



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 8, 2023 – 02:59 PM EST

PDB ID : 2HWB  
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 : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

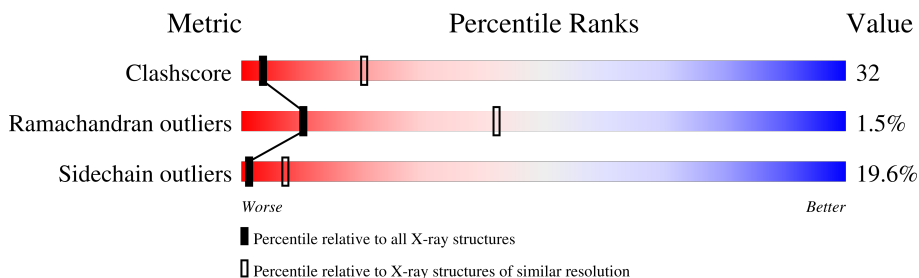
# 1 Overall quality at a glance

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            | 141614                      | 2416 (3.00-3.00)                                      |
| Ramachandran outliers | 138981                      | 2333 (3.00-3.00)                                      |
| Sidechain outliers    | 138945                      | 2336 (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    |                  |
| 2   | 2     | 262    |                  |
| 3   | 3     | 236    |                  |
| 4   | 4     | 68     |                  |

## 2 Entry composition [i](#)

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 |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
|     |       |          | Total | C    | N   | O   | S |         |         |       |
| 1   | 1     | 273      | 2170  | 1373 | 375 | 414 | 8 | 0       | 0       | 0     |

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

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

There is a discrepancy between the modelled and reference sequences:

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

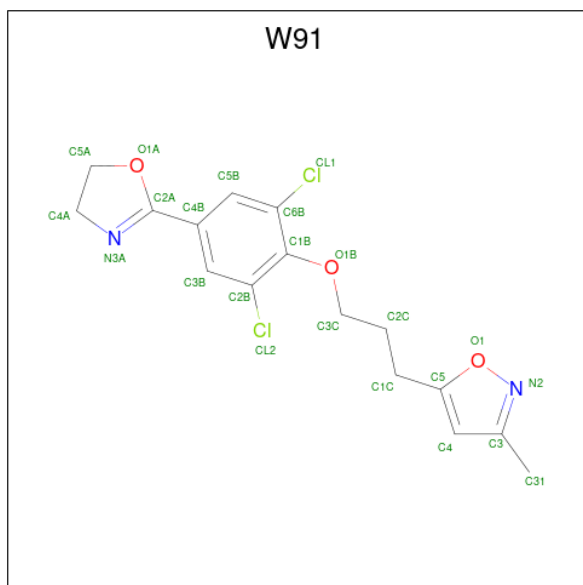
- Molecule 3 is a protein called HUMAN RHINOVIRUS 14 COAT PROTEIN (SUBUNIT VP3).

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

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

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

- Molecule 5 is 5-(3-(2,6-DICHLORO-4-(4,5-DIHYDRO-2-OXAZOLYL)PHENOXY)PROPYL)-3-METHYL ISOXAZOLE (three-letter code: 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 |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
|     |       |          | Total | C  | Cl | N | O |         |         |
| 5   | 1     | 1        | 23    | 16 | 2  | 2 | 3 | 0       | 0       |

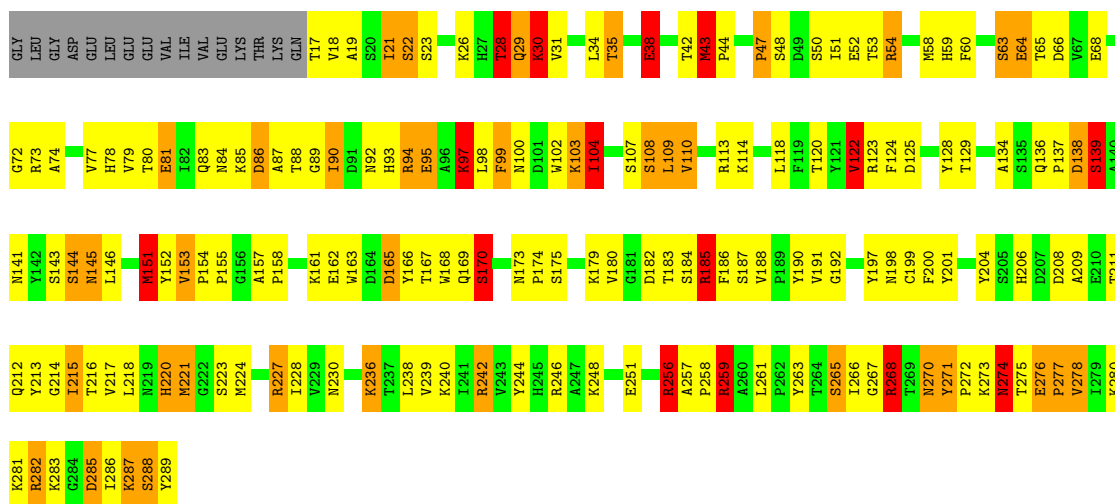
### 3 Residue-property plots [i](#)

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

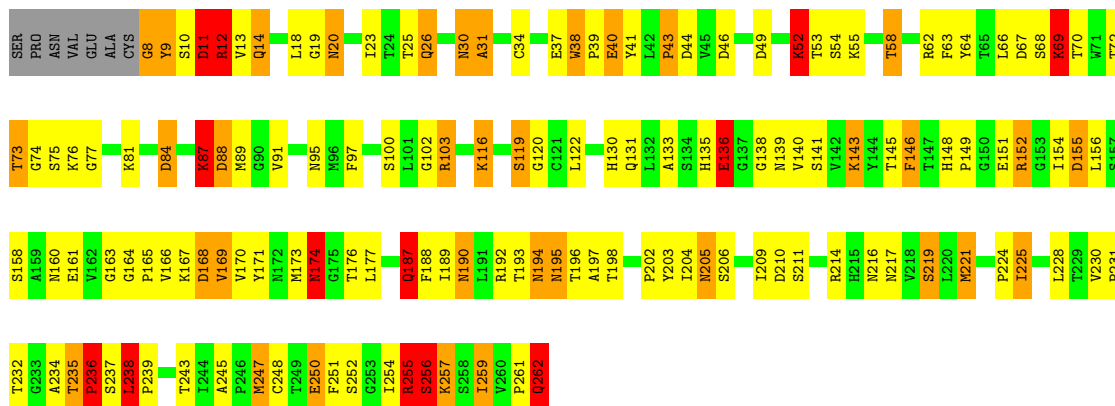
- Molecule 1: HUMAN RHINOVIRUS 14 COAT PROTEIN (SUBUNIT VP1)

Chain 1: 



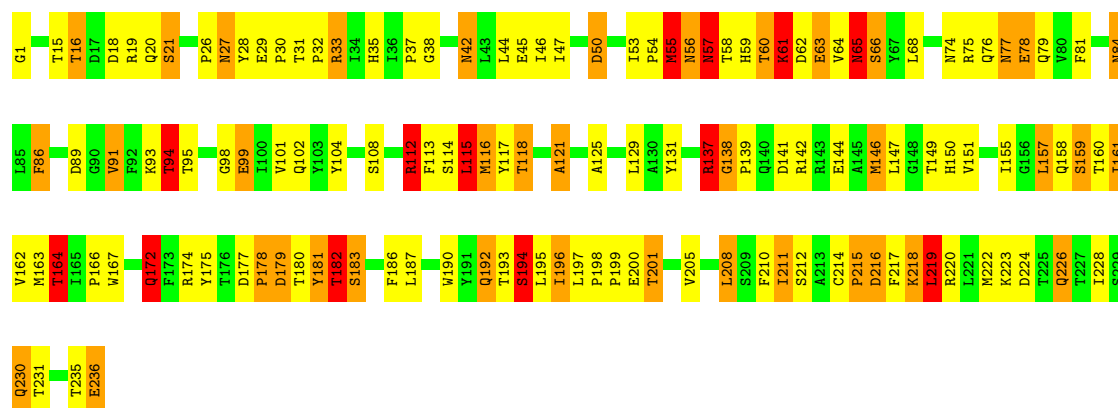
- Molecule 2: HUMAN RHINOVIRUS 14 COAT PROTEIN (SUBUNIT VP2)

Chain 2: 



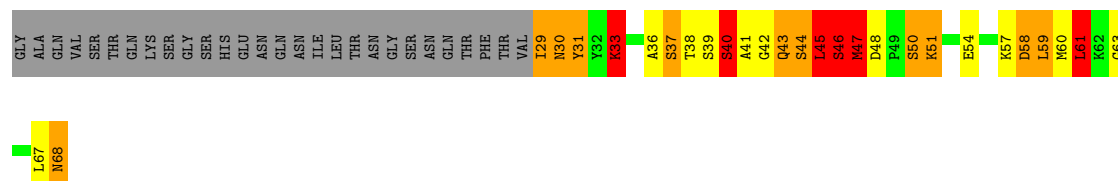
- Molecule 3: HUMAN RHINOVIRUS 14 COAT PROTEIN (SUBUNIT VP3)

Chain 3: 42% 36% 17% 6%



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

Chain 4: 18% 16% 16% 9% 41%



## 4 Data and refinement statistics

Xtrriage (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.                          | Xtrriage  |
| Total number of atoms                                    | 6290  | wwPDB-VP  |
| Average B, all atoms (Å <sup>2</sup> )                   | 0.0   | wwPDB-VP  |

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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     | 1.67         | 32/2228 (1.4%)  | 2.13        | 93/3031 (3.1%)  |
| 2   | 2     | 1.86         | 34/2000 (1.7%)  | 2.16        | 76/2734 (2.8%)  |
| 3   | 3     | 1.77         | 21/1898 (1.1%)  | 2.16        | 73/2597 (2.8%)  |
| 4   | 4     | 2.30         | 13/302 (4.3%)   | 2.46        | 21/406 (5.2%)   |
| All | All   | 1.80         | 100/6428 (1.6%) | 2.16        | 263/8768 (3.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | 1     | 0                   | 2                   |
| 2   | 2     | 0                   | 2                   |
| All | All   | 0                   | 4                   |

All (100) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | 1     | 285 | ASP  | CA-CB | 11.83 | 1.79        | 1.53     |
| 4   | 4     | 42  | GLY  | N-CA  | 11.70 | 1.63        | 1.46     |
| 4   | 4     | 40  | SER  | CB-OG | 10.77 | 1.56        | 1.42     |
| 2   | 2     | 256 | SER  | CB-OG | 10.25 | 1.55        | 1.42     |
| 1   | 1     | 95  | GLU  | CB-CG | 10.12 | 1.71        | 1.52     |
| 4   | 4     | 44  | SER  | CB-OG | 9.95  | 1.55        | 1.42     |
| 1   | 1     | 188 | VAL  | C-N   | 9.75  | 1.52        | 1.34     |
| 2   | 2     | 169 | VAL  | C-N   | -9.74 | 1.11        | 1.34     |
| 4   | 4     | 41  | ALA  | C-O   | 9.37  | 1.41        | 1.23     |
| 1   | 1     | 38  | GLU  | CB-CG | -9.03 | 1.34        | 1.52     |
| 1   | 1     | 63  | SER  | CB-OG | -8.77 | 1.30        | 1.42     |
| 3   | 3     | 21  | SER  | CA-CB | 8.68  | 1.66        | 1.52     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | 2     | 248 | CYS  | CB-SG  | -8.67 | 1.67        | 1.82     |
| 3   | 3     | 57  | ASN  | CA-CB  | 8.43  | 1.75        | 1.53     |
| 2   | 2     | 40  | GLU  | CD-OE1 | 8.22  | 1.34        | 1.25     |
| 1   | 1     | 288 | SER  | CA-CB  | 8.03  | 1.65        | 1.52     |
| 2   | 2     | 52  | LYS  | CE-NZ  | 7.95  | 1.69        | 1.49     |
| 3   | 3     | 1   | GLY  | N-CA   | 7.89  | 1.57        | 1.46     |
| 2   | 2     | 219 | SER  | CA-CB  | -7.73 | 1.41        | 1.52     |
| 3   | 3     | 63  | GLU  | CD-OE1 | 7.66  | 1.34        | 1.25     |
| 1   | 1     | 283 | LYS  | N-CA   | 7.63  | 1.61        | 1.46     |
| 2   | 2     | 136 | GLU  | CB-CG  | 7.55  | 1.66        | 1.52     |
| 3   | 3     | 108 | SER  | CB-OG  | 7.47  | 1.51        | 1.42     |
| 4   | 4     | 33  | LYS  | CE-NZ  | 7.39  | 1.67        | 1.49     |
| 1   | 1     | 282 | ARG  | CD-NE  | 7.28  | 1.58        | 1.46     |
| 1   | 1     | 139 | SER  | CB-OG  | 7.26  | 1.51        | 1.42     |
| 2   | 2     | 152 | ARG  | CD-NE  | 7.23  | 1.58        | 1.46     |
| 2   | 2     | 152 | ARG  | CZ-NH2 | 7.03  | 1.42        | 1.33     |
| 2   | 2     | 194 | ASN  | CA-CB  | 6.97  | 1.71        | 1.53     |
| 3   | 3     | 164 | THR  | C-O    | 6.91  | 1.36        | 1.23     |
| 4   | 4     | 46  | SER  | CB-OG  | 6.87  | 1.51        | 1.42     |
| 1   | 1     | 143 | SER  | CB-OG  | 6.79  | 1.51        | 1.42     |
| 4   | 4     | 51  | LYS  | CE-NZ  | 6.77  | 1.66        | 1.49     |
| 3   | 3     | 61  | LYS  | CE-NZ  | 6.71  | 1.65        | 1.49     |
| 2   | 2     | 256 | SER  | C-O    | 6.68  | 1.36        | 1.23     |
| 1   | 1     | 72  | GLY  | C-O    | 6.52  | 1.34        | 1.23     |
| 1   | 1     | 30  | LYS  | CE-NZ  | 6.50  | 1.65        | 1.49     |
| 2   | 2     | 8   | GLY  | N-CA   | 6.43  | 1.55        | 1.46     |
| 1   | 1     | 81  | GLU  | CD-OE1 | 6.42  | 1.32        | 1.25     |
| 2   | 2     | 12  | ARG  | NE-CZ  | 6.36  | 1.41        | 1.33     |
| 1   | 1     | 283 | LYS  | CE-NZ  | 6.35  | 1.65        | 1.49     |
| 3   | 3     | 138 | GLY  | N-CA   | 6.33  | 1.55        | 1.46     |
| 1   | 1     | 52  | GLU  | C-O    | 6.32  | 1.35        | 1.23     |
| 2   | 2     | 87  | LYS  | CB-CG  | -6.30 | 1.35        | 1.52     |
| 3   | 3     | 194 | SER  | CB-OG  | -6.29 | 1.34        | 1.42     |
| 1   | 1     | 30  | LYS  | CD-CE  | 6.28  | 1.67        | 1.51     |
| 4   | 4     | 33  | LYS  | CD-CE  | 6.19  | 1.66        | 1.51     |
| 3   | 3     | 50  | ASP  | CA-CB  | -6.08 | 1.40        | 1.53     |
| 3   | 3     | 108 | SER  | CA-CB  | -6.04 | 1.43        | 1.52     |
| 1   | 1     | 144 | SER  | N-CA   | 6.01  | 1.58        | 1.46     |
| 1   | 1     | 94  | ARG  | CD-NE  | 6.00  | 1.56        | 1.46     |
| 2   | 2     | 102 | GLY  | N-CA   | 5.97  | 1.55        | 1.46     |
| 4   | 4     | 54  | GLU  | CD-OE1 | 5.94  | 1.32        | 1.25     |
| 3   | 3     | 99  | GLU  | CB-CG  | -5.92 | 1.41        | 1.52     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | 1     | 285 | ASP  | N-CA   | -5.83 | 1.34        | 1.46     |
| 2   | 2     | 11  | ASP  | CA-CB  | 5.65  | 1.66        | 1.53     |
| 3   | 3     | 172 | GLN  | CG-CD  | -5.65 | 1.38        | 1.51     |
| 4   | 4     | 37  | SER  | CB-OG  | -5.64 | 1.34        | 1.42     |
| 2   | 2     | 168 | ASP  | C-O    | 5.63  | 1.34        | 1.23     |
| 2   | 2     | 235 | THR  | C-N    | -5.62 | 1.23        | 1.34     |
| 1   | 1     | 97  | LYS  | CD-CE  | 5.61  | 1.65        | 1.51     |
| 2   | 2     | 187 | GLN  | N-CA   | 5.61  | 1.57        | 1.46     |
| 3   | 3     | 45  | GLU  | CD-OE1 | 5.59  | 1.31        | 1.25     |
| 4   | 4     | 63  | GLY  | N-CA   | 5.58  | 1.54        | 1.46     |
| 1   | 1     | 139 | SER  | CA-CB  | 5.57  | 1.61        | 1.52     |
| 4   | 4     | 45  | LEU  | C-N    | 5.56  | 1.46        | 1.34     |
| 3   | 3     | 222 | MET  | CG-SD  | 5.54  | 1.95        | 1.81     |
| 2   | 2     | 219 | SER  | CB-OG  | -5.47 | 1.35        | 1.42     |
| 4   | 4     | 50  | SER  | CB-OG  | 5.45  | 1.49        | 1.42     |
| 2   | 2     | 236 | PRO  | C-O    | 5.43  | 1.34        | 1.23     |
| 1   | 1     | 276 | GLU  | CD-OE1 | 5.42  | 1.31        | 1.25     |
| 2   | 2     | 54  | SER  | CA-CB  | -5.41 | 1.44        | 1.52     |
| 2   | 2     | 262 | GLN  | CD-OE1 | 5.40  | 1.35        | 1.24     |
| 1   | 1     | 73  | ARG  | C-O    | 5.39  | 1.33        | 1.23     |
| 2   | 2     | 187 | GLN  | CB-CG  | -5.35 | 1.38        | 1.52     |
| 1   | 1     | 267 | GLY  | C-O    | 5.35  | 1.32        | 1.23     |
| 1   | 1     | 94  | ARG  | NE-CZ  | 5.33  | 1.40        | 1.33     |
| 2   | 2     | 40  | GLU  | CB-CG  | 5.28  | 1.62        | 1.52     |
| 1   | 1     | 251 | GLU  | CA-CB  | -5.26 | 1.42        | 1.53     |
| 2   | 2     | 68  | SER  | CB-OG  | -5.26 | 1.35        | 1.42     |
| 2   | 2     | 120 | GLY  | N-CA   | 5.25  | 1.53        | 1.46     |
| 3   | 3     | 33  | ARG  | CZ-NH2 | 5.25  | 1.39        | 1.33     |
| 1   | 1     | 246 | ARG  | CZ-NH2 | 5.24  | 1.39        | 1.33     |
| 2   | 2     | 74  | GLY  | C-O    | 5.21  | 1.31        | 1.23     |
| 1   | 1     | 143 | SER  | C-O    | 5.18  | 1.33        | 1.23     |
| 2   | 2     | 161 | GLU  | CA-CB  | -5.16 | 1.42        | 1.53     |
| 3   | 3     | 118 | THR  | CB-OG1 | 5.14  | 1.53        | 1.43     |
| 1   | 1     | 283 | LYS  | CD-CE  | 5.11  | 1.64        | 1.51     |
| 3   | 3     | 77  | ASN  | C-O    | 5.11  | 1.33        | 1.23     |
| 2   | 2     | 136 | GLU  | CD-OE1 | 5.11  | 1.31        | 1.25     |
| 1   | 1     | 68  | GLU  | CD-OE2 | -5.10 | 1.20        | 1.25     |
| 2   | 2     | 12  | ARG  | CZ-NH2 | 5.10  | 1.39        | 1.33     |
| 2   | 2     | 38  | TRP  | CG-CD1 | 5.08  | 1.43        | 1.36     |
| 1   | 1     | 26  | LYS  | CB-CG  | -5.07 | 1.38        | 1.52     |
| 2   | 2     | 58  | THR  | C-O    | 5.07  | 1.32        | 1.23     |
| 3   | 3     | 38  | GLY  | CA-C   | -5.04 | 1.43        | 1.51     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | 1     | 288 | SER  | C-O   | 5.03  | 1.32        | 1.23     |
| 2   | 2     | 100 | SER  | CB-OG | -5.02 | 1.35        | 1.42     |
| 3   | 3     | 30  | PRO  | N-CD  | -5.02 | 1.40        | 1.47     |
| 3   | 3     | 86  | PHE  | CA-CB | -5.01 | 1.43        | 1.53     |

All (263) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1   | 1     | 246 | ARG  | NE-CZ-NH1 | 22.48  | 131.54      | 120.30   |
| 1   | 1     | 256 | ARG  | NE-CZ-NH2 | 20.36  | 130.48      | 120.30   |
| 1   | 1     | 123 | ARG  | NE-CZ-NH1 | 19.07  | 129.84      | 120.30   |
| 2   | 2     | 255 | ARG  | NE-CZ-NH2 | -18.82 | 110.89      | 120.30   |
| 2   | 2     | 87  | LYS  | CA-CB-CG  | 17.61  | 152.15      | 113.40   |
| 1   | 1     | 285 | ASP  | CB-CG-OD1 | -17.57 | 102.49      | 118.30   |
| 3   | 3     | 137 | ARG  | NE-CZ-NH1 | -16.89 | 111.86      | 120.30   |
| 1   | 1     | 256 | ARG  | NE-CZ-NH1 | -16.88 | 111.86      | 120.30   |
| 1   | 1     | 94  | ARG  | NE-CZ-NH2 | -16.50 | 112.05      | 120.30   |
| 3   | 3     | 216 | ASP  | CB-CG-OD2 | 16.07  | 132.76      | 118.30   |
| 2   | 2     | 255 | ARG  | NE-CZ-NH1 | 14.25  | 127.43      | 120.30   |
| 1   | 1     | 282 | ARG  | NE-CZ-NH2 | -14.09 | 113.25      | 120.30   |
| 2   | 2     | 168 | ASP  | CB-CG-OD1 | -12.85 | 106.73      | 118.30   |
| 3   | 3     | 50  | ASP  | CA-CB-CG  | 12.24  | 140.32      | 113.40   |
| 1   | 1     | 94  | ARG  | CD-NE-CZ  | -12.04 | 106.75      | 123.60   |
| 2   | 2     | 11  | ASP  | CB-CG-OD1 | -11.73 | 107.74      | 118.30   |
| 2   | 2     | 194 | ASN  | N-CA-CB   | -11.55 | 89.81       | 110.60   |
| 2   | 2     | 193 | THR  | C-N-CA    | 11.39  | 150.18      | 121.70   |
| 3   | 3     | 215 | PRO  | C-N-CA    | 11.01  | 149.22      | 121.70   |
| 2   | 2     | 152 | ARG  | NE-CZ-NH2 | -10.99 | 114.81      | 120.30   |
| 4   | 4     | 41  | ALA  | CA-C-N    | 10.88  | 137.96      | 116.20   |
| 4   | 4     | 48  | ASP  | CB-CG-OD1 | -10.80 | 108.58      | 118.30   |
| 3   | 3     | 19  | ARG  | NE-CZ-NH2 | 10.77  | 125.68      | 120.30   |
| 3   | 3     | 33  | ARG  | NE-CZ-NH2 | -10.70 | 114.95      | 120.30   |
| 1   | 1     | 285 | ASP  | CB-CG-OD2 | 10.58  | 127.82      | 118.30   |
| 1   | 1     | 285 | ASP  | CA-CB-CG  | -10.48 | 90.35       | 113.40   |
| 3   | 3     | 50  | ASP  | CB-CG-OD1 | 10.44  | 127.70      | 118.30   |
| 2   | 2     | 151 | GLU  | CA-CB-CG  | 10.40  | 136.29      | 113.40   |
| 1   | 1     | 246 | ARG  | NE-CZ-NH2 | -10.07 | 115.27      | 120.30   |
| 1   | 1     | 246 | ARG  | CD-NE-CZ  | 10.04  | 137.65      | 123.60   |
| 1   | 1     | 282 | ARG  | CD-NE-CZ  | -9.96  | 109.65      | 123.60   |
| 3   | 3     | 57  | ASN  | N-CA-CB   | -9.82  | 92.92       | 110.60   |
| 3   | 3     | 146 | MET  | CG-SD-CE  | 9.81   | 115.90      | 100.20   |
| 3   | 3     | 216 | ASP  | CB-CG-OD1 | -9.72  | 109.55      | 118.30   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | 2     | 88  | ASP  | CB-CG-OD1  | -9.69 | 109.58      | 118.30   |
| 1   | 1     | 242 | ARG  | NE-CZ-NH2  | -9.36 | 115.62      | 120.30   |
| 1   | 1     | 54  | ARG  | CD-NE-CZ   | -9.35 | 110.51      | 123.60   |
| 1   | 1     | 66  | ASP  | CB-CG-OD2  | -9.19 | 110.03      | 118.30   |
| 3   | 3     | 57  | ASN  | CB-CA-C    | -9.03 | 92.34       | 110.40   |
| 2   | 2     | 11  | ASP  | CA-CB-CG   | -8.99 | 93.63       | 113.40   |
| 3   | 3     | 137 | ARG  | NE-CZ-NH2  | 8.92  | 124.76      | 120.30   |
| 1   | 1     | 38  | GLU  | CA-CB-CG   | 8.90  | 132.97      | 113.40   |
| 3   | 3     | 112 | ARG  | NE-CZ-NH2  | -8.71 | 115.95      | 120.30   |
| 3   | 3     | 182 | THR  | CA-CB-CG2  | 8.55  | 124.37      | 112.40   |
| 1   | 1     | 285 | ASP  | N-CA-CB    | -8.51 | 95.28       | 110.60   |
| 1   | 1     | 268 | ARG  | CD-NE-CZ   | -8.45 | 111.77      | 123.60   |
| 1   | 1     | 123 | ARG  | CD-NE-CZ   | 8.39  | 135.35      | 123.60   |
| 1   | 1     | 63  | SER  | CB-CA-C    | -8.38 | 94.19       | 110.10   |
| 2   | 2     | 250 | GLU  | CA-CB-CG   | 8.33  | 131.72      | 113.40   |
| 1   | 1     | 285 | ASP  | CB-CA-C    | -8.30 | 93.79       | 110.40   |
| 3   | 3     | 172 | GLN  | CB-CG-CD   | 8.23  | 133.00      | 111.60   |
| 2   | 2     | 152 | ARG  | NE-CZ-NH1  | 8.19  | 124.39      | 120.30   |
| 1   | 1     | 251 | GLU  | CA-CB-CG   | 8.19  | 131.41      | 113.40   |
| 4   | 4     | 45  | LEU  | N-CA-CB    | -8.16 | 94.08       | 110.40   |
| 3   | 3     | 224 | ASP  | CB-CG-OD1  | -8.06 | 111.05      | 118.30   |
| 2   | 2     | 255 | ARG  | CA-CB-CG   | 8.04  | 131.08      | 113.40   |
| 2   | 2     | 11  | ASP  | OD1-CG-OD2 | 8.02  | 138.54      | 123.30   |
| 4   | 4     | 48  | ASP  | OD1-CG-OD2 | 8.00  | 138.50      | 123.30   |
| 1   | 1     | 95  | GLU  | OE1-CD-OE2 | 7.98  | 132.88      | 123.30   |
| 1   | 1     | 38  | GLU  | CB-CG-CD   | 7.98  | 135.74      | 114.20   |
| 3   | 3     | 181 | TYR  | CB-CG-CD2  | -7.98 | 116.22      | 121.00   |
| 4   | 4     | 47  | MET  | CA-CB-CG   | -7.87 | 99.92       | 113.30   |
| 2   | 2     | 219 | SER  | CA-CB-OG   | 7.83  | 132.35      | 111.20   |
| 1   | 1     | 145 | ASN  | OD1-CG-ND2 | 7.79  | 139.81      | 121.90   |
| 3   | 3     | 21  | SER  | CB-CA-C    | -7.69 | 95.49       | 110.10   |
| 2   | 2     | 155 | ASP  | CB-CG-OD1  | -7.65 | 111.42      | 118.30   |
| 2   | 2     | 187 | GLN  | CA-CB-CG   | 7.60  | 130.13      | 113.40   |
| 3   | 3     | 78  | GLU  | OE1-CD-OE2 | 7.58  | 132.40      | 123.30   |
| 2   | 2     | 11  | ASP  | C-N-CA     | 7.55  | 140.58      | 121.70   |
| 1   | 1     | 277 | PRO  | N-CD-CG    | -7.54 | 91.88       | 103.20   |
| 2   | 2     | 187 | GLN  | CB-CA-C    | 7.50  | 125.39      | 110.40   |
| 1   | 1     | 123 | ARG  | NE-CZ-NH2  | -7.47 | 116.56      | 120.30   |
| 3   | 3     | 236 | GLU  | CA-CB-CG   | 7.43  | 129.75      | 113.40   |
| 1   | 1     | 259 | ARG  | CA-CB-CG   | -7.34 | 97.25       | 113.40   |
| 2   | 2     | 214 | ARG  | NE-CZ-NH1  | 7.32  | 123.96      | 120.30   |
| 1   | 1     | 282 | ARG  | NH1-CZ-NH2 | 7.30  | 127.43      | 119.40   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | 1     | 227 | ARG  | NE-CZ-NH2  | 7.24  | 123.92      | 120.30   |
| 3   | 3     | 142 | ARG  | CA-CB-CG   | 7.23  | 129.31      | 113.40   |
| 1   | 1     | 113 | ARG  | NE-CZ-NH2  | 7.22  | 123.91      | 120.30   |
| 3   | 3     | 112 | ARG  | NE-CZ-NH1  | 7.22  | 123.91      | 120.30   |
| 2   | 2     | 194 | ASN  | CA-CB-CG   | -7.15 | 97.67       | 113.40   |
| 2   | 2     | 190 | ASN  | CA-CB-CG   | 7.09  | 129.00      | 113.40   |
| 3   | 3     | 121 | ALA  | CB-CA-C    | -7.03 | 99.55       | 110.10   |
| 3   | 3     | 28  | TYR  | CB-CG-CD1  | -7.02 | 116.79      | 121.00   |
| 2   | 2     | 168 | ASP  | N-CA-CB    | -7.02 | 97.97       | 110.60   |
| 1   | 1     | 68  | GLU  | CG-CD-OE2  | 7.01  | 132.32      | 118.30   |
| 3   | 3     | 137 | ARG  | CD-NE-CZ   | -7.01 | 113.79      | 123.60   |
| 2   | 2     | 256 | SER  | CA-C-O     | -7.01 | 105.38      | 120.10   |
| 4   | 4     | 41  | ALA  | CA-C-O     | -6.96 | 105.47      | 120.10   |
| 1   | 1     | 42  | THR  | CA-CB-CG2  | 6.93  | 122.10      | 112.40   |
| 1   | 1     | 125 | ASP  | CB-CG-OD1  | -6.90 | 112.09      | 118.30   |
| 1   | 1     | 28  | THR  | CB-CA-C    | -6.89 | 92.98       | 111.60   |
| 1   | 1     | 26  | LYS  | CA-CB-CG   | 6.85  | 128.47      | 113.40   |
| 4   | 4     | 37  | SER  | CB-CA-C    | 6.77  | 122.96      | 110.10   |
| 2   | 2     | 136 | GLU  | CG-CD-OE1  | -6.76 | 104.78      | 118.30   |
| 3   | 3     | 163 | MET  | CA-CB-CG   | -6.74 | 101.85      | 113.30   |
| 3   | 3     | 194 | SER  | N-CA-CB    | -6.73 | 100.40      | 110.50   |
| 3   | 3     | 216 | ASP  | N-CA-CB    | -6.68 | 98.57       | 110.60   |
| 2   | 2     | 146 | PHE  | CB-CG-CD1  | -6.67 | 116.13      | 120.80   |
| 1   | 1     | 265 | SER  | N-CA-CB    | -6.66 | 100.52      | 110.50   |
| 2   | 2     | 103 | ARG  | CD-NE-CZ   | -6.64 | 114.30      | 123.60   |
| 3   | 3     | 57  | ASN  | CA-CB-CG   | -6.61 | 98.86       | 113.40   |
| 1   | 1     | 94  | ARG  | NH1-CZ-NH2 | 6.60  | 126.66      | 119.40   |
| 2   | 2     | 87  | LYS  | CB-CG-CD   | 6.58  | 128.71      | 111.60   |
| 3   | 3     | 27  | ASN  | CB-CA-C    | -6.58 | 97.24       | 110.40   |
| 3   | 3     | 45  | GLU  | CG-CD-OE2  | 6.57  | 131.44      | 118.30   |
| 1   | 1     | 68  | GLU  | CG-CD-OE1  | -6.57 | 105.17      | 118.30   |
| 1   | 1     | 276 | GLU  | OE1-CD-OE2 | 6.56  | 131.17      | 123.30   |
| 1   | 1     | 288 | SER  | CB-CA-C    | -6.52 | 97.71       | 110.10   |
| 2   | 2     | 203 | TYR  | CB-CG-CD2  | 6.51  | 124.91      | 121.00   |
| 1   | 1     | 53  | THR  | CA-CB-OG1  | -6.51 | 95.33       | 109.00   |
| 1   | 1     | 288 | SER  | N-CA-CB    | -6.49 | 100.77      | 110.50   |
| 4   | 4     | 45  | LEU  | CB-CA-C    | 6.48  | 122.51      | 110.20   |
| 3   | 3     | 74  | ASN  | CA-CB-CG   | -6.47 | 99.17       | 113.40   |
| 1   | 1     | 22  | SER  | N-CA-CB    | -6.46 | 100.81      | 110.50   |
| 1   | 1     | 144 | SER  | N-CA-CB    | -6.45 | 100.82      | 110.50   |
| 3   | 3     | 55  | MET  | CA-CB-CG   | -6.45 | 102.34      | 113.30   |
| 3   | 3     | 183 | SER  | N-CA-CB    | -6.44 | 100.84      | 110.50   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | 2     | 168 | ASP  | OD1-CG-OD2 | 6.43  | 135.51      | 123.30   |
| 3   | 3     | 29  | GLU  | CB-CG-CD   | 6.40  | 131.47      | 114.20   |
| 2   | 2     | 97  | PHE  | CB-CG-CD1  | -6.38 | 116.34      | 120.80   |
| 1   | 1     | 274 | ASN  | O-C-N      | 6.34  | 132.85      | 122.70   |
| 1   | 1     | 187 | SER  | C-N-CA     | -6.33 | 105.89      | 121.70   |
| 1   | 1     | 138 | ASP  | CB-CG-OD1  | 6.30  | 123.97      | 118.30   |
| 3   | 3     | 65  | ASN  | CA-CB-CG   | -6.30 | 99.55       | 113.40   |
| 3   | 3     | 16  | THR  | N-CA-CB    | -6.29 | 98.34       | 110.30   |
| 1   | 1     | 95  | GLU  | CB-CG-CD   | -6.28 | 97.25       | 114.20   |
| 1   | 1     | 271 | TYR  | CB-CG-CD1  | 6.27  | 124.77      | 121.00   |
| 2   | 2     | 38  | TRP  | N-CA-CB    | -6.27 | 99.31       | 110.60   |
| 4   | 4     | 44  | SER  | CA-C-N     | -6.25 | 103.45      | 117.20   |
| 1   | 1     | 145 | ASN  | CA-CB-CG   | -6.23 | 99.69       | 113.40   |
| 3   | 3     | 19  | ARG  | CA-CB-CG   | 6.22  | 127.09      | 113.40   |
| 3   | 3     | 27  | ASN  | CA-CB-CG   | -6.21 | 99.74       | 113.40   |
| 3   | 3     | 63  | GLU  | CG-CD-OE1  | -6.21 | 105.89      | 118.30   |
| 1   | 1     | 151 | MET  | CG-SD-CE   | 6.20  | 110.11      | 100.20   |
| 1   | 1     | 122 | VAL  | N-CA-CB    | -6.18 | 97.90       | 111.50   |
| 2   | 2     | 69  | LYS  | CA-CB-CG   | 6.16  | 126.94      | 113.40   |
| 2   | 2     | 136 | GLU  | CB-CG-CD   | -6.15 | 97.58       | 114.20   |
| 2   | 2     | 203 | TYR  | CB-CG-CD1  | -6.14 | 117.32      | 121.00   |
| 1   | 1     | 224 | MET  | CG-SD-CE   | 6.13  | 110.01      | 100.20   |
| 1   | 1     | 221 | MET  | CG-SD-CE   | 6.10  | 109.96      | 100.20   |
| 1   | 1     | 97  | LYS  | CD-CE-NZ   | -6.10 | 97.67       | 111.70   |
| 3   | 3     | 219 | LEU  | CA-CB-CG   | 6.09  | 129.30      | 115.30   |
| 2   | 2     | 219 | SER  | CB-CA-C    | 6.09  | 121.66      | 110.10   |
| 3   | 3     | 222 | MET  | CG-SD-CE   | -6.09 | 90.46       | 100.20   |
| 1   | 1     | 86  | ASP  | CB-CG-OD1  | 6.06  | 123.75      | 118.30   |
| 3   | 3     | 66  | SER  | CB-CA-C    | 6.06  | 121.61      | 110.10   |
| 2   | 2     | 119 | SER  | N-CA-CB    | 6.04  | 119.55      | 110.50   |
| 2   | 2     | 235 | THR  | CA-CB-CG2  | -6.03 | 103.96      | 112.40   |
| 2   | 2     | 67  | ASP  | CA-CB-CG   | -6.02 | 100.15      | 113.40   |
| 4   | 4     | 61  | LEU  | CB-CG-CD2  | -6.01 | 100.78      | 111.00   |
| 2   | 2     | 247 | MET  | CB-CA-C    | 6.01  | 122.43      | 110.40   |
| 2   | 2     | 169 | VAL  | CA-C-N     | 6.01  | 130.42      | 117.20   |
| 4   | 4     | 48  | ASP  | CB-CG-OD2  | -6.01 | 112.89      | 118.30   |
| 3   | 3     | 1   | GLY  | N-CA-C     | 5.97  | 128.03      | 113.10   |
| 2   | 2     | 103 | ARG  | CA-CB-CG   | 5.97  | 126.54      | 113.40   |
| 2   | 2     | 12  | ARG  | NE-CZ-NH2  | -5.97 | 117.32      | 120.30   |
| 1   | 1     | 257 | ALA  | N-CA-CB    | -5.92 | 101.81      | 110.10   |
| 3   | 3     | 58  | THR  | CA-CB-CG2  | -5.92 | 104.11      | 112.40   |
| 1   | 1     | 256 | ARG  | CD-NE-CZ   | -5.91 | 115.33      | 123.60   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | 1     | 35  | THR  | N-CA-CB    | -5.89 | 99.10       | 110.30   |
| 1   | 1     | 94  | ARG  | CG-CD-NE   | -5.88 | 99.46       | 111.80   |
| 2   | 2     | 256 | SER  | CA-C-N     | 5.86  | 130.10      | 117.20   |
| 4   | 4     | 30  | ASN  | CA-CB-CG   | -5.86 | 100.52      | 113.40   |
| 1   | 1     | 268 | ARG  | NE-CZ-NH2  | -5.85 | 117.37      | 120.30   |
| 1   | 1     | 236 | LYS  | CD-CE-NZ   | -5.85 | 98.25       | 111.70   |
| 4   | 4     | 33  | LYS  | CD-CE-NZ   | -5.85 | 98.25       | 111.70   |
| 3   | 3     | 45  | GLU  | CG-CD-OE1  | -5.84 | 106.63      | 118.30   |
| 2   | 2     | 31  | ALA  | N-CA-CB    | 5.83  | 118.25      | 110.10   |
| 2   | 2     | 238 | LEU  | N-CA-CB    | -5.82 | 98.76       | 110.40   |
| 3   | 3     | 27  | ASN  | O-C-N      | 5.82  | 132.01      | 122.70   |
| 1   | 1     | 28  | THR  | OG1-CB-CG2 | 5.78  | 123.29      | 110.00   |
| 2   | 2     | 255 | ARG  | CB-CG-CD   | 5.77  | 126.60      | 111.60   |
| 2   | 2     | 68  | SER  | N-CA-CB    | -5.75 | 101.88      | 110.50   |
| 2   | 2     | 214 | ARG  | NE-CZ-NH2  | -5.74 | 117.43      | 120.30   |
| 3   | 3     | 77  | ASN  | CA-C-N     | 5.74  | 129.82      | 117.20   |
| 2   | 2     | 73  | THR  | CA-CB-OG1  | -5.74 | 96.95       | 109.00   |
| 1   | 1     | 95  | GLU  | CA-CB-CG   | -5.72 | 100.82      | 113.40   |
| 1   | 1     | 48  | SER  | CA-C-O     | -5.71 | 108.11      | 120.10   |
| 3   | 3     | 147 | LEU  | CA-CB-CG   | 5.71  | 128.43      | 115.30   |
| 1   | 1     | 246 | ARG  | NH1-CZ-NH2 | -5.70 | 113.13      | 119.40   |
| 2   | 2     | 52  | LYS  | CD-CE-NZ   | -5.69 | 98.61       | 111.70   |
| 1   | 1     | 274 | ASN  | N-CA-CB    | 5.69  | 120.84      | 110.60   |
| 2   | 2     | 161 | GLU  | CA-CB-CG   | 5.68  | 125.90      | 113.40   |
| 2   | 2     | 75  | SER  | N-CA-CB    | -5.68 | 101.98      | 110.50   |
| 3   | 3     | 1   | GLY  | O-C-N      | -5.67 | 113.62      | 122.70   |
| 1   | 1     | 244 | TYR  | CB-CG-CD2  | -5.64 | 117.61      | 121.00   |
| 3   | 3     | 164 | THR  | N-CA-CB    | -5.64 | 99.58       | 110.30   |
| 4   | 4     | 44  | SER  | O-C-N      | 5.61  | 131.68      | 122.70   |
| 3   | 3     | 177 | ASP  | CB-CG-OD1  | -5.59 | 113.27      | 118.30   |
| 2   | 2     | 210 | ASP  | N-CA-CB    | -5.58 | 100.57      | 110.60   |
| 3   | 3     | 94  | THR  | O-C-N      | 5.54  | 131.56      | 122.70   |
| 2   | 2     | 84  | ASP  | CB-CG-OD2  | -5.53 | 113.32      | 118.30   |
| 1   | 1     | 122 | VAL  | CB-CA-C    | 5.51  | 121.87      | 111.40   |
| 2   | 2     | 9   | TYR  | CB-CA-C    | 5.50  | 121.41      | 110.40   |
| 2   | 2     | 43  | PRO  | N-CD-CG    | -5.50 | 94.95       | 103.20   |
| 4   | 4     | 44  | SER  | C-N-CA     | -5.49 | 107.97      | 121.70   |
| 3   | 3     | 186 | PHE  | CB-CG-CD1  | -5.49 | 116.96      | 120.80   |
| 1   | 1     | 81  | GLU  | CG-CD-OE1  | -5.48 | 107.34      | 118.30   |
| 3   | 3     | 112 | ARG  | CA-CB-CG   | 5.48  | 125.46      | 113.40   |
| 2   | 2     | 12  | ARG  | CD-NE-CZ   | -5.48 | 115.93      | 123.60   |
| 1   | 1     | 26  | LYS  | CD-CE-NZ   | -5.46 | 99.15       | 111.70   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | 1     | 43  | MET  | CG-SD-CE   | 5.44  | 108.91      | 100.20   |
| 3   | 3     | 60  | THR  | CA-CB-OG1  | -5.43 | 97.60       | 109.00   |
| 2   | 2     | 174 | ASN  | CA-C-N     | 5.42  | 127.04      | 116.20   |
| 2   | 2     | 44  | ASP  | CA-CB-CG   | 5.41  | 125.29      | 113.40   |
| 1   | 1     | 270 | ASN  | O-C-N      | 5.40  | 131.35      | 122.70   |
| 3   | 3     | 161 | ILE  | CA-CB-CG1  | -5.40 | 100.73      | 111.00   |
| 4   | 4     | 44  | SER  | N-CA-CB    | 5.40  | 118.61      | 110.50   |
| 3   | 3     | 115 | LEU  | CA-CB-CG   | 5.38  | 127.67      | 115.30   |
| 2   | 2     | 169 | VAL  | CB-CA-C    | -5.38 | 101.18      | 111.40   |
| 3   | 3     | 231 | THR  | CA-CB-OG1  | -5.38 | 97.71       | 109.00   |
| 3   | 3     | 65  | ASN  | N-CA-CB    | -5.36 | 100.95      | 110.60   |
| 1   | 1     | 123 | ARG  | NH1-CZ-NH2 | -5.35 | 113.52      | 119.40   |
| 2   | 2     | 262 | GLN  | CA-C-O     | -5.35 | 108.87      | 120.10   |
| 1   | 1     | 64  | GLU  | CA-CB-CG   | 5.34  | 125.15      | 113.40   |
| 2   | 2     | 259 | ILE  | CB-CG1-CD1 | -5.32 | 99.01       | 113.90   |
| 3   | 3     | 42  | ASN  | CB-CG-OD1  | -5.30 | 111.00      | 121.60   |
| 2   | 2     | 88  | ASP  | CA-CB-CG   | -5.30 | 101.75      | 113.40   |
| 1   | 1     | 187 | SER  | O-C-N      | 5.29  | 131.16      | 122.70   |
| 3   | 3     | 116 | MET  | CB-CG-SD   | -5.27 | 96.59       | 112.40   |
| 2   | 2     | 143 | LYS  | CD-CE-NZ   | -5.26 | 99.59       | 111.70   |
| 3   | 3     | 33  | ARG  | CB-CG-CD   | -5.26 | 97.91       | 111.60   |
| 3   | 3     | 74  | ASN  | OD1-CG-ND2 | 5.23  | 133.92      | 121.90   |
| 2   | 2     | 38  | TRP  | CA-CB-CG   | -5.22 | 103.77      | 113.70   |
| 1   | 1     | 275 | THR  | CA-C-O     | -5.22 | 109.14      | 120.10   |
| 2   | 2     | 203 | TYR  | CZ-CE2-CD2 | -5.22 | 115.10      | 119.80   |
| 1   | 1     | 275 | THR  | CA-C-N     | 5.21  | 128.67      | 117.20   |
| 2   | 2     | 219 | SER  | N-CA-CB    | 5.21  | 118.31      | 110.50   |
| 3   | 3     | 78  | GLU  | CA-CB-CG   | 5.21  | 124.86      | 113.40   |
| 4   | 4     | 48  | ASP  | CA-CB-CG   | -5.21 | 101.95      | 113.40   |
| 1   | 1     | 242 | ARG  | CD-NE-CZ   | -5.20 | 116.32      | 123.60   |
| 1   | 1     | 271 | TYR  | CB-CG-CD2  | -5.19 | 117.88      | 121.00   |
| 4   | 4     | 36  | ALA  | C-N-CA     | -5.19 | 108.72      | 121.70   |
| 1   | 1     | 187 | SER  | CB-CA-C    | 5.19  | 119.96      | 110.10   |
| 3   | 3     | 222 | MET  | CB-CG-SD   | -5.19 | 96.83       | 112.40   |
| 1   | 1     | 21  | ILE  | CA-CB-CG1  | -5.16 | 101.19      | 111.00   |
| 2   | 2     | 52  | LYS  | CA-C-N     | 5.16  | 128.55      | 117.20   |
| 2   | 2     | 11  | ASP  | CB-CG-OD2  | -5.16 | 113.66      | 118.30   |
| 2   | 2     | 14  | GLN  | OE1-CD-NE2 | 5.15  | 133.75      | 121.90   |
| 2   | 2     | 221 | MET  | CA-CB-CG   | -5.15 | 104.55      | 113.30   |
| 1   | 1     | 50  | SER  | CA-C-N     | 5.14  | 128.50      | 117.20   |
| 2   | 2     | 203 | TYR  | CG-CD2-CE2 | 5.13  | 125.40      | 121.30   |
| 1   | 1     | 282 | ARG  | CG-CD-NE   | -5.12 | 101.05      | 111.80   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4   | 4     | 31  | TYR  | CG-CD2-CE2 | -5.12 | 117.21      | 121.30   |
| 1   | 1     | 141 | ASN  | CA-CB-CG   | -5.11 | 102.16      | 113.40   |
| 2   | 2     | 14  | GLN  | CA-CB-CG   | -5.11 | 102.17      | 113.40   |
| 4   | 4     | 39  | SER  | O-C-N      | 5.10  | 130.85      | 122.70   |
| 3   | 3     | 144 | GLU  | CA-CB-CG   | 5.09  | 124.61      | 113.40   |
| 1   | 1     | 17  | THR  | CA-CB-CG2  | -5.09 | 105.27      | 112.40   |
| 4   | 4     | 58  | ASP  | O-C-N      | 5.09  | 130.85      | 122.70   |
| 3   | 3     | 141 | ASP  | CB-CG-OD1  | 5.08  | 122.87      | 118.30   |
| 2   | 2     | 18  | LEU  | CB-CA-C    | 5.07  | 119.84      | 110.20   |
| 3   | 3     | 172 | GLN  | CG-CD-NE2  | 5.06  | 128.84      | 116.70   |
| 3   | 3     | 86  | PHE  | CB-CA-C    | 5.04  | 120.48      | 110.40   |
| 1   | 1     | 270 | ASN  | CB-CA-C    | -5.04 | 100.32      | 110.40   |
| 1   | 1     | 282 | ARG  | CB-CA-C    | -5.04 | 100.33      | 110.40   |
| 3   | 3     | 178 | PRO  | O-C-N      | 5.04  | 130.76      | 122.70   |
| 1   | 1     | 185 | ARG  | NE-CZ-NH2  | 5.03  | 122.82      | 120.30   |
| 1   | 1     | 274 | ASN  | CA-C-N     | -5.01 | 106.17      | 117.20   |
| 3   | 3     | 57  | ASN  | N-CA-C     | 5.01  | 124.53      | 111.00   |
| 3   | 3     | 187 | LEU  | N-CA-CB    | -5.01 | 100.38      | 110.40   |
| 1   | 1     | 22  | SER  | CA-C-O     | -5.01 | 109.58      | 120.10   |

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 [i](#)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | 1     | 2170  | 0        | 2106     | 167     | 0            |
| 2   | 2     | 1951  | 0        | 1923     | 127     | 0            |
| 3   | 3     | 1849  | 0        | 1831     | 138     | 0            |
| 4   | 4     | 297   | 0        | 294      | 36      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 5   | 1     | 23    | 0        | 16       | 2       | 0            |
| All | All   | 6290  | 0        | 6170     | 396     | 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 32.

All (396) 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              |
| 2:2:136:GLU:HB3  | 2:2:140:VAL:HG21 | 1.44                     | 0.97              |
| 3:3:57:ASN:CB    | 3:3:57:ASN:N     | 2.28                     | 0.97              |
| 1:1:191:VAL:HG23 | 1:1:191:VAL:O    | 1.66                     | 0.96              |
| 1:1:58:MET:HE1   | 3:3:216:ASP:HA   | 1.49                     | 0.95              |
| 1:1:83:GLN:HG3   | 1:1:85:LYS:HE2   | 1.47                     | 0.94              |
| 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              |
| 3:3:57:ASN:CB    | 3:3:57:ASN:C     | 2.37                     | 0.92              |
| 1:1:285:ASP:CB   | 1:1:285:ASP:N    | 2.34                     | 0.91              |
| 1:1:285:ASP:CA   | 1:1:285:ASP:CG   | 2.37                     | 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              |
| 2:2:11:ASP:HB2   | 4:4:68:ASN:OD1   | 1.71                     | 0.90              |
| 1:1:285:ASP:CB   | 1:1:285:ASP:C    | 2.40                     | 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              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 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              |
| 3:3:57:ASN:CA    | 3:3:57:ASN:CG    | 2.45                     | 0.84              |
| 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              |
| 2:2:9:TYR:HD1    | 2:2:9:TYR:N      | 1.77                     | 0.80              |
| 1:1:58:MET:CE    | 3:3:216:ASP:HA   | 2.11                     | 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:CA   | 2.13                     | 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              |
| 3:3:197:LEU:HB3  | 3:3:201:THR:CG2  | 2.18                     | 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              |
| 2:2:262:GLN:HE21 | 2:2:262:GLN:C    | 1.91                     | 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              |
| 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              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 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              |
| 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              |
| 2:2:174:ASN:C    | 2:2:174:ASN:HD22 | 1.93                     | 0.70              |
| 1:1:170:SER:OG   | 1:1:170:SER:O    | 2.09                     | 0.70              |
| 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              |
| 1:1:89:GLY:C     | 1:1:90:ILE:HD13  | 2.13                     | 0.68              |
| 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              |
| 2:2:195:ASN:HD22 | 2:2:195:ASN:C    | 1.99                     | 0.66              |
| 3:3:89:ASP:HA    | 3:3:93:LYS:HD2   | 1.78                     | 0.66              |
| 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              |
| 1:1:163: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              |
| 2:2:205:ASN:ND2  | 2:2:206:SER:H    | 1.97                     | 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              |
| 2:2:155:ASP:C    | 2:2:155:ASP:OD1  | 2.37                     | 0.62              |
| 3:3:75:ARG:O     | 3:3:194:SER:HB2  | 1.99                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 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              |
| 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              |
| 1:1:58:MET:HE1   | 3:3:216:ASP:C    | 2.23                     | 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              |
| 2:2:11:ASP:H     | 4:4:68:ASN:CG    | 2.06                     | 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              |
| 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              |
| 2:2:64:TYR:CD1   | 2:2:89:MET:HB3   | 2.39                     | 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              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 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              |
| 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              |
| 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              |
| 2:2:77:GLY:O     | 2:2:156:LEU:HB2  | 2.07                     | 0.55              |
| 2:2:235:THR:HG22 | 2:2:236:PRO:N    | 2.22                     | 0.55              |
| 1:1:38:GLU:CD    | 3:3:116:MET:HE1  | 2.27                     | 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              |
| 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              |
| 1:1:151:MET:HE1  | 1:1:168:TRP:HA   | 1.90                     | 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              |
| 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              |
| 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              |
| 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              |
| 2:2:235: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              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 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              |
| 3:3:57:ASN:HB3   | 3:3:57:ASN:C     | 2.28                     | 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              |
| 1:1:236:LYS:NZ   | 1:1:238:LEU:HD11 | 2.25                     | 0.52              |
| 2:2:174:ASN:C    | 2:2:174:ASN:ND2  | 2.63                     | 0.52              |
| 3:3:216:ASP:O    | 3:3:218:LYS:HE3  | 2.09                     | 0.52              |
| 1:1:43:MET:HE3   | 1:1:43:MET:HA    | 1.92                     | 0.51              |
| 1:1:122:VAL:HG13 | 1:1:124:PHE:CE2  | 2.45                     | 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              |
| 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              |
| 4:4:44:SER:O     | 4:4:45:LEU:C     | 2.48                     | 0.51              |
| 1:1:153:VAL:HG12 | 1:1:157:ALA:HB3  | 1.91                     | 0.51              |
| 1:1:114:LYS:NZ   | 3:3:99:GLU:OE2   | 2.43                     | 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              |
| 1:1:65: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              |
| 1:1:58:MET:HE1   | 3:3:216:ASP:O    | 2.12                     | 0.50              |
| 1:1:58:MET:CE    | 3:3:216:ASP:O    | 2.60                     | 0.50              |
| 1:1:60:PHE:CD2   | 3:3:218:LYS:HB3  | 2.46                     | 0.50              |
| 1:1:208:ASP:C    | 2:2:261:PRO:HG2  | 2.32                     | 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              |
| 2:2:8:GLY:C      | 2:2:9:TYR:HD1    | 2.14                     | 0.50              |
| 1:1:151:MET:CE   | 1:1:167:THR:O    | 2.60                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 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              |
| 3:3:63:GLU:C     | 3:3:65:ASN:H     | 2.14                     | 0.49              |
| 2:2:205:ASN:HD22 | 2:2:206:SER:N    | 2.09                     | 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              |
| 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              |
| 1:1:273:LYS:O    | 1:1:274:ASN:C    | 2.52                     | 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              |
| 4:4:59:LEU:HG    | 4:4:60:MET:N     | 2.27                     | 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              |
| 1:1:174: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              |
| 4:4:29:ILE:O     | 4:4:29:ILE:CG2   | 2.62                     | 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              |
| 4:4:44:SER:C     | 4:4:46:SER:N     | 2.68                     | 0.47              |
| 2:2:195:ASN:ND2  | 2:2:195:ASN:C    | 2.66                     | 0.47              |
| 3:3:84:ASN:ND2   | 3:3:84:ASN:C     | 2.69                     | 0.46              |
| 1:1:74:ALA:HB3   | 3:3:15:THR:HB    | 1.97                     | 0.46              |
| 2:2:130:HIS:ND1  | 2:2:219:SER:OG   | 2.47                     | 0.46              |
| 1:1:92:ASN:C     | 1:1:92:ASN:ND2   | 2.67                     | 0.46              |
| 1:1:200:PHE:CE2  | 1:1:256:ARG:HD2  | 2.50                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:4:61:LEU:HD12  | 4:4:61:LEU:HA    | 1.63                     | 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              |
| 1:1:92:ASN:CG    | 1:1:95:GLU:HB2   | 2.36                     | 0.46              |
| 2:2:158:SER:HG   | 2:2:167:LYS:CE   | 2.26                     | 0.46              |
| 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              |
| 1:1:215:ILE:C    | 1:1:217:VAL:H    | 2.20                     | 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              |
| 4:4:30:ASN:HA    | 4:4:30:ASN:HD22  | 1.40                     | 0.45              |
| 3:3:84:ASN:HD22  | 3:3:84:ASN:C     | 2.20                     | 0.45              |
| 2:2:37:GLU:CD    | 3:3:35:HIS:HE2   | 2.19                     | 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              |
| 2:2:13:VAL:C     | 2:2:14:GLN:CG    | 2.85                     | 0.45              |
| 2:2:91:VAL:HG12  | 2:2:95:ASN:HD22  | 1.82                     | 0.45              |
| 2:2:235:THR:CG2  | 2:2:236:PRO:N    | 2.79                     | 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              |
| 1:1:77:VAL:C     | 1:1:109:LEU:CD2  | 2.86                     | 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              |
| 1:1:215:ILE:C    | 1:1:217:VAL:N    | 2.71                     | 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              |
| 3:3:55:MET:HE2   | 3:3:91:VAL:HG21  | 1.99                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:3:181:TYR:CD1  | 3:3:181:TYR:C    | 2.91                     | 0.44              |
| 1:1:47:PRO:HB3   | 3:3:166:PRO:HB3  | 1.99                     | 0.44              |
| 3:3:197:LEU:HD21 | 3:3:205:VAL:HG11 | 1.99                     | 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              |
| 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              |
| 3:3:57:ASN:HD21  | 3:3:91:VAL:HG13  | 1.83                     | 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              |
| 2:2:262:GLN:C    | 2:2:262:GLN:NE2  | 2.66                     | 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              |
| 1:1:110:VAL:HG13 | 3:3:230:GLN:CD   | 2.39                     | 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              |
| 3:3:195:LEU:C    | 3:3:196:ILE:HG12 | 2.40                     | 0.43              |
| 1:1:214:GLY:O    | 1:1:217:VAL:CG1  | 2.67                     | 0.42              |
| 1:1:146:LEU:HD13 | 1:1:228:ILE:CD1  | 2.50                     | 0.42              |
| 2:2:13:VAL:C     | 2:2:14:GLN:HG2   | 2.39                     | 0.42              |
| 1:1:151:MET:HE1  | 1:1:167:THR:O    | 2.19                     | 0.42              |
| 1:1:87:ALA:HB2   | 1:1:98:LEU:HD11  | 2.02                     | 0.42              |
| 2:2:10:SER:OG    | 4:4:68:ASN:OXT   | 2.35                     | 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              |
| 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              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:3:44:LEU:HA    | 3:3:44:LEU:HD23  | 1.79                     | 0.42              |
| 4:4:43:GLN:O     | 4:4:44:SER:C     | 2.58                     | 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              |
| 1:1:103:LYS:O    | 1:1:103:LYS:CG   | 2.67                     | 0.42              |
| 1:1:103:LYS:O    | 1:1:104:ILE:C    | 2.57                     | 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              |
| 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              |
| 3:3:18:ASP:CG    | 4:4:40:SER:HB2   | 2.41                     | 0.41              |
| 2:2:43:PRO:HG2   | 2:2:46:ASP:HB2   | 2.03                     | 0.41              |
| 3:3:64:VAL:HG12  | 3:3:64:VAL:O     | 2.21                     | 0.41              |
| 3:3:137:ARG:HH11 | 3:3:137:ARG:HD3  | 1.23                     | 0.41              |
| 1:1:38:GLU:CD    | 3:3:116:MET:CE   | 2.88                     | 0.41              |
| 1:1:54:ARG:HH11  | 1:1:54:ARG:HD2   | 1.55                     | 0.41              |
| 1:1:97:LYS:C     | 1:1:99:PHE:N     | 2.71                     | 0.41              |
| 1:1:169:GLN:O    | 1:1:170:SER:C    | 2.59                     | 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              |
| 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%)   | 5           | 27 |
| 2   | 2     | 253/262 (97%) | 234 (92%) | 17 (7%) | 2 (1%)   | 19          | 57 |
| 3   | 3     | 234/236 (99%) | 217 (93%) | 15 (6%) | 2 (1%)   | 17          | 55 |
| 4   | 4     | 38/68 (56%)   | 34 (90%)  | 3 (8%)  | 1 (3%)   | 5           | 27 |
| All | All   | 796/855 (93%) | 726 (91%) | 58 (7%) | 12 (2%)  | 10          | 42 |

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 [i](#)

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

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

| Mol | Chain | Analysed       | Rotameric | Outliers  | Percentiles |   |
|-----|-------|----------------|-----------|-----------|-------------|---|
| 1   | 1     | 239/253 (94%)  | 195 (82%) | 44 (18%)  | 1           | 9 |
| 2   | 2     | 223/229 (97%)  | 180 (81%) | 43 (19%)  | 1           | 8 |
| 3   | 3     | 209/209 (100%) | 171 (82%) | 38 (18%)  | 1           | 9 |
| 4   | 4     | 33/57 (58%)    | 20 (61%)  | 13 (39%)  | 0           | 0 |
| All | All   | 704/748 (94%)  | 566 (80%) | 138 (20%) | 1           | 7 |

All (138) 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     | 63  | SER  |
| 1   | 1     | 81  | GLU  |
| 1   | 1     | 90  | ILE  |
| 1   | 1     | 97  | LYS  |
| 1   | 1     | 100 | ASN  |
| 1   | 1     | 104 | ILE  |
| 1   | 1     | 107 | SER  |
| 1   | 1     | 108 | SER  |
| 1   | 1     | 109 | LEU  |
| 1   | 1     | 110 | VAL  |
| 1   | 1     | 122 | VAL  |
| 1   | 1     | 136 | GLN  |
| 1   | 1     | 137 | PRO  |
| 1   | 1     | 138 | ASP  |
| 1   | 1     | 139 | SER  |
| 1   | 1     | 144 | SER  |
| 1   | 1     | 145 | ASN  |
| 1   | 1     | 151 | MET  |
| 1   | 1     | 153 | VAL  |
| 1   | 1     | 161 | LYS  |
| 1   | 1     | 170 | SER  |
| 1   | 1     | 183 | THR  |
| 1   | 1     | 184 | SER  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | 1            | 185        | ARG         |
| 1          | 1            | 215        | ILE         |
| 1          | 1            | 216        | THR         |
| 1          | 1            | 220        | HIS         |
| 1          | 1            | 221        | MET         |
| 1          | 1            | 240        | LYS         |
| 1          | 1            | 256        | ARG         |
| 1          | 1            | 268        | ARG         |
| 1          | 1            | 274        | ASN         |
| 1          | 1            | 278        | VAL         |
| 1          | 1            | 287        | LYS         |
| 2          | 2            | 11         | ASP         |
| 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            | 88         | ASP         |
| 2          | 2            | 103        | ARG         |
| 2          | 2            | 116        | LYS         |
| 2          | 2            | 119        | SER         |
| 2          | 2            | 136        | GLU         |
| 2          | 2            | 141        | SER         |
| 2          | 2            | 145        | THR         |
| 2          | 2            | 152        | ARG         |
| 2          | 2            | 165        | PRO         |
| 2          | 2            | 168        | ASP         |
| 2          | 2            | 169        | VAL         |
| 2          | 2            | 174        | ASN         |
| 2          | 2            | 187        | GLN         |
| 2          | 2            | 192        | ARG         |
| 2          | 2            | 195        | ASN         |
| 2          | 2            | 205        | ASN         |
| 2          | 2            | 209        | ILE         |
| 2          | 2            | 211        | SER         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 2          | 2            | 217        | ASN         |
| 2          | 2            | 221        | MET         |
| 2          | 2            | 225        | ILE         |
| 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            | 262        | GLN         |
| 3          | 3            | 16         | THR         |
| 3          | 3            | 33         | ARG         |
| 3          | 3            | 46         | ILE         |
| 3          | 3            | 55         | MET         |
| 3          | 3            | 56         | ASN         |
| 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            | 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         |
| 3          | 3            | 196        | ILE         |
| 3          | 3            | 201        | THR         |
| 3          | 3            | 208        | LEU         |
| 3          | 3            | 211        | ILE         |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | 3     | 217 | PHE  |
| 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 (29) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1     | 61  | ASN  |
| 1   | 1     | 92  | ASN  |
| 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     | 131 | GLN  |
| 2   | 2     | 174 | ASN  |
| 2   | 2     | 187 | GLN  |
| 2   | 2     | 190 | ASN  |
| 2   | 2     | 195 | ASN  |
| 2   | 2     | 205 | ASN  |
| 2   | 2     | 216 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | 2     | 217 | ASN  |
| 2   | 2     | 262 | GLN  |
| 3   | 3     | 20  | GLN  |
| 3   | 3     | 41  | HIS  |
| 3   | 3     | 42  | ASN  |
| 3   | 3     | 56  | ASN  |
| 3   | 3     | 84  | ASN  |
| 3   | 3     | 102 | GLN  |
| 3   | 3     | 140 | GLN  |
| 3   | 3     | 192 | GLN  |
| 3   | 3     | 226 | GLN  |
| 4   | 4     | 30  | ASN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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 | -    | 22,25,25     | 3.18 | 5 (22%)  | 29,34,34    | 2.70 | 7 (24%)  |

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 | -    | -       | 1/10/18/18 | 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 | 11.99 | 1.43        | 1.27     |
| 5   | 1     | 700 | W91  | C4A-N3A | -6.42 | 1.36        | 1.47     |
| 5   | 1     | 700 | W91  | C4-C5   | -3.24 | 1.35        | 1.39     |
| 5   | 1     | 700 | W91  | O1A-C5A | -3.03 | 1.38        | 1.46     |
| 5   | 1     | 700 | W91  | O1A-C2A | -2.82 | 1.31        | 1.36     |

All (7) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 5   | 1     | 700 | W91  | O1A-C2A-N3A | -9.55 | 110.02      | 118.23   |
| 5   | 1     | 700 | W91  | C4A-N3A-C2A | 6.30  | 112.40      | 106.77   |
| 5   | 1     | 700 | W91  | O1A-C2A-C4B | 5.83  | 123.57      | 115.85   |
| 5   | 1     | 700 | W91  | O1A-C5A-C4A | 3.74  | 111.89      | 104.28   |
| 5   | 1     | 700 | W91  | C1C-C5-C4   | 2.58  | 135.28      | 128.60   |
| 5   | 1     | 700 | W91  | C3C-O1B-C1B | 2.55  | 121.95      | 114.23   |
| 5   | 1     | 700 | W91  | C5A-C4A-N3A | -2.06 | 99.44       | 104.35   |

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 |

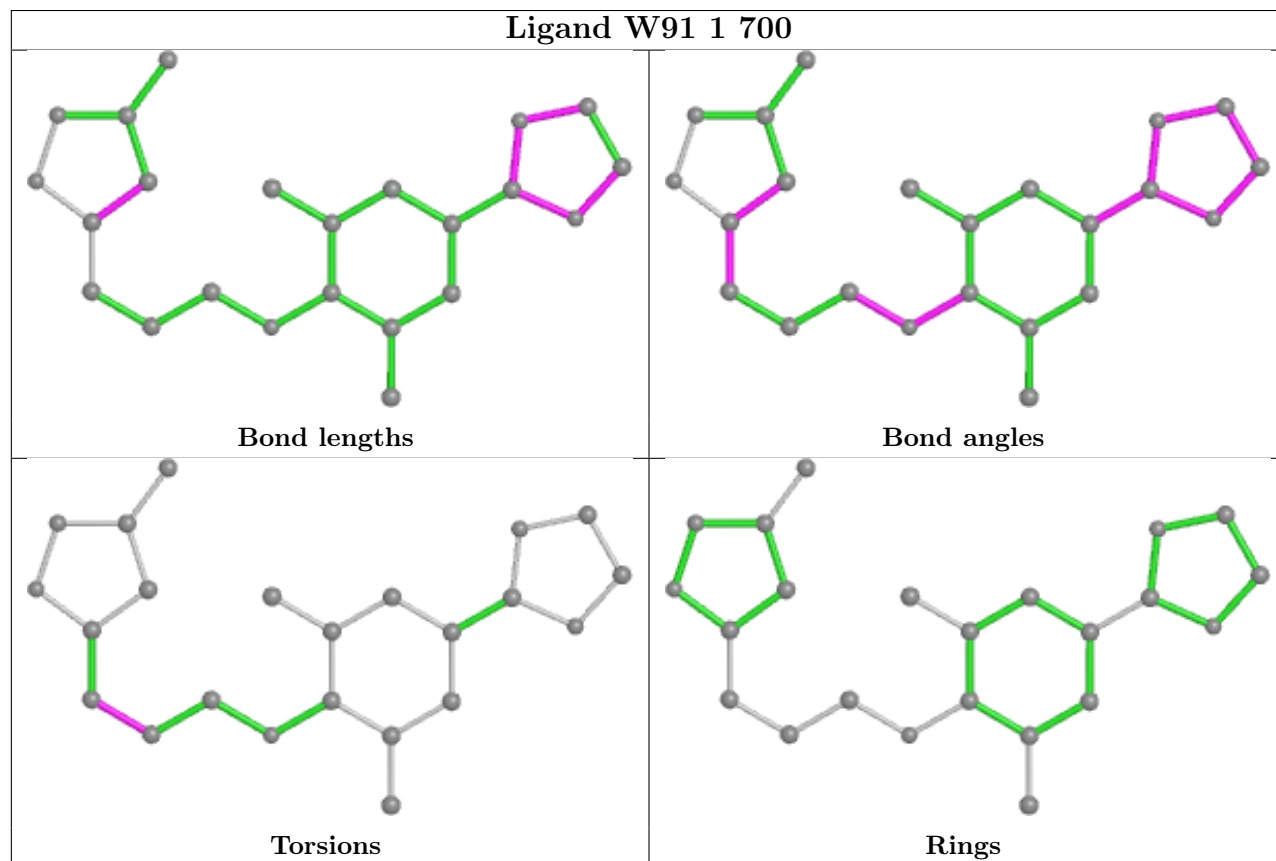
There are no ring outliers.

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 [i](#)

There are no such residues in this entry.

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

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.