     |
| 1   | C     | 154 | TYR  | C-O     | 7.06  | 1.36        | 1.23     |
| 1   | A     | 128 | GLU  | CG-CD   | 7.05  | 1.62        | 1.51     |
| 1   | A     | 118 | VAL  | CB-CG1  | 7.05  | 1.67        | 1.52     |
| 1   | A     | 80  | HIS  | C-O     | 7.04  | 1.36        | 1.23     |
| 1   | C     | 389 | ILE  | CA-CB   | -7.04 | 1.38        | 1.54     |
| 1   | C     | 269 | GLU  | CD-OE1  | 7.02  | 1.33        | 1.25     |
| 1   | A     | 336 | MET  | CG-SD   | 7.02  | 1.99        | 1.81     |
| 1   | A     | 193 | PHE  | CG-CD1  | -6.99 | 1.28        | 1.38     |
| 1   | C     | 363 | ALA  | CA-CB   | -6.97 | 1.37        | 1.52     |
| 1   | A     | 232 | PRO  | CG-CD   | 6.96  | 1.73        | 1.50     |
| 1   | C     | 107 | GLU  | CG-CD   | 6.94  | 1.62        | 1.51     |
| 1   | A     | 179 | TYR  | CG-CD2  | -6.94 | 1.30        | 1.39     |
| 1   | C     | 311 | GLN  | CB-CG   | 6.94  | 1.71        | 1.52     |
| 1   | A     | 283 | ALA  | N-CA    | 6.93  | 1.60        | 1.46     |
| 1   | C     | 366 | GLU  | CG-CD   | 6.93  | 1.62        | 1.51     |
| 1   | A     | 128 | GLU  | CD-OE1  | -6.93 | 1.18        | 1.25     |
| 1   | C     | 327 | LEU  | N-CA    | -6.92 | 1.32        | 1.46     |
| 1   | A     | 113 | ALA  | N-CA    | 6.90  | 1.60        | 1.46     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | A     | 44  | VAL  | CB-CG2 | 6.90  | 1.67        | 1.52     |
| 1   | C     | 130 | ARG  | C-O    | 6.89  | 1.36        | 1.23     |
| 1   | A     | 186 | ARG  | CG-CD  | 6.89  | 1.69        | 1.51     |
| 1   | C     | 250 | LEU  | C-O    | 6.89  | 1.36        | 1.23     |
| 1   | C     | 228 | VAL  | CB-CG2 | -6.89 | 1.38        | 1.52     |
| 1   | C     | 354 | SER  | N-CA   | 6.89  | 1.60        | 1.46     |
| 1   | A     | 254 | VAL  | N-CA   | -6.89 | 1.32        | 1.46     |
| 1   | A     | 203 | TYR  | CE2-CZ | -6.88 | 1.29        | 1.38     |
| 1   | A     | 392 | LYS  | CE-NZ  | 6.87  | 1.66        | 1.49     |
| 1   | A     | 258 | SER  | CB-OG  | 6.87  | 1.51        | 1.42     |
| 1   | C     | 155 | ALA  | N-CA   | 6.86  | 1.60        | 1.46     |
| 1   | C     | 90  | ARG  | CG-CD  | 6.85  | 1.69        | 1.51     |
| 1   | A     | 350 | PHE  | CG-CD1 | 6.84  | 1.49        | 1.38     |
| 1   | A     | 135 | ALA  | CA-CB  | 6.83  | 1.66        | 1.52     |
| 1   | C     | 16  | PRO  | CA-C   | -6.82 | 1.39        | 1.52     |
| 1   | A     | 66  | THR  | CA-CB  | 6.81  | 1.71        | 1.53     |
| 1   | A     | 223 | VAL  | CB-CG2 | 6.79  | 1.67        | 1.52     |
| 1   | C     | 292 | PHE  | CG-CD1 | 6.77  | 1.49        | 1.38     |
| 1   | A     | 276 | GLU  | CG-CD  | -6.75 | 1.41        | 1.51     |
| 1   | A     | 140 | GLU  | CB-CG  | -6.74 | 1.39        | 1.52     |
| 1   | A     | 107 | GLU  | CB-CG  | 6.72  | 1.65        | 1.52     |
| 1   | A     | 369 | VAL  | CB-CG1 | -6.72 | 1.38        | 1.52     |
| 1   | C     | 236 | ASP  | C-O    | -6.71 | 1.10        | 1.23     |
| 1   | A     | 57  | ARG  | CB-CG  | 6.71  | 1.70        | 1.52     |
| 1   | C     | 41  | ALA  | N-CA   | 6.70  | 1.59        | 1.46     |
| 1   | A     | 188 | ASP  | C-O    | 6.70  | 1.36        | 1.23     |
| 1   | C     | 258 | SER  | N-CA   | 6.69  | 1.59        | 1.46     |
| 1   | C     | 40  | GLU  | CD-OE2 | 6.69  | 1.33        | 1.25     |
| 1   | A     | 175 | PRO  | CG-CD  | 6.68  | 1.72        | 1.50     |
| 1   | A     | 298 | GLY  | C-O    | 6.68  | 1.34        | 1.23     |
| 1   | C     | 182 | ASP  | C-O    | 6.68  | 1.36        | 1.23     |
| 1   | A     | 276 | GLU  | CB-CG  | -6.67 | 1.39        | 1.52     |
| 1   | C     | 97  | ASP  | C-O    | 6.67  | 1.36        | 1.23     |
| 1   | C     | 240 | ARG  | CZ-NH1 | -6.67 | 1.24        | 1.33     |
| 1   | A     | 252 | THR  | C-O    | 6.65  | 1.35        | 1.23     |
| 1   | A     | 404 | LEU  | CG-CD1 | 6.64  | 1.76        | 1.51     |
| 1   | C     | 138 | LEU  | N-CA   | 6.60  | 1.59        | 1.46     |
| 1   | C     | 245 | LEU  | CA-CB  | -6.60 | 1.38        | 1.53     |
| 1   | C     | 90  | ARG  | N-CA   | 6.60  | 1.59        | 1.46     |
| 1   | C     | 225 | ASN  | C-O    | -6.60 | 1.10        | 1.23     |
| 1   | C     | 223 | VAL  | CA-CB  | -6.58 | 1.41        | 1.54     |
| 1   | C     | 276 | GLU  | CD-OE1 | 6.56  | 1.32        | 1.25     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | C     | 364 | ARG  | CG-CD   | 6.56  | 1.68        | 1.51     |
| 1   | A     | 24  | PHE  | CA-C    | 6.56  | 1.70        | 1.52     |
| 1   | A     | 179 | TYR  | CD2-CE2 | 6.53  | 1.49        | 1.39     |
| 1   | A     | 401 | ALA  | CA-CB   | 6.53  | 1.66        | 1.52     |
| 1   | C     | 159 | PRO  | C-O     | 6.51  | 1.36        | 1.23     |
| 1   | A     | 108 | GLN  | CB-CG   | -6.50 | 1.35        | 1.52     |
| 1   | A     | 310 | VAL  | CA-CB   | 6.49  | 1.68        | 1.54     |
| 1   | C     | 387 | ALA  | CA-CB   | -6.48 | 1.38        | 1.52     |
| 1   | A     | 350 | PHE  | C-O     | 6.47  | 1.35        | 1.23     |
| 1   | C     | 22  | LEU  | C-O     | 6.47  | 1.35        | 1.23     |
| 1   | C     | 131 | ILE  | CA-CB   | 6.46  | 1.69        | 1.54     |
| 1   | C     | 179 | TYR  | CE1-CZ  | 6.46  | 1.47        | 1.38     |
| 1   | A     | 338 | VAL  | C-O     | -6.46 | 1.11        | 1.23     |
| 1   | A     | 163 | PHE  | CE1-CZ  | 6.46  | 1.49        | 1.37     |
| 1   | C     | 78  | TYR  | C-O     | 6.46  | 1.35        | 1.23     |
| 1   | C     | 162 | ILE  | CB-CG2  | -6.46 | 1.32        | 1.52     |
| 1   | C     | 171 | GLU  | CD-OE2  | 6.45  | 1.32        | 1.25     |
| 1   | C     | 379 | PRO  | CG-CD   | 6.45  | 1.72        | 1.50     |
| 1   | C     | 150 | PHE  | C-O     | -6.44 | 1.11        | 1.23     |
| 1   | A     | 161 | ARG  | CZ-NH2  | 6.43  | 1.41        | 1.33     |
| 1   | C     | 196 | ALA  | CA-CB   | -6.42 | 1.39        | 1.52     |
| 1   | C     | 140 | GLU  | CD-OE2  | 6.41  | 1.32        | 1.25     |
| 1   | C     | 356 | LEU  | CB-CG   | 6.40  | 1.71        | 1.52     |
| 1   | A     | 219 | ALA  | CA-CB   | -6.39 | 1.39        | 1.52     |
| 1   | A     | 256 | PHE  | CG-CD2  | 6.39  | 1.48        | 1.38     |
| 1   | A     | 263 | PHE  | CE2-CZ  | 6.39  | 1.49        | 1.37     |
| 1   | C     | 73  | GLU  | CG-CD   | 6.39  | 1.61        | 1.51     |
| 1   | A     | 146 | GLY  | N-CA    | -6.32 | 1.36        | 1.46     |
| 1   | C     | 158 | PHE  | C-O     | 6.32  | 1.35        | 1.23     |
| 1   | C     | 197 | LYS  | CD-CE   | 6.32  | 1.67        | 1.51     |
| 1   | C     | 40  | GLU  | CG-CD   | 6.30  | 1.61        | 1.51     |
| 1   | A     | 350 | PHE  | CE2-CZ  | 6.29  | 1.49        | 1.37     |
| 1   | C     | 148 | CYS  | CB-SG   | -6.29 | 1.71        | 1.82     |
| 1   | C     | 144 | PRO  | N-CD    | -6.28 | 1.39        | 1.47     |
| 1   | C     | 231 | ARG  | CZ-NH1  | 6.27  | 1.41        | 1.33     |
| 1   | C     | 197 | LYS  | CB-CG   | 6.25  | 1.69        | 1.52     |
| 1   | C     | 307 | PHE  | C-O     | -6.25 | 1.11        | 1.23     |
| 1   | C     | 263 | PHE  | CG-CD1  | 6.24  | 1.48        | 1.38     |
| 1   | C     | 159 | PRO  | CA-CB   | 6.24  | 1.66        | 1.53     |
| 1   | C     | 356 | LEU  | CG-CD1  | 6.23  | 1.75        | 1.51     |
| 1   | C     | 296 | ALA  | CA-CB   | 6.23  | 1.65        | 1.52     |
| 1   | C     | 209 | GLU  | CD-OE1  | 6.22  | 1.32        | 1.25     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 89  | PRO  | CA-C    | 6.22  | 1.65        | 1.52     |
| 1   | C     | 18  | VAL  | CB-CG2  | 6.20  | 1.65        | 1.52     |
| 1   | A     | 406 | TRP  | CE2-CZ2 | -6.19 | 1.29        | 1.39     |
| 1   | A     | 257 | LEU  | CG-CD2  | -6.19 | 1.28        | 1.51     |
| 1   | C     | 284 | ALA  | C-O     | 6.19  | 1.35        | 1.23     |
| 1   | A     | 68  | GLY  | C-O     | 6.18  | 1.33        | 1.23     |
| 1   | A     | 155 | ALA  | CA-CB   | -6.18 | 1.39        | 1.52     |
| 1   | C     | 273 | GLU  | N-CA    | -6.17 | 1.34        | 1.46     |
| 1   | A     | 357 | CYS  | C-O     | 6.17  | 1.35        | 1.23     |
| 1   | A     | 273 | GLU  | CB-CG   | 6.16  | 1.63        | 1.52     |
| 1   | A     | 227 | GLN  | CB-CG   | -6.16 | 1.35        | 1.52     |
| 1   | A     | 314 | LYS  | CB-CG   | 6.16  | 1.69        | 1.52     |
| 1   | A     | 231 | ARG  | N-CA    | 6.15  | 1.58        | 1.46     |
| 1   | C     | 128 | GLU  | CG-CD   | 6.15  | 1.61        | 1.51     |
| 1   | C     | 55  | TRP  | CZ3-CH2 | -6.14 | 1.30        | 1.40     |
| 1   | A     | 84  | GLU  | CG-CD   | 6.14  | 1.61        | 1.51     |
| 1   | C     | 158 | PHE  | CD2-CE2 | 6.14  | 1.51        | 1.39     |
| 1   | C     | 317 | GLN  | CB-CG   | 6.13  | 1.69        | 1.52     |
| 1   | A     | 305 | TYR  | CD2-CE2 | -6.13 | 1.30        | 1.39     |
| 1   | A     | 311 | GLN  | CG-CD   | 6.12  | 1.65        | 1.51     |
| 1   | A     | 372 | LYS  | CE-NZ   | 6.12  | 1.64        | 1.49     |
| 1   | C     | 86  | PRO  | CA-C    | 6.11  | 1.65        | 1.52     |
| 1   | A     | 99  | ILE  | CA-CB   | 6.11  | 1.69        | 1.54     |
| 1   | A     | 154 | TYR  | CB-CG   | 6.11  | 1.60        | 1.51     |
| 1   | C     | 277 | ARG  | C-N     | 6.11  | 1.45        | 1.34     |
| 1   | C     | 253 | VAL  | CA-CB   | 6.09  | 1.67        | 1.54     |
| 1   | A     | 183 | GLN  | CB-CG   | 6.08  | 1.69        | 1.52     |
| 1   | C     | 338 | VAL  | N-CA    | 6.07  | 1.58        | 1.46     |
| 1   | A     | 379 | PRO  | CB-CG   | 6.06  | 1.80        | 1.50     |
| 1   | C     | 103 | MET  | CA-C    | -6.05 | 1.37        | 1.52     |
| 1   | A     | 263 | PHE  | CD1-CE1 | 6.05  | 1.51        | 1.39     |
| 1   | A     | 256 | PHE  | CE2-CZ  | -6.04 | 1.25        | 1.37     |
| 1   | C     | 80  | HIS  | CA-CB   | 6.01  | 1.67        | 1.53     |
| 1   | A     | 251 | ASP  | CB-CG   | 6.01  | 1.64        | 1.51     |
| 1   | C     | 208 | ILE  | CB-CG2  | 6.01  | 1.71        | 1.52     |
| 1   | C     | 93  | GLY  | C-O     | -5.99 | 1.14        | 1.23     |
| 1   | C     | 163 | PHE  | CE2-CZ  | -5.99 | 1.25        | 1.37     |
| 1   | A     | 75  | TYR  | CD1-CE1 | 5.98  | 1.48        | 1.39     |
| 1   | C     | 307 | PHE  | CG-CD2  | 5.98  | 1.47        | 1.38     |
| 1   | C     | 388 | GLN  | CB-CG   | 5.97  | 1.68        | 1.52     |
| 1   | A     | 160 | ILE  | CB-CG2  | -5.96 | 1.34        | 1.52     |
| 1   | A     | 87  | PHE  | CG-CD2  | 5.96  | 1.47        | 1.38     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | C     | 305 | TYR  | CG-CD1  | 5.95  | 1.46        | 1.39     |
| 1   | A     | 307 | PHE  | C-O     | -5.95 | 1.12        | 1.23     |
| 1   | C     | 253 | VAL  | CB-CG1  | 5.95  | 1.65        | 1.52     |
| 1   | C     | 135 | ALA  | CA-CB   | 5.95  | 1.65        | 1.52     |
| 1   | C     | 365 | ARG  | CZ-NH2  | -5.95 | 1.25        | 1.33     |
| 1   | A     | 118 | VAL  | N-CA    | -5.94 | 1.34        | 1.46     |
| 1   | C     | 98  | PHE  | CE1-CZ  | 5.94  | 1.48        | 1.37     |
| 1   | A     | 151 | THR  | N-CA    | 5.92  | 1.58        | 1.46     |
| 1   | C     | 279 | GLU  | CG-CD   | 5.92  | 1.60        | 1.51     |
| 1   | A     | 71  | ILE  | C-O     | 5.92  | 1.34        | 1.23     |
| 1   | C     | 203 | TYR  | CD1-CE1 | -5.91 | 1.30        | 1.39     |
| 1   | A     | 106 | PRO  | C-O     | 5.91  | 1.35        | 1.23     |
| 1   | C     | 286 | GLU  | CB-CG   | 5.91  | 1.63        | 1.52     |
| 1   | A     | 333 | ALA  | N-CA    | 5.91  | 1.58        | 1.46     |
| 1   | C     | 112 | ARG  | CZ-NH1  | 5.91  | 1.40        | 1.33     |
| 1   | A     | 145 | GLN  | CD-NE2  | 5.89  | 1.47        | 1.32     |
| 1   | A     | 402 | LEU  | CA-CB   | 5.88  | 1.67        | 1.53     |
| 1   | C     | 156 | GLU  | C-O     | 5.88  | 1.34        | 1.23     |
| 1   | C     | 90  | ARG  | CB-CG   | 5.88  | 1.68        | 1.52     |
| 1   | C     | 102 | SER  | CB-OG   | 5.86  | 1.49        | 1.42     |
| 1   | C     | 132 | GLN  | C-O     | 5.85  | 1.34        | 1.23     |
| 1   | A     | 103 | MET  | N-CA    | 5.85  | 1.58        | 1.46     |
| 1   | A     | 380 | ASP  | N-CA    | -5.85 | 1.34        | 1.46     |
| 1   | A     | 47  | GLU  | CG-CD   | 5.84  | 1.60        | 1.51     |
| 1   | A     | 81  | PHE  | N-CA    | 5.82  | 1.57        | 1.46     |
| 1   | C     | 104 | ASP  | N-CA    | 5.81  | 1.57        | 1.46     |
| 1   | A     | 76  | GLU  | CD-OE1  | 5.81  | 1.32        | 1.25     |
| 1   | C     | 34  | LEU  | CG-CD1  | 5.80  | 1.73        | 1.51     |
| 1   | A     | 203 | TYR  | CD2-CE2 | -5.79 | 1.30        | 1.39     |
| 1   | C     | 104 | ASP  | CB-CG   | 5.79  | 1.64        | 1.51     |
| 1   | C     | 28  | MET  | CA-C    | 5.78  | 1.68        | 1.52     |
| 1   | A     | 29  | TYR  | CD2-CE2 | 5.77  | 1.48        | 1.39     |
| 1   | A     | 96  | TYR  | C-O     | 5.77  | 1.34        | 1.23     |
| 1   | C     | 168 | GLY  | N-CA    | 5.77  | 1.54        | 1.46     |
| 1   | C     | 362 | LEU  | C-N     | -5.77 | 1.20        | 1.34     |
| 1   | A     | 250 | LEU  | CG-CD1  | 5.76  | 1.73        | 1.51     |
| 1   | A     | 280 | ARG  | CA-C    | 5.76  | 1.68        | 1.52     |
| 1   | A     | 125 | ASP  | CA-C    | -5.76 | 1.38        | 1.52     |
| 1   | A     | 163 | PHE  | CB-CG   | -5.75 | 1.41        | 1.51     |
| 1   | A     | 101 | THR  | C-O     | 5.74  | 1.34        | 1.23     |
| 1   | A     | 178 | LYS  | CE-NZ   | 5.74  | 1.63        | 1.49     |
| 1   | C     | 239 | LYS  | CE-NZ   | 5.74  | 1.63        | 1.49     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 406 | TRP  | CE3-CZ3 | -5.73 | 1.28        | 1.38     |
| 1   | A     | 307 | PHE  | CE2-CZ  | 5.73  | 1.48        | 1.37     |
| 1   | A     | 83  | SER  | CB-OG   | 5.72  | 1.49        | 1.42     |
| 1   | C     | 159 | PRO  | CG-CD   | 5.72  | 1.69        | 1.50     |
| 1   | A     | 178 | LYS  | CD-CE   | 5.71  | 1.65        | 1.51     |
| 1   | A     | 55  | TRP  | CE3-CZ3 | -5.71 | 1.28        | 1.38     |
| 1   | C     | 367 | ILE  | CB-CG2  | 5.71  | 1.70        | 1.52     |
| 1   | C     | 365 | ARG  | N-CA    | 5.70  | 1.57        | 1.46     |
| 1   | A     | 184 | MET  | CG-SD   | -5.68 | 1.66        | 1.81     |
| 1   | C     | 133 | GLU  | CG-CD   | 5.68  | 1.60        | 1.51     |
| 1   | A     | 387 | ALA  | C-O     | 5.67  | 1.34        | 1.23     |
| 1   | C     | 335 | PRO  | N-CA    | 5.67  | 1.56        | 1.47     |
| 1   | A     | 305 | TYR  | C-O     | 5.66  | 1.34        | 1.23     |
| 1   | A     | 149 | ASN  | CB-CG   | 5.65  | 1.64        | 1.51     |
| 1   | C     | 366 | GLU  | CD-OE2  | 5.64  | 1.31        | 1.25     |
| 1   | A     | 360 | GLN  | CB-CG   | 5.64  | 1.67        | 1.52     |
| 1   | C     | 359 | GLY  | N-CA    | 5.64  | 1.54        | 1.46     |
| 1   | C     | 314 | LYS  | CD-CE   | 5.63  | 1.65        | 1.51     |
| 1   | A     | 111 | PHE  | CB-CG   | 5.62  | 1.60        | 1.51     |
| 1   | C     | 179 | TYR  | CD2-CE2 | -5.62 | 1.30        | 1.39     |
| 1   | C     | 179 | TYR  | CG-CD1  | 5.61  | 1.46        | 1.39     |
| 1   | A     | 107 | GLU  | CG-CD   | -5.61 | 1.43        | 1.51     |
| 1   | A     | 340 | PHE  | CB-CG   | 5.60  | 1.60        | 1.51     |
| 1   | C     | 150 | PHE  | CD1-CE1 | 5.60  | 1.50        | 1.39     |
| 1   | C     | 342 | ARG  | CG-CD   | 5.60  | 1.66        | 1.51     |
| 1   | C     | 78  | TYR  | CA-C    | 5.60  | 1.67        | 1.52     |
| 1   | A     | 373 | GLU  | CB-CG   | -5.59 | 1.41        | 1.52     |
| 1   | C     | 204 | LEU  | N-CA    | -5.59 | 1.35        | 1.46     |
| 1   | A     | 356 | LEU  | CG-CD1  | 5.59  | 1.72        | 1.51     |
| 1   | C     | 79  | ARG  | CG-CD   | 5.58  | 1.66        | 1.51     |
| 1   | A     | 259 | PHE  | CA-CB   | -5.58 | 1.41        | 1.53     |
| 1   | C     | 86  | PRO  | CG-CD   | 5.57  | 1.69        | 1.50     |
| 1   | A     | 235 | SER  | CB-OG   | 5.56  | 1.49        | 1.42     |
| 1   | A     | 405 | VAL  | CA-CB   | 5.56  | 1.66        | 1.54     |
| 1   | A     | 106 | PRO  | CB-CG   | 5.55  | 1.77        | 1.50     |
| 1   | C     | 165 | LEU  | CG-CD2  | 5.53  | 1.72        | 1.51     |
| 1   | C     | 401 | ALA  | N-CA    | -5.53 | 1.35        | 1.46     |
| 1   | C     | 256 | PHE  | CD2-CE2 | 5.52  | 1.50        | 1.39     |
| 1   | C     | 186 | ARG  | CG-CD   | -5.51 | 1.38        | 1.51     |
| 1   | A     | 247 | VAL  | N-CA    | 5.50  | 1.57        | 1.46     |
| 1   | A     | 256 | PHE  | C-O     | 5.50  | 1.33        | 1.23     |
| 1   | A     | 266 | LYS  | N-CA    | 5.50  | 1.57        | 1.46     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | C     | 86  | PRO  | N-CA   | -5.49 | 1.38        | 1.47     |
| 1   | A     | 193 | PHE  | CB-CG  | -5.49 | 1.42        | 1.51     |
| 1   | C     | 89  | PRO  | N-CA   | 5.49  | 1.56        | 1.47     |
| 1   | C     | 153 | ASP  | CB-CG  | 5.48  | 1.63        | 1.51     |
| 1   | C     | 202 | ASP  | CB-CG  | 5.48  | 1.63        | 1.51     |
| 1   | C     | 103 | MET  | N-CA   | 5.47  | 1.57        | 1.46     |
| 1   | C     | 279 | GLU  | CB-CG  | 5.47  | 1.62        | 1.52     |
| 1   | A     | 157 | PRO  | C-O    | -5.46 | 1.12        | 1.23     |
| 1   | A     | 195 | GLU  | CD-OE1 | 5.46  | 1.31        | 1.25     |
| 1   | A     | 237 | GLU  | CG-CD  | -5.46 | 1.43        | 1.51     |
| 1   | A     | 359 | GLY  | N-CA   | 5.46  | 1.54        | 1.46     |
| 1   | A     | 141 | SER  | C-O    | 5.46  | 1.33        | 1.23     |
| 1   | C     | 285 | CYS  | CA-CB  | 5.46  | 1.66        | 1.53     |
| 1   | A     | 392 | LYS  | CD-CE  | 5.45  | 1.64        | 1.51     |
| 1   | C     | 175 | PRO  | CA-C   | 5.44  | 1.63        | 1.52     |
| 1   | C     | 19  | PRO  | N-CA   | -5.44 | 1.38        | 1.47     |
| 1   | A     | 154 | TYR  | CE1-CZ | 5.44  | 1.45        | 1.38     |
| 1   | A     | 108 | GLN  | CA-C   | -5.43 | 1.38        | 1.52     |
| 1   | C     | 350 | PHE  | CE1-CZ | 5.43  | 1.47        | 1.37     |
| 1   | C     | 265 | ALA  | N-CA   | 5.43  | 1.57        | 1.46     |
| 1   | C     | 277 | ARG  | N-CA   | -5.43 | 1.35        | 1.46     |
| 1   | A     | 172 | GLU  | CD-OE1 | 5.43  | 1.31        | 1.25     |
| 1   | C     | 398 | GLY  | N-CA   | 5.42  | 1.54        | 1.46     |
| 1   | C     | 175 | PRO  | C-O    | 5.42  | 1.34        | 1.23     |
| 1   | A     | 18  | VAL  | CB-CG2 | 5.42  | 1.64        | 1.52     |
| 1   | A     | 40  | GLU  | CD-OE2 | 5.41  | 1.31        | 1.25     |
| 1   | C     | 304 | ASP  | CB-CG  | -5.40 | 1.40        | 1.51     |
| 1   | A     | 279 | GLU  | CG-CD  | -5.40 | 1.43        | 1.51     |
| 1   | C     | 225 | ASN  | C-N    | -5.39 | 1.23        | 1.33     |
| 1   | A     | 269 | GLU  | CD-OE1 | 5.39  | 1.31        | 1.25     |
| 1   | C     | 340 | PHE  | C-O    | -5.39 | 1.13        | 1.23     |
| 1   | A     | 72  | ARG  | CB-CG  | 5.39  | 1.67        | 1.52     |
| 1   | C     | 61  | GLY  | CA-C   | -5.39 | 1.43        | 1.51     |
| 1   | C     | 84  | GLU  | CA-C   | 5.39  | 1.67        | 1.52     |
| 1   | C     | 263 | PHE  | C-O    | -5.38 | 1.13        | 1.23     |
| 1   | A     | 385 | PRO  | C-O    | 5.38  | 1.34        | 1.23     |
| 1   | C     | 274 | LEU  | CG-CD2 | 5.38  | 1.71        | 1.51     |
| 1   | C     | 108 | GLN  | CB-CG  | -5.38 | 1.38        | 1.52     |
| 1   | C     | 84  | GLU  | CB-CG  | 5.38  | 1.62        | 1.52     |
| 1   | A     | 240 | ARG  | CZ-NH2 | 5.37  | 1.40        | 1.33     |
| 1   | A     | 244 | ALA  | C-O    | 5.37  | 1.33        | 1.23     |
| 1   | C     | 246 | LEU  | N-CA   | 5.37  | 1.57        | 1.46     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | C     | 397 | SER  | C-O     | 5.36  | 1.33        | 1.23     |
| 1   | C     | 220 | ILE  | N-CA    | 5.36  | 1.57        | 1.46     |
| 1   | A     | 228 | VAL  | CA-C    | -5.35 | 1.39        | 1.52     |
| 1   | A     | 26  | PHE  | CE2-CZ  | 5.35  | 1.47        | 1.37     |
| 1   | A     | 124 | VAL  | CB-CG2  | -5.35 | 1.41        | 1.52     |
| 1   | A     | 127 | LEU  | CG-CD2  | 5.35  | 1.71        | 1.51     |
| 1   | A     | 132 | GLN  | CB-CG   | 5.35  | 1.67        | 1.52     |
| 1   | C     | 47  | GLU  | CD-OE1  | 5.35  | 1.31        | 1.25     |
| 1   | C     | 133 | GLU  | CD-OE1  | 5.34  | 1.31        | 1.25     |
| 1   | A     | 150 | PHE  | CD2-CE2 | 5.34  | 1.50        | 1.39     |
| 1   | A     | 382 | SER  | CA-CB   | 5.34  | 1.60        | 1.52     |
| 1   | C     | 61  | GLY  | C-O     | -5.34 | 1.15        | 1.23     |
| 1   | A     | 402 | LEU  | CB-CG   | 5.33  | 1.68        | 1.52     |
| 1   | A     | 244 | ALA  | CA-CB   | -5.33 | 1.41        | 1.52     |
| 1   | C     | 188 | ASP  | C-O     | 5.33  | 1.33        | 1.23     |
| 1   | A     | 147 | GLN  | CB-CG   | -5.33 | 1.38        | 1.52     |
| 1   | C     | 301 | LEU  | CA-C    | 5.33  | 1.66        | 1.52     |
| 1   | A     | 227 | GLN  | CA-CB   | -5.33 | 1.42        | 1.53     |
| 1   | A     | 313 | LYS  | CB-CG   | 5.32  | 1.67        | 1.52     |
| 1   | C     | 302 | THR  | C-O     | 5.32  | 1.33        | 1.23     |
| 1   | A     | 323 | MET  | CB-CG   | 5.32  | 1.68        | 1.51     |
| 1   | C     | 234 | THR  | CA-CB   | 5.32  | 1.67        | 1.53     |
| 1   | A     | 337 | HIS  | CA-CB   | 5.32  | 1.65        | 1.53     |
| 1   | C     | 243 | GLY  | C-O     | -5.32 | 1.15        | 1.23     |
| 1   | A     | 221 | SER  | CB-OG   | -5.31 | 1.35        | 1.42     |
| 1   | C     | 42  | TRP  | CG-CD1  | -5.31 | 1.29        | 1.36     |
| 1   | A     | 409 | ALA  | CA-C    | 5.31  | 1.66        | 1.52     |
| 1   | C     | 147 | GLN  | CG-CD   | 5.31  | 1.63        | 1.51     |
| 1   | C     | 286 | GLU  | CG-CD   | 5.31  | 1.59        | 1.51     |
| 1   | C     | 385 | PRO  | C-O     | 5.31  | 1.33        | 1.23     |
| 1   | C     | 143 | ARG  | CG-CD   | 5.30  | 1.65        | 1.51     |
| 1   | A     | 372 | LYS  | CG-CD   | 5.30  | 1.70        | 1.52     |
| 1   | A     | 316 | ASP  | CB-CG   | -5.29 | 1.40        | 1.51     |
| 1   | C     | 20  | GLU  | CD-OE1  | 5.28  | 1.31        | 1.25     |
| 1   | A     | 98  | PHE  | CE1-CZ  | 5.28  | 1.47        | 1.37     |
| 1   | C     | 181 | THR  | CB-CG2  | 5.28  | 1.69        | 1.52     |
| 1   | C     | 27  | ASP  | CB-CG   | 5.27  | 1.62        | 1.51     |
| 1   | C     | 75  | TYR  | CD1-CE1 | -5.27 | 1.31        | 1.39     |
| 1   | C     | 47  | GLU  | CG-CD   | 5.27  | 1.59        | 1.51     |
| 1   | A     | 78  | TYR  | CE1-CZ  | 5.26  | 1.45        | 1.38     |
| 1   | C     | 372 | LYS  | C-O     | 5.26  | 1.33        | 1.23     |
| 1   | C     | 295 | VAL  | CB-CG2  | 5.25  | 1.63        | 1.52     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 377 | ARG  | C-O     | 5.25  | 1.33        | 1.23     |
| 1   | C     | 237 | GLU  | CA-CB   | -5.24 | 1.42        | 1.53     |
| 1   | C     | 269 | GLU  | CB-CG   | -5.23 | 1.42        | 1.52     |
| 1   | C     | 331 | GLU  | C-O     | 5.23  | 1.33        | 1.23     |
| 1   | A     | 67  | ARG  | N-CA    | 5.23  | 1.56        | 1.46     |
| 1   | C     | 206 | PRO  | C-O     | -5.22 | 1.12        | 1.23     |
| 1   | A     | 262 | GLU  | N-CA    | -5.22 | 1.35        | 1.46     |
| 1   | A     | 81  | PHE  | CG-CD2  | 5.22  | 1.46        | 1.38     |
| 1   | C     | 43  | ALA  | CA-CB   | -5.22 | 1.41        | 1.52     |
| 1   | C     | 84  | GLU  | CD-OE1  | -5.21 | 1.20        | 1.25     |
| 1   | C     | 292 | PHE  | CE1-CZ  | 5.21  | 1.47        | 1.37     |
| 1   | C     | 88  | ILE  | C-N     | 5.21  | 1.44        | 1.34     |
| 1   | C     | 292 | PHE  | CA-C    | 5.20  | 1.66        | 1.52     |
| 1   | A     | 264 | LEU  | C-O     | 5.19  | 1.33        | 1.23     |
| 1   | C     | 237 | GLU  | CG-CD   | -5.19 | 1.44        | 1.51     |
| 1   | A     | 111 | PHE  | N-CA    | -5.19 | 1.35        | 1.46     |
| 1   | A     | 299 | ARG  | CZ-NH1  | 5.19  | 1.39        | 1.33     |
| 1   | A     | 316 | ASP  | N-CA    | 5.19  | 1.56        | 1.46     |
| 1   | A     | 346 | SER  | C-O     | -5.18 | 1.13        | 1.23     |
| 1   | A     | 296 | ALA  | C-O     | -5.18 | 1.13        | 1.23     |
| 1   | C     | 124 | VAL  | CB-CG2  | 5.18  | 1.63        | 1.52     |
| 1   | C     | 150 | PHE  | CD2-CE2 | 5.18  | 1.49        | 1.39     |
| 1   | C     | 54  | VAL  | CB-CG2  | -5.17 | 1.42        | 1.52     |
| 1   | C     | 113 | ALA  | C-O     | 5.17  | 1.33        | 1.23     |
| 1   | A     | 65  | ALA  | C-O     | 5.17  | 1.33        | 1.23     |
| 1   | A     | 311 | GLN  | CB-CG   | 5.17  | 1.66        | 1.52     |
| 1   | C     | 98  | PHE  | CG-CD1  | 5.17  | 1.46        | 1.38     |
| 1   | A     | 25  | ASP  | CB-CG   | 5.16  | 1.62        | 1.51     |
| 1   | A     | 254 | VAL  | CA-C    | -5.16 | 1.39        | 1.52     |
| 1   | C     | 119 | VAL  | CB-CG1  | 5.16  | 1.63        | 1.52     |
| 1   | A     | 192 | THR  | N-CA    | 5.16  | 1.56        | 1.46     |
| 1   | C     | 364 | ARG  | CZ-NH2  | -5.16 | 1.26        | 1.33     |
| 1   | A     | 276 | GLU  | CA-CB   | -5.16 | 1.42        | 1.53     |
| 1   | C     | 114 | LEU  | N-CA    | 5.16  | 1.56        | 1.46     |
| 1   | A     | 36  | ALA  | CA-CB   | 5.15  | 1.63        | 1.52     |
| 1   | A     | 342 | ARG  | CA-C    | -5.15 | 1.39        | 1.52     |
| 1   | C     | 367 | ILE  | C-O     | -5.15 | 1.13        | 1.23     |
| 1   | C     | 147 | GLN  | CD-OE1  | -5.14 | 1.12        | 1.24     |
| 1   | A     | 79  | ARG  | C-O     | -5.14 | 1.13        | 1.23     |
| 1   | C     | 202 | ASP  | C-O     | 5.14  | 1.33        | 1.23     |
| 1   | A     | 112 | ARG  | C-O     | 5.14  | 1.33        | 1.23     |
| 1   | C     | 257 | LEU  | C-O     | 5.12  | 1.33        | 1.23     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 227 | GLN  | C-O     | 5.12  | 1.33        | 1.23     |
| 1   | A     | 110 | GLN  | C-O     | 5.11  | 1.33        | 1.23     |
| 1   | A     | 384 | ALA  | CA-CB   | 5.11  | 1.63        | 1.52     |
| 1   | C     | 66  | THR  | CB-CG2  | -5.11 | 1.35        | 1.52     |
| 1   | A     | 157 | PRO  | N-CA    | 5.11  | 1.55        | 1.47     |
| 1   | C     | 259 | PHE  | CG-CD2  | -5.11 | 1.31        | 1.38     |
| 1   | C     | 181 | THR  | CA-CB   | -5.11 | 1.40        | 1.53     |
| 1   | A     | 377 | ARG  | CZ-NH2  | 5.10  | 1.39        | 1.33     |
| 1   | C     | 39  | GLN  | C-O     | 5.10  | 1.33        | 1.23     |
| 1   | C     | 408 | PRO  | CA-C    | 5.10  | 1.63        | 1.52     |
| 1   | C     | 73  | GLU  | CB-CG   | 5.09  | 1.61        | 1.52     |
| 1   | A     | 266 | LYS  | C-O     | 5.09  | 1.33        | 1.23     |
| 1   | C     | 179 | TYR  | CG-CD2  | 5.08  | 1.45        | 1.39     |
| 1   | C     | 206 | PRO  | N-CA    | -5.08 | 1.38        | 1.47     |
| 1   | C     | 377 | ARG  | CA-C    | 5.08  | 1.66        | 1.52     |
| 1   | A     | 201 | TYR  | CB-CG   | 5.07  | 1.59        | 1.51     |
| 1   | C     | 129 | ASN  | N-CA    | -5.07 | 1.36        | 1.46     |
| 1   | C     | 42  | TRP  | CA-C    | -5.07 | 1.39        | 1.52     |
| 1   | C     | 132 | GLN  | CD-OE1  | 5.07  | 1.35        | 1.24     |
| 1   | A     | 67  | ARG  | CZ-NH1  | 5.07  | 1.39        | 1.33     |
| 1   | C     | 199 | ALA  | CA-CB   | -5.06 | 1.41        | 1.52     |
| 1   | A     | 169 | LEU  | C-O     | -5.06 | 1.13        | 1.23     |
| 1   | A     | 410 | THR  | N-CA    | 5.05  | 1.56        | 1.46     |
| 1   | C     | 409 | ALA  | C-O     | 5.05  | 1.32        | 1.23     |
| 1   | A     | 348 | THR  | N-CA    | -5.05 | 1.36        | 1.46     |
| 1   | C     | 152 | GLU  | CD-OE2  | 5.05  | 1.31        | 1.25     |
| 1   | C     | 348 | THR  | C-O     | 5.05  | 1.32        | 1.23     |
| 1   | A     | 289 | LEU  | CG-CD2  | 5.05  | 1.70        | 1.51     |
| 1   | A     | 176 | HIS  | C-O     | 5.04  | 1.32        | 1.23     |
| 1   | A     | 50  | VAL  | CB-CG2  | 5.04  | 1.63        | 1.52     |
| 1   | C     | 205 | ILE  | N-CA    | -5.04 | 1.36        | 1.46     |
| 1   | C     | 290 | ARG  | CZ-NH1  | 5.04  | 1.39        | 1.33     |
| 1   | A     | 135 | ALA  | C-O     | -5.04 | 1.13        | 1.23     |
| 1   | A     | 192 | THR  | C-O     | 5.04  | 1.32        | 1.23     |
| 1   | A     | 195 | GLU  | CG-CD   | -5.04 | 1.44        | 1.51     |
| 1   | A     | 50  | VAL  | CA-CB   | -5.04 | 1.44        | 1.54     |
| 1   | C     | 72  | ARG  | CZ-NH2  | -5.03 | 1.26        | 1.33     |
| 1   | A     | 81  | PHE  | CD1-CE1 | 5.03  | 1.49        | 1.39     |
| 1   | A     | 262 | GLU  | CD-OE1  | -5.03 | 1.20        | 1.25     |
| 1   | C     | 76  | GLU  | CG-CD   | 5.03  | 1.59        | 1.51     |
| 1   | A     | 83  | SER  | N-CA    | 5.02  | 1.56        | 1.46     |
| 1   | A     | 101 | THR  | CB-OG1  | -5.02 | 1.33        | 1.43     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | A     | 104 | ASP  | C-O    | -5.02 | 1.13        | 1.23     |
| 1   | C     | 109 | ARG  | CZ-NH2 | 5.02  | 1.39        | 1.33     |
| 1   | C     | 86  | PRO  | N-CD   | 5.02  | 1.54        | 1.47     |
| 1   | C     | 110 | GLN  | CG-CD  | 5.02  | 1.62        | 1.51     |
| 1   | C     | 205 | ILE  | CA-C   | 5.01  | 1.66        | 1.52     |
| 1   | C     | 306 | GLU  | C-O    | -5.01 | 1.13        | 1.23     |
| 1   | C     | 227 | GLN  | C-O    | 5.00  | 1.32        | 1.23     |

All (353) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 1   | C     | 290 | ARG  | NE-CZ-NH1  | -24.41 | 108.09      | 120.30   |
| 1   | C     | 130 | ARG  | NE-CZ-NH1  | -23.85 | 108.37      | 120.30   |
| 1   | A     | 77  | ASP  | CB-CG-OD2  | 20.89  | 137.10      | 118.30   |
| 1   | C     | 130 | ARG  | NE-CZ-NH2  | 20.79  | 130.70      | 120.30   |
| 1   | C     | 377 | ARG  | NE-CZ-NH1  | -19.19 | 110.70      | 120.30   |
| 1   | C     | 112 | ARG  | NE-CZ-NH1  | 16.40  | 128.50      | 120.30   |
| 1   | C     | 112 | ARG  | NE-CZ-NH2  | -15.12 | 112.74      | 120.30   |
| 1   | C     | 188 | ASP  | CB-CG-OD2  | -14.79 | 104.99      | 118.30   |
| 1   | A     | 151 | THR  | CA-CB-CG2  | -14.36 | 92.29       | 112.40   |
| 1   | C     | 299 | ARG  | NE-CZ-NH2  | -14.35 | 113.12      | 120.30   |
| 1   | A     | 184 | MET  | CG-SD-CE   | -13.84 | 78.06       | 100.20   |
| 1   | A     | 72  | ARG  | NE-CZ-NH1  | -13.17 | 113.72      | 120.30   |
| 1   | C     | 231 | ARG  | NE-CZ-NH2  | -13.06 | 113.77      | 120.30   |
| 1   | C     | 299 | ARG  | NE-CZ-NH1  | 12.88  | 126.74      | 120.30   |
| 1   | C     | 290 | ARG  | NE-CZ-NH2  | 12.56  | 126.58      | 120.30   |
| 1   | A     | 371 | LEU  | CB-CG-CD2  | -12.54 | 89.68       | 111.00   |
| 1   | C     | 280 | ARG  | NE-CZ-NH2  | -12.07 | 114.27      | 120.30   |
| 1   | C     | 304 | ASP  | CB-CG-OD1  | -12.01 | 107.49      | 118.30   |
| 1   | C     | 231 | ARG  | NE-CZ-NH1  | 11.91  | 126.26      | 120.30   |
| 1   | C     | 72  | ARG  | NE-CZ-NH2  | -11.51 | 114.55      | 120.30   |
| 1   | C     | 356 | LEU  | CB-CG-CD1  | 11.21  | 130.06      | 111.00   |
| 1   | C     | 364 | ARG  | NE-CZ-NH2  | 11.10  | 125.85      | 120.30   |
| 1   | C     | 99  | ILE  | CG1-CB-CG2 | 10.98  | 135.56      | 111.40   |
| 1   | A     | 299 | ARG  | NE-CZ-NH2  | -10.93 | 114.83      | 120.30   |
| 1   | C     | 327 | LEU  | CB-CG-CD1  | -10.69 | 92.83       | 111.00   |
| 1   | C     | 240 | ARG  | NE-CZ-NH1  | -10.40 | 115.10      | 120.30   |
| 1   | C     | 316 | ASP  | CB-CG-OD2  | -10.32 | 109.01      | 118.30   |
| 1   | A     | 67  | ARG  | NE-CZ-NH1  | 10.32  | 125.46      | 120.30   |
| 1   | C     | 143 | ARG  | C-N-CD     | 9.99   | 149.39      | 128.40   |
| 1   | C     | 143 | ARG  | CB-CG-CD   | -9.90  | 85.86       | 111.60   |
| 1   | C     | 260 | SER  | N-CA-CB    | 9.81   | 125.22      | 110.50   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | C     | 257 | LEU  | CB-CG-CD1  | 9.77  | 127.62      | 111.00   |
| 1   | C     | 291 | ARG  | NE-CZ-NH2  | 9.73  | 125.17      | 120.30   |
| 1   | A     | 377 | ARG  | NE-CZ-NH1  | -9.73 | 115.44      | 120.30   |
| 1   | C     | 304 | ASP  | CB-CG-OD2  | 9.71  | 127.03      | 118.30   |
| 1   | A     | 254 | VAL  | CB-CA-C    | -9.68 | 93.00       | 111.40   |
| 1   | A     | 163 | PHE  | CZ-CE2-CD2 | -9.44 | 108.77      | 120.10   |
| 1   | A     | 205 | ILE  | CG1-CB-CG2 | 9.41  | 132.10      | 111.40   |
| 1   | A     | 90  | ARG  | NE-CZ-NH2  | -9.41 | 115.59      | 120.30   |
| 1   | C     | 369 | VAL  | CG1-CB-CG2 | -9.33 | 95.97       | 110.90   |
| 1   | C     | 404 | LEU  | CB-CG-CD2  | 9.22  | 126.67      | 111.00   |
| 1   | A     | 339 | ASP  | CB-CG-OD2  | -9.21 | 110.01      | 118.30   |
| 1   | C     | 67  | ARG  | NE-CZ-NH1  | 9.19  | 124.90      | 120.30   |
| 1   | C     | 364 | ARG  | NE-CZ-NH1  | -9.10 | 115.75      | 120.30   |
| 1   | C     | 165 | LEU  | CB-CG-CD2  | 9.09  | 126.46      | 111.00   |
| 1   | A     | 70  | LEU  | CA-CB-CG   | 9.05  | 136.12      | 115.30   |
| 1   | C     | 118 | VAL  | CG1-CB-CG2 | -8.97 | 96.55       | 110.90   |
| 1   | A     | 134 | LEU  | CB-CA-C    | -8.95 | 93.20       | 110.20   |
| 1   | C     | 11  | LEU  | CB-CG-CD1  | -8.95 | 95.79       | 111.00   |
| 1   | A     | 236 | ASP  | CB-CG-OD1  | -8.81 | 110.37      | 118.30   |
| 1   | A     | 142 | LEU  | CD1-CG-CD2 | -8.78 | 84.15       | 110.50   |
| 1   | A     | 280 | ARG  | CG-CD-NE   | -8.78 | 93.35       | 111.80   |
| 1   | A     | 52  | ASP  | CB-CG-OD2  | -8.78 | 110.40      | 118.30   |
| 1   | C     | 82  | SER  | N-CA-CB    | -8.66 | 97.51       | 110.50   |
| 1   | A     | 297 | ASP  | CB-CG-OD2  | -8.65 | 110.52      | 118.30   |
| 1   | C     | 280 | ARG  | NE-CZ-NH1  | 8.61  | 124.60      | 120.30   |
| 1   | C     | 105 | PRO  | C-N-CD     | -8.61 | 101.67      | 120.60   |
| 1   | A     | 174 | ILE  | C-N-CD     | 8.58  | 146.42      | 128.40   |
| 1   | A     | 134 | LEU  | CB-CG-CD1  | 8.56  | 125.55      | 111.00   |
| 1   | A     | 123 | VAL  | CG1-CB-CG2 | -8.54 | 97.24       | 110.90   |
| 1   | A     | 245 | LEU  | CA-CB-CG   | 8.49  | 134.84      | 115.30   |
| 1   | A     | 251 | ASP  | CB-CG-OD2  | 8.45  | 125.91      | 118.30   |
| 1   | A     | 312 | LEU  | CB-CG-CD2  | -8.43 | 96.67       | 111.00   |
| 1   | A     | 316 | ASP  | CB-CG-OD2  | -8.32 | 110.81      | 118.30   |
| 1   | C     | 188 | ASP  | N-CA-CB    | -8.28 | 95.70       | 110.60   |
| 1   | C     | 330 | ARG  | NE-CZ-NH2  | -8.28 | 116.16      | 120.30   |
| 1   | C     | 402 | LEU  | CA-CB-CG   | 8.25  | 134.28      | 115.30   |
| 1   | A     | 67  | ARG  | NE-CZ-NH2  | -8.24 | 116.18      | 120.30   |
| 1   | A     | 177 | LEU  | CB-CG-CD1  | -8.19 | 97.07       | 111.00   |
| 1   | A     | 365 | ARG  | NE-CZ-NH1  | -8.13 | 116.23      | 120.30   |
| 1   | C     | 371 | LEU  | CA-CB-CG   | 8.12  | 133.98      | 115.30   |
| 1   | C     | 111 | PHE  | C-N-CA     | -8.08 | 101.51      | 121.70   |
| 1   | C     | 200 | LEU  | CB-CG-CD2  | -8.07 | 97.28       | 111.00   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | C     | 211 | ARG  | CA-CB-CG   | 8.01  | 131.01      | 113.40   |
| 1   | A     | 240 | ARG  | NE-CZ-NH1  | -7.99 | 116.31      | 120.30   |
| 1   | C     | 142 | LEU  | CB-CG-CD1  | 7.94  | 124.50      | 111.00   |
| 1   | A     | 211 | ARG  | NE-CZ-NH1  | -7.91 | 116.34      | 120.30   |
| 1   | C     | 96  | TYR  | CB-CA-C    | -7.90 | 94.61       | 110.40   |
| 1   | C     | 264 | LEU  | N-CA-C     | -7.89 | 89.70       | 111.00   |
| 1   | A     | 138 | LEU  | CA-CB-CG   | 7.88  | 133.44      | 115.30   |
| 1   | C     | 263 | PHE  | CB-CG-CD1  | -7.88 | 115.29      | 120.80   |
| 1   | C     | 264 | LEU  | CB-CG-CD2  | 7.83  | 124.32      | 111.00   |
| 1   | C     | 356 | LEU  | CA-CB-CG   | -7.83 | 97.30       | 115.30   |
| 1   | C     | 240 | ARG  | CG-CD-NE   | -7.81 | 95.40       | 111.80   |
| 1   | A     | 154 | TYR  | CZ-CE2-CD2 | -7.79 | 112.79      | 119.80   |
| 1   | A     | 257 | LEU  | CB-CG-CD2  | 7.68  | 124.06      | 111.00   |
| 1   | C     | 402 | LEU  | N-CA-C     | 7.68  | 131.73      | 111.00   |
| 1   | A     | 246 | LEU  | CA-CB-CG   | 7.64  | 132.88      | 115.30   |
| 1   | A     | 85  | CYS  | N-CA-CB    | -7.63 | 96.86       | 110.60   |
| 1   | A     | 290 | ARG  | NE-CZ-NH2  | 7.62  | 124.11      | 120.30   |
| 1   | A     | 77  | ASP  | OD1-CG-OD2 | -7.55 | 108.94      | 123.30   |
| 1   | C     | 90  | ARG  | NE-CZ-NH1  | -7.55 | 116.52      | 120.30   |
| 1   | A     | 402 | LEU  | CB-CG-CD2  | 7.53  | 123.80      | 111.00   |
| 1   | C     | 188 | ASP  | CB-CG-OD1  | 7.51  | 125.06      | 118.30   |
| 1   | A     | 191 | MET  | CA-CB-CG   | 7.47  | 126.00      | 113.30   |
| 1   | C     | 165 | LEU  | CA-CB-CG   | 7.45  | 132.44      | 115.30   |
| 1   | A     | 112 | ARG  | NE-CZ-NH1  | -7.43 | 116.58      | 120.30   |
| 1   | A     | 143 | ARG  | NE-CZ-NH2  | 7.42  | 124.01      | 120.30   |
| 1   | C     | 80  | HIS  | N-CA-CB    | 7.41  | 123.94      | 110.60   |
| 1   | A     | 70  | LEU  | CB-CG-CD2  | 7.41  | 123.59      | 111.00   |
| 1   | A     | 173 | ASP  | CB-CG-OD2  | -7.41 | 111.63      | 118.30   |
| 1   | A     | 265 | ALA  | N-CA-C     | 7.35  | 130.85      | 111.00   |
| 1   | C     | 75  | TYR  | CB-CG-CD2  | 7.33  | 125.40      | 121.00   |
| 1   | A     | 130 | ARG  | NE-CZ-NH1  | -7.33 | 116.64      | 120.30   |
| 1   | C     | 99  | ILE  | CB-CA-C    | -7.30 | 96.99       | 111.60   |
| 1   | C     | 75  | TYR  | CB-CG-CD1  | -7.30 | 116.62      | 121.00   |
| 1   | C     | 358 | LEU  | CB-CG-CD2  | -7.25 | 98.67       | 111.00   |
| 1   | A     | 70  | LEU  | CB-CG-CD1  | 7.22  | 123.27      | 111.00   |
| 1   | C     | 53  | LEU  | CB-CA-C    | -7.21 | 96.50       | 110.20   |
| 1   | A     | 401 | ALA  | CB-CA-C    | 7.13  | 120.79      | 110.10   |
| 1   | C     | 251 | ASP  | CB-CG-OD2  | 7.12  | 124.70      | 118.30   |
| 1   | C     | 404 | LEU  | CB-CG-CD1  | -7.11 | 98.91       | 111.00   |
| 1   | C     | 186 | ARG  | NE-CZ-NH1  | -7.09 | 116.75      | 120.30   |
| 1   | A     | 356 | LEU  | CB-CG-CD2  | 7.03  | 122.95      | 111.00   |
| 1   | A     | 277 | ARG  | CA-CB-CG   | -7.03 | 97.94       | 113.40   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 267 | SER  | CB-CA-C    | 7.01  | 123.42      | 110.10   |
| 1   | C     | 294 | LEU  | CB-CG-CD1  | 7.01  | 122.91      | 111.00   |
| 1   | C     | 90  | ARG  | NE-CZ-NH2  | 6.96  | 123.78      | 120.30   |
| 1   | C     | 338 | VAL  | CA-CB-CG1  | 6.95  | 121.32      | 110.90   |
| 1   | A     | 231 | ARG  | NE-CZ-NH2  | -6.94 | 116.83      | 120.30   |
| 1   | C     | 340 | PHE  | CB-CG-CD2  | 6.94  | 125.66      | 120.80   |
| 1   | C     | 143 | ARG  | CG-CD-NE   | -6.94 | 97.23       | 111.80   |
| 1   | C     | 342 | ARG  | CG-CD-NE   | 6.90  | 126.29      | 111.80   |
| 1   | A     | 161 | ARG  | NE-CZ-NH2  | -6.90 | 116.85      | 120.30   |
| 1   | C     | 251 | ASP  | CB-CG-OD1  | -6.88 | 112.11      | 118.30   |
| 1   | A     | 385 | PRO  | N-CA-C     | 6.86  | 129.93      | 112.10   |
| 1   | C     | 28  | MET  | CG-SD-CE   | -6.85 | 89.25       | 100.20   |
| 1   | A     | 86  | PRO  | CB-CA-C    | -6.84 | 94.91       | 112.00   |
| 1   | C     | 184 | MET  | CG-SD-CE   | -6.83 | 89.27       | 100.20   |
| 1   | C     | 123 | VAL  | CG1-CB-CG2 | -6.83 | 99.98       | 110.90   |
| 1   | A     | 364 | ARG  | NE-CZ-NH1  | 6.82  | 123.71      | 120.30   |
| 1   | A     | 250 | LEU  | CB-CG-CD1  | 6.80  | 122.56      | 111.00   |
| 1   | A     | 142 | LEU  | CB-CG-CD1  | 6.80  | 122.56      | 111.00   |
| 1   | C     | 114 | LEU  | CB-CG-CD2  | 6.79  | 122.54      | 111.00   |
| 1   | C     | 97  | ASP  | CB-CG-OD2  | -6.79 | 112.19      | 118.30   |
| 1   | A     | 105 | PRO  | N-CD-CG    | -6.78 | 93.03       | 103.20   |
| 1   | C     | 88  | ILE  | C-N-CD     | -6.78 | 105.69      | 120.60   |
| 1   | C     | 272 | GLN  | CA-CB-CG   | -6.76 | 98.54       | 113.40   |
| 1   | A     | 61  | GLY  | N-CA-C     | -6.71 | 96.31       | 113.10   |
| 1   | C     | 223 | VAL  | CB-CA-C    | -6.70 | 98.67       | 111.40   |
| 1   | A     | 161 | ARG  | NE-CZ-NH1  | -6.68 | 116.96      | 120.30   |
| 1   | C     | 191 | MET  | CA-CB-CG   | 6.66  | 124.63      | 113.30   |
| 1   | C     | 134 | LEU  | CB-CG-CD1  | 6.66  | 122.31      | 111.00   |
| 1   | A     | 246 | LEU  | CB-CG-CD1  | 6.65  | 122.31      | 111.00   |
| 1   | A     | 358 | LEU  | CB-CG-CD1  | 6.61  | 122.24      | 111.00   |
| 1   | C     | 131 | ILE  | N-CA-CB    | 6.58  | 125.92      | 110.80   |
| 1   | A     | 290 | ARG  | NE-CZ-NH1  | -6.56 | 117.02      | 120.30   |
| 1   | A     | 409 | ALA  | O-C-N      | -6.56 | 112.21      | 122.70   |
| 1   | C     | 103 | MET  | CB-CA-C    | -6.53 | 97.34       | 110.40   |
| 1   | C     | 238 | ALA  | CB-CA-C    | 6.53  | 119.89      | 110.10   |
| 1   | C     | 147 | GLN  | CG-CD-OE1  | -6.52 | 108.57      | 121.60   |
| 1   | A     | 395 | ILE  | CB-CA-C    | -6.50 | 98.60       | 111.60   |
| 1   | A     | 247 | VAL  | CG1-CB-CG2 | -6.45 | 100.58      | 110.90   |
| 1   | A     | 96  | TYR  | O-C-N      | -6.44 | 112.40      | 122.70   |
| 1   | A     | 270 | HIS  | N-CA-C     | -6.44 | 93.62       | 111.00   |
| 1   | A     | 402 | LEU  | CB-CG-CD1  | 6.41  | 121.90      | 111.00   |
| 1   | A     | 250 | LEU  | CB-CA-C    | 6.40  | 122.37      | 110.20   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | C     | 186 | ARG  | CB-CG-CD   | 6.40  | 128.24      | 111.60   |
| 1   | A     | 151 | THR  | N-CA-C     | 6.39  | 128.25      | 111.00   |
| 1   | C     | 356 | LEU  | CB-CG-CD2  | -6.39 | 100.14      | 111.00   |
| 1   | A     | 404 | LEU  | CB-CG-CD1  | 6.38  | 121.85      | 111.00   |
| 1   | C     | 377 | ARG  | NE-CZ-NH2  | 6.34  | 123.47      | 120.30   |
| 1   | C     | 244 | ALA  | N-CA-CB    | 6.31  | 118.93      | 110.10   |
| 1   | A     | 389 | ILE  | CB-CA-C    | -6.30 | 98.99       | 111.60   |
| 1   | A     | 127 | LEU  | CB-CG-CD1  | -6.28 | 100.33      | 111.00   |
| 1   | C     | 61  | GLY  | N-CA-C     | -6.28 | 97.41       | 113.10   |
| 1   | A     | 14  | LEU  | CB-CG-CD1  | -6.26 | 100.36      | 111.00   |
| 1   | A     | 163 | PHE  | CG-CD1-CE1 | -6.25 | 113.92      | 120.80   |
| 1   | A     | 139 | ILE  | CA-CB-CG1  | -6.25 | 99.13       | 111.00   |
| 1   | C     | 344 | LYS  | N-CA-C     | -6.21 | 94.24       | 111.00   |
| 1   | A     | 228 | VAL  | CA-CB-CG2  | -6.20 | 101.60      | 110.90   |
| 1   | A     | 271 | ARG  | NE-CZ-NH2  | 6.20  | 123.40      | 120.30   |
| 1   | C     | 40  | GLU  | CB-CA-C    | 6.18  | 122.75      | 110.40   |
| 1   | C     | 266 | LYS  | CB-CG-CD   | -6.15 | 95.60       | 111.60   |
| 1   | A     | 28  | MET  | CG-SD-CE   | -6.14 | 90.37       | 100.20   |
| 1   | C     | 288 | LEU  | CA-CB-CG   | -6.14 | 101.18      | 115.30   |
| 1   | A     | 207 | ILE  | N-CA-CB    | -6.11 | 96.75       | 110.80   |
| 1   | A     | 323 | MET  | CG-SD-CE   | 6.10  | 109.96      | 100.20   |
| 1   | C     | 399 | VAL  | CG1-CB-CG2 | 6.09  | 120.64      | 110.90   |
| 1   | C     | 301 | LEU  | CB-CG-CD2  | 6.07  | 121.32      | 111.00   |
| 1   | C     | 225 | ASN  | C-N-CA     | -6.06 | 109.57      | 122.30   |
| 1   | A     | 143 | ARG  | NE-CZ-NH1  | -6.06 | 117.27      | 120.30   |
| 1   | C     | 52  | ASP  | CB-CG-OD1  | -6.05 | 112.86      | 118.30   |
| 1   | C     | 335 | PRO  | CB-CA-C    | -6.04 | 96.89       | 112.00   |
| 1   | A     | 339 | ASP  | CB-CG-OD1  | 6.02  | 123.72      | 118.30   |
| 1   | A     | 409 | ALA  | CB-CA-C    | 6.02  | 119.13      | 110.10   |
| 1   | C     | 137 | SER  | CA-CB-OG   | -6.01 | 94.96       | 111.20   |
| 1   | C     | 293 | SER  | C-N-CA     | -6.01 | 106.68      | 121.70   |
| 1   | A     | 365 | ARG  | NE-CZ-NH2  | 6.00  | 123.30      | 120.30   |
| 1   | A     | 271 | ARG  | NE-CZ-NH1  | -6.00 | 117.30      | 120.30   |
| 1   | A     | 263 | PHE  | CB-CG-CD1  | -5.99 | 116.60      | 120.80   |
| 1   | A     | 276 | GLU  | OE1-CD-OE2 | 5.99  | 130.49      | 123.30   |
| 1   | A     | 134 | LEU  | CB-CG-CD2  | -5.99 | 100.81      | 111.00   |
| 1   | C     | 138 | LEU  | CB-CG-CD2  | 5.98  | 121.17      | 111.00   |
| 1   | A     | 384 | ALA  | N-CA-C     | -5.98 | 94.86       | 111.00   |
| 1   | A     | 14  | LEU  | CB-CG-CD2  | 5.97  | 121.16      | 111.00   |
| 1   | C     | 303 | SER  | CB-CA-C    | 5.96  | 121.42      | 110.10   |
| 1   | C     | 365 | ARG  | NE-CZ-NH2  | -5.96 | 117.32      | 120.30   |
| 1   | A     | 220 | ILE  | CB-CA-C    | -5.93 | 99.75       | 111.60   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | C     | 27  | ASP  | CB-CG-OD2  | 5.92  | 123.63      | 118.30   |
| 1   | A     | 188 | ASP  | CB-CG-OD2  | -5.92 | 112.97      | 118.30   |
| 1   | C     | 305 | TYR  | CB-CG-CD2  | -5.92 | 117.45      | 121.00   |
| 1   | A     | 369 | VAL  | CB-CA-C    | -5.92 | 100.16      | 111.40   |
| 1   | A     | 298 | GLY  | N-CA-C     | 5.91  | 127.88      | 113.10   |
| 1   | C     | 147 | GLN  | CB-CG-CD   | 5.91  | 126.97      | 111.60   |
| 1   | C     | 110 | GLN  | O-C-N      | -5.90 | 113.26      | 122.70   |
| 1   | A     | 278 | PRO  | C-N-CA     | -5.89 | 106.96      | 121.70   |
| 1   | A     | 285 | CYS  | CA-CB-SG   | -5.89 | 103.40      | 114.00   |
| 1   | C     | 164 | MET  | CB-CG-SD   | 5.85  | 129.94      | 112.40   |
| 1   | A     | 346 | SER  | CB-CA-C    | 5.84  | 121.20      | 110.10   |
| 1   | C     | 202 | ASP  | CB-CG-OD1  | 5.84  | 123.55      | 118.30   |
| 1   | C     | 79  | ARG  | O-C-N      | 5.84  | 132.04      | 122.70   |
| 1   | C     | 405 | VAL  | CB-CA-C    | -5.83 | 100.32      | 111.40   |
| 1   | C     | 377 | ARG  | NH1-CZ-NH2 | 5.83  | 125.81      | 119.40   |
| 1   | A     | 342 | ARG  | NE-CZ-NH1  | -5.82 | 117.39      | 120.30   |
| 1   | A     | 36  | ALA  | CB-CA-C    | 5.82  | 118.82      | 110.10   |
| 1   | A     | 109 | ARG  | CB-CA-C    | 5.82  | 122.03      | 110.40   |
| 1   | C     | 173 | ASP  | N-CA-C     | 5.81  | 126.69      | 111.00   |
| 1   | A     | 87  | PHE  | CB-CG-CD1  | -5.81 | 116.73      | 120.80   |
| 1   | C     | 239 | LYS  | CB-CA-C    | -5.80 | 98.79       | 110.40   |
| 1   | A     | 96  | TYR  | CB-CG-CD1  | 5.80  | 124.48      | 121.00   |
| 1   | A     | 284 | ALA  | N-CA-C     | 5.79  | 126.65      | 111.00   |
| 1   | A     | 195 | GLU  | OE1-CD-OE2 | 5.78  | 130.24      | 123.30   |
| 1   | C     | 261 | MET  | CG-SD-CE   | -5.77 | 90.97       | 100.20   |
| 1   | C     | 85  | CYS  | CB-CA-C    | -5.77 | 98.86       | 110.40   |
| 1   | C     | 195 | GLU  | OE1-CD-OE2 | 5.77  | 130.22      | 123.30   |
| 1   | C     | 130 | ARG  | O-C-N      | 5.75  | 131.89      | 122.70   |
| 1   | C     | 357 | CYS  | O-C-N      | -5.73 | 113.53      | 122.70   |
| 1   | C     | 261 | MET  | CB-CA-C    | 5.73  | 121.86      | 110.40   |
| 1   | A     | 302 | THR  | N-CA-C     | 5.72  | 126.46      | 111.00   |
| 1   | C     | 364 | ARG  | CG-CD-NE   | 5.72  | 123.81      | 111.80   |
| 1   | C     | 250 | LEU  | N-CA-C     | 5.70  | 126.38      | 111.00   |
| 1   | C     | 22  | LEU  | CB-CG-CD2  | 5.69  | 120.68      | 111.00   |
| 1   | A     | 392 | LYS  | N-CA-C     | -5.69 | 95.64       | 111.00   |
| 1   | A     | 380 | ASP  | CB-CG-OD2  | 5.69  | 123.42      | 118.30   |
| 1   | C     | 254 | VAL  | CB-CA-C    | -5.68 | 100.61      | 111.40   |
| 1   | C     | 337 | HIS  | CB-CA-C    | 5.67  | 121.74      | 110.40   |
| 1   | A     | 173 | ASP  | CB-CG-OD1  | 5.65  | 123.39      | 118.30   |
| 1   | A     | 201 | TYR  | N-CA-CB    | -5.65 | 100.43      | 110.60   |
| 1   | C     | 340 | PHE  | CB-CG-CD1  | -5.65 | 116.85      | 120.80   |
| 1   | A     | 94  | GLU  | N-CA-C     | -5.64 | 95.76       | 111.00   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | C     | 271 | ARG  | NE-CZ-NH2  | -5.64 | 117.48      | 120.30   |
| 1   | A     | 110 | GLN  | N-CA-CB    | -5.64 | 100.45      | 110.60   |
| 1   | C     | 204 | LEU  | CD1-CG-CD2 | -5.64 | 93.59       | 110.50   |
| 1   | C     | 377 | ARG  | CD-NE-CZ   | -5.64 | 115.71      | 123.60   |
| 1   | C     | 130 | ARG  | CB-CA-C    | -5.63 | 99.13       | 110.40   |
| 1   | A     | 91  | GLU  | CB-CA-C    | -5.63 | 99.13       | 110.40   |
| 1   | C     | 112 | ARG  | CD-NE-CZ   | 5.63  | 131.48      | 123.60   |
| 1   | C     | 130 | ARG  | CG-CD-NE   | 5.62  | 123.61      | 111.80   |
| 1   | C     | 75  | TYR  | CE1-CZ-OH  | -5.62 | 104.92      | 120.10   |
| 1   | C     | 266 | LYS  | CD-CE-NZ   | 5.62  | 124.63      | 111.70   |
| 1   | C     | 165 | LEU  | CB-CG-CD1  | -5.62 | 101.45      | 111.00   |
| 1   | C     | 233 | ILE  | N-CA-C     | -5.62 | 95.84       | 111.00   |
| 1   | A     | 373 | GLU  | CA-CB-CG   | -5.61 | 101.06      | 113.40   |
| 1   | C     | 203 | TYR  | CD1-CE1-CZ | -5.60 | 114.76      | 119.80   |
| 1   | C     | 245 | LEU  | CB-CG-CD1  | -5.60 | 101.48      | 111.00   |
| 1   | A     | 142 | LEU  | CB-CG-CD2  | 5.59  | 120.51      | 111.00   |
| 1   | A     | 236 | ASP  | CB-CG-OD2  | 5.59  | 123.34      | 118.30   |
| 1   | A     | 90  | ARG  | NE-CZ-NH1  | 5.58  | 123.09      | 120.30   |
| 1   | A     | 350 | PHE  | N-CA-CB    | -5.56 | 100.59      | 110.60   |
| 1   | C     | 79  | ARG  | NE-CZ-NH2  | 5.56  | 123.08      | 120.30   |
| 1   | A     | 350 | PHE  | CB-CA-C    | 5.54  | 121.48      | 110.40   |
| 1   | A     | 399 | VAL  | CA-CB-CG1  | 5.54  | 119.21      | 110.90   |
| 1   | A     | 410 | THR  | OG1-CB-CG2 | -5.54 | 97.25       | 110.00   |
| 1   | A     | 79  | ARG  | NE-CZ-NH1  | -5.54 | 117.53      | 120.30   |
| 1   | A     | 125 | ASP  | CB-CG-OD2  | 5.54  | 123.28      | 118.30   |
| 1   | A     | 141 | SER  | N-CA-CB    | -5.51 | 102.23      | 110.50   |
| 1   | C     | 96  | TYR  | C-N-CA     | -5.50 | 107.94      | 121.70   |
| 1   | C     | 372 | LYS  | CD-CE-NZ   | 5.50  | 124.36      | 111.70   |
| 1   | A     | 261 | MET  | CA-CB-CG   | 5.50  | 122.65      | 113.30   |
| 1   | A     | 30  | ASN  | C-N-CD     | 5.49  | 139.94      | 128.40   |
| 1   | A     | 371 | LEU  | N-CA-C     | -5.49 | 96.17       | 111.00   |
| 1   | A     | 380 | ASP  | N-CA-CB    | -5.49 | 100.71      | 110.60   |
| 1   | A     | 371 | LEU  | CB-CG-CD1  | 5.48  | 120.31      | 111.00   |
| 1   | C     | 288 | LEU  | CB-CG-CD2  | 5.48  | 120.31      | 111.00   |
| 1   | A     | 278 | PRO  | O-C-N      | -5.47 | 113.95      | 122.70   |
| 1   | C     | 197 | LYS  | CD-CE-NZ   | -5.46 | 99.15       | 111.70   |
| 1   | C     | 180 | LEU  | CB-CG-CD1  | -5.45 | 101.73      | 111.00   |
| 1   | C     | 110 | GLN  | C-N-CA     | -5.45 | 108.08      | 121.70   |
| 1   | C     | 290 | ARG  | CA-CB-CG   | -5.45 | 101.41      | 113.40   |
| 1   | C     | 272 | GLN  | N-CA-C     | 5.45  | 125.70      | 111.00   |
| 1   | C     | 368 | ILE  | C-N-CA     | 5.44  | 135.30      | 121.70   |
| 1   | A     | 277 | ARG  | CB-CA-C    | 5.43  | 121.27      | 110.40   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 373 | GLU  | N-CA-C     | 5.43  | 125.66      | 111.00   |
| 1   | A     | 251 | ASP  | OD1-CG-OD2 | -5.42 | 113.00      | 123.30   |
| 1   | A     | 382 | SER  | CB-CA-C    | 5.42  | 120.40      | 110.10   |
| 1   | C     | 300 | ILE  | C-N-CA     | -5.41 | 108.18      | 121.70   |
| 1   | A     | 247 | VAL  | CA-CB-CG1  | 5.40  | 119.00      | 110.90   |
| 1   | A     | 299 | ARG  | NH1-CZ-NH2 | 5.39  | 125.33      | 119.40   |
| 1   | A     | 79  | ARG  | O-C-N      | -5.39 | 114.08      | 122.70   |
| 1   | C     | 237 | GLU  | CA-C-N     | -5.39 | 105.34      | 117.20   |
| 1   | C     | 130 | ARG  | N-CA-CB    | 5.39  | 120.30      | 110.60   |
| 1   | A     | 117 | GLN  | N-CA-CB    | 5.38  | 120.29      | 110.60   |
| 1   | A     | 367 | ILE  | CG1-CB-CG2 | -5.38 | 99.55       | 111.40   |
| 1   | C     | 371 | LEU  | CB-CG-CD2  | 5.37  | 120.13      | 111.00   |
| 1   | C     | 87  | PHE  | N-CA-C     | 5.37  | 125.49      | 111.00   |
| 1   | C     | 290 | ARG  | NH1-CZ-NH2 | 5.36  | 125.29      | 119.40   |
| 1   | A     | 25  | ASP  | CB-CG-OD1  | 5.35  | 123.11      | 118.30   |
| 1   | A     | 197 | LYS  | CA-CB-CG   | 5.35  | 125.16      | 113.40   |
| 1   | A     | 330 | ARG  | CG-CD-NE   | -5.32 | 100.62      | 111.80   |
| 1   | C     | 251 | ASP  | O-C-N      | -5.32 | 114.19      | 122.70   |
| 1   | C     | 119 | VAL  | CG1-CB-CG2 | 5.32  | 119.41      | 110.90   |
| 1   | C     | 142 | LEU  | CB-CA-C    | -5.32 | 100.10      | 110.20   |
| 1   | A     | 57  | ARG  | NE-CZ-NH2  | 5.30  | 122.95      | 120.30   |
| 1   | A     | 99  | ILE  | CB-CA-C    | -5.30 | 101.00      | 111.60   |
| 1   | C     | 239 | LYS  | CB-CG-CD   | -5.30 | 97.83       | 111.60   |
| 1   | C     | 124 | VAL  | CG1-CB-CG2 | 5.29  | 119.36      | 110.90   |
| 1   | A     | 290 | ARG  | CD-NE-CZ   | -5.28 | 116.21      | 123.60   |
| 1   | A     | 324 | LEU  | N-CA-C     | 5.26  | 125.21      | 111.00   |
| 1   | A     | 207 | ILE  | CG1-CB-CG2 | 5.26  | 122.97      | 111.40   |
| 1   | C     | 362 | LEU  | CB-CG-CD1  | 5.25  | 119.93      | 111.00   |
| 1   | A     | 121 | MET  | CB-CG-SD   | 5.25  | 128.15      | 112.40   |
| 1   | C     | 305 | TYR  | OH-CZ-CE2  | -5.24 | 105.95      | 120.10   |
| 1   | A     | 195 | GLU  | CB-CA-C    | -5.24 | 99.92       | 110.40   |
| 1   | A     | 187 | PRO  | N-CD-CG    | -5.24 | 95.35       | 103.20   |
| 1   | C     | 342 | ARG  | NE-CZ-NH1  | 5.23  | 122.92      | 120.30   |
| 1   | C     | 179 | TYR  | CB-CG-CD2  | -5.22 | 117.87      | 121.00   |
| 1   | C     | 112 | ARG  | N-CA-C     | -5.22 | 96.90       | 111.00   |
| 1   | C     | 242 | CYS  | C-N-CA     | 5.22  | 133.26      | 122.30   |
| 1   | C     | 11  | LEU  | CB-CG-CD2  | -5.20 | 102.16      | 111.00   |
| 1   | C     | 113 | ALA  | C-N-CA     | 5.19  | 134.67      | 121.70   |
| 1   | A     | 101 | THR  | N-CA-C     | 5.19  | 125.01      | 111.00   |
| 1   | A     | 330 | ARG  | CB-CA-C    | -5.19 | 100.03      | 110.40   |
| 1   | A     | 40  | GLU  | N-CA-C     | 5.17  | 124.97      | 111.00   |
| 1   | A     | 174 | ILE  | C-N-CA     | -5.17 | 100.28      | 122.00   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 290 | ARG  | N-CA-CB    | -5.17 | 101.29      | 110.60   |
| 1   | C     | 211 | ARG  | NE-CZ-NH1  | -5.17 | 117.72      | 120.30   |
| 1   | A     | 131 | ILE  | CG1-CB-CG2 | -5.16 | 100.06      | 111.40   |
| 1   | A     | 165 | LEU  | CA-CB-CG   | 5.15  | 127.15      | 115.30   |
| 1   | C     | 97  | ASP  | CB-CG-OD1  | 5.15  | 122.93      | 118.30   |
| 1   | A     | 222 | ILE  | CB-CA-C    | -5.15 | 101.31      | 111.60   |
| 1   | C     | 271 | ARG  | CG-CD-NE   | -5.14 | 101.01      | 111.80   |
| 1   | A     | 337 | HIS  | CB-CA-C    | 5.13  | 120.67      | 110.40   |
| 1   | C     | 336 | MET  | CA-CB-CG   | 5.13  | 122.02      | 113.30   |
| 1   | C     | 268 | PRO  | C-N-CA     | -5.13 | 108.89      | 121.70   |
| 1   | A     | 78  | TYR  | CG-CD2-CE2 | 5.10  | 125.38      | 121.30   |
| 1   | A     | 413 | ALA  | CB-CA-C    | 5.09  | 117.74      | 110.10   |
| 1   | A     | 186 | ARG  | NE-CZ-NH1  | 5.09  | 122.84      | 120.30   |
| 1   | A     | 368 | ILE  | CA-CB-CG1  | -5.09 | 101.33      | 111.00   |
| 1   | C     | 105 | PRO  | C-N-CA     | 5.09  | 143.37      | 122.00   |
| 1   | C     | 257 | LEU  | CA-CB-CG   | 5.09  | 127.00      | 115.30   |
| 1   | C     | 102 | SER  | O-C-N      | 5.07  | 130.81      | 122.70   |
| 1   | A     | 127 | LEU  | CB-CG-CD2  | 5.06  | 119.61      | 111.00   |
| 1   | C     | 254 | VAL  | CA-CB-CG1  | -5.06 | 103.31      | 110.90   |
| 1   | A     | 383 | ILE  | N-CA-C     | 5.05  | 124.63      | 111.00   |
| 1   | A     | 396 | VAL  | CG1-CB-CG2 | -5.05 | 102.82      | 110.90   |
| 1   | A     | 387 | ALA  | CB-CA-C    | 5.04  | 117.65      | 110.10   |
| 1   | A     | 378 | ILE  | CB-CA-C    | -5.03 | 101.53      | 111.60   |
| 1   | C     | 70  | LEU  | CB-CG-CD2  | 5.02  | 119.54      | 111.00   |
| 1   | A     | 50  | VAL  | CG1-CB-CG2 | 5.02  | 118.93      | 110.90   |
| 1   | A     | 72  | ARG  | NH1-CZ-NH2 | 5.02  | 124.92      | 119.40   |
| 1   | C     | 142 | LEU  | CB-CG-CD2  | -5.02 | 102.47      | 111.00   |
| 1   | C     | 178 | LYS  | N-CA-CB    | -5.00 | 101.59      | 110.60   |

There are no chirality outliers.

All (17) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | A     | 107 | GLU  | Peptide   |
| 1   | A     | 108 | GLN  | Peptide   |
| 1   | A     | 120 | GLY  | Peptide   |
| 1   | A     | 258 | SER  | Mainchain |
| 1   | A     | 261 | MET  | Mainchain |
| 1   | A     | 303 | SER  | Peptide   |
| 1   | A     | 382 | SER  | Peptide   |
| 1   | A     | 81  | PHE  | Peptide   |
| 1   | C     | 204 | LEU  | Peptide   |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | C     | 205 | ILE  | Mainchain |
| 1   | C     | 238 | ALA  | Mainchain |
| 1   | C     | 263 | PHE  | Mainchain |
| 1   | C     | 270 | HIS  | Peptide   |
| 1   | C     | 303 | SER  | Peptide   |
| 1   | C     | 359 | GLY  | Peptide   |
| 1   | C     | 379 | PRO  | Peptide   |
| 1   | C     | 403 | PRO  | Mainchain |

## 5.2 Too-close contacts [i](#)

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     | 3201  | 0        | 3148     | 418     | 11           |
| 1   | C     | 3199  | 0        | 3137     | 392     | 12           |
| 2   | A     | 43    | 0        | 32       | 19      | 0            |
| 2   | C     | 43    | 0        | 32       | 9       | 0            |
| 3   | A     | 111   | 0        | 0        | 9       | 0            |
| 3   | C     | 99    | 0        | 0        | 9       | 0            |
| All | All   | 6696  | 0        | 6349     | 797     | 23           |

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 62.

All (797) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:C:356:LEU:CD1 | 1:C:356:LEU:CG  | 1.74                     | 1.61              |
| 1:A:404:LEU:CG  | 1:A:404:LEU:CD1 | 1.76                     | 1.58              |
| 1:A:151:THR:CG2 | 1:A:151:THR:CB  | 1.75                     | 1.58              |
| 1:C:373:GLU:CG  | 1:C:373:GLU:CB  | 1.75                     | 1.58              |
| 1:C:131:ILE:CB  | 1:C:131:ILE:CG2 | 1.78                     | 1.56              |
| 1:C:369:VAL:CB  | 1:C:369:VAL:CA  | 1.78                     | 1.56              |
| 1:C:389:ILE:CB  | 1:C:389:ILE:CG2 | 1.82                     | 1.56              |
| 1:A:139:ILE:CG2 | 1:A:139:ILE:CB  | 1.75                     | 1.56              |
| 1:A:240:ARG:CG  | 1:A:240:ARG:CD  | 1.79                     | 1.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:409:ALA:CA   | 1:A:409:ALA:CB   | 1.75                     | 1.55              |
| 1:C:254:VAL:CB   | 1:C:254:VAL:CG1  | 1.80                     | 1.55              |
| 1:A:389:ILE:CB   | 1:A:389:ILE:CG2  | 1.84                     | 1.54              |
| 1:C:112:ARG:CD   | 1:C:112:ARG:CG   | 1.80                     | 1.53              |
| 1:A:96:TYR:C     | 1:A:96:TYR:CA    | 1.76                     | 1.53              |
| 1:C:143:ARG:HH11 | 1:C:143:ARG:CG   | 1.22                     | 1.52              |
| 1:A:134:LEU:CG   | 1:A:134:LEU:CD1  | 1.86                     | 1.52              |
| 1:A:205:ILE:CB   | 1:A:205:ILE:CG2  | 1.79                     | 1.52              |
| 1:A:257:LEU:C    | 1:A:257:LEU:CA   | 1.75                     | 1.51              |
| 1:A:264:LEU:CG   | 1:A:264:LEU:CD2  | 1.83                     | 1.51              |
| 1:A:367:ILE:N    | 1:A:367:ILE:CA   | 1.70                     | 1.51              |
| 1:A:105:PRO:CD   | 1:A:105:PRO:CG   | 1.75                     | 1.50              |
| 1:C:399:VAL:CB   | 1:C:399:VAL:CG2  | 1.87                     | 1.49              |
| 1:A:379:PRO:CB   | 1:A:379:PRO:CG   | 1.80                     | 1.47              |
| 1:A:106:PRO:CG   | 1:A:106:PRO:CB   | 1.77                     | 1.44              |
| 1:A:385:PRO:CB   | 1:A:385:PRO:CG   | 1.88                     | 1.43              |
| 1:C:335:PRO:CB   | 1:C:335:PRO:CG   | 2.00                     | 1.39              |
| 1:A:20:GLU:CD    | 1:C:165:LEU:HG   | 1.39                     | 1.38              |
| 1:A:277:ARG:NH2  | 1:A:280:ARG:HH21 | 1.27                     | 1.28              |
| 1:A:247:VAL:HG12 | 3:A:519:HOH:O    | 1.29                     | 1.25              |
| 1:A:20:GLU:CD    | 1:C:165:LEU:CG   | 2.10                     | 1.18              |
| 1:C:277:ARG:HE   | 1:C:280:ARG:NH2  | 1.42                     | 1.16              |
| 2:C:415:HEC:HBB3 | 2:C:415:HEC:HMB1 | 1.26                     | 1.15              |
| 1:A:20:GLU:OE2   | 1:C:165:LEU:HG   | 1.44                     | 1.14              |
| 1:C:143:ARG:NH1  | 1:C:143:ARG:HG2  | 1.17                     | 1.14              |
| 1:C:205:ILE:CG2  | 1:C:206:PRO:HD3  | 1.79                     | 1.11              |
| 1:C:56:THR:HG22  | 1:C:64:ILE:HD11  | 1.19                     | 1.10              |
| 1:C:40:GLU:HG3   | 1:C:336:MET:CE   | 1.80                     | 1.10              |
| 1:A:277:ARG:NH2  | 1:A:280:ARG:NH2  | 1.98                     | 1.10              |
| 1:C:99:ILE:HG22  | 1:C:99:ILE:O     | 1.45                     | 1.09              |
| 1:C:143:ARG:CG   | 1:C:143:ARG:NH1  | 1.88                     | 1.08              |
| 1:A:39:GLN:H     | 1:A:39:GLN:NE2   | 1.50                     | 1.08              |
| 1:A:151:THR:CG2  | 1:A:151:THR:CA   | 2.31                     | 1.08              |
| 1:A:151:THR:HG23 | 1:A:151:THR:H    | 1.22                     | 1.04              |
| 1:C:130:ARG:NH1  | 1:C:165:LEU:HD21 | 1.71                     | 1.04              |
| 1:C:277:ARG:NE   | 1:C:280:ARG:HH21 | 1.55                     | 1.04              |
| 1:A:298:GLY:O    | 1:A:299:ARG:HD3  | 1.53                     | 1.04              |
| 1:C:160:ILE:HG12 | 1:C:250:LEU:HG   | 1.37                     | 1.04              |
| 1:C:41:ALA:O     | 1:C:44:VAL:HG13  | 1.59                     | 1.02              |
| 1:C:228:VAL:O    | 1:C:231:ARG:HD2  | 1.59                     | 1.02              |
| 1:A:384:ALA:HA   | 1:A:405:VAL:HG22 | 1.42                     | 1.01              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:277:ARG:CZ   | 1:A:280:ARG:NH2  | 2.24                     | 1.00              |
| 1:A:237:GLU:HG2  | 1:A:240:ARG:NH2  | 1.74                     | 1.00              |
| 1:C:205:ILE:HG22 | 1:C:206:PRO:HD3  | 1.03                     | 1.00              |
| 1:C:40:GLU:HG3   | 1:C:336:MET:HE2  | 1.42                     | 0.99              |
| 1:C:414:VAL:CG1  | 1:C:414:VAL:OXT  | 2.11                     | 0.98              |
| 1:A:277:ARG:HH21 | 1:A:280:ARG:NH2  | 1.56                     | 0.98              |
| 1:A:277:ARG:HE   | 1:A:280:ARG:CZ   | 1.75                     | 0.98              |
| 1:A:277:ARG:NE   | 1:A:280:ARG:NH2  | 2.12                     | 0.97              |
| 1:C:166:LEU:HD12 | 1:C:166:LEU:O    | 1.64                     | 0.97              |
| 1:C:267:SER:HG   | 1:C:270:HIS:HD1  | 1.11                     | 0.96              |
| 1:A:205:ILE:CG2  | 1:A:205:ILE:HB   | 1.94                     | 0.96              |
| 1:A:69:GLN:O     | 1:A:73:GLU:HG3   | 1.66                     | 0.96              |
| 1:A:77:ASP:OD2   | 1:A:80:HIS:ND1   | 1.98                     | 0.95              |
| 1:C:277:ARG:NE   | 1:C:280:ARG:NH2  | 2.11                     | 0.95              |
| 1:A:277:ARG:O    | 1:A:279:GLU:N    | 2.00                     | 0.95              |
| 1:C:143:ARG:HH11 | 1:C:143:ARG:HG3  | 1.28                     | 0.94              |
| 1:C:205:ILE:HG22 | 1:C:206:PRO:CD   | 1.96                     | 0.93              |
| 1:C:185:THR:HA   | 1:C:395:ILE:HD13 | 1.47                     | 0.92              |
| 1:A:96:TYR:OH    | 1:A:101:THR:OG1  | 1.86                     | 0.92              |
| 1:A:151:THR:CG2  | 1:A:151:THR:N    | 2.33                     | 0.92              |
| 1:A:242:CYS:O    | 1:A:246:LEU:HD23 | 1.70                     | 0.91              |
| 1:A:131:ILE:HD12 | 1:A:162:ILE:HD12 | 1.51                     | 0.91              |
| 1:C:111:PHE:CE2  | 1:C:228:VAL:HG21 | 2.05                     | 0.91              |
| 1:A:151:THR:HG23 | 1:A:151:THR:N    | 1.86                     | 0.89              |
| 1:C:46:GLN:O     | 1:C:67:ARG:NH2   | 2.04                     | 0.89              |
| 1:A:384:ALA:HA   | 1:A:405:VAL:CG2  | 2.02                     | 0.89              |
| 1:C:356:LEU:CD1  | 1:C:356:LEU:HG   | 2.01                     | 0.89              |
| 1:A:39:GLN:H     | 1:A:39:GLN:HE21  | 1.19                     | 0.88              |
| 1:C:134:LEU:HD11 | 1:C:138:LEU:HD11 | 1.56                     | 0.88              |
| 1:A:209:GLU:O    | 1:A:213:GLN:HG3  | 1.74                     | 0.87              |
| 1:A:96:TYR:HH    | 1:A:101:THR:HG1  | 1.17                     | 0.87              |
| 1:A:237:GLU:HG2  | 1:A:240:ARG:HH21 | 1.39                     | 0.87              |
| 1:C:322:GLN:HB3  | 1:C:348:THR:O    | 1.74                     | 0.87              |
| 1:C:254:VAL:CG1  | 1:C:254:VAL:C    | 2.42                     | 0.87              |
| 1:C:205:ILE:N    | 1:C:206:PRO:CD   | 2.38                     | 0.86              |
| 1:A:181:THR:HA   | 1:A:184:MET:CE   | 2.06                     | 0.86              |
| 1:A:277:ARG:HE   | 1:A:280:ARG:NH2  | 1.70                     | 0.86              |
| 1:A:192:THR:OG1  | 1:A:195:GLU:HG2  | 1.76                     | 0.85              |
| 1:C:56:THR:CG2   | 1:C:64:ILE:HD11  | 2.06                     | 0.85              |
| 1:A:103:MET:CE   | 1:A:107:GLU:OE1  | 2.25                     | 0.84              |
| 1:C:254:VAL:CG1  | 1:C:254:VAL:CA   | 2.56                     | 0.84              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:277:ARG:HE   | 1:C:280:ARG:HH21 | 0.88                     | 0.84              |
| 1:C:99:ILE:CG2   | 1:C:241:MET:HB2  | 2.06                     | 0.83              |
| 1:C:220:ILE:HD13 | 1:C:242:CYS:SG   | 2.17                     | 0.83              |
| 1:A:138:LEU:HD23 | 1:A:154:TYR:CD2  | 2.13                     | 0.83              |
| 1:A:378:ILE:N    | 1:A:379:PRO:HD3  | 1.92                     | 0.83              |
| 1:A:17:HIS:HA    | 1:C:217:THR:HG23 | 1.61                     | 0.83              |
| 1:C:356:LEU:CD1  | 1:C:356:LEU:CD2  | 2.57                     | 0.82              |
| 1:A:127:LEU:O    | 1:A:131:ILE:HD13 | 1.80                     | 0.82              |
| 1:A:121:MET:N    | 1:A:122:PRO:HD2  | 1.94                     | 0.82              |
| 1:C:131:ILE:HG22 | 1:C:369:VAL:HG11 | 1.62                     | 0.82              |
| 1:C:56:THR:HG22  | 1:C:64:ILE:CD1   | 2.08                     | 0.81              |
| 1:A:20:GLU:OE1   | 1:C:165:LEU:CA   | 2.28                     | 0.81              |
| 1:A:274:LEU:HD22 | 1:A:281:ILE:HD13 | 1.61                     | 0.81              |
| 1:A:277:ARG:O    | 1:A:280:ARG:N    | 2.13                     | 0.81              |
| 1:C:91:GLU:H     | 1:C:91:GLU:CD    | 1.84                     | 0.81              |
| 1:C:295:VAL:HG22 | 1:C:396:VAL:HG22 | 1.61                     | 0.81              |
| 1:C:390:GLN:O    | 1:C:400:GLN:N    | 2.13                     | 0.81              |
| 1:C:40:GLU:HG3   | 1:C:336:MET:HE3  | 1.61                     | 0.81              |
| 1:A:237:GLU:CG   | 1:A:240:ARG:HH21 | 1.93                     | 0.81              |
| 1:C:395:ILE:H    | 1:C:395:ILE:HD12 | 1.44                     | 0.81              |
| 1:A:103:MET:SD   | 1:A:107:GLU:OE1  | 2.39                     | 0.80              |
| 1:A:233:ILE:HD13 | 1:A:237:GLU:HB2  | 1.62                     | 0.80              |
| 1:C:414:VAL:OXT  | 1:C:414:VAL:HG13 | 1.82                     | 0.79              |
| 1:C:135:ALA:O    | 1:C:139:ILE:HG12 | 1.82                     | 0.79              |
| 1:C:383:ILE:HD13 | 1:C:389:ILE:HD11 | 1.62                     | 0.79              |
| 1:A:389:ILE:HD12 | 1:A:389:ILE:H    | 1.47                     | 0.79              |
| 1:C:400:GLN:O    | 1:C:401:ALA:HB2  | 1.81                     | 0.79              |
| 1:A:40:GLU:OE1   | 1:A:40:GLU:N     | 2.15                     | 0.78              |
| 1:A:177:LEU:HD13 | 1:A:246:LEU:CD1  | 2.13                     | 0.78              |
| 1:C:192:THR:OG1  | 1:C:195:GLU:HG2  | 1.83                     | 0.78              |
| 1:A:21:HIS:HA    | 1:C:130:ARG:HD3  | 1.65                     | 0.77              |
| 1:A:40:GLU:HG3   | 1:A:336:MET:HE1  | 1.66                     | 0.77              |
| 1:A:404:LEU:CD1  | 1:A:404:LEU:HG   | 2.10                     | 0.77              |
| 1:A:20:GLU:OE1   | 1:C:165:LEU:C    | 2.23                     | 0.77              |
| 1:C:99:ILE:HG22  | 1:C:241:MET:HB2  | 1.67                     | 0.77              |
| 1:A:253:VAL:HG12 | 1:A:253:VAL:O    | 1.85                     | 0.76              |
| 1:C:337:HIS:O    | 1:C:342:ARG:NH2  | 2.16                     | 0.76              |
| 1:A:276:GLU:C    | 1:A:277:ARG:HG3  | 2.06                     | 0.76              |
| 1:C:166:LEU:HD12 | 1:C:166:LEU:C    | 2.06                     | 0.76              |
| 1:A:134:LEU:CD1  | 1:A:134:LEU:HG   | 2.10                     | 0.76              |
| 1:A:203:TYR:O    | 1:A:207:ILE:HD13 | 1.85                     | 0.75              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:276:GLU:O    | 1:C:277:ARG:HG3  | 1.86                     | 0.75              |
| 1:A:139:ILE:CG2  | 1:A:139:ILE:HB   | 2.12                     | 0.75              |
| 1:A:40:GLU:HG3   | 1:A:336:MET:CE   | 2.16                     | 0.75              |
| 1:A:389:ILE:CG2  | 1:A:389:ILE:CA   | 2.65                     | 0.75              |
| 1:C:273:GLU:O    | 1:C:277:ARG:HB2  | 1.87                     | 0.75              |
| 1:A:98:PHE:CE2   | 1:A:243:GLY:O    | 2.39                     | 0.75              |
| 1:A:277:ARG:O    | 1:A:278:PRO:C    | 2.24                     | 0.75              |
| 1:C:11:LEU:N     | 1:C:11:LEU:HD12  | 2.02                     | 0.75              |
| 1:A:39:GLN:HE21  | 1:A:39:GLN:N     | 1.85                     | 0.75              |
| 1:A:209:GLU:O    | 1:A:213:GLN:NE2  | 2.21                     | 0.74              |
| 1:C:113:ALA:O    | 1:C:116:ASN:HB3  | 1.88                     | 0.74              |
| 1:A:103:MET:HE1  | 1:A:107:GLU:OE1  | 1.86                     | 0.74              |
| 1:A:233:ILE:CD1  | 1:A:237:GLU:HB2  | 2.17                     | 0.74              |
| 1:C:267:SER:O    | 1:C:270:HIS:N    | 2.19                     | 0.74              |
| 1:A:86:PRO:O     | 1:A:298:GLY:N    | 2.21                     | 0.74              |
| 1:C:244:ALA:O    | 1:C:245:LEU:C    | 2.25                     | 0.74              |
| 1:A:384:ALA:CA   | 1:A:405:VAL:HG22 | 2.18                     | 0.73              |
| 1:C:201:TYR:CG   | 1:C:239:LYS:HD2  | 2.23                     | 0.73              |
| 1:C:205:ILE:H    | 1:C:206:PRO:CD   | 2.01                     | 0.73              |
| 1:C:254:VAL:C    | 1:C:254:VAL:HG12 | 2.07                     | 0.73              |
| 1:C:191:MET:CE   | 1:C:196:ALA:HA   | 2.18                     | 0.73              |
| 1:C:290:ARG:NH2  | 1:C:335:PRO:O    | 2.21                     | 0.73              |
| 1:A:322:GLN:HG2  | 1:A:351:GLY:HA2  | 1.69                     | 0.73              |
| 1:A:20:GLU:OE1   | 1:C:165:LEU:CG   | 2.36                     | 0.73              |
| 1:A:205:ILE:N    | 1:A:206:PRO:CD   | 2.52                     | 0.72              |
| 1:A:143:ARG:HG3  | 1:A:411:THR:HB   | 1.71                     | 0.72              |
| 1:A:17:HIS:CD2   | 1:A:313:LYS:CD   | 2.72                     | 0.72              |
| 1:C:357:CYS:SG   | 2:C:415:HEC:CHB  | 2.74                     | 0.72              |
| 1:C:39:GLN:H     | 1:C:39:GLN:HE21  | 1.37                     | 0.72              |
| 1:C:99:ILE:HG23  | 1:C:100:PRO:N    | 2.05                     | 0.72              |
| 1:A:125:ASP:O    | 1:A:128:GLU:HB2  | 1.88                     | 0.72              |
| 1:A:139:ILE:HD12 | 1:A:374:TRP:CZ3  | 2.25                     | 0.72              |
| 1:A:181:THR:HG23 | 1:A:247:VAL:HG22 | 1.71                     | 0.71              |
| 1:A:205:ILE:HG22 | 1:A:206:PRO:HD3  | 1.70                     | 0.71              |
| 1:A:257:LEU:C    | 1:A:257:LEU:HA   | 2.06                     | 0.71              |
| 1:C:278:PRO:O    | 1:C:281:ILE:HG13 | 1.90                     | 0.71              |
| 1:C:389:ILE:CG2  | 1:C:389:ILE:CA   | 2.66                     | 0.71              |
| 1:A:139:ILE:CG2  | 1:A:139:ILE:CA   | 2.65                     | 0.71              |
| 1:A:223:VAL:HG12 | 1:A:224:ALA:N    | 2.05                     | 0.71              |
| 1:C:183:GLN:O    | 1:C:187:PRO:HG3  | 1.90                     | 0.71              |
| 1:A:96:TYR:C     | 1:A:96:TYR:HA    | 2.05                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:395:ILE:O    | 1:A:395:ILE:HG22 | 1.90                     | 0.70              |
| 1:C:108:GLN:O    | 1:C:108:GLN:HG2  | 1.85                     | 0.70              |
| 1:A:20:GLU:OE2   | 1:C:165:LEU:CG   | 2.32                     | 0.70              |
| 1:C:184:MET:HE2  | 1:C:200:LEU:HD22 | 1.74                     | 0.70              |
| 1:C:195:GLU:HA   | 1:C:195:GLU:OE1  | 1.91                     | 0.70              |
| 1:C:191:MET:HE1  | 1:C:196:ALA:HA   | 1.73                     | 0.70              |
| 1:A:298:GLY:O    | 1:A:299:ARG:NH1  | 2.18                     | 0.69              |
| 1:C:257:LEU:CD2  | 1:C:367:ILE:HD13 | 2.22                     | 0.69              |
| 1:C:130:ARG:HH11 | 1:C:165:LEU:HD21 | 1.56                     | 0.69              |
| 1:A:39:GLN:NE2   | 1:A:39:GLN:N     | 2.33                     | 0.69              |
| 1:C:195:GLU:OE1  | 1:C:195:GLU:CA   | 2.38                     | 0.69              |
| 1:A:12:ALA:O     | 1:A:57:ARG:HB3   | 1.92                     | 0.69              |
| 1:A:20:GLU:CG    | 1:C:165:LEU:HG   | 2.23                     | 0.69              |
| 1:A:167:ALA:O    | 1:A:220:ILE:HD13 | 1.93                     | 0.69              |
| 1:A:191:MET:HE1  | 1:A:196:ALA:HA   | 1.73                     | 0.69              |
| 1:C:228:VAL:O    | 1:C:231:ARG:CD   | 2.40                     | 0.69              |
| 1:A:115:ALA:HB3  | 1:A:358:LEU:HD13 | 1.74                     | 0.69              |
| 1:A:291:ARG:HG3  | 1:A:292:PHE:CE1  | 2.28                     | 0.69              |
| 1:C:201:TYR:CD2  | 1:C:239:LYS:HD2  | 2.28                     | 0.69              |
| 1:A:115:ALA:HB3  | 1:A:358:LEU:CD1  | 2.23                     | 0.69              |
| 1:C:29:TYR:HE2   | 1:C:89:PRO:HD3   | 1.56                     | 0.69              |
| 1:A:20:GLU:OE1   | 1:C:165:LEU:CB   | 2.41                     | 0.69              |
| 1:A:277:ARG:NE   | 1:A:280:ARG:CZ   | 2.53                     | 0.69              |
| 1:C:103:MET:HG2  | 1:C:107:GLU:OE1  | 1.92                     | 0.69              |
| 1:C:134:LEU:CD1  | 1:C:138:LEU:CD1  | 2.71                     | 0.69              |
| 1:A:407:ASP:HB3  | 1:A:410:THR:HG23 | 1.74                     | 0.68              |
| 1:A:139:ILE:HD11 | 1:A:154:TYR:CE2  | 2.28                     | 0.68              |
| 1:C:56:THR:O     | 1:C:61:GLY:HA2   | 1.93                     | 0.68              |
| 1:A:139:ILE:O    | 1:A:142:LEU:HB2  | 1.94                     | 0.68              |
| 1:A:359:GLY:HA3  | 2:A:415:HEC:C3C  | 2.23                     | 0.68              |
| 1:A:373:GLU:HB3  | 1:A:377:ARG:NH1  | 2.09                     | 0.68              |
| 1:C:99:ILE:HG21  | 1:C:241:MET:HB2  | 1.73                     | 0.68              |
| 1:C:209:GLU:O    | 1:C:213:GLN:HG3  | 1.94                     | 0.68              |
| 1:A:191:MET:CE   | 1:A:196:ALA:HA   | 2.23                     | 0.68              |
| 1:C:130:ARG:HH12 | 1:C:165:LEU:HD11 | 1.58                     | 0.68              |
| 1:A:29:TYR:OH    | 1:A:88:ILE:O     | 2.06                     | 0.68              |
| 1:A:208:ILE:O    | 1:A:212:ARG:HG3  | 1.94                     | 0.68              |
| 1:C:61:GLY:O     | 1:C:62:HIS:HB3   | 1.93                     | 0.68              |
| 1:A:292:PHE:O    | 1:A:293:SER:C    | 2.32                     | 0.68              |
| 1:A:378:ILE:HG22 | 1:A:378:ILE:O    | 1.93                     | 0.68              |
| 1:A:19:PRO:HB2   | 1:A:21:HIS:ND1   | 2.10                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:203:TYR:O    | 1:A:206:PRO:HD2  | 1.93                     | 0.67              |
| 1:A:268:PRO:O    | 1:A:271:ARG:HB2  | 1.93                     | 0.67              |
| 1:A:414:VAL:CG1  | 1:A:414:VAL:OXT  | 2.42                     | 0.67              |
| 1:C:99:ILE:HG13  | 1:C:103:MET:HE1  | 1.76                     | 0.67              |
| 1:C:158:PHE:O    | 1:C:162:ILE:HD13 | 1.94                     | 0.67              |
| 1:C:287:GLU:OE1  | 1:C:342:ARG:HD2  | 1.94                     | 0.67              |
| 1:A:19:PRO:HB2   | 1:A:21:HIS:CE1   | 2.28                     | 0.67              |
| 1:C:205:ILE:N    | 1:C:206:PRO:HD2  | 2.08                     | 0.67              |
| 2:C:415:HEC:HMB1 | 2:C:415:HEC:CBB  | 1.89                     | 0.67              |
| 1:A:39:GLN:H     | 1:A:39:GLN:CD    | 1.96                     | 0.67              |
| 1:C:29:TYR:HE2   | 1:C:89:PRO:CD    | 2.07                     | 0.67              |
| 1:A:258:SER:O    | 1:A:259:PHE:C    | 2.32                     | 0.67              |
| 1:A:56:THR:O     | 1:A:61:GLY:HA2   | 1.95                     | 0.67              |
| 1:A:181:THR:HA   | 1:A:184:MET:HE3  | 1.77                     | 0.67              |
| 1:A:220:ILE:HG22 | 1:A:220:ILE:O    | 1.92                     | 0.67              |
| 1:A:377:ARG:HB3  | 1:A:412:LYS:O    | 1.95                     | 0.67              |
| 1:A:17:HIS:CD2   | 1:A:313:LYS:HD3  | 2.31                     | 0.66              |
| 1:A:98:PHE:CE2   | 1:A:243:GLY:C    | 2.69                     | 0.66              |
| 1:C:78:TYR:CE1   | 1:C:79:ARG:HD2   | 2.29                     | 0.66              |
| 1:C:103:MET:CE   | 1:C:107:GLU:OE1  | 2.44                     | 0.66              |
| 1:A:277:ARG:HH21 | 1:A:280:ARG:HH21 | 0.70                     | 0.66              |
| 1:C:257:LEU:HD21 | 1:C:367:ILE:HD13 | 1.78                     | 0.66              |
| 1:A:17:HIS:CD2   | 1:A:313:LYS:HD2  | 2.31                     | 0.65              |
| 1:A:112:ARG:NH1  | 2:A:415:HEC:O1D  | 2.26                     | 0.65              |
| 1:A:365:ARG:HD3  | 3:A:423:HOH:O    | 1.95                     | 0.65              |
| 1:A:384:ALA:CB   | 1:A:403:PRO:HB2  | 2.26                     | 0.65              |
| 1:A:363:ALA:HB1  | 2:A:415:HEC:HBB2 | 1.77                     | 0.65              |
| 1:A:277:ARG:HA   | 3:A:438:HOH:O    | 1.96                     | 0.65              |
| 1:C:290:ARG:NH1  | 1:C:335:PRO:O    | 2.30                     | 0.65              |
| 1:A:281:ILE:HG23 | 1:A:371:LEU:HD12 | 1.79                     | 0.65              |
| 1:C:130:ARG:HG3  | 1:C:165:LEU:HD21 | 1.79                     | 0.65              |
| 1:C:294:LEU:HD12 | 1:C:397:SER:O    | 1.97                     | 0.65              |
| 1:A:139:ILE:HD12 | 1:A:374:TRP:CE3  | 2.32                     | 0.65              |
| 1:C:88:ILE:HA    | 1:C:89:PRO:O     | 1.96                     | 0.65              |
| 1:A:151:THR:HG22 | 1:A:258:SER:OG   | 1.97                     | 0.64              |
| 1:A:269:GLU:HA   | 1:A:272:GLN:HB2  | 1.79                     | 0.64              |
| 1:C:287:GLU:OE1  | 1:C:345:VAL:HG13 | 1.97                     | 0.64              |
| 1:C:67:ARG:NH1   | 3:C:498:HOH:O    | 2.30                     | 0.64              |
| 1:C:100:PRO:HG3  | 1:C:112:ARG:HA   | 1.80                     | 0.64              |
| 1:C:131:ILE:CG2  | 1:C:131:ILE:CA   | 2.74                     | 0.64              |
| 1:C:365:ARG:O    | 1:C:369:VAL:HB   | 1.97                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:115:ALA:CB   | 1:A:358:LEU:HD13 | 2.28                     | 0.64              |
| 1:C:414:VAL:OXT  | 1:C:414:VAL:HG12 | 1.94                     | 0.64              |
| 1:C:149:ASN:ND2  | 1:C:151:THR:OG1  | 2.31                     | 0.64              |
| 1:C:112:ARG:CZ   | 1:C:358:LEU:HD21 | 2.26                     | 0.64              |
| 1:A:136:CYS:O    | 1:A:137:SER:C    | 2.35                     | 0.64              |
| 1:A:15:PRO:HG2   | 1:A:18:VAL:HG23  | 1.80                     | 0.64              |
| 1:A:177:LEU:HD13 | 1:A:246:LEU:HD12 | 1.79                     | 0.64              |
| 1:C:103:MET:HE2  | 1:C:107:GLU:OE1  | 1.98                     | 0.64              |
| 1:A:138:LEU:O    | 1:A:142:LEU:HG   | 1.97                     | 0.64              |
| 1:A:237:GLU:O    | 1:A:241:MET:N    | 2.31                     | 0.63              |
| 1:A:277:ARG:HB3  | 1:A:280:ARG:HG3  | 1.78                     | 0.63              |
| 1:C:205:ILE:CG2  | 1:C:206:PRO:CD   | 2.66                     | 0.63              |
| 1:A:71:ILE:HG21  | 1:A:325:SER:OG   | 1.97                     | 0.63              |
| 1:C:391:HIS:N    | 1:C:391:HIS:CD2  | 2.61                     | 0.63              |
| 1:C:204:LEU:O    | 1:C:207:ILE:HB   | 1.98                     | 0.63              |
| 1:C:99:ILE:HD11  | 1:C:240:ARG:NH2  | 2.14                     | 0.63              |
| 1:C:172:GLU:N    | 1:C:172:GLU:OE1  | 2.30                     | 0.63              |
| 1:A:33:ASN:HD22  | 1:A:44:VAL:HG11  | 1.61                     | 0.63              |
| 1:C:103:MET:SD   | 1:C:107:GLU:OE1  | 2.57                     | 0.63              |
| 1:C:369:VAL:CA   | 1:C:369:VAL:HB   | 2.15                     | 0.63              |
| 1:A:191:MET:HE2  | 1:A:196:ALA:N    | 2.14                     | 0.63              |
| 1:A:374:TRP:NE1  | 1:A:381:PHE:CE1  | 2.65                     | 0.63              |
| 1:A:216:GLY:H    | 1:A:221:SER:HB3  | 1.64                     | 0.62              |
| 1:A:205:ILE:N    | 1:A:206:PRO:HD2  | 2.14                     | 0.62              |
| 1:C:108:GLN:HE22 | 1:C:354:SER:HB2  | 1.64                     | 0.62              |
| 1:A:358:LEU:CD1  | 2:A:415:HEC:HBD2 | 2.30                     | 0.62              |
| 1:A:14:LEU:O     | 1:A:15:PRO:C     | 2.36                     | 0.62              |
| 1:C:262:GLU:HB2  | 1:C:402:LEU:HD13 | 1.81                     | 0.62              |
| 1:C:262:GLU:O    | 1:C:265:ALA:HB3  | 1.99                     | 0.62              |
| 1:C:301:LEU:N    | 1:C:301:LEU:CD2  | 2.62                     | 0.62              |
| 1:A:20:GLU:CD    | 1:C:165:LEU:CB   | 2.68                     | 0.62              |
| 1:C:144:PRO:HG2  | 1:C:145:GLN:N    | 2.15                     | 0.62              |
| 1:A:19:PRO:HD2   | 1:A:22:LEU:HD12  | 1.82                     | 0.62              |
| 1:A:20:GLU:OE1   | 1:C:165:LEU:O    | 2.17                     | 0.62              |
| 1:C:149:ASN:O    | 1:C:153:ASP:HB2  | 2.00                     | 0.62              |
| 1:A:20:GLU:OE1   | 1:C:165:LEU:HD12 | 2.00                     | 0.61              |
| 1:C:178:LYS:NZ   | 1:C:250:LEU:O    | 2.29                     | 0.61              |
| 1:C:273:GLU:OE2  | 1:C:280:ARG:NH1  | 2.32                     | 0.61              |
| 1:A:118:VAL:HG12 | 1:A:222:ILE:HD12 | 1.82                     | 0.61              |
| 1:A:377:ARG:C    | 1:A:379:PRO:HD3  | 2.21                     | 0.61              |
| 1:A:253:VAL:O    | 1:A:253:VAL:CG1  | 2.47                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:99:ILE:O     | 1:C:99:ILE:CG2   | 2.15                     | 0.61              |
| 1:C:277:ARG:HE   | 1:C:280:ARG:CZ   | 2.10                     | 0.61              |
| 1:A:88:ILE:HD13  | 1:A:319:LEU:HD13 | 1.82                     | 0.61              |
| 1:C:242:CYS:O    | 1:C:246:LEU:HD23 | 2.01                     | 0.61              |
| 1:A:72:ARG:HG3   | 1:A:72:ARG:HH11  | 1.64                     | 0.61              |
| 1:A:96:TYR:CZ    | 1:A:98:PHE:HB2   | 2.36                     | 0.61              |
| 1:C:181:THR:HA   | 1:C:184:MET:HE3  | 1.82                     | 0.61              |
| 1:C:341:SER:C    | 1:C:342:ARG:O    | 2.35                     | 0.61              |
| 1:A:149:ASN:ND2  | 1:A:151:THR:OG1  | 2.33                     | 0.61              |
| 1:C:173:ASP:HB3  | 1:C:177:LEU:HD11 | 1.82                     | 0.61              |
| 1:A:205:ILE:HG22 | 1:A:206:PRO:CD   | 2.30                     | 0.60              |
| 1:C:134:LEU:HD11 | 1:C:138:LEU:CD1  | 2.27                     | 0.60              |
| 1:C:159:PRO:HG3  | 1:C:257:LEU:HD12 | 1.83                     | 0.60              |
| 1:C:254:VAL:CG1  | 1:C:254:VAL:CG2  | 2.72                     | 0.60              |
| 1:C:267:SER:O    | 1:C:268:PRO:C    | 2.37                     | 0.60              |
| 1:C:290:ARG:NH2  | 1:C:337:HIS:O    | 2.34                     | 0.60              |
| 1:A:205:ILE:CG2  | 1:A:205:ILE:C    | 2.69                     | 0.60              |
| 1:A:206:PRO:HB2  | 1:A:207:ILE:HD12 | 1.83                     | 0.60              |
| 1:A:374:TRP:CD1  | 1:A:381:PHE:CE1  | 2.89                     | 0.60              |
| 1:A:404:LEU:CD1  | 1:A:404:LEU:CD2  | 2.76                     | 0.60              |
| 1:A:209:GLU:C    | 1:A:213:GLN:HE21 | 2.05                     | 0.60              |
| 1:A:251:ASP:O    | 1:A:396:VAL:HG11 | 2.02                     | 0.60              |
| 1:A:304:ASP:HA   | 1:A:313:LYS:HA   | 1.83                     | 0.60              |
| 1:A:358:LEU:HG   | 2:A:415:HEC:HBD2 | 1.83                     | 0.60              |
| 1:A:17:HIS:CG    | 1:A:313:LYS:HD3  | 2.37                     | 0.60              |
| 1:A:151:THR:CG2  | 1:A:151:THR:H    | 1.96                     | 0.60              |
| 1:A:240:ARG:CD   | 1:A:240:ARG:CB   | 2.77                     | 0.60              |
| 1:C:389:ILE:CG2  | 1:C:389:ILE:HB   | 2.19                     | 0.60              |
| 1:C:281:ILE:HB   | 1:C:282:PRO:HD3  | 1.84                     | 0.60              |
| 1:C:373:GLU:CG   | 1:C:373:GLU:CA   | 2.73                     | 0.60              |
| 1:A:277:ARG:N    | 1:A:278:PRO:CD   | 2.65                     | 0.59              |
| 1:C:111:PHE:O    | 1:C:112:ARG:C    | 2.28                     | 0.59              |
| 1:A:110:GLN:HE21 | 1:A:229:ASN:HA   | 1.66                     | 0.59              |
| 1:A:231:ARG:O    | 1:A:231:ARG:HD3  | 2.01                     | 0.59              |
| 1:A:272:GLN:CA   | 1:A:272:GLN:HE21 | 2.16                     | 0.59              |
| 1:C:257:LEU:HD23 | 1:C:367:ILE:CD1  | 2.32                     | 0.59              |
| 1:C:268:PRO:O    | 1:C:269:GLU:C    | 2.36                     | 0.59              |
| 1:A:237:GLU:HG2  | 1:A:240:ARG:HH22 | 1.63                     | 0.59              |
| 1:A:15:PRO:HG2   | 1:A:18:VAL:CG2   | 2.31                     | 0.59              |
| 1:A:96:TYR:CE1   | 1:A:102:SER:HB3  | 2.38                     | 0.59              |
| 1:C:177:LEU:HD21 | 1:C:203:TYR:CE2  | 2.38                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:39:GLN:H     | 1:C:39:GLN:NE2   | 2.00                     | 0.59              |
| 1:C:75:TYR:CZ    | 1:C:320:LEU:HB2  | 2.38                     | 0.59              |
| 1:C:142:LEU:HD22 | 1:C:148:CYS:HB3  | 1.84                     | 0.58              |
| 1:C:214:LYS:N    | 1:C:215:PRO:HD3  | 2.18                     | 0.58              |
| 1:C:287:GLU:HA   | 1:C:345:VAL:HG11 | 1.85                     | 0.58              |
| 1:C:395:ILE:H    | 1:C:395:ILE:CD1  | 2.16                     | 0.58              |
| 1:A:277:ARG:N    | 1:A:278:PRO:HD2  | 2.18                     | 0.58              |
| 1:C:11:LEU:N     | 1:C:11:LEU:CD1   | 2.66                     | 0.58              |
| 1:C:139:ILE:HD12 | 1:C:374:TRP:CE3  | 2.38                     | 0.58              |
| 1:A:99:ILE:HG12  | 1:A:103:MET:HE3  | 1.85                     | 0.58              |
| 1:A:220:ILE:O    | 1:A:220:ILE:CG2  | 2.52                     | 0.58              |
| 1:A:85:CYS:SG    | 1:A:317:GLN:NE2  | 2.77                     | 0.58              |
| 1:A:88:ILE:HD12  | 1:A:88:ILE:N     | 2.19                     | 0.58              |
| 1:A:88:ILE:HG23  | 1:A:89:PRO:HA    | 1.84                     | 0.58              |
| 1:A:209:GLU:O    | 1:A:213:GLN:CG   | 2.48                     | 0.58              |
| 1:A:407:ASP:OD1  | 1:A:409:ALA:HB3  | 2.04                     | 0.58              |
| 1:A:130:ARG:NH2  | 1:A:165:LEU:HD11 | 2.18                     | 0.58              |
| 1:A:121:MET:N    | 1:A:122:PRO:CD   | 2.67                     | 0.57              |
| 1:A:277:ARG:CB   | 1:A:280:ARG:HG3  | 2.34                     | 0.57              |
| 1:C:290:ARG:CZ   | 1:C:335:PRO:O    | 2.52                     | 0.57              |
| 1:A:181:THR:HA   | 1:A:184:MET:HE1  | 1.86                     | 0.57              |
| 1:A:201:TYR:CD1  | 1:A:239:LYS:HG2  | 2.39                     | 0.57              |
| 1:A:201:TYR:OH   | 1:A:240:ARG:HG2  | 2.03                     | 0.57              |
| 1:A:46:GLN:O     | 1:A:67:ARG:NH2   | 2.33                     | 0.57              |
| 1:A:143:ARG:HG3  | 1:A:411:THR:CB   | 2.33                     | 0.57              |
| 1:A:184:MET:HB3  | 1:A:193:PHE:HE1  | 1.70                     | 0.57              |
| 1:C:193:PHE:CD2  | 1:C:193:PHE:C    | 2.78                     | 0.57              |
| 1:C:205:ILE:H    | 1:C:206:PRO:HD3  | 1.67                     | 0.57              |
| 1:C:373:GLU:CB   | 1:C:373:GLU:CD   | 2.70                     | 0.57              |
| 1:A:288:LEU:CD2  | 1:A:292:PHE:HE2  | 2.18                     | 0.57              |
| 1:C:130:ARG:HH11 | 1:C:130:ARG:HG3  | 1.70                     | 0.57              |
| 1:C:148:CYS:SG   | 1:C:404:LEU:HD12 | 2.45                     | 0.57              |
| 1:A:341:SER:O    | 1:A:342:ARG:C    | 2.40                     | 0.56              |
| 1:A:378:ILE:O    | 1:A:381:PHE:HD1  | 1.88                     | 0.56              |
| 1:C:63:TRP:C     | 1:C:64:ILE:HD12  | 2.26                     | 0.56              |
| 1:C:96:TYR:HD2   | 1:C:193:PHE:CZ   | 2.22                     | 0.56              |
| 1:C:266:LYS:HD2  | 1:C:383:ILE:CD1  | 2.35                     | 0.56              |
| 1:A:207:ILE:HD12 | 1:A:207:ILE:N    | 2.20                     | 0.56              |
| 1:A:22:LEU:HD22  | 1:A:53:LEU:O     | 2.05                     | 0.56              |
| 1:A:237:GLU:CG   | 1:A:240:ARG:NH2  | 2.54                     | 0.56              |
| 1:A:256:PHE:HZ   | 1:A:288:LEU:C    | 2.09                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:272:GLN:CA   | 1:A:272:GLN:NE2  | 2.68                     | 0.56              |
| 1:C:356:LEU:HG   | 1:C:357:CYS:N    | 2.20                     | 0.56              |
| 1:A:156:GLU:O    | 1:A:160:ILE:HD12 | 2.05                     | 0.56              |
| 1:A:195:GLU:HA   | 1:A:195:GLU:OE1  | 2.06                     | 0.56              |
| 1:A:384:ALA:HB2  | 1:A:403:PRO:HB2  | 1.88                     | 0.56              |
| 1:C:174:ILE:O    | 1:C:175:PRO:C    | 2.41                     | 0.56              |
| 1:A:277:ARG:HD2  | 3:A:495:HOH:O    | 2.05                     | 0.56              |
| 1:A:100:PRO:HB2  | 2:A:415:HEC:O2D  | 2.06                     | 0.56              |
| 1:A:240:ARG:CG   | 1:A:240:ARG:NE   | 2.63                     | 0.56              |
| 1:A:205:ILE:CG2  | 1:A:205:ILE:CA   | 2.76                     | 0.56              |
| 1:C:377:ARG:C    | 1:C:378:ILE:HD12 | 2.25                     | 0.56              |
| 1:A:287:GLU:OE1  | 1:A:342:ARG:HD2  | 2.06                     | 0.56              |
| 1:C:235:SER:O    | 1:C:238:ALA:HB3  | 2.06                     | 0.56              |
| 1:C:355:HIS:ND1  | 2:C:415:HEC:O2D  | 2.39                     | 0.56              |
| 1:C:64:ILE:HD12  | 1:C:64:ILE:N     | 2.21                     | 0.56              |
| 1:C:184:MET:CE   | 1:C:200:LEU:HD22 | 2.35                     | 0.56              |
| 1:A:75:TYR:OH    | 1:A:322:GLN:NE2  | 2.39                     | 0.55              |
| 1:A:134:LEU:CD1  | 1:A:134:LEU:CD2  | 2.79                     | 0.55              |
| 1:C:29:TYR:CE2   | 1:C:89:PRO:HD3   | 2.40                     | 0.55              |
| 1:A:24:PHE:O     | 1:A:56:THR:HB    | 2.06                     | 0.55              |
| 1:C:369:VAL:CA   | 1:C:369:VAL:CG2  | 2.75                     | 0.55              |
| 1:C:100:PRO:CG   | 1:C:112:ARG:HA   | 2.36                     | 0.55              |
| 1:C:256:PHE:HD2  | 1:C:367:ILE:CD1  | 2.18                     | 0.55              |
| 1:C:14:LEU:HD11  | 1:C:18:VAL:HB    | 1.88                     | 0.55              |
| 1:C:29:TYR:CE2   | 1:C:89:PRO:CD    | 2.89                     | 0.55              |
| 1:C:191:MET:HE2  | 1:C:196:ALA:HA   | 1.88                     | 0.55              |
| 1:C:289:LEU:HD13 | 1:C:350:PHE:HE2  | 1.72                     | 0.55              |
| 1:A:228:VAL:O    | 1:A:231:ARG:CD   | 2.55                     | 0.55              |
| 1:A:20:GLU:OE1   | 1:C:165:LEU:CD1  | 2.55                     | 0.55              |
| 1:A:216:GLY:H    | 1:A:221:SER:CB   | 2.19                     | 0.55              |
| 1:C:131:ILE:HG23 | 1:C:158:PHE:CZ   | 2.42                     | 0.55              |
| 1:C:305:TYR:N    | 3:C:505:HOH:O    | 2.35                     | 0.55              |
| 1:A:409:ALA:CB   | 1:A:409:ALA:N    | 2.63                     | 0.54              |
| 1:A:205:ILE:HD11 | 1:A:239:LYS:HD2  | 1.89                     | 0.54              |
| 1:C:88:ILE:HD11  | 1:C:317:GLN:HB3  | 1.90                     | 0.54              |
| 1:A:20:GLU:CG    | 1:C:165:LEU:CG   | 2.83                     | 0.54              |
| 1:C:87:PHE:CD1   | 1:C:87:PHE:N     | 2.76                     | 0.54              |
| 1:A:372:LYS:O    | 1:A:376:THR:HB   | 2.08                     | 0.54              |
| 1:C:87:PHE:N     | 1:C:87:PHE:HD1   | 2.06                     | 0.54              |
| 1:C:147:GLN:HA   | 1:C:406:TRP:CZ3  | 2.43                     | 0.54              |
| 1:C:277:ARG:HB3  | 1:C:280:ARG:HG3  | 1.90                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:362:LEU:O    | 1:A:363:ALA:C    | 2.46                     | 0.54              |
| 1:A:409:ALA:CB   | 1:A:409:ALA:HA   | 2.18                     | 0.54              |
| 1:C:63:TRP:CE2   | 1:C:312:LEU:CD2  | 2.91                     | 0.54              |
| 1:C:407:ASP:O    | 1:C:410:THR:HG23 | 2.08                     | 0.54              |
| 1:A:184:MET:HB3  | 1:A:193:PHE:CE1  | 2.44                     | 0.53              |
| 1:A:127:LEU:HB3  | 1:A:131:ILE:CD1  | 2.39                     | 0.53              |
| 1:A:244:ALA:O    | 1:A:245:LEU:C    | 2.46                     | 0.53              |
| 1:A:264:LEU:CD2  | 1:A:264:LEU:CD1  | 2.84                     | 0.53              |
| 1:A:276:GLU:O    | 1:A:277:ARG:HG3  | 2.06                     | 0.53              |
| 1:A:358:LEU:HG   | 2:A:415:HEC:CBD  | 2.37                     | 0.53              |
| 1:A:288:LEU:HD23 | 1:A:292:PHE:CE2  | 2.43                     | 0.53              |
| 1:A:322:GLN:CG   | 1:A:351:GLY:HA2  | 2.38                     | 0.53              |
| 1:C:96:TYR:HD2   | 1:C:193:PHE:HZ   | 1.57                     | 0.53              |
| 1:C:121:MET:HB3  | 3:C:426:HOH:O    | 2.08                     | 0.53              |
| 1:A:99:ILE:HD11  | 1:A:240:ARG:NH2  | 2.24                     | 0.53              |
| 1:A:134:LEU:O    | 1:A:138:LEU:HB2  | 2.08                     | 0.53              |
| 1:A:138:LEU:HD22 | 1:A:158:PHE:HB2  | 1.90                     | 0.53              |
| 1:A:383:ILE:HD11 | 1:A:402:LEU:HD11 | 1.90                     | 0.53              |
| 1:C:377:ARG:NH1  | 1:C:377:ARG:HG3  | 2.23                     | 0.53              |
| 1:A:366:GLU:C    | 1:A:367:ILE:CA   | 2.64                     | 0.53              |
| 1:C:113:ALA:O    | 1:C:116:ASN:CB   | 2.56                     | 0.53              |
| 1:A:177:LEU:HD13 | 1:A:246:LEU:HD13 | 1.90                     | 0.53              |
| 1:C:78:TYR:CZ    | 1:C:79:ARG:NH1   | 2.76                     | 0.53              |
| 1:C:177:LEU:HD21 | 1:C:203:TYR:CD2  | 2.43                     | 0.53              |
| 1:A:139:ILE:HD11 | 1:A:154:TYR:CD2  | 2.44                     | 0.53              |
| 1:A:103:MET:HE1  | 1:A:107:GLU:CD   | 2.30                     | 0.52              |
| 1:A:205:ILE:CG2  | 1:A:206:PRO:HD3  | 2.38                     | 0.52              |
| 1:A:38:VAL:N     | 1:A:391:HIS:ND1  | 2.56                     | 0.52              |
| 1:A:125:ASP:HA   | 3:A:497:HOH:O    | 2.08                     | 0.52              |
| 1:C:106:PRO:O    | 1:C:107:GLU:C    | 2.47                     | 0.52              |
| 1:C:115:ALA:HB2  | 1:C:241:MET:HE1  | 1.92                     | 0.52              |
| 1:A:266:LYS:O    | 1:A:267:SER:HB2  | 2.08                     | 0.52              |
| 1:C:204:LEU:C    | 1:C:208:ILE:HD13 | 2.29                     | 0.52              |
| 1:A:182:ASP:OD2  | 1:A:186:ARG:NH2  | 2.42                     | 0.52              |
| 1:C:51:PRO:HD2   | 1:C:54:VAL:HG12  | 1.91                     | 0.52              |
| 1:C:63:TRP:CE2   | 1:C:312:LEU:HD23 | 2.44                     | 0.52              |
| 1:A:22:LEU:HD11  | 1:A:310:VAL:HG22 | 1.90                     | 0.52              |
| 1:C:253:VAL:HG23 | 2:C:415:HEC:HMC3 | 1.92                     | 0.52              |
| 1:A:389:ILE:CG2  | 1:A:389:ILE:CG1  | 2.78                     | 0.52              |
| 1:C:131:ILE:HG23 | 1:C:158:PHE:CE1  | 2.45                     | 0.52              |
| 1:C:134:LEU:CD1  | 1:C:138:LEU:HD11 | 2.26                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:119:VAL:HG11 | 2:A:415:HEC:HBC1 | 1.92                     | 0.52              |
| 1:A:167:ALA:HB1  | 1:A:220:ILE:HD11 | 1.92                     | 0.52              |
| 1:C:14:LEU:HD12  | 1:C:15:PRO:HG2   | 1.91                     | 0.52              |
| 1:C:185:THR:CA   | 1:C:395:ILE:HD13 | 2.30                     | 0.52              |
| 1:C:201:TYR:O    | 1:C:205:ILE:HB   | 2.10                     | 0.52              |
| 1:C:276:GLU:O    | 1:C:277:ARG:CG   | 2.56                     | 0.52              |
| 1:C:98:PHE:HA    | 1:C:240:ARG:O    | 2.10                     | 0.52              |
| 1:C:130:ARG:NH1  | 1:C:165:LEU:CD2  | 2.60                     | 0.52              |
| 1:C:204:LEU:O    | 1:C:208:ILE:HD13 | 2.10                     | 0.52              |
| 1:C:341:SER:O    | 1:C:342:ARG:O    | 2.27                     | 0.52              |
| 1:C:273:GLU:O    | 1:C:277:ARG:CB   | 2.56                     | 0.51              |
| 1:A:272:GLN:O    | 1:A:276:GLU:HG2  | 2.10                     | 0.51              |
| 1:A:312:LEU:HD23 | 1:A:312:LEU:N    | 2.25                     | 0.51              |
| 1:C:289:LEU:HD13 | 1:C:350:PHE:CE2  | 2.44                     | 0.51              |
| 1:A:118:VAL:CG1  | 1:A:219:ALA:HA   | 2.41                     | 0.51              |
| 1:A:288:LEU:HD23 | 1:A:292:PHE:HE2  | 1.75                     | 0.51              |
| 1:A:383:ILE:CD1  | 1:A:402:LEU:HD11 | 2.40                     | 0.51              |
| 1:C:100:PRO:CG   | 1:C:112:ARG:HB2  | 2.41                     | 0.51              |
| 1:C:313:LYS:O    | 1:C:316:ASP:HB2  | 2.10                     | 0.51              |
| 1:C:350:PHE:O    | 1:C:357:CYS:HB2  | 2.09                     | 0.51              |
| 1:C:109:ARG:HD3  | 3:C:443:HOH:O    | 2.11                     | 0.51              |
| 1:C:13:PRO:O     | 1:C:15:PRO:HD2   | 2.11                     | 0.51              |
| 1:C:191:MET:HE2  | 1:C:196:ALA:CA   | 2.40                     | 0.51              |
| 1:C:156:GLU:O    | 1:C:160:ILE:HB   | 2.11                     | 0.51              |
| 1:C:377:ARG:NH1  | 1:C:377:ARG:CG   | 2.73                     | 0.51              |
| 1:C:83:SER:HB3   | 1:C:101:THR:O    | 2.11                     | 0.51              |
| 1:C:106:PRO:HA   | 3:C:443:HOH:O    | 2.09                     | 0.51              |
| 1:A:276:GLU:C    | 1:A:278:PRO:HD2  | 2.31                     | 0.51              |
| 1:C:87:PHE:CE2   | 1:C:395:ILE:HG12 | 2.46                     | 0.51              |
| 1:A:211:ARG:HG3  | 1:A:221:SER:OG   | 2.11                     | 0.51              |
| 1:A:218:ASP:O    | 1:A:219:ALA:C    | 2.48                     | 0.51              |
| 1:A:276:GLU:O    | 1:A:277:ARG:CG   | 2.59                     | 0.50              |
| 1:C:40:GLU:CG    | 1:C:336:MET:HE2  | 2.30                     | 0.50              |
| 1:C:97:ASP:O     | 1:C:99:ILE:HD13  | 2.11                     | 0.50              |
| 1:C:294:LEU:O    | 1:C:294:LEU:HG   | 2.10                     | 0.50              |
| 1:A:24:PHE:HB3   | 1:A:54:VAL:HG21  | 1.94                     | 0.50              |
| 1:A:143:ARG:HH11 | 1:A:143:ARG:HG2  | 1.76                     | 0.50              |
| 1:A:276:GLU:C    | 1:A:277:ARG:CG   | 2.78                     | 0.50              |
| 1:A:207:ILE:N    | 1:A:207:ILE:CD1  | 2.75                     | 0.50              |
| 1:A:237:GLU:CB   | 1:A:240:ARG:HH21 | 2.23                     | 0.50              |
| 1:C:358:LEU:HG   | 2:C:415:HEC:HBD2 | 1.93                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:256:PHE:HZ   | 1:C:288:LEU:HB3  | 1.75                     | 0.50              |
| 1:A:97:ASP:OD1   | 1:A:97:ASP:N     | 2.28                     | 0.50              |
| 1:A:384:ALA:HA   | 1:A:405:VAL:HG21 | 1.90                     | 0.50              |
| 1:C:97:ASP:OD2   | 1:C:240:ARG:HD2  | 2.11                     | 0.50              |
| 1:A:23:VAL:HG12  | 1:A:23:VAL:O     | 2.11                     | 0.50              |
| 1:A:75:TYR:HE1   | 1:A:299:ARG:CZ   | 2.24                     | 0.50              |
| 1:C:18:VAL:HG11  | 1:C:55:TRP:CG    | 2.46                     | 0.50              |
| 1:C:88:ILE:CA    | 1:C:89:PRO:O     | 2.59                     | 0.50              |
| 1:C:112:ARG:O    | 1:C:113:ALA:C    | 2.49                     | 0.50              |
| 1:A:96:TYR:CZ    | 1:A:101:THR:OG1  | 2.64                     | 0.50              |
| 1:C:10:ASN:C     | 1:C:11:LEU:HD12  | 2.32                     | 0.50              |
| 1:C:137:SER:O    | 1:C:139:ILE:N    | 2.45                     | 0.50              |
| 1:C:191:MET:HE2  | 1:C:196:ALA:N    | 2.26                     | 0.50              |
| 1:A:88:ILE:HD12  | 1:A:88:ILE:H     | 1.77                     | 0.50              |
| 1:A:297:ASP:OD2  | 2:A:415:HEC:O2A  | 2.30                     | 0.50              |
| 1:A:384:ALA:HB3  | 1:A:403:PRO:HB2  | 1.93                     | 0.50              |
| 1:C:134:LEU:CD1  | 1:C:138:LEU:HD13 | 2.42                     | 0.50              |
| 1:A:72:ARG:HH11  | 1:A:72:ARG:CG    | 2.21                     | 0.49              |
| 1:C:377:ARG:HB3  | 1:C:378:ILE:HD12 | 1.93                     | 0.49              |
| 1:A:131:ILE:CD1  | 1:A:162:ILE:HD12 | 2.35                     | 0.49              |
| 1:C:111:PHE:CD2  | 1:C:228:VAL:HG21 | 2.44                     | 0.49              |
| 1:A:57:ARG:HA    | 1:A:61:GLY:HA2   | 1.94                     | 0.49              |
| 1:A:140:GLU:O    | 1:A:144:PRO:HD2  | 2.12                     | 0.49              |
| 1:C:15:PRO:HG3   | 1:C:55:TRP:CZ2   | 2.47                     | 0.49              |
| 1:C:91:GLU:HG2   | 3:C:472:HOH:O    | 2.12                     | 0.49              |
| 1:C:395:ILE:HD12 | 1:C:395:ILE:N    | 2.22                     | 0.49              |
| 1:A:17:HIS:CG    | 1:A:313:LYS:CD   | 2.95                     | 0.49              |
| 1:A:154:TYR:O    | 1:A:155:ALA:C    | 2.47                     | 0.49              |
| 1:C:114:LEU:HD23 | 1:C:233:ILE:HD12 | 1.94                     | 0.49              |
| 1:C:160:ILE:HG22 | 1:C:160:ILE:O    | 2.12                     | 0.49              |
| 1:C:251:ASP:O    | 1:C:255:ASN:ND2  | 2.45                     | 0.49              |
| 1:C:383:ILE:CD1  | 1:C:389:ILE:HD11 | 2.38                     | 0.49              |
| 1:A:98:PHE:CD2   | 1:A:244:ALA:N    | 2.81                     | 0.49              |
| 1:A:395:ILE:O    | 1:A:395:ILE:CG2  | 2.60                     | 0.49              |
| 1:A:228:VAL:O    | 1:A:231:ARG:HD2  | 2.13                     | 0.49              |
| 1:A:291:ARG:HG3  | 1:A:292:PHE:CZ   | 2.48                     | 0.49              |
| 1:C:29:TYR:CE2   | 1:C:89:PRO:HD2   | 2.48                     | 0.49              |
| 1:C:134:LEU:HD23 | 1:C:158:PHE:HA   | 1.94                     | 0.49              |
| 2:A:415:HEC:HMB1 | 2:A:415:HEC:HBB3 | 1.94                     | 0.49              |
| 1:C:257:LEU:CD2  | 1:C:367:ILE:CD1  | 2.88                     | 0.49              |
| 1:A:72:ARG:HD3   | 1:A:352:HIS:CE1  | 2.47                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:88:ILE:HD13  | 1:A:319:LEU:CD1  | 2.42                     | 0.49              |
| 1:C:131:ILE:HG22 | 1:C:131:ILE:O    | 2.13                     | 0.49              |
| 1:C:152:GLU:O    | 1:C:157:PRO:HD3  | 2.12                     | 0.49              |
| 1:A:362:LEU:HD23 | 2:A:415:HEC:HMC1 | 1.94                     | 0.48              |
| 1:C:33:ASN:O     | 1:C:36:ALA:HB3   | 2.13                     | 0.48              |
| 1:A:158:PHE:HD2  | 1:A:159:PRO:HD3  | 1.77                     | 0.48              |
| 1:C:49:ASN:H     | 1:C:49:ASN:HD22  | 1.61                     | 0.48              |
| 1:C:130:ARG:HH11 | 1:C:130:ARG:CG   | 2.18                     | 0.48              |
| 1:A:19:PRO:C     | 1:A:21:HIS:N     | 2.66                     | 0.48              |
| 1:C:256:PHE:HD2  | 1:C:367:ILE:HD11 | 1.76                     | 0.48              |
| 1:C:340:PHE:N    | 1:C:340:PHE:CD1  | 2.76                     | 0.48              |
| 1:C:389:ILE:CG2  | 1:C:399:VAL:HG13 | 2.43                     | 0.48              |
| 1:A:41:ALA:O     | 1:A:44:VAL:HG22  | 2.13                     | 0.48              |
| 1:A:92:ALA:O     | 1:A:96:TYR:N     | 2.34                     | 0.48              |
| 1:A:414:VAL:OXT  | 1:A:414:VAL:HG12 | 2.13                     | 0.48              |
| 1:A:127:LEU:HB3  | 1:A:131:ILE:HD11 | 1.95                     | 0.48              |
| 1:A:195:GLU:OE1  | 1:A:195:GLU:CA   | 2.60                     | 0.48              |
| 1:C:266:LYS:HD2  | 1:C:383:ILE:HD12 | 1.95                     | 0.48              |
| 1:A:118:VAL:HG23 | 1:A:119:VAL:HG13 | 1.96                     | 0.48              |
| 1:A:291:ARG:HD2  | 1:A:291:ARG:O    | 2.14                     | 0.48              |
| 1:A:359:GLY:HA3  | 2:A:415:HEC:C4C  | 2.43                     | 0.48              |
| 1:C:91:GLU:CD    | 1:C:91:GLU:N     | 2.59                     | 0.48              |
| 1:C:99:ILE:HG23  | 1:C:100:PRO:CD   | 2.43                     | 0.48              |
| 1:A:143:ARG:HH11 | 1:A:143:ARG:CG   | 2.25                     | 0.48              |
| 1:C:130:ARG:HG3  | 1:C:165:LEU:CD2  | 2.43                     | 0.48              |
| 1:C:392:LYS:HD2  | 1:C:392:LYS:HA   | 1.50                     | 0.48              |
| 1:A:61:GLY:O     | 1:A:62:HIS:HB3   | 2.13                     | 0.47              |
| 1:A:100:PRO:HG3  | 1:A:112:ARG:HA   | 1.96                     | 0.47              |
| 1:A:166:LEU:O    | 1:A:166:LEU:HD12 | 2.14                     | 0.47              |
| 1:A:191:MET:HE2  | 1:A:196:ALA:CA   | 2.44                     | 0.47              |
| 1:C:290:ARG:O    | 1:C:290:ARG:HG2  | 1.98                     | 0.47              |
| 1:A:20:GLU:CD    | 1:C:165:LEU:CD1  | 2.83                     | 0.47              |
| 1:A:383:ILE:HD13 | 1:A:404:LEU:CD2  | 2.44                     | 0.47              |
| 1:C:99:ILE:HD11  | 1:C:240:ARG:CZ   | 2.45                     | 0.47              |
| 1:C:100:PRO:O    | 1:C:355:HIS:HE1  | 1.97                     | 0.47              |
| 1:C:160:ILE:HG23 | 1:C:250:LEU:HD11 | 1.96                     | 0.47              |
| 1:A:143:ARG:HG2  | 1:A:143:ARG:NH1  | 2.30                     | 0.47              |
| 1:A:338:VAL:HG12 | 1:A:338:VAL:O    | 2.13                     | 0.47              |
| 1:C:234:THR:OG1  | 1:C:237:GLU:HG3  | 2.14                     | 0.47              |
| 1:A:267:SER:O    | 1:A:268:PRO:C    | 2.53                     | 0.47              |
| 1:A:167:ALA:HB1  | 1:A:220:ILE:CD1  | 2.45                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:414:VAL:OXT  | 1:A:414:VAL:HG13 | 2.15                     | 0.47              |
| 1:A:201:TYR:O    | 1:A:205:ILE:N    | 2.47                     | 0.47              |
| 1:A:364:ARG:O    | 1:A:365:ARG:C    | 2.53                     | 0.47              |
| 1:C:80:HIS:CD2   | 1:C:305:TYR:CG   | 3.03                     | 0.47              |
| 1:C:257:LEU:HD23 | 1:C:367:ILE:HD12 | 1.96                     | 0.47              |
| 1:A:11:LEU:HD21  | 1:A:25:ASP:OD2   | 2.15                     | 0.47              |
| 1:C:100:PRO:O    | 1:C:355:HIS:CE1  | 2.68                     | 0.47              |
| 1:A:121:MET:HB2  | 1:A:122:PRO:HD3  | 1.97                     | 0.47              |
| 1:A:150:PHE:CE1  | 1:A:261:MET:HG2  | 2.50                     | 0.47              |
| 1:A:313:LYS:HE2  | 3:A:505:HOH:O    | 2.13                     | 0.47              |
| 2:A:415:HEC:HHD  | 2:A:415:HEC:HAC  | 1.62                     | 0.47              |
| 1:C:295:VAL:O    | 1:C:322:GLN:N    | 2.46                     | 0.47              |
| 1:A:39:GLN:HB3   | 1:A:327:LEU:HD11 | 1.97                     | 0.46              |
| 1:A:213:GLN:O    | 1:A:215:PRO:HD3  | 2.15                     | 0.46              |
| 1:C:103:MET:CG   | 1:C:107:GLU:OE1  | 2.60                     | 0.46              |
| 1:C:265:ALA:HA   | 1:C:381:PHE:CE2  | 2.50                     | 0.46              |
| 1:A:115:ALA:CB   | 1:A:358:LEU:CD1  | 2.88                     | 0.46              |
| 1:A:164:MET:HE1  | 1:A:169:LEU:HB3  | 1.97                     | 0.46              |
| 1:C:261:MET:HB2  | 1:C:261:MET:HE3  | 1.58                     | 0.46              |
| 1:A:363:ALA:CB   | 2:A:415:HEC:HBB2 | 2.43                     | 0.46              |
| 1:C:391:HIS:N    | 1:C:391:HIS:HD2  | 2.11                     | 0.46              |
| 1:A:334:ALA:O    | 1:A:335:PRO:C    | 2.53                     | 0.46              |
| 1:C:256:PHE:CD2  | 1:C:367:ILE:CD1  | 2.98                     | 0.46              |
| 1:A:67:ARG:HD2   | 1:A:330:ARG:CZ   | 2.46                     | 0.46              |
| 1:A:266:LYS:O    | 1:A:267:SER:CB   | 2.63                     | 0.46              |
| 1:A:272:GLN:HE21 | 1:A:272:GLN:C    | 2.18                     | 0.46              |
| 1:A:378:ILE:O    | 1:A:381:PHE:CD1  | 2.68                     | 0.46              |
| 1:C:155:ALA:O    | 1:C:254:VAL:HG22 | 2.15                     | 0.46              |
| 1:A:201:TYR:CG   | 1:A:239:LYS:HE3  | 2.51                     | 0.46              |
| 1:C:42:TRP:C     | 1:C:44:VAL:N     | 2.68                     | 0.46              |
| 1:C:114:LEU:CD2  | 1:C:233:ILE:HD12 | 2.45                     | 0.46              |
| 1:C:205:ILE:N    | 1:C:206:PRO:HD3  | 2.23                     | 0.46              |
| 1:C:377:ARG:CG   | 1:C:377:ARG:HH11 | 2.24                     | 0.46              |
| 1:A:19:PRO:C     | 1:A:21:HIS:H     | 2.18                     | 0.46              |
| 1:C:186:ARG:O    | 1:C:187:PRO:C    | 2.51                     | 0.46              |
| 1:A:82:SER:HB2   | 1:A:104:ASP:OD2  | 2.16                     | 0.46              |
| 1:A:257:LEU:CA   | 1:A:258:SER:N    | 2.64                     | 0.46              |
| 1:C:88:ILE:C     | 1:C:89:PRO:O     | 2.54                     | 0.46              |
| 1:C:266:LYS:HD2  | 1:C:383:ILE:HD11 | 1.96                     | 0.46              |
| 1:C:149:ASN:O    | 1:C:153:ASP:CB   | 2.63                     | 0.46              |
| 1:C:243:GLY:O    | 1:C:244:ALA:O    | 2.34                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:301:LEU:N    | 1:C:301:LEU:HD23 | 2.31                     | 0.45              |
| 1:A:98:PHE:CD2   | 1:A:243:GLY:C    | 2.90                     | 0.45              |
| 1:A:207:ILE:O    | 1:A:208:ILE:C    | 2.50                     | 0.45              |
| 1:C:100:PRO:HG2  | 1:C:112:ARG:HB2  | 1.98                     | 0.45              |
| 1:A:15:PRO:HA    | 1:A:16:PRO:HD2   | 1.79                     | 0.45              |
| 1:A:373:GLU:HB3  | 1:A:377:ARG:HH12 | 1.80                     | 0.45              |
| 1:C:294:LEU:N    | 1:C:294:LEU:HD23 | 2.30                     | 0.45              |
| 1:C:402:LEU:HA   | 1:C:403:PRO:HD3  | 1.85                     | 0.45              |
| 1:A:38:VAL:HG11  | 1:A:397:SER:HB3  | 1.98                     | 0.45              |
| 1:A:39:GLN:N     | 1:A:39:GLN:CD    | 2.67                     | 0.45              |
| 1:A:15:PRO:CG    | 1:A:18:VAL:HG23  | 2.47                     | 0.45              |
| 1:A:108:GLN:HE22 | 1:A:354:SER:HB2  | 1.80                     | 0.45              |
| 1:A:358:LEU:CG   | 2:A:415:HEC:HBD2 | 2.47                     | 0.45              |
| 1:A:367:ILE:N    | 1:A:367:ILE:CB   | 2.64                     | 0.45              |
| 1:C:10:ASN:C     | 1:C:10:ASN:OD1   | 2.55                     | 0.45              |
| 1:C:18:VAL:HA    | 1:C:19:PRO:HD3   | 1.57                     | 0.45              |
| 1:C:249:GLY:C    | 1:C:250:LEU:HD12 | 2.37                     | 0.45              |
| 1:C:134:LEU:HD12 | 1:C:138:LEU:CD1  | 2.47                     | 0.45              |
| 1:C:143:ARG:O    | 1:C:144:PRO:C    | 2.51                     | 0.45              |
| 1:A:359:GLY:HA3  | 2:A:415:HEC:C2C  | 2.46                     | 0.45              |
| 1:C:293:SER:HB2  | 1:C:349:THR:OG1  | 2.17                     | 0.45              |
| 1:C:201:TYR:O    | 1:C:204:LEU:N    | 2.40                     | 0.45              |
| 1:C:205:ILE:H    | 1:C:206:PRO:HD2  | 1.72                     | 0.45              |
| 1:C:311:GLN:CD   | 3:C:505:HOH:O    | 2.55                     | 0.45              |
| 1:C:359:GLY:HA3  | 2:C:415:HEC:C3C  | 2.46                     | 0.45              |
| 1:A:136:CYS:SG   | 1:A:377:ARG:NH2  | 2.90                     | 0.45              |
| 1:C:14:LEU:HA    | 1:C:15:PRO:HD2   | 1.54                     | 0.45              |
| 1:A:20:GLU:OE2   | 1:C:165:LEU:CB   | 2.65                     | 0.44              |
| 1:C:134:LEU:O    | 1:C:134:LEU:HG   | 2.17                     | 0.44              |
| 1:C:233:ILE:O    | 1:C:233:ILE:HG23 | 2.17                     | 0.44              |
| 1:A:130:ARG:HG3  | 1:A:165:LEU:HD21 | 1.99                     | 0.44              |
| 1:A:261:MET:HG3  | 1:A:404:LEU:CD1  | 2.47                     | 0.44              |
| 1:C:43:ALA:C     | 1:C:45:LEU:N     | 2.68                     | 0.44              |
| 1:C:137:SER:O    | 1:C:138:LEU:C    | 2.55                     | 0.44              |
| 1:A:71:ILE:HG21  | 1:A:325:SER:HG   | 1.81                     | 0.44              |
| 1:A:164:MET:CE   | 1:A:169:LEU:HB3  | 2.47                     | 0.44              |
| 1:C:114:LEU:HD22 | 1:C:228:VAL:CG1  | 2.47                     | 0.44              |
| 1:C:245:LEU:O    | 1:C:247:VAL:N    | 2.51                     | 0.44              |
| 1:C:327:LEU:O    | 1:C:335:PRO:HB3  | 2.18                     | 0.44              |
| 1:A:19:PRO:CB    | 1:A:21:HIS:CE1   | 2.98                     | 0.44              |
| 1:C:98:PHE:CD1   | 1:C:98:PHE:N     | 2.85                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:253:VAL:CG2  | 2:C:415:HEC:HMC3 | 2.47                     | 0.44              |
| 1:C:395:ILE:O    | 1:C:396:VAL:HG23 | 2.17                     | 0.44              |
| 1:A:99:ILE:HG12  | 1:A:103:MET:CE   | 2.48                     | 0.44              |
| 1:C:19:PRO:HG2   | 1:C:22:LEU:HD12  | 2.00                     | 0.44              |
| 1:C:75:TYR:CE2   | 1:C:320:LEU:HB2  | 2.53                     | 0.44              |
| 1:C:99:ILE:HG12  | 1:C:240:ARG:HH21 | 1.82                     | 0.44              |
| 1:A:187:PRO:HD2  | 3:A:440:HOH:O    | 2.17                     | 0.44              |
| 1:A:392:LYS:HE3  | 1:A:392:LYS:HB3  | 1.87                     | 0.44              |
| 1:C:99:ILE:CD1   | 1:C:240:ARG:NH2  | 2.79                     | 0.44              |
| 1:C:304:ASP:N    | 1:C:314:LYS:H    | 2.16                     | 0.44              |
| 1:A:261:MET:HG3  | 1:A:404:LEU:HD11 | 1.99                     | 0.44              |
| 1:C:83:SER:O     | 1:C:86:PRO:HD3   | 2.17                     | 0.44              |
| 1:A:131:ILE:CD1  | 1:A:131:ILE:N    | 2.81                     | 0.44              |
| 1:A:358:LEU:HD12 | 2:A:415:HEC:HBD2 | 1.99                     | 0.44              |
| 1:A:171:GLU:C    | 1:A:173:ASP:H    | 2.21                     | 0.44              |
| 1:A:191:MET:HE2  | 1:A:196:ALA:HA   | 1.96                     | 0.44              |
| 1:A:354:SER:OG   | 1:A:355:HIS:CD2  | 2.71                     | 0.44              |
| 1:C:243:GLY:O    | 1:C:244:ALA:C    | 2.49                     | 0.44              |
| 1:C:378:ILE:N    | 1:C:379:PRO:HD3  | 2.32                     | 0.44              |
| 1:A:149:ASN:C    | 1:A:149:ASN:HD22 | 2.22                     | 0.43              |
| 1:C:365:ARG:O    | 1:C:369:VAL:CB   | 2.65                     | 0.43              |
| 1:A:121:MET:HB2  | 1:A:122:PRO:CD   | 2.48                     | 0.43              |
| 1:A:258:SER:O    | 1:A:262:GLU:HB2  | 2.18                     | 0.43              |
| 1:C:204:LEU:O    | 1:C:208:ILE:CD1  | 2.65                     | 0.43              |
| 1:C:209:GLU:O    | 1:C:213:GLN:CG   | 2.64                     | 0.43              |
| 1:C:406:TRP:O    | 1:C:408:PRO:HD3  | 2.18                     | 0.43              |
| 1:A:72:ARG:HG3   | 1:A:72:ARG:NH1   | 2.32                     | 0.43              |
| 1:A:269:GLU:H    | 1:A:269:GLU:HG3  | 1.66                     | 0.43              |
| 1:C:364:ARG:HG3  | 1:C:364:ARG:HH11 | 1.84                     | 0.43              |
| 1:A:112:ARG:HD2  | 2:A:415:HEC:O1D  | 2.18                     | 0.43              |
| 1:A:187:PRO:HB3  | 3:A:472:HOH:O    | 2.19                     | 0.43              |
| 1:A:205:ILE:O    | 1:A:209:GLU:HG3  | 2.19                     | 0.43              |
| 1:C:112:ARG:CD   | 1:C:112:ARG:CB   | 2.83                     | 0.43              |
| 1:C:334:ALA:HA   | 1:C:335:PRO:HD2  | 1.89                     | 0.43              |
| 1:A:107:GLU:O    | 1:A:108:GLN:C    | 2.54                     | 0.43              |
| 1:C:239:LYS:HE3  | 1:C:239:LYS:HB3  | 1.70                     | 0.43              |
| 1:A:158:PHE:O    | 1:A:162:ILE:HG12 | 2.19                     | 0.43              |
| 1:C:395:ILE:C    | 1:C:396:VAL:HG23 | 2.39                     | 0.43              |
| 1:A:72:ARG:O     | 1:A:76:GLU:HG3   | 2.18                     | 0.43              |
| 1:A:149:ASN:HB3  | 1:A:152:GLU:HG3  | 2.00                     | 0.43              |
| 1:C:99:ILE:O     | 1:C:241:MET:HA   | 2.19                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:389:ILE:H    | 1:C:389:ILE:HG13 | 1.49                     | 0.43              |
| 1:A:78:TYR:CZ    | 1:A:105:PRO:HB2  | 2.53                     | 0.43              |
| 1:A:96:TYR:CD1   | 1:A:102:SER:HB3  | 2.54                     | 0.43              |
| 1:A:108:GLN:HE21 | 1:A:108:GLN:HB3  | 1.23                     | 0.43              |
| 1:A:298:GLY:C    | 1:A:299:ARG:HD3  | 2.35                     | 0.43              |
| 1:A:389:ILE:CG2  | 1:A:389:ILE:C    | 2.87                     | 0.43              |
| 1:C:143:ARG:HG3  | 1:C:411:THR:HG21 | 2.00                     | 0.43              |
| 1:C:205:ILE:CB   | 1:C:206:PRO:HD3  | 2.42                     | 0.43              |
| 1:A:67:ARG:HD2   | 1:A:330:ARG:NH1  | 2.34                     | 0.42              |
| 1:A:228:VAL:C    | 1:A:230:GLY:H    | 2.22                     | 0.42              |
| 1:C:63:TRP:CZ2   | 1:C:312:LEU:HD23 | 2.54                     | 0.42              |
| 1:C:139:ILE:CD1  | 1:C:374:TRP:HE3  | 2.32                     | 0.42              |
| 1:A:19:PRO:CD    | 1:A:22:LEU:HD12  | 2.47                     | 0.42              |
| 1:A:45:LEU:HD12  | 1:A:324:LEU:HD11 | 2.01                     | 0.42              |
| 1:C:71:ILE:HD13  | 1:C:321:PRO:O    | 2.19                     | 0.42              |
| 1:C:405:VAL:O    | 1:C:406:TRP:HB3  | 2.18                     | 0.42              |
| 1:A:138:LEU:HD23 | 1:A:154:TYR:HD2  | 1.78                     | 0.42              |
| 1:A:186:ARG:O    | 1:A:187:PRO:C    | 2.55                     | 0.42              |
| 1:C:81:PHE:HB3   | 1:C:299:ARG:HG3  | 2.01                     | 0.42              |
| 1:A:322:GLN:NE2  | 2:A:415:HEC:HBA2 | 2.34                     | 0.42              |
| 1:A:51:PRO:HD2   | 1:A:54:VAL:HG12  | 2.01                     | 0.42              |
| 1:A:262:GLU:HA   | 1:A:402:LEU:HD21 | 2.01                     | 0.42              |
| 1:A:272:GLN:NE2  | 1:A:272:GLN:HA   | 2.33                     | 0.42              |
| 1:C:58:CYS:O     | 1:C:59:ASN:C     | 2.57                     | 0.42              |
| 1:C:125:ASP:O    | 1:C:126:LYS:C    | 2.52                     | 0.42              |
| 1:C:163:PHE:CG   | 1:C:249:GLY:HA3  | 2.55                     | 0.42              |
| 1:A:130:ARG:CZ   | 1:A:165:LEU:HD11 | 2.50                     | 0.42              |
| 1:A:135:ALA:O    | 1:A:139:ILE:HG12 | 2.19                     | 0.42              |
| 1:A:139:ILE:HG23 | 1:A:378:ILE:HD12 | 2.01                     | 0.42              |
| 1:A:220:ILE:N    | 1:A:220:ILE:HD12 | 2.34                     | 0.42              |
| 1:C:275:ILE:CD1  | 1:C:379:PRO:HB3  | 2.50                     | 0.42              |
| 1:A:254:VAL:O    | 1:A:254:VAL:HG12 | 2.18                     | 0.42              |
| 1:A:375:LEU:O    | 1:A:379:PRO:HG3  | 2.19                     | 0.42              |
| 1:C:254:VAL:CG1  | 1:C:254:VAL:O    | 2.68                     | 0.42              |
| 1:C:324:LEU:O    | 1:C:325:SER:C    | 2.55                     | 0.42              |
| 1:C:356:LEU:HG   | 1:C:357:CYS:H    | 1.81                     | 0.42              |
| 1:A:131:ILE:HD12 | 1:A:162:ILE:CD1  | 2.36                     | 0.42              |
| 1:C:143:ARG:HD2  | 1:C:411:THR:HB   | 2.02                     | 0.42              |
| 1:A:56:THR:OG1   | 1:A:58:CYS:HB2   | 2.20                     | 0.42              |
| 1:A:363:ALA:O    | 1:A:367:ILE:HD12 | 2.19                     | 0.42              |
| 1:C:239:LYS:HE2  | 1:C:239:LYS:HB2  | 1.84                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:140:GLU:CD   | 1:A:143:ARG:HE   | 2.23                     | 0.41              |
| 1:A:171:GLU:C    | 1:A:173:ASP:N    | 2.72                     | 0.41              |
| 1:A:330:ARG:H    | 1:A:330:ARG:HG3  | 1.63                     | 0.41              |
| 1:C:84:GLU:HA    | 1:C:102:SER:O    | 2.20                     | 0.41              |
| 1:C:134:LEU:HD12 | 1:C:138:LEU:HD13 | 2.02                     | 0.41              |
| 1:C:274:LEU:HD23 | 1:C:274:LEU:HA   | 1.78                     | 0.41              |
| 1:C:110:GLN:H    | 1:C:110:GLN:HG2  | 1.71                     | 0.41              |
| 1:C:112:ARG:HG3  | 1:C:358:LEU:HD11 | 2.02                     | 0.41              |
| 1:C:134:LEU:O    | 1:C:138:LEU:HD13 | 2.20                     | 0.41              |
| 1:C:131:ILE:CG2  | 1:C:158:PHE:CZ   | 3.03                     | 0.41              |
| 1:C:166:LEU:C    | 1:C:166:LEU:CD1  | 2.80                     | 0.41              |
| 1:C:181:THR:HA   | 1:C:184:MET:CE   | 2.48                     | 0.41              |
| 1:C:281:ILE:HB   | 1:C:282:PRO:CD   | 2.50                     | 0.41              |
| 1:C:285:CYS:SG   | 1:C:367:ILE:HG21 | 2.60                     | 0.41              |
| 1:C:311:GLN:NE2  | 3:C:505:HOH:O    | 2.53                     | 0.41              |
| 1:A:364:ARG:O    | 1:A:368:ILE:HG12 | 2.19                     | 0.41              |
| 1:C:322:GLN:N    | 1:C:322:GLN:OE1  | 2.54                     | 0.41              |
| 1:C:109:ARG:O    | 1:C:110:GLN:C    | 2.58                     | 0.41              |
| 1:C:173:ASP:HB3  | 1:C:177:LEU:CD1  | 2.50                     | 0.41              |
| 1:C:399:VAL:CG2  | 1:C:399:VAL:CA   | 2.89                     | 0.41              |
| 1:C:131:ILE:CG2  | 1:C:131:ILE:O    | 2.68                     | 0.41              |
| 1:A:256:PHE:HZ   | 1:A:289:LEU:N    | 2.18                     | 0.41              |
| 1:C:233:ILE:H    | 1:C:233:ILE:HG22 | 1.60                     | 0.41              |
| 1:A:14:LEU:HA    | 1:A:14:LEU:HD12  | 1.72                     | 0.41              |
| 1:A:78:TYR:CG    | 1:A:105:PRO:HD2  | 2.56                     | 0.41              |
| 1:A:88:ILE:CG2   | 1:A:89:PRO:HA    | 2.50                     | 0.41              |
| 1:A:150:PHE:HB3  | 1:A:402:LEU:HB3  | 2.02                     | 0.41              |
| 1:C:99:ILE:HG21  | 1:C:241:MET:HE3  | 2.02                     | 0.41              |
| 1:C:131:ILE:CG2  | 1:C:131:ILE:C    | 2.89                     | 0.41              |
| 1:C:369:VAL:CA   | 1:C:369:VAL:CG1  | 2.83                     | 0.41              |
| 1:A:254:VAL:HG23 | 3:A:494:HOH:O    | 2.21                     | 0.40              |
| 1:A:256:PHE:CE1  | 1:A:292:PHE:HB2  | 2.56                     | 0.40              |
| 1:C:201:TYR:HB3  | 1:C:239:LYS:HD2  | 2.03                     | 0.40              |
| 1:C:277:ARG:CZ   | 1:C:280:ARG:HH21 | 2.28                     | 0.40              |
| 1:C:365:ARG:HE   | 1:C:369:VAL:HG23 | 1.86                     | 0.40              |
| 1:C:395:ILE:O    | 1:C:396:VAL:CG2  | 2.69                     | 0.40              |
| 1:A:75:TYR:CE1   | 1:A:299:ARG:CZ   | 3.04                     | 0.40              |
| 1:A:160:ILE:HG23 | 1:A:250:LEU:HG   | 2.03                     | 0.40              |
| 1:A:270:HIS:O    | 1:A:271:ARG:C    | 2.59                     | 0.40              |
| 1:A:407:ASP:HB3  | 1:A:410:THR:CG2  | 2.46                     | 0.40              |
| 1:C:155:ALA:O    | 1:C:159:PRO:CD   | 2.69                     | 0.40              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:C:262:GLU:HA  | 1:C:402:LEU:HD11 | 2.03                     | 0.40              |
| 1:C:109:ARG:NH1 | 3:C:443:HOH:O    | 2.54                     | 0.40              |
| 2:C:415:HEC:HHB | 2:C:415:HEC:HMA1 | 1.86                     | 0.40              |
| 1:A:130:ARG:HD2 | 1:A:130:ARG:HA   | 1.50                     | 0.40              |
| 1:A:229:ASN:HA  | 1:A:229:ASN:HD22 | 1.47                     | 0.40              |
| 1:A:262:GLU:HG3 | 1:A:402:LEU:HD13 | 2.04                     | 0.40              |
| 1:A:291:ARG:HG3 | 1:A:292:PHE:CD1  | 2.56                     | 0.40              |
| 1:C:256:PHE:HD2 | 1:C:367:ILE:HD12 | 1.87                     | 0.40              |
| 1:A:298:GLY:O   | 1:A:299:ARG:CD   | 2.46                     | 0.40              |

All (23) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:A:109:ARG:NH2 | 1:A:176:HIS:CB[2_545]  | 1.02                     | 1.18              |
| 1:C:109:ARG:NH2 | 1:C:176:HIS:CB[2_546]  | 1.05                     | 1.15              |
| 1:C:107:GLU:OE2 | 1:C:410:THR:CG2[1_455] | 1.48                     | 0.72              |
| 1:C:110:GLN:OE1 | 1:C:176:HIS:ND1[2_546] | 1.54                     | 0.66              |
| 1:A:110:GLN:OE1 | 1:A:176:HIS:ND1[2_545] | 1.59                     | 0.61              |
| 1:A:110:GLN:OE1 | 1:A:176:HIS:CE1[2_545] | 1.63                     | 0.57              |
| 1:C:110:GLN:OE1 | 1:C:176:HIS:CE1[2_546] | 1.77                     | 0.43              |
| 1:A:109:ARG:CZ  | 1:A:176:HIS:CB[2_545]  | 1.82                     | 0.38              |
| 1:C:109:ARG:CZ  | 1:C:176:HIS:CB[2_546]  | 1.82                     | 0.38              |
| 1:A:107:GLU:OE2 | 1:A:410:THR:CG2[1_455] | 1.83                     | 0.37              |
| 1:C:110:GLN:CD  | 1:C:176:HIS:ND1[2_546] | 1.89                     | 0.31              |
| 1:C:172:GLU:OE2 | 1:C:276:GLU:OE2[2_656] | 1.89                     | 0.31              |
| 1:C:116:ASN:ND2 | 1:C:202:ASP:OD2[2_546] | 1.93                     | 0.27              |
| 1:A:109:ARG:NH2 | 1:A:176:HIS:CA[2_545]  | 1.94                     | 0.26              |
| 1:C:109:ARG:NH2 | 1:C:176:HIS:CA[2_546]  | 1.95                     | 0.25              |
| 1:A:172:GLU:OE2 | 1:A:276:GLU:OE2[2_655] | 2.03                     | 0.17              |
| 1:A:109:ARG:NH2 | 1:A:176:HIS:CG[2_545]  | 2.06                     | 0.14              |
| 1:A:116:ASN:ND2 | 1:A:202:ASP:OD2[2_545] | 2.07                     | 0.13              |
| 1:C:109:ARG:NE  | 1:C:176:HIS:CD2[2_546] | 2.09                     | 0.11              |
| 1:C:109:ARG:CZ  | 1:C:176:HIS:CG[2_546]  | 2.12                     | 0.08              |
| 1:C:107:GLU:OE2 | 1:C:410:THR:CB[1_455]  | 2.13                     | 0.07              |
| 1:A:116:ASN:ND2 | 1:A:202:ASP:OD1[2_545] | 2.17                     | 0.03              |
| 1:A:209:GLU:OE2 | 1:A:356:LEU:CD2[2_555] | 2.17                     | 0.03              |

## 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     | 403/414 (97%) | 345 (86%) | 38 (9%)  | 20 (5%)  | 2           | 0 |
| 1   | C     | 403/414 (97%) | 336 (83%) | 49 (12%) | 18 (4%)  | 2           | 0 |
| All | All   | 806/828 (97%) | 681 (84%) | 87 (11%) | 38 (5%)  | 2           | 0 |

All (38) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 90  | ARG  |
| 1   | A     | 246 | LEU  |
| 1   | A     | 278 | PRO  |
| 1   | A     | 282 | PRO  |
| 1   | A     | 293 | SER  |
| 1   | C     | 47  | GLU  |
| 1   | C     | 52  | ASP  |
| 1   | C     | 98  | PHE  |
| 1   | C     | 137 | SER  |
| 1   | C     | 244 | ALA  |
| 1   | C     | 246 | LEU  |
| 1   | C     | 271 | ARG  |
| 1   | A     | 52  | ASP  |
| 1   | A     | 168 | GLY  |
| 1   | A     | 329 | GLU  |
| 1   | C     | 89  | PRO  |
| 1   | C     | 245 | LEU  |
| 1   | C     | 314 | LYS  |
| 1   | C     | 342 | ARG  |
| 1   | A     | 110 | GLN  |
| 1   | A     | 137 | SER  |
| 1   | A     | 172 | GLU  |
| 1   | A     | 251 | ASP  |
| 1   | A     | 268 | PRO  |
| 1   | C     | 138 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 36  | ALA  |
| 1   | A     | 138 | LEU  |
| 1   | A     | 244 | ALA  |
| 1   | A     | 338 | VAL  |
| 1   | A     | 365 | ARG  |
| 1   | C     | 229 | ASN  |
| 1   | C     | 293 | SER  |
| 1   | C     | 356 | LEU  |
| 1   | A     | 16  | PRO  |
| 1   | C     | 363 | ALA  |
| 1   | C     | 369 | VAL  |
| 1   | A     | 277 | ARG  |
| 1   | C     | 174 | ILE  |

### 5.3.2 Protein sidechains [i](#)

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     | 347/356 (98%) | 309 (89%) | 38 (11%) | 6           | 3 |
| 1   | C     | 347/356 (98%) | 303 (87%) | 44 (13%) | 4           | 1 |
| All | All   | 694/712 (98%) | 612 (88%) | 82 (12%) | 5           | 2 |

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

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 16  | PRO  |
| 1   | A     | 39  | GLN  |
| 1   | A     | 47  | GLU  |
| 1   | A     | 57  | ARG  |
| 1   | A     | 70  | LEU  |
| 1   | A     | 82  | SER  |
| 1   | A     | 83  | SER  |
| 1   | A     | 88  | ILE  |
| 1   | A     | 99  | ILE  |
| 1   | A     | 101 | THR  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | A            | 105        | PRO         |
| 1          | A            | 108        | GLN         |
| 1          | A            | 109        | ARG         |
| 1          | A            | 118        | VAL         |
| 1          | A            | 131        | ILE         |
| 1          | A            | 141        | SER         |
| 1          | A            | 143        | ARG         |
| 1          | A            | 149        | ASN         |
| 1          | A            | 158        | PHE         |
| 1          | A            | 166        | LEU         |
| 1          | A            | 223        | VAL         |
| 1          | A            | 231        | ARG         |
| 1          | A            | 232        | PRO         |
| 1          | A            | 233        | ILE         |
| 1          | A            | 261        | MET         |
| 1          | A            | 268        | PRO         |
| 1          | A            | 269        | GLU         |
| 1          | A            | 291        | ARG         |
| 1          | A            | 313        | LYS         |
| 1          | A            | 335        | PRO         |
| 1          | A            | 342        | ARG         |
| 1          | A            | 344        | LYS         |
| 1          | A            | 365        | ARG         |
| 1          | A            | 380        | ASP         |
| 1          | A            | 382        | SER         |
| 1          | A            | 388        | GLN         |
| 1          | A            | 392        | LYS         |
| 1          | A            | 412        | LYS         |
| 1          | C            | 16         | PRO         |
| 1          | C            | 39         | GLN         |
| 1          | C            | 49         | ASN         |
| 1          | C            | 79         | ARG         |
| 1          | C            | 86         | PRO         |
| 1          | C            | 87         | PHE         |
| 1          | C            | 91         | GLU         |
| 1          | C            | 99         | ILE         |
| 1          | C            | 101        | THR         |
| 1          | C            | 121        | MET         |
| 1          | C            | 126        | LYS         |
| 1          | C            | 133        | GLU         |
| 1          | C            | 138        | LEU         |
| 1          | C            | 140        | GLU         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | C            | 143        | ARG         |
| 1          | C            | 144        | PRO         |
| 1          | C            | 147        | GLN         |
| 1          | C            | 149        | ASN         |
| 1          | C            | 166        | LEU         |
| 1          | C            | 182        | ASP         |
| 1          | C            | 193        | PHE         |
| 1          | C            | 211        | ARG         |
| 1          | C            | 212        | ARG         |
| 1          | C            | 213        | GLN         |
| 1          | C            | 229        | ASN         |
| 1          | C            | 231        | ARG         |
| 1          | C            | 232        | PRO         |
| 1          | C            | 239        | LYS         |
| 1          | C            | 241        | MET         |
| 1          | C            | 246        | LEU         |
| 1          | C            | 264        | LEU         |
| 1          | C            | 268        | PRO         |
| 1          | C            | 272        | GLN         |
| 1          | C            | 276        | GLU         |
| 1          | C            | 301        | LEU         |
| 1          | C            | 312        | LEU         |
| 1          | C            | 323        | MET         |
| 1          | C            | 325        | SER         |
| 1          | C            | 344        | LYS         |
| 1          | C            | 385        | PRO         |
| 1          | C            | 388        | GLN         |
| 1          | C            | 395        | ILE         |
| 1          | C            | 405        | VAL         |
| 1          | C            | 410        | THR         |

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

| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | A            | 17         | HIS         |
| 1          | A            | 33         | ASN         |
| 1          | A            | 39         | GLN         |
| 1          | A            | 46         | GLN         |
| 1          | A            | 108        | GLN         |
| 1          | A            | 110        | GLN         |
| 1          | A            | 149        | ASN         |
| 1          | A            | 229        | ASN         |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 272 | GLN  |
| 1   | A     | 317 | GLN  |
| 1   | A     | 343 | GLN  |
| 1   | A     | 355 | HIS  |
| 1   | C     | 30  | ASN  |
| 1   | C     | 39  | GLN  |
| 1   | C     | 46  | GLN  |
| 1   | C     | 49  | ASN  |
| 1   | C     | 59  | ASN  |
| 1   | C     | 80  | HIS  |
| 1   | C     | 108 | GLN  |
| 1   | C     | 129 | ASN  |
| 1   | C     | 149 | ASN  |
| 1   | C     | 272 | GLN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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



| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 2   | HEC  | C     | 415 | 3,1  | 32,50,50     | 3.89 | 19 (59%) | 24,82,82    | 4.24 | 12 (50%) |
| 2   | HEC  | A     | 415 | 3,1  | 32,50,50     | 3.46 | 16 (50%) | 24,82,82    | 3.00 | 10 (41%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings |
|-----|------|-------|-----|------|---------|------------|-------|
| 2   | HEC  | C     | 415 | 3,1  | -       | 2/10/54/54 | -     |
| 2   | HEC  | A     | 415 | 3,1  | -       | 6/10/54/54 | -     |

All (35) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 2   | C     | 415 | HEC  | C2B-C3B | -12.78 | 1.27        | 1.40     |
| 2   | A     | 415 | HEC  | C2B-C3B | -11.37 | 1.28        | 1.40     |
| 2   | C     | 415 | HEC  | CMD-C2D | 8.01   | 1.68        | 1.51     |
| 2   | A     | 415 | HEC  | CAD-C3D | 6.81   | 1.62        | 1.52     |
| 2   | A     | 415 | HEC  | CAA-C2A | 5.69   | 1.62        | 1.52     |
| 2   | C     | 415 | HEC  | CAD-C3D | 5.68   | 1.60        | 1.52     |
| 2   | C     | 415 | HEC  | C4D-CHA | -5.47  | 1.25        | 1.41     |
| 2   | C     | 415 | HEC  | C3D-C2D | 5.03   | 1.52        | 1.37     |
| 2   | A     | 415 | HEC  | CBB-CAB | -4.68  | 1.31        | 1.49     |
| 2   | C     | 415 | HEC  | CBC-CAC | -4.37  | 1.33        | 1.49     |
| 2   | A     | 415 | HEC  | C4B-C3B | 4.28   | 1.50        | 1.43     |
| 2   | C     | 415 | HEC  | C1D-CHD | -4.25  | 1.29        | 1.41     |
| 2   | C     | 415 | HEC  | CMC-C2C | 4.24   | 1.61        | 1.51     |
| 2   | C     | 415 | HEC  | C1B-CHB | -4.09  | 1.29        | 1.41     |
| 2   | A     | 415 | HEC  | C3D-C2D | 4.06   | 1.49        | 1.37     |
| 2   | C     | 415 | HEC  | CBB-CAB | -3.81  | 1.35        | 1.49     |
| 2   | A     | 415 | HEC  | O1A-CGA | -3.70  | 1.09        | 1.22     |
| 2   | A     | 415 | HEC  | CMD-C2D | 3.67   | 1.59        | 1.51     |
| 2   | A     | 415 | HEC  | CBC-CAC | -3.64  | 1.35        | 1.49     |
| 2   | C     | 415 | HEC  | C1B-NB  | -3.59  | 1.28        | 1.36     |
| 2   | A     | 415 | HEC  | C3C-C2C | -3.50  | 1.37        | 1.40     |
| 2   | C     | 415 | HEC  | C1D-ND  | -3.24  | 1.29        | 1.36     |
| 2   | C     | 415 | HEC  | CMB-C2B | 3.09   | 1.58        | 1.51     |
| 2   | A     | 415 | HEC  | C1D-CHD | -2.99  | 1.32        | 1.41     |
| 2   | A     | 415 | HEC  | C2A-C1A | 2.93   | 1.49        | 1.42     |
| 2   | A     | 415 | HEC  | O2D-CGD | -2.91  | 1.21        | 1.30     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | A     | 415 | HEC  | C1C-NC  | 2.78  | 1.41        | 1.36     |
| 2   | C     | 415 | HEC  | CBD-CGD | 2.62  | 1.56        | 1.50     |
| 2   | A     | 415 | HEC  | CBD-CGD | 2.51  | 1.56        | 1.50     |
| 2   | C     | 415 | HEC  | C3C-C4C | 2.43  | 1.47        | 1.43     |
| 2   | C     | 415 | HEC  | C4D-ND  | 2.38  | 1.41        | 1.36     |
| 2   | C     | 415 | HEC  | O2A-CGA | -2.29 | 1.23        | 1.30     |
| 2   | C     | 415 | HEC  | C1C-CHC | -2.21 | 1.34        | 1.41     |
| 2   | A     | 415 | HEC  | CMC-C2C | 2.20  | 1.56        | 1.51     |
| 2   | C     | 415 | HEC  | C1C-NC  | -2.04 | 1.32        | 1.36     |

All (22) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 2   | C     | 415 | HEC  | CMB-C2B-C3B | -11.70 | 112.06      | 125.82   |
| 2   | C     | 415 | HEC  | CMB-C2B-C1B | 9.76   | 143.47      | 128.46   |
| 2   | C     | 415 | HEC  | CMC-C2C-C3C | 6.67   | 133.66      | 125.82   |
| 2   | A     | 415 | HEC  | CMC-C2C-C3C | 6.06   | 132.95      | 125.82   |
| 2   | A     | 415 | HEC  | O2A-CGA-CBA | 5.87   | 132.88      | 114.03   |
| 2   | C     | 415 | HEC  | C4C-C3C-C2C | 5.86   | 112.68      | 106.35   |
| 2   | C     | 415 | HEC  | O2D-CGD-O1D | -5.72  | 109.05      | 123.30   |
| 2   | A     | 415 | HEC  | O1A-CGA-CBA | -5.28  | 106.11      | 123.08   |
| 2   | C     | 415 | HEC  | O2D-CGD-CBD | 4.95   | 129.94      | 114.03   |
| 2   | A     | 415 | HEC  | CMA-C3A-C2A | 4.85   | 134.09      | 124.94   |
| 2   | A     | 415 | HEC  | CMB-C2B-C3B | -4.55  | 120.47      | 125.82   |
| 2   | A     | 415 | HEC  | CMC-C2C-C1C | -4.14  | 122.10      | 128.46   |
| 2   | A     | 415 | HEC  | C3B-C4B-NB  | -4.06  | 103.28      | 110.94   |
| 2   | C     | 415 | HEC  | CAA-C2A-C3A | -3.80  | 116.32      | 127.25   |
| 2   | C     | 415 | HEC  | CAD-C3D-C2D | 3.11   | 136.19      | 127.25   |
| 2   | A     | 415 | HEC  | O2D-CGD-O1D | -3.02  | 115.78      | 123.30   |
| 2   | A     | 415 | HEC  | C2B-C3B-C4B | 2.92   | 109.50      | 106.35   |
| 2   | C     | 415 | HEC  | O2A-CGA-O1A | -2.78  | 116.36      | 123.30   |
| 2   | C     | 415 | HEC  | C3B-C4B-NB  | 2.69   | 116.02      | 110.94   |
| 2   | C     | 415 | HEC  | C3C-C4C-NC  | -2.66  | 105.93      | 110.94   |
| 2   | C     | 415 | HEC  | CBA-CAA-C2A | -2.53  | 108.33      | 112.60   |
| 2   | A     | 415 | HEC  | CMD-C2D-C3D | -2.12  | 120.95      | 124.94   |

There are no chirality outliers.

All (8) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | A     | 415 | HEC  | C1A-C2A-CAA-CBA |
| 2   | A     | 415 | HEC  | C3A-C2A-CAA-CBA |

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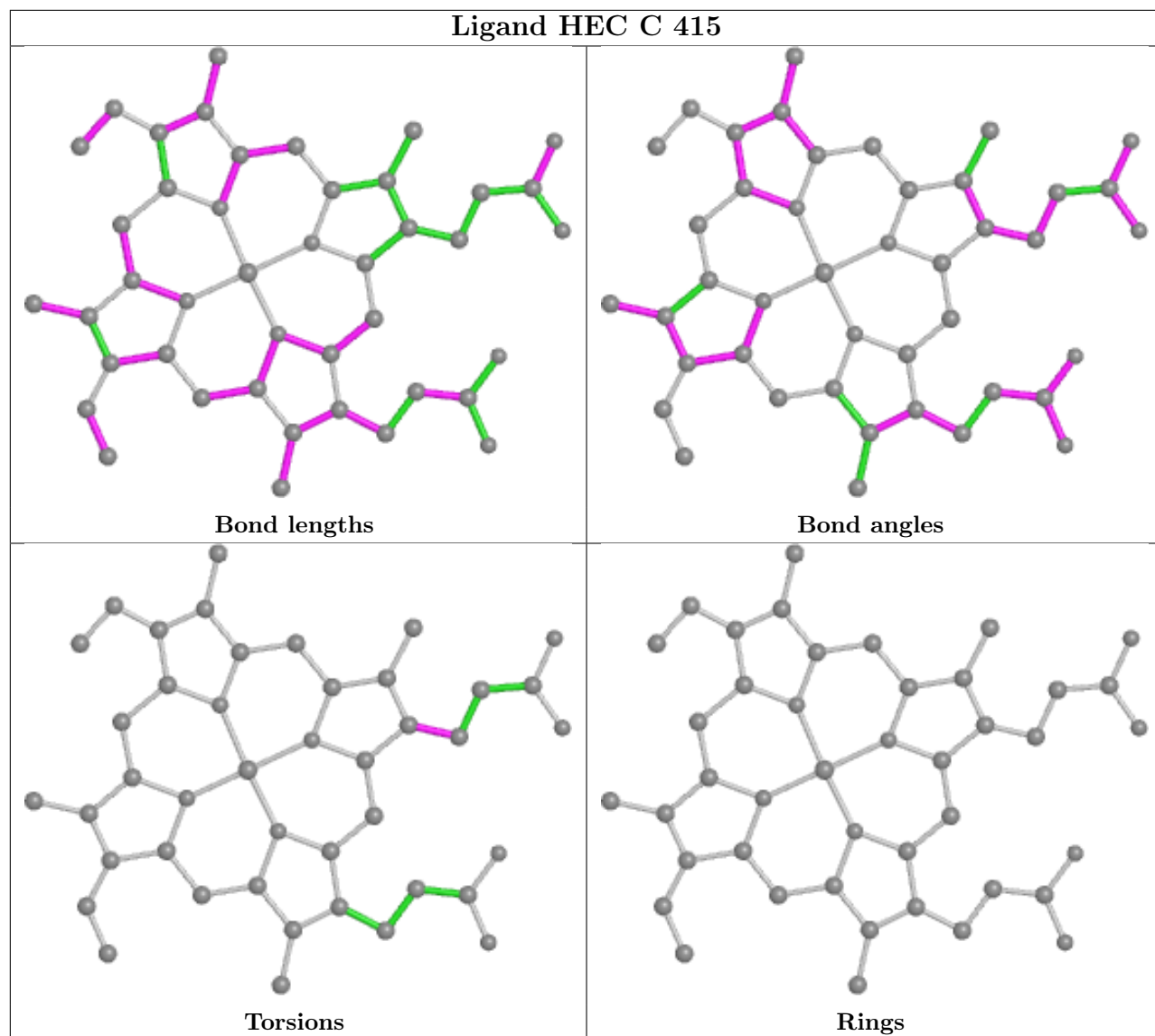
| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | C     | 415 | HEC  | C1A-C2A-CAA-CBA |
| 2   | C     | 415 | HEC  | C3A-C2A-CAA-CBA |
| 2   | A     | 415 | HEC  | CAA-CBA-CGA-O1A |
| 2   | A     | 415 | HEC  | CAA-CBA-CGA-O2A |
| 2   | A     | 415 | HEC  | CAD-CBD-CGD-O2D |
| 2   | A     | 415 | HEC  | CAD-CBD-CGD-O1D |

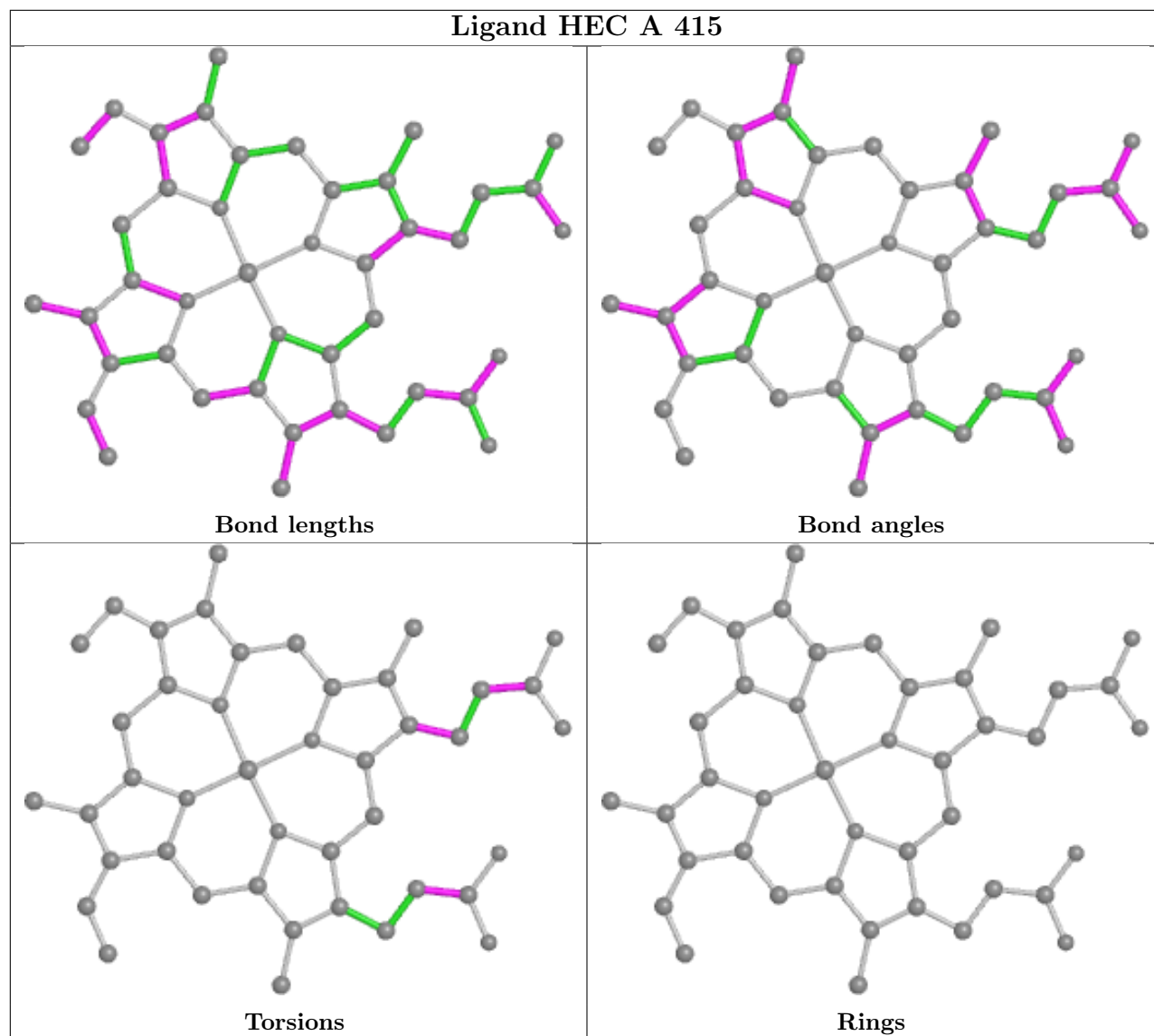
There are no ring outliers.

2 monomers are involved in 28 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2   | C     | 415 | HEC  | 9       | 0            |
| 2   | A     | 415 | HEC  | 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.





## 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     | 405/414 (97%) | 0.77   | 30 (7%) 14 20 | 8, 24, 36, 49         | 0     |
| 1   | C     | 405/414 (97%) | 0.73   | 23 (5%) 23 32 | 11, 24, 34, 44        | 0     |
| All | All   | 810/828 (97%) | 0.75   | 53 (6%) 18 25 | 8, 24, 36, 49         | 0     |

All (53) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 414 | VAL  | 7.6  |
| 1   | A     | 214 | LYS  | 6.0  |
| 1   | C     | 246 | LEU  | 5.9  |
| 1   | C     | 229 | ASN  | 5.8  |
| 1   | C     | 19  | PRO  | 4.4  |
| 1   | A     | 229 | ASN  | 4.3  |
| 1   | A     | 246 | LEU  | 4.1  |
| 1   | A     | 230 | GLY  | 4.1  |
| 1   | A     | 389 | ILE  | 4.1  |
| 1   | C     | 414 | VAL  | 3.8  |
| 1   | A     | 215 | PRO  | 3.7  |
| 1   | A     | 278 | PRO  | 3.5  |
| 1   | A     | 121 | MET  | 3.4  |
| 1   | A     | 213 | GLN  | 3.3  |
| 1   | A     | 228 | VAL  | 3.2  |
| 1   | C     | 121 | MET  | 3.2  |
| 1   | A     | 19  | PRO  | 3.2  |
| 1   | C     | 214 | LYS  | 3.2  |
| 1   | C     | 220 | ILE  | 3.2  |
| 1   | A     | 10  | ASN  | 3.1  |
| 1   | A     | 264 | LEU  | 3.0  |
| 1   | A     | 383 | ILE  | 2.9  |
| 1   | A     | 313 | LYS  | 2.9  |
| 1   | A     | 88  | ILE  | 2.9  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 70  | LEU  | 2.9  |
| 1   | C     | 10  | ASN  | 2.7  |
| 1   | C     | 122 | PRO  | 2.6  |
| 1   | A     | 343 | GLN  | 2.6  |
| 1   | C     | 230 | GLY  | 2.6  |
| 1   | C     | 274 | LEU  | 2.5  |
| 1   | A     | 165 | LEU  | 2.4  |
| 1   | C     | 133 | GLU  | 2.4  |
| 1   | A     | 18  | VAL  | 2.4  |
| 1   | A     | 101 | THR  | 2.3  |
| 1   | A     | 205 | ILE  | 2.3  |
| 1   | C     | 395 | ILE  | 2.3  |
| 1   | A     | 200 | LEU  | 2.3  |
| 1   | C     | 213 | GLN  | 2.3  |
| 1   | C     | 234 | THR  | 2.2  |
| 1   | A     | 109 | ARG  | 2.2  |
| 1   | A     | 350 | PHE  | 2.2  |
| 1   | A     | 244 | ALA  | 2.2  |
| 1   | A     | 386 | GLY  | 2.2  |
| 1   | C     | 215 | PRO  | 2.2  |
| 1   | C     | 278 | PRO  | 2.2  |
| 1   | A     | 250 | LEU  | 2.1  |
| 1   | C     | 227 | GLN  | 2.1  |
| 1   | C     | 383 | ILE  | 2.1  |
| 1   | C     | 208 | ILE  | 2.1  |
| 1   | C     | 257 | LEU  | 2.1  |
| 1   | C     | 333 | ALA  | 2.1  |
| 1   | A     | 202 | ASP  | 2.0  |
| 1   | C     | 235 | SER  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

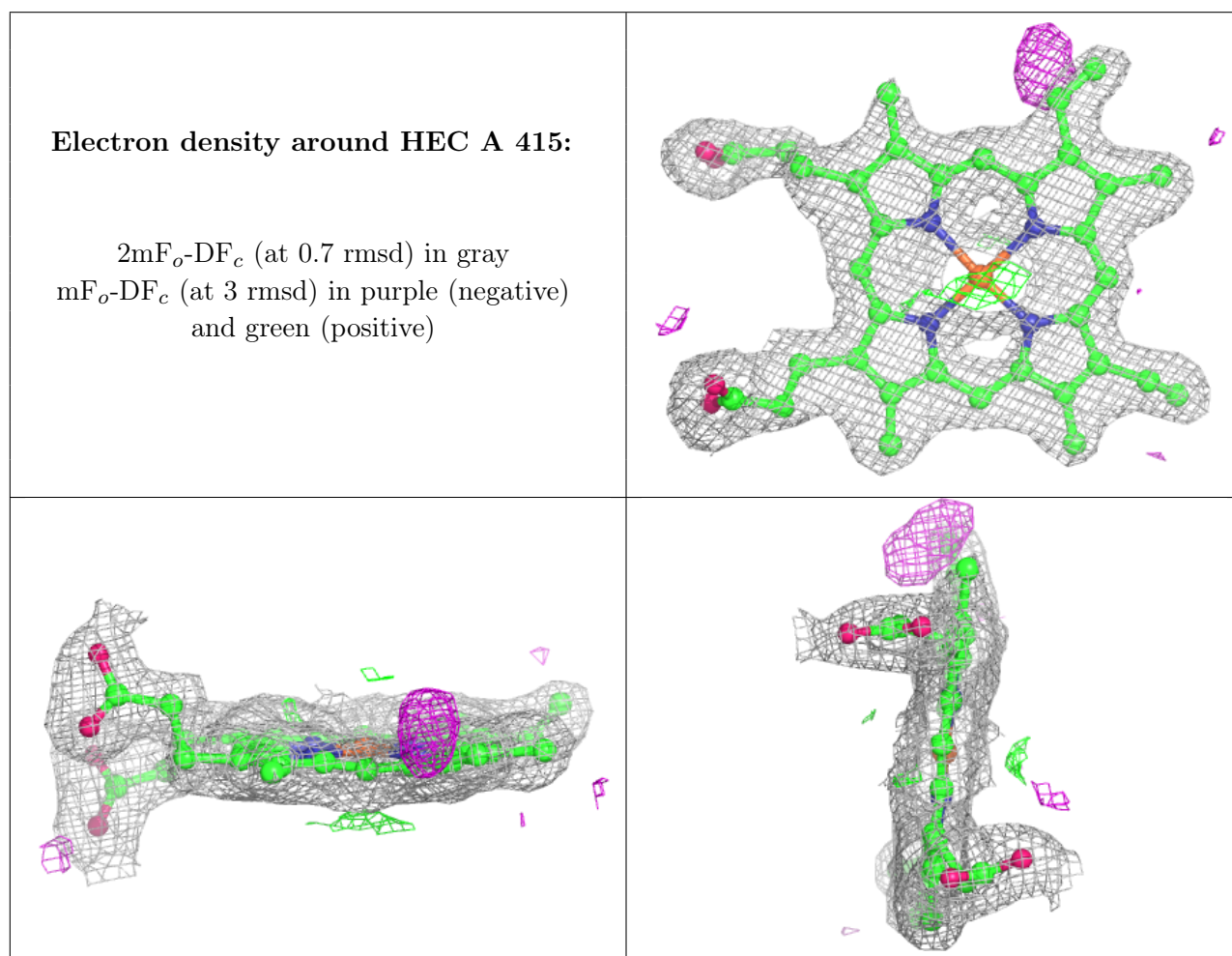
There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

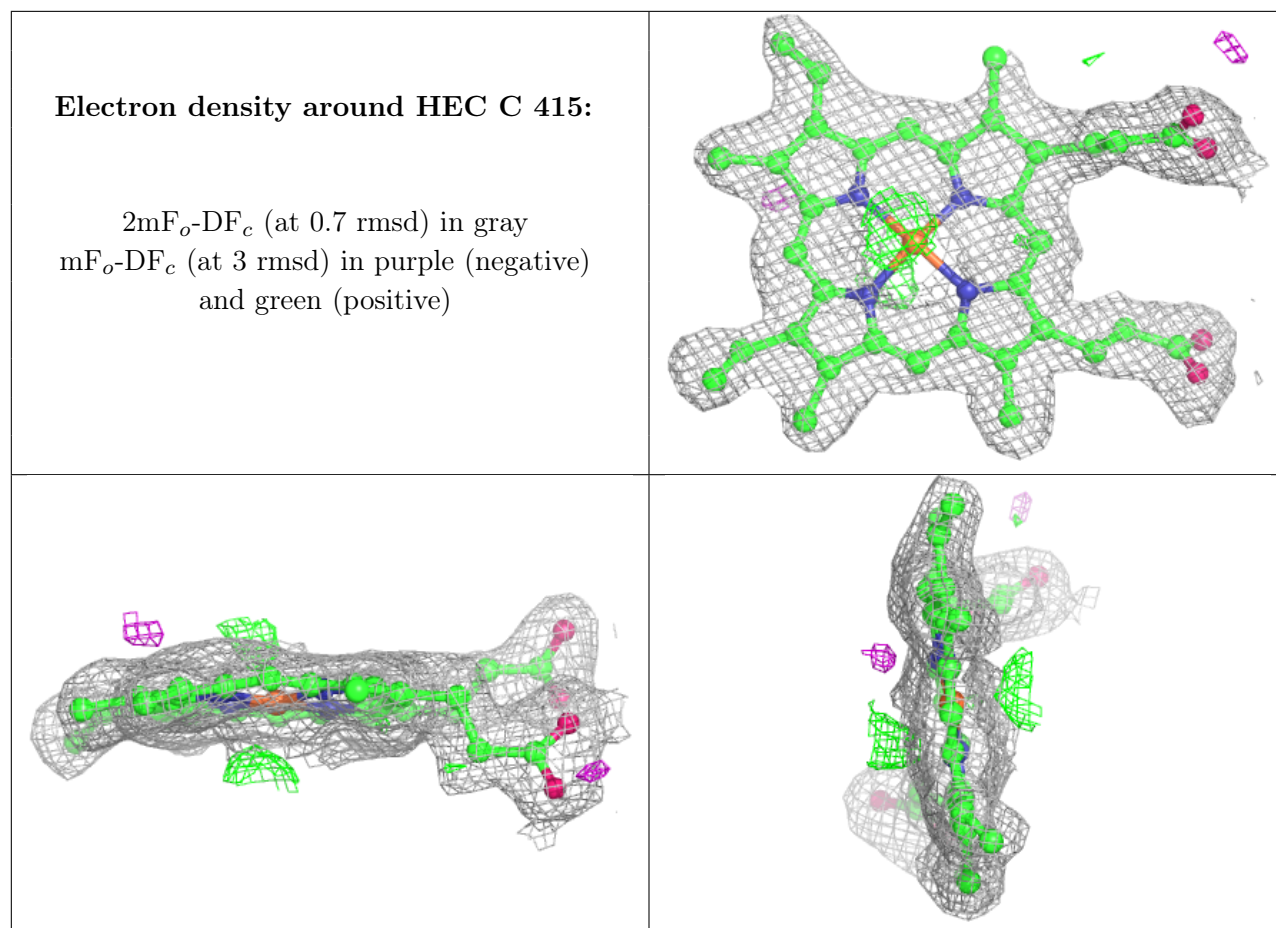
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 2   | HEC  | A     | 415 | 43/43 | 0.94 | 0.16 | 13,15,17,18                | 0     |
| 2   | HEC  | C     | 415 | 43/43 | 0.94 | 0.14 | 13,18,20,21                | 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.







## 6.5 Other polymers [i](#)

There are no such residues in this entry.