



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 10:29 PM UTC

PDB ID : 2HWB / pdb\_00002hwb  
Title : A comparison of the anti-rhinoviral drug binding pocket in hrv14 and hrv1a  
Authors : Kim, K.H.; Rossmann, M.G.  
Deposited on : 1994-01-25  
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                     |
| Xtriage (Phenix)               | : | NOT EXECUTED                                                     |
| EDS                            | : | NOT EXECUTED                                                     |
| Buster-report                  | : | wwPDB partial adaption of 1.1.7 (2018)                           |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

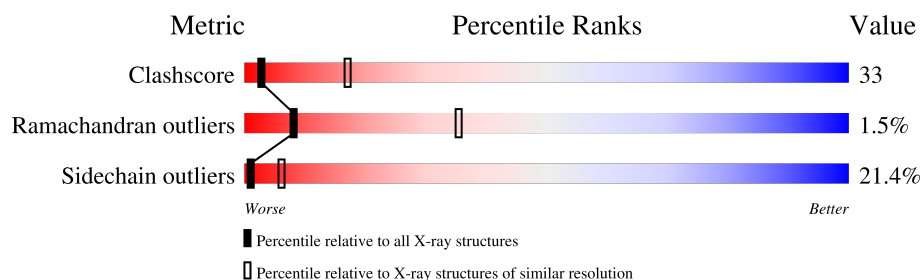
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| Clashscore            | 190562                      | 2977 (3.00-3.00)                                      |
| Ramachandran outliers | 187476                      | 2877 (3.00-3.00)                                      |
| Sidechain outliers    | 187428                      | 2880 (3.00-3.00)                                      |

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

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain    |
|-----|-------|--------|---------------------|
| 1   | 1     | 289    | 25% 40% 23% 6% 6%   |
| 2   | 2     | 262    | 25% 37% 27% 8% .    |
| 3   | 3     | 236    | 25% 38% 29% 8%      |
| 4   | 4     | 68     | 13% 21% 15% 10% 41% |

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6290 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 HUMAN RHINOVIRUS 14 COAT PROTEIN (SUBUNIT VP1).

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | 1     | 273      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2170  | 1373 | 375 | 414 | 8 |         |         |       |

- Molecule 2 is a protein called HUMAN RHINOVIRUS 14 COAT PROTEIN (SUBUNIT VP2).

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 2   | 2     | 255      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1951  | 1237 | 330 | 372 | 12 |         |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| 2     | 170     | VAL      | ILE    | conflict | UNP P03303 |

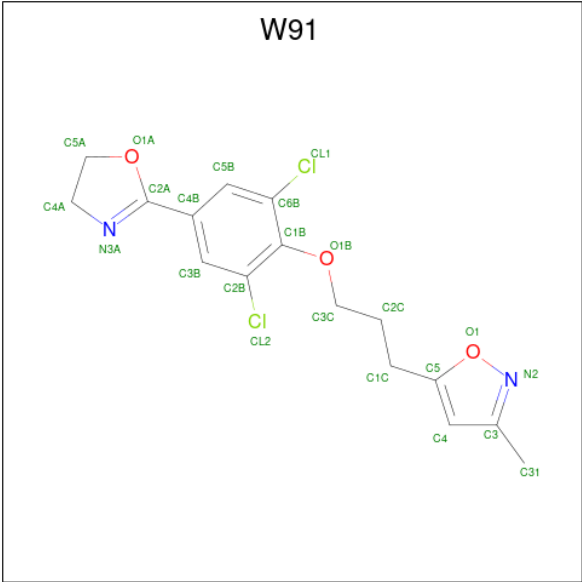
- Molecule 3 is a protein called HUMAN RHINOVIRUS 14 COAT PROTEIN (SUBUNIT VP3).

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3   | 3     | 236      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1849  | 1184 | 305 | 353 | 7 |         |         |       |

- Molecule 4 is a protein called HUMAN RHINOVIRUS 14 COAT PROTEIN (SUBUNIT VP4).

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 4   | 4     | 40       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 297   | 186 | 47 | 62 | 2 |         |         |       |

- Molecule 5 is 5-(3-(2,6-DICHLORO-4-(4,5-DIHYDRO-2-OXAZOLYL)PHENOXY)PROPYL)-3-METHYL ISOXAZOLE (CCD ID: W91) (formula: C<sub>16</sub>H<sub>16</sub>Cl<sub>2</sub>N<sub>2</sub>O<sub>3</sub>).



| Mol | Chain | Residues | Atoms |    |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 5   | 1     | 1        | Total | C  | Cl | N | O | 0       | 0       |
|     |       |          | 23    | 16 | 2  | 2 | 3 |         |         |

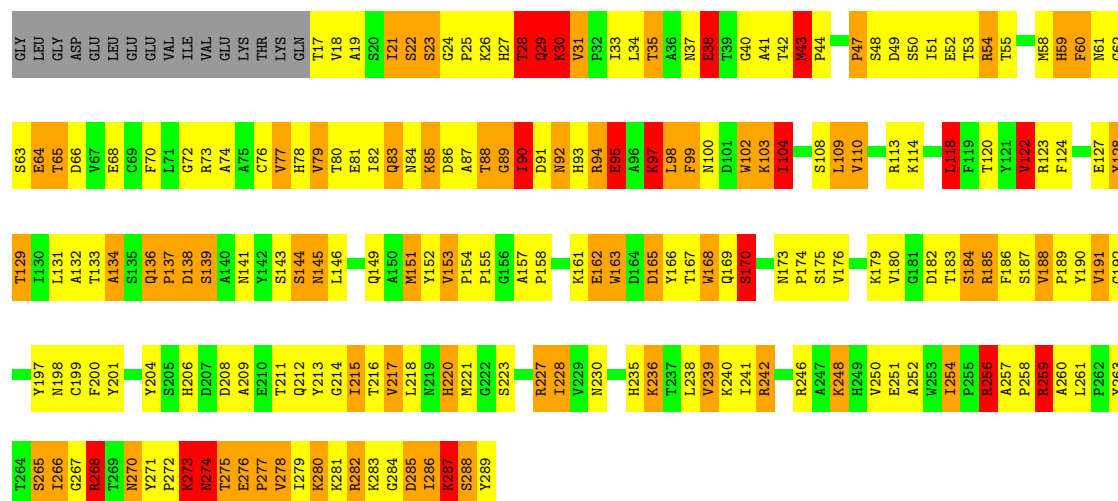
### 3 Residue-property plots

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

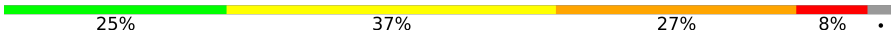
Note EDS was not executed.

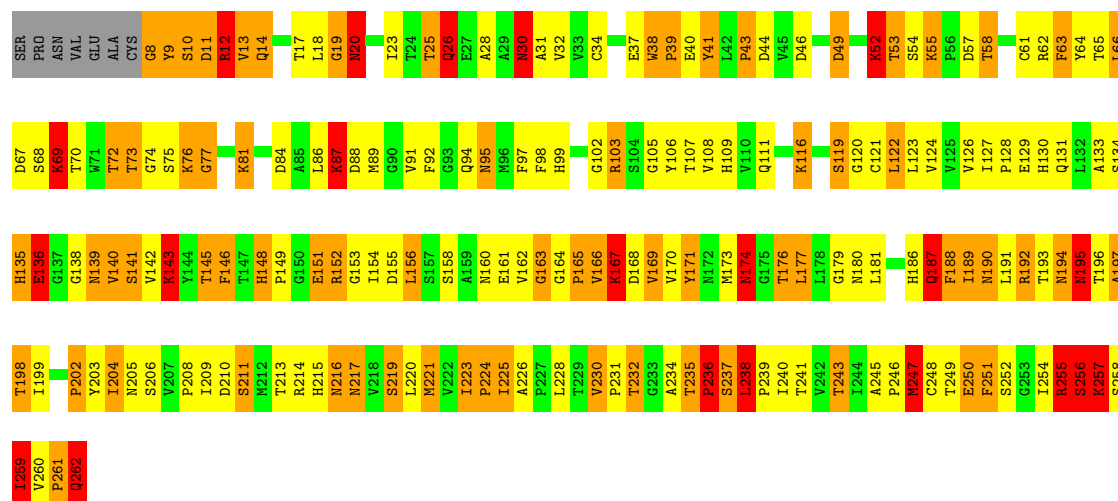
#### • Molecule 1: HUMAN RHINOVIRUS 14 COAT PROTEIN (SUBUNIT VP1)

Chain 1: 

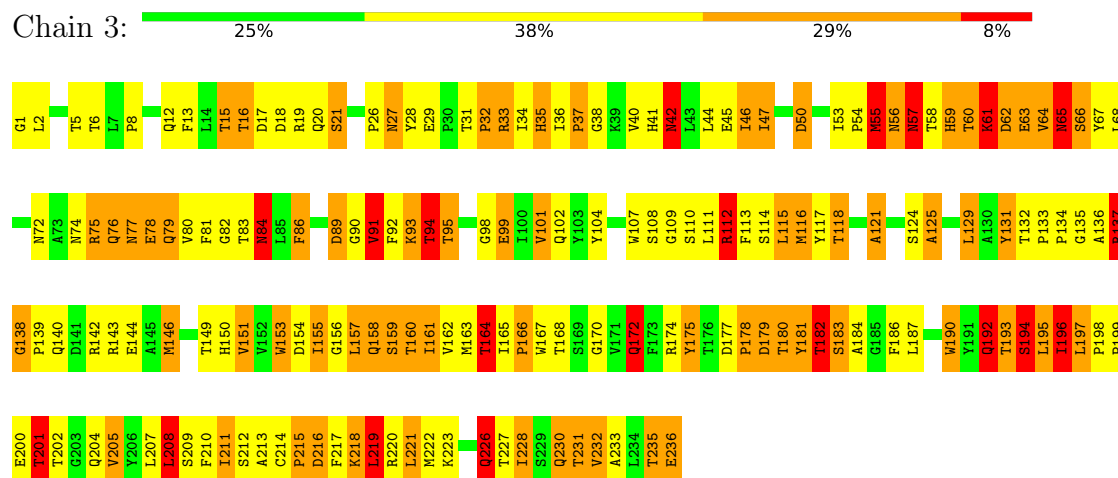


#### • Molecule 2: HUMAN RHINOVIRUS 14 COAT PROTEIN (SUBUNIT VP2)

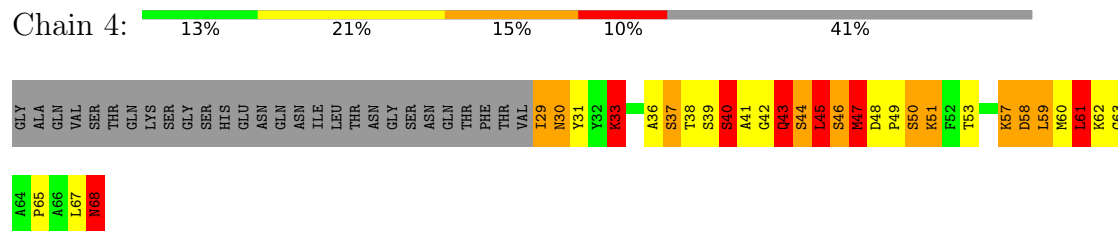
Chain 2: 



• Molecule 3: HUMAN RHINOVIRUS 14 COAT PROTEIN (SUBUNIT VP3)



• Molecule 4: HUMAN RHINOVIRUS 14 COAT PROTEIN (SUBUNIT VP4)



## 4 Data and refinement statistics

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

| Property                                                 | Value                                           | Source    |
|----------------------------------------------------------|-------------------------------------------------|-----------|
| Space group                                              | P 21 3                                          | Depositor |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$ | 445.10Å 445.10Å 445.10Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å)                                           | (Not available) – 3.00                          | Depositor |
| % Data completeness<br>(in resolution range)             | (Not available) ((Not available)-3.00)          | Depositor |
| $R_{merge}$                                              | (Not available)                                 | Depositor |
| $R_{sym}$                                                | (Not available)                                 | Depositor |
| Refinement program                                       | unknown                                         | Depositor |
| R, $R_{free}$                                            | (Not available) , (Not available)               | Depositor |
| Estimated twinning fraction                              | No twinning to report.                          | Xtriage   |
| Total number of atoms                                    | 6290                                            | wwPDB-VP  |
| Average B, all atoms (Å <sup>2</sup> )                   | 0.0                                             | wwPDB-VP  |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: W91

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   | 1     | 2.06         | 72/2228 (3.2%)  | 2.43        | 167/3031 (5.5%) |
| 2   | 2     | 2.43         | 94/2000 (4.7%)  | 2.77        | 192/2734 (7.0%) |
| 3   | 3     | 2.31         | 80/1898 (4.2%)  | 2.79        | 191/2597 (7.4%) |
| 4   | 4     | 2.64         | 14/302 (4.6%)   | 3.14        | 34/406 (8.4%)   |
| All | All   | 2.28         | 260/6428 (4.0%) | 2.68        | 584/8768 (6.7%) |

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   | 1     | 0                   | 2                   |
| 2   | 2     | 0                   | 2                   |
| All | All   | 0                   | 4                   |

All (260) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 1   | 1     | 285 | ASP  | CA-CB | 17.81  | 1.79        | 1.53     |
| 2   | 2     | 169 | VAL  | C-N   | -16.17 | 1.11        | 1.33     |
| 1   | 1     | 188 | VAL  | C-N   | 15.46  | 1.52        | 1.33     |
| 4   | 4     | 41  | ALA  | C-O   | 13.29  | 1.41        | 1.24     |
| 3   | 3     | 57  | ASN  | CA-CB | 12.78  | 1.75        | 1.53     |
| 4   | 4     | 42  | GLY  | N-CA  | 12.57  | 1.63        | 1.45     |
| 2   | 2     | 194 | ASN  | CA-CB | 11.51  | 1.71        | 1.53     |
| 1   | 1     | 283 | LYS  | N-CA  | 10.84  | 1.61        | 1.46     |
| 1   | 1     | 144 | SER  | N-CA  | 10.33  | 1.58        | 1.45     |
| 3   | 3     | 164 | THR  | C-O   | 10.30  | 1.36        | 1.24     |
| 4   | 4     | 45  | LEU  | C-N   | 9.39   | 1.46        | 1.33     |
| 2   | 2     | 187 | GLN  | N-CA  | 9.31   | 1.57        | 1.45     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | 2     | 256 | SER  | C-O     | 9.29  | 1.36        | 1.24     |
| 1   | 1     | 52  | GLU  | C-O     | 9.12  | 1.35        | 1.24     |
| 2   | 2     | 102 | GLY  | N-CA    | 9.00  | 1.55        | 1.45     |
| 1   | 1     | 282 | ARG  | CD-NE   | 8.98  | 1.58        | 1.46     |
| 2   | 2     | 152 | ARG  | CD-NE   | 8.92  | 1.58        | 1.46     |
| 2   | 2     | 168 | ASP  | C-O     | 8.77  | 1.34        | 1.24     |
| 2   | 2     | 174 | ASN  | C-O     | 8.59  | 1.30        | 1.23     |
| 3   | 3     | 21  | SER  | CA-CB   | 8.55  | 1.66        | 1.54     |
| 3   | 3     | 50  | ASP  | CA-CB   | -8.28 | 1.40        | 1.53     |
| 3   | 3     | 232 | VAL  | N-CA    | 8.27  | 1.55        | 1.46     |
| 1   | 1     | 73  | ARG  | C-O     | 7.95  | 1.33        | 1.23     |
| 3   | 3     | 138 | GLY  | N-CA    | 7.91  | 1.55        | 1.44     |
| 2   | 2     | 77  | GLY  | N-CA    | 7.86  | 1.53        | 1.45     |
| 1   | 1     | 285 | ASP  | N-CA    | -7.83 | 1.34        | 1.45     |
| 2   | 2     | 236 | PRO  | C-O     | 7.80  | 1.34        | 1.24     |
| 2   | 2     | 161 | GLU  | CA-CB   | -7.78 | 1.42        | 1.53     |
| 2   | 2     | 135 | HIS  | CE1-NE2 | -7.73 | 1.24        | 1.32     |
| 3   | 3     | 1   | GLY  | N-CA    | 7.71  | 1.57        | 1.45     |
| 1   | 1     | 122 | VAL  | N-CA    | 7.58  | 1.55        | 1.46     |
| 2   | 2     | 52  | LYS  | N-CA    | 7.57  | 1.55        | 1.46     |
| 1   | 1     | 72  | GLY  | C-O     | 7.53  | 1.34        | 1.23     |
| 2   | 2     | 12  | ARG  | NE-CZ   | 7.52  | 1.41        | 1.33     |
| 1   | 1     | 143 | SER  | C-O     | 7.50  | 1.33        | 1.24     |
| 2   | 2     | 108 | VAL  | C-O     | 7.43  | 1.32        | 1.24     |
| 3   | 3     | 215 | PRO  | C-N     | -7.43 | 1.23        | 1.33     |
| 1   | 1     | 94  | ARG  | CD-NE   | 7.42  | 1.56        | 1.46     |
| 1   | 1     | 288 | SER  | C-O     | 7.31  | 1.32        | 1.23     |
| 2   | 2     | 11  | ASP  | CA-CB   | 7.31  | 1.66        | 1.53     |
| 1   | 1     | 28  | THR  | CA-CB   | 7.29  | 1.64        | 1.53     |
| 2   | 2     | 120 | GLY  | N-CA    | 7.27  | 1.53        | 1.45     |
| 1   | 1     | 132 | ALA  | C-O     | 7.27  | 1.32        | 1.24     |
| 3   | 3     | 77  | ASN  | C-O     | 7.20  | 1.33        | 1.24     |
| 3   | 3     | 60  | THR  | CA-CB   | 7.17  | 1.65        | 1.54     |
| 2   | 2     | 260 | VAL  | N-CA    | 7.12  | 1.55        | 1.46     |
| 4   | 4     | 40  | SER  | CB-OG   | 7.05  | 1.56        | 1.42     |
| 2   | 2     | 9   | TYR  | C-O     | 7.04  | 1.32        | 1.23     |
| 2   | 2     | 219 | SER  | CA-CB   | -7.04 | 1.41        | 1.53     |
| 2   | 2     | 74  | GLY  | C-O     | 7.00  | 1.31        | 1.23     |
| 2   | 2     | 58  | THR  | C-O     | 6.99  | 1.32        | 1.24     |
| 1   | 1     | 276 | GLU  | C-O     | 6.95  | 1.30        | 1.24     |
| 4   | 4     | 49  | PRO  | C-N     | -6.91 | 1.24        | 1.34     |
| 1   | 1     | 30  | LYS  | C-O     | 6.88  | 1.31        | 1.23     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | 1     | 133 | THR  | N-CA    | 6.84  | 1.54        | 1.45     |
| 1   | 1     | 288 | SER  | CA-CB   | 6.83  | 1.65        | 1.53     |
| 2   | 2     | 223 | ILE  | CA-CB   | 6.80  | 1.59        | 1.54     |
| 3   | 3     | 86  | PHE  | CA-CB   | -6.79 | 1.43        | 1.52     |
| 1   | 1     | 91  | ASP  | N-CA    | 6.78  | 1.55        | 1.46     |
| 3   | 3     | 6   | THR  | N-CA    | 6.77  | 1.54        | 1.45     |
| 2   | 2     | 197 | ALA  | C-O     | 6.76  | 1.31        | 1.23     |
| 3   | 3     | 216 | ASP  | CA-CB   | 6.76  | 1.64        | 1.53     |
| 1   | 1     | 23  | SER  | N-CA    | 6.74  | 1.54        | 1.45     |
| 2   | 2     | 243 | THR  | C-O     | 6.74  | 1.32        | 1.24     |
| 2   | 2     | 193 | THR  | C-N     | -6.73 | 1.23        | 1.33     |
| 2   | 2     | 152 | ARG  | CZ-NH2  | 6.73  | 1.42        | 1.33     |
| 2   | 2     | 256 | SER  | CB-OG   | 6.71  | 1.55        | 1.42     |
| 2   | 2     | 194 | ASN  | N-CA    | -6.70 | 1.37        | 1.45     |
| 1   | 1     | 188 | VAL  | N-CA    | 6.69  | 1.54        | 1.46     |
| 2   | 2     | 10  | SER  | C-N     | -6.66 | 1.25        | 1.33     |
| 1   | 1     | 251 | GLU  | CA-CB   | -6.65 | 1.42        | 1.53     |
| 1   | 1     | 280 | LYS  | C-O     | 6.62  | 1.31        | 1.24     |
| 1   | 1     | 85  | LYS  | C-O     | 6.60  | 1.31        | 1.23     |
| 1   | 1     | 73  | ARG  | N-CA    | 6.59  | 1.53        | 1.45     |
| 3   | 3     | 57  | ASN  | N-CA    | -6.57 | 1.37        | 1.46     |
| 3   | 3     | 156 | GLY  | C-O     | -6.54 | 1.18        | 1.24     |
| 2   | 2     | 9   | TYR  | N-CA    | 6.54  | 1.53        | 1.46     |
| 1   | 1     | 79  | VAL  | C-N     | -6.53 | 1.24        | 1.33     |
| 2   | 2     | 39  | PRO  | C-O     | 6.52  | 1.31        | 1.23     |
| 2   | 2     | 52  | LYS  | CE-NZ   | 6.52  | 1.69        | 1.49     |
| 4   | 4     | 44  | SER  | CB-OG   | 6.51  | 1.55        | 1.42     |
| 2   | 2     | 190 | ASN  | CA-CB   | -6.50 | 1.44        | 1.53     |
| 4   | 4     | 62  | LYS  | C-O     | 6.50  | 1.31        | 1.24     |
| 2   | 2     | 217 | ASN  | C-O     | 6.48  | 1.32        | 1.24     |
| 2   | 2     | 109 | HIS  | CE1-NE2 | -6.47 | 1.26        | 1.32     |
| 2   | 2     | 262 | GLN  | CD-OE1  | 6.47  | 1.35        | 1.23     |
| 3   | 3     | 15  | THR  | C-O     | 6.44  | 1.32        | 1.24     |
| 1   | 1     | 134 | ALA  | CA-CB   | -6.43 | 1.42        | 1.53     |
| 3   | 3     | 57  | ASN  | C-N     | -6.42 | 1.25        | 1.33     |
| 4   | 4     | 62  | LYS  | N-CA    | 6.42  | 1.54        | 1.46     |
| 2   | 2     | 30  | ASN  | N-CA    | 6.36  | 1.54        | 1.46     |
| 3   | 3     | 165 | ILE  | N-CA    | 6.35  | 1.54        | 1.46     |
| 2   | 2     | 8   | GLY  | N-CA    | 6.34  | 1.55        | 1.45     |
| 1   | 1     | 22  | SER  | C-N     | -6.33 | 1.25        | 1.33     |
| 1   | 1     | 95  | GLU  | CB-CG   | 6.31  | 1.71        | 1.52     |
| 3   | 3     | 205 | VAL  | N-CA    | 6.30  | 1.53        | 1.46     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | 1     | 94  | ARG  | NE-CZ  | 6.29  | 1.40        | 1.33     |
| 3   | 3     | 5   | THR  | C-O    | 6.28  | 1.31        | 1.24     |
| 4   | 4     | 63  | GLY  | N-CA   | 6.24  | 1.54        | 1.45     |
| 1   | 1     | 184 | SER  | C-O    | 6.23  | 1.32        | 1.23     |
| 3   | 3     | 182 | THR  | CA-CB  | 6.21  | 1.62        | 1.53     |
| 2   | 2     | 259 | ILE  | C-O    | 6.20  | 1.31        | 1.24     |
| 1   | 1     | 251 | GLU  | N-CA   | 6.19  | 1.53        | 1.46     |
| 3   | 3     | 75  | ARG  | C-N    | -6.18 | 1.24        | 1.33     |
| 3   | 3     | 178 | PRO  | CA-CB  | -6.17 | 1.45        | 1.53     |
| 2   | 2     | 121 | CYS  | C-O    | 6.16  | 1.31        | 1.23     |
| 1   | 1     | 24  | GLY  | N-CA   | 6.13  | 1.53        | 1.44     |
| 3   | 3     | 16  | THR  | CA-CB  | 6.12  | 1.63        | 1.53     |
| 3   | 3     | 118 | THR  | CB-OG1 | 6.11  | 1.53        | 1.43     |
| 2   | 2     | 257 | LYS  | N-CA   | 6.11  | 1.54        | 1.46     |
| 4   | 4     | 45  | LEU  | N-CA   | 6.11  | 1.55        | 1.46     |
| 3   | 3     | 164 | THR  | N-CA   | 6.10  | 1.53        | 1.46     |
| 1   | 1     | 274 | ASN  | N-CA   | 6.09  | 1.54        | 1.46     |
| 4   | 4     | 33  | LYS  | CE-NZ  | 6.06  | 1.67        | 1.49     |
| 3   | 3     | 155 | ILE  | N-CA   | 6.05  | 1.53        | 1.46     |
| 1   | 1     | 28  | THR  | N-CA   | -6.05 | 1.37        | 1.45     |
| 2   | 2     | 162 | VAL  | N-CA   | 6.05  | 1.53        | 1.46     |
| 2   | 2     | 190 | ASN  | N-CA   | 6.04  | 1.54        | 1.46     |
| 1   | 1     | 131 | LEU  | C-O    | 6.04  | 1.31        | 1.23     |
| 2   | 2     | 19  | GLY  | C-N    | -6.03 | 1.25        | 1.33     |
| 2   | 2     | 168 | ASP  | CA-CB  | 6.03  | 1.60        | 1.53     |
| 3   | 3     | 215 | PRO  | CA-CB  | -6.03 | 1.44        | 1.53     |
| 3   | 3     | 57  | ASN  | C-O    | 6.03  | 1.31        | 1.24     |
| 2   | 2     | 208 | PRO  | C-N    | -6.02 | 1.28        | 1.33     |
| 3   | 3     | 110 | SER  | N-CA   | 6.02  | 1.52        | 1.45     |
| 3   | 3     | 36  | ILE  | N-CA   | 5.99  | 1.53        | 1.46     |
| 1   | 1     | 88  | THR  | CB-OG1 | 5.93  | 1.53        | 1.43     |
| 3   | 3     | 222 | MET  | CG-SD  | 5.92  | 1.95        | 1.80     |
| 3   | 3     | 175 | TYR  | CA-C   | 5.88  | 1.60        | 1.52     |
| 2   | 2     | 17  | THR  | C-N    | -5.87 | 1.25        | 1.33     |
| 3   | 3     | 135 | GLY  | C-O    | 5.87  | 1.30        | 1.24     |
| 3   | 3     | 116 | MET  | N-CA   | 5.87  | 1.53        | 1.46     |
| 2   | 2     | 176 | THR  | N-CA   | 5.86  | 1.53        | 1.45     |
| 2   | 2     | 180 | ASN  | C-N    | -5.85 | 1.25        | 1.33     |
| 2   | 2     | 103 | ARG  | C-O    | 5.85  | 1.31        | 1.23     |
| 3   | 3     | 219 | LEU  | C-N    | -5.84 | 1.26        | 1.33     |
| 3   | 3     | 213 | ALA  | C-O    | 5.83  | 1.30        | 1.23     |
| 1   | 1     | 38  | GLU  | CB-CG  | -5.82 | 1.34        | 1.52     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | 3     | 27  | ASN  | C-N     | -5.81 | 1.25        | 1.33     |
| 2   | 2     | 135 | HIS  | CG-CD2  | -5.79 | 1.29        | 1.35     |
| 1   | 1     | 276 | GLU  | N-CA    | 5.79  | 1.54        | 1.45     |
| 1   | 1     | 239 | VAL  | C-O     | 5.78  | 1.30        | 1.24     |
| 1   | 1     | 287 | LYS  | C-O     | 5.75  | 1.31        | 1.24     |
| 3   | 3     | 33  | ARG  | NE-CZ   | 5.73  | 1.39        | 1.33     |
| 2   | 2     | 88  | ASP  | C-O     | 5.72  | 1.32        | 1.24     |
| 2   | 2     | 152 | ARG  | NE-CZ   | 5.72  | 1.39        | 1.33     |
| 3   | 3     | 41  | HIS  | CE1-NE2 | 5.72  | 1.38        | 1.32     |
| 2   | 2     | 63  | PHE  | C-O     | 5.71  | 1.31        | 1.24     |
| 2   | 2     | 55  | LYS  | N-CA    | 5.71  | 1.53        | 1.46     |
| 2   | 2     | 54  | SER  | CA-CB   | -5.71 | 1.44        | 1.53     |
| 3   | 3     | 35  | HIS  | C-N     | -5.70 | 1.26        | 1.33     |
| 2   | 2     | 208 | PRO  | C-O     | 5.70  | 1.30        | 1.24     |
| 4   | 4     | 45  | LEU  | C-O     | 5.69  | 1.31        | 1.23     |
| 3   | 3     | 158 | GLN  | C-O     | 5.69  | 1.30        | 1.24     |
| 2   | 2     | 103 | ARG  | N-CA    | 5.67  | 1.52        | 1.46     |
| 1   | 1     | 268 | ARG  | N-CA    | 5.66  | 1.52        | 1.45     |
| 1   | 1     | 63  | SER  | CB-OG   | -5.65 | 1.30        | 1.42     |
| 3   | 3     | 38  | GLY  | CA-C    | -5.65 | 1.43        | 1.51     |
| 3   | 3     | 201 | THR  | C-O     | 5.64  | 1.30        | 1.23     |
| 2   | 2     | 87  | LYS  | CB-CG   | -5.64 | 1.35        | 1.52     |
| 2   | 2     | 195 | ASN  | CA-CB   | -5.63 | 1.44        | 1.54     |
| 3   | 3     | 82  | GLY  | C-N     | -5.63 | 1.26        | 1.33     |
| 3   | 3     | 82  | GLY  | N-CA    | 5.62  | 1.50        | 1.45     |
| 2   | 2     | 259 | ILE  | N-CA    | 5.62  | 1.53        | 1.46     |
| 1   | 1     | 274 | ASN  | CA-C    | 5.61  | 1.60        | 1.52     |
| 1   | 1     | 25  | PRO  | CA-CB   | -5.61 | 1.45        | 1.53     |
| 1   | 1     | 267 | GLY  | C-O     | 5.61  | 1.32        | 1.24     |
| 3   | 3     | 172 | GLN  | CG-CD   | -5.60 | 1.38        | 1.52     |
| 1   | 1     | 285 | ASP  | C-N     | 5.59  | 1.40        | 1.33     |
| 3   | 3     | 108 | SER  | CA-CB   | -5.58 | 1.43        | 1.53     |
| 1   | 1     | 137 | PRO  | C-O     | 5.58  | 1.31        | 1.24     |
| 1   | 1     | 254 | ILE  | CA-CB   | 5.57  | 1.61        | 1.54     |
| 2   | 2     | 168 | ASP  | C-N     | -5.56 | 1.26        | 1.33     |
| 2   | 2     | 237 | SER  | C-O     | 5.55  | 1.30        | 1.23     |
| 4   | 4     | 51  | LYS  | CE-NZ   | 5.54  | 1.66        | 1.49     |
| 2   | 2     | 151 | GLU  | CA-CB   | -5.53 | 1.43        | 1.53     |
| 2   | 2     | 75  | SER  | C-O     | 5.53  | 1.30        | 1.23     |
| 3   | 3     | 231 | THR  | CB-OG1  | 5.53  | 1.52        | 1.43     |
| 2   | 2     | 223 | ILE  | CA-C    | -5.52 | 1.48        | 1.52     |
| 2   | 2     | 194 | ASN  | C-O     | 5.52  | 1.30        | 1.23     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | 2     | 109 | HIS  | C-O     | 5.52  | 1.30        | 1.24     |
| 3   | 3     | 140 | GLN  | C-N     | -5.52 | 1.26        | 1.33     |
| 3   | 3     | 66  | SER  | N-CA    | 5.51  | 1.53        | 1.46     |
| 2   | 2     | 237 | SER  | N-CA    | 5.51  | 1.52        | 1.46     |
| 3   | 3     | 61  | LYS  | CE-NZ   | 5.50  | 1.65        | 1.49     |
| 3   | 3     | 77  | ASN  | CG-OD1  | 5.48  | 1.33        | 1.23     |
| 1   | 1     | 187 | SER  | C-O     | 5.48  | 1.30        | 1.23     |
| 3   | 3     | 91  | VAL  | C-O     | 5.48  | 1.30        | 1.24     |
| 2   | 2     | 153 | GLY  | C-N     | -5.47 | 1.25        | 1.33     |
| 3   | 3     | 40  | VAL  | C-O     | 5.47  | 1.30        | 1.24     |
| 3   | 3     | 75  | ARG  | N-CA    | 5.45  | 1.52        | 1.45     |
| 2   | 2     | 141 | SER  | N-CA    | 5.45  | 1.52        | 1.45     |
| 1   | 1     | 163 | TRP  | NE1-CE2 | -5.44 | 1.31        | 1.37     |
| 1   | 1     | 279 | ILE  | C-O     | 5.44  | 1.29        | 1.24     |
| 1   | 1     | 277 | PRO  | N-CA    | 5.41  | 1.53        | 1.47     |
| 3   | 3     | 209 | SER  | N-CA    | 5.41  | 1.52        | 1.46     |
| 2   | 2     | 211 | SER  | C-O     | 5.41  | 1.30        | 1.23     |
| 1   | 1     | 25  | PRO  | C-N     | -5.40 | 1.25        | 1.33     |
| 2   | 2     | 171 | TYR  | C-O     | 5.38  | 1.31        | 1.24     |
| 2   | 2     | 61  | CYS  | CA-C    | -5.37 | 1.47        | 1.53     |
| 3   | 3     | 17  | ASP  | CG-OD1  | 5.37  | 1.35        | 1.25     |
| 3   | 3     | 37  | PRO  | CA-CB   | -5.36 | 1.45        | 1.53     |
| 4   | 4     | 61  | LEU  | C-O     | 5.36  | 1.30        | 1.24     |
| 2   | 2     | 148 | HIS  | ND1-CE1 | 5.36  | 1.38        | 1.32     |
| 1   | 1     | 33  | ILE  | C-O     | 5.36  | 1.30        | 1.24     |
| 3   | 3     | 74  | ASN  | CA-CB   | 5.35  | 1.61        | 1.53     |
| 2   | 2     | 68  | SER  | CA-C    | -5.34 | 1.45        | 1.52     |
| 3   | 3     | 228 | ILE  | C-O     | 5.34  | 1.30        | 1.24     |
| 1   | 1     | 102 | TRP  | NE1-CE2 | -5.34 | 1.31        | 1.37     |
| 1   | 1     | 127 | GLU  | CA-CB   | -5.33 | 1.46        | 1.53     |
| 1   | 1     | 30  | LYS  | CE-NZ   | 5.32  | 1.65        | 1.49     |
| 2   | 2     | 256 | SER  | C-N     | -5.32 | 1.26        | 1.33     |
| 3   | 3     | 209 | SER  | C-O     | 5.32  | 1.30        | 1.23     |
| 1   | 1     | 122 | VAL  | C-O     | 5.31  | 1.29        | 1.24     |
| 2   | 2     | 103 | ARG  | CA-CB   | -5.29 | 1.45        | 1.53     |
| 2   | 2     | 72  | THR  | CB-OG1  | 5.29  | 1.52        | 1.43     |
| 2   | 2     | 14  | GLN  | CD-NE2  | 5.29  | 1.44        | 1.33     |
| 2   | 2     | 123 | LEU  | C-N     | -5.28 | 1.26        | 1.33     |
| 2   | 2     | 99  | HIS  | C-N     | -5.27 | 1.26        | 1.34     |
| 2   | 2     | 219 | SER  | N-CA    | 5.26  | 1.52        | 1.46     |
| 2   | 2     | 246 | PRO  | C-O     | 5.25  | 1.29        | 1.23     |
| 3   | 3     | 2   | LEU  | CA-CB   | 5.25  | 1.63        | 1.53     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | 1     | 270 | ASN  | CA-C    | 5.24  | 1.59        | 1.52     |
| 1   | 1     | 54  | ARG  | C-O     | 5.24  | 1.30        | 1.23     |
| 2   | 2     | 38  | TRP  | CA-C    | -5.23 | 1.45        | 1.52     |
| 1   | 1     | 168 | TRP  | NE1-CE2 | -5.23 | 1.31        | 1.37     |
| 3   | 3     | 64  | VAL  | C-N     | -5.22 | 1.26        | 1.33     |
| 3   | 3     | 146 | MET  | C-O     | 5.22  | 1.30        | 1.24     |
| 3   | 3     | 164 | THR  | CA-CB   | 5.21  | 1.61        | 1.53     |
| 1   | 1     | 283 | LYS  | CE-NZ   | 5.19  | 1.65        | 1.49     |
| 3   | 3     | 77  | ASN  | C-N     | -5.19 | 1.26        | 1.33     |
| 3   | 3     | 58  | THR  | CA-CB   | 5.18  | 1.62        | 1.53     |
| 2   | 2     | 202 | PRO  | C-N     | -5.18 | 1.26        | 1.33     |
| 2   | 2     | 204 | ILE  | C-N     | -5.16 | 1.26        | 1.33     |
| 1   | 1     | 42  | THR  | C-O     | 5.16  | 1.29        | 1.23     |
| 1   | 1     | 85  | LYS  | N-CA    | 5.16  | 1.52        | 1.46     |
| 3   | 3     | 153 | TRP  | C-O     | 5.16  | 1.30        | 1.24     |
| 2   | 2     | 202 | PRO  | C-O     | 5.15  | 1.29        | 1.23     |
| 3   | 3     | 133 | PRO  | CA-CB   | -5.14 | 1.47        | 1.54     |
| 1   | 1     | 252 | ALA  | C-O     | 5.14  | 1.30        | 1.23     |
| 3   | 3     | 205 | VAL  | C-O     | 5.13  | 1.30        | 1.23     |
| 2   | 2     | 248 | CYS  | C-N     | -5.11 | 1.26        | 1.33     |
| 3   | 3     | 136 | ALA  | C-O     | 5.10  | 1.30        | 1.23     |
| 1   | 1     | 48  | SER  | C-N     | -5.09 | 1.26        | 1.33     |
| 3   | 3     | 112 | ARG  | CA-CB   | -5.08 | 1.45        | 1.53     |
| 2   | 2     | 128 | PRO  | CA-CB   | -5.07 | 1.47        | 1.53     |
| 2   | 2     | 220 | LEU  | C-N     | -5.07 | 1.26        | 1.33     |
| 1   | 1     | 275 | THR  | C-O     | 5.05  | 1.30        | 1.23     |
| 3   | 3     | 65  | ASN  | CA-CB   | 5.05  | 1.62        | 1.53     |
| 3   | 3     | 232 | VAL  | C-O     | 5.05  | 1.29        | 1.23     |
| 1   | 1     | 246 | ARG  | CD-NE   | -5.05 | 1.39        | 1.46     |
| 3   | 3     | 164 | THR  | CA-C    | -5.05 | 1.46        | 1.52     |
| 3   | 3     | 84  | ASN  | N-CA    | 5.04  | 1.51        | 1.45     |
| 1   | 1     | 129 | THR  | N-CA    | 5.03  | 1.52        | 1.46     |
| 1   | 1     | 89  | GLY  | C-O     | 5.03  | 1.31        | 1.24     |
| 2   | 2     | 186 | HIS  | C-O     | 5.03  | 1.29        | 1.23     |
| 3   | 3     | 109 | GLY  | C-N     | 5.02  | 1.40        | 1.33     |
| 3   | 3     | 216 | ASP  | N-CA    | -5.02 | 1.40        | 1.46     |
| 2   | 2     | 12  | ARG  | N-CA    | -5.01 | 1.40        | 1.46     |
| 3   | 3     | 154 | ASP  | N-CA    | 5.01  | 1.52        | 1.46     |

All (584) bond angle outliers are listed below:

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| Mol | Chain | Res | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 3   | 3     | 50  | ASP  | CA-CB-CG   | 27.72  | 140.32      | 112.60   |
| 1   | 1     | 285 | ASP  | CA-CB-CG   | -22.25 | 90.35       | 112.60   |
| 3   | 3     | 215 | PRO  | CA-C-N     | 20.37  | 149.22      | 120.29   |
| 3   | 3     | 215 | PRO  | C-N-CA     | 20.37  | 149.22      | 120.29   |
| 2   | 2     | 87  | LYS  | CA-CB-CG   | 19.02  | 152.15      | 114.10   |
| 2   | 2     | 11  | ASP  | CA-CB-CG   | -18.97 | 93.63       | 112.60   |
| 1   | 1     | 145 | ASN  | OD1-CG-ND2 | 17.21  | 139.81      | 122.60   |
| 2   | 2     | 193 | THR  | CA-C-N     | 16.44  | 150.18      | 122.07   |
| 2   | 2     | 193 | THR  | C-N-CA     | 16.44  | 150.18      | 122.07   |
| 2   | 2     | 190 | ASN  | CA-CB-CG   | 16.40  | 129.00      | 112.60   |
| 2   | 2     | 194 | ASN  | CA-CB-CG   | -14.93 | 97.67       | 112.60   |
| 2   | 2     | 11  | ASP  | CA-C-N     | 14.81  | 140.58      | 120.44   |
| 2   | 2     | 11  | ASP  | C-N-CA     | 14.81  | 140.58      | 120.44   |
| 3   | 3     | 57  | ASN  | CA-CB-CG   | -13.74 | 98.86       | 112.60   |
| 1   | 1     | 38  | GLU  | CB-CG-CD   | 13.61  | 135.74      | 112.60   |
| 3   | 3     | 74  | ASN  | CA-CB-CG   | -13.43 | 99.17       | 112.60   |
| 3   | 3     | 65  | ASN  | CA-CB-CG   | -13.05 | 99.55       | 112.60   |
| 1   | 1     | 145 | ASN  | CA-CB-CG   | -12.91 | 99.69       | 112.60   |
| 3   | 3     | 27  | ASN  | CA-CB-CG   | -12.86 | 99.74       | 112.60   |
| 2   | 2     | 44  | ASP  | CA-CB-CG   | 12.69  | 125.29      | 112.60   |
| 2   | 2     | 194 | ASN  | N-CA-CB    | -12.64 | 89.81       | 110.41   |
| 1   | 1     | 94  | ARG  | CD-NE-CZ   | -12.61 | 106.75      | 124.40   |
| 1   | 1     | 256 | ARG  | NE-CZ-NH2  | 12.54  | 130.48      | 119.20   |
| 2   | 2     | 67  | ASP  | CA-CB-CG   | -12.45 | 100.15      | 112.60   |
| 2   | 2     | 256 | SER  | CA-C-O     | -12.21 | 105.38      | 119.79   |
| 4   | 4     | 30  | ASN  | CA-CB-CG   | -12.08 | 100.52      | 112.60   |
| 3   | 3     | 172 | GLN  | CB-CG-CD   | 12.00  | 133.00      | 112.60   |
| 4   | 4     | 45  | LEU  | N-CA-CB    | -11.92 | 94.08       | 111.84   |
| 3   | 3     | 74  | ASN  | OD1-CG-ND2 | 11.32  | 133.92      | 122.60   |
| 4   | 4     | 41  | ALA  | CA-C-O     | -11.31 | 105.47      | 119.38   |
| 2   | 2     | 14  | GLN  | OE1-CD-NE2 | 11.15  | 133.75      | 122.60   |
| 3   | 3     | 29  | GLU  | CB-CG-CD   | 11.10  | 131.47      | 112.60   |
| 2   | 2     | 151 | GLU  | CA-CB-CG   | 11.09  | 136.29      | 114.10   |
| 1   | 1     | 285 | ASP  | N-CA-CB    | -11.04 | 95.28       | 110.29   |
| 1   | 1     | 25  | PRO  | CA-C-O     | -10.87 | 108.95      | 121.56   |
| 2   | 2     | 88  | ASP  | CA-CB-CG   | -10.85 | 101.75      | 112.60   |
| 4   | 4     | 48  | ASP  | CA-CB-CG   | -10.65 | 101.95      | 112.60   |
| 2   | 2     | 219 | SER  | CA-CB-OG   | 10.62  | 132.35      | 111.10   |
| 2   | 2     | 97  | PHE  | CA-CB-CG   | -10.60 | 103.20      | 113.80   |
| 1   | 1     | 282 | ARG  | CD-NE-CZ   | -10.53 | 109.65      | 124.40   |
| 1   | 1     | 141 | ASN  | CA-CB-CG   | -10.44 | 102.16      | 112.60   |

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| Mol | Chain | Res | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 3   | 3     | 57  | ASN  | N-CA-CB   | -10.40 | 92.92       | 110.49   |
| 3   | 3     | 72  | ASN  | CA-CB-CG  | -10.18 | 102.42      | 112.60   |
| 4   | 4     | 48  | ASP  | O-C-N     | 10.06  | 128.27      | 121.23   |
| 1   | 1     | 246 | ARG  | NE-CZ-NH1 | 10.04  | 131.54      | 121.50   |
| 1   | 1     | 63  | SER  | CB-CA-C   | -10.00 | 94.19       | 110.79   |
| 1   | 1     | 54  | ARG  | CD-NE-CZ  | -9.92  | 110.51      | 124.40   |
| 4   | 4     | 44  | SER  | CA-C-N    | -9.86  | 107.97      | 122.07   |
| 4   | 4     | 44  | SER  | C-N-CA    | -9.86  | 107.97      | 122.07   |
| 1   | 1     | 91  | ASP  | CA-CB-CG  | -9.85  | 102.75      | 112.60   |
| 1   | 1     | 275 | THR  | CA-C-O    | -9.80  | 109.14      | 121.88   |
| 1   | 1     | 285 | ASP  | N-CA-C    | 9.79   | 122.95      | 110.33   |
| 1   | 1     | 22  | SER  | CA-C-O    | -9.74  | 109.58      | 120.69   |
| 1   | 1     | 28  | THR  | CB-CA-C   | -9.68  | 92.98       | 111.48   |
| 3   | 3     | 137 | ARG  | NE-CZ-NH1 | -9.64  | 111.86      | 121.50   |
| 1   | 1     | 256 | ARG  | NE-CZ-NH1 | -9.64  | 111.86      | 121.50   |
| 3   | 3     | 33  | ARG  | CA-C-O    | -9.63  | 110.08      | 121.05   |
| 1   | 1     | 79  | VAL  | CA-C-O    | -9.56  | 110.45      | 120.39   |
| 1   | 1     | 53  | THR  | CA-CB-OG1 | -9.51  | 95.33       | 109.60   |
| 1   | 1     | 246 | ARG  | CD-NE-CZ  | 9.46   | 137.65      | 124.40   |
| 1   | 1     | 38  | GLU  | CA-CB-CG  | 9.44   | 132.97      | 114.10   |
| 3   | 3     | 86  | PHE  | CA-CB-CG  | 9.42   | 123.22      | 113.80   |
| 3   | 3     | 89  | ASP  | CA-CB-CG  | -9.35  | 103.25      | 112.60   |
| 2   | 2     | 255 | ARG  | NE-CZ-NH2 | -9.23  | 110.89      | 119.20   |
| 3   | 3     | 57  | ASN  | CB-CA-C   | -9.09  | 92.34       | 110.42   |
| 2   | 2     | 195 | ASN  | CA-CB-CG  | 9.03   | 121.63      | 112.60   |
| 1   | 1     | 95  | GLU  | CB-CG-CD  | -9.03  | 97.25       | 112.60   |
| 1   | 1     | 268 | ARG  | CD-NE-CZ  | -9.02  | 111.77      | 124.40   |
| 4   | 4     | 50  | SER  | CA-C-O    | -9.01  | 109.92      | 120.10   |
| 3   | 3     | 196 | ILE  | CA-C-O    | -8.97  | 111.21      | 120.27   |
| 2   | 2     | 136 | GLU  | CB-CG-CD  | -8.83  | 97.58       | 112.60   |
| 2   | 2     | 250 | GLU  | CA-CB-CG  | 8.81   | 131.72      | 114.10   |
| 1   | 1     | 187 | SER  | CA-C-N    | -8.78  | 105.89      | 122.13   |
| 1   | 1     | 187 | SER  | C-N-CA    | -8.78  | 105.89      | 122.13   |
| 4   | 4     | 68  | ASN  | CA-CB-CG  | -8.77  | 103.83      | 112.60   |
| 1   | 1     | 270 | ASN  | CA-CB-CG  | 8.72   | 121.32      | 112.60   |
| 1   | 1     | 251 | GLU  | CA-CB-CG  | 8.66   | 131.41      | 114.10   |
| 2   | 2     | 255 | ARG  | CA-CB-CG  | 8.49   | 131.08      | 114.10   |
| 2   | 2     | 139 | ASN  | CA-CB-CG  | -8.48  | 104.12      | 112.60   |
| 2   | 2     | 73  | THR  | CA-CB-OG1 | -8.43  | 96.95       | 109.60   |
| 1   | 1     | 259 | ARG  | CA-CB-CG  | -8.43  | 97.25       | 114.10   |
| 2   | 2     | 169 | VAL  | CB-CA-C   | -8.43  | 101.18      | 111.97   |
| 2   | 2     | 168 | ASP  | CA-C-O    | -8.41  | 110.61      | 120.62   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | 2     | 68  | SER  | N-CA-C     | 8.38  | 122.88      | 110.48   |
| 2   | 2     | 169 | VAL  | CA-C-O     | -8.38 | 112.29      | 121.17   |
| 4   | 4     | 36  | ALA  | CA-C-N     | -8.38 | 108.72      | 122.54   |
| 4   | 4     | 36  | ALA  | C-N-CA     | -8.38 | 108.72      | 122.54   |
| 4   | 4     | 41  | ALA  | N-CA-C     | 8.34  | 122.72      | 112.54   |
| 1   | 1     | 123 | ARG  | NE-CZ-NH1  | 8.34  | 129.84      | 121.50   |
| 3   | 3     | 74  | ASN  | CA-C-O     | -8.31 | 109.92      | 120.55   |
| 3   | 3     | 172 | GLN  | CG-CD-NE2  | 8.29  | 128.84      | 116.40   |
| 3   | 3     | 57  | ASN  | OD1-CG-ND2 | 8.27  | 130.87      | 122.60   |
| 3   | 3     | 5   | THR  | CA-C-O     | -8.26 | 111.15      | 120.32   |
| 1   | 1     | 122 | VAL  | N-CA-CB    | -8.26 | 97.90       | 111.45   |
| 3   | 3     | 219 | LEU  | CA-C-O     | -8.21 | 111.22      | 120.66   |
| 1   | 1     | 82  | ILE  | CA-C-O     | -8.20 | 113.06      | 121.67   |
| 3   | 3     | 182 | THR  | CA-CB-CG2  | 8.16  | 124.37      | 110.50   |
| 2   | 2     | 49  | ASP  | CA-CB-CG   | 8.15  | 120.75      | 112.60   |
| 3   | 3     | 21  | SER  | CB-CA-C    | -8.14 | 95.49       | 108.91   |
| 1   | 1     | 29  | GLN  | N-CA-C     | -8.13 | 102.40      | 113.30   |
| 3   | 3     | 16  | THR  | N-CA-CB    | -8.12 | 98.34       | 110.61   |
| 4   | 4     | 57  | LYS  | CA-C-O     | -8.12 | 112.33      | 120.70   |
| 2   | 2     | 187 | GLN  | CA-CB-CG   | 8.01  | 130.13      | 114.10   |
| 3   | 3     | 27  | ASN  | O-C-N      | 8.01  | 132.01      | 122.00   |
| 3   | 3     | 233 | ALA  | CA-C-O     | -8.00 | 112.39      | 121.19   |
| 3   | 3     | 60  | THR  | CA-CB-OG1  | -8.00 | 97.60       | 109.60   |
| 2   | 2     | 248 | CYS  | CA-C-O     | -7.99 | 112.27      | 121.54   |
| 1   | 1     | 288 | SER  | CA-C-O     | -7.99 | 113.09      | 121.55   |
| 3   | 3     | 78  | GLU  | N-CA-C     | 7.98  | 120.83      | 110.53   |
| 3   | 3     | 111 | LEU  | CA-C-N     | -7.95 | 111.79      | 123.00   |
| 3   | 3     | 111 | LEU  | C-N-CA     | -7.95 | 111.79      | 123.00   |
| 1   | 1     | 94  | ARG  | NE-CZ-NH2  | -7.95 | 112.05      | 119.20   |
| 3   | 3     | 231 | THR  | CA-CB-OG1  | -7.93 | 97.71       | 109.60   |
| 2   | 2     | 223 | ILE  | N-CA-CB    | -7.92 | 101.50      | 112.27   |
| 1   | 1     | 37  | ASN  | CB-CG-ND2  | 7.90  | 128.25      | 116.40   |
| 2   | 2     | 216 | ASN  | CA-C-O     | -7.84 | 112.10      | 120.80   |
| 3   | 3     | 216 | ASP  | N-CA-CB    | -7.83 | 98.57       | 110.16   |
| 3   | 3     | 236 | GLU  | CA-CB-CG   | 7.83  | 129.75      | 114.10   |
| 1   | 1     | 123 | ARG  | CD-NE-CZ   | 7.82  | 135.35      | 124.40   |
| 3   | 3     | 62  | ASP  | CA-CB-CG   | 7.81  | 120.41      | 112.60   |
| 2   | 2     | 95  | ASN  | CA-CB-CG   | -7.80 | 104.80      | 112.60   |
| 2   | 2     | 109 | HIS  | CA-C-O     | -7.76 | 110.79      | 120.57   |
| 4   | 4     | 45  | LEU  | CA-C-O     | 7.76  | 130.54      | 121.54   |
| 1   | 1     | 282 | ARG  | CA-C-N     | -7.73 | 111.51      | 122.41   |
| 1   | 1     | 282 | ARG  | C-N-CA     | -7.73 | 111.51      | 122.41   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | 1     | 274 | ASN  | O-C-N      | 7.71  | 132.85      | 122.59   |
| 4   | 4     | 37  | SER  | CB-CA-C    | 7.71  | 122.96      | 110.09   |
| 1   | 1     | 64  | GLU  | CB-CG-CD   | 7.69  | 125.67      | 112.60   |
| 2   | 2     | 240 | ILE  | CA-C-O     | -7.65 | 112.36      | 120.39   |
| 2   | 2     | 190 | ASN  | OD1-CG-ND2 | -7.64 | 114.96      | 122.60   |
| 3   | 3     | 142 | ARG  | CA-CB-CG   | 7.61  | 129.31      | 114.10   |
| 3   | 3     | 59  | HIS  | CA-C-O     | 7.60  | 130.47      | 121.88   |
| 3   | 3     | 137 | ARG  | CD-NE-CZ   | -7.58 | 113.79      | 124.40   |
| 1   | 1     | 61  | ASN  | CA-CB-CG   | -7.58 | 105.03      | 112.60   |
| 1   | 1     | 17  | THR  | CA-C-N     | -7.57 | 110.38      | 122.50   |
| 1   | 1     | 17  | THR  | C-N-CA     | -7.57 | 110.38      | 122.50   |
| 2   | 2     | 87  | LYS  | CB-CG-CD   | 7.57  | 128.71      | 111.30   |
| 3   | 3     | 184 | ALA  | N-CA-C     | 7.57  | 122.71      | 113.17   |
| 3   | 3     | 27  | ASN  | N-CA-C     | 7.56  | 124.07      | 113.56   |
| 1   | 1     | 277 | PRO  | N-CD-CG    | -7.54 | 91.88       | 103.20   |
| 3   | 3     | 79  | GLN  | OE1-CD-NE2 | -7.48 | 115.12      | 122.60   |
| 1   | 1     | 288 | SER  | N-CA-C     | 7.39  | 120.40      | 110.35   |
| 4   | 4     | 30  | ASN  | CA-C-O     | -7.37 | 112.28      | 120.69   |
| 2   | 2     | 98  | PHE  | CA-C-O     | -7.35 | 111.00      | 119.60   |
| 2   | 2     | 140 | VAL  | CA-C-O     | -7.35 | 113.37      | 121.23   |
| 1   | 1     | 188 | VAL  | CA-C-N     | -7.33 | 113.17      | 120.21   |
| 1   | 1     | 188 | VAL  | C-N-CA     | -7.33 | 113.17      | 120.21   |
| 4   | 4     | 45  | LEU  | CB-CA-C    | 7.33  | 122.51      | 111.80   |
| 3   | 3     | 129 | LEU  | CA-C-O     | -7.32 | 112.95      | 120.71   |
| 3   | 3     | 27  | ASN  | CB-CA-C    | -7.31 | 97.24       | 111.06   |
| 3   | 3     | 118 | THR  | CA-CB-OG1  | -7.31 | 98.64       | 109.60   |
| 3   | 3     | 61  | LYS  | CA-C-O     | -7.30 | 112.60      | 121.06   |
| 2   | 2     | 39  | PRO  | CA-C-O     | -7.29 | 113.03      | 121.34   |
| 2   | 2     | 107 | THR  | CA-C-O     | -7.29 | 112.30      | 120.32   |
| 2   | 2     | 77  | GLY  | CA-C-O     | -7.26 | 114.79      | 122.05   |
| 2   | 2     | 187 | GLN  | CB-CA-C    | 7.25  | 125.39      | 109.94   |
| 2   | 2     | 180 | ASN  | CA-CB-CG   | -7.25 | 105.35      | 112.60   |
| 2   | 2     | 103 | ARG  | CD-NE-CZ   | -7.22 | 114.30      | 124.40   |
| 2   | 2     | 68  | SER  | O-C-N      | -7.21 | 114.81      | 122.96   |
| 3   | 3     | 124 | SER  | CA-C-O     | -7.21 | 113.55      | 121.33   |
| 3   | 3     | 19  | ARG  | NE-CZ-NH2  | 7.20  | 125.68      | 119.20   |
| 1   | 1     | 275 | THR  | CA-CB-OG1  | -7.20 | 98.80       | 109.60   |
| 2   | 2     | 52  | LYS  | CA-C-O     | -7.20 | 113.27      | 121.19   |
| 1   | 1     | 26  | LYS  | CA-CB-CG   | 7.19  | 128.47      | 114.10   |
| 2   | 2     | 169 | VAL  | N-CA-C     | 7.18  | 117.32      | 110.42   |
| 3   | 3     | 46  | ILE  | CA-C-O     | -7.17 | 112.50      | 120.25   |
| 1   | 1     | 284 | GLY  | CA-C-N     | 7.13  | 133.64      | 120.95   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | 1     | 284 | GLY  | C-N-CA     | 7.13  | 133.64      | 120.95   |
| 4   | 4     | 30  | ASN  | OD1-CG-ND2 | 7.13  | 129.73      | 122.60   |
| 2   | 2     | 146 | PHE  | CA-CB-CG   | -7.13 | 106.67      | 113.80   |
| 1   | 1     | 59  | HIS  | CA-C-O     | -7.09 | 112.01      | 120.81   |
| 2   | 2     | 168 | ASP  | N-CA-CB    | -7.09 | 97.97       | 109.60   |
| 4   | 4     | 47  | MET  | CA-CB-CG   | -7.09 | 99.92       | 114.10   |
| 2   | 2     | 134 | SER  | CA-C-O     | -7.06 | 113.01      | 121.05   |
| 1   | 1     | 285 | ASP  | CB-CA-C    | -7.05 | 93.79       | 110.02   |
| 2   | 2     | 259 | ILE  | CB-CG1-CD1 | -7.04 | 99.01       | 113.80   |
| 3   | 3     | 13  | PHE  | CA-CB-CG   | 7.04  | 120.84      | 113.80   |
| 3   | 3     | 164 | THR  | N-CA-CB    | -7.00 | 99.58       | 110.57   |
| 1   | 1     | 85  | LYS  | CA-C-O     | -7.00 | 113.96      | 121.38   |
| 1   | 1     | 28  | THR  | OG1-CB-CG2 | 7.00  | 123.29      | 109.30   |
| 3   | 3     | 35  | HIS  | CA-C-O     | -7.00 | 112.87      | 120.92   |
| 1   | 1     | 43  | MET  | CA-C-O     | 6.99  | 126.32      | 119.75   |
| 3   | 3     | 94  | THR  | O-C-N      | 6.98  | 131.56      | 122.42   |
| 3   | 3     | 77  | ASN  | OD1-CG-ND2 | -6.96 | 115.64      | 122.60   |
| 3   | 3     | 121 | ALA  | CA-C-O     | -6.95 | 112.25      | 120.10   |
| 1   | 1     | 187 | SER  | O-C-N      | 6.94  | 131.16      | 123.25   |
| 1   | 1     | 285 | ASP  | CB-CG-OD1  | -6.92 | 102.49      | 118.40   |
| 3   | 3     | 109 | GLY  | CA-C-N     | -6.90 | 110.91      | 122.64   |
| 3   | 3     | 109 | GLY  | C-N-CA     | -6.90 | 110.91      | 122.64   |
| 3   | 3     | 66  | SER  | CB-CA-C    | 6.90  | 121.61      | 110.09   |
| 1   | 1     | 138 | ASP  | CA-CB-CG   | 6.88  | 119.48      | 112.60   |
| 2   | 2     | 9   | TYR  | CB-CA-C    | 6.88  | 121.41      | 109.65   |
| 2   | 2     | 186 | HIS  | CA-CB-CG   | -6.87 | 106.93      | 113.80   |
| 1   | 1     | 270 | ASN  | O-C-N      | 6.87  | 131.35      | 122.97   |
| 3   | 3     | 65  | ASN  | OD1-CG-ND2 | 6.86  | 129.46      | 122.60   |
| 1   | 1     | 89  | GLY  | CA-C-N     | -6.86 | 114.29      | 122.93   |
| 1   | 1     | 89  | GLY  | C-N-CA     | -6.86 | 114.29      | 122.93   |
| 2   | 2     | 57  | ASP  | CB-CA-C    | -6.84 | 108.69      | 116.63   |
| 1   | 1     | 35  | THR  | CA-CB-OG1  | -6.84 | 99.33       | 109.60   |
| 4   | 4     | 44  | SER  | O-C-N      | 6.83  | 131.68      | 122.59   |
| 1   | 1     | 42  | THR  | CA-CB-CG2  | 6.82  | 122.10      | 110.50   |
| 2   | 2     | 219 | SER  | CB-CA-C    | 6.82  | 121.66      | 109.38   |
| 3   | 3     | 202 | THR  | CA-C-O     | 6.82  | 128.53      | 121.23   |
| 2   | 2     | 193 | THR  | O-C-N      | -6.82 | 115.11      | 121.79   |
| 3   | 3     | 146 | MET  | CG-SD-CE   | 6.82  | 115.90      | 100.90   |
| 2   | 2     | 14  | GLN  | CB-CG-CD   | -6.81 | 101.03      | 112.60   |
| 3   | 3     | 187 | LEU  | CA-C-O     | -6.80 | 113.03      | 120.24   |
| 2   | 2     | 238 | LEU  | N-CA-CB    | -6.80 | 98.76       | 110.72   |
| 3   | 3     | 231 | THR  | CA-C-O     | -6.78 | 110.58      | 119.06   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 3   | 3     | 143 | ARG  | N-CA-C     | -6.77 | 103.98      | 111.36   |
| 1   | 1     | 49  | ASP  | N-CA-C     | -6.75 | 105.33      | 113.97   |
| 1   | 1     | 35  | THR  | N-CA-CB    | -6.74 | 99.10       | 110.49   |
| 3   | 3     | 178 | PRO  | O-C-N      | 6.74  | 130.76      | 123.01   |
| 3   | 3     | 151 | VAL  | CA-C-O     | -6.73 | 113.58      | 120.25   |
| 2   | 2     | 224 | PRO  | CA-C-O     | -6.72 | 114.04      | 121.23   |
| 2   | 2     | 124 | VAL  | CA-C-O     | -6.71 | 112.81      | 120.66   |
| 2   | 2     | 249 | THR  | CA-CB-OG1  | -6.70 | 99.55       | 109.60   |
| 1   | 1     | 62  | GLY  | CA-C-N     | 6.69  | 129.25      | 120.28   |
| 1   | 1     | 62  | GLY  | C-N-CA     | 6.69  | 129.25      | 120.28   |
| 4   | 4     | 58  | ASP  | O-C-N      | 6.69  | 130.85      | 123.22   |
| 3   | 3     | 227 | THR  | CA-CB-OG1  | -6.65 | 99.62       | 109.60   |
| 1   | 1     | 288 | SER  | CB-CA-C    | -6.65 | 97.71       | 109.62   |
| 2   | 2     | 255 | ARG  | CB-CG-CD   | 6.65  | 126.60      | 111.30   |
| 1   | 1     | 98  | LEU  | N-CA-C     | -6.65 | 105.03      | 113.01   |
| 1   | 1     | 95  | GLU  | CA-CB-CG   | -6.64 | 100.82      | 114.10   |
| 3   | 3     | 134 | PRO  | CA-C-N     | -6.64 | 116.27      | 123.30   |
| 3   | 3     | 134 | PRO  | C-N-CA     | -6.64 | 116.27      | 123.30   |
| 1   | 1     | 259 | ARG  | CA-C-O     | -6.63 | 113.19      | 120.81   |
| 1   | 1     | 90  | ILE  | CA-C-N     | -6.63 | 109.73      | 122.06   |
| 1   | 1     | 90  | ILE  | C-N-CA     | -6.63 | 109.73      | 122.06   |
| 1   | 1     | 60  | PHE  | CA-C-O     | -6.62 | 113.61      | 120.89   |
| 3   | 3     | 187 | LEU  | N-CA-CB    | -6.62 | 100.38      | 110.77   |
| 1   | 1     | 282 | ARG  | NE-CZ-NH2  | -6.61 | 113.25      | 119.20   |
| 3   | 3     | 202 | THR  | CA-CB-OG1  | -6.58 | 99.73       | 109.60   |
| 1   | 1     | 25  | PRO  | CA-C-N     | 6.58  | 133.39      | 122.73   |
| 1   | 1     | 25  | PRO  | C-N-CA     | 6.58  | 133.39      | 122.73   |
| 2   | 2     | 161 | GLU  | CA-C-N     | -6.56 | 114.50      | 122.90   |
| 2   | 2     | 161 | GLU  | C-N-CA     | -6.56 | 114.50      | 122.90   |
| 2   | 2     | 198 | THR  | CA-C-O     | -6.56 | 113.04      | 120.32   |
| 3   | 3     | 42  | ASN  | CA-C-O     | -6.55 | 113.12      | 120.66   |
| 2   | 2     | 145 | THR  | CA-CB-OG1  | -6.55 | 99.78       | 109.60   |
| 2   | 2     | 38  | TRP  | N-CA-CB    | -6.54 | 99.31       | 110.11   |
| 2   | 2     | 12  | ARG  | N-CA-C     | 6.53  | 118.19      | 111.14   |
| 2   | 2     | 148 | HIS  | CA-CB-CG   | 6.52  | 120.32      | 113.80   |
| 2   | 2     | 11  | ASP  | OD1-CG-OD2 | 6.52  | 138.54      | 122.90   |
| 1   | 1     | 97  | LYS  | CB-CA-C    | -6.51 | 102.48      | 111.73   |
| 2   | 2     | 18  | LEU  | CB-CA-C    | 6.51  | 119.84      | 110.79   |
| 4   | 4     | 48  | ASP  | OD1-CG-OD2 | 6.50  | 138.50      | 122.90   |
| 2   | 2     | 163 | GLY  | O-C-N      | 6.50  | 130.17      | 122.50   |
| 3   | 3     | 19  | ARG  | CA-CB-CG   | 6.50  | 127.09      | 114.10   |
| 4   | 4     | 39  | SER  | O-C-N      | 6.49  | 130.85      | 122.23   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 3   | 3     | 74  | ASN  | N-CA-C     | 6.48  | 120.51      | 112.47   |
| 1   | 1     | 188 | VAL  | O-C-N      | 6.48  | 128.49      | 121.10   |
| 1   | 1     | 256 | ARG  | CD-NE-CZ   | -6.48 | 115.33      | 124.40   |
| 2   | 2     | 142 | VAL  | CA-C-O     | -6.48 | 113.08      | 120.66   |
| 4   | 4     | 36  | ALA  | N-CA-C     | -6.47 | 105.25      | 113.01   |
| 2   | 2     | 193 | THR  | CA-C-O     | 6.47  | 126.51      | 119.40   |
| 2   | 2     | 226 | ALA  | N-CA-C     | -6.47 | 99.21       | 109.04   |
| 3   | 3     | 182 | THR  | CA-CB-OG1  | -6.46 | 99.91       | 109.60   |
| 3   | 3     | 205 | VAL  | CB-CA-C    | 6.46  | 120.20      | 110.90   |
| 1   | 1     | 122 | VAL  | CB-CA-C    | 6.45  | 121.87      | 110.71   |
| 2   | 2     | 194 | ASN  | N-CA-C     | 6.45  | 120.58      | 110.32   |
| 2   | 2     | 241 | THR  | CA-C-O     | -6.45 | 113.87      | 120.71   |
| 3   | 3     | 57  | ASN  | N-CA-C     | 6.45  | 124.53      | 110.80   |
| 2   | 2     | 111 | GLN  | OE1-CD-NE2 | -6.44 | 116.16      | 122.60   |
| 2   | 2     | 247 | MET  | CB-CA-C    | 6.44  | 122.43      | 109.68   |
| 2   | 2     | 223 | ILE  | CA-C-O     | -6.43 | 116.59      | 119.94   |
| 3   | 3     | 65  | ASN  | N-CA-CB    | -6.43 | 100.95      | 110.53   |
| 2   | 2     | 69  | LYS  | CA-CB-CG   | 6.42  | 126.94      | 114.10   |
| 3   | 3     | 172 | GLN  | OE1-CD-NE2 | -6.41 | 116.19      | 122.60   |
| 1   | 1     | 277 | PRO  | CB-CA-C    | 6.41  | 119.78      | 111.64   |
| 3   | 3     | 99  | GLU  | CB-CG-CD   | 6.41  | 123.49      | 112.60   |
| 1   | 1     | 239 | VAL  | CB-CA-C    | 6.41  | 120.11      | 110.63   |
| 3   | 3     | 164 | THR  | CA-CB-OG1  | -6.39 | 100.01      | 109.60   |
| 3   | 3     | 216 | ASP  | CA-C-N     | 6.39  | 129.79      | 120.71   |
| 3   | 3     | 216 | ASP  | C-N-CA     | 6.39  | 129.79      | 120.71   |
| 2   | 2     | 203 | TYR  | CA-C-O     | -6.39 | 113.17      | 120.58   |
| 3   | 3     | 204 | GLN  | O-C-N      | 6.38  | 130.21      | 123.06   |
| 4   | 4     | 44  | SER  | CA-CB-OG   | -6.38 | 98.34       | 111.10   |
| 1   | 1     | 50  | SER  | CA-C-O     | -6.37 | 110.47      | 118.43   |
| 3   | 3     | 226 | GLN  | CB-CG-CD   | -6.36 | 101.80      | 112.60   |
| 2   | 2     | 235 | THR  | CB-CA-C    | -6.34 | 99.50       | 109.52   |
| 1   | 1     | 137 | PRO  | CA-C-N     | -6.33 | 113.02      | 122.39   |
| 1   | 1     | 137 | PRO  | C-N-CA     | -6.33 | 113.02      | 122.39   |
| 3   | 3     | 83  | THR  | CA-CB-OG1  | -6.33 | 100.11      | 109.60   |
| 2   | 2     | 145 | THR  | CA-C-O     | -6.32 | 113.80      | 120.63   |
| 1   | 1     | 265 | SER  | O-C-N      | -6.32 | 115.94      | 123.27   |
| 1   | 1     | 144 | SER  | N-CA-CB    | -6.31 | 100.82      | 110.42   |
| 1   | 1     | 288 | SER  | N-CA-CB    | -6.31 | 100.77      | 110.04   |
| 3   | 3     | 41  | HIS  | CA-C-O     | -6.30 | 112.43      | 119.67   |
| 1   | 1     | 250 | VAL  | N-CA-C     | 6.30  | 117.78      | 109.21   |
| 3   | 3     | 63  | GLU  | CB-CG-CD   | -6.29 | 101.90      | 112.60   |
| 3   | 3     | 202 | THR  | N-CA-C     | 6.27  | 118.39      | 108.79   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4   | 4     | 65  | PRO  | CB-CA-C    | -6.27 | 103.37      | 111.46   |
| 1   | 1     | 282 | ARG  | NH1-CZ-NH2 | 6.26  | 127.43      | 119.30   |
| 3   | 3     | 193 | THR  | CA-C-O     | -6.25 | 111.57      | 120.51   |
| 3   | 3     | 181 | TYR  | O-C-N      | 6.25  | 128.75      | 122.12   |
| 2   | 2     | 143 | LYS  | O-C-N      | 6.24  | 130.49      | 122.81   |
| 3   | 3     | 216 | ASP  | CB-CG-OD2  | 6.24  | 132.76      | 118.40   |
| 3   | 3     | 80  | VAL  | CA-C-O     | -6.24 | 114.03      | 120.71   |
| 1   | 1     | 70  | PHE  | CA-CB-CG   | 6.23  | 120.03      | 113.80   |
| 1   | 1     | 48  | SER  | CA-C-O     | -6.22 | 108.11      | 119.36   |
| 2   | 2     | 103 | ARG  | CA-CB-CG   | 6.22  | 126.54      | 114.10   |
| 3   | 3     | 183 | SER  | N-CA-CB    | -6.22 | 100.84      | 110.29   |
| 2   | 2     | 28  | ALA  | CA-C-O     | -6.21 | 114.80      | 121.94   |
| 3   | 3     | 196 | ILE  | N-CA-CB    | -6.21 | 103.38      | 111.82   |
| 1   | 1     | 260 | ALA  | CA-C-O     | -6.20 | 111.44      | 120.13   |
| 3   | 3     | 132 | THR  | CA-C-O     | -6.20 | 113.89      | 119.59   |
| 3   | 3     | 27  | ASN  | N-CA-CB    | -6.18 | 103.07      | 113.15   |
| 3   | 3     | 161 | ILE  | CA-C-O     | -6.18 | 113.90      | 120.39   |
| 1   | 1     | 31  | VAL  | N-CA-CB    | -6.18 | 102.56      | 111.21   |
| 3   | 3     | 137 | ARG  | NE-CZ-NH2  | 6.18  | 124.76      | 119.20   |
| 4   | 4     | 43  | GLN  | OE1-CD-NE2 | -6.17 | 116.43      | 122.60   |
| 3   | 3     | 6   | THR  | CB-CA-C    | 6.15  | 120.03      | 109.51   |
| 1   | 1     | 274 | ASN  | N-CA-CB    | 6.12  | 120.84      | 110.49   |
| 3   | 3     | 163 | MET  | CA-CB-CG   | -6.12 | 101.85      | 114.10   |
| 1   | 1     | 236 | LYS  | CA-C-O     | -6.12 | 114.25      | 121.16   |
| 1   | 1     | 252 | ALA  | CA-C-O     | -6.12 | 113.63      | 120.66   |
| 3   | 3     | 170 | GLY  | CA-C-N     | 6.12  | 128.69      | 120.50   |
| 3   | 3     | 170 | GLY  | C-N-CA     | 6.12  | 128.69      | 120.50   |
| 2   | 2     | 11  | ASP  | O-C-N      | 6.10  | 130.32      | 122.39   |
| 2   | 2     | 111 | GLN  | CB-CG-CD   | 6.09  | 122.96      | 112.60   |
| 2   | 2     | 179 | GLY  | CA-C-O     | -6.09 | 114.24      | 120.45   |
| 1   | 1     | 141 | ASN  | O-C-N      | 6.08  | 129.75      | 122.27   |
| 2   | 2     | 194 | ASN  | OD1-CG-ND2 | 6.08  | 128.68      | 122.60   |
| 3   | 3     | 193 | THR  | CA-CB-OG1  | -6.08 | 100.49      | 109.60   |
| 2   | 2     | 195 | ASN  | OD1-CG-ND2 | -6.06 | 116.54      | 122.60   |
| 1   | 1     | 68  | GLU  | CG-CD-OE2  | 6.05  | 132.32      | 118.40   |
| 1   | 1     | 52  | GLU  | CA-C-O     | -6.05 | 113.65      | 120.43   |
| 2   | 2     | 12  | ARG  | CD-NE-CZ   | -6.05 | 115.93      | 124.40   |
| 1   | 1     | 136 | GLN  | CG-CD-NE2  | -6.04 | 107.33      | 116.40   |
| 3   | 3     | 8   | PRO  | CA-C-O     | -6.04 | 114.54      | 121.36   |
| 2   | 2     | 241 | THR  | CA-CB-OG1  | -6.03 | 100.55      | 109.60   |
| 3   | 3     | 137 | ARG  | CA-C-O     | -6.02 | 115.01      | 121.94   |
| 3   | 3     | 36  | ILE  | CA-C-O     | -6.01 | 111.89      | 119.95   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | 1     | 77  | VAL  | CA-C-O     | -6.01 | 113.25      | 118.96   |
| 2   | 2     | 86  | LEU  | CA-C-N     | 6.00  | 130.30      | 120.63   |
| 2   | 2     | 86  | LEU  | C-N-CA     | 6.00  | 130.30      | 120.63   |
| 3   | 3     | 47  | ILE  | CB-CG1-CD1 | -6.00 | 101.19      | 113.80   |
| 3   | 3     | 121 | ALA  | CB-CA-C    | -5.99 | 99.55       | 110.63   |
| 2   | 2     | 169 | VAL  | N-CA-CB    | 5.99  | 117.56      | 110.55   |
| 3   | 3     | 41  | HIS  | N-CA-CB    | 5.99  | 119.08      | 110.40   |
| 1   | 1     | 41  | ALA  | CA-C-O     | -5.98 | 114.66      | 121.72   |
| 3   | 3     | 194 | SER  | N-CA-CB    | -5.97 | 100.40      | 110.49   |
| 1   | 1     | 133 | THR  | CA-CB-OG1  | -5.97 | 100.65      | 109.60   |
| 2   | 2     | 14  | GLN  | CA-CB-CG   | -5.97 | 102.17      | 114.10   |
| 1   | 1     | 55  | THR  | CA-CB-OG1  | -5.93 | 100.71      | 109.60   |
| 2   | 2     | 255 | ARG  | NE-CZ-NH1  | 5.93  | 127.43      | 121.50   |
| 2   | 2     | 136 | GLU  | CG-CD-OE1  | -5.92 | 104.78      | 118.40   |
| 3   | 3     | 92  | PHE  | CA-CB-CG   | -5.92 | 107.88      | 113.80   |
| 1   | 1     | 265 | SER  | N-CA-CB    | -5.92 | 100.52      | 111.53   |
| 2   | 2     | 41  | TYR  | N-CA-CB    | 5.92  | 118.49      | 110.38   |
| 3   | 3     | 160 | THR  | CA-CB-OG1  | -5.92 | 100.72      | 109.60   |
| 1   | 1     | 259 | ARG  | CB-CA-C    | -5.91 | 100.44      | 109.89   |
| 3   | 3     | 77  | ASN  | O-C-N      | -5.91 | 114.74      | 122.59   |
| 2   | 2     | 161 | GLU  | CA-CB-CG   | 5.90  | 125.90      | 114.10   |
| 1   | 1     | 22  | SER  | N-CA-CB    | -5.90 | 100.81      | 109.95   |
| 2   | 2     | 105 | GLY  | N-CA-C     | -5.89 | 102.39      | 112.64   |
| 3   | 3     | 158 | GLN  | CA-C-O     | 5.89  | 127.63      | 120.62   |
| 3   | 3     | 55  | MET  | CA-CB-CG   | -5.88 | 102.34      | 114.10   |
| 3   | 3     | 207 | LEU  | CA-C-O     | -5.87 | 114.28      | 120.80   |
| 3   | 3     | 1   | GLY  | O-C-N      | -5.86 | 113.62      | 123.00   |
| 1   | 1     | 280 | LYS  | CB-CA-C    | -5.85 | 101.74      | 110.16   |
| 3   | 3     | 57  | ASN  | O-C-N      | -5.85 | 114.81      | 122.59   |
| 2   | 2     | 88  | ASP  | CA-C-O     | -5.84 | 112.58      | 119.48   |
| 2   | 2     | 226 | ALA  | O-C-N      | 5.83  | 127.83      | 121.36   |
| 1   | 1     | 270 | ASN  | CB-CA-C    | -5.82 | 100.32      | 109.70   |
| 2   | 2     | 105 | GLY  | CA-C-O     | -5.82 | 112.95      | 122.56   |
| 3   | 3     | 33  | ARG  | CB-CG-CD   | -5.82 | 97.91       | 111.30   |
| 3   | 3     | 93  | LYS  | N-CA-C     | 5.82  | 118.40      | 111.71   |
| 1   | 1     | 145 | ASN  | CB-CG-ND2  | -5.81 | 107.68      | 116.40   |
| 3   | 3     | 59  | HIS  | CA-CB-CG   | -5.80 | 108.00      | 113.80   |
| 3   | 3     | 197 | LEU  | CB-CA-C    | 5.80  | 117.21      | 108.86   |
| 3   | 3     | 131 | TYR  | CA-C-O     | -5.78 | 114.13      | 120.43   |
| 2   | 2     | 235 | THR  | OG1-CB-CG2 | 5.78  | 120.86      | 109.30   |
| 1   | 1     | 267 | GLY  | CA-C-N     | -5.78 | 113.10      | 122.81   |
| 1   | 1     | 267 | GLY  | C-N-CA     | -5.78 | 113.10      | 122.81   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | 2     | 54  | SER  | CA-C-N     | -5.77 | 115.08      | 122.98   |
| 2   | 2     | 54  | SER  | C-N-CA     | -5.77 | 115.08      | 122.98   |
| 1   | 1     | 242 | ARG  | CD-NE-CZ   | -5.77 | 116.32      | 124.40   |
| 4   | 4     | 65  | PRO  | CA-C-O     | -5.76 | 114.78      | 121.34   |
| 1   | 1     | 68  | GLU  | CG-CD-OE1  | -5.75 | 105.17      | 118.40   |
| 2   | 2     | 198 | THR  | O-C-N      | 5.73  | 130.01      | 123.31   |
| 2   | 2     | 210 | ASP  | N-CA-CB    | -5.72 | 100.57      | 110.87   |
| 2   | 2     | 86  | LEU  | CA-C-O     | -5.71 | 112.88      | 119.56   |
| 1   | 1     | 129 | THR  | CA-C-O     | -5.70 | 114.54      | 120.70   |
| 1   | 1     | 94  | ARG  | CG-CD-NE   | -5.70 | 99.46       | 112.00   |
| 3   | 3     | 66  | SER  | N-CA-C     | -5.70 | 105.99      | 113.17   |
| 3   | 3     | 137 | ARG  | O-C-N      | 5.69  | 129.65      | 122.65   |
| 3   | 3     | 161 | ILE  | CA-CB-CG1  | -5.69 | 100.73      | 110.40   |
| 1   | 1     | 83  | GLN  | CB-CG-CD   | -5.68 | 102.94      | 112.60   |
| 2   | 2     | 189 | ILE  | CA-C-O     | -5.68 | 113.30      | 120.69   |
| 3   | 3     | 112 | ARG  | CA-CB-CG   | 5.68  | 125.46      | 114.10   |
| 3   | 3     | 45  | GLU  | CG-CD-OE2  | 5.67  | 131.44      | 118.40   |
| 1   | 1     | 139 | SER  | CA-CB-OG   | -5.67 | 99.77       | 111.10   |
| 3   | 3     | 38  | GLY  | N-CA-C     | 5.66  | 123.70      | 115.32   |
| 1   | 1     | 94  | ARG  | NH1-CZ-NH2 | 5.66  | 126.66      | 119.30   |
| 2   | 2     | 190 | ASN  | CB-CA-C    | 5.65  | 120.00      | 110.79   |
| 2   | 2     | 99  | HIS  | CA-CB-CG   | -5.64 | 108.16      | 113.80   |
| 1   | 1     | 241 | ILE  | N-CA-CB    | -5.64 | 104.23      | 110.99   |
| 1   | 1     | 28  | THR  | N-CA-C     | 5.63  | 118.06      | 109.95   |
| 2   | 2     | 199 | ILE  | CA-C-O     | -5.62 | 114.40      | 120.36   |
| 3   | 3     | 235 | THR  | CA-CB-OG1  | -5.61 | 101.18      | 109.60   |
| 2   | 2     | 106 | TYR  | CA-C-O     | -5.61 | 115.27      | 121.33   |
| 2   | 2     | 217 | ASN  | CB-CA-C    | 5.60  | 118.96      | 109.55   |
| 3   | 3     | 180 | THR  | CA-CB-OG1  | -5.59 | 101.22      | 109.60   |
| 4   | 4     | 58  | ASP  | CA-C-N     | 5.57  | 129.02      | 121.05   |
| 4   | 4     | 58  | ASP  | C-N-CA     | 5.57  | 129.02      | 121.05   |
| 3   | 3     | 190 | TRP  | CA-C-O     | -5.57 | 115.11      | 121.40   |
| 1   | 1     | 27  | HIS  | CA-CB-CG   | 5.57  | 119.36      | 113.80   |
| 3   | 3     | 166 | PRO  | CB-CA-C    | 5.56  | 118.63      | 111.46   |
| 2   | 2     | 9   | TYR  | CA-CB-CG   | -5.54 | 103.92      | 113.90   |
| 1   | 1     | 273 | LYS  | CG-CD-CE   | -5.54 | 98.56       | 111.30   |
| 2   | 2     | 94  | GLN  | CG-CD-NE2  | -5.54 | 108.09      | 116.40   |
| 2   | 2     | 68  | SER  | N-CA-CB    | -5.53 | 101.88      | 110.29   |
| 3   | 3     | 42  | ASN  | CB-CG-ND2  | 5.53  | 124.70      | 116.40   |
| 2   | 2     | 215 | HIS  | CA-C-O     | -5.53 | 112.53      | 120.11   |
| 2   | 2     | 262 | GLN  | OE1-CD-NE2 | -5.53 | 117.07      | 122.60   |
| 2   | 2     | 99  | HIS  | CA-C-N     | 5.53  | 128.24      | 120.28   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | 2     | 99  | HIS  | C-N-CA     | 5.53  | 128.24      | 120.28   |
| 1   | 1     | 64  | GLU  | CA-CB-CG   | 5.53  | 125.15      | 114.10   |
| 1   | 1     | 235 | HIS  | CA-CB-CG   | -5.53 | 108.28      | 113.80   |
| 2   | 2     | 168 | ASP  | CA-C-N     | 5.52  | 127.52      | 120.56   |
| 2   | 2     | 168 | ASP  | C-N-CA     | 5.52  | 127.52      | 120.56   |
| 2   | 2     | 251 | PHE  | CA-C-O     | -5.52 | 114.87      | 121.11   |
| 3   | 3     | 76  | GLN  | CA-C-O     | -5.50 | 115.18      | 121.68   |
| 2   | 2     | 188 | PHE  | CA-C-O     | -5.50 | 114.95      | 121.66   |
| 3   | 3     | 140 | GLN  | CA-CB-CG   | -5.50 | 103.10      | 114.10   |
| 2   | 2     | 43  | PRO  | N-CD-CG    | -5.50 | 94.95       | 103.20   |
| 2   | 2     | 167 | LYS  | CA-C-O     | 5.49  | 126.15      | 119.78   |
| 1   | 1     | 63  | SER  | O-C-N      | 5.48  | 127.93      | 122.12   |
| 3   | 3     | 107 | TRP  | CA-C-O     | -5.48 | 115.20      | 121.40   |
| 3   | 3     | 84  | ASN  | OD1-CG-ND2 | 5.47  | 128.07      | 122.60   |
| 2   | 2     | 192 | ARG  | CA-C-O     | -5.47 | 111.94      | 119.05   |
| 2   | 2     | 258 | SER  | O-C-N      | 5.47  | 129.54      | 122.81   |
| 4   | 4     | 50  | SER  | CA-CB-OG   | -5.46 | 100.18      | 111.10   |
| 2   | 2     | 38  | TRP  | CB-CA-C    | 5.46  | 116.27      | 108.68   |
| 3   | 3     | 57  | ASN  | CA-C-N     | 5.45  | 131.98      | 121.18   |
| 3   | 3     | 57  | ASN  | C-N-CA     | 5.45  | 131.98      | 121.18   |
| 3   | 3     | 164 | THR  | CB-CA-C    | 5.45  | 119.14      | 109.72   |
| 2   | 2     | 63  | PHE  | CA-CB-CG   | 5.44  | 119.24      | 113.80   |
| 1   | 1     | 144 | SER  | CA-C-N     | -5.44 | 115.38      | 123.11   |
| 1   | 1     | 144 | SER  | C-N-CA     | -5.44 | 115.38      | 123.11   |
| 2   | 2     | 26  | GLN  | OE1-CD-NE2 | -5.44 | 117.16      | 122.60   |
| 3   | 3     | 63  | GLU  | CG-CD-OE1  | -5.44 | 105.89      | 118.40   |
| 1   | 1     | 50  | SER  | CB-CA-C    | 5.43  | 117.49      | 109.29   |
| 2   | 2     | 221 | MET  | CA-C-O     | -5.43 | 114.30      | 120.32   |
| 3   | 3     | 168 | THR  | CA-CB-OG1  | -5.43 | 101.46      | 109.60   |
| 2   | 2     | 232 | THR  | CA-CB-OG1  | -5.42 | 101.47      | 109.60   |
| 3   | 3     | 195 | LEU  | CA-C-O     | -5.42 | 114.88      | 121.05   |
| 1   | 1     | 21  | ILE  | CA-CB-CG1  | -5.42 | 101.19      | 110.40   |
| 2   | 2     | 13  | VAL  | CA-C-O     | -5.41 | 114.56      | 120.84   |
| 2   | 2     | 123 | LEU  | CA-C-O     | -5.41 | 114.54      | 120.43   |
| 2   | 2     | 219 | SER  | N-CA-C     | -5.41 | 100.88      | 109.59   |
| 2   | 2     | 129 | GLU  | CB-CA-C    | -5.41 | 104.21      | 111.89   |
| 2   | 2     | 92  | PHE  | N-CA-C     | -5.41 | 105.08      | 110.97   |
| 3   | 3     | 90  | GLY  | CA-C-O     | -5.41 | 114.87      | 121.68   |
| 2   | 2     | 53  | THR  | CA-C-O     | -5.40 | 115.57      | 121.89   |
| 2   | 2     | 187 | GLN  | CA-C-O     | -5.38 | 114.96      | 120.99   |
| 3   | 3     | 78  | GLU  | CA-CB-CG   | 5.38  | 124.86      | 114.10   |
| 3   | 3     | 34  | ILE  | CA-C-O     | -5.37 | 114.07      | 120.78   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 3   | 3     | 116 | MET  | CB-CG-SD   | -5.37 | 96.59       | 112.70   |
| 3   | 3     | 143 | ARG  | O-C-N      | 5.36  | 128.26      | 122.15   |
| 2   | 2     | 81  | LYS  | CB-CG-CD   | 5.36  | 123.63      | 111.30   |
| 1   | 1     | 282 | ARG  | O-C-N      | 5.36  | 129.40      | 122.81   |
| 3   | 3     | 38  | GLY  | O-C-N      | -5.35 | 116.01      | 122.38   |
| 2   | 2     | 120 | GLY  | CA-C-O     | -5.34 | 114.43      | 122.54   |
| 3   | 3     | 221 | LEU  | O-C-N      | 5.33  | 129.68      | 122.59   |
| 2   | 2     | 12  | ARG  | CB-CG-CD   | -5.33 | 99.04       | 111.30   |
| 3   | 3     | 112 | ARG  | CB-CA-C    | 5.33  | 119.00      | 110.16   |
| 3   | 3     | 226 | GLN  | N-CA-C     | -5.33 | 106.73      | 113.18   |
| 1   | 1     | 92  | ASN  | O-C-N      | 5.32  | 129.46      | 123.28   |
| 2   | 2     | 102 | GLY  | CA-C-O     | -5.32 | 115.46      | 121.68   |
| 1   | 1     | 26  | LYS  | CG-CD-CE   | -5.31 | 99.08       | 111.30   |
| 2   | 2     | 210 | ASP  | CA-CB-CG   | -5.31 | 107.29      | 112.60   |
| 2   | 2     | 177 | LEU  | N-CA-CB    | -5.31 | 101.63      | 110.23   |
| 3   | 3     | 192 | GLN  | N-CA-C     | -5.30 | 105.08      | 112.45   |
| 1   | 1     | 288 | SER  | CA-CB-OG   | -5.30 | 100.50      | 111.10   |
| 2   | 2     | 76  | LYS  | CA-C-O     | -5.29 | 113.43      | 119.41   |
| 2   | 2     | 262 | GLN  | CG-CD-NE2  | 5.29  | 124.33      | 116.40   |
| 3   | 3     | 222 | MET  | CB-CG-SD   | -5.29 | 96.83       | 112.70   |
| 4   | 4     | 58  | ASP  | N-CA-CB    | 5.28  | 119.03      | 110.42   |
| 3   | 3     | 204 | GLN  | CA-C-O     | -5.28 | 115.03      | 121.36   |
| 1   | 1     | 60  | PHE  | N-CA-CB    | -5.27 | 102.17      | 111.39   |
| 1   | 1     | 286 | ILE  | O-C-N      | 5.27  | 127.75      | 121.80   |
| 3   | 3     | 16  | THR  | OG1-CB-CG2 | 5.27  | 119.84      | 109.30   |
| 3   | 3     | 86  | PHE  | CB-CA-C    | 5.27  | 120.48      | 111.68   |
| 3   | 3     | 28  | TYR  | N-CA-CB    | -5.26 | 102.23      | 109.97   |
| 3   | 3     | 161 | ILE  | N-CA-CB    | 5.26  | 118.67      | 111.41   |
| 3   | 3     | 56  | ASN  | CA-C-N     | 5.26  | 131.59      | 121.54   |
| 3   | 3     | 56  | ASN  | C-N-CA     | 5.26  | 131.59      | 121.54   |
| 2   | 2     | 168 | ASP  | OD1-CG-OD2 | 5.25  | 135.51      | 122.90   |
| 3   | 3     | 144 | GLU  | CA-CB-CG   | 5.25  | 124.61      | 114.10   |
| 2   | 2     | 214 | ARG  | CD-NE-CZ   | -5.25 | 117.05      | 124.40   |
| 3   | 3     | 77  | ASN  | CA-CB-CG   | -5.25 | 107.35      | 112.60   |
| 4   | 4     | 53  | THR  | CA-CB-OG1  | -5.25 | 101.73      | 109.60   |
| 2   | 2     | 72  | THR  | CA-CB-OG1  | -5.25 | 101.73      | 109.60   |
| 1   | 1     | 227 | ARG  | NE-CZ-NH2  | 5.24  | 123.92      | 119.20   |
| 2   | 2     | 122 | LEU  | CA-C-O     | -5.24 | 115.09      | 121.28   |
| 1   | 1     | 136 | GLN  | OE1-CD-NE2 | 5.24  | 127.84      | 122.60   |
| 1   | 1     | 259 | ARG  | N-CA-CB    | 5.24  | 117.65      | 109.85   |
| 3   | 3     | 186 | PHE  | CA-CB-CG   | -5.24 | 108.56      | 113.80   |
| 1   | 1     | 113 | ARG  | NE-CZ-NH2  | 5.23  | 123.91      | 119.20   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2   | 2     | 195 | ASN  | N-CA-C    | -5.23 | 106.69      | 114.64   |
| 2   | 2     | 20  | ASN  | CA-CB-CG  | 5.23  | 117.83      | 112.60   |
| 3   | 3     | 158 | GLN  | CG-CD-OE1 | 5.23  | 131.26      | 120.80   |
| 2   | 2     | 243 | THR  | CA-C-O    | -5.22 | 114.69      | 120.38   |
| 2   | 2     | 257 | LYS  | N-CA-CB   | 5.22  | 119.31      | 110.49   |
| 3   | 3     | 94  | THR  | CA-C-O    | -5.22 | 113.20      | 119.15   |
| 3   | 3     | 208 | LEU  | CA-C-O    | -5.22 | 115.01      | 120.80   |
| 1   | 1     | 257 | ALA  | N-CA-CB   | -5.21 | 101.81      | 109.98   |
| 3   | 3     | 138 | GLY  | N-CA-C    | -5.20 | 101.72      | 112.34   |
| 1   | 1     | 127 | GLU  | CA-C-O    | -5.20 | 114.60      | 120.32   |
| 2   | 2     | 75  | SER  | N-CA-CB   | -5.20 | 101.98      | 109.83   |
| 1   | 1     | 268 | ARG  | CB-CA-C   | 5.20  | 119.74      | 109.66   |
| 2   | 2     | 8   | GLY  | CA-C-N    | -5.20 | 113.49      | 120.87   |
| 2   | 2     | 8   | GLY  | C-N-CA    | -5.20 | 113.49      | 120.87   |
| 1   | 1     | 23  | SER  | CA-C-O    | -5.19 | 115.04      | 121.06   |
| 2   | 2     | 259 | ILE  | CA-C-O    | -5.19 | 114.99      | 120.39   |
| 1   | 1     | 282 | ARG  | CB-CA-C   | -5.19 | 100.33      | 109.62   |
| 1   | 1     | 279 | ILE  | CA-C-N    | 5.18  | 128.69      | 121.02   |
| 1   | 1     | 279 | ILE  | C-N-CA    | 5.18  | 128.69      | 121.02   |
| 1   | 1     | 63  | SER  | N-CA-C    | 5.18  | 116.92      | 111.28   |
| 3   | 3     | 231 | THR  | CA-C-N    | -5.18 | 115.34      | 122.69   |
| 3   | 3     | 231 | THR  | C-N-CA    | -5.18 | 115.34      | 122.69   |
| 2   | 2     | 38  | TRP  | CA-CB-CG  | -5.17 | 103.77      | 113.60   |
| 2   | 2     | 181 | LEU  | N-CA-C    | -5.17 | 106.23      | 112.54   |
| 3   | 3     | 215 | PRO  | CB-CA-C   | 5.17  | 119.25      | 111.44   |
| 3   | 3     | 233 | ALA  | O-C-N     | 5.17  | 129.23      | 122.87   |
| 2   | 2     | 18  | LEU  | N-CA-CB   | -5.17 | 102.80      | 110.71   |
| 3   | 3     | 109 | GLY  | N-CA-C    | 5.17  | 117.57      | 111.63   |
| 2   | 2     | 213 | THR  | CA-CB-OG1 | -5.16 | 101.86      | 109.60   |
| 2   | 2     | 127 | ILE  | CA-C-O    | -5.16 | 114.27      | 119.89   |
| 2   | 2     | 119 | SER  | O-C-N     | 5.13  | 129.38      | 123.17   |
| 2   | 2     | 143 | LYS  | CA-C-N    | 5.13  | 131.34      | 121.54   |
| 2   | 2     | 143 | LYS  | C-N-CA    | 5.13  | 131.34      | 121.54   |
| 3   | 3     | 186 | PHE  | O-C-N     | 5.12  | 129.81      | 123.15   |
| 3   | 3     | 67  | TYR  | N-CA-C    | -5.12 | 106.88      | 113.23   |
| 1   | 1     | 145 | ASN  | O-C-N     | 5.12  | 129.58      | 123.13   |
| 3   | 3     | 45  | GLU  | CG-CD-OE1 | -5.12 | 106.63      | 118.40   |
| 2   | 2     | 152 | ARG  | CD-NE-CZ  | -5.12 | 117.24      | 124.40   |
| 1   | 1     | 128 | TYR  | CA-CB-CG  | -5.11 | 104.70      | 113.90   |
| 3   | 3     | 82  | GLY  | N-CA-C    | -5.11 | 103.00      | 110.87   |
| 2   | 2     | 165 | PRO  | CA-C-O    | -5.11 | 115.41      | 122.15   |
| 3   | 3     | 75  | ARG  | CD-NE-CZ  | -5.10 | 117.26      | 124.40   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | 2     | 32  | VAL  | O-C-N      | 5.10  | 128.34      | 123.14   |
| 1   | 1     | 40  | GLY  | N-CA-C     | -5.09 | 108.09      | 115.27   |
| 2   | 2     | 169 | VAL  | O-C-N      | -5.09 | 116.92      | 121.91   |
| 3   | 3     | 1   | GLY  | N-CA-C     | 5.08  | 128.03      | 113.30   |
| 1   | 1     | 285 | ASP  | CA-C-N     | -5.08 | 111.98      | 120.30   |
| 1   | 1     | 285 | ASP  | C-N-CA     | -5.08 | 111.98      | 120.30   |
| 2   | 2     | 127 | ILE  | O-C-N      | 5.08  | 125.59      | 120.92   |
| 1   | 1     | 27  | HIS  | CA-C-O     | -5.07 | 113.13      | 122.62   |
| 2   | 2     | 119 | SER  | CA-C-O     | -5.07 | 115.67      | 121.40   |
| 2   | 2     | 168 | ASP  | CB-CG-OD1  | -5.07 | 106.73      | 118.40   |
| 3   | 3     | 125 | ALA  | CA-C-O     | -5.07 | 115.52      | 121.10   |
| 3   | 3     | 177 | ASP  | N-CA-CB    | -5.07 | 103.00      | 110.14   |
| 2   | 2     | 65  | THR  | CA-CB-OG1  | -5.06 | 102.01      | 109.60   |
| 1   | 1     | 66  | ASP  | CA-C-O     | -5.06 | 115.62      | 121.19   |
| 2   | 2     | 259 | ILE  | CA-C-N     | -5.06 | 112.77      | 122.13   |
| 2   | 2     | 259 | ILE  | C-N-CA     | -5.06 | 112.77      | 122.13   |
| 1   | 1     | 76  | CYS  | CA-C-O     | -5.05 | 115.00      | 120.81   |
| 1   | 1     | 189 | PRO  | CA-C-O     | -5.05 | 115.19      | 122.31   |
| 1   | 1     | 68  | GLU  | N-CA-C     | -5.04 | 105.97      | 111.82   |
| 3   | 3     | 32  | PRO  | CA-C-O     | -5.04 | 115.71      | 121.56   |
| 1   | 1     | 270 | ASN  | N-CA-CB    | 5.04  | 117.71      | 109.69   |
| 1   | 1     | 118 | LEU  | N-CA-C     | -5.04 | 107.08      | 113.18   |
| 2   | 2     | 25  | THR  | CA-C-O     | 5.04  | 126.45      | 120.66   |
| 3   | 3     | 217 | PHE  | N-CA-C     | 5.04  | 117.53      | 110.23   |
| 1   | 1     | 65  | THR  | N-CA-C     | -5.04 | 106.06      | 113.61   |
| 2   | 2     | 126 | VAL  | CA-C-O     | -5.03 | 115.14      | 120.53   |
| 1   | 1     | 189 | PRO  | CB-CA-C    | -5.03 | 103.62      | 111.22   |
| 2   | 2     | 235 | THR  | CA-C-O     | 5.03  | 125.40      | 120.17   |
| 2   | 2     | 215 | HIS  | CA-CB-CG   | 5.02  | 118.82      | 113.80   |
| 2   | 2     | 261 | PRO  | CA-C-N     | 5.02  | 130.74      | 121.70   |
| 2   | 2     | 261 | PRO  | C-N-CA     | 5.02  | 130.74      | 121.70   |
| 2   | 2     | 236 | PRO  | N-CA-CB    | -5.02 | 97.98       | 103.25   |
| 3   | 3     | 217 | PHE  | CA-C-O     | -5.02 | 115.67      | 121.19   |
| 3   | 3     | 158 | GLN  | CB-CA-C    | 5.01  | 118.29      | 110.67   |
| 3   | 3     | 146 | MET  | CB-CA-C    | 5.01  | 120.39      | 110.17   |
| 3   | 3     | 95  | THR  | CA-CB-OG1  | -5.01 | 102.09      | 109.60   |
| 3   | 3     | 155 | ILE  | CB-CG1-CD1 | 5.01  | 124.31      | 113.80   |
| 4   | 4     | 57  | LYS  | N-CA-CB    | 5.01  | 117.33      | 110.07   |
| 3   | 3     | 118 | THR  | CA-CB-CG2  | 5.00  | 119.01      | 110.50   |

There are no chirality outliers.

All (4) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | 1     | 259 | ARG  | Sidechain |
| 1   | 1     | 268 | ARG  | Sidechain |
| 2   | 2     | 12  | ARG  | Sidechain |
| 2   | 2     | 255 | ARG  | Sidechain |

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | 1     | 2170  | 0        | 2107     | 174     | 0            |
| 2   | 2     | 1951  | 0        | 1923     | 132     | 0            |
| 3   | 3     | 1849  | 0        | 1832     | 142     | 0            |
| 4   | 4     | 297   | 0        | 294      | 36      | 0            |
| 5   | 1     | 23    | 0        | 16       | 2       | 0            |
| All | All   | 6290  | 0        | 6172     | 411     | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 33.

All (411) 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) |
|-----------------|------------------|--------------------------|-------------------|
| 3:3:57:ASN:CB   | 3:3:57:ASN:CA    | 1.75                     | 1.58              |
| 4:4:33:LYS:CE   | 4:4:33:LYS:NZ    | 1.67                     | 1.55              |
| 2:2:52:LYS:NZ   | 2:2:52:LYS:CE    | 1.68                     | 1.54              |
| 1:1:285:ASP:CB  | 1:1:285:ASP:CA   | 1.80                     | 1.54              |
| 3:3:179:ASP:OD2 | 3:3:182:THR:HB   | 1.40                     | 1.17              |
| 2:2:158:SER:OG  | 2:2:167:LYS:HE2  | 1.46                     | 1.14              |
| 3:3:21:SER:O    | 4:4:37:SER:HB2   | 1.54                     | 1.07              |
| 1:1:285:ASP:CA  | 1:1:285:ASP:OD1  | 2.00                     | 1.07              |
| 1:1:258:PRO:HG2 | 3:3:99:GLU:HG2   | 1.36                     | 1.06              |
| 1:1:47:PRO:HA   | 3:3:164:THR:HG21 | 1.34                     | 1.05              |
| 2:2:12:ARG:NH1  | 2:2:12:ARG:HG3   | 1.69                     | 1.05              |
| 2:2:255:ARG:HG2 | 2:2:256:SER:H    | 1.24                     | 1.03              |
| 1:1:282:ARG:HG3 | 3:3:57:ASN:HB3   | 1.41                     | 1.02              |
| 1:1:151:MET:HE1 | 1:1:167:THR:O    | 1.64                     | 0.98              |
| 2:2:136:GLU:HB3 | 2:2:140:VAL:HG21 | 1.44                     | 0.97              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:3:57:ASN:CB    | 3:3:57:ASN:N     | 2.28                     | 0.97              |
| 3:3:57:ASN:CB    | 3:3:57:ASN:C     | 2.37                     | 0.96              |
| 1:1:191:VAL:HG23 | 1:1:191:VAL:O    | 1.66                     | 0.96              |
| 1:1:285:ASP:CA   | 1:1:285:ASP:CG   | 2.37                     | 0.95              |
| 1:1:83:GLN:HG3   | 1:1:85:LYS:HE2   | 1.47                     | 0.94              |
| 1:1:285:ASP:CB   | 1:1:285:ASP:C    | 2.40                     | 0.93              |
| 1:1:152:TYR:O    | 1:1:154:PRO:HD3  | 1.69                     | 0.93              |
| 2:2:41:TYR:CE2   | 2:2:55:LYS:HD3   | 2.05                     | 0.92              |
| 1:1:285:ASP:CB   | 1:1:285:ASP:N    | 2.34                     | 0.91              |
| 2:2:12:ARG:HG3   | 2:2:12:ARG:HH11  | 1.27                     | 0.91              |
| 2:2:235:THR:HG23 | 2:2:236:PRO:HD2  | 1.53                     | 0.91              |
| 1:1:28:THR:HB    | 1:1:30:LYS:H     | 1.35                     | 0.90              |
| 1:1:58:MET:HE1   | 3:3:216:ASP:O    | 1.71                     | 0.90              |
| 2:2:11:ASP:HB2   | 4:4:68:ASN:OD1   | 1.71                     | 0.90              |
| 3:3:57:ASN:CA    | 3:3:57:ASN:CG    | 2.45                     | 0.89              |
| 1:1:285:ASP:OD1  | 1:1:285:ASP:HA   | 1.73                     | 0.88              |
| 3:3:198:PRO:HD2  | 3:3:201:THR:HG21 | 1.55                     | 0.88              |
| 2:2:20:ASN:ND2   | 2:2:62:ARG:HE    | 1.72                     | 0.87              |
| 1:1:47:PRO:HA    | 3:3:164:THR:CG2  | 2.03                     | 0.87              |
| 1:1:162:GLU:HB2  | 1:1:165:ASP:OD1  | 1.75                     | 0.86              |
| 2:2:195:ASN:ND2  | 2:2:196:THR:HG23 | 1.90                     | 0.86              |
| 2:2:12:ARG:HH11  | 2:2:12:ARG:CG    | 1.89                     | 0.85              |
| 2:2:116:LYS:HB3  | 3:3:121:ALA:HB3  | 1.58                     | 0.85              |
| 1:1:90:ILE:HD13  | 1:1:90:ILE:N     | 1.92                     | 0.84              |
| 1:1:282:ARG:HD2  | 1:1:285:ASP:O    | 1.78                     | 0.84              |
| 2:2:158:SER:OG   | 2:2:167:LYS:CE   | 2.27                     | 0.82              |
| 1:1:102:TRP:O    | 1:1:104:ILE:N    | 2.12                     | 0.82              |
| 2:2:30:ASN:HD22  | 2:2:31:ALA:H     | 1.27                     | 0.82              |
| 2:2:52:LYS:NZ    | 2:2:52:LYS:CD    | 2.43                     | 0.82              |
| 1:1:191:VAL:O    | 1:1:191:VAL:CG2  | 2.27                     | 0.82              |
| 1:1:248:LYS:HE3  | 4:4:38:THR:O     | 1.80                     | 0.82              |
| 2:2:10:SER:OG    | 2:2:12:ARG:HB2   | 1.78                     | 0.82              |
| 2:2:136:GLU:CB   | 2:2:140:VAL:HG21 | 2.09                     | 0.82              |
| 4:4:59:LEU:HD21  | 4:4:61:LEU:HD13  | 1.61                     | 0.81              |
| 1:1:38:GLU:CD    | 3:3:116:MET:HE2  | 2.05                     | 0.81              |
| 1:1:58:MET:CE    | 3:3:216:ASP:HA   | 2.11                     | 0.80              |
| 2:2:9:TYR:HD1    | 2:2:9:TYR:N      | 1.77                     | 0.80              |
| 2:2:195:ASN:HD22 | 2:2:196:THR:HG23 | 1.47                     | 0.79              |
| 4:4:68:ASN:OD1   | 4:4:68:ASN:N     | 2.11                     | 0.79              |
| 2:2:9:TYR:N      | 2:2:9:TYR:CD1    | 2.43                     | 0.79              |
| 1:1:58:MET:HE1   | 3:3:216:ASP:C    | 2.08                     | 0.78              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:2:262:GLN:HE21 | 2:2:262:GLN:C    | 1.91                     | 0.78              |
| 1:1:282:ARG:HG3  | 3:3:57:ASN:CB    | 2.15                     | 0.77              |
| 2:2:255:ARG:HG2  | 2:2:256:SER:N    | 2.00                     | 0.77              |
| 3:3:79:GLN:HB2   | 3:3:190:TRP:CZ3  | 2.20                     | 0.76              |
| 1:1:94:ARG:NH1   | 1:1:94:ARG:HG2   | 2.00                     | 0.76              |
| 1:1:103:LYS:HA   | 1:1:223:SER:HB3  | 1.68                     | 0.76              |
| 1:1:220:HIS:CG   | 1:1:220:HIS:O    | 2.39                     | 0.75              |
| 1:1:270:ASN:HA   | 2:2:133:ALA:HB1  | 1.68                     | 0.75              |
| 3:3:179:ASP:OD2  | 3:3:182:THR:CB   | 2.31                     | 0.74              |
| 2:2:174:ASN:C    | 2:2:174:ASN:HD22 | 1.93                     | 0.74              |
| 3:3:197:LEU:HB3  | 3:3:201:THR:CG2  | 2.18                     | 0.74              |
| 1:1:89:GLY:C     | 1:1:90:ILE:HD13  | 2.13                     | 0.74              |
| 4:4:43:GLN:HG2   | 4:4:45:LEU:HB2   | 1.70                     | 0.73              |
| 2:2:188:PHE:O    | 2:2:194:ASN:ND2  | 2.22                     | 0.73              |
| 3:3:26:PRO:O     | 3:3:27:ASN:HB2   | 1.89                     | 0.73              |
| 1:1:92:ASN:OD1   | 1:1:95:GLU:HB2   | 1.87                     | 0.73              |
| 1:1:282:ARG:CG   | 3:3:57:ASN:HB3   | 2.18                     | 0.73              |
| 1:1:47:PRO:CA    | 3:3:164:THR:HG21 | 2.15                     | 0.72              |
| 1:1:58:MET:HE1   | 3:3:216:ASP:HA   | 1.71                     | 0.71              |
| 2:2:53:THR:HG22  | 2:2:252:SER:HB2  | 1.71                     | 0.71              |
| 1:1:258:PRO:CG   | 3:3:99:GLU:HG2   | 2.16                     | 0.71              |
| 4:4:33:LYS:NZ    | 4:4:33:LYS:CD    | 2.52                     | 0.71              |
| 2:2:20:ASN:HD21  | 2:2:62:ARG:HE    | 1.39                     | 0.71              |
| 2:2:230:VAL:CG2  | 2:2:234:ALA:HB3  | 2.20                     | 0.71              |
| 2:2:195:ASN:HD22 | 2:2:195:ASN:C    | 1.99                     | 0.71              |
| 1:1:19:ALA:HB2   | 1:1:58:MET:HG2   | 1.72                     | 0.71              |
| 3:3:57:ASN:CA    | 3:3:57:ASN:OD1   | 2.38                     | 0.70              |
| 1:1:170:SER:O    | 1:1:170:SER:OG   | 2.09                     | 0.70              |
| 2:2:39:PRO:HG2   | 2:2:247:MET:HE2  | 1.74                     | 0.69              |
| 2:2:235:THR:CG2  | 2:2:236:PRO:HD2  | 2.21                     | 0.69              |
| 2:2:136:GLU:HB3  | 2:2:140:VAL:CG2  | 2.21                     | 0.69              |
| 3:3:98:GLY:O     | 3:3:102:GLN:HG3  | 1.92                     | 0.69              |
| 2:2:230:VAL:HG23 | 2:2:234:ALA:HB3  | 1.74                     | 0.69              |
| 4:4:29:ILE:HG22  | 4:4:29:ILE:O     | 1.94                     | 0.68              |
| 1:1:83:GLN:CG    | 1:1:85:LYS:HE2   | 2.24                     | 0.67              |
| 3:3:20:GLN:HE22  | 4:4:31:TYR:H     | 1.42                     | 0.67              |
| 1:1:278:VAL:HG12 | 3:3:62:ASP:OD2   | 1.95                     | 0.67              |
| 3:3:61:LYS:HD3   | 3:3:63:GLU:OE2   | 1.95                     | 0.67              |
| 2:2:84:ASP:OD1   | 2:2:87:LYS:HE2   | 1.94                     | 0.67              |
| 2:2:155:ASP:C    | 2:2:155:ASP:OD1  | 2.37                     | 0.66              |
| 3:3:89:ASP:HA    | 3:3:93:LYS:HD2   | 1.78                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:3:42:ASN:HD22  | 3:3:44:LEU:H     | 1.43                     | 0.66              |
| 3:3:197:LEU:HB3  | 3:3:201:THR:HG22 | 1.77                     | 0.65              |
| 1:1:151:MET:SD   | 1:1:170:SER:HB2  | 2.35                     | 0.65              |
| 1:1:201:TYR:HD2  | 1:1:214:GLY:O    | 1.80                     | 0.65              |
| 1:1:285:ASP:CB   | 1:1:285:ASP:H    | 2.09                     | 0.65              |
| 2:2:190:ASN:HD21 | 3:3:118:THR:HA   | 1.62                     | 0.65              |
| 2:2:256:SER:O    | 2:2:257:LYS:HB3  | 1.96                     | 0.65              |
| 2:2:149:PRO:HG3  | 2:2:154:ILE:HG13 | 1.78                     | 0.64              |
| 2:2:205:ASN:HD22 | 2:2:206:SER:H    | 1.45                     | 0.64              |
| 1:1:58:MET:HE1   | 3:3:216:ASP:CA   | 2.27                     | 0.64              |
| 1:1:163:TRP:O    | 1:1:227:ARG:NH1  | 2.30                     | 0.64              |
| 2:2:12:ARG:HH21  | 3:3:157:LEU:HD21 | 1.63                     | 0.64              |
| 3:3:79:GLN:HB2   | 3:3:190:TRP:CE3  | 2.32                     | 0.64              |
| 1:1:78:HIS:NE2   | 1:1:102:TRP:HB2  | 2.13                     | 0.64              |
| 2:2:30:ASN:HD22  | 2:2:31:ALA:N     | 1.94                     | 0.64              |
| 2:2:23:ILE:HD11  | 2:2:243:THR:HG21 | 1.79                     | 0.64              |
| 2:2:12:ARG:NH1   | 4:4:68:ASN:O     | 2.31                     | 0.64              |
| 1:1:60:PHE:CE2   | 3:3:218:LYS:HB3  | 2.33                     | 0.64              |
| 2:2:11:ASP:H     | 4:4:68:ASN:CG    | 2.06                     | 0.63              |
| 1:1:151:MET:HE1  | 1:1:167:THR:C    | 2.24                     | 0.63              |
| 2:2:205:ASN:ND2  | 2:2:206:SER:H    | 1.97                     | 0.63              |
| 2:2:39:PRO:CG    | 2:2:247:MET:HE2  | 2.29                     | 0.63              |
| 2:2:187:GLN:HE21 | 2:2:197:ALA:HA   | 1.64                     | 0.63              |
| 1:1:87:ALA:HA    | 1:1:90:ILE:HG12  | 1.81                     | 0.62              |
| 3:3:75:ARG:O     | 3:3:194:SER:HB2  | 1.99                     | 0.62              |
| 1:1:185:ARG:HG3  | 1:1:186:PHE:N    | 2.10                     | 0.62              |
| 2:2:40:GLU:HG3   | 2:2:41:TYR:O     | 2.00                     | 0.62              |
| 1:1:120:THR:O    | 1:1:199:CYS:HB2  | 1.99                     | 0.62              |
| 1:1:103:LYS:O    | 1:1:104:ILE:O    | 2.17                     | 0.62              |
| 1:1:166:TYR:O    | 1:1:169:GLN:HB2  | 1.99                     | 0.62              |
| 3:3:84:ASN:ND2   | 3:3:86:PHE:H     | 1.98                     | 0.62              |
| 2:2:170:VAL:CG1  | 2:2:170:VAL:O    | 2.47                     | 0.61              |
| 2:2:13:VAL:O     | 2:2:14:GLN:HG2   | 1.99                     | 0.61              |
| 2:2:38:TRP:CZ3   | 4:4:57:LYS:HD2   | 2.36                     | 0.61              |
| 3:3:57:ASN:ND2   | 3:3:91:VAL:HG13  | 2.15                     | 0.61              |
| 2:2:133:ALA:O    | 2:2:166:VAL:HG12 | 2.01                     | 0.61              |
| 1:1:281:LYS:HD2  | 3:3:59:HIS:O     | 2.01                     | 0.61              |
| 1:1:204:TYR:CE2  | 1:1:213:TYR:HB2  | 2.36                     | 0.61              |
| 1:1:103:LYS:HA   | 1:1:223:SER:CB   | 2.30                     | 0.61              |
| 3:3:55:MET:HG3   | 3:3:55:MET:O     | 1.99                     | 0.61              |
| 1:1:90:ILE:N     | 1:1:90:ILE:CD1   | 2.62                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:1:265:SER:HB3  | 1:1:268:ARG:HG2  | 1.83                     | 0.60              |
| 3:3:76:GLN:O     | 3:3:78:GLU:N     | 2.34                     | 0.60              |
| 3:3:56:ASN:HB3   | 3:3:66:SER:HA    | 1.83                     | 0.60              |
| 1:1:51:ILE:HD13  | 3:3:166:PRO:HG3  | 1.82                     | 0.59              |
| 1:1:204:TYR:HD2  | 1:1:212:GLN:O    | 1.85                     | 0.59              |
| 3:3:131:TYR:HB3  | 3:3:149:THR:HB   | 1.82                     | 0.59              |
| 1:1:259:ARG:HD2  | 1:1:263:TYR:CE1  | 2.38                     | 0.59              |
| 2:2:256:SER:O    | 2:2:257:LYS:CB   | 2.50                     | 0.59              |
| 1:1:94:ARG:NH1   | 1:1:94:ARG:CG    | 2.60                     | 0.59              |
| 3:3:175:TYR:H    | 3:3:182:THR:HG21 | 1.68                     | 0.59              |
| 3:3:84:ASN:HD22  | 3:3:86:PHE:H     | 1.49                     | 0.59              |
| 2:2:30:ASN:HD21  | 4:4:58:ASP:H     | 1.51                     | 0.59              |
| 1:1:206:HIS:CE1  | 1:1:208:ASP:HB2  | 2.38                     | 0.58              |
| 3:3:180:THR:O    | 3:3:183:SER:HB3  | 2.02                     | 0.58              |
| 1:1:209:ALA:HB2  | 2:2:261:PRO:HB3  | 1.85                     | 0.58              |
| 1:1:155:PRO:HB3  | 1:1:220:HIS:HE1  | 1.69                     | 0.58              |
| 1:1:43:MET:HE3   | 1:1:43:MET:HA    | 1.85                     | 0.58              |
| 2:2:177:LEU:HD11 | 3:3:94:THR:HG21  | 1.86                     | 0.57              |
| 2:2:204:ILE:HG12 | 3:3:37:PRO:HG2   | 1.86                     | 0.57              |
| 1:1:151:MET:HB2  | 1:1:175:SER:OG   | 2.04                     | 0.57              |
| 1:1:285:ASP:HB3  | 1:1:287:LYS:N    | 2.18                     | 0.57              |
| 2:2:221:MET:HE2  | 2:2:223:ILE:HD11 | 1.87                     | 0.57              |
| 2:2:64:TYR:CD1   | 2:2:89:MET:HB3   | 2.39                     | 0.57              |
| 3:3:57:ASN:HB3   | 3:3:57:ASN:C     | 2.28                     | 0.57              |
| 3:3:179:ASP:OD2  | 3:3:182:THR:CG2  | 2.52                     | 0.57              |
| 1:1:93:HIS:CE1   | 1:1:163:TRP:HD1  | 2.22                     | 0.57              |
| 1:1:58:MET:HE3   | 3:3:216:ASP:HA   | 1.85                     | 0.56              |
| 2:2:52:LYS:NZ    | 2:2:52:LYS:HD3   | 2.20                     | 0.56              |
| 1:1:43:MET:HG3   | 1:1:44:PRO:HD2   | 1.87                     | 0.56              |
| 1:1:85:LYS:HB3   | 1:1:236:LYS:HG3  | 1.87                     | 0.56              |
| 2:2:174:ASN:C    | 2:2:174:ASN:ND2  | 2.63                     | 0.56              |
| 3:3:31:THR:CG2   | 3:3:32:PRO:HD2   | 2.34                     | 0.56              |
| 1:1:93:HIS:CE1   | 1:1:162:GLU:HG2  | 2.41                     | 0.56              |
| 3:3:53:ILE:HD11  | 3:3:211:ILE:HB   | 1.87                     | 0.56              |
| 4:4:44:SER:O     | 4:4:45:LEU:C     | 2.48                     | 0.56              |
| 2:2:10:SER:OG    | 2:2:12:ARG:CB    | 2.53                     | 0.56              |
| 1:1:155:PRO:HB3  | 1:1:220:HIS:CE1  | 2.41                     | 0.56              |
| 1:1:236:LYS:HE3  | 1:1:238:LEU:HD13 | 1.88                     | 0.55              |
| 2:2:170:VAL:O    | 2:2:170:VAL:HG12 | 2.05                     | 0.55              |
| 2:2:189:ILE:HA   | 2:2:194:ASN:ND2  | 2.21                     | 0.55              |
| 4:4:43:GLN:O     | 4:4:45:LEU:HB3   | 2.05                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:2:77:GLY:O     | 2:2:156:LEU:HB2  | 2.07                     | 0.55              |
| 1:1:208:ASP:O    | 2:2:261:PRO:HG2  | 2.07                     | 0.55              |
| 1:1:204:TYR:HE2  | 1:1:213:TYR:HB2  | 1.72                     | 0.55              |
| 2:2:230:VAL:HG23 | 2:2:231:PRO:O    | 2.05                     | 0.55              |
| 3:3:199:PRO:O    | 3:3:200:GLU:HB2  | 2.04                     | 0.55              |
| 2:2:38:TRP:CD1   | 2:2:39:PRO:HD2   | 2.42                     | 0.55              |
| 1:1:266:ILE:HD12 | 3:3:235:THR:HA   | 1.88                     | 0.54              |
| 1:1:79:VAL:HG22  | 1:1:242:ARG:HG2  | 1.89                     | 0.54              |
| 2:2:8:GLY:C      | 2:2:9:TYR:HD1    | 2.14                     | 0.54              |
| 3:3:31:THR:HG23  | 3:3:32:PRO:HD2   | 1.87                     | 0.54              |
| 3:3:198:PRO:O    | 3:3:201:THR:HB   | 2.07                     | 0.54              |
| 1:1:208:ASP:HB3  | 1:1:211:THR:HB   | 1.89                     | 0.54              |
| 3:3:175:TYR:H    | 3:3:182:THR:CG2  | 2.21                     | 0.54              |
| 1:1:158:PRO:HB2  | 1:1:167:THR:HG22 | 1.90                     | 0.54              |
| 4:4:59:LEU:HD21  | 4:4:61:LEU:CD1   | 2.34                     | 0.54              |
| 2:2:38:TRP:HZ3   | 4:4:57:LYS:HD2   | 1.70                     | 0.54              |
| 2:2:230:VAL:HB   | 2:2:231:PRO:HD2  | 1.89                     | 0.54              |
| 3:3:63:GLU:C     | 3:3:65:ASN:H     | 2.14                     | 0.54              |
| 1:1:35:THR:HG23  | 3:3:160:THR:HB   | 1.90                     | 0.54              |
| 3:3:20:GLN:HE22  | 4:4:31:TYR:N     | 2.04                     | 0.54              |
| 1:1:208:ASP:C    | 2:2:261:PRO:HG2  | 2.32                     | 0.54              |
| 3:3:193:THR:O    | 3:3:194:SER:CB   | 2.55                     | 0.54              |
| 3:3:197:LEU:HB3  | 3:3:201:THR:HG21 | 1.87                     | 0.54              |
| 3:3:117:TYR:CD1  | 3:3:155:ILE:HD13 | 2.44                     | 0.54              |
| 1:1:273:LYS:O    | 1:1:274:ASN:C    | 2.52                     | 0.53              |
| 3:3:55:MET:HA    | 3:3:91:VAL:HG11  | 1.91                     | 0.53              |
| 1:1:271:TYR:HB2  | 1:1:272:PRO:HD2  | 1.89                     | 0.53              |
| 2:2:195:ASN:ND2  | 2:2:195:ASN:C    | 2.66                     | 0.53              |
| 2:2:235:THR:CG2  | 2:2:236:PRO:CD   | 2.86                     | 0.53              |
| 3:3:18:ASP:OD2   | 4:4:40:SER:HB2   | 2.09                     | 0.53              |
| 3:3:86:PHE:CD1   | 3:3:178:PRO:HB3  | 2.44                     | 0.53              |
| 2:2:12:ARG:NH2   | 3:3:157:LEU:HD21 | 2.24                     | 0.53              |
| 1:1:88:THR:O     | 1:1:90:ILE:HD13  | 2.09                     | 0.52              |
| 1:1:83:GLN:HG3   | 1:1:85:LYS:CE    | 2.31                     | 0.52              |
| 1:1:104:ILE:HD12 | 5:1:700:W91:H3C2 | 1.90                     | 0.52              |
| 1:1:88:THR:O     | 1:1:90:ILE:CD1   | 2.58                     | 0.52              |
| 3:3:175:TYR:HB2  | 3:3:182:THR:HG21 | 1.92                     | 0.52              |
| 1:1:276:GLU:HB3  | 1:1:277:PRO:CD   | 2.39                     | 0.52              |
| 1:1:92:ASN:C     | 1:1:92:ASN:ND2   | 2.67                     | 0.52              |
| 1:1:236:LYS:NZ   | 1:1:238:LEU:HD11 | 2.25                     | 0.52              |
| 3:3:216:ASP:O    | 3:3:218:LYS:HE3  | 2.09                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:2:66:LEU:HD12  | 2:2:89:MET:HE3   | 1.91                     | 0.52              |
| 1:1:114:LYS:NZ   | 3:3:99:GLU:OE2   | 2.43                     | 0.51              |
| 1:1:122:VAL:HG13 | 1:1:124:PHE:CE2  | 2.45                     | 0.51              |
| 2:2:262:GLN:C    | 2:2:262:GLN:NE2  | 2.66                     | 0.51              |
| 4:4:44:SER:C     | 4:4:46:SER:N     | 2.68                     | 0.51              |
| 1:1:273:LYS:O    | 1:1:274:ASN:O    | 2.27                     | 0.51              |
| 2:2:177:LEU:CD1  | 3:3:94:THR:HG21  | 2.40                     | 0.51              |
| 3:3:75:ARG:NH1   | 3:3:78:GLU:OE2   | 2.41                     | 0.51              |
| 1:1:236:LYS:HE3  | 1:1:238:LEU:CD1  | 2.40                     | 0.51              |
| 3:3:193:THR:O    | 3:3:194:SER:HB3  | 2.08                     | 0.51              |
| 3:3:84:ASN:ND2   | 3:3:84:ASN:C     | 2.69                     | 0.51              |
| 1:1:84:ASN:HB2   | 1:1:228:ILE:HD12 | 1.91                     | 0.51              |
| 1:1:129:THR:OG1  | 1:1:185:ARG:NH1  | 2.41                     | 0.51              |
| 2:2:34:CYS:HB2   | 2:2:202:PRO:CD   | 2.41                     | 0.51              |
| 3:3:214:CYS:HB3  | 3:3:215:PRO:HD2  | 1.92                     | 0.51              |
| 1:1:38:GLU:OE1   | 3:3:116:MET:HE2  | 2.10                     | 0.51              |
| 1:1:153:VAL:HG12 | 1:1:157:ALA:HB3  | 1.91                     | 0.51              |
| 1:1:265:SER:HB2  | 2:2:138:GLY:O    | 2.11                     | 0.51              |
| 1:1:94:ARG:CG    | 1:1:94:ARG:HH11  | 2.24                     | 0.51              |
| 3:3:210:PHE:N    | 3:3:210:PHE:CD1  | 2.78                     | 0.51              |
| 3:3:84:ASN:HD22  | 3:3:86:PHE:N     | 2.08                     | 0.51              |
| 1:1:92:ASN:CG    | 1:1:95:GLU:HB2   | 2.36                     | 0.50              |
| 1:1:65:THR:HG22  | 3:3:104:TYR:CZ   | 2.46                     | 0.50              |
| 2:2:171:TYR:HA   | 2:2:176:THR:O    | 2.11                     | 0.50              |
| 2:2:255:ARG:CG   | 2:2:256:SER:H    | 1.99                     | 0.50              |
| 2:2:139:ASN:N    | 2:2:139:ASN:OD1  | 2.44                     | 0.50              |
| 1:1:60:PHE:CD2   | 3:3:218:LYS:HB3  | 2.46                     | 0.50              |
| 1:1:215:ILE:C    | 1:1:217:VAL:H    | 2.20                     | 0.50              |
| 2:2:158:SER:HG   | 2:2:167:LYS:HE2  | 1.71                     | 0.50              |
| 1:1:190:TYR:HD1  | 1:1:197:TYR:CZ   | 2.30                     | 0.50              |
| 3:3:84:ASN:HD22  | 3:3:84:ASN:C     | 2.20                     | 0.49              |
| 2:2:13:VAL:C     | 2:2:14:GLN:CG    | 2.85                     | 0.49              |
| 2:2:37:GLU:CD    | 3:3:35:HIS:HE2   | 2.19                     | 0.49              |
| 2:2:143:LYS:HG2  | 2:2:163:GLY:O    | 2.12                     | 0.49              |
| 1:1:58:MET:O     | 1:1:59:HIS:HB2   | 2.12                     | 0.49              |
| 2:2:235:THR:HG22 | 2:2:236:PRO:N    | 2.22                     | 0.49              |
| 2:2:205:ASN:HD22 | 2:2:206:SER:N    | 2.09                     | 0.49              |
| 1:1:77:VAL:C     | 1:1:109:LEU:CD2  | 2.86                     | 0.49              |
| 1:1:179:LYS:O    | 1:1:182:ASP:HB2  | 2.12                     | 0.49              |
| 2:2:19:GLY:HA2   | 2:2:58:THR:HG22  | 1.94                     | 0.49              |
| 3:3:95:THR:O     | 3:3:99:GLU:HB2   | 2.13                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:2:34:CYS:HB2   | 2:2:202:PRO:HD2  | 1.94                     | 0.49              |
| 3:3:20:GLN:NE2   | 4:4:31:TYR:H     | 2.11                     | 0.49              |
| 3:3:181:TYR:CD1  | 3:3:181:TYR:C    | 2.91                     | 0.49              |
| 2:2:30:ASN:ND2   | 2:2:31:ALA:H     | 2.05                     | 0.48              |
| 1:1:134:ALA:HB2  | 1:1:180:VAL:HG11 | 1.95                     | 0.48              |
| 3:3:129:LEU:O    | 3:3:150:HIS:HA   | 2.13                     | 0.48              |
| 3:3:54:PRO:O     | 3:3:91:VAL:HG12  | 2.13                     | 0.48              |
| 3:3:125:ALA:HB3  | 3:3:155:ILE:HD12 | 1.95                     | 0.48              |
| 2:2:10:SER:CB    | 4:4:68:ASN:OXT   | 2.61                     | 0.48              |
| 2:2:135:HIS:CD2  | 2:2:160:ASN:HB3  | 2.49                     | 0.48              |
| 3:3:115:LEU:HD22 | 3:3:129:LEU:HD21 | 1.96                     | 0.48              |
| 1:1:280:LYS:HE3  | 3:3:89:ASP:OD1   | 2.13                     | 0.48              |
| 3:3:20:GLN:HE22  | 4:4:30:ASN:HA    | 1.78                     | 0.48              |
| 3:3:61:LYS:O     | 3:3:61:LYS:HG2   | 2.07                     | 0.48              |
| 3:3:112:ARG:NH1  | 3:3:112:ARG:HG2  | 2.27                     | 0.48              |
| 3:3:190:TRP:CD1  | 3:3:190:TRP:N    | 2.81                     | 0.48              |
| 1:1:110:VAL:HG13 | 3:3:230:GLN:CD   | 2.39                     | 0.47              |
| 1:1:174:PRO:O    | 5:1:700:W91:H4A2 | 2.14                     | 0.47              |
| 1:1:87:ALA:CA    | 1:1:90:ILE:HG12  | 2.44                     | 0.47              |
| 3:3:112:ARG:HD3  | 3:3:162:VAL:CG1  | 2.44                     | 0.47              |
| 3:3:195:LEU:C    | 3:3:196:ILE:HG12 | 2.40                     | 0.47              |
| 2:2:13:VAL:C     | 2:2:14:GLN:HG2   | 2.39                     | 0.47              |
| 1:1:83:GLN:OE1   | 1:1:236:LYS:HD2  | 2.15                     | 0.47              |
| 1:1:268:ARG:CZ   | 2:2:139:ASN:HB2  | 2.44                     | 0.47              |
| 2:2:177:LEU:CD1  | 3:3:94:THR:CG2   | 2.93                     | 0.47              |
| 1:1:228:ILE:HD11 | 1:1:239:VAL:HG21 | 1.97                     | 0.47              |
| 2:2:13:VAL:HA    | 2:2:25:THR:O     | 2.15                     | 0.47              |
| 2:2:63:PHE:CD1   | 2:2:245:ALA:HB2  | 2.50                     | 0.47              |
| 4:4:43:GLN:O     | 4:4:44:SER:C     | 2.58                     | 0.47              |
| 1:1:74:ALA:HB3   | 3:3:15:THR:HB    | 1.97                     | 0.46              |
| 1:1:103:LYS:O    | 1:1:104:ILE:C    | 2.57                     | 0.46              |
| 2:2:130:HIS:ND1  | 2:2:219:SER:OG   | 2.47                     | 0.46              |
| 1:1:200:PHE:CE2  | 1:1:256:ARG:HD2  | 2.50                     | 0.46              |
| 4:4:59:LEU:HG    | 4:4:60:MET:N     | 2.27                     | 0.46              |
| 4:4:61:LEU:HD12  | 4:4:61:LEU:HA    | 1.63                     | 0.46              |
| 1:1:215:ILE:C    | 1:1:217:VAL:N    | 2.71                     | 0.46              |
| 1:1:236:LYS:HE2  | 1:1:236:LYS:HB3  | 1.83                     | 0.46              |
| 2:2:156:LEU:HD11 | 2:2:173:MET:SD   | 2.56                     | 0.46              |
| 3:3:101:VAL:HG22 | 3:3:219:LEU:HD11 | 1.98                     | 0.46              |
| 2:2:158:SER:HG   | 2:2:167:LYS:CE   | 2.26                     | 0.46              |
| 3:3:18:ASP:CG    | 4:4:40:SER:HB2   | 2.41                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:2:148:HIS:N    | 2:2:149:PRO:CD   | 2.79                     | 0.46              |
| 3:3:55:MET:CE    | 3:3:91:VAL:HG21  | 2.46                     | 0.46              |
| 1:1:169:GLN:O    | 1:1:170:SER:C    | 2.59                     | 0.45              |
| 1:1:97:LYS:C     | 1:1:99:PHE:N     | 2.71                     | 0.45              |
| 3:3:57:ASN:CB    | 3:3:57:ASN:H     | 2.26                     | 0.45              |
| 1:1:198:ASN:ND2  | 2:2:206:SER:OG   | 2.40                     | 0.45              |
| 2:2:228:LEU:CD1  | 2:2:238:LEU:HD22 | 2.47                     | 0.45              |
| 2:2:190:ASN:H    | 2:2:194:ASN:CB   | 2.30                     | 0.45              |
| 1:1:31:VAL:HG11  | 1:1:34:LEU:HD12  | 1.98                     | 0.45              |
| 2:2:187:GLN:NE2  | 2:2:198:THR:H    | 2.14                     | 0.45              |
| 3:3:55:MET:HE2   | 3:3:91:VAL:HG21  | 1.98                     | 0.45              |
| 4:4:30:ASN:HA    | 4:4:30:ASN:HD22  | 1.40                     | 0.45              |
| 3:3:50:ASP:HA    | 3:3:212:SER:HB3  | 1.98                     | 0.45              |
| 1:1:28:THR:HG22  | 1:1:29:GLN:H     | 1.81                     | 0.45              |
| 1:1:64:GLU:O     | 1:1:64:GLU:HG2   | 2.17                     | 0.45              |
| 1:1:285:ASP:HB3  | 1:1:288:SER:H    | 1.82                     | 0.45              |
| 2:2:91:VAL:HG12  | 2:2:95:ASN:HD22  | 1.82                     | 0.45              |
| 2:2:259:ILE:HG21 | 2:2:259:ILE:HD13 | 1.74                     | 0.45              |
| 1:1:43:MET:HA    | 1:1:43:MET:CE    | 2.46                     | 0.45              |
| 3:3:192:GLN:HE21 | 3:3:192:GLN:HA   | 1.81                     | 0.45              |
| 1:1:201:TYR:H    | 2:2:131:GLN:HE21 | 1.66                     | 0.44              |
| 1:1:215:ILE:O    | 1:1:218:LEU:N    | 2.43                     | 0.44              |
| 2:2:190:ASN:H    | 2:2:194:ASN:HB3  | 1.82                     | 0.44              |
| 1:1:92:ASN:C     | 1:1:92:ASN:HD22  | 2.26                     | 0.44              |
| 1:1:268:ARG:NH1  | 3:3:236:GLU:O    | 2.46                     | 0.44              |
| 3:3:57:ASN:N     | 3:3:57:ASN:HB2   | 2.25                     | 0.44              |
| 3:3:61:LYS:O     | 3:3:63:GLU:HG3   | 2.17                     | 0.44              |
| 3:3:116:MET:HG3  | 3:3:159:SER:OG   | 2.17                     | 0.44              |
| 1:1:289:TYR:CE2  | 3:3:138:GLY:HA3  | 2.53                     | 0.44              |
| 4:4:43:GLN:O     | 4:4:45:LEU:CB    | 2.66                     | 0.44              |
| 4:4:59:LEU:CD2   | 4:4:61:LEU:HD13  | 2.41                     | 0.44              |
| 1:1:47:PRO:HB3   | 3:3:166:PRO:HB3  | 1.99                     | 0.44              |
| 2:2:10:SER:OG    | 4:4:68:ASN:OXT   | 2.35                     | 0.44              |
| 3:3:197:LEU:HD21 | 3:3:205:VAL:HG11 | 1.99                     | 0.44              |
| 3:3:221:LEU:C    | 3:3:221:LEU:HD23 | 2.43                     | 0.44              |
| 1:1:154:PRO:HD2  | 1:1:173:ASN:HD21 | 1.83                     | 0.44              |
| 1:1:282:ARG:CG   | 3:3:57:ASN:CB    | 2.89                     | 0.44              |
| 1:1:286:ILE:HG23 | 3:3:81:PHE:HA    | 2.00                     | 0.44              |
| 2:2:146:PHE:CG   | 2:2:164:GLY:HA2  | 2.52                     | 0.44              |
| 1:1:98:LEU:O     | 1:1:99:PHE:HB3   | 2.18                     | 0.44              |
| 1:1:289:TYR:CD2  | 3:3:138:GLY:HA3  | 2.53                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:4:43:GLN:HG3   | 4:4:45:LEU:H     | 1.82                     | 0.44              |
| 1:1:87:ALA:HB2   | 1:1:98:LEU:CD1   | 2.48                     | 0.43              |
| 1:1:128:TYR:HB2  | 1:1:186:PHE:CZ   | 2.53                     | 0.43              |
| 3:3:208:LEU:HA   | 3:3:208:LEU:HD12 | 1.73                     | 0.43              |
| 2:2:190:ASN:O    | 2:2:191:LEU:C    | 2.61                     | 0.43              |
| 3:3:57:ASN:HD21  | 3:3:91:VAL:HG13  | 1.83                     | 0.43              |
| 1:1:38:GLU:N     | 3:3:116:MET:HE1  | 2.34                     | 0.43              |
| 1:1:146:LEU:HD13 | 1:1:228:ILE:HD13 | 1.99                     | 0.43              |
| 1:1:104:ILE:HG12 | 1:1:223:SER:HA   | 2.00                     | 0.43              |
| 1:1:146:LEU:HA   | 1:1:230:ASN:OD1  | 2.18                     | 0.43              |
| 3:3:61:LYS:HG2   | 3:3:63:GLU:HG3   | 2.00                     | 0.43              |
| 2:2:70:THR:HG22  | 2:2:72:THR:HG22  | 2.01                     | 0.43              |
| 2:2:91:VAL:HG12  | 2:2:95:ASN:ND2   | 2.34                     | 0.43              |
| 3:3:112:ARG:HG2  | 3:3:112:ARG:HH11 | 1.83                     | 0.43              |
| 1:1:285:ASP:C    | 1:1:285:ASP:HB3  | 2.38                     | 0.43              |
| 2:2:10:SER:CB    | 2:2:12:ARG:HB2   | 2.49                     | 0.43              |
| 3:3:151:VAL:HG11 | 3:3:161:ILE:HD11 | 2.01                     | 0.43              |
| 2:2:95:ASN:HB3   | 2:2:251:PHE:CE2  | 2.53                     | 0.43              |
| 2:2:205:ASN:ND2  | 2:2:206:SER:N    | 2.66                     | 0.43              |
| 1:1:214:GLY:O    | 1:1:217:VAL:CG1  | 2.67                     | 0.42              |
| 1:1:77:VAL:C     | 1:1:109:LEU:HD22 | 2.44                     | 0.42              |
| 1:1:146:LEU:HD13 | 1:1:228:ILE:CD1  | 2.50                     | 0.42              |
| 4:4:43:GLN:C     | 4:4:45:LEU:N     | 2.74                     | 0.42              |
| 1:1:87:ALA:HB2   | 1:1:98:LEU:HD11  | 2.02                     | 0.42              |
| 1:1:89:GLY:C     | 1:1:90:ILE:CD1   | 2.89                     | 0.42              |
| 3:3:153:TRP:CD1  | 3:3:153:TRP:C    | 2.97                     | 0.42              |
| 3:3:226:GLN:HE21 | 3:3:226:GLN:HB2  | 1.21                     | 0.42              |
| 2:2:225:ILE:O    | 3:3:68:LEU:HD21  | 2.19                     | 0.42              |
| 1:1:285:ASP:HB3  | 1:1:288:SER:N    | 2.34                     | 0.42              |
| 2:2:40:GLU:O     | 2:2:40:GLU:CG    | 2.61                     | 0.42              |
| 2:2:228:LEU:HD11 | 2:2:238:LEU:HD22 | 2.02                     | 0.42              |
| 2:2:235:THR:CG2  | 2:2:236:PRO:N    | 2.79                     | 0.42              |
| 1:1:190:TYR:CD1  | 1:1:197:TYR:CZ   | 3.07                     | 0.42              |
| 2:2:122:LEU:HD23 | 2:2:224:PRO:HA   | 2.02                     | 0.42              |
| 3:3:44:LEU:HA    | 3:3:44:LEU:HD23  | 1.79                     | 0.42              |
| 1:1:165:ASP:N    | 1:1:168:TRP:HD1  | 2.18                     | 0.42              |
| 1:1:261:LEU:HD11 | 2:2:171:TYR:CD2  | 2.55                     | 0.42              |
| 1:1:289:TYR:CZ   | 3:3:139:PRO:HD2  | 2.55                     | 0.42              |
| 1:1:286:ILE:HD13 | 1:1:286:ILE:HG21 | 1.77                     | 0.42              |
| 2:2:69:LYS:O     | 2:2:239:PRO:HA   | 2.20                     | 0.41              |
| 4:4:43:GLN:HG2   | 4:4:43:GLN:O     | 2.18                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:1:86:ASP:OD1   | 1:1:88:THR:HB    | 2.20                     | 0.41              |
| 1:1:98:LEU:HD23  | 1:1:98:LEU:HA    | 1.80                     | 0.41              |
| 1:1:102:TRP:O    | 1:1:102:TRP:CG   | 2.73                     | 0.41              |
| 2:2:235:THR:HG22 | 2:2:237:SER:N    | 2.35                     | 0.41              |
| 3:3:47:ILE:HG21  | 3:3:47:ILE:HD13  | 1.51                     | 0.41              |
| 3:3:113:PHE:CE2  | 3:3:115:LEU:HD13 | 2.55                     | 0.41              |
| 3:3:167:TRP:HZ2  | 3:3:172:GLN:HA   | 1.86                     | 0.41              |
| 1:1:87:ALA:C     | 1:1:90:ILE:HG12  | 2.46                     | 0.41              |
| 2:2:43:PRO:HG2   | 2:2:46:ASP:HB2   | 2.03                     | 0.41              |
| 3:3:64:VAL:O     | 3:3:64:VAL:HG12  | 2.21                     | 0.41              |
| 1:1:97:LYS:C     | 1:1:99:PHE:H     | 2.23                     | 0.41              |
| 3:3:137:ARG:HH11 | 3:3:137:ARG:HD3  | 1.23                     | 0.41              |
| 1:1:54:ARG:HH11  | 1:1:54:ARG:HD2   | 1.55                     | 0.41              |
| 1:1:102:TRP:C    | 1:1:104:ILE:N    | 2.78                     | 0.41              |
| 1:1:103:LYS:O    | 1:1:103:LYS:CG   | 2.67                     | 0.41              |
| 2:2:84:ASP:HB2   | 2:2:216:ASN:HD21 | 1.86                     | 0.41              |
| 1:1:78:HIS:NE2   | 1:1:80:THR:HB    | 2.36                     | 0.41              |
| 2:2:13:VAL:HG22  | 2:2:26:GLN:HA    | 2.03                     | 0.41              |
| 3:3:157:LEU:HD23 | 3:3:157:LEU:O    | 2.21                     | 0.40              |
| 3:3:20:GLN:NE2   | 4:4:30:ASN:HA    | 2.36                     | 0.40              |
| 1:1:104:ILE:CG1  | 1:1:223:SER:HA   | 2.50                     | 0.40              |
| 1:1:118:LEU:HD12 | 1:1:118:LEU:HA   | 1.91                     | 0.40              |
| 3:3:231:THR:C    | 3:3:232:VAL:HG13 | 2.45                     | 0.40              |
| 1:1:190:TYR:CE1  | 1:1:192:GLY:HA3  | 2.56                     | 0.40              |
| 1:1:265:SER:OG   | 2:2:139:ASN:HB3  | 2.21                     | 0.40              |
| 3:3:214:CYS:HB3  | 3:3:215:PRO:CD   | 2.51                     | 0.40              |
| 1:1:285:ASP:HB3  | 1:1:287:LYS:H    | 1.87                     | 0.40              |

There are no symmetry-related clashes.

## 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   | 1     | 271/289 (94%) | 241 (89%) | 23 (8%) | 7 (3%)   | 4           | 23 |
| 2   | 2     | 253/262 (97%) | 234 (92%) | 17 (7%) | 2 (1%)   | 16          | 50 |
| 3   | 3     | 234/236 (99%) | 217 (93%) | 15 (6%) | 2 (1%)   | 14          | 48 |
| 4   | 4     | 38/68 (56%)   | 34 (90%)  | 3 (8%)  | 1 (3%)   | 4           | 23 |
| All | All   | 796/855 (93%) | 726 (91%) | 58 (7%) | 12 (2%)  | 8           | 35 |

All (12) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1     | 103 | LYS  |
| 1   | 1     | 104 | ILE  |
| 1   | 1     | 139 | SER  |
| 3   | 3     | 57  | ASN  |
| 3   | 3     | 77  | ASN  |
| 2   | 2     | 255 | ARG  |
| 2   | 2     | 257 | LYS  |
| 1   | 1     | 165 | ASP  |
| 1   | 1     | 108 | SER  |
| 1   | 1     | 170 | SER  |
| 4   | 4     | 47  | MET  |
| 1   | 1     | 99  | PHE  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed       | Rotameric | Outliers  | Percentiles |   |
|-----|-------|----------------|-----------|-----------|-------------|---|
| 1   | 1     | 239/253 (94%)  | 185 (77%) | 54 (23%)  | 1           | 5 |
| 2   | 2     | 223/229 (97%)  | 178 (80%) | 45 (20%)  | 1           | 7 |
| 3   | 3     | 209/209 (100%) | 170 (81%) | 39 (19%)  | 1           | 9 |
| 4   | 4     | 33/57 (58%)    | 20 (61%)  | 13 (39%)  | 0           | 1 |
| All | All   | 704/748 (94%)  | 553 (79%) | 151 (21%) | 1           | 6 |

All (151) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1     | 18  | VAL  |
| 1   | 1     | 21  | ILE  |
| 1   | 1     | 22  | SER  |
| 1   | 1     | 23  | SER  |
| 1   | 1     | 28  | THR  |
| 1   | 1     | 29  | GLN  |
| 1   | 1     | 30  | LYS  |
| 1   | 1     | 38  | GLU  |
| 1   | 1     | 43  | MET  |
| 1   | 1     | 47  | PRO  |
| 1   | 1     | 81  | GLU  |
| 1   | 1     | 90  | ILE  |
| 1   | 1     | 95  | GLU  |
| 1   | 1     | 97  | LYS  |
| 1   | 1     | 100 | ASN  |
| 1   | 1     | 104 | ILE  |
| 1   | 1     | 109 | LEU  |
| 1   | 1     | 110 | VAL  |
| 1   | 1     | 118 | LEU  |
| 1   | 1     | 122 | VAL  |
| 1   | 1     | 136 | GLN  |
| 1   | 1     | 137 | PRO  |
| 1   | 1     | 138 | ASP  |
| 1   | 1     | 144 | SER  |
| 1   | 1     | 145 | ASN  |
| 1   | 1     | 149 | GLN  |
| 1   | 1     | 151 | MET  |
| 1   | 1     | 153 | VAL  |
| 1   | 1     | 161 | LYS  |
| 1   | 1     | 162 | GLU  |
| 1   | 1     | 170 | SER  |
| 1   | 1     | 176 | VAL  |
| 1   | 1     | 183 | THR  |
| 1   | 1     | 184 | SER  |
| 1   | 1     | 185 | ARG  |
| 1   | 1     | 188 | VAL  |
| 1   | 1     | 191 | VAL  |
| 1   | 1     | 215 | ILE  |
| 1   | 1     | 216 | THR  |
| 1   | 1     | 217 | VAL  |
| 1   | 1     | 220 | HIS  |
| 1   | 1     | 221 | MET  |
| 1   | 1     | 228 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1     | 240 | LYS  |
| 1   | 1     | 248 | LYS  |
| 1   | 1     | 254 | ILE  |
| 1   | 1     | 256 | ARG  |
| 1   | 1     | 266 | ILE  |
| 1   | 1     | 268 | ARG  |
| 1   | 1     | 273 | LYS  |
| 1   | 1     | 274 | ASN  |
| 1   | 1     | 275 | THR  |
| 1   | 1     | 278 | VAL  |
| 1   | 1     | 287 | LYS  |
| 2   | 2     | 12  | ARG  |
| 2   | 2     | 20  | ASN  |
| 2   | 2     | 26  | GLN  |
| 2   | 2     | 30  | ASN  |
| 2   | 2     | 49  | ASP  |
| 2   | 2     | 52  | LYS  |
| 2   | 2     | 66  | LEU  |
| 2   | 2     | 69  | LYS  |
| 2   | 2     | 73  | THR  |
| 2   | 2     | 76  | LYS  |
| 2   | 2     | 81  | LYS  |
| 2   | 2     | 87  | LYS  |
| 2   | 2     | 103 | ARG  |
| 2   | 2     | 116 | LYS  |
| 2   | 2     | 119 | SER  |
| 2   | 2     | 136 | GLU  |
| 2   | 2     | 141 | SER  |
| 2   | 2     | 143 | LYS  |
| 2   | 2     | 145 | THR  |
| 2   | 2     | 151 | GLU  |
| 2   | 2     | 152 | ARG  |
| 2   | 2     | 156 | LEU  |
| 2   | 2     | 165 | PRO  |
| 2   | 2     | 166 | VAL  |
| 2   | 2     | 167 | LYS  |
| 2   | 2     | 169 | VAL  |
| 2   | 2     | 174 | ASN  |
| 2   | 2     | 187 | GLN  |
| 2   | 2     | 192 | ARG  |
| 2   | 2     | 195 | ASN  |
| 2   | 2     | 209 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | 2     | 211 | SER  |
| 2   | 2     | 217 | ASN  |
| 2   | 2     | 225 | ILE  |
| 2   | 2     | 230 | VAL  |
| 2   | 2     | 232 | THR  |
| 2   | 2     | 236 | PRO  |
| 2   | 2     | 238 | LEU  |
| 2   | 2     | 247 | MET  |
| 2   | 2     | 250 | GLU  |
| 2   | 2     | 254 | ILE  |
| 2   | 2     | 255 | ARG  |
| 2   | 2     | 256 | SER  |
| 2   | 2     | 259 | ILE  |
| 2   | 2     | 262 | GLN  |
| 3   | 3     | 12  | GLN  |
| 3   | 3     | 16  | THR  |
| 3   | 3     | 33  | ARG  |
| 3   | 3     | 42  | ASN  |
| 3   | 3     | 46  | ILE  |
| 3   | 3     | 55  | MET  |
| 3   | 3     | 60  | THR  |
| 3   | 3     | 61  | LYS  |
| 3   | 3     | 65  | ASN  |
| 3   | 3     | 84  | ASN  |
| 3   | 3     | 91  | VAL  |
| 3   | 3     | 94  | THR  |
| 3   | 3     | 101 | VAL  |
| 3   | 3     | 112 | ARG  |
| 3   | 3     | 114 | SER  |
| 3   | 3     | 115 | LEU  |
| 3   | 3     | 137 | ARG  |
| 3   | 3     | 146 | MET  |
| 3   | 3     | 157 | LEU  |
| 3   | 3     | 158 | GLN  |
| 3   | 3     | 159 | SER  |
| 3   | 3     | 164 | THR  |
| 3   | 3     | 172 | GLN  |
| 3   | 3     | 174 | ARG  |
| 3   | 3     | 179 | ASP  |
| 3   | 3     | 182 | THR  |
| 3   | 3     | 192 | GLN  |
| 3   | 3     | 194 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | 3     | 196 | ILE  |
| 3   | 3     | 201 | THR  |
| 3   | 3     | 208 | LEU  |
| 3   | 3     | 211 | ILE  |
| 3   | 3     | 218 | LYS  |
| 3   | 3     | 219 | LEU  |
| 3   | 3     | 220 | ARG  |
| 3   | 3     | 223 | LYS  |
| 3   | 3     | 226 | GLN  |
| 3   | 3     | 228 | ILE  |
| 3   | 3     | 230 | GLN  |
| 4   | 4     | 29  | ILE  |
| 4   | 4     | 33  | LYS  |
| 4   | 4     | 40  | SER  |
| 4   | 4     | 43  | GLN  |
| 4   | 4     | 45  | LEU  |
| 4   | 4     | 46  | SER  |
| 4   | 4     | 47  | MET  |
| 4   | 4     | 50  | SER  |
| 4   | 4     | 51  | LYS  |
| 4   | 4     | 59  | LEU  |
| 4   | 4     | 61  | LEU  |
| 4   | 4     | 67  | LEU  |
| 4   | 4     | 68  | ASN  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1     | 61  | ASN  |
| 1   | 1     | 92  | ASN  |
| 1   | 1     | 93  | HIS  |
| 1   | 1     | 100 | ASN  |
| 1   | 1     | 136 | GLN  |
| 1   | 1     | 173 | ASN  |
| 1   | 1     | 198 | ASN  |
| 1   | 1     | 220 | HIS  |
| 2   | 2     | 15  | GLN  |
| 2   | 2     | 20  | ASN  |
| 2   | 2     | 30  | ASN  |
| 2   | 2     | 94  | GLN  |
| 2   | 2     | 111 | GLN  |
| 2   | 2     | 131 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | 2     | 135 | HIS  |
| 2   | 2     | 174 | ASN  |
| 2   | 2     | 187 | GLN  |
| 2   | 2     | 190 | ASN  |
| 2   | 2     | 195 | ASN  |
| 2   | 2     | 205 | ASN  |
| 2   | 2     | 216 | ASN  |
| 2   | 2     | 262 | GLN  |
| 3   | 3     | 20  | GLN  |
| 3   | 3     | 27  | ASN  |
| 3   | 3     | 42  | ASN  |
| 3   | 3     | 56  | ASN  |
| 3   | 3     | 65  | ASN  |
| 3   | 3     | 74  | ASN  |
| 3   | 3     | 84  | ASN  |
| 3   | 3     | 140 | GLN  |
| 3   | 3     | 192 | GLN  |
| 3   | 3     | 226 | GLN  |
| 4   | 4     | 30  | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 5   | W91  | 1     | 700 | -    | 25,25,25     | 3.13 | 5 (20%)     | 33,34,34    | 2.81 | 9 (27%)     |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 5   | W91  | 1     | 700 | -    | -       | 1/11/18/18 | 0/3/3/3 |

All (5) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 5   | 1     | 700 | W91  | C2A-N3A | 12.92 | 1.43        | 1.27     |
| 5   | 1     | 700 | W91  | C4A-N3A | -6.95 | 1.36        | 1.47     |
| 5   | 1     | 700 | W91  | O1A-C5A | -3.02 | 1.38        | 1.46     |
| 5   | 1     | 700 | W91  | O1A-C2A | -2.92 | 1.31        | 1.36     |
| 5   | 1     | 700 | W91  | C4-C3   | -2.50 | 1.36        | 1.40     |

All (9) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 5   | 1     | 700 | W91  | O1A-C2A-N3A | -9.52 | 110.02      | 118.25   |
| 5   | 1     | 700 | W91  | C4A-N3A-C2A | 6.37  | 112.40      | 106.75   |
| 5   | 1     | 700 | W91  | O1A-C2A-C4B | 6.11  | 123.57      | 115.85   |
| 5   | 1     | 700 | W91  | C5-O1-N2    | -4.69 | 104.77      | 108.30   |
| 5   | 1     | 700 | W91  | C4-C3-N2    | -4.19 | 108.50      | 111.54   |
| 5   | 1     | 700 | W91  | O1A-C5A-C4A | 4.12  | 111.89      | 104.24   |
| 5   | 1     | 700 | W91  | C3C-O1B-C1B | 2.58  | 121.95      | 114.22   |
| 5   | 1     | 700 | W91  | O1-N2-C3    | 2.31  | 109.02      | 105.18   |
| 5   | 1     | 700 | W91  | C5A-C4A-N3A | -2.28 | 99.44       | 104.42   |

There are no chirality outliers.

All (1) torsion outliers are listed below:

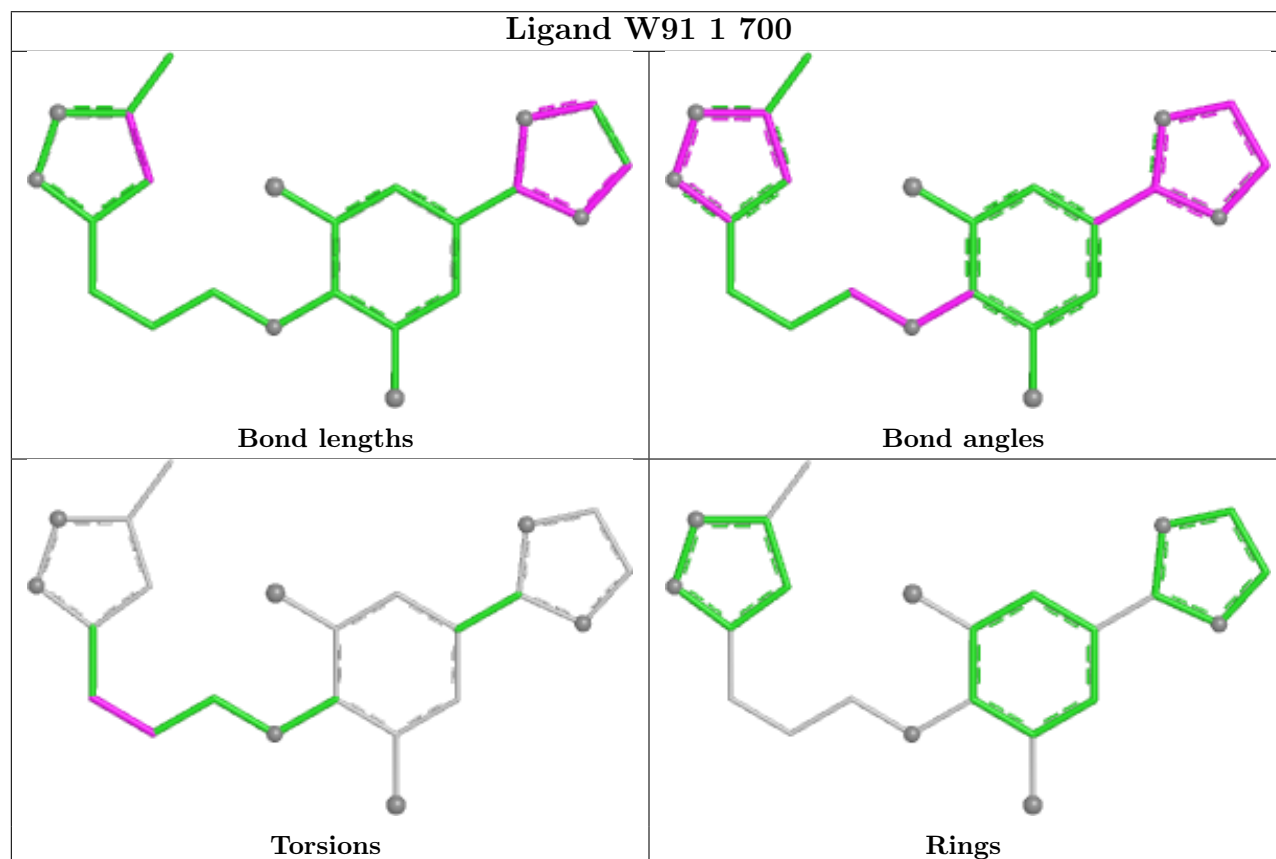
| Mol | Chain | Res | Type | Atoms          |
|-----|-------|-----|------|----------------|
| 5   | 1     | 700 | W91  | C5-C1C-C2C-C3C |

There are no ring outliers.

1 monomer is involved in 2 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 5   | 1     | 700 | W91  | 2       | 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 ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 2   | 2     | 1                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | 2     | 169:VAL   | C      | 170:VAL   | N      | 1.11         |

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.