



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 01:03 PM EDT

PDB ID : 3KBP / pdb\_00003kbp  
Title : KIDNEY BEAN PURPLE ACID PHOSPHATASE  
Authors : Klabunde, T.; Strater, N.; Krebs, B.  
Deposited on : 1995-10-02  
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                     |
| Xtriage (Phenix)               | : | NOT EXECUTED                                                     |
| EDS                            | : | NOT EXECUTED                                                     |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.50                                                             |

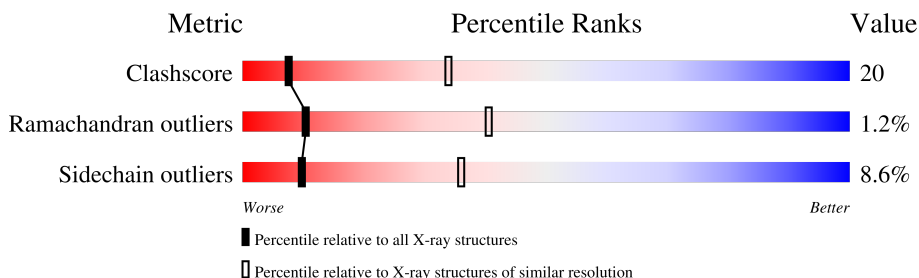
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

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



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

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

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 432    |                  |
| 1   | B     | 432    |                  |
| 1   | C     | 432    |                  |
| 1   | D     | 432    |                  |

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14284 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 PURPLE ACID PHOSPHATASE.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 424      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3494  | 2243 | 605 | 636 | 10 |         |         |       |
| 1   | B     | 424      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3494  | 2243 | 605 | 636 | 10 |         |         |       |
| 1   | C     | 424      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3494  | 2243 | 605 | 636 | 10 |         |         |       |
| 1   | D     | 424      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3494  | 2243 | 605 | 636 | 10 |         |         |       |

There are 8 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| A     | 253     | TYR      | HIS    | conflict | UNP P80366 |
| A     | 254     | SER      | ILE    | conflict | UNP P80366 |
| B     | 253     | TYR      | HIS    | conflict | UNP P80366 |
| B     | 254     | SER      | ILE    | conflict | UNP P80366 |
| C     | 253     | TYR      | HIS    | conflict | UNP P80366 |
| C     | 254     | SER      | ILE    | conflict | UNP P80366 |
| D     | 253     | TYR      | HIS    | conflict | UNP P80366 |
| D     | 254     | SER      | ILE    | conflict | UNP P80366 |

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



| Mol | Chain | Residues | Atoms |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 2   | A     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 2   | A     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 2   | A     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 2   | A     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 2   | B     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 2   | B     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 2   | B     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 2   | B     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 2   | C     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 2   | C     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 2   | C     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |

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| Mol | Chain | Residues | Atoms |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 2   | C     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 2   | D     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 2   | D     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 2   | D     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 2   | D     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |

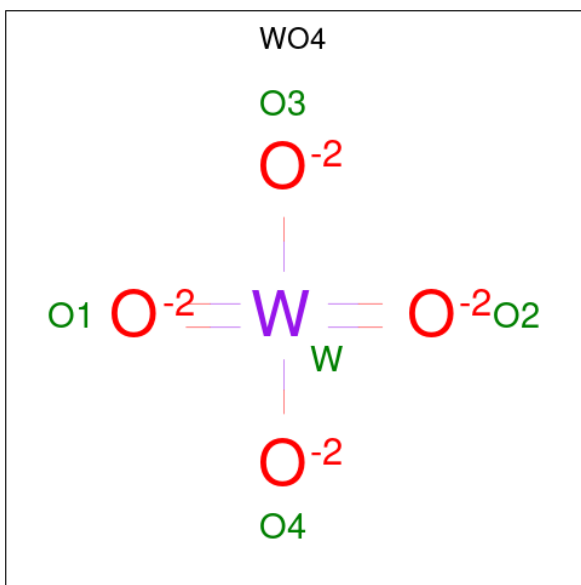
- Molecule 3 is FE (III) ION (CCD ID: FE) (formula: Fe).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 3   | A     | 1        | Total | Fe | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 3   | B     | 1        | Total | Fe | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 3   | C     | 1        | Total | Fe | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 3   | D     | 1        | Total | Fe | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 4   | A     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 4   | B     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 4   | C     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 4   | D     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 5 is TUNGSTATE(VI)ION (CCD ID: WO4) (formula: O<sub>4</sub>W).



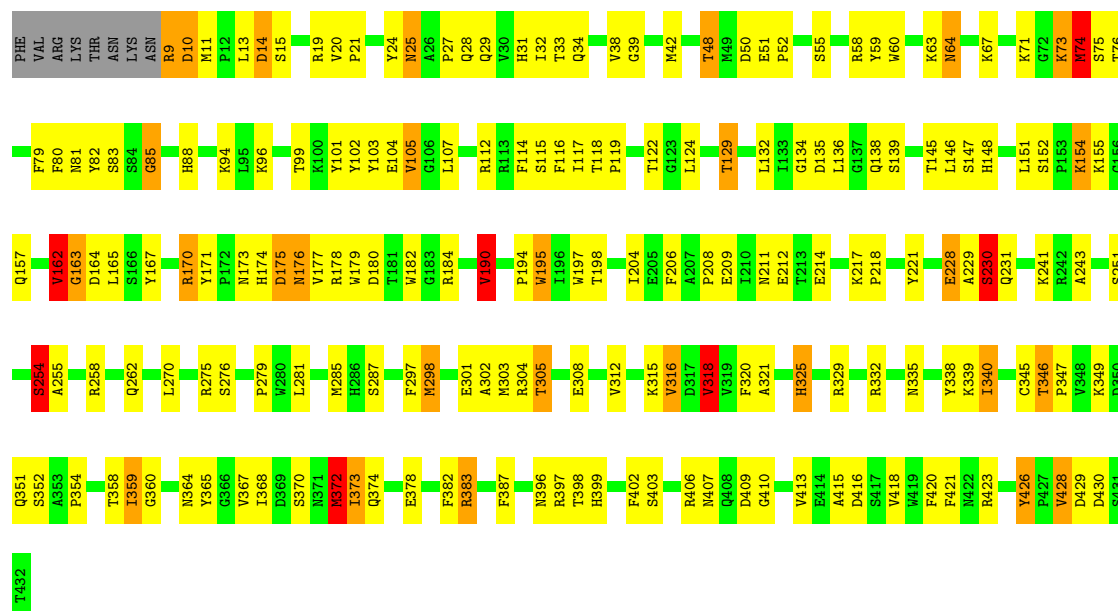
| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 5   | A     | 1        | Total | O | W | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 5   | B     | 1        | Total | O | W | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 5   | C     | 1        | Total | O | W | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 5   | D     | 1        | Total | O | W | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |





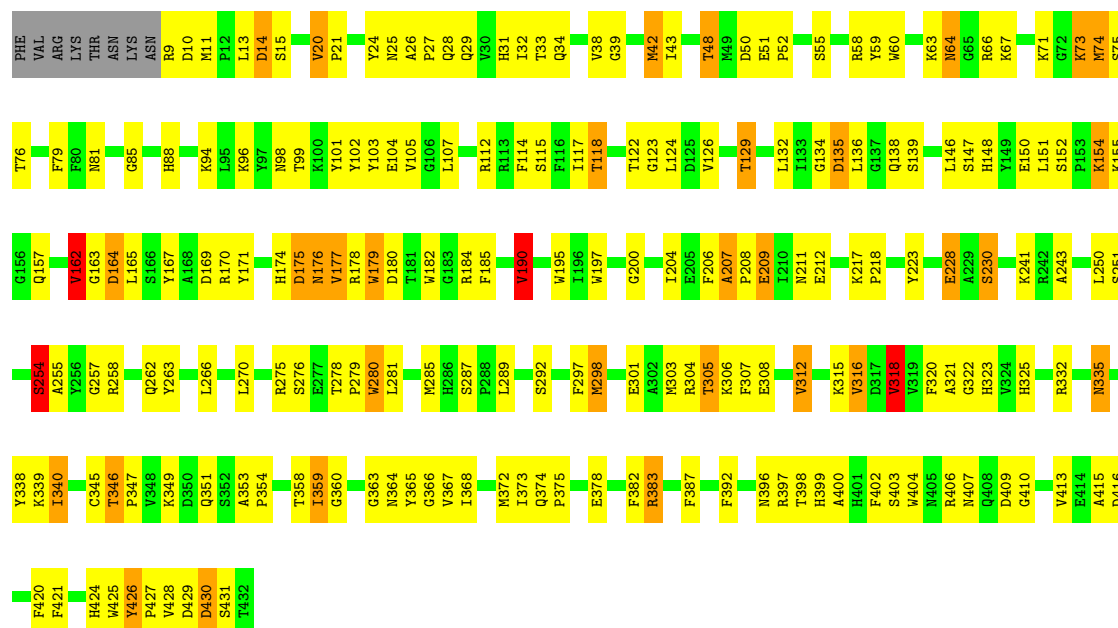
• Molecule 1: PURPLE ACID PHOSPHATASE

Chain C: 54% 36% 6% ..



• Molecule 1: PURPLE ACID PHOSPHATASE

Chain D: 50% 40% 7% ..



## 4 Data and refinement statistics

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

| Property                                                 | Value                                           | Source    |
|----------------------------------------------------------|-------------------------------------------------|-----------|
| Space group                                              | C 2 2 21                                        | Depositor |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$ | 132.70Å 347.30Å 128.70Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å)                                           | 10.00 – 3.00                                    | Depositor |
| % Data completeness<br>(in resolution range)             | 69.1 (10.00-3.00)                               | Depositor |
| $R_{merge}$                                              | 0.08                                            | Depositor |
| $R_{sym}$                                                | (Not available)                                 | Depositor |
| Refinement program                                       | X-PLOR 3.1                                      | Depositor |
| R, $R_{free}$                                            | 0.189 , 0.220                                   | Depositor |
| Estimated twinning fraction                              | No twinning to report.                          | Xtriage   |
| Total number of atoms                                    | 14284                                           | wwPDB-VP  |
| Average B, all atoms (Å <sup>2</sup> )                   | 35.0                                            | 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: NAG, FE, ZN, WO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths |                 | Bond angles |                  |
|-----|-------|--------------|-----------------|-------------|------------------|
|     |       | RMSZ         | $\# Z  > 5$     | RMSZ        | $\# Z  > 5$      |
| 1   | A     | 1.10         | 8/3613 (0.2%)   | 1.34        | 41/4912 (0.8%)   |
| 1   | B     | 1.00         | 2/3613 (0.1%)   | 1.31        | 38/4912 (0.8%)   |
| 1   | C     | 1.04         | 2/3613 (0.1%)   | 1.30        | 45/4912 (0.9%)   |
| 1   | D     | 1.06         | 2/3613 (0.1%)   | 1.31        | 46/4912 (0.9%)   |
| All | All   | 1.05         | 14/14452 (0.1%) | 1.32        | 170/19648 (0.9%) |

All (14) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | A     | 74  | MET  | SD-CE | -8.45 | 1.58        | 1.79     |
| 1   | A     | 43  | ILE  | CA-CB | -7.21 | 1.45        | 1.54     |
| 1   | A     | 92  | ILE  | CA-CB | -6.34 | 1.46        | 1.54     |
| 1   | C     | 74  | MET  | SD-CE | -6.25 | 1.64        | 1.79     |
| 1   | B     | 210 | ILE  | CA-CB | -5.72 | 1.47        | 1.54     |
| 1   | B     | 74  | MET  | SD-CE | -5.58 | 1.65        | 1.79     |
| 1   | A     | 337 | ALA  | CA-CB | -5.38 | 1.46        | 1.54     |
| 1   | D     | 118 | THR  | CA-CB | -5.31 | 1.45        | 1.53     |
| 1   | A     | 132 | LEU  | CA-C  | -5.28 | 1.46        | 1.52     |
| 1   | A     | 226 | PRO  | CA-C  | -5.20 | 1.48        | 1.53     |
| 1   | A     | 87  | ILE  | CA-CB | -5.19 | 1.47        | 1.54     |
| 1   | A     | 373 | ILE  | CA-CB | -5.11 | 1.47        | 1.53     |
| 1   | C     | 373 | ILE  | CA-CB | -5.11 | 1.48        | 1.54     |
| 1   | D     | 42  | MET  | SD-CE | -5.10 | 1.66        | 1.79     |

All (170) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 1   | A     | 154 | LYS  | N-CA-C | -11.38 | 92.86       | 109.59   |
| 1   | D     | 154 | LYS  | N-CA-C | -11.05 | 93.34       | 109.59   |
| 1   | B     | 230 | SER  | N-CA-C | -10.49 | 93.43       | 109.79   |

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| Mol | Chain | Res | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 1   | C     | 154 | LYS  | N-CA-C | -10.35 | 94.38       | 109.59   |
| 1   | B     | 154 | LYS  | N-CA-C | -10.15 | 94.54       | 109.15   |
| 1   | A     | 230 | SER  | N-CA-C | -9.92  | 94.32       | 109.79   |
| 1   | D     | 230 | SER  | N-CA-C | -9.70  | 94.66       | 109.79   |
| 1   | B     | 163 | GLY  | N-CA-C | 9.69   | 121.16      | 111.95   |
| 1   | A     | 230 | SER  | CA-C-N | -9.56  | 108.93      | 123.17   |
| 1   | A     | 230 | SER  | C-N-CA | -9.56  | 108.93      | 123.17   |
| 1   | B     | 38  | VAL  | N-CA-C | 9.48   | 121.16      | 112.43   |
| 1   | D     | 230 | SER  | CA-C-N | -9.48  | 109.05      | 123.17   |
| 1   | D     | 230 | SER  | C-N-CA | -9.48  | 109.05      | 123.17   |
| 1   | A     | 163 | GLY  | N-CA-C | 9.27   | 120.75      | 111.95   |
| 1   | B     | 230 | SER  | CA-C-N | -9.16  | 109.52      | 123.17   |
| 1   | B     | 230 | SER  | C-N-CA | -9.16  | 109.52      | 123.17   |
| 1   | D     | 426 | TYR  | CA-C-N | 8.87   | 130.92      | 119.84   |
| 1   | D     | 426 | TYR  | C-N-CA | 8.87   | 130.92      | 119.84   |
| 1   | C     | 230 | SER  | CA-C-N | -8.71  | 110.19      | 123.17   |
| 1   | C     | 230 | SER  | C-N-CA | -8.71  | 110.19      | 123.17   |
| 1   | C     | 38  | VAL  | N-CA-C | 8.33   | 120.10      | 112.43   |
| 1   | C     | 230 | SER  | N-CA-C | -8.09  | 93.57       | 110.80   |
| 1   | B     | 85  | GLY  | N-CA-C | -8.00  | 98.48       | 112.55   |
| 1   | A     | 21  | PRO  | CA-C-N | 7.95   | 127.88      | 119.85   |
| 1   | A     | 21  | PRO  | C-N-CA | 7.95   | 127.88      | 119.85   |
| 1   | C     | 81  | ASN  | N-CA-C | -7.69  | 103.95      | 112.72   |
| 1   | B     | 81  | ASN  | N-CA-C | -7.66  | 103.99      | 112.72   |
| 1   | D     | 163 | GLY  | N-CA-C | 7.65   | 119.22      | 111.95   |
| 1   | C     | 163 | GLY  | N-CA-C | 7.50   | 120.69      | 112.29   |
| 1   | C     | 107 | LEU  | N-CA-C | 7.36   | 119.30      | 111.28   |
| 1   | D     | 85  | GLY  | N-CA-C | -7.30  | 99.70       | 112.55   |
| 1   | D     | 81  | ASN  | N-CA-C | -7.26  | 104.44      | 112.72   |
| 1   | D     | 38  | VAL  | N-CA-C | 7.04   | 119.93      | 113.10   |
| 1   | A     | 254 | SER  | N-CA-C | -7.04  | 98.89       | 109.94   |
| 1   | C     | 332 | ARG  | N-CA-C | -6.96  | 99.36       | 109.59   |
| 1   | D     | 410 | GLY  | N-CA-C | -6.94  | 101.99      | 113.02   |
| 1   | C     | 254 | SER  | N-CA-C | -6.92  | 99.07       | 109.94   |
| 1   | C     | 21  | PRO  | CA-C-N | 6.83   | 126.75      | 119.85   |
| 1   | C     | 21  | PRO  | C-N-CA | 6.83   | 126.75      | 119.85   |
| 1   | C     | 136 | LEU  | N-CA-C | 6.82   | 118.40      | 110.97   |
| 1   | D     | 21  | PRO  | CA-C-N | 6.81   | 126.57      | 119.76   |
| 1   | D     | 21  | PRO  | C-N-CA | 6.81   | 126.57      | 119.76   |
| 1   | B     | 346 | THR  | CA-C-N | 6.78   | 127.19      | 119.93   |
| 1   | B     | 346 | THR  | C-N-CA | 6.78   | 127.19      | 119.93   |
| 1   | A     | 136 | LEU  | N-CA-C | 6.78   | 118.36      | 110.97   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 332 | ARG  | N-CA-C  | -6.77 | 99.40       | 109.15   |
| 1   | B     | 21  | PRO  | CA-C-N  | 6.76  | 126.67      | 119.85   |
| 1   | B     | 21  | PRO  | C-N-CA  | 6.76  | 126.67      | 119.85   |
| 1   | A     | 81  | ASN  | N-CA-C  | -6.73 | 105.05      | 112.72   |
| 1   | B     | 197 | TRP  | N-CA-C  | 6.72  | 121.26      | 109.96   |
| 1   | B     | 332 | ARG  | N-CA-C  | -6.72 | 99.48       | 109.15   |
| 1   | A     | 287 | SER  | CA-C-N  | 6.71  | 126.47      | 119.76   |
| 1   | A     | 287 | SER  | C-N-CA  | 6.71  | 126.47      | 119.76   |
| 1   | C     | 287 | SER  | CA-C-N  | 6.70  | 127.70      | 120.13   |
| 1   | C     | 287 | SER  | C-N-CA  | 6.70  | 127.70      | 120.13   |
| 1   | D     | 287 | SER  | CA-C-N  | 6.63  | 127.15      | 119.99   |
| 1   | D     | 287 | SER  | C-N-CA  | 6.63  | 127.15      | 119.99   |
| 1   | B     | 254 | SER  | N-CA-C  | -6.62 | 99.55       | 109.94   |
| 1   | D     | 430 | ASP  | N-CA-C  | -6.60 | 105.36      | 113.41   |
| 1   | A     | 410 | GLY  | N-CA-C  | -6.59 | 103.72      | 112.82   |
| 1   | D     | 332 | ARG  | N-CA-C  | -6.58 | 99.67       | 109.15   |
| 1   | C     | 170 | ARG  | N-CA-C  | -6.54 | 104.33      | 112.90   |
| 1   | A     | 346 | THR  | CA-C-N  | 6.54  | 126.92      | 119.93   |
| 1   | A     | 346 | THR  | C-N-CA  | 6.54  | 126.92      | 119.93   |
| 1   | B     | 190 | VAL  | N-CA-C  | 6.53  | 121.29      | 111.89   |
| 1   | B     | 287 | SER  | CA-C-N  | 6.52  | 127.03      | 119.99   |
| 1   | B     | 287 | SER  | C-N-CA  | 6.52  | 127.03      | 119.99   |
| 1   | A     | 204 | ILE  | CB-CA-C | -6.49 | 103.57      | 111.88   |
| 1   | A     | 197 | TRP  | N-CA-C  | 6.44  | 120.79      | 109.96   |
| 1   | C     | 85  | GLY  | N-CA-C  | -6.42 | 101.59      | 112.77   |
| 1   | D     | 197 | TRP  | N-CA-C  | 6.39  | 120.70      | 109.96   |
| 1   | A     | 85  | GLY  | N-CA-C  | -6.39 | 101.31      | 112.55   |
| 1   | C     | 241 | LYS  | N-CA-C  | -6.37 | 99.34       | 109.59   |
| 1   | C     | 397 | ARG  | N-CA-C  | -6.36 | 105.28      | 113.16   |
| 1   | D     | 136 | LEU  | N-CA-C  | 6.35  | 117.89      | 110.97   |
| 1   | D     | 241 | LYS  | N-CA-C  | -6.30 | 99.45       | 109.59   |
| 1   | B     | 13  | LEU  | N-CA-C  | 6.24  | 118.88      | 111.71   |
| 1   | D     | 204 | ILE  | CB-CA-C | -6.23 | 103.90      | 111.88   |
| 1   | A     | 190 | VAL  | N-CA-C  | 6.22  | 120.84      | 111.89   |
| 1   | B     | 136 | LEU  | N-CA-C  | 6.21  | 117.73      | 110.97   |
| 1   | D     | 312 | VAL  | N-CA-C  | -6.20 | 104.59      | 110.42   |
| 1   | A     | 331 | GLU  | N-CA-C  | -6.18 | 101.37      | 110.52   |
| 1   | C     | 346 | THR  | CA-C-N  | 6.13  | 126.49      | 119.93   |
| 1   | C     | 346 | THR  | C-N-CA  | 6.13  | 126.49      | 119.93   |
| 1   | C     | 197 | TRP  | N-CA-C  | 6.13  | 120.25      | 109.96   |
| 1   | B     | 241 | LYS  | N-CA-C  | -6.05 | 99.84       | 109.59   |
| 1   | A     | 38  | VAL  | N-CA-C  | 6.03  | 118.94      | 113.10   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | D     | 254 | SER  | N-CA-C  | -6.02 | 100.49      | 109.94   |
| 1   | C     | 204 | ILE  | CB-CA-C | -6.01 | 104.19      | 111.88   |
| 1   | C     | 426 | TYR  | CA-C-N  | 6.00  | 127.34      | 119.84   |
| 1   | C     | 426 | TYR  | C-N-CA  | 6.00  | 127.34      | 119.84   |
| 1   | D     | 318 | VAL  | CB-CA-C | -5.98 | 102.99      | 111.19   |
| 1   | B     | 204 | ILE  | CB-CA-C | -5.95 | 104.26      | 111.88   |
| 1   | B     | 20  | VAL  | N-CA-C  | 5.95  | 113.76      | 107.76   |
| 1   | A     | 353 | ALA  | CA-C-N  | 5.94  | 126.40      | 120.52   |
| 1   | A     | 353 | ALA  | C-N-CA  | 5.94  | 126.40      | 120.52   |
| 1   | A     | 298 | MET  | N-CA-C  | 5.89  | 120.42      | 113.23   |
| 1   | D     | 162 | VAL  | N-CA-C  | 5.86  | 121.52      | 109.34   |
| 1   | A     | 20  | VAL  | N-CA-C  | 5.82  | 113.64      | 107.76   |
| 1   | B     | 410 | GLY  | N-CA-C  | -5.82 | 103.77      | 113.02   |
| 1   | A     | 318 | VAL  | CB-CA-C | -5.79 | 101.74      | 110.55   |
| 1   | B     | 163 | GLY  | CA-C-O  | -5.79 | 118.46      | 122.22   |
| 1   | D     | 39  | GLY  | N-CA-C  | 5.79  | 122.67      | 114.85   |
| 1   | C     | 39  | GLY  | N-CA-C  | 5.79  | 122.66      | 114.85   |
| 1   | A     | 39  | GLY  | N-CA-C  | 5.77  | 122.64      | 114.85   |
| 1   | D     | 190 | VAL  | N-CA-C  | 5.75  | 121.30      | 109.34   |
| 1   | B     | 373 | ILE  | N-CA-C  | -5.73 | 100.33      | 108.58   |
| 1   | D     | 346 | THR  | CA-C-N  | 5.73  | 126.06      | 119.93   |
| 1   | D     | 346 | THR  | C-N-CA  | 5.73  | 126.06      | 119.93   |
| 1   | D     | 322 | GLY  | N-CA-C  | -5.69 | 99.69       | 113.18   |
| 1   | C     | 173 | ASN  | N-CA-C  | -5.68 | 104.97      | 112.24   |
| 1   | D     | 48  | THR  | N-CA-C  | -5.67 | 100.15      | 109.40   |
| 1   | D     | 397 | ARG  | N-CA-C  | -5.62 | 106.19      | 113.16   |
| 1   | B     | 322 | GLY  | N-CA-C  | -5.62 | 99.86       | 113.18   |
| 1   | B     | 214 | GLU  | CA-C-N  | 5.62  | 125.63      | 119.90   |
| 1   | B     | 214 | GLU  | C-N-CA  | 5.62  | 125.63      | 119.90   |
| 1   | C     | 410 | GLY  | N-CA-C  | -5.61 | 105.08      | 112.82   |
| 1   | C     | 335 | ASN  | N-CA-C  | -5.60 | 98.87       | 110.80   |
| 1   | A     | 207 | ALA  | CA-C-N  | 5.59  | 125.70      | 119.32   |
| 1   | A     | 207 | ALA  | C-N-CA  | 5.59  | 125.70      | 119.32   |
| 1   | B     | 78  | ARG  | N-CA-C  | -5.58 | 100.30      | 109.40   |
| 1   | B     | 177 | VAL  | N-CA-C  | -5.58 | 104.93      | 110.62   |
| 1   | B     | 39  | GLY  | N-CA-C  | 5.58  | 122.45      | 114.64   |
| 1   | D     | 280 | TRP  | N-CA-C  | 5.57  | 117.37      | 108.41   |
| 1   | A     | 307 | PHE  | N-CA-C  | 5.56  | 120.95      | 113.72   |
| 1   | C     | 214 | GLU  | CA-C-N  | 5.54  | 125.56      | 119.90   |
| 1   | C     | 214 | GLU  | C-N-CA  | 5.54  | 125.56      | 119.90   |
| 1   | A     | 170 | ARG  | N-CA-C  | -5.53 | 105.66      | 112.90   |
| 1   | D     | 20  | VAL  | N-CA-C  | 5.52  | 113.34      | 107.76   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | C     | 190 | VAL  | N-CA-C  | 5.46  | 119.75      | 111.89   |
| 1   | D     | 179 | TRP  | N-CA-C  | -5.44 | 105.00      | 111.69   |
| 1   | A     | 177 | VAL  | N-CA-C  | -5.40 | 105.11      | 110.62   |
| 1   | C     | 135 | ASP  | N-CA-CB | -5.39 | 103.98      | 112.13   |
| 1   | D     | 298 | MET  | N-CA-C  | 5.39  | 119.81      | 113.23   |
| 1   | B     | 280 | TRP  | N-CA-C  | 5.37  | 117.50      | 108.96   |
| 1   | B     | 335 | ASN  | N-CA-C  | -5.34 | 99.43       | 110.80   |
| 1   | A     | 241 | LYS  | N-CA-C  | -5.34 | 101.00      | 109.59   |
| 1   | C     | 195 | TRP  | N-CA-C  | -5.32 | 99.76       | 108.76   |
| 1   | D     | 353 | ALA  | CA-C-N  | 5.32  | 125.52      | 120.31   |
| 1   | D     | 353 | ALA  | C-N-CA  | 5.32  | 125.52      | 120.31   |
| 1   | C     | 298 | MET  | N-CA-C  | 5.31  | 119.71      | 113.23   |
| 1   | D     | 13  | LEU  | N-CA-C  | 5.27  | 117.77      | 111.71   |
| 1   | A     | 425 | TRP  | CA-C-N  | -5.26 | 117.47      | 122.37   |
| 1   | A     | 425 | TRP  | C-N-CA  | -5.26 | 117.47      | 122.37   |
| 1   | C     | 162 | VAL  | N-CA-C  | 5.26  | 120.27      | 109.34   |
| 1   | A     | 109 | ASN  | CA-C-N  | -5.25 | 115.65      | 123.11   |
| 1   | A     | 109 | ASN  | C-N-CA  | -5.25 | 115.65      | 123.11   |
| 1   | B     | 48  | THR  | N-CA-C  | -5.25 | 100.85      | 109.40   |
| 1   | C     | 352 | SER  | N-CA-C  | -5.24 | 106.93      | 113.38   |
| 1   | B     | 397 | ARG  | N-CA-C  | -5.24 | 106.84      | 113.18   |
| 1   | D     | 307 | PHE  | N-CA-C  | 5.23  | 120.52      | 113.72   |
| 1   | A     | 160 | LEU  | N-CA-C  | -5.21 | 100.67      | 108.96   |
| 1   | A     | 317 | ASP  | N-CA-C  | 5.21  | 116.81      | 111.03   |
| 1   | D     | 107 | LEU  | N-CA-C  | 5.20  | 117.69      | 111.71   |
| 1   | B     | 298 | MET  | N-CA-C  | 5.19  | 119.57      | 113.23   |
| 1   | D     | 207 | ALA  | CA-C-N  | 5.19  | 125.23      | 119.32   |
| 1   | D     | 207 | ALA  | C-N-CA  | 5.19  | 125.23      | 119.32   |
| 1   | C     | 318 | VAL  | CB-CA-C | -5.17 | 102.69      | 110.55   |
| 1   | B     | 162 | VAL  | N-CA-C  | 5.17  | 120.09      | 109.34   |
| 1   | D     | 135 | ASP  | N-CA-CB | -5.16 | 104.34      | 112.13   |
| 1   | D     | 335 | ASN  | N-CA-C  | -5.15 | 99.83       | 110.80   |
| 1   | C     | 80  | PHE  | N-CA-C  | -5.15 | 99.83       | 110.80   |
| 1   | C     | 372 | MET  | N-CA-C  | 5.14  | 117.69      | 110.14   |
| 1   | C     | 19  | ARG  | N-CA-C  | 5.10  | 117.63      | 110.23   |
| 1   | D     | 177 | VAL  | N-CA-C  | -5.08 | 105.44      | 110.62   |
| 1   | A     | 135 | ASP  | N-CA-CB | -5.07 | 104.51      | 112.46   |
| 1   | C     | 13  | LEU  | N-CA-C  | 5.06  | 116.79      | 111.28   |
| 1   | C     | 11  | MET  | CA-C-N  | 5.03  | 125.75      | 120.11   |
| 1   | C     | 11  | MET  | C-N-CA  | 5.03  | 125.75      | 120.11   |
| 1   | C     | 48  | THR  | N-CA-C  | -5.01 | 101.24      | 109.40   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 3494  | 0        | 3307     | 126     | 0            |
| 1   | B     | 3494  | 0        | 3306     | 150     | 0            |
| 1   | C     | 3494  | 0        | 3306     | 139     | 0            |
| 1   | D     | 3494  | 0        | 3307     | 151     | 0            |
| 2   | A     | 70    | 0        | 65       | 2       | 0            |
| 2   | B     | 70    | 0        | 65       | 2       | 0            |
| 2   | C     | 70    | 0        | 65       | 2       | 0            |
| 2   | D     | 70    | 0        | 65       | 1       | 0            |
| 3   | A     | 1     | 0        | 0        | 0       | 0            |
| 3   | B     | 1     | 0        | 0        | 0       | 0            |
| 3   | C     | 1     | 0        | 0        | 0       | 0            |
| 3   | D     | 1     | 0        | 0        | 0       | 0            |
| 4   | A     | 1     | 0        | 0        | 0       | 0            |
| 4   | B     | 1     | 0        | 0        | 0       | 0            |
| 4   | C     | 1     | 0        | 0        | 0       | 0            |
| 4   | D     | 1     | 0        | 0        | 0       | 0            |
| 5   | A     | 5     | 0        | 0        | 0       | 0            |
| 5   | B     | 5     | 0        | 0        | 0       | 0            |
| 5   | C     | 5     | 0        | 0        | 0       | 0            |
| 5   | D     | 5     | 0        | 0        | 1       | 0            |
| All | All   | 14284 | 0        | 13486    | 561     | 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 20.

All (561) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1          | Atom-2         | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|----------------|--------------------------|-------------------|
| 1:B:63:LYS:HZ3  | 1:B:64:ASN:HB3 | 1.28                     | 0.94              |
| 1:D:63:LYS:HZ3  | 1:D:64:ASN:HB3 | 1.38                     | 0.88              |
| 1:C:55:SER:H    | 1:C:71:LYS:HZ3 | 1.25                     | 0.84              |
| 1:D:374:GLN:NE2 | 1:D:375:PRO:HA | 1.92                     | 0.83              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:398:THR:HG22 | 1:D:426:TYR:HB2  | 1.58                     | 0.83              |
| 1:A:63:LYS:HZ3   | 1:A:64:ASN:HB3   | 1.47                     | 0.80              |
| 1:A:55:SER:H     | 1:A:71:LYS:HZ3   | 1.29                     | 0.79              |
| 1:A:134:GLY:HA3  | 1:A:162:VAL:HG12 | 1.63                     | 0.79              |
| 1:C:134:GLY:HA3  | 1:C:162:VAL:HG12 | 1.63                     | 0.79              |
| 1:D:421:PHE:CD2  | 1:D:428:VAL:HG23 | 2.17                     | 0.78              |
| 1:C:63:LYS:HZ3   | 1:C:64:ASN:HB3   | 1.49                     | 0.78              |
| 1:A:338:TYR:CZ   | 1:A:340:ILE:HA   | 2.20                     | 0.76              |
| 1:B:63:LYS:NZ    | 1:B:64:ASN:HB3   | 1.99                     | 0.76              |
| 1:B:325:HIS:HA   | 1:B:360:GLY:O    | 1.85                     | 0.75              |
| 1:C:398:THR:HG22 | 1:C:426:TYR:HB2  | 1.68                     | 0.75              |
| 1:D:374:GLN:HE21 | 1:D:375:PRO:HA   | 1.50                     | 0.75              |
| 1:B:338:TYR:CZ   | 1:B:340:ILE:HA   | 2.21                     | 0.75              |
| 1:B:10:ASP:HA    | 1:B:139:SER:HA   | 1.68                     | 0.75              |
| 1:B:372:MET:HE2  | 1:B:383:ARG:HD3  | 1.67                     | 0.74              |
| 1:C:9:ARG:HH11   | 1:C:9:ARG:HG2    | 1.51                     | 0.74              |
| 1:C:63:LYS:NZ    | 1:C:64:ASN:HB3   | 2.03                     | 0.74              |
| 1:D:134:GLY:HA3  | 1:D:162:VAL:HG12 | 1.69                     | 0.74              |
| 1:D:426:TYR:N    | 1:D:427:PRO:HD3  | 2.00                     | 0.74              |
| 1:A:301:GLU:O    | 1:A:305:THR:HG23 | 1.87                     | 0.73              |
| 1:B:285:MET:SD   | 1:B:303:MET:HE3  | 2.27                     | 0.73              |
| 1:D:74:MET:CE    | 1:D:76:THR:HG23  | 2.17                     | 0.73              |
| 1:D:338:TYR:CZ   | 1:D:340:ILE:HA   | 2.23                     | 0.73              |
| 1:B:33:THR:HG22  | 1:B:34:GLN:H     | 1.54                     | 0.73              |
| 1:D:409:ASP:HB3  | 1:D:413:VAL:HB   | 1.69                     | 0.73              |
| 1:B:74:MET:CE    | 1:B:76:THR:HG23  | 2.19                     | 0.72              |
| 1:B:138:GLN:NE2  | 1:B:178:ARG:HH11 | 1.88                     | 0.72              |
| 1:A:74:MET:CE    | 1:A:76:THR:HG23  | 2.20                     | 0.71              |
| 1:D:63:LYS:NZ    | 1:D:64:ASN:HB3   | 2.04                     | 0.71              |
| 1:C:325:HIS:HA   | 1:C:360:GLY:O    | 1.91                     | 0.71              |
| 1:B:134:GLY:HA3  | 1:B:162:VAL:HG12 | 1.72                     | 0.71              |
| 1:C:338:TYR:CZ   | 1:C:340:ILE:HA   | 2.25                     | 0.70              |
| 1:C:73:LYS:HD3   | 1:C:74:MET:N     | 2.06                     | 0.70              |
| 1:D:138:GLN:NE2  | 1:D:178:ARG:HH11 | 1.90                     | 0.69              |
| 1:C:421:PHE:CD2  | 1:C:428:VAL:HG22 | 2.27                     | 0.69              |
| 1:B:409:ASP:HB3  | 1:B:413:VAL:HB   | 1.74                     | 0.69              |
| 1:A:63:LYS:NZ    | 1:A:64:ASN:HB3   | 2.08                     | 0.69              |
| 1:C:63:LYS:HZ2   | 1:C:96:LYS:HE2   | 1.58                     | 0.69              |
| 1:C:359:ILE:HD13 | 1:C:359:ILE:N    | 2.07                     | 0.69              |
| 1:D:275:ARG:NH2  | 1:D:315:LYS:O    | 2.22                     | 0.69              |
| 1:D:368:ILE:HG12 | 1:D:387:PHE:CZ   | 2.29                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:10:ASP:HA    | 1:A:139:SER:HA   | 1.75                     | 0.68              |
| 1:C:409:ASP:HB3  | 1:C:413:VAL:HB   | 1.75                     | 0.68              |
| 1:D:359:ILE:HD13 | 1:D:359:ILE:N    | 2.08                     | 0.68              |
| 1:B:275:ARG:NH2  | 1:B:315:LYS:O    | 2.26                     | 0.68              |
| 1:B:316:VAL:HG22 | 1:B:354:PRO:HB3  | 1.76                     | 0.68              |
| 1:D:79:PHE:CZ    | 1:D:212:GLU:HG3  | 2.28                     | 0.68              |
| 1:A:138:GLN:NE2  | 1:A:178:ARG:HH11 | 1.91                     | 0.68              |
| 1:C:33:THR:HG22  | 1:C:34:GLN:H     | 1.59                     | 0.68              |
| 1:C:138:GLN:NE2  | 1:C:178:ARG:HH11 | 1.91                     | 0.68              |
| 1:B:421:PHE:CD2  | 1:B:430:ASP:HB3  | 2.29                     | 0.68              |
| 1:C:421:PHE:CD2  | 1:C:430:ASP:HB3  | 2.29                     | 0.68              |
| 1:D:258:ARG:HG3  | 1:D:258:ARG:HH11 | 1.58                     | 0.68              |
| 1:A:359:ILE:HD13 | 1:A:359:ILE:N    | 2.10                     | 0.67              |
| 1:B:258:ARG:HG3  | 1:B:258:ARG:HH11 | 1.59                     | 0.67              |
| 1:D:281:LEU:HD23 | 1:D:316:VAL:HA   | 1.75                     | 0.67              |
| 1:A:398:THR:HG22 | 1:A:426:TYR:HB2  | 1.77                     | 0.66              |
| 1:A:73:LYS:HD3   | 1:A:74:MET:N     | 2.09                     | 0.66              |
| 1:D:217:LYS:HB3  | 1:D:218:PRO:HD3  | 1.77                     | 0.66              |
| 1:D:325:HIS:HA   | 1:D:360:GLY:O    | 1.96                     | 0.66              |
| 1:B:359:ILE:N    | 1:B:359:ILE:HD13 | 2.10                     | 0.66              |
| 1:C:370:SER:O    | 1:C:372:MET:HE2  | 1.97                     | 0.65              |
| 1:D:190:VAL:HG13 | 1:D:195:TRP:CD1  | 2.31                     | 0.65              |
| 1:C:74:MET:CE    | 1:C:76:THR:HG23  | 2.27                     | 0.65              |
| 1:B:124:LEU:O    | 1:B:279:PRO:HG3  | 1.97                     | 0.65              |
| 1:C:28:GLN:HE22  | 1:C:184:ARG:HE   | 1.45                     | 0.65              |
| 1:C:426:TYR:O    | 1:C:428:VAL:HG13 | 1.95                     | 0.65              |
| 1:B:368:ILE:HG12 | 1:B:387:PHE:CZ   | 2.32                     | 0.64              |
| 1:D:33:THR:HG22  | 1:D:34:GLN:H     | 1.61                     | 0.64              |
| 1:D:292:SER:C    | 1:D:373:ILE:HD12 | 2.22                     | 0.64              |
| 1:A:409:ASP:HB3  | 1:A:413:VAL:HB   | 1.78                     | 0.64              |
| 1:D:258:ARG:HG3  | 1:D:258:ARG:NH1  | 2.13                     | 0.64              |
| 1:A:275:ARG:NH2  | 1:A:315:LYS:O    | 2.30                     | 0.64              |
| 1:A:258:ARG:HH11 | 1:A:258:ARG:HG3  | 1.63                     | 0.63              |
| 1:B:190:VAL:HG13 | 1:B:195:TRP:CD1  | 2.33                     | 0.63              |
| 1:C:368:ILE:HG12 | 1:C:387:PHE:CZ   | 2.34                     | 0.63              |
| 1:A:285:MET:O    | 1:A:321:ALA:HA   | 1.99                     | 0.63              |
| 1:D:63:LYS:HZ2   | 1:D:96:LYS:HE2   | 1.64                     | 0.63              |
| 1:A:63:LYS:HZ2   | 1:A:96:LYS:HE2   | 1.61                     | 0.63              |
| 1:D:28:GLN:HE22  | 1:D:184:ARG:HE   | 1.47                     | 0.63              |
| 1:B:292:SER:O    | 1:B:373:ILE:HG12 | 1.98                     | 0.62              |
| 1:D:28:GLN:NE2   | 1:D:184:ARG:HE   | 1.97                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:281:LEU:HD23 | 1:B:316:VAL:HA   | 1.80                     | 0.62              |
| 1:A:28:GLN:NE2   | 1:A:184:ARG:HE   | 1.97                     | 0.62              |
| 1:A:33:THR:HG22  | 1:A:34:GLN:H     | 1.65                     | 0.61              |
| 1:A:190:VAL:HG13 | 1:A:195:TRP:CD1  | 2.36                     | 0.61              |
| 1:D:55:SER:OG    | 1:D:88:HIS:HD2   | 1.81                     | 0.61              |
| 1:D:424:HIS:HD2  | 1:D:425:TRP:CD1  | 2.18                     | 0.61              |
| 1:B:33:THR:HG22  | 1:B:34:GLN:N     | 2.15                     | 0.61              |
| 1:B:59:TYR:HA    | 1:B:102:TYR:O    | 2.00                     | 0.61              |
| 1:C:285:MET:SD   | 1:C:303:MET:HE3  | 2.41                     | 0.61              |
| 1:A:368:ILE:HG12 | 1:A:387:PHE:CZ   | 2.36                     | 0.61              |
| 1:C:28:GLN:NE2   | 1:C:184:ARG:HE   | 1.99                     | 0.60              |
| 1:C:174:HIS:O    | 1:C:175:ASP:C    | 2.42                     | 0.60              |
| 1:A:74:MET:HE1   | 1:A:76:THR:HG23  | 1.83                     | 0.60              |
| 1:C:258:ARG:HG3  | 1:C:258:ARG:HH11 | 1.64                     | 0.60              |
| 1:A:134:GLY:O    | 1:A:135:ASP:HB2  | 2.00                     | 0.60              |
| 1:B:301:GLU:O    | 1:B:305:THR:HG23 | 2.01                     | 0.60              |
| 1:D:316:VAL:HG22 | 1:D:354:PRO:HB3  | 1.83                     | 0.60              |
| 1:B:73:LYS:HD3   | 1:B:74:MET:N     | 2.16                     | 0.60              |
| 1:C:359:ILE:HD13 | 1:C:359:ILE:H    | 1.66                     | 0.60              |
| 1:D:285:MET:SD   | 1:D:303:MET:HE3  | 2.41                     | 0.60              |
| 1:B:74:MET:HE1   | 1:B:76:THR:HG23  | 1.83                     | 0.59              |
| 1:D:406:ARG:HG3  | 1:D:415:ALA:CB   | 2.32                     | 0.59              |
| 1:A:258:ARG:HG3  | 1:A:258:ARG:NH1  | 2.18                     | 0.59              |
| 1:B:258:ARG:HG3  | 1:B:258:ARG:NH1  | 2.14                     | 0.59              |
| 1:B:25:ASN:ND2   | 1:B:51:GLU:H     | 2.00                     | 0.59              |
| 1:C:364:ASN:HD21 | 1:C:367:VAL:H    | 1.51                     | 0.59              |
| 1:D:74:MET:HE2   | 1:D:75:SER:C     | 2.27                     | 0.59              |
| 1:D:292:SER:O    | 1:D:373:ILE:HD12 | 2.02                     | 0.59              |
| 1:D:301:GLU:O    | 1:D:305:THR:HG23 | 2.03                     | 0.59              |
| 1:D:74:MET:HE1   | 1:D:76:THR:HG23  | 1.85                     | 0.58              |
| 1:A:174:HIS:O    | 1:A:175:ASP:C    | 2.46                     | 0.58              |
| 1:A:285:MET:SD   | 1:A:303:MET:HE3  | 2.43                     | 0.58              |
| 1:D:132:LEU:HD22 | 1:D:320:PHE:CD1  | 2.38                     | 0.58              |
| 1:C:74:MET:HE2   | 1:C:75:SER:N     | 2.19                     | 0.58              |
| 1:C:351:GLN:OE1  | 1:C:429:ASP:HA   | 2.04                     | 0.58              |
| 1:B:174:HIS:O    | 1:B:175:ASP:C    | 2.46                     | 0.58              |
| 1:C:285:MET:O    | 1:C:321:ALA:HA   | 2.04                     | 0.58              |
| 1:A:132:LEU:HD22 | 1:A:320:PHE:CD1  | 2.38                     | 0.58              |
| 1:A:406:ARG:HG3  | 1:A:415:ALA:CB   | 2.33                     | 0.58              |
| 1:B:398:THR:HG22 | 1:B:426:TYR:HB2  | 1.84                     | 0.58              |
| 1:D:9:ARG:HG2    | 1:D:366:GLY:HA3  | 1.85                     | 0.58              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:A:325:HIS:HA   | 1:A:360:GLY:O   | 2.04                     | 0.58              |
| 1:A:58:ARG:O     | 1:A:103:TYR:HA  | 2.04                     | 0.58              |
| 1:D:146:LEU:O    | 1:D:150:GLU:HG3 | 2.04                     | 0.58              |
| 1:D:10:ASP:HA    | 1:D:139:SER:HA  | 1.84                     | 0.57              |
| 1:C:33:THR:HG22  | 1:C:34:GLN:N    | 2.18                     | 0.57              |
| 1:A:167:TYR:HD2  | 1:A:170:ARG:HD2 | 1.68                     | 0.57              |
| 1:A:79:PHE:CZ    | 1:A:212:GLU:HG3 | 2.38                     | 0.57              |
| 1:B:124:LEU:HD12 | 1:B:279:PRO:HD3 | 1.86                     | 0.57              |
| 1:B:359:ILE:HD13 | 1:B:359:ILE:H   | 1.68                     | 0.57              |
| 1:C:10:ASP:HA    | 1:C:139:SER:HA  | 1.85                     | 0.57              |
| 1:C:29:GLN:O     | 1:C:31:HIS:HD2  | 1.88                     | 0.57              |
| 1:B:285:MET:O    | 1:B:321:ALA:HA  | 2.05                     | 0.57              |
| 1:C:33:THR:HG23  | 1:C:195:TRP:O   | 2.05                     | 0.57              |
| 1:D:359:ILE:HD13 | 1:D:359:ILE:H   | 1.69                     | 0.57              |
| 1:B:132:LEU:HD22 | 1:B:320:PHE:CD1 | 2.39                     | 0.57              |
| 1:B:171:TYR:CE1  | 1:B:178:ARG:HG3 | 2.39                     | 0.57              |
| 1:B:364:ASN:HD22 | 1:B:365:TYR:H   | 1.53                     | 0.57              |
| 1:C:124:LEU:HD12 | 1:C:279:PRO:HD3 | 1.86                     | 0.57              |
| 1:D:58:ARG:O     | 1:D:103:TYR:HA  | 2.05                     | 0.57              |
| 1:D:59:TYR:HA    | 1:D:102:TYR:O   | 2.05                     | 0.57              |
| 1:A:251:SER:HB3  | 1:A:254:SER:HB2 | 1.87                     | 0.57              |
| 1:B:28:GLN:NE2   | 1:B:184:ARG:HE  | 2.03                     | 0.57              |
| 1:C:338:TYR:O    | 1:C:339:LYS:HD2 | 2.05                     | 0.57              |
| 1:D:73:LYS:HD3   | 1:D:74:MET:N    | 2.20                     | 0.57              |
| 1:C:48:THR:OG1   | 1:C:88:HIS:HE1  | 1.88                     | 0.56              |
| 1:B:79:PHE:CZ    | 1:B:212:GLU:HG3 | 2.40                     | 0.56              |
| 1:D:174:HIS:O    | 1:D:175:ASP:C   | 2.48                     | 0.56              |
| 1:D:251:SER:HB3  | 1:D:254:SER:HB2 | 1.87                     | 0.56              |
| 1:B:29:GLN:O     | 1:B:31:HIS:HD2  | 1.88                     | 0.56              |
| 1:A:281:LEU:HD23 | 1:A:316:VAL:HA  | 1.86                     | 0.56              |
| 1:B:55:SER:OG    | 1:B:88:HIS:HD2  | 1.89                     | 0.56              |
| 1:C:124:LEU:O    | 1:C:279:PRO:HG3 | 2.06                     | 0.56              |
| 1:D:364:ASN:HD22 | 1:D:365:TYR:H   | 1.54                     | 0.56              |
| 1:C:281:LEU:HD23 | 1:C:316:VAL:HA  | 1.87                     | 0.56              |
| 1:C:316:VAL:HG22 | 1:C:354:PRO:HB3 | 1.87                     | 0.56              |
| 1:C:258:ARG:HG3  | 1:C:258:ARG:NH1 | 2.19                     | 0.56              |
| 1:A:60:TRP:HB3   | 1:A:67:LYS:HA   | 1.88                     | 0.56              |
| 1:D:29:GLN:O     | 1:D:31:HIS:HD2  | 1.89                     | 0.56              |
| 1:A:74:MET:HE2   | 1:A:75:SER:C    | 2.30                     | 0.56              |
| 1:A:359:ILE:HD13 | 1:A:359:ILE:H   | 1.70                     | 0.56              |
| 1:C:297:PHE:CE2  | 1:C:298:MET:HG3 | 2.41                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:33:THR:HG22  | 1:A:34:GLN:N     | 2.21                     | 0.55              |
| 1:B:58:ARG:O     | 1:B:103:TYR:HA   | 2.06                     | 0.55              |
| 1:C:190:VAL:HG13 | 1:C:195:TRP:CD1  | 2.41                     | 0.55              |
| 1:A:124:LEU:HD12 | 1:A:279:PRO:HD3  | 1.88                     | 0.55              |
| 1:A:129:THR:H    | 1:A:157:GLN:HE21 | 1.53                     | 0.55              |
| 1:A:28:GLN:HE22  | 1:A:184:ARG:HE   | 1.53                     | 0.55              |
| 1:B:251:SER:HB3  | 1:B:254:SER:HB2  | 1.88                     | 0.55              |
| 1:B:316:VAL:O    | 1:B:354:PRO:HB3  | 2.06                     | 0.55              |
| 1:A:316:VAL:HG22 | 1:A:354:PRO:HB3  | 1.87                     | 0.55              |
| 1:C:9:ARG:HH11   | 1:C:9:ARG:CG     | 2.18                     | 0.55              |
| 1:C:79:PHE:CZ    | 1:C:212:GLU:HG3  | 2.42                     | 0.55              |
| 1:B:364:ASN:HD21 | 1:B:367:VAL:H    | 1.54                     | 0.55              |
| 1:C:275:ARG:NH2  | 1:C:315:LYS:O    | 2.39                     | 0.55              |
| 1:C:301:GLU:O    | 1:C:305:THR:HG23 | 2.06                     | 0.55              |
| 1:D:33:THR:HG22  | 1:D:34:GLN:N     | 2.21                     | 0.55              |
| 1:A:374:GLN:HA   | 1:A:374:GLN:NE2  | 2.22                     | 0.54              |
| 1:A:217:LYS:HB3  | 1:A:218:PRO:HD3  | 1.88                     | 0.54              |
| 1:A:251:SER:CB   | 1:A:254:SER:HB2  | 2.38                     | 0.54              |
| 1:B:101:TYR:O    | 1:B:115:SER:HA   | 2.08                     | 0.54              |
| 1:A:59:TYR:HA    | 1:A:102:TYR:O    | 2.07                     | 0.54              |
| 1:D:364:ASN:HD21 | 1:D:367:VAL:H    | 1.56                     | 0.54              |
| 1:B:24:TYR:OH    | 1:B:51:GLU:HG2   | 2.08                     | 0.54              |
| 1:C:167:TYR:HD2  | 1:C:170:ARG:HD2  | 1.73                     | 0.54              |
| 1:A:74:MET:HE2   | 1:A:75:SER:N     | 2.22                     | 0.54              |
| 1:C:117:ILE:HG22 | 1:C:118:THR:O    | 2.07                     | 0.54              |
| 1:D:124:LEU:O    | 1:D:279:PRO:HG3  | 2.07                     | 0.54              |
| 1:A:74:MET:HE2   | 1:A:75:SER:CA    | 2.37                     | 0.53              |
| 1:D:74:MET:HE2   | 1:D:75:SER:CA    | 2.37                     | 0.53              |
| 1:D:124:LEU:HD12 | 1:D:279:PRO:HD3  | 1.90                     | 0.53              |
| 1:B:74:MET:HE2   | 1:B:75:SER:C     | 2.34                     | 0.53              |
| 1:B:250:LEU:HD21 | 1:B:266:LEU:HD13 | 1.91                     | 0.53              |
| 1:A:29:GLN:O     | 1:A:31:HIS:HD2   | 1.91                     | 0.53              |
| 1:D:117:ILE:HG22 | 1:D:118:THR:O    | 2.08                     | 0.53              |
| 1:D:171:TYR:CE1  | 1:D:178:ARG:HG3  | 2.43                     | 0.53              |
| 1:A:117:ILE:HG22 | 1:A:118:THR:O    | 2.08                     | 0.53              |
| 1:B:165:LEU:O    | 1:B:182:TRP:CE2  | 2.62                     | 0.53              |
| 1:B:421:PHE:HB3  | 1:B:426:TYR:O    | 2.08                     | 0.53              |
| 1:C:74:MET:HE2   | 1:C:75:SER:CA    | 2.39                     | 0.53              |
| 1:B:306:LYS:HD3  | 1:C:302:ALA:HB2  | 1.91                     | 0.53              |
| 1:D:338:TYR:O    | 1:D:339:LYS:HD2  | 2.08                     | 0.53              |
| 1:A:364:ASN:HD22 | 1:A:365:TYR:H    | 1.57                     | 0.52              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:73:LYS:HD3   | 1:C:74:MET:H      | 1.73                     | 0.52              |
| 1:D:167:TYR:HD2  | 1:D:170:ARG:HD2   | 1.73                     | 0.52              |
| 1:C:74:MET:HE2   | 1:C:75:SER:C      | 2.33                     | 0.52              |
| 1:C:251:SER:OG   | 1:C:254:SER:HB2   | 2.10                     | 0.52              |
| 1:B:251:SER:CB   | 1:B:254:SER:HB2   | 2.39                     | 0.52              |
| 1:D:24:TYR:OH    | 1:D:51:GLU:HG2    | 2.09                     | 0.52              |
| 1:D:101:TYR:O    | 1:D:115:SER:HA    | 2.09                     | 0.52              |
| 1:D:151:LEU:O    | 1:D:152:SER:C     | 2.53                     | 0.52              |
| 1:D:74:MET:HE2   | 1:D:75:SER:N      | 2.24                     | 0.52              |
| 1:D:297:PHE:CD1  | 1:D:373:ILE:HD11  | 2.45                     | 0.52              |
| 1:B:167:TYR:HD2  | 1:B:170:ARG:HD2   | 1.75                     | 0.52              |
| 1:B:122:THR:HA   | 1:B:243:ALA:O     | 2.09                     | 0.52              |
| 1:B:382:PHE:CE2  | 1:B:416:ASP:HB2   | 2.44                     | 0.52              |
| 1:D:162:VAL:HG13 | 1:D:162:VAL:O     | 2.10                     | 0.52              |
| 1:B:151:LEU:O    | 1:B:152:SER:C     | 2.53                     | 0.52              |
| 1:D:206:PHE:C    | 1:D:208:PRO:HD3   | 2.34                     | 0.52              |
| 1:D:285:MET:O    | 1:D:321:ALA:HA    | 2.10                     | 0.52              |
| 1:A:364:ASN:HD21 | 1:A:367:VAL:H     | 1.57                     | 0.51              |
| 1:C:251:SER:CB   | 1:C:254:SER:HB2   | 2.40                     | 0.51              |
| 1:A:431:SER:O    | 1:A:432:THR:HG23  | 2.10                     | 0.51              |
| 1:A:228:GLU:CD   | 1:A:228:GLU:H     | 2.18                     | 0.51              |
| 1:B:406:ARG:HG3  | 1:B:415:ALA:CB    | 2.40                     | 0.51              |
| 1:D:25:ASN:HD22  | 1:D:50:ASP:H      | 1.57                     | 0.51              |
| 1:D:308:GLU:O    | 1:D:312:VAL:HG23  | 2.10                     | 0.51              |
| 1:A:297:PHE:CE2  | 1:A:298:MET:HG3   | 2.46                     | 0.51              |
| 1:A:374:GLN:HA   | 1:A:374:GLN:HE21  | 1.74                     | 0.51              |
| 1:A:382:PHE:CE2  | 1:A:416:ASP:HB2   | 2.46                     | 0.51              |
| 1:D:48:THR:OG1   | 1:D:88:HIS:HE1    | 1.94                     | 0.51              |
| 1:A:24:TYR:OH    | 1:A:51:GLU:HG2    | 2.10                     | 0.51              |
| 1:B:425:TRP:O    | 1:B:426:TYR:HB2   | 2.10                     | 0.51              |
| 1:D:25:ASN:ND2   | 1:D:51:GLU:H      | 2.08                     | 0.51              |
| 1:B:200:GLY:O    | 1:B:203:GLU:HB2   | 2.11                     | 0.50              |
| 1:C:171:TYR:CE1  | 1:C:178:ARG:HG3   | 2.46                     | 0.50              |
| 1:A:211:ASN:OD1  | 2:A:436(A):NAG:C2 | 2.59                     | 0.50              |
| 1:B:422:ASN:OD1  | 1:B:425:TRP:HD1   | 1.94                     | 0.50              |
| 1:C:316:VAL:O    | 1:C:354:PRO:HB3   | 2.11                     | 0.50              |
| 1:D:122:THR:HA   | 1:D:243:ALA:O     | 2.12                     | 0.50              |
| 1:C:25:ASN:ND2   | 1:C:51:GLU:H      | 2.09                     | 0.50              |
| 1:A:101:TYR:O    | 1:A:115:SER:HA    | 2.12                     | 0.50              |
| 1:B:99:THR:O     | 1:B:117:ILE:HA    | 2.12                     | 0.50              |
| 1:D:129:THR:HG23 | 1:D:157:GLN:HE21  | 1.77                     | 0.50              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:171:TYR:CE1  | 1:A:178:ARG:HG3   | 2.46                     | 0.50              |
| 1:A:421:PHE:CD2  | 1:A:430:ASP:HB3   | 2.46                     | 0.50              |
| 1:A:308:GLU:O    | 1:A:312:VAL:HG23  | 2.11                     | 0.50              |
| 1:B:399:HIS:CE1  | 1:B:421:PHE:HE1   | 2.28                     | 0.50              |
| 1:D:318:VAL:HG11 | 1:D:320:PHE:CZ    | 2.46                     | 0.50              |
| 1:B:285:MET:SD   | 1:B:303:MET:CE    | 3.00                     | 0.50              |
| 1:B:318:VAL:HG21 | 1:B:392:PHE:CE2   | 2.46                     | 0.50              |
| 1:C:406:ARG:HG3  | 1:C:415:ALA:CB    | 2.40                     | 0.50              |
| 1:D:346:THR:HG23 | 1:D:347:PRO:HD2   | 1.93                     | 0.50              |
| 1:A:55:SER:OG    | 1:A:88:HIS:HD2    | 1.95                     | 0.50              |
| 1:A:251:SER:OG   | 1:A:254:SER:HB2   | 2.12                     | 0.50              |
| 1:B:179:TRP:CZ3  | 1:B:223:TYR:HE2   | 2.30                     | 0.50              |
| 1:B:28:GLN:HE22  | 1:B:184:ARG:HE    | 1.59                     | 0.50              |
| 1:B:117:ILE:HG22 | 1:B:118:THR:O     | 2.12                     | 0.50              |
| 1:C:162:VAL:O    | 1:C:162:VAL:HG13  | 2.10                     | 0.50              |
| 1:D:60:TRP:HB3   | 1:D:67:LYS:HA     | 1.94                     | 0.50              |
| 1:A:151:LEU:O    | 1:A:152:SER:C     | 2.55                     | 0.49              |
| 1:B:129:THR:H    | 1:B:157:GLN:HE21  | 1.59                     | 0.49              |
| 1:A:97:TYR:CE1   | 1:A:121:GLN:HA    | 2.47                     | 0.49              |
| 1:C:101:TYR:O    | 1:C:115:SER:HA    | 2.12                     | 0.49              |
| 1:B:211:ASN:OD1  | 2:B:436(A):NAG:C2 | 2.61                     | 0.49              |
| 1:D:251:SER:CB   | 1:D:254:SER:HB2   | 2.41                     | 0.49              |
| 1:A:351:GLN:OE1  | 1:A:429:ASP:HA    | 2.13                     | 0.49              |
| 1:B:177:VAL:O    | 1:B:180:ASP:N     | 2.46                     | 0.49              |
| 1:C:59:TYR:HA    | 1:C:102:TYR:O     | 2.12                     | 0.49              |
| 1:C:76:THR:HG22  | 1:C:85:GLY:O      | 2.13                     | 0.49              |
| 1:B:27:PRO:HG3   | 1:B:105:VAL:O     | 2.13                     | 0.49              |
| 1:B:228:GLU:H    | 1:B:228:GLU:CD    | 2.20                     | 0.49              |
| 1:C:217:LYS:HB3  | 1:C:218:PRO:HD3   | 1.95                     | 0.49              |
| 1:A:346:THR:HG23 | 1:A:347:PRO:HD2   | 1.94                     | 0.49              |
| 1:C:29:GLN:NE2   | 1:C:180:ASP:HA    | 2.28                     | 0.49              |
| 1:C:382:PHE:CE2  | 1:C:416:ASP:HB2   | 2.48                     | 0.49              |
| 1:B:217:LYS:HB3  | 1:B:218:PRO:HD3   | 1.95                     | 0.49              |
| 1:C:251:SER:HB3  | 1:C:254:SER:HB2   | 1.93                     | 0.49              |
| 1:D:79:PHE:CE1   | 1:D:212:GLU:HG3   | 2.48                     | 0.49              |
| 1:B:338:TYR:O    | 1:B:339:LYS:HD2   | 2.12                     | 0.48              |
| 1:C:32:ILE:HD12  | 1:C:42:MET:HE3    | 1.95                     | 0.48              |
| 1:B:308:GLU:O    | 1:B:312:VAL:HG23  | 2.13                     | 0.48              |
| 1:B:426:TYR:N    | 1:B:427:PRO:CD    | 2.76                     | 0.48              |
| 1:B:63:LYS:HZ2   | 1:B:96:LYS:HE2    | 1.78                     | 0.48              |
| 1:B:165:LEU:O    | 1:B:182:TRP:NE1   | 2.46                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:29:GLN:NE2   | 1:A:180:ASP:HA   | 2.28                     | 0.48              |
| 1:C:374:GLN:HE22 | 1:C:383:ARG:HH12 | 1.60                     | 0.48              |
| 1:B:190:VAL:HG13 | 1:B:195:TRP:CG   | 2.48                     | 0.48              |
| 1:B:382:PHE:HE2  | 1:B:416:ASP:HB2  | 1.78                     | 0.48              |
| 1:C:134:GLY:CA   | 1:C:162:VAL:HG12 | 2.40                     | 0.48              |
| 1:C:364:ASN:HD22 | 1:C:365:TYR:H    | 1.62                     | 0.48              |
| 1:A:146:LEU:O    | 1:A:150:GLU:HG3  | 2.14                     | 0.48              |
| 1:C:308:GLU:O    | 1:C:312:VAL:HG23 | 2.13                     | 0.48              |
| 1:B:25:ASN:HD22  | 1:B:50:ASP:H     | 1.60                     | 0.48              |
| 1:C:129:THR:H    | 1:C:157:GLN:HE21 | 1.62                     | 0.48              |
| 1:D:185:PHE:CD1  | 1:D:185:PHE:C    | 2.90                     | 0.48              |
| 1:B:251:SER:OG   | 1:B:254:SER:HB2  | 2.14                     | 0.48              |
| 1:C:421:PHE:CD2  | 1:C:428:VAL:CG2  | 2.94                     | 0.48              |
| 1:D:190:VAL:HG13 | 1:D:195:TRP:CG   | 2.48                     | 0.48              |
| 1:B:29:GLN:NE2   | 1:B:180:ASP:HA   | 2.29                     | 0.48              |
| 1:D:297:PHE:CE2  | 1:D:298:MET:HG3  | 2.49                     | 0.48              |
| 1:B:292:SER:O    | 1:B:373:ILE:CG1  | 2.61                     | 0.47              |
| 1:C:58:ARG:O     | 1:C:103:TYR:HA   | 2.14                     | 0.47              |
| 1:D:289:LEU:HB3  | 1:D:304:ARG:HG3  | 1.96                     | 0.47              |
| 1:A:338:TYR:O    | 1:A:339:LYS:HD2  | 2.14                     | 0.47              |
| 1:A:338:TYR:CE2  | 1:A:340:ILE:HA   | 2.48                     | 0.47              |
| 1:B:175:ASP:O    | 1:B:177:VAL:N    | 2.47                     | 0.47              |
| 1:C:24:TYR:OH    | 1:C:51:GLU:HG2   | 2.14                     | 0.47              |
| 1:C:63:LYS:HG3   | 1:C:64:ASN:H     | 1.79                     | 0.47              |
| 1:A:190:VAL:HG13 | 1:A:195:TRP:CG   | 2.50                     | 0.47              |
| 1:D:228:GLU:CD   | 1:D:228:GLU:H    | 2.22                     | 0.47              |
| 1:D:373:ILE:O    | 1:D:383:ARG:NH2  | 2.43                     | 0.47              |
| 1:B:320:PHE:HB3  | 1:B:359:ILE:HD11 | 1.95                     | 0.47              |
| 1:B:364:ASN:ND2  | 1:B:367:VAL:H    | 2.12                     | 0.47              |
| 1:C:301:GLU:OE2  | 1:C:304:ARG:NH1  | 2.48                     | 0.47              |
| 1:D:382:PHE:CE2  | 1:D:416:ASP:HB2  | 2.49                     | 0.47              |
| 1:D:409:ASP:HB3  | 1:D:413:VAL:CB   | 2.42                     | 0.47              |
| 1:A:73:LYS:HD3   | 1:A:74:MET:H     | 1.79                     | 0.47              |
| 1:B:60:TRP:HB3   | 1:B:67:LYS:HA    | 1.97                     | 0.47              |
| 1:B:74:MET:HE2   | 1:B:75:SER:CA    | 2.44                     | 0.47              |
| 1:B:148:HIS:CE1  | 1:B:407:ASN:HA   | 2.50                     | 0.47              |
| 1:B:346:THR:HG23 | 1:B:347:PRO:HD2  | 1.96                     | 0.47              |
| 1:C:190:VAL:HG13 | 1:C:195:TRP:CG   | 2.49                     | 0.47              |
| 1:B:146:LEU:O    | 1:B:150:GLU:HG3  | 2.15                     | 0.47              |
| 1:C:74:MET:HE1   | 1:C:76:THR:HG23  | 1.97                     | 0.47              |
| 1:D:129:THR:H    | 1:D:157:GLN:HE21 | 1.62                     | 0.47              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:48:THR:OG1   | 1:A:88:HIS:HE1    | 1.97                     | 0.47              |
| 1:B:63:LYS:HG3   | 1:B:64:ASN:H      | 1.80                     | 0.47              |
| 1:B:185:PHE:CD1  | 1:B:185:PHE:C     | 2.92                     | 0.47              |
| 1:C:25:ASN:HD22  | 1:C:50:ASP:H      | 1.62                     | 0.47              |
| 1:C:176:ASN:N    | 1:C:176:ASN:HD22  | 2.13                     | 0.47              |
| 1:B:25:ASN:ND2   | 1:B:50:ASP:HB2    | 2.30                     | 0.46              |
| 1:B:55:SER:H     | 1:B:71:LYS:NZ     | 2.13                     | 0.46              |
| 1:B:134:GLY:O    | 1:B:135:ASP:HB2   | 2.15                     | 0.46              |
| 1:A:163:GLY:HA2  | 1:A:198:THR:O     | 2.15                     | 0.46              |
| 1:B:351:GLN:OE1  | 1:B:429:ASP:HA    | 2.15                     | 0.46              |
| 1:D:323:HIS:CE1  | 5:D:440:WO4:O3    | 2.68                     | 0.46              |
| 1:B:217:LYS:O    | 1:B:218:PRO:C     | 2.57                     | 0.46              |
| 1:C:151:LEU:O    | 1:C:152:SER:C     | 2.58                     | 0.46              |
| 1:A:185:PHE:C    | 1:A:185:PHE:CD1   | 2.94                     | 0.46              |
| 1:A:124:LEU:O    | 1:A:279:PRO:HG3   | 2.15                     | 0.46              |
| 1:B:25:ASN:HD21  | 1:B:51:GLU:H      | 1.64                     | 0.46              |
| 1:C:217:LYS:HG3  | 1:C:221:TYR:CE2   | 2.51                     | 0.46              |
| 1:C:423:ARG:HA   | 1:C:423:ARG:NE    | 2.30                     | 0.46              |
| 1:D:207:ALA:HA   | 1:D:209:GLU:OE2   | 2.16                     | 0.46              |
| 1:C:132:LEU:HD22 | 1:C:320:PHE:CD1   | 2.50                     | 0.46              |
| 1:C:167:TYR:CD2  | 1:C:170:ARG:HD2   | 2.50                     | 0.46              |
| 1:C:338:TYR:CE2  | 1:C:340:ILE:HA    | 2.50                     | 0.46              |
| 1:A:176:ASN:N    | 1:A:176:ASN:HD22  | 2.14                     | 0.46              |
| 1:B:297:PHE:CE2  | 1:B:298:MET:HG3   | 2.50                     | 0.46              |
| 1:A:211:ASN:OD1  | 2:A:436(A):NAG:H2 | 2.16                     | 0.46              |
| 1:A:346:THR:HA   | 1:A:347:PRO:HD3   | 1.75                     | 0.46              |
| 1:B:207:ALA:HB3  | 1:B:212:GLU:HB2   | 1.97                     | 0.46              |
| 1:C:116:PHE:CD1  | 1:C:116:PHE:C     | 2.94                     | 0.46              |
| 1:C:27:PRO:HG3   | 1:C:105:VAL:O     | 2.16                     | 0.45              |
| 1:D:167:TYR:CD2  | 1:D:170:ARG:HD2   | 2.50                     | 0.45              |
| 1:B:296:HIS:CD2  | 1:B:323:HIS:O     | 2.69                     | 0.45              |
| 1:D:373:ILE:HG22 | 1:D:374:GLN:N     | 2.30                     | 0.45              |
| 1:B:33:THR:HG23  | 1:B:195:TRP:O     | 2.15                     | 0.45              |
| 1:B:176:ASN:N    | 1:B:176:ASN:HD22  | 2.14                     | 0.45              |
| 1:D:351:GLN:OE1  | 1:D:429:ASP:HA    | 2.16                     | 0.45              |
| 1:C:270:LEU:HD23 | 1:C:270:LEU:HA    | 1.83                     | 0.45              |
| 1:C:409:ASP:HB3  | 1:C:413:VAL:CB    | 2.45                     | 0.45              |
| 1:D:103:TYR:CZ   | 1:D:114:PHE:HB2   | 2.52                     | 0.45              |
| 1:D:424:HIS:CD2  | 1:D:425:TRP:CD1   | 3.02                     | 0.45              |
| 1:B:74:MET:HE2   | 1:B:75:SER:N      | 2.31                     | 0.45              |
| 1:B:124:LEU:HD11 | 1:B:425:TRP:CZ2   | 2.52                     | 0.45              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:423:ARG:HA   | 1:B:423:ARG:NE    | 2.30                     | 0.45              |
| 1:D:99:THR:O     | 1:D:117:ILE:HA    | 2.16                     | 0.45              |
| 1:C:60:TRP:HB3   | 1:C:67:LYS:HA     | 1.99                     | 0.45              |
| 1:D:134:GLY:CA   | 1:D:162:VAL:HG12  | 2.42                     | 0.45              |
| 1:A:14:ASP:O     | 1:A:15:SER:C      | 2.59                     | 0.45              |
| 1:A:25:ASN:ND2   | 1:A:51:GLU:H      | 2.14                     | 0.45              |
| 1:B:55:SER:H     | 1:B:71:LYS:HZ3    | 1.65                     | 0.45              |
| 1:B:211:ASN:OD1  | 2:B:436(A):NAG:H2 | 2.16                     | 0.45              |
| 1:D:338:TYR:CE2  | 1:D:340:ILE:HA    | 2.51                     | 0.45              |
| 1:A:129:THR:HG23 | 1:A:157:GLN:HE21  | 1.82                     | 0.45              |
| 1:A:240:ILE:O    | 1:A:240:ILE:HG13  | 2.15                     | 0.45              |
| 1:D:25:ASN:ND2   | 1:D:50:ASP:HB2    | 2.32                     | 0.45              |
| 1:D:255:ALA:O    | 1:D:262:GLN:HB3   | 2.17                     | 0.45              |
| 1:D:10:ASP:O     | 1:D:11:MET:C      | 2.58                     | 0.44              |
| 1:A:329:ARG:NE   | 1:A:418:VAL:HG21  | 2.32                     | 0.44              |
| 1:B:14:ASP:O     | 1:B:15:SER:C      | 2.60                     | 0.44              |
| 1:A:167:TYR:CD2  | 1:A:170:ARG:HD2   | 2.51                     | 0.44              |
| 1:A:174:HIS:O    | 1:A:176:ASN:N     | 2.50                     | 0.44              |
| 1:C:27:PRO:HG2   | 1:C:112:ARG:HD3   | 1.99                     | 0.44              |
| 1:D:134:GLY:O    | 1:D:135:ASP:HB2   | 2.16                     | 0.44              |
| 1:B:48:THR:OG1   | 1:B:88:HIS:HE1    | 2.00                     | 0.44              |
| 1:C:206:PHE:C    | 1:C:208:PRO:HD3   | 2.43                     | 0.44              |
| 1:C:364:ASN:ND2  | 1:C:367:VAL:H     | 2.13                     | 0.44              |
| 1:D:33:THR:HG23  | 1:D:195:TRP:O     | 2.17                     | 0.44              |
| 1:B:365:TYR:CD1  | 1:B:365:TYR:N     | 2.84                     | 0.44              |
| 1:C:217:LYS:HG3  | 1:C:221:TYR:HE2   | 1.81                     | 0.44              |
| 1:B:206:PHE:C    | 1:B:208:PRO:HD3   | 2.42                     | 0.44              |
| 1:B:331:GLU:OE1  | 1:B:431:SER:HB3   | 2.18                     | 0.44              |
| 1:B:346:THR:HA   | 1:B:347:PRO:HD3   | 1.72                     | 0.44              |
| 1:C:99:THR:N     | 1:C:118:THR:OG1   | 2.51                     | 0.44              |
| 1:C:175:ASP:O    | 1:C:177:VAL:N     | 2.50                     | 0.44              |
| 1:D:211:ASN:OD1  | 2:D:436(A):NAG:C2 | 2.66                     | 0.44              |
| 1:D:346:THR:HA   | 1:D:347:PRO:HD3   | 1.76                     | 0.44              |
| 1:C:406:ARG:HB2  | 1:C:409:ASP:OD2   | 2.18                     | 0.44              |
| 1:B:217:LYS:HG3  | 1:B:221:TYR:HE2   | 1.83                     | 0.43              |
| 1:D:250:LEU:HD21 | 1:D:266:LEU:HD13  | 1.99                     | 0.43              |
| 1:C:211:ASN:OD1  | 2:C:436(A):NAG:C2 | 2.66                     | 0.43              |
| 1:C:396:ASN:HB2  | 1:C:398:THR:H     | 1.83                     | 0.43              |
| 1:D:148:HIS:CE1  | 1:D:407:ASN:HA    | 2.54                     | 0.43              |
| 1:A:364:ASN:ND2  | 1:A:367:VAL:H     | 2.16                     | 0.43              |
| 1:B:174:HIS:O    | 1:B:176:ASN:N     | 2.51                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:148:HIS:CE1  | 1:C:407:ASN:HA   | 2.53                     | 0.43              |
| 1:C:228:GLU:CD   | 1:C:228:GLU:H    | 2.26                     | 0.43              |
| 1:C:399:HIS:CE1  | 1:C:421:PHE:HE1  | 2.36                     | 0.43              |
| 1:D:25:ASN:ND2   | 1:D:50:ASP:H     | 2.16                     | 0.43              |
| 1:D:169:ASP:N    | 1:D:169:ASP:OD1  | 2.52                     | 0.43              |
| 1:D:318:VAL:HG21 | 1:D:392:PHE:CE1  | 2.53                     | 0.43              |
| 1:A:122:THR:HA   | 1:A:243:ALA:O    | 2.18                     | 0.43              |
| 1:B:294:ASN:HD22 | 1:B:371:ASN:HB3  | 1.84                     | 0.43              |
| 1:C:25:ASN:ND2   | 1:C:50:ASP:HB2   | 2.33                     | 0.43              |
| 1:D:32:ILE:HA    | 1:D:43:ILE:O     | 2.19                     | 0.43              |
| 1:A:231:GLN:N    | 1:A:231:GLN:OE1  | 2.51                     | 0.43              |
| 1:B:167:TYR:CD2  | 1:B:170:ARG:HD2  | 2.54                     | 0.43              |
| 1:D:363:GLY:O    | 1:D:364:ASN:C    | 2.60                     | 0.43              |
| 1:B:338:TYR:CE2  | 1:B:340:ILE:HA   | 2.53                     | 0.43              |
| 1:D:372:MET:SD   | 1:D:383:ARG:HD3  | 2.59                     | 0.43              |
| 1:D:406:ARG:HG3  | 1:D:415:ALA:HB3  | 2.01                     | 0.43              |
| 1:A:25:ASN:HD22  | 1:A:50:ASP:H     | 1.66                     | 0.43              |
| 1:A:42:MET:HE1   | 1:A:194:PRO:HD3  | 2.00                     | 0.43              |
| 1:A:103:TYR:CZ   | 1:A:114:PHE:HB2  | 2.54                     | 0.43              |
| 1:A:116:PHE:CD1  | 1:A:116:PHE:C    | 2.96                     | 0.43              |
| 1:C:402:PHE:HB3  | 1:C:420:PHE:HE1  | 1.84                     | 0.43              |
| 1:D:175:ASP:O    | 1:D:177:VAL:N    | 2.51                     | 0.43              |
| 1:D:409:ASP:CB   | 1:D:413:VAL:HB   | 2.44                     | 0.43              |
| 1:B:217:LYS:HG3  | 1:B:221:TYR:CE2  | 2.53                     | 0.43              |
| 1:B:409:ASP:HB3  | 1:B:413:VAL:CB   | 2.45                     | 0.43              |
| 1:C:174:HIS:O    | 1:C:176:ASN:N    | 2.52                     | 0.43              |
| 1:D:9:ARG:O      | 1:D:9:ARG:HG3    | 2.17                     | 0.43              |
| 1:A:123:GLY:HA3  | 1:A:126:VAL:HG23 | 1.99                     | 0.43              |
| 1:A:365:TYR:CD1  | 1:A:365:TYR:N    | 2.87                     | 0.43              |
| 1:B:80:PHE:CD1   | 1:B:210:ILE:HB   | 2.54                     | 0.43              |
| 1:B:103:TYR:CZ   | 1:B:114:PHE:HB2  | 2.54                     | 0.43              |
| 1:B:345:CYS:SG   | 1:C:338:TYR:CE1  | 3.12                     | 0.43              |
| 1:A:134:GLY:CA   | 1:A:162:VAL:HG12 | 2.42                     | 0.43              |
| 1:A:229:ALA:C    | 1:A:230:SER:O    | 2.61                     | 0.43              |
| 1:B:296:HIS:HD2  | 1:B:323:HIS:O    | 2.02                     | 0.43              |
| 1:B:171:TYR:CD1  | 1:B:178:ARG:HG3  | 2.54                     | 0.42              |
| 1:D:257:GLY:O    | 1:D:263:TYR:HB2  | 2.19                     | 0.42              |
| 1:A:175:ASP:O    | 1:A:177:VAL:N    | 2.52                     | 0.42              |
| 1:D:98:ASN:HA    | 1:D:118:THR:O    | 2.19                     | 0.42              |
| 1:C:104:GLU:HA   | 1:C:112:ARG:O    | 2.20                     | 0.42              |
| 1:D:365:TYR:CD1  | 1:D:365:TYR:N    | 2.87                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:207:ALA:HA   | 1:A:209:GLU:OE2   | 2.19                     | 0.42              |
| 1:A:320:PHE:HB3  | 1:A:359:ILE:HD11  | 2.01                     | 0.42              |
| 1:C:318:VAL:HG11 | 1:C:320:PHE:CZ    | 2.54                     | 0.42              |
| 1:C:373:ILE:O    | 1:C:383:ARG:NH2   | 2.43                     | 0.42              |
| 1:D:63:LYS:HG3   | 1:D:64:ASN:H      | 1.83                     | 0.42              |
| 1:D:123:GLY:HA3  | 1:D:126:VAL:HG23  | 2.01                     | 0.42              |
| 1:A:63:LYS:NZ    | 1:A:96:LYS:HE2    | 2.33                     | 0.42              |
| 1:A:409:ASP:HB3  | 1:A:413:VAL:CB    | 2.48                     | 0.42              |
| 1:D:14:ASP:O     | 1:D:15:SER:C      | 2.63                     | 0.42              |
| 1:D:55:SER:H     | 1:D:71:LYS:NZ     | 2.16                     | 0.42              |
| 1:D:280:TRP:CZ2  | 1:D:400:ALA:HB2   | 2.55                     | 0.42              |
| 1:D:316:VAL:O    | 1:D:354:PRO:HB3   | 2.19                     | 0.42              |
| 1:B:409:ASP:OD2  | 1:B:415:ALA:HB2   | 2.20                     | 0.42              |
| 1:C:14:ASP:O     | 1:C:15:SER:C      | 2.60                     | 0.42              |
| 1:C:211:ASN:OD1  | 2:C:436(A):NAG:H2 | 2.20                     | 0.42              |
| 1:D:404:TRP:HB3  | 1:D:416:ASP:HB3   | 2.01                     | 0.42              |
| 1:B:27:PRO:HG2   | 1:B:112:ARG:HD3   | 2.02                     | 0.42              |
| 1:B:162:VAL:O    | 1:B:162:VAL:HG13  | 2.19                     | 0.42              |
| 1:C:176:ASN:O    | 1:C:179:TRP:HB2   | 2.20                     | 0.42              |
| 1:D:99:THR:N     | 1:D:118:THR:OG1   | 2.52                     | 0.42              |
| 1:D:402:PHE:HB2  | 1:D:420:PHE:CE1   | 2.55                     | 0.42              |
| 1:B:42:MET:HE1   | 1:B:194:PRO:HD3   | 2.01                     | 0.42              |
| 1:B:97:TYR:CE1   | 1:B:121:GLN:HA    | 2.55                     | 0.42              |
| 1:C:174:HIS:CD2  | 1:C:174:HIS:N     | 2.88                     | 0.42              |
| 1:C:229:ALA:C    | 1:C:230:SER:O     | 2.56                     | 0.42              |
| 1:C:255:ALA:O    | 1:C:262:GLN:HB3   | 2.20                     | 0.42              |
| 1:D:64:ASN:HD21  | 1:D:66:ARG:HB2    | 1.85                     | 0.42              |
| 1:D:409:ASP:OD2  | 1:D:415:ALA:HB2   | 2.20                     | 0.42              |
| 1:C:402:PHE:CB   | 1:C:420:PHE:HE1   | 2.33                     | 0.42              |
| 1:D:270:LEU:HD23 | 1:D:270:LEU:HA    | 1.87                     | 0.42              |
| 1:D:382:PHE:HE2  | 1:D:416:ASP:HB2   | 1.84                     | 0.42              |
| 1:A:25:ASN:ND2   | 1:A:50:ASP:HB2    | 2.35                     | 0.41              |
| 1:A:32:ILE:HG12  | 1:A:190:VAL:O     | 2.20                     | 0.41              |
| 1:A:162:VAL:O    | 1:A:162:VAL:HG13  | 2.20                     | 0.41              |
| 1:A:270:LEU:HD23 | 1:A:270:LEU:HA    | 1.86                     | 0.41              |
| 1:B:104:GLU:HB3  | 1:B:111:THR:CG2   | 2.50                     | 0.41              |
| 1:C:231:GLN:OE1  | 1:C:231:GLN:N     | 2.53                     | 0.41              |
| 1:D:251:SER:OG   | 1:D:254:SER:HB2   | 2.20                     | 0.41              |
| 1:B:207:ALA:HA   | 1:B:209:GLU:OE2   | 2.20                     | 0.41              |
| 1:B:255:ALA:O    | 1:B:262:GLN:HB3   | 2.20                     | 0.41              |
| 1:B:258:ARG:HA   | 1:B:263:TYR:CD2   | 2.55                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:178:ARG:HD3  | 1:C:178:ARG:HA   | 1.94                     | 0.41              |
| 1:D:364:ASN:ND2  | 1:D:367:VAL:H    | 2.16                     | 0.41              |
| 1:A:64:ASN:HD21  | 1:A:66:ARG:HB2   | 1.85                     | 0.41              |
| 1:B:318:VAL:HG11 | 1:B:320:PHE:CZ   | 2.55                     | 0.41              |
| 1:C:29:GLN:HE22  | 1:C:180:ASP:HA   | 1.86                     | 0.41              |
| 1:C:103:TYR:CZ   | 1:C:114:PHE:HB2  | 2.54                     | 0.41              |
| 1:C:145:THR:O    | 1:C:146:LEU:C    | 2.61                     | 0.41              |
| 1:C:372:MET:HG3  | 1:C:383:ARG:NH1  | 2.35                     | 0.41              |
| 1:D:104:GLU:HA   | 1:D:112:ARG:O    | 2.21                     | 0.41              |
| 1:A:398:THR:CG2  | 1:A:426:TYR:HB2  | 2.49                     | 0.41              |
| 1:B:338:TYR:CE1  | 1:C:345:CYS:O    | 2.73                     | 0.41              |
| 1:C:129:THR:HG23 | 1:C:157:GLN:HE21 | 1.85                     | 0.41              |
| 1:C:409:ASP:CB   | 1:C:413:VAL:HB   | 2.49                     | 0.41              |
| 1:D:25:ASN:HD21  | 1:D:51:GLU:H     | 1.69                     | 0.41              |
| 1:D:174:HIS:O    | 1:D:176:ASN:N    | 2.52                     | 0.41              |
| 1:D:177:VAL:O    | 1:D:180:ASP:N    | 2.53                     | 0.41              |
| 1:D:165:LEU:O    | 1:D:182:TRP:CE2  | 2.73                     | 0.41              |
| 1:A:345:CYS:O    | 1:A:345:CYS:SG   | 2.79                     | 0.41              |
| 1:B:409:ASP:CB   | 1:B:413:VAL:HB   | 2.47                     | 0.41              |
| 1:D:396:ASN:HB2  | 1:D:398:THR:H    | 1.86                     | 0.41              |
| 1:B:145:THR:O    | 1:B:146:LEU:C    | 2.61                     | 0.41              |
| 1:B:222:ARG:HH11 | 1:B:222:ARG:HG2  | 1.86                     | 0.41              |
| 1:B:255:ALA:HB2  | 1:C:255:ALA:HB2  | 2.02                     | 0.41              |
| 1:C:163:GLY:HA2  | 1:C:198:THR:O    | 2.20                     | 0.41              |
| 1:D:164:ASP:H    | 1:D:200:GLY:HA3  | 1.86                     | 0.41              |
| 1:C:122:THR:HA   | 1:C:243:ALA:O    | 2.21                     | 0.41              |
| 1:D:278:THR:HA   | 1:D:279:PRO:HD2  | 1.92                     | 0.41              |
| 1:D:402:PHE:CB   | 1:D:420:PHE:HE1  | 2.34                     | 0.41              |
| 1:A:25:ASN:HD22  | 1:A:25:ASN:HA    | 1.68                     | 0.41              |
| 1:A:207:ALA:HB1  | 1:A:210:ILE:HG12 | 2.03                     | 0.41              |
| 1:A:242:ARG:O    | 1:A:243:ALA:C    | 2.64                     | 0.41              |
| 1:C:42:MET:HE1   | 1:C:194:PRO:HD3  | 2.03                     | 0.41              |
| 1:D:26:ALA:HA    | 1:D:27:PRO:HD2   | 1.95                     | 0.41              |
| 1:D:28:GLN:HG3   | 1:D:29:GLN:HG3   | 2.02                     | 0.41              |
| 1:D:73:LYS:HD3   | 1:D:74:MET:H     | 1.85                     | 0.41              |
| 1:D:217:LYS:O    | 1:D:218:PRO:C    | 2.62                     | 0.41              |
| 1:D:345:CYS:O    | 1:D:345:CYS:SG   | 2.77                     | 0.41              |
| 1:D:399:HIS:CE1  | 1:D:421:PHE:HE1  | 2.39                     | 0.41              |
| 1:A:33:THR:HG23  | 1:A:195:TRP:O    | 2.21                     | 0.41              |
| 1:A:95:LEU:HB3   | 1:A:118:THR:HG21 | 2.02                     | 0.41              |
| 1:A:104:GLU:HA   | 1:A:112:ARG:O    | 2.20                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:165:LEU:O    | 1:A:182:TRP:CE2  | 2.74                     | 0.41              |
| 1:A:171:TYR:CD1  | 1:A:178:ARG:HG3  | 2.56                     | 0.41              |
| 1:B:149:TYR:OH   | 1:B:156:GLY:HA3  | 2.21                     | 0.41              |
| 1:C:329:ARG:NE   | 1:C:418:VAL:HG21 | 2.36                     | 0.41              |
| 1:C:346:THR:HG23 | 1:C:347:PRO:HD2  | 2.03                     | 0.41              |
| 1:D:32:ILE:HD12  | 1:D:42:MET:HE3   | 2.03                     | 0.41              |
| 1:A:129:THR:H    | 1:A:157:GLN:NE2  | 2.19                     | 0.40              |
| 1:B:338:TYR:HE1  | 1:C:345:CYS:O    | 2.03                     | 0.40              |
| 1:B:364:ASN:HD22 | 1:B:365:TYR:N    | 2.17                     | 0.40              |
| 1:C:345:CYS:O    | 1:C:345:CYS:SG   | 2.79                     | 0.40              |
| 1:D:373:ILE:CG2  | 1:D:374:GLN:N    | 2.84                     | 0.40              |
| 1:A:295:HIS:O    | 1:A:296:HIS:HB2  | 2.19                     | 0.40              |
| 1:A:423:ARG:NE   | 1:A:423:ARG:HA   | 2.36                     | 0.40              |
| 1:B:29:GLN:HE22  | 1:B:180:ASP:HA   | 1.87                     | 0.40              |
| 1:C:138:GLN:NE2  | 1:C:178:ARG:HD2  | 2.36                     | 0.40              |
| 1:D:179:TRP:CZ3  | 1:D:223:TYR:HE2  | 2.39                     | 0.40              |
| 1:D:304:ARG:C    | 1:D:306:LYS:N    | 2.79                     | 0.40              |
| 1:A:145:THR:O    | 1:A:146:LEU:C    | 2.63                     | 0.40              |
| 1:B:129:THR:HG23 | 1:B:157:GLN:HE21 | 1.84                     | 0.40              |
| 1:C:82:TYR:CG    | 1:C:83:SER:N     | 2.90                     | 0.40              |
| 1:C:165:LEU:O    | 1:C:182:TRP:CE2  | 2.75                     | 0.40              |
| 1:A:161:PHE:HD1  | 1:A:163:GLY:H    | 1.69                     | 0.40              |
| 1:A:174:HIS:CD2  | 1:A:174:HIS:N    | 2.90                     | 0.40              |
| 1:B:154:LYS:HG2  | 1:B:154:LYS:O    | 2.22                     | 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   | A     | 422/432 (98%) | 374 (89%) | 45 (11%) | 3 (1%)   | 18 53       |

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| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|-----------|----------|-------------|----|
| 1   | B     | 422/432 (98%)   | 371 (88%)  | 45 (11%)  | 6 (1%)   | 9           | 36 |
| 1   | C     | 422/432 (98%)   | 369 (87%)  | 48 (11%)  | 5 (1%)   | 10          | 40 |
| 1   | D     | 422/432 (98%)   | 369 (87%)  | 47 (11%)  | 6 (1%)   | 9           | 36 |
| All | All   | 1688/1728 (98%) | 1483 (88%) | 185 (11%) | 20 (1%)  | 10          | 40 |

All (20) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 175 | ASP  |
| 1   | B     | 175 | ASP  |
| 1   | C     | 175 | ASP  |
| 1   | D     | 175 | ASP  |
| 1   | D     | 431 | SER  |
| 1   | A     | 176 | ASN  |
| 1   | B     | 176 | ASN  |
| 1   | C     | 176 | ASN  |
| 1   | C     | 325 | HIS  |
| 1   | D     | 176 | ASN  |
| 1   | B     | 426 | TYR  |
| 1   | D     | 164 | ASP  |
| 1   | D     | 335 | ASN  |
| 1   | D     | 340 | ILE  |
| 1   | A     | 340 | ILE  |
| 1   | B     | 164 | ASP  |
| 1   | B     | 340 | ILE  |
| 1   | B     | 343 | GLY  |
| 1   | C     | 164 | ASP  |
| 1   | C     | 340 | ILE  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|-------------|----|
| 1   | A     | 373/381 (98%) | 341 (91%) | 32 (9%)  | 10          | 36 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1   | B     | 373/381 (98%)   | 340 (91%)  | 33 (9%)  | 9           | 35 |
| 1   | C     | 373/381 (98%)   | 339 (91%)  | 34 (9%)  | 9           | 33 |
| 1   | D     | 373/381 (98%)   | 344 (92%)  | 29 (8%)  | 11          | 39 |
| All | All   | 1492/1524 (98%) | 1364 (91%) | 128 (9%) | 10          | 36 |

All (128) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 14  | ASP  |
| 1   | A     | 20  | VAL  |
| 1   | A     | 25  | ASN  |
| 1   | A     | 52  | PRO  |
| 1   | A     | 64  | ASN  |
| 1   | A     | 73  | LYS  |
| 1   | A     | 74  | MET  |
| 1   | A     | 94  | LYS  |
| 1   | A     | 105 | VAL  |
| 1   | A     | 119 | PRO  |
| 1   | A     | 129 | THR  |
| 1   | A     | 147 | SER  |
| 1   | A     | 154 | LYS  |
| 1   | A     | 155 | LYS  |
| 1   | A     | 162 | VAL  |
| 1   | A     | 176 | ASN  |
| 1   | A     | 190 | VAL  |
| 1   | A     | 209 | GLU  |
| 1   | A     | 228 | GLU  |
| 1   | A     | 230 | SER  |
| 1   | A     | 254 | SER  |
| 1   | A     | 276 | SER  |
| 1   | A     | 316 | VAL  |
| 1   | A     | 318 | VAL  |
| 1   | A     | 349 | LYS  |
| 1   | A     | 358 | THR  |
| 1   | A     | 359 | ILE  |
| 1   | A     | 378 | GLU  |
| 1   | A     | 383 | ARG  |
| 1   | A     | 403 | SER  |
| 1   | A     | 428 | VAL  |
| 1   | A     | 430 | ASP  |
| 1   | B     | 14  | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 20  | VAL  |
| 1   | B     | 25  | ASN  |
| 1   | B     | 52  | PRO  |
| 1   | B     | 64  | ASN  |
| 1   | B     | 73  | LYS  |
| 1   | B     | 74  | MET  |
| 1   | B     | 75  | SER  |
| 1   | B     | 94  | LYS  |
| 1   | B     | 105 | VAL  |
| 1   | B     | 119 | PRO  |
| 1   | B     | 129 | THR  |
| 1   | B     | 147 | SER  |
| 1   | B     | 154 | LYS  |
| 1   | B     | 155 | LYS  |
| 1   | B     | 162 | VAL  |
| 1   | B     | 176 | ASN  |
| 1   | B     | 190 | VAL  |
| 1   | B     | 209 | GLU  |
| 1   | B     | 228 | GLU  |
| 1   | B     | 230 | SER  |
| 1   | B     | 254 | SER  |
| 1   | B     | 276 | SER  |
| 1   | B     | 316 | VAL  |
| 1   | B     | 318 | VAL  |
| 1   | B     | 349 | LYS  |
| 1   | B     | 358 | THR  |
| 1   | B     | 359 | ILE  |
| 1   | B     | 371 | ASN  |
| 1   | B     | 372 | MET  |
| 1   | B     | 378 | GLU  |
| 1   | B     | 383 | ARG  |
| 1   | B     | 403 | SER  |
| 1   | C     | 9   | ARG  |
| 1   | C     | 10  | ASP  |
| 1   | C     | 14  | ASP  |
| 1   | C     | 20  | VAL  |
| 1   | C     | 25  | ASN  |
| 1   | C     | 52  | PRO  |
| 1   | C     | 64  | ASN  |
| 1   | C     | 73  | LYS  |
| 1   | C     | 74  | MET  |
| 1   | C     | 94  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 105 | VAL  |
| 1   | C     | 119 | PRO  |
| 1   | C     | 129 | THR  |
| 1   | C     | 147 | SER  |
| 1   | C     | 154 | LYS  |
| 1   | C     | 155 | LYS  |
| 1   | C     | 162 | VAL  |
| 1   | C     | 190 | VAL  |
| 1   | C     | 209 | GLU  |
| 1   | C     | 228 | GLU  |
| 1   | C     | 230 | SER  |
| 1   | C     | 254 | SER  |
| 1   | C     | 276 | SER  |
| 1   | C     | 305 | THR  |
| 1   | C     | 316 | VAL  |
| 1   | C     | 318 | VAL  |
| 1   | C     | 349 | LYS  |
| 1   | C     | 358 | THR  |
| 1   | C     | 359 | ILE  |
| 1   | C     | 372 | MET  |
| 1   | C     | 378 | GLU  |
| 1   | C     | 383 | ARG  |
| 1   | C     | 403 | SER  |
| 1   | C     | 428 | VAL  |
| 1   | D     | 14  | ASP  |
| 1   | D     | 20  | VAL  |
| 1   | D     | 52  | PRO  |
| 1   | D     | 64  | ASN  |
| 1   | D     | 73  | LYS  |
| 1   | D     | 74  | MET  |
| 1   | D     | 94  | LYS  |
| 1   | D     | 105 | VAL  |
| 1   | D     | 129 | THR  |
| 1   | D     | 147 | SER  |
| 1   | D     | 154 | LYS  |
| 1   | D     | 155 | LYS  |
| 1   | D     | 162 | VAL  |
| 1   | D     | 190 | VAL  |
| 1   | D     | 209 | GLU  |
| 1   | D     | 228 | GLU  |
| 1   | D     | 230 | SER  |
| 1   | D     | 254 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 276 | SER  |
| 1   | D     | 305 | THR  |
| 1   | D     | 316 | VAL  |
| 1   | D     | 318 | VAL  |
| 1   | D     | 349 | LYS  |
| 1   | D     | 358 | THR  |
| 1   | D     | 359 | ILE  |
| 1   | D     | 378 | GLU  |
| 1   | D     | 383 | ARG  |
| 1   | D     | 403 | SER  |
| 1   | D     | 430 | ASP  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 25  | ASN  |
| 1   | A     | 28  | GLN  |
| 1   | A     | 29  | GLN  |
| 1   | A     | 31  | HIS  |
| 1   | A     | 34  | GLN  |
| 1   | A     | 64  | ASN  |
| 1   | A     | 88  | HIS  |
| 1   | A     | 138 | GLN  |
| 1   | A     | 157 | GLN  |
| 1   | A     | 176 | ASN  |
| 1   | A     | 364 | ASN  |
| 1   | A     | 371 | ASN  |
| 1   | A     | 374 | GLN  |
| 1   | A     | 389 | HIS  |
| 1   | A     | 399 | HIS  |
| 1   | A     | 424 | HIS  |
| 1   | B     | 25  | ASN  |
| 1   | B     | 28  | GLN  |
| 1   | B     | 29  | GLN  |
| 1   | B     | 31  | HIS  |
| 1   | B     | 34  | GLN  |
| 1   | B     | 64  | ASN  |
| 1   | B     | 88  | HIS  |
| 1   | B     | 138 | GLN  |
| 1   | B     | 157 | GLN  |
| 1   | B     | 176 | ASN  |
| 1   | B     | 294 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 364 | ASN  |
| 1   | B     | 389 | HIS  |
| 1   | B     | 399 | HIS  |
| 1   | B     | 424 | HIS  |
| 1   | C     | 25  | ASN  |
| 1   | C     | 28  | GLN  |
| 1   | C     | 29  | GLN  |
| 1   | C     | 31  | HIS  |
| 1   | C     | 34  | GLN  |
| 1   | C     | 64  | ASN  |
| 1   | C     | 88  | HIS  |
| 1   | C     | 138 | GLN  |
| 1   | C     | 157 | GLN  |
| 1   | C     | 176 | ASN  |
| 1   | C     | 294 | ASN  |
| 1   | C     | 364 | ASN  |
| 1   | C     | 389 | HIS  |
| 1   | C     | 399 | HIS  |
| 1   | C     | 424 | HIS  |
| 1   | D     | 25  | ASN  |
| 1   | D     | 28  | GLN  |
| 1   | D     | 29  | GLN  |
| 1   | D     | 31  | HIS  |
| 1   | D     | 34  | GLN  |
| 1   | D     | 64  | ASN  |
| 1   | D     | 88  | HIS  |
| 1   | D     | 138 | GLN  |
| 1   | D     | 157 | GLN  |
| 1   | D     | 176 | ASN  |
| 1   | D     | 193 | GLN  |
| 1   | D     | 224 | HIS  |
| 1   | D     | 364 | ASN  |
| 1   | D     | 389 | HIS  |
| 1   | D     | 399 | HIS  |
| 1   | D     | 424 | HIS  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 32 ligands modelled in this entry, 8 are monoatomic - leaving 24 for Mogul analysis.

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

| Mol | Type | Chain | Res    | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|--------|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |        |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 5   | WO4  | A     | 440    | 3,4  | 2,4,4        | 2.52 | 1 (50%)     | -           |      |             |
| 2   | NAG  | D     | 433(A) | 1    | 14,14,15     | 0.93 | 1 (7%)      | 17,19,21    | 1.26 | 2 (11%)     |
| 2   | NAG  | A     | 436(A) | 1    | 14,14,15     | 1.33 | 3 (21%)     | 17,19,21    | 1.25 | 2 (11%)     |
| 2   | NAG  | A     | 434(A) | 1    | 14,14,15     | 0.85 | 0           | 17,19,21    | 1.44 | 1 (5%)      |
| 2   | NAG  | C     | 435(A) | 1    | 14,14,15     | 0.50 | 0           | 17,19,21    | 0.83 | 0           |
| 2   | NAG  | C     | 434(A) | 1    | 14,14,15     | 1.00 | 1 (7%)      | 17,19,21    | 1.61 | 4 (23%)     |
| 2   | NAG  | A     | 435(A) | 1    | 14,14,15     | 0.57 | 0           | 17,19,21    | 1.00 | 1 (5%)      |
| 2   | NAG  | C     | 436(A) | 1    | 14,14,15     | 1.43 | 3 (21%)     | 17,19,21    | 1.24 | 3 (17%)     |
| 2   | NAG  | D     | 434(A) | 1    | 14,14,15     | 0.85 | 0           | 17,19,21    | 1.51 | 2 (11%)     |
| 2   | NAG  | B     | 435(A) | 1    | 14,14,15     | 0.79 | 0           | 17,19,21    | 0.61 | 0           |
| 2   | NAG  | C     | 433(A) | 1    | 14,14,15     | 1.14 | 1 (7%)      | 17,19,21    | 1.10 | 1 (5%)      |
| 2   | NAG  | C     | 437(A) | 1    | 14,14,15     | 1.13 | 2 (14%)     | 17,19,21    | 1.09 | 2 (11%)     |
| 2   | NAG  | A     | 433(A) | 1    | 14,14,15     | 0.95 | 0           | 17,19,21    | 1.22 | 2 (11%)     |
| 5   | WO4  | C     | 440    | 3,4  | 2,4,4        | 4.78 | 2 (100%)    | -           |      |             |
| 2   | NAG  | B     | 433(A) | 1    | 14,14,15     | 1.18 | 1 (7%)      | 17,19,21    | 1.29 | 2 (11%)     |
| 2   | NAG  | B     | 434(A) | 1    | 14,14,15     | 0.67 | 0           | 17,19,21    | 1.23 | 2 (11%)     |
| 5   | WO4  | D     | 440    | 3,4  | 2,4,4        | 2.55 | 1 (50%)     | -           |      |             |
| 5   | WO4  | B     | 440    | 3,4  | 2,4,4        | 3.32 | 1 (50%)     | -           |      |             |

| Mol | Type | Chain | Res    | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|--------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |        |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 2   | NAG  | A     | 437(A) | 1    | 14,14,15     | 0.91 | 0        | 17,19,21    | 1.12 | 2 (11%)  |
| 2   | NAG  | B     | 436(A) | 1    | 14,14,15     | 1.49 | 3 (21%)  | 17,19,21    | 1.23 | 3 (17%)  |
| 2   | NAG  | D     | 436(A) | 1    | 14,14,15     | 1.34 | 2 (14%)  | 17,19,21    | 1.13 | 2 (11%)  |
| 2   | NAG  | D     | 437(A) | 1    | 14,14,15     | 1.23 | 2 (14%)  | 17,19,21    | 1.11 | 1 (5%)   |
| 2   | NAG  | B     | 437(A) | 1    | 14,14,15     | 1.01 | 0        | 17,19,21    | 0.90 | 1 (5%)   |
| 2   | NAG  | D     | 435(A) | 1    | 14,14,15     | 0.61 | 0        | 17,19,21    | 0.84 | 0        |

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

| Mol | Type | Chain | Res    | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|--------|------|---------|-----------|---------|
| 2   | NAG  | D     | 433(A) | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 2   | NAG  | A     | 436(A) | 1    | -       | 4/6/23/26 | 0/1/1/1 |
| 2   | NAG  | A     | 434(A) | 1    | -       | 4/6/23/26 | 0/1/1/1 |
| 2   | NAG  | C     | 435(A) | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 2   | NAG  | C     | 434(A) | 1    | -       | 4/6/23/26 | 0/1/1/1 |
| 2   | NAG  | A     | 435(A) | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 2   | NAG  | C     | 436(A) | 1    | -       | 4/6/23/26 | 0/1/1/1 |
| 2   | NAG  | D     | 434(A) | 1    | -       | 4/6/23/26 | 0/1/1/1 |
| 2   | NAG  | B     | 435(A) | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 2   | NAG  | C     | 433(A) | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 2   | NAG  | C     | 437(A) | 1    | -       | 0/6/23/26 | 0/1/1/1 |
| 2   | NAG  | A     | 433(A) | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 2   | NAG  | B     | 433(A) | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 2   | NAG  | B     | 434(A) | 1    | -       | 4/6/23/26 | 0/1/1/1 |
| 2   | NAG  | A     | 437(A) | 1    | -       | 0/6/23/26 | 0/1/1/1 |
| 2   | NAG  | B     | 436(A) | 1    | -       | 4/6/23/26 | 0/1/1/1 |
| 2   | NAG  | D     | 436(A) | 1    | -       | 4/6/23/26 | 0/1/1/1 |
| 2   | NAG  | D     | 437(A) | 1    | -       | 0/6/23/26 | 0/1/1/1 |
| 2   | NAG  | B     | 437(A) | 1    | -       | 0/6/23/26 | 0/1/1/1 |
| 2   | NAG  | D     | 435(A) | 1    | -       | 2/6/23/26 | 0/1/1/1 |

All (24) bond length outliers are listed below:

| Mol | Chain | Res    | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|-------|-------|-------------|----------|
| 5   | C     | 440    | WO4  | W-O2  | -5.39 | 1.65        | 1.77     |
| 5   | B     | 440    | WO4  | W-O2  | -4.40 | 1.67        | 1.77     |
| 5   | C     | 440    | WO4  | W-O1  | -4.09 | 1.68        | 1.77     |
| 2   | B     | 436(A) | NAG  | C1-C2 | 3.65  | 1.57        | 1.52     |
| 5   | D     | 440    | WO4  | W-O2  | -3.51 | 1.69        | 1.77     |
| 5   | A     | 440    | WO4  | W-O2  | -3.33 | 1.69        | 1.77     |
| 2   | D     | 436(A) | NAG  | C1-C2 | 3.14  | 1.56        | 1.52     |
| 2   | C     | 436(A) | NAG  | C1-C2 | 3.07  | 1.56        | 1.52     |
| 2   | C     | 433(A) | NAG  | C1-C2 | 2.92  | 1.56        | 1.52     |
| 2   | B     | 433(A) | NAG  | C1-C2 | 2.91  | 1.56        | 1.52     |
| 2   | A     | 436(A) | NAG  | C1-C2 | 2.85  | 1.56        | 1.52     |
| 2   | C     | 437(A) | NAG  | C3-C2 | 2.52  | 1.57        | 1.52     |
| 2   | D     | 433(A) | NAG  | C1-C2 | 2.51  | 1.55        | 1.52     |
| 2   | D     | 437(A) | NAG  | C4-C3 | 2.37  | 1.58        | 1.52     |
| 2   | B     | 436(A) | NAG  | C4-C5 | 2.37  | 1.58        | 1.53     |
| 2   | C     | 436(A) | NAG  | O5-C5 | 2.35  | 1.48        | 1.43     |
| 2   | C     | 436(A) | NAG  | C4-C5 | 2.29  | 1.57        | 1.53     |
| 2   | A     | 436(A) | NAG  | O5-C5 | 2.27  | 1.47        | 1.43     |
| 2   | D     | 436(A) | NAG  | O5-C5 | 2.21  | 1.47        | 1.43     |
| 2   | C     | 434(A) | NAG  | C3-C2 | 2.15  | 1.57        | 1.52     |
| 2   | D     | 437(A) | NAG  | C3-C2 | 2.12  | 1.57        | 1.52     |
| 2   | A     | 436(A) | NAG  | C4-C5 | 2.07  | 1.57        | 1.53     |
| 2   | B     | 436(A) | NAG  | O5-C5 | 2.05  | 1.47        | 1.43     |
| 2   | C     | 437(A) | NAG  | C4-C3 | 2.04  | 1.57        | 1.52     |

All (33) bond angle outliers are listed below:

| Mol | Chain | Res    | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|----------|-------|-------------|----------|
| 2   | C     | 434(A) | NAG  | C4-C3-C2 | -4.61 | 104.26      | 111.02   |
| 2   | A     | 434(A) | NAG  | C4-C3-C2 | -4.39 | 104.59      | 111.02   |
| 2   | D     | 434(A) | NAG  | C4-C3-C2 | -4.38 | 104.61      | 111.02   |
| 2   | B     | 434(A) | NAG  | C4-C3-C2 | -3.41 | 106.02      | 111.02   |
| 2   | D     | 437(A) | NAG  | C4-C3-C2 | -2.95 | 106.70      | 111.02   |
| 2   | A     | 436(A) | NAG  | C4-C3-C2 | -2.94 | 106.71      | 111.02   |
| 2   | D     | 433(A) | NAG  | C4-C3-C2 | -2.84 | 106.85      | 111.02   |
| 2   | C     | 436(A) | NAG  | C4-C3-C2 | -2.80 | 106.92      | 111.02   |
| 2   | A     | 435(A) | NAG  | C2-N2-C7 | -2.79 | 119.16      | 122.90   |
| 2   | D     | 433(A) | NAG  | C2-N2-C7 | -2.77 | 119.19      | 122.90   |
| 2   | B     | 433(A) | NAG  | C4-C3-C2 | -2.73 | 107.02      | 111.02   |
| 2   | A     | 437(A) | NAG  | C2-N2-C7 | -2.69 | 119.29      | 122.90   |
| 2   | B     | 436(A) | NAG  | C4-C3-C2 | -2.67 | 107.11      | 111.02   |
| 2   | A     | 433(A) | NAG  | C4-C3-C2 | -2.58 | 107.23      | 111.02   |
| 2   | A     | 433(A) | NAG  | C2-N2-C7 | -2.57 | 119.46      | 122.90   |

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| Mol | Chain | Res    | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|----------|-------|-------------|----------|
| 2   | A     | 437(A) | NAG  | C4-C3-C2 | -2.51 | 107.34      | 111.02   |
| 2   | C     | 437(A) | NAG  | C4-C3-C2 | -2.50 | 107.35      | 111.02   |
| 2   | D     | 436(A) | NAG  | C4-C3-C2 | -2.49 | 107.37      | 111.02   |
| 2   | C     | 434(A) | NAG  | O5-C1-C2 | -2.48 | 107.45      | 111.29   |
| 2   | B     | 433(A) | NAG  | C2-N2-C7 | -2.42 | 119.66      | 122.90   |
| 2   | C     | 437(A) | NAG  | C2-N2-C7 | -2.40 | 119.68      | 122.90   |
| 2   | D     | 436(A) | NAG  | C1-O5-C5 | 2.39  | 115.39      | 112.19   |
| 2   | B     | 437(A) | NAG  | C4-C3-C2 | -2.39 | 107.52      | 111.02   |
| 2   | A     | 436(A) | NAG  | C1-O5-C5 | 2.34  | 115.32      | 112.19   |
| 2   | C     | 436(A) | NAG  | C1-C2-N2 | 2.33  | 114.10      | 110.43   |
| 2   | C     | 433(A) | NAG  | C4-C3-C2 | -2.31 | 107.63      | 111.02   |
| 2   | B     | 436(A) | NAG  | C1-C2-N2 | 2.31  | 114.07      | 110.43   |
| 2   | C     | 436(A) | NAG  | C1-O5-C5 | 2.31  | 115.28      | 112.19   |
| 2   | D     | 434(A) | NAG  | O5-C1-C2 | -2.26 | 107.79      | 111.29   |
| 2   | B     | 436(A) | NAG  | C1-O5-C5 | 2.22  | 115.16      | 112.19   |
| 2   | C     | 434(A) | NAG  | C2-N2-C7 | -2.21 | 119.94      | 122.90   |
| 2   | C     | 434(A) | NAG  | O3-C3-C2 | 2.14  | 113.85      | 109.40   |
| 2   | B     | 434(A) | NAG  | O5-C1-C2 | -2.10 | 108.05      | 111.29   |

There are no chirality outliers.

All (48) torsion outliers are listed below:

| Mol | Chain | Res    | Type | Atoms       |
|-----|-------|--------|------|-------------|
| 2   | A     | 434(A) | NAG  | C1-C2-N2-C7 |
| 2   | B     | 434(A) | NAG  | C1-C2-N2-C7 |
| 2   | D     | 434(A) | NAG  | C1-C2-N2-C7 |
| 2   | A     | 436(A) | NAG  | O5-C5-C6-O6 |
| 2   | C     | 435(A) | NAG  | O5-C5-C6-O6 |
| 2   | D     | 435(A) | NAG  | O5-C5-C6-O6 |
| 2   | D     | 436(A) | NAG  | O5-C5-C6-O6 |
| 2   | C     | 436(A) | NAG  | O5-C5-C6-O6 |
| 2   | A     | 435(A) | NAG  | O5-C5-C6-O6 |
| 2   | B     | 435(A) | NAG  | O5-C5-C6-O6 |
| 2   | B     | 436(A) | NAG  | O5-C5-C6-O6 |
| 2   | D     | 436(A) | NAG  | C4-C5-C6-O6 |
| 2   | B     | 436(A) | NAG  | C4-C5-C6-O6 |
| 2   | C     | 434(A) | NAG  | O5-C5-C6-O6 |
| 2   | C     | 435(A) | NAG  | C4-C5-C6-O6 |
| 2   | A     | 436(A) | NAG  | C4-C5-C6-O6 |
| 2   | C     | 434(A) | NAG  | C4-C5-C6-O6 |
| 2   | B     | 434(A) | NAG  | O5-C5-C6-O6 |
| 2   | D     | 434(A) | NAG  | O5-C5-C6-O6 |

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| Mol | Chain | Res    | Type | Atoms       |
|-----|-------|--------|------|-------------|
| 2   | A     | 434(A) | NAG  | O5-C5-C6-O6 |
| 2   | B     | 433(A) | NAG  | O5-C5-C6-O6 |
| 2   | A     | 435(A) | NAG  | C4-C5-C6-O6 |
| 2   | B     | 435(A) | NAG  | C4-C5-C6-O6 |
| 2   | D     | 435(A) | NAG  | C4-C5-C6-O6 |
| 2   | D     | 434(A) | NAG  | C4-C5-C6-O6 |
| 2   | A     | 434(A) | NAG  | C4-C5-C6-O6 |
| 2   | B     | 434(A) | NAG  | C4-C5-C6-O6 |
| 2   | D     | 433(A) | NAG  | O5-C5-C6-O6 |
| 2   | C     | 436(A) | NAG  | C4-C5-C6-O6 |
| 2   | A     | 433(A) | NAG  | O5-C5-C6-O6 |
| 2   | C     | 433(A) | NAG  | O5-C5-C6-O6 |
| 2   | B     | 433(A) | NAG  | C4-C5-C6-O6 |
| 2   | A     | 436(A) | NAG  | C1-C2-N2-C7 |
| 2   | B     | 436(A) | NAG  | C1-C2-N2-C7 |
| 2   | C     | 434(A) | NAG  | C1-C2-N2-C7 |
| 2   | C     | 436(A) | NAG  | C1-C2-N2-C7 |
| 2   | D     | 436(A) | NAG  | C1-C2-N2-C7 |
| 2   | C     | 433(A) | NAG  | C4-C5-C6-O6 |
| 2   | D     | 433(A) | NAG  | C4-C5-C6-O6 |
| 2   | A     | 433(A) | NAG  | C4-C5-C6-O6 |
| 2   | A     | 434(A) | NAG  | C3-C2-N2-C7 |
| 2   | A     | 436(A) | NAG  | C3-C2-N2-C7 |
| 2   | B     | 434(A) | NAG  | C3-C2-N2-C7 |
| 2   | B     | 436(A) | NAG  | C3-C2-N2-C7 |
| 2   | C     | 434(A) | NAG  | C3-C2-N2-C7 |
| 2   | C     | 436(A) | NAG  | C3-C2-N2-C7 |
| 2   | D     | 434(A) | NAG  | C3-C2-N2-C7 |
| 2   | D     | 436(A) | NAG  | C3-C2-N2-C7 |

There are no ring outliers.

5 monomers are involved in 8 short contacts:

| Mol | Chain | Res    | Type | Clashes | Symm-Clashes |
|-----|-------|--------|------|---------|--------------|
| 2   | A     | 436(A) | NAG  | 2       | 0            |
| 2   | C     | 436(A) | NAG  | 2       | 0            |
| 5   | D     | 440    | WO4  | 1       | 0            |
| 2   | B     | 436(A) | NAG  | 2       | 0            |
| 2   | D     | 436(A) | NAG  | 1       | 0            |

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.