



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 04:04 AM UTC

PDB ID : 1BU6 / pdb\_00001bu6  
Title : CRYSTAL STRUCTURES OF ESCHERICHIA COLI GLYCEROL KINASE AND THE MUTANT A65T IN AN INACTIVE TETRAMER: CONFORMATIONAL CHANGES AND IMPLICATIONS FOR ALLOSTERIC REGULATION  
Authors : Feese, M.D.; Faber, H.R.; Bystrom, C.E.; Pettigrew, D.W.; Remington, S.J.  
Deposited on : 1998-08-30  
Resolution : 2.37 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                     |
| Xtriage (Phenix)               | : | 2.0                                                              |
| EDS                            | : | 3.0                                                              |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| CCP4                           | : | 9.0.010 (Gargrove)                                               |
| Density-Fitness                | : | 1.0.12                                                           |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

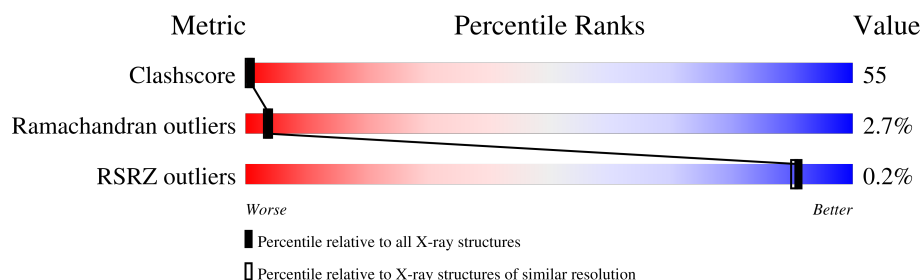
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.37 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                      | 7722 (2.40-2.36)                                      |
| Ramachandran outliers | 187476                      | 7626 (2.40-2.36)                                      |
| RSRZ outliers         | 180081                      | 7170 (2.40-2.36)                                      |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | O     | 501    |                  |
| 1   | X     | 501    |                  |
| 1   | Y     | 501    |                  |
| 1   | Z     | 501    |                  |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 2   | SO4  | O     | 502 | -         | -        | X       | -                |
| 3   | GOL  | Z     | 504 | -         | -        | X       | -                |

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15815 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.

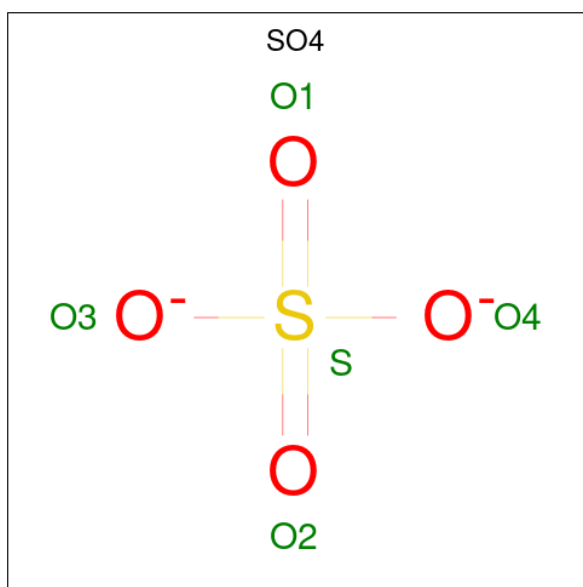
- Molecule 1 is a protein called PROTEIN (GLYCEROL KINASE).

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | O     | 497      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3891  | 2452 | 680 | 740 | 19 |         |         |       |
| 1   | Y     | 499      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3921  | 2471 | 686 | 745 | 19 |         |         |       |
| 1   | Z     | 498      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3913  | 2465 | 686 | 743 | 19 |         |         |       |
| 1   | X     | 498      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3896  | 2456 | 681 | 740 | 19 |         |         |       |

There are 4 discrepancies between the modelled and reference sequences:

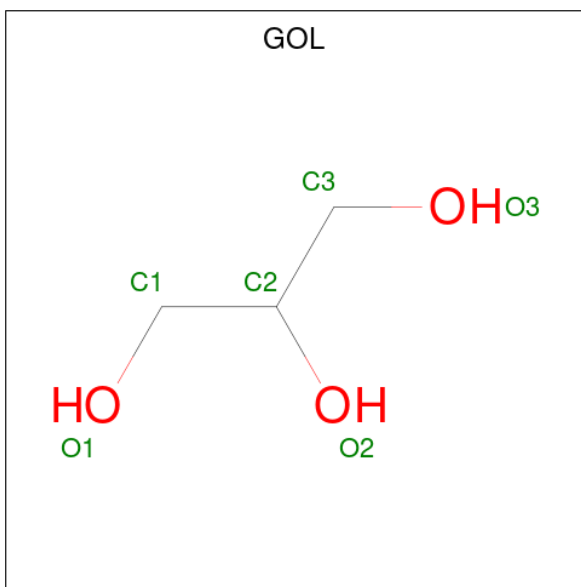
| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| O     | 65      | THR      | ALA    | engineered mutation | UNP P0A6F3 |
| Y     | 65      | THR      | ALA    | engineered mutation | UNP P0A6F3 |
| Z     | 65      | THR      | ALA    | engineered mutation | UNP P0A6F3 |
| X     | 65      | THR      | ALA    | engineered mutation | UNP P0A6F3 |

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 2   | O     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | O     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | Y     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | Z     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | Z     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | X     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 3   | O     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 3   | Y     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 3   | Z     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 3   | X     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |

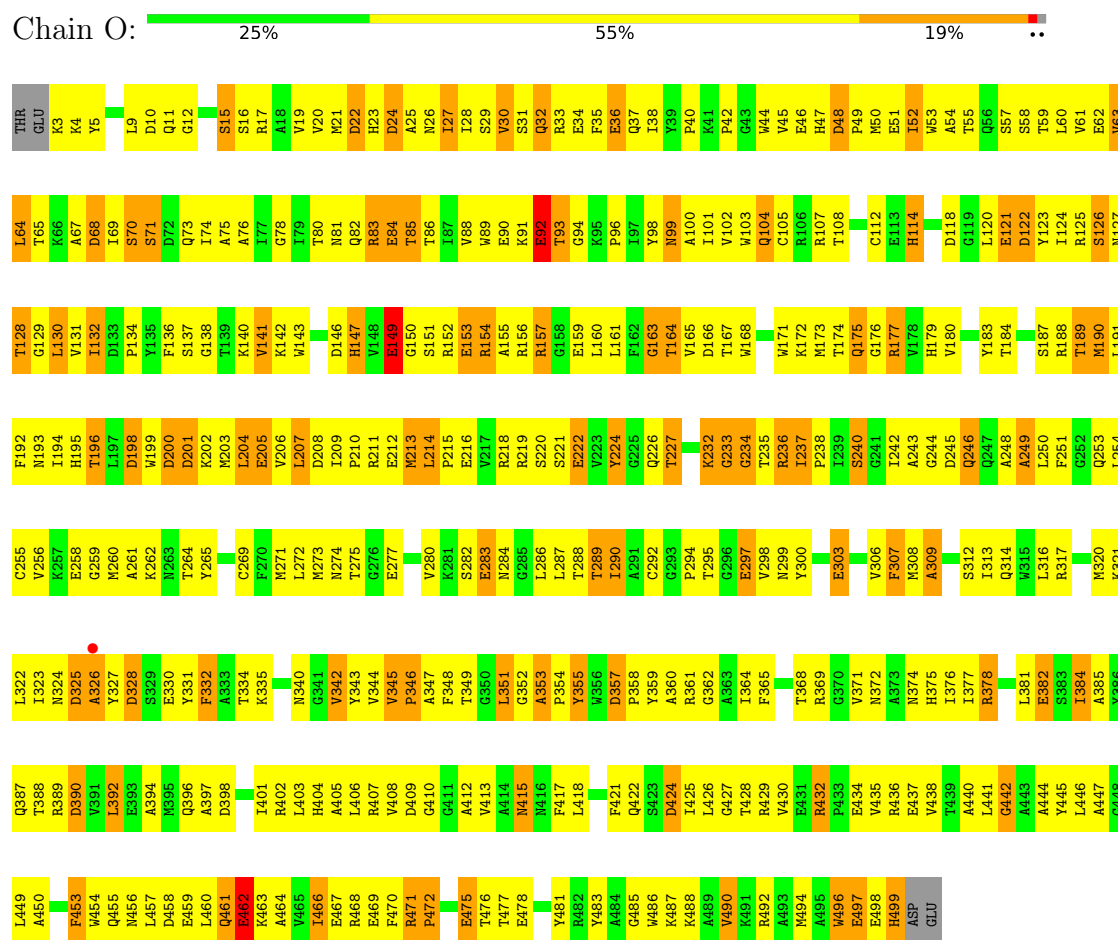
- Molecule 4 is water.

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 4   | O     | 29       | Total | O  | 0       | 0       |
|     |       |          | 29    | 29 |         |         |
| 4   | Y     | 38       | Total | O  | 0       | 0       |
|     |       |          | 38    | 38 |         |         |
| 4   | Z     | 31       | Total | O  | 0       | 0       |
|     |       |          | 31    | 31 |         |         |
| 4   | X     | 42       | Total | O  | 0       | 0       |
|     |       |          | 42    | 42 |         |         |

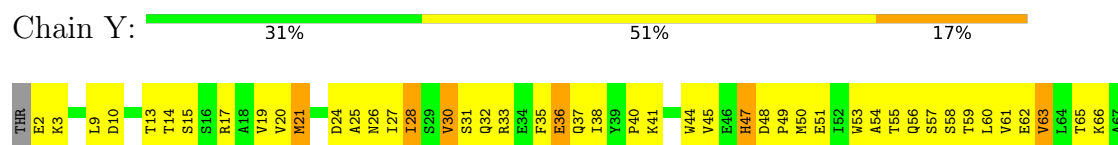
### 3 Residue-property plots

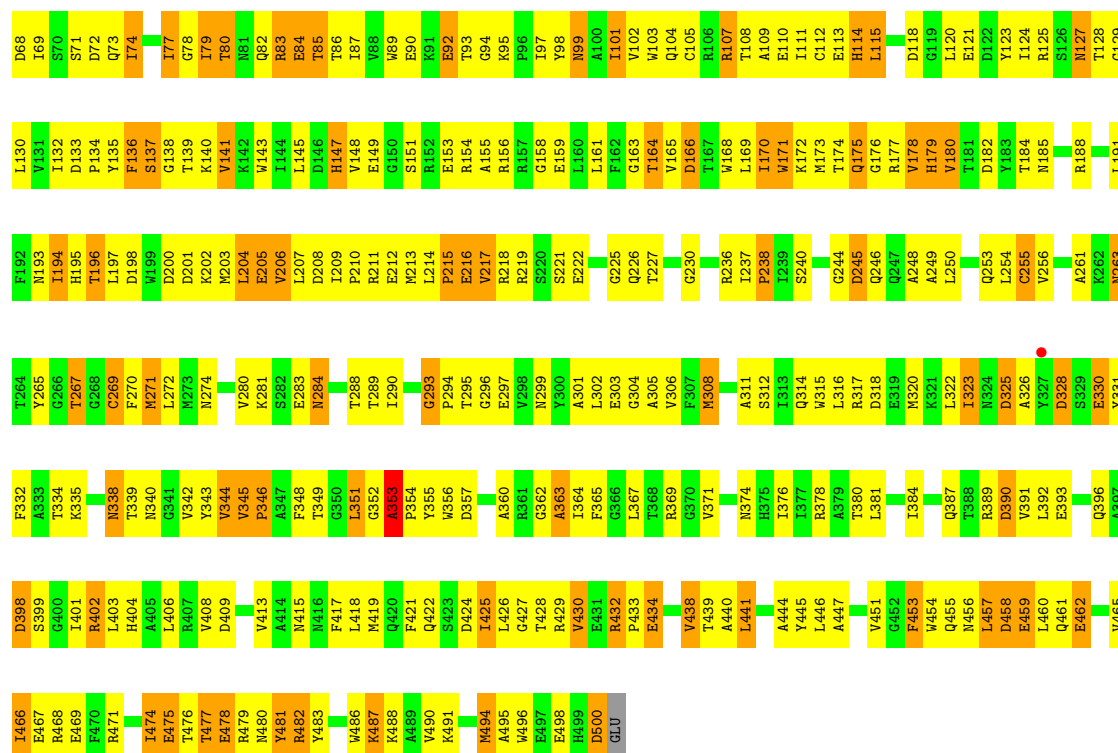
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

#### • Molecule 1: PROTEIN (GLYCEROL KINASE)

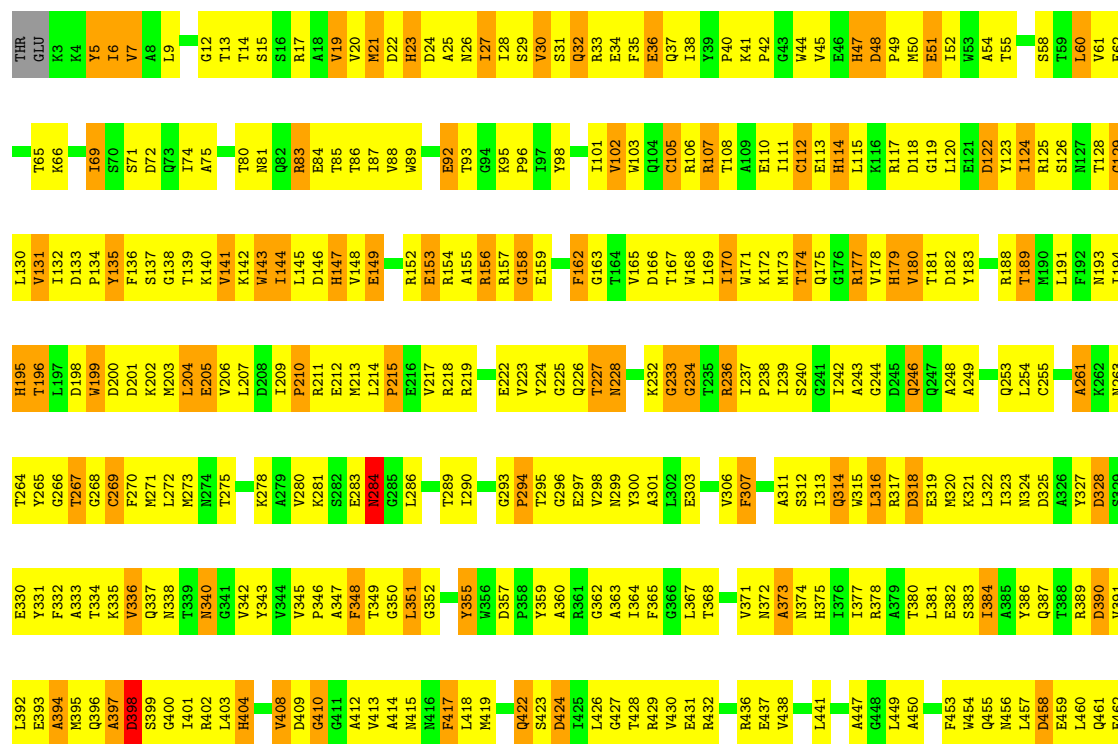
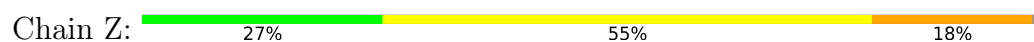


#### • Molecule 1: PROTEIN (GLYCEROL KINASE)

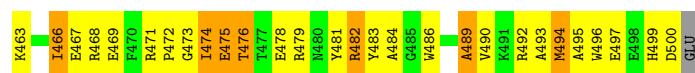




### • Molecule 1: PROTEIN (GLYCEROL KINASE)

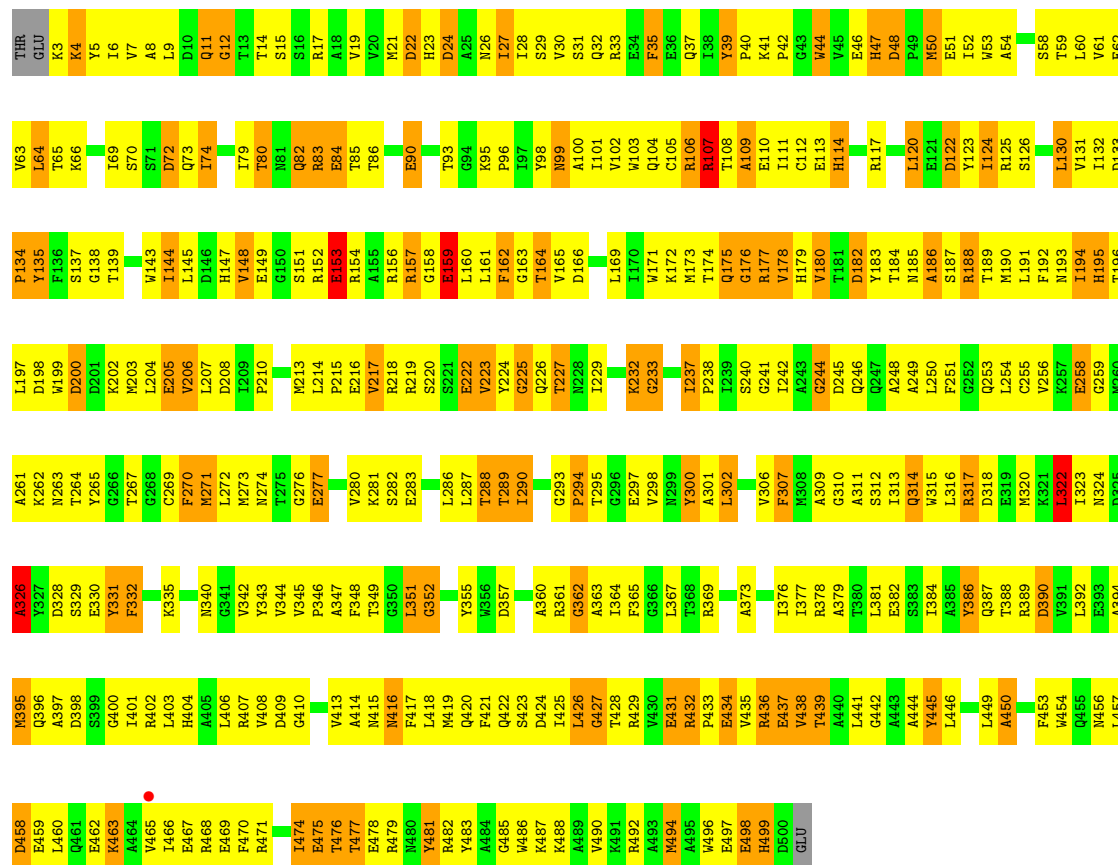






• Molecule 1: PROTEIN (GLYCEROL KINASE)

Chain X: 27% 52% 20%



## 4 Data and refinement statistics

| Property                                                                | Value                                                        | Source           |
|-------------------------------------------------------------------------|--------------------------------------------------------------|------------------|
| Space group                                                             | P 1 21 1                                                     | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 91.90Å 119.00Å 109.30Å<br>90.00° 103.40° 90.00°              | Depositor        |
| Resolution (Å)                                                          | 20.00 – 2.37<br>20.00 – 2.37                                 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 74.0 (20.00-2.37)<br>72.2 (20.00-2.37)                       | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.07                                                         | Depositor        |
| $R_{sym}$                                                               | (Not available)                                              | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 0.49 (at 2.37Å)                                              | Xtriage          |
| Refinement program                                                      | TNT 5F-6                                                     | Depositor        |
| R, $R_{free}$                                                           | 0.167 , (Not available)<br>(Not available) , (Not available) | Depositor<br>DCC |
| $R_{free}$ test set                                                     | No test flags present.                                       | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 31.5                                                         | Xtriage          |
| Anisotropy                                                              | 0.469                                                        | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.32 , 148.6                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$  | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                       | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.96                                                         | EDS              |
| Total number of atoms                                                   | 15815                                                        | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 38.0                                                         | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 32.80 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.8628e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, GOL

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   | O     | 1.64         | 43/3970 (1.1%)   | 2.07        | 127/5387 (2.4%)  |
| 1   | X     | 1.63         | 36/3975 (0.9%)   | 2.11        | 163/5393 (3.0%)  |
| 1   | Y     | 1.58         | 30/4001 (0.7%)   | 2.06        | 124/5427 (2.3%)  |
| 1   | Z     | 1.60         | 37/3992 (0.9%)   | 2.04        | 121/5413 (2.2%)  |
| All | All   | 1.61         | 146/15938 (0.9%) | 2.07        | 535/21620 (2.5%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | X     | 2                   | 0                   |
| 1   | Z     | 1                   | 0                   |
| All | All   | 3                   | 0                   |

All (146) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | X     | 475 | GLU  | CD-OE2 | 9.83  | 1.44        | 1.25     |
| 1   | X     | 84  | GLU  | N-CA   | 8.63  | 1.56        | 1.46     |
| 1   | X     | 117 | ARG  | NE-CZ  | 8.40  | 1.42        | 1.33     |
| 1   | X     | 237 | ILE  | CA-C   | -8.17 | 1.44        | 1.52     |
| 1   | Y     | 475 | GLU  | CD-OE2 | 7.25  | 1.39        | 1.25     |
| 1   | O     | 357 | ASP  | C-N    | -7.18 | 1.27        | 1.33     |
| 1   | X     | 53  | TRP  | C-O    | 6.95  | 1.32        | 1.24     |
| 1   | Z     | 236 | ARG  | C-N    | 6.91  | 1.41        | 1.33     |
| 1   | Y     | 345 | VAL  | CA-CB  | -6.83 | 1.48        | 1.54     |
| 1   | Z     | 384 | ILE  | CA-CB  | -6.81 | 1.46        | 1.54     |
| 1   | Z     | 131 | VAL  | CA-CB  | -6.77 | 1.48        | 1.55     |
| 1   | O     | 130 | LEU  | CA-C   | -6.72 | 1.46        | 1.53     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | O     | 353 | ALA  | CA-C   | -6.52 | 1.45        | 1.53     |
| 1   | Z     | 424 | ASP  | C-O    | -6.50 | 1.16        | 1.24     |
| 1   | Y     | 482 | ARG  | NE-CZ  | 6.45  | 1.40        | 1.33     |
| 1   | Y     | 402 | ARG  | NE-CZ  | 6.43  | 1.40        | 1.33     |
| 1   | O     | 157 | ARG  | NE-CZ  | 6.37  | 1.40        | 1.33     |
| 1   | Z     | 38  | ILE  | CA-CB  | -6.37 | 1.46        | 1.54     |
| 1   | Z     | 36  | GLU  | CD-OE2 | 6.32  | 1.37        | 1.25     |
| 1   | X     | 117 | ARG  | CD-NE  | 6.27  | 1.55        | 1.46     |
| 1   | Z     | 264 | THR  | N-CA   | -6.22 | 1.38        | 1.46     |
| 1   | Y     | 217 | VAL  | CA-C   | -6.20 | 1.45        | 1.52     |
| 1   | Y     | 323 | ILE  | CA-C   | -6.17 | 1.45        | 1.52     |
| 1   | X     | 227 | THR  | CA-C   | -6.13 | 1.45        | 1.52     |
| 1   | Y     | 84  | GLU  | CD-OE1 | 6.08  | 1.36        | 1.25     |
| 1   | O     | 10  | ASP  | CA-C   | -6.08 | 1.45        | 1.53     |
| 1   | O     | 224 | TYR  | C-N    | 6.07  | 1.39        | 1.33     |
| 1   | Y     | 434 | GLU  | CD-OE2 | 6.03  | 1.36        | 1.25     |
| 1   | X     | 386 | TYR  | CA-C   | -5.99 | 1.45        | 1.52     |
| 1   | O     | 160 | LEU  | CA-C   | -5.93 | 1.45        | 1.52     |
| 1   | X     | 390 | ASP  | CG-OD1 | 5.92  | 1.36        | 1.25     |
| 1   | X     | 362 | GLY  | CA-C   | 5.91  | 1.59        | 1.52     |
| 1   | O     | 153 | GLU  | CA-C   | -5.91 | 1.44        | 1.52     |
| 1   | Y     | 195 | HIS  | CA-C   | -5.90 | 1.46        | 1.52     |
| 1   | X     | 298 | VAL  | N-CA   | -5.90 | 1.39        | 1.46     |
| 1   | O     | 244 | GLY  | C-O    | 5.89  | 1.29        | 1.23     |
| 1   | O     | 475 | GLU  | CD-OE1 | 5.89  | 1.36        | 1.25     |
| 1   | X     | 39  | TYR  | N-CA   | -5.88 | 1.40        | 1.46     |
| 1   | X     | 83  | ARG  | N-CA   | -5.87 | 1.39        | 1.46     |
| 1   | Y     | 500 | ASP  | CG-OD1 | 5.87  | 1.36        | 1.25     |
| 1   | Z     | 149 | GLU  | CD-OE1 | 5.87  | 1.36        | 1.25     |
| 1   | Z     | 205 | GLU  | CA-C   | -5.82 | 1.45        | 1.52     |
| 1   | X     | 277 | GLU  | CD-OE2 | 5.74  | 1.36        | 1.25     |
| 1   | Z     | 264 | THR  | CA-C   | -5.72 | 1.45        | 1.52     |
| 1   | Y     | 83  | ARG  | CA-C   | -5.72 | 1.44        | 1.52     |
| 1   | X     | 83  | ARG  | CA-C   | -5.70 | 1.45        | 1.52     |
| 1   | Z     | 32  | GLN  | CA-C   | -5.68 | 1.45        | 1.52     |
| 1   | Z     | 34  | GLU  | CD-OE1 | 5.65  | 1.36        | 1.25     |
| 1   | Z     | 143 | TRP  | CA-C   | -5.64 | 1.45        | 1.52     |
| 1   | Z     | 475 | GLU  | CD-OE2 | 5.62  | 1.36        | 1.25     |
| 1   | X     | 122 | ASP  | CG-OD2 | 5.61  | 1.36        | 1.25     |
| 1   | Z     | 246 | GLN  | CA-C   | -5.61 | 1.45        | 1.52     |
| 1   | O     | 27  | ILE  | C-N    | -5.60 | 1.28        | 1.33     |
| 1   | Z     | 144 | ILE  | CA-CB  | -5.57 | 1.47        | 1.54     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | O     | 84  | GLU  | N-CA    | 5.57  | 1.53        | 1.46     |
| 1   | Z     | 48  | ASP  | CG-OD1  | 5.56  | 1.35        | 1.25     |
| 1   | O     | 92  | GLU  | CD-OE1  | 5.56  | 1.35        | 1.25     |
| 1   | O     | 346 | PRO  | C-N     | -5.54 | 1.26        | 1.33     |
| 1   | Y     | 205 | GLU  | N-CA    | -5.54 | 1.39        | 1.46     |
| 1   | O     | 130 | LEU  | C-N     | -5.53 | 1.26        | 1.33     |
| 1   | Y     | 101 | ILE  | CA-CB   | -5.51 | 1.47        | 1.54     |
| 1   | Z     | 424 | ASP  | C-N     | -5.51 | 1.27        | 1.33     |
| 1   | Z     | 6   | ILE  | N-CA    | -5.51 | 1.39        | 1.46     |
| 1   | O     | 154 | ARG  | N-CA    | -5.50 | 1.39        | 1.46     |
| 1   | Z     | 156 | ARG  | NE-CZ   | 5.49  | 1.39        | 1.33     |
| 1   | Y     | 170 | ILE  | CA-CB   | -5.48 | 1.48        | 1.54     |
| 1   | Z     | 69  | ILE  | CA-CB   | -5.47 | 1.47        | 1.54     |
| 1   | X     | 82  | GLN  | CA-C    | -5.47 | 1.45        | 1.52     |
| 1   | Y     | 205 | GLU  | CA-C    | -5.47 | 1.46        | 1.52     |
| 1   | X     | 395 | MET  | N-CA    | -5.47 | 1.39        | 1.46     |
| 1   | O     | 205 | GLU  | N-CA    | -5.46 | 1.39        | 1.46     |
| 1   | Y     | 216 | GLU  | CD-OE1  | 5.45  | 1.35        | 1.25     |
| 1   | O     | 300 | TYR  | CA-C    | -5.44 | 1.46        | 1.52     |
| 1   | O     | 121 | GLU  | CD-OE1  | 5.43  | 1.35        | 1.25     |
| 1   | Y     | 92  | GLU  | CD-OE1  | 5.41  | 1.35        | 1.25     |
| 1   | Z     | 255 | CYS  | CA-C    | -5.41 | 1.47        | 1.53     |
| 1   | Y     | 171 | TRP  | N-CA    | -5.39 | 1.39        | 1.46     |
| 1   | O     | 326 | ALA  | CA-C    | 5.39  | 1.59        | 1.52     |
| 1   | X     | 162 | PHE  | N-CA    | -5.38 | 1.39        | 1.45     |
| 1   | Z     | 38  | ILE  | N-CA    | -5.37 | 1.39        | 1.46     |
| 1   | X     | 153 | GLU  | CD-OE2  | 5.36  | 1.35        | 1.25     |
| 1   | O     | 36  | GLU  | CD-OE2  | 5.36  | 1.35        | 1.25     |
| 1   | O     | 384 | ILE  | CA-CB   | -5.34 | 1.48        | 1.54     |
| 1   | O     | 15  | SER  | N-CA    | -5.33 | 1.39        | 1.45     |
| 1   | O     | 434 | GLU  | CD-OE2  | 5.33  | 1.35        | 1.25     |
| 1   | O     | 355 | TYR  | CA-C    | -5.32 | 1.45        | 1.52     |
| 1   | Y     | 143 | TRP  | N-CA    | -5.32 | 1.40        | 1.46     |
| 1   | Y     | 346 | PRO  | N-CA    | -5.32 | 1.43        | 1.47     |
| 1   | Y     | 356 | TRP  | NE1-CE2 | 5.32  | 1.43        | 1.37     |
| 1   | Y     | 111 | ILE  | N-CA    | -5.32 | 1.40        | 1.46     |
| 1   | X     | 143 | TRP  | CA-C    | -5.31 | 1.46        | 1.52     |
| 1   | X     | 404 | HIS  | CG-ND1  | 5.30  | 1.44        | 1.38     |
| 1   | O     | 377 | ILE  | CA-CB   | -5.30 | 1.47        | 1.54     |
| 1   | Y     | 204 | LEU  | C-N     | -5.29 | 1.27        | 1.33     |
| 1   | O     | 204 | LEU  | C-N     | -5.29 | 1.26        | 1.33     |
| 1   | X     | 84  | GLU  | CA-C    | -5.29 | 1.46        | 1.52     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | O     | 277 | GLU  | CD-OE2 | 5.29  | 1.35        | 1.25     |
| 1   | X     | 258 | GLU  | CD-OE2 | 5.28  | 1.35        | 1.25     |
| 1   | Z     | 199 | TRP  | CA-C   | -5.27 | 1.46        | 1.52     |
| 1   | O     | 189 | THR  | CA-C   | -5.26 | 1.45        | 1.52     |
| 1   | X     | 82  | GLN  | N-CA   | -5.26 | 1.39        | 1.46     |
| 1   | Z     | 355 | TYR  | CA-C   | -5.23 | 1.46        | 1.52     |
| 1   | Z     | 122 | ASP  | CA-C   | -5.22 | 1.46        | 1.52     |
| 1   | Z     | 110 | GLU  | CD-OE2 | 5.21  | 1.35        | 1.25     |
| 1   | O     | 249 | ALA  | CA-C   | -5.20 | 1.46        | 1.52     |
| 1   | O     | 290 | ILE  | CA-C   | -5.20 | 1.46        | 1.52     |
| 1   | X     | 22  | ASP  | CG-OD1 | 5.19  | 1.35        | 1.25     |
| 1   | X     | 205 | GLU  | CD-OE2 | 5.18  | 1.35        | 1.25     |
| 1   | Y     | 194 | ILE  | CA-C   | -5.18 | 1.46        | 1.52     |
| 1   | O     | 22  | ASP  | CG-OD1 | 5.17  | 1.35        | 1.25     |
| 1   | O     | 175 | GLN  | CA-C   | -5.17 | 1.46        | 1.53     |
| 1   | X     | 437 | GLU  | CD-OE2 | 5.16  | 1.35        | 1.25     |
| 1   | Z     | 27  | ILE  | CA-C   | -5.16 | 1.47        | 1.53     |
| 1   | X     | 27  | ILE  | C-N    | -5.15 | 1.29        | 1.33     |
| 1   | Z     | 69  | ILE  | CA-C   | -5.15 | 1.46        | 1.52     |
| 1   | O     | 32  | GLN  | CA-C   | -5.14 | 1.46        | 1.52     |
| 1   | Y     | 265 | TYR  | CA-C   | -5.13 | 1.47        | 1.53     |
| 1   | X     | 434 | GLU  | CD-OE1 | 5.13  | 1.35        | 1.25     |
| 1   | O     | 462 | GLU  | CD-OE1 | 5.12  | 1.35        | 1.25     |
| 1   | Z     | 92  | GLU  | CD-OE2 | 5.12  | 1.35        | 1.25     |
| 1   | X     | 431 | GLU  | CD-OE1 | 5.10  | 1.35        | 1.25     |
| 1   | O     | 388 | THR  | N-CA   | -5.10 | 1.39        | 1.46     |
| 1   | Y     | 462 | GLU  | CD-OE1 | 5.09  | 1.35        | 1.25     |
| 1   | Z     | 170 | ILE  | CA-CB  | -5.09 | 1.48        | 1.54     |
| 1   | X     | 200 | ASP  | CG-OD2 | 5.09  | 1.35        | 1.25     |
| 1   | Z     | 462 | GLU  | CD-OE2 | 5.08  | 1.35        | 1.25     |
| 1   | X     | 31  | SER  | CA-C   | -5.08 | 1.46        | 1.52     |
| 1   | Y     | 153 | GLU  | CD-OE1 | 5.08  | 1.34        | 1.25     |
| 1   | O     | 163 | GLY  | N-CA   | -5.07 | 1.40        | 1.45     |
| 1   | Z     | 314 | GLN  | N-CA   | -5.07 | 1.39        | 1.46     |
| 1   | O     | 34  | GLU  | CD-OE1 | 5.06  | 1.34        | 1.25     |
| 1   | Z     | 437 | GLU  | CD-OE2 | 5.06  | 1.34        | 1.25     |
| 1   | X     | 283 | GLU  | CD-OE1 | 5.06  | 1.34        | 1.25     |
| 1   | O     | 63  | VAL  | CA-C   | -5.05 | 1.46        | 1.52     |
| 1   | Y     | 58  | SER  | CA-C   | -5.05 | 1.45        | 1.52     |
| 1   | O     | 246 | GLN  | CA-C   | -5.04 | 1.46        | 1.52     |
| 1   | Y     | 255 | CYS  | CA-C   | -5.03 | 1.48        | 1.53     |
| 1   | Z     | 124 | ILE  | C-N    | -5.03 | 1.27        | 1.33     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | X     | 326 | ALA  | CA-C   | 5.03  | 1.59        | 1.52     |
| 1   | Y     | 404 | HIS  | CG-ND1 | 5.02  | 1.43        | 1.38     |
| 1   | Z     | 51  | GLU  | CD-OE1 | 5.01  | 1.34        | 1.25     |
| 1   | O     | 236 | ARG  | C-N    | 5.01  | 1.36        | 1.33     |
| 1   | Z     | 410 | GLY  | CA-C   | -5.01 | 1.47        | 1.52     |
| 1   | O     | 30  | VAL  | C-O    | -5.00 | 1.17        | 1.23     |
| 1   | X     | 12  | GLY  | N-CA   | 5.00  | 1.49        | 1.44     |
| 1   | O     | 68  | ASP  | CG-OD1 | 5.00  | 1.34        | 1.25     |

All (535) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|--------|-------------|----------|
| 1   | X     | 83  | ARG  | CA-C-N   | -12.87 | 100.98      | 121.44   |
| 1   | X     | 83  | ARG  | C-N-CA   | -12.87 | 100.98      | 121.44   |
| 1   | X     | 83  | ARG  | N-CA-C   | 12.50  | 126.08      | 111.71   |
| 1   | Y     | 83  | ARG  | N-CA-C   | 12.21  | 127.27      | 112.38   |
| 1   | Y     | 147 | HIS  | CA-CB-CG | -12.08 | 101.72      | 113.80   |
| 1   | Z     | 83  | ARG  | N-CA-C   | 11.88  | 127.12      | 112.87   |
| 1   | O     | 147 | HIS  | CA-CB-CG | -11.60 | 102.20      | 113.80   |
| 1   | O     | 83  | ARG  | N-CA-C   | 11.27  | 126.39      | 112.87   |
| 1   | O     | 83  | ARG  | CA-C-N   | -10.94 | 100.64      | 121.54   |
| 1   | O     | 83  | ARG  | C-N-CA   | -10.94 | 100.64      | 121.54   |
| 1   | Z     | 147 | HIS  | CA-CB-CG | -10.47 | 103.33      | 113.80   |
| 1   | Z     | 83  | ARG  | CA-C-N   | -10.33 | 102.51      | 121.41   |
| 1   | Z     | 83  | ARG  | C-N-CA   | -10.33 | 102.51      | 121.41   |
| 1   | Y     | 83  | ARG  | CA-C-N   | -10.26 | 102.63      | 121.41   |
| 1   | Y     | 83  | ARG  | C-N-CA   | -10.26 | 102.63      | 121.41   |
| 1   | X     | 351 | LEU  | CA-C-N   | -10.16 | 105.56      | 122.43   |
| 1   | X     | 351 | LEU  | C-N-CA   | -10.16 | 105.56      | 122.43   |
| 1   | Y     | 118 | ASP  | CA-CB-CG | -9.93  | 102.67      | 112.60   |
| 1   | X     | 148 | VAL  | CB-CA-C  | -9.86  | 99.17       | 110.41   |
| 1   | Y     | 466 | ILE  | N-CA-CB  | 9.84   | 121.99      | 111.46   |
| 1   | O     | 163 | GLY  | O-C-N    | 9.68   | 130.62      | 123.27   |
| 1   | O     | 324 | ASN  | CA-CB-CG | -9.65  | 102.95      | 112.60   |
| 1   | X     | 332 | PHE  | CA-CB-CG | -9.61  | 104.19      | 113.80   |
| 1   | Y     | 94  | GLY  | N-CA-C   | -9.51  | 102.09      | 115.30   |
| 1   | Y     | 351 | LEU  | CA-C-N   | -9.42  | 102.94      | 121.41   |
| 1   | Y     | 351 | LEU  | C-N-CA   | -9.42  | 102.94      | 121.41   |
| 1   | Z     | 195 | HIS  | CA-CB-CG | -9.39  | 104.41      | 113.80   |
| 1   | O     | 122 | ASP  | CA-CB-CG | -9.20  | 103.40      | 112.60   |
| 1   | Z     | 47  | HIS  | CA-CB-CG | 9.11   | 122.91      | 113.80   |
| 1   | Z     | 307 | PHE  | CA-CB-CG | 8.98   | 122.78      | 113.80   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | O     | 390 | ASP  | CA-CB-CG | 8.90  | 121.50      | 112.60   |
| 1   | X     | 244 | GLY  | N-CA-C   | -8.86 | 100.72      | 112.14   |
| 1   | X     | 14  | THR  | N-CA-CB  | -8.79 | 98.31       | 111.15   |
| 1   | Y     | 208 | ASP  | CA-C-N   | -8.70 | 115.28      | 122.85   |
| 1   | Y     | 208 | ASP  | C-N-CA   | -8.70 | 115.28      | 122.85   |
| 1   | O     | 30  | VAL  | CB-CA-C  | -8.61 | 99.83       | 111.80   |
| 1   | Z     | 114 | HIS  | CA-CB-CG | -8.58 | 105.22      | 113.80   |
| 1   | Y     | 180 | VAL  | N-CA-CB  | -8.26 | 101.94      | 112.60   |
| 1   | X     | 182 | ASP  | CA-CB-CG | -8.21 | 104.39      | 112.60   |
| 1   | O     | 327 | TYR  | N-CA-C   | -8.20 | 103.40      | 113.41   |
| 1   | O     | 129 | GLY  | N-CA-C   | -8.19 | 103.91      | 115.30   |
| 1   | Y     | 481 | TYR  | N-CA-CB  | -8.18 | 97.75       | 109.94   |
| 1   | Y     | 206 | VAL  | N-CA-CB  | -8.18 | 101.43      | 110.51   |
| 1   | X     | 237 | ILE  | O-C-N    | 8.12  | 130.35      | 121.10   |
| 1   | Z     | 328 | ASP  | N-CA-C   | -8.11 | 102.41      | 111.82   |
| 1   | X     | 120 | LEU  | N-CA-C   | 8.10  | 122.94      | 112.89   |
| 1   | Z     | 148 | VAL  | CB-CA-C  | 8.04  | 120.68      | 110.96   |
| 1   | Y     | 267 | THR  | CA-C-N   | 8.02  | 129.31      | 122.17   |
| 1   | Y     | 267 | THR  | C-N-CA   | 8.02  | 129.31      | 122.17   |
| 1   | O     | 36  | GLU  | N-CA-C   | 7.92  | 121.91      | 110.10   |
| 1   | Z     | 351 | LEU  | CA-C-N   | -7.86 | 109.09      | 122.21   |
| 1   | Z     | 351 | LEU  | C-N-CA   | -7.86 | 109.09      | 122.21   |
| 1   | Z     | 404 | HIS  | CA-CB-CG | -7.84 | 105.96      | 113.80   |
| 1   | Y     | 263 | ASN  | CA-CB-CG | -7.80 | 104.80      | 112.60   |
| 1   | X     | 317 | ARG  | N-CA-C   | 7.78  | 119.54      | 111.14   |
| 1   | O     | 284 | ASN  | N-CA-C   | 7.77  | 122.39      | 113.15   |
| 1   | O     | 325 | ASP  | CB-CA-C  | 7.69  | 121.47      | 110.24   |
| 1   | Z     | 180 | VAL  | N-CA-C   | 7.67  | 119.86      | 108.96   |
| 1   | Y     | 136 | PHE  | N-CA-C   | 7.67  | 122.52      | 110.32   |
| 1   | Z     | 417 | PHE  | CA-CB-CG | -7.60 | 106.20      | 113.80   |
| 1   | Y     | 323 | ILE  | N-CA-C   | -7.57 | 97.19       | 108.85   |
| 1   | X     | 318 | ASP  | CA-CB-CG | 7.56  | 120.16      | 112.60   |
| 1   | X     | 90  | GLU  | CB-CG-CD | -7.54 | 99.78       | 112.60   |
| 1   | Y     | 404 | HIS  | CA-CB-CG | -7.52 | 106.28      | 113.80   |
| 1   | Z     | 107 | ARG  | N-CA-C   | 7.47  | 121.31      | 111.75   |
| 1   | X     | 137 | SER  | N-CA-CB  | 7.45  | 121.05      | 109.94   |
| 1   | O     | 83  | ARG  | O-C-N    | -7.40 | 112.59      | 122.43   |
| 1   | O     | 415 | ASN  | CB-CA-C  | -7.38 | 99.08       | 110.88   |
| 1   | Z     | 284 | ASN  | N-CA-C   | 7.37  | 126.51      | 110.80   |
| 1   | Z     | 205 | GLU  | O-C-N    | 7.37  | 130.66      | 122.11   |
| 1   | X     | 404 | HIS  | N-CA-CB  | 7.35  | 121.22      | 110.26   |
| 1   | O     | 132 | ILE  | N-CA-C   | 7.34  | 118.38      | 107.15   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | Z     | 373 | ALA  | N-CA-C     | 7.32  | 119.89      | 111.11   |
| 1   | O     | 85  | THR  | CB-CA-C    | 7.31  | 121.16      | 109.61   |
| 1   | Y     | 475 | GLU  | N-CA-CB    | -7.29 | 98.10       | 109.69   |
| 1   | Y     | 204 | LEU  | CA-C-O     | 7.28  | 128.35      | 119.97   |
| 1   | Y     | 79  | ILE  | N-CA-C     | 7.28  | 118.85      | 107.28   |
| 1   | Z     | 318 | ASP  | CA-CB-CG   | 7.25  | 119.85      | 112.60   |
| 1   | Z     | 45  | VAL  | CA-C-O     | 7.25  | 127.42      | 120.25   |
| 1   | O     | 499 | HIS  | CA-CB-CG   | 7.24  | 121.04      | 113.80   |
| 1   | O     | 357 | ASP  | CA-C-O     | 7.22  | 128.31      | 120.08   |
| 1   | O     | 289 | THR  | N-CA-CB    | 7.21  | 122.67      | 110.49   |
| 1   | X     | 82  | GLN  | N-CA-C     | -7.20 | 99.17       | 109.96   |
| 1   | Y     | 345 | VAL  | CB-CA-C    | 7.17  | 117.89      | 111.08   |
| 1   | Z     | 42  | PRO  | N-CA-CB    | 7.14  | 109.53      | 103.17   |
| 1   | X     | 172 | LYS  | N-CA-CB    | 7.14  | 120.83      | 110.20   |
| 1   | Y     | 195 | HIS  | CA-CB-CG   | -7.14 | 106.66      | 113.80   |
| 1   | Z     | 148 | VAL  | N-CA-CB    | 7.12  | 119.12      | 111.00   |
| 1   | X     | 159 | GLU  | N-CA-C     | 7.11  | 125.95      | 110.80   |
| 1   | X     | 53  | TRP  | CA-C-O     | 7.10  | 128.46      | 121.00   |
| 1   | X     | 386 | TYR  | O-C-N      | 7.08  | 129.36      | 122.07   |
| 1   | Z     | 23  | HIS  | CA-CB-CG   | -7.06 | 106.74      | 113.80   |
| 1   | Z     | 327 | TYR  | N-CA-C     | -7.05 | 104.67      | 113.28   |
| 1   | Y     | 353 | ALA  | N-CA-CB    | 7.05  | 122.91      | 110.37   |
| 1   | Y     | 205 | GLU  | O-C-N      | 7.04  | 129.63      | 122.03   |
| 1   | X     | 186 | ALA  | O-C-N      | 7.03  | 129.40      | 122.09   |
| 1   | X     | 499 | HIS  | N-CA-CB    | 7.03  | 121.32      | 109.87   |
| 1   | O     | 126 | SER  | N-CA-CB    | 7.01  | 120.71      | 110.47   |
| 1   | O     | 237 | ILE  | N-CA-CB    | 7.01  | 119.80      | 112.37   |
| 1   | O     | 122 | ASP  | N-CA-CB    | 7.00  | 120.41      | 110.12   |
| 1   | O     | 284 | ASN  | CA-CB-CG   | -6.99 | 105.61      | 112.60   |
| 1   | Y     | 14  | THR  | OG1-CB-CG2 | 6.95  | 123.20      | 109.30   |
| 1   | O     | 93  | THR  | N-CA-CB    | -6.95 | 99.60       | 110.44   |
| 1   | X     | 47  | HIS  | CA-CB-CG   | 6.95  | 120.75      | 113.80   |
| 1   | O     | 408 | VAL  | N-CA-CB    | -6.94 | 100.78      | 112.44   |
| 1   | X     | 281 | LYS  | CB-CA-C    | 6.91  | 120.93      | 109.53   |
| 1   | Y     | 465 | VAL  | N-CA-C     | 6.91  | 118.25      | 108.17   |
| 1   | X     | 226 | GLN  | N-CA-C     | 6.91  | 119.57      | 109.07   |
| 1   | O     | 15  | SER  | N-CA-CB    | -6.90 | 100.65      | 111.56   |
| 1   | Y     | 494 | MET  | N-CA-C     | 6.90  | 120.49      | 110.28   |
| 1   | Y     | 328 | ASP  | N-CA-C     | -6.89 | 103.78      | 111.71   |
| 1   | Z     | 348 | PHE  | CA-CB-CG   | -6.89 | 106.91      | 113.80   |
| 1   | Z     | 269 | CYS  | CB-CA-C    | -6.88 | 97.25       | 109.70   |
| 1   | X     | 474 | ILE  | N-CA-C     | 6.88  | 118.02      | 108.12   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | O     | 314 | GLN  | CB-CA-C   | -6.88 | 99.38       | 110.79   |
| 1   | Y     | 284 | ASN  | CA-CB-CG  | -6.86 | 105.74      | 112.60   |
| 1   | O     | 90  | GLU  | N-CA-CB   | 6.84  | 121.66      | 110.37   |
| 1   | X     | 114 | HIS  | CA-CB-CG  | -6.84 | 106.96      | 113.80   |
| 1   | Y     | 209 | ILE  | N-CA-CB   | -6.82 | 102.99      | 112.27   |
| 1   | X     | 188 | ARG  | CG-CD-NE  | 6.82  | 127.00      | 112.00   |
| 1   | Y     | 458 | ASP  | CA-CB-CG  | -6.80 | 105.80      | 112.60   |
| 1   | Y     | 99  | ASN  | CA-CB-CG  | -6.77 | 105.83      | 112.60   |
| 1   | Z     | 410 | GLY  | N-CA-C    | -6.75 | 105.26      | 112.08   |
| 1   | Y     | 163 | GLY  | O-C-N     | 6.74  | 128.39      | 123.27   |
| 1   | Z     | 198 | ASP  | CA-CB-CG  | 6.73  | 119.33      | 112.60   |
| 1   | O     | 204 | LEU  | CA-C-O    | 6.70  | 127.65      | 120.55   |
| 1   | X     | 426 | LEU  | N-CA-C    | -6.69 | 104.14      | 112.90   |
| 1   | X     | 5   | TYR  | N-CA-C    | 6.69  | 119.88      | 109.52   |
| 1   | X     | 388 | THR  | N-CA-CB   | -6.69 | 99.92       | 110.28   |
| 1   | Z     | 489 | ALA  | O-C-N     | 6.68  | 128.98      | 122.03   |
| 1   | Y     | 195 | HIS  | N-CA-C    | -6.68 | 104.05      | 112.93   |
| 1   | O     | 454 | TRP  | N-CA-CB   | 6.68  | 122.45      | 110.83   |
| 1   | Z     | 380 | THR  | CA-CB-OG1 | -6.67 | 99.60       | 109.60   |
| 1   | X     | 30  | VAL  | N-CA-C    | 6.66  | 117.14      | 108.35   |
| 1   | Y     | 363 | ALA  | N-CA-C    | 6.66  | 118.67      | 108.42   |
| 1   | Z     | 324 | ASN  | CA-CB-CG  | -6.64 | 105.96      | 112.60   |
| 1   | O     | 163 | GLY  | CA-C-N    | 6.63  | 135.25      | 121.32   |
| 1   | O     | 163 | GLY  | C-N-CA    | 6.63  | 135.25      | 121.32   |
| 1   | Z     | 30  | VAL  | N-CA-C    | 6.63  | 117.10      | 108.35   |
| 1   | X     | 28  | ILE  | CB-CA-C   | -6.62 | 104.40      | 110.63   |
| 1   | X     | 188 | ARG  | CD-NE-CZ  | 6.62  | 133.66      | 124.40   |
| 1   | Y     | 384 | ILE  | CA-C-N    | 6.61  | 129.46      | 120.54   |
| 1   | Y     | 384 | ILE  | C-N-CA    | 6.61  | 129.46      | 120.54   |
| 1   | Z     | 236 | ARG  | N-CA-CB   | -6.61 | 99.31       | 111.13   |
| 1   | Z     | 408 | VAL  | CB-CA-C   | -6.60 | 101.05      | 110.82   |
| 1   | Y     | 114 | HIS  | CA-CB-CG  | -6.60 | 107.20      | 113.80   |
| 1   | Y     | 459 | GLU  | N-CA-C    | -6.60 | 104.01      | 111.07   |
| 1   | Y     | 441 | LEU  | CB-CA-C   | -6.59 | 100.26      | 110.81   |
| 1   | O     | 351 | LEU  | CA-C-N    | -6.58 | 111.43      | 122.62   |
| 1   | O     | 351 | LEU  | C-N-CA    | -6.58 | 111.43      | 122.62   |
| 1   | O     | 136 | PHE  | CA-C-N    | 6.58  | 128.99      | 120.44   |
| 1   | O     | 136 | PHE  | C-N-CA    | 6.58  | 128.99      | 120.44   |
| 1   | Y     | 107 | ARG  | N-CA-C    | 6.54  | 119.24      | 111.71   |
| 1   | Z     | 261 | ALA  | N-CA-C    | 6.52  | 120.15      | 109.85   |
| 1   | Z     | 144 | ILE  | CB-CA-C   | -6.51 | 103.34      | 112.14   |
| 1   | Y     | 238 | PRO  | CB-CA-C   | -6.51 | 103.49      | 111.11   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | O     | 490 | VAL  | CA-CB-CG1 | -6.49 | 99.36       | 110.40   |
| 1   | Z     | 333 | ALA  | CA-C-N    | -6.49 | 112.27      | 122.65   |
| 1   | Z     | 333 | ALA  | C-N-CA    | -6.49 | 112.27      | 122.65   |
| 1   | Y     | 404 | HIS  | CB-CA-C   | 6.48  | 122.56      | 110.70   |
| 1   | Y     | 141 | VAL  | CB-CA-C   | -6.47 | 103.42      | 111.70   |
| 1   | Z     | 466 | ILE  | N-CA-CB   | 6.47  | 118.00      | 110.82   |
| 1   | O     | 201 | ASP  | O-C-N     | 6.46  | 128.97      | 122.12   |
| 1   | Y     | 453 | PHE  | CA-CB-CG  | -6.46 | 107.34      | 113.80   |
| 1   | O     | 114 | HIS  | CA-C-N    | -6.45 | 109.71      | 120.68   |
| 1   | O     | 114 | HIS  | C-N-CA    | -6.45 | 109.71      | 120.68   |
| 1   | O     | 136 | PHE  | CA-CB-CG  | -6.45 | 107.35      | 113.80   |
| 1   | X     | 147 | HIS  | CB-CA-C   | 6.45  | 122.78      | 110.27   |
| 1   | Z     | 122 | ASP  | CA-CB-CG  | -6.44 | 106.16      | 112.60   |
| 1   | O     | 200 | ASP  | CA-CB-CG  | 6.44  | 119.04      | 112.60   |
| 1   | X     | 490 | VAL  | CB-CA-C   | -6.42 | 103.48      | 111.70   |
| 1   | Y     | 36  | GLU  | N-CA-C    | 6.42  | 120.33      | 110.20   |
| 1   | O     | 432 | ARG  | CA-C-N    | 6.41  | 127.85      | 119.84   |
| 1   | O     | 432 | ARG  | C-N-CA    | 6.41  | 127.85      | 119.84   |
| 1   | Y     | 344 | VAL  | CA-C-N    | -6.40 | 116.21      | 123.25   |
| 1   | Y     | 344 | VAL  | C-N-CA    | -6.40 | 116.21      | 123.25   |
| 1   | X     | 180 | VAL  | CA-CB-CG1 | 6.39  | 121.26      | 110.40   |
| 1   | X     | 427 | GLY  | N-CA-C    | -6.39 | 103.88      | 114.48   |
| 1   | X     | 147 | HIS  | N-CA-C    | 6.39  | 120.79      | 113.19   |
| 1   | O     | 35  | PHE  | CA-CB-CG  | -6.38 | 107.42      | 113.80   |
| 1   | Z     | 112 | CYS  | N-CA-CB   | 6.38  | 119.49      | 110.12   |
| 1   | O     | 449 | LEU  | CA-C-N    | 6.36  | 129.13      | 120.54   |
| 1   | O     | 449 | LEU  | C-N-CA    | 6.36  | 129.13      | 120.54   |
| 1   | Y     | 474 | ILE  | CA-C-N    | 6.36  | 129.87      | 120.90   |
| 1   | Y     | 474 | ILE  | C-N-CA    | 6.36  | 129.87      | 120.90   |
| 1   | Y     | 432 | ARG  | O-C-N     | 6.34  | 129.08      | 121.60   |
| 1   | Z     | 350 | GLY  | CA-C-N    | -6.34 | 112.59      | 122.42   |
| 1   | Z     | 350 | GLY  | C-N-CA    | -6.34 | 112.59      | 122.42   |
| 1   | O     | 35  | PHE  | CA-C-N    | 6.33  | 129.74      | 120.82   |
| 1   | O     | 35  | PHE  | C-N-CA    | 6.33  | 129.74      | 120.82   |
| 1   | Z     | 72  | ASP  | CA-C-N    | -6.32 | 112.73      | 122.60   |
| 1   | Z     | 72  | ASP  | C-N-CA    | -6.32 | 112.73      | 122.60   |
| 1   | X     | 177 | ARG  | N-CA-CB   | 6.32  | 121.17      | 110.49   |
| 1   | O     | 307 | PHE  | N-CA-C    | 6.31  | 117.82      | 111.07   |
| 1   | Y     | 72  | ASP  | CA-CB-CG  | 6.31  | 118.91      | 112.60   |
| 1   | X     | 24  | ASP  | CA-CB-CG  | -6.29 | 106.31      | 112.60   |
| 1   | X     | 86  | THR  | N-CA-CB   | -6.29 | 100.57      | 110.69   |
| 1   | X     | 161 | LEU  | CA-C-N    | -6.27 | 112.77      | 122.87   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | X     | 161 | LEU  | C-N-CA    | -6.27 | 112.77      | 122.87   |
| 1   | X     | 176 | GLY  | N-CA-C    | -6.27 | 106.39      | 114.85   |
| 1   | Z     | 141 | VAL  | CB-CA-C   | -6.26 | 103.99      | 111.81   |
| 1   | X     | 35  | PHE  | CA-C-N    | 6.24  | 129.57      | 120.71   |
| 1   | X     | 35  | PHE  | C-N-CA    | 6.24  | 129.57      | 120.71   |
| 1   | O     | 52  | ILE  | CB-CA-C   | -6.22 | 104.00      | 111.97   |
| 1   | O     | 332 | PHE  | CA-CB-CG  | -6.22 | 107.58      | 113.80   |
| 1   | X     | 11  | GLN  | CB-CA-C   | 6.22  | 121.57      | 111.05   |
| 1   | Y     | 86  | THR  | N-CA-C    | 6.21  | 118.53      | 108.41   |
| 1   | O     | 376 | ILE  | CB-CA-C   | -6.20 | 103.66      | 112.22   |
| 1   | X     | 84  | GLU  | N-CA-CB   | 6.20  | 120.69      | 111.01   |
| 1   | X     | 445 | TYR  | CB-CA-C   | -6.20 | 100.45      | 110.74   |
| 1   | Z     | 196 | THR  | N-CA-CB   | -6.20 | 100.38      | 110.42   |
| 1   | Y     | 35  | PHE  | CA-CB-CG  | -6.19 | 107.61      | 113.80   |
| 1   | X     | 158 | GLY  | CA-C-N    | 6.17  | 133.32      | 121.54   |
| 1   | X     | 158 | GLY  | C-N-CA    | 6.17  | 133.32      | 121.54   |
| 1   | X     | 50  | MET  | N-CA-C    | 6.16  | 117.66      | 111.07   |
| 1   | Y     | 318 | ASP  | CA-CB-CG  | 6.16  | 118.76      | 112.60   |
| 1   | Y     | 85  | THR  | CA-CB-OG1 | -6.15 | 100.38      | 109.60   |
| 1   | X     | 352 | GLY  | N-CA-C    | -6.14 | 104.90      | 112.33   |
| 1   | Y     | 171 | TRP  | N-CA-CB   | -6.13 | 101.10      | 110.12   |
| 1   | X     | 137 | SER  | O-C-N     | 6.11  | 128.44      | 122.09   |
| 1   | Y     | 296 | GLY  | N-CA-C    | -6.11 | 106.21      | 115.00   |
| 1   | X     | 270 | PHE  | CA-CB-CG  | -6.11 | 107.69      | 113.80   |
| 1   | X     | 82  | GLN  | O-C-N     | 6.10  | 130.44      | 122.93   |
| 1   | Y     | 498 | GLU  | N-CA-C    | 6.09  | 118.61      | 108.20   |
| 1   | Y     | 487 | LYS  | CB-CA-C   | 6.08  | 120.42      | 110.88   |
| 1   | Y     | 14  | THR  | N-CA-CB   | -6.08 | 102.92      | 111.00   |
| 1   | Y     | 261 | ALA  | N-CA-C    | 6.07  | 118.63      | 109.23   |
| 1   | Y     | 77  | ILE  | CB-CA-C   | -6.06 | 101.59      | 110.81   |
| 1   | X     | 439 | THR  | N-CA-CB   | 6.06  | 118.80      | 110.01   |
| 1   | X     | 280 | VAL  | N-CA-CB   | -6.06 | 104.11      | 110.72   |
| 1   | X     | 172 | LYS  | N-CA-C    | -6.06 | 104.24      | 111.69   |
| 1   | O     | 153 | GLU  | CA-CB-CG  | -6.05 | 102.00      | 114.10   |
| 1   | Z     | 177 | ARG  | CB-CA-C   | 6.05  | 120.28      | 110.96   |
| 1   | X     | 80  | THR  | N-CA-CB   | 6.05  | 122.37      | 111.37   |
| 1   | Z     | 394 | ALA  | CA-C-N    | 6.04  | 128.70      | 120.54   |
| 1   | Z     | 394 | ALA  | C-N-CA    | 6.04  | 128.70      | 120.54   |
| 1   | X     | 195 | HIS  | N-CA-C    | -6.04 | 104.64      | 112.68   |
| 1   | X     | 59  | THR  | N-CA-CB   | 6.04  | 118.76      | 110.01   |
| 1   | Y     | 263 | ASN  | N-CA-CB   | 6.03  | 120.80      | 110.68   |
| 1   | Y     | 466 | ILE  | CB-CA-C   | 6.02  | 117.92      | 111.35   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | Y     | 80  | THR  | N-CA-CB    | 6.02  | 120.47      | 110.85   |
| 1   | O     | 196 | THR  | N-CA-CB    | -6.00 | 100.43      | 110.39   |
| 1   | O     | 237 | ILE  | N-CA-C     | 5.96  | 114.71      | 107.61   |
| 1   | O     | 487 | LYS  | N-CA-C     | 5.96  | 117.78      | 111.28   |
| 1   | Z     | 215 | PRO  | CB-CA-C    | -5.96 | 102.22      | 111.22   |
| 1   | X     | 283 | GLU  | N-CA-C     | -5.96 | 105.32      | 112.59   |
| 1   | Y     | 164 | THR  | N-CA-CB    | 5.96  | 118.60      | 110.38   |
| 1   | Y     | 478 | GLU  | CB-CA-C    | -5.96 | 101.79      | 110.96   |
| 1   | X     | 394 | ALA  | CA-C-O     | 5.95  | 127.07      | 120.82   |
| 1   | O     | 136 | PHE  | O-C-N      | 5.95  | 129.72      | 123.06   |
| 1   | Y     | 10  | ASP  | CA-CB-CG   | 5.95  | 118.55      | 112.60   |
| 1   | X     | 222 | GLU  | O-C-N      | -5.95 | 116.98      | 123.52   |
| 1   | X     | 322 | LEU  | N-CA-C     | 5.95  | 123.46      | 110.80   |
| 1   | Z     | 449 | LEU  | N-CA-C     | -5.94 | 104.80      | 111.28   |
| 1   | Y     | 500 | ASP  | CA-CB-CG   | 5.94  | 118.54      | 112.60   |
| 1   | Y     | 390 | ASP  | CA-CB-CG   | 5.93  | 118.53      | 112.60   |
| 1   | X     | 400 | GLY  | N-CA-C     | -5.93 | 107.06      | 115.30   |
| 1   | O     | 453 | PHE  | N-CA-C     | -5.93 | 104.82      | 111.28   |
| 1   | Y     | 430 | VAL  | CA-C-N     | -5.93 | 114.63      | 122.99   |
| 1   | Y     | 430 | VAL  | C-N-CA     | -5.93 | 114.63      | 122.99   |
| 1   | O     | 24  | ASP  | CA-CB-CG   | -5.92 | 106.68      | 112.60   |
| 1   | Y     | 345 | VAL  | CA-CB-CG2  | -5.92 | 100.34      | 110.40   |
| 1   | O     | 303 | GLU  | N-CA-C     | 5.91  | 118.53      | 108.90   |
| 1   | X     | 288 | THR  | CA-CB-CG2  | -5.91 | 100.46      | 110.50   |
| 1   | X     | 232 | LYS  | N-CA-C     | 5.91  | 119.08      | 107.98   |
| 1   | Z     | 147 | HIS  | CB-CA-C    | 5.90  | 122.42      | 110.38   |
| 1   | Z     | 390 | ASP  | CB-CA-C    | -5.90 | 101.54      | 110.92   |
| 1   | O     | 213 | MET  | N-CA-C     | -5.90 | 105.92      | 114.12   |
| 1   | O     | 300 | TYR  | CA-CB-CG   | -5.89 | 103.29      | 113.90   |
| 1   | O     | 440 | ALA  | N-CA-CB    | 5.89  | 119.17      | 110.33   |
| 1   | O     | 196 | THR  | N-CA-C     | -5.89 | 105.36      | 112.54   |
| 1   | Z     | 340 | ASN  | OD1-CG-ND2 | 5.88  | 128.48      | 122.60   |
| 1   | O     | 27  | ILE  | N-CA-CB    | 5.88  | 118.32      | 110.26   |
| 1   | Z     | 390 | ASP  | CA-CB-CG   | 5.88  | 118.48      | 112.60   |
| 1   | X     | 225 | GLY  | N-CA-C     | 5.87  | 117.90      | 110.38   |
| 1   | X     | 107 | ARG  | N-CA-C     | 5.86  | 123.28      | 110.80   |
| 1   | X     | 48  | ASP  | CA-C-N     | 5.85  | 127.16      | 119.84   |
| 1   | X     | 48  | ASP  | C-N-CA     | 5.85  | 127.16      | 119.84   |
| 1   | Z     | 422 | GLN  | O-C-N      | 5.84  | 128.09      | 122.07   |
| 1   | X     | 144 | ILE  | O-C-N      | 5.84  | 127.64      | 121.91   |
| 1   | Y     | 28  | ILE  | N-CA-C     | -5.82 | 105.41      | 111.58   |
| 1   | Z     | 458 | ASP  | CA-CB-CG   | -5.80 | 106.80      | 112.60   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | O     | 104 | GLN  | CA-C-O    | -5.79 | 113.55      | 120.10   |
| 1   | X     | 200 | ASP  | CA-CB-CG  | -5.79 | 106.81      | 112.60   |
| 1   | Y     | 178 | VAL  | CA-C-N    | 5.79  | 130.79      | 123.03   |
| 1   | Y     | 178 | VAL  | C-N-CA    | 5.79  | 130.79      | 123.03   |
| 1   | X     | 302 | LEU  | CA-C-N    | -5.79 | 112.60      | 122.33   |
| 1   | X     | 302 | LEU  | C-N-CA    | -5.79 | 112.60      | 122.33   |
| 1   | O     | 153 | GLU  | O-C-N     | 5.79  | 130.29      | 122.59   |
| 1   | X     | 290 | ILE  | N-CA-CB   | 5.79  | 117.43      | 110.95   |
| 1   | O     | 93  | THR  | CA-CB-OG1 | -5.78 | 100.92      | 109.60   |
| 1   | Z     | 227 | THR  | CA-CB-OG1 | 5.78  | 118.28      | 109.60   |
| 1   | Y     | 149 | GLU  | N-CA-C    | 5.78  | 123.11      | 110.80   |
| 1   | Y     | 245 | ASP  | N-CA-C    | 5.77  | 118.03      | 111.11   |
| 1   | Y     | 269 | CYS  | CB-CA-C   | -5.77 | 99.15       | 109.71   |
| 1   | X     | 84  | GLU  | O-C-N     | 5.77  | 128.38      | 122.09   |
| 1   | Z     | 283 | GLU  | N-CA-C    | -5.76 | 103.74      | 112.04   |
| 1   | X     | 324 | ASN  | N-CA-CB   | 5.75  | 118.64      | 110.13   |
| 1   | X     | 298 | VAL  | O-C-N     | 5.75  | 128.72      | 122.63   |
| 1   | X     | 44  | TRP  | N-CA-C    | 5.74  | 119.18      | 109.76   |
| 1   | O     | 118 | ASP  | CB-CA-C   | 5.74  | 121.84      | 110.42   |
| 1   | O     | 497 | GLU  | N-CA-C    | 5.74  | 118.88      | 109.76   |
| 1   | X     | 175 | GLN  | CA-C-N    | -5.74 | 114.54      | 122.63   |
| 1   | X     | 175 | GLN  | C-N-CA    | -5.74 | 114.54      | 122.63   |
| 1   | O     | 378 | ARG  | CA-C-O    | 5.74  | 126.57      | 119.97   |
| 1   | Y     | 314 | GLN  | CB-CA-C   | 5.74  | 122.30      | 110.31   |
| 1   | O     | 342 | VAL  | N-CA-C    | 5.73  | 117.46      | 109.55   |
| 1   | O     | 42  | PRO  | N-CA-CB   | 5.73  | 109.27      | 103.25   |
| 1   | Z     | 404 | HIS  | CB-CA-C   | 5.73  | 120.72      | 109.72   |
| 1   | O     | 149 | GLU  | N-CA-C    | 5.72  | 122.99      | 110.80   |
| 1   | Y     | 63  | VAL  | CB-CA-C   | -5.71 | 103.31      | 112.16   |
| 1   | O     | 227 | THR  | N-CA-CB   | 5.71  | 119.20      | 110.70   |
| 1   | Z     | 340 | ASN  | CB-CA-C   | -5.70 | 103.64      | 111.73   |
| 1   | X     | 33  | ARG  | N-CA-CB   | 5.70  | 120.06      | 110.77   |
| 1   | O     | 297 | GLU  | CA-CB-CG  | -5.70 | 102.70      | 114.10   |
| 1   | Z     | 239 | ILE  | N-CA-CB   | -5.70 | 105.16      | 111.66   |
| 1   | X     | 340 | ASN  | CB-CA-C   | -5.69 | 102.73      | 111.66   |
| 1   | O     | 424 | ASP  | CB-CA-C   | -5.69 | 101.40      | 110.84   |
| 1   | Y     | 330 | GLU  | N-CA-CB   | -5.67 | 101.77      | 110.16   |
| 1   | X     | 390 | ASP  | CA-CB-CG  | 5.67  | 118.27      | 112.60   |
| 1   | X     | 205 | GLU  | O-C-N     | 5.67  | 127.92      | 122.03   |
| 1   | O     | 328 | ASP  | N-CA-C    | -5.66 | 105.20      | 111.71   |
| 1   | O     | 234 | GLY  | N-CA-C    | -5.66 | 107.85      | 115.21   |
| 1   | O     | 120 | LEU  | N-CA-C    | 5.66  | 119.80      | 113.01   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | X     | 48  | ASP  | CA-CB-CG  | 5.66  | 118.26      | 112.60   |
| 1   | Z     | 105 | CYS  | CB-CA-C   | 5.65  | 118.54      | 109.61   |
| 1   | O     | 198 | ASP  | CA-C-O    | -5.65 | 115.19      | 121.23   |
| 1   | Y     | 180 | VAL  | N-CA-C    | 5.64  | 116.96      | 108.96   |
| 1   | X     | 416 | ASN  | O-C-N     | 5.63  | 127.87      | 122.07   |
| 1   | Y     | 425 | ILE  | N-CA-C    | 5.63  | 116.36      | 110.62   |
| 1   | Z     | 107 | ARG  | NE-CZ-NH1 | 5.62  | 127.12      | 121.50   |
| 1   | Z     | 69  | ILE  | O-C-N     | 5.62  | 128.87      | 123.14   |
| 1   | X     | 162 | PHE  | CA-CB-CG  | -5.62 | 108.18      | 113.80   |
| 1   | Z     | 38  | ILE  | CA-C-N    | -5.61 | 116.26      | 123.16   |
| 1   | Z     | 38  | ILE  | C-N-CA    | -5.61 | 116.26      | 123.16   |
| 1   | X     | 481 | TYR  | CA-CB-CG  | -5.60 | 103.81      | 113.90   |
| 1   | Z     | 14  | THR  | N-CA-CB   | -5.60 | 103.14      | 110.59   |
| 1   | O     | 63  | VAL  | O-C-N     | 5.60  | 127.60      | 121.83   |
| 1   | X     | 134 | PRO  | N-CA-CB   | 5.60  | 108.67      | 103.41   |
| 1   | O     | 164 | THR  | N-CA-C    | -5.60 | 103.00      | 110.55   |
| 1   | Z     | 417 | PHE  | N-CA-C    | -5.59 | 104.88      | 110.97   |
| 1   | O     | 70  | SER  | N-CA-CB   | 5.58  | 119.27      | 110.23   |
| 1   | X     | 64  | LEU  | CB-CA-C   | -5.58 | 100.92      | 110.24   |
| 1   | X     | 397 | ALA  | N-CA-C    | -5.58 | 104.84      | 111.03   |
| 1   | X     | 439 | THR  | CB-CA-C   | 5.57  | 119.62      | 110.88   |
| 1   | Z     | 263 | ASN  | CA-CB-CG  | -5.57 | 107.03      | 112.60   |
| 1   | X     | 33  | ARG  | CB-CA-C   | 5.57  | 118.71      | 110.14   |
| 1   | Z     | 307 | PHE  | N-CA-C    | 5.56  | 118.86      | 111.75   |
| 1   | Z     | 175 | GLN  | CB-CG-CD  | 5.55  | 122.03      | 112.60   |
| 1   | X     | 62  | GLU  | N-CA-CB   | 5.54  | 118.26      | 110.12   |
| 1   | O     | 236 | ARG  | CA-C-N    | -5.54 | 118.51      | 123.33   |
| 1   | O     | 236 | ARG  | C-N-CA    | -5.54 | 118.51      | 123.33   |
| 1   | Z     | 234 | GLY  | N-CA-C    | -5.54 | 106.38      | 114.90   |
| 1   | Y     | 179 | HIS  | CB-CA-C   | -5.53 | 103.72      | 111.85   |
| 1   | O     | 128 | THR  | CA-CB-CG2 | -5.52 | 101.11      | 110.50   |
| 1   | X     | 474 | ILE  | CA-C-N    | 5.52  | 129.53      | 121.31   |
| 1   | X     | 474 | ILE  | C-N-CA    | 5.52  | 129.53      | 121.31   |
| 1   | O     | 392 | LEU  | CB-CA-C   | -5.51 | 101.32      | 110.68   |
| 1   | O     | 471 | ARG  | CA-C-N    | 5.50  | 126.72      | 119.84   |
| 1   | O     | 471 | ARG  | C-N-CA    | 5.50  | 126.72      | 119.84   |
| 1   | Z     | 129 | GLY  | CA-C-O    | 5.50  | 125.13      | 119.02   |
| 1   | O     | 141 | VAL  | CB-CA-C   | -5.50 | 104.66      | 111.70   |
| 1   | X     | 135 | TYR  | N-CA-CB   | -5.50 | 101.82      | 110.06   |
| 1   | Y     | 47  | HIS  | CA-CB-CG  | 5.49  | 119.29      | 113.80   |
| 1   | Y     | 185 | ASN  | CA-CB-CG  | -5.49 | 107.11      | 112.60   |
| 1   | X     | 117 | ARG  | CD-NE-CZ  | 5.49  | 132.09      | 124.40   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | O     | 382 | GLU  | N-CA-CB   | 5.49  | 118.18      | 110.12   |
| 1   | Y     | 14  | THR  | CA-CB-CG2 | 5.48  | 119.82      | 110.50   |
| 1   | X     | 386 | TYR  | CA-CB-CG  | -5.48 | 104.03      | 113.90   |
| 1   | Z     | 7   | VAL  | CB-CA-C   | -5.48 | 102.66      | 110.83   |
| 1   | X     | 124 | ILE  | N-CA-CB   | -5.47 | 104.14      | 110.55   |
| 1   | Y     | 215 | PRO  | CA-C-N    | -5.47 | 115.28      | 122.99   |
| 1   | Y     | 215 | PRO  | C-N-CA    | -5.47 | 115.28      | 122.99   |
| 1   | Z     | 158 | GLY  | N-CA-C    | 5.47  | 121.46      | 113.48   |
| 1   | Z     | 204 | LEU  | CA-C-O    | 5.46  | 126.25      | 119.97   |
| 1   | X     | 331 | TYR  | CB-CA-C   | -5.46 | 102.24      | 110.92   |
| 1   | Z     | 318 | ASP  | N-CA-C    | 5.45  | 118.05      | 111.40   |
| 1   | X     | 289 | THR  | N-CA-C    | 5.45  | 117.26      | 109.14   |
| 1   | Y     | 115 | LEU  | O-C-N     | 5.45  | 127.68      | 122.07   |
| 1   | Y     | 293 | GLY  | N-CA-C    | -5.45 | 105.47      | 112.00   |
| 1   | Z     | 174 | THR  | N-CA-C    | -5.44 | 105.08      | 112.26   |
| 1   | O     | 345 | VAL  | CA-C-N    | 5.43  | 126.62      | 119.84   |
| 1   | O     | 345 | VAL  | C-N-CA    | 5.43  | 126.62      | 119.84   |
| 1   | X     | 195 | HIS  | CA-CB-CG  | -5.43 | 108.37      | 113.80   |
| 1   | Y     | 89  | TRP  | N-CA-C    | 5.42  | 117.65      | 109.41   |
| 1   | X     | 227 | THR  | O-C-N     | 5.42  | 129.56      | 123.27   |
| 1   | X     | 322 | LEU  | CA-C-N    | -5.42 | 114.08      | 122.69   |
| 1   | X     | 322 | LEU  | C-N-CA    | -5.42 | 114.08      | 122.69   |
| 1   | O     | 177 | ARG  | N-CA-CB   | 5.40  | 117.80      | 109.91   |
| 1   | X     | 498 | GLU  | N-CA-C    | 5.39  | 118.03      | 109.24   |
| 1   | X     | 208 | ASP  | CB-CA-C   | -5.39 | 103.79      | 112.09   |
| 1   | X     | 205 | GLU  | N-CA-C    | -5.39 | 105.10      | 110.97   |
| 1   | O     | 236 | ARG  | CD-NE-CZ  | -5.38 | 116.86      | 124.40   |
| 1   | Y     | 308 | MET  | N-CA-C    | 5.38  | 117.60      | 108.02   |
| 1   | X     | 164 | THR  | N-CA-CB   | 5.38  | 117.69      | 109.94   |
| 1   | Y     | 457 | LEU  | N-CA-C    | 5.38  | 117.83      | 111.33   |
| 1   | Z     | 189 | THR  | CA-CB-OG1 | -5.38 | 101.54      | 109.60   |
| 1   | X     | 217 | VAL  | N-CA-CB   | 5.38  | 117.62      | 110.26   |
| 1   | Z     | 136 | PHE  | CA-CB-CG  | -5.37 | 108.43      | 113.80   |
| 1   | Z     | 328 | ASP  | CA-CB-CG  | 5.37  | 117.97      | 112.60   |
| 1   | Z     | 149 | GLU  | N-CA-C    | 5.37  | 122.24      | 110.80   |
| 1   | O     | 183 | TYR  | O-C-N     | 5.36  | 127.82      | 122.03   |
| 1   | X     | 72  | ASP  | CA-C-N    | -5.36 | 112.99      | 122.26   |
| 1   | X     | 72  | ASP  | C-N-CA    | -5.36 | 112.99      | 122.26   |
| 1   | Z     | 129 | GLY  | N-CA-C    | -5.35 | 108.25      | 115.36   |
| 1   | Y     | 74  | ILE  | N-CA-C    | 5.35  | 115.33      | 107.15   |
| 1   | Z     | 147 | HIS  | CA-C-N    | -5.34 | 115.69      | 122.37   |
| 1   | Z     | 147 | HIS  | C-N-CA    | -5.34 | 115.69      | 122.37   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | Y     | 482 | ARG  | N-CA-C   | -5.34 | 105.46      | 111.28   |
| 1   | Z     | 156 | ARG  | CB-CA-C  | -5.34 | 102.43      | 110.92   |
| 1   | O     | 427 | GLY  | N-CA-C   | -5.33 | 103.49      | 114.16   |
| 1   | X     | 185 | ASN  | N-CA-C   | 5.33  | 116.77      | 111.07   |
| 1   | Z     | 198 | ASP  | CA-C-O   | -5.33 | 115.58      | 121.28   |
| 1   | X     | 74  | ILE  | N-CA-C   | 5.33  | 114.93      | 107.37   |
| 1   | Z     | 234 | GLY  | O-C-N    | 5.32  | 128.82      | 122.34   |
| 1   | X     | 131 | VAL  | O-C-N    | -5.31 | 117.72      | 123.14   |
| 1   | O     | 244 | GLY  | N-CA-C   | -5.31 | 104.31      | 111.54   |
| 1   | Z     | 60  | LEU  | N-CA-CB  | -5.31 | 102.03      | 109.94   |
| 1   | X     | 436 | ARG  | CB-CA-C  | 5.30  | 119.56      | 110.01   |
| 1   | Z     | 5   | TYR  | CB-CA-C  | -5.30 | 98.92       | 109.79   |
| 1   | Y     | 178 | VAL  | O-C-N    | 5.30  | 128.98      | 122.83   |
| 1   | Y     | 267 | THR  | O-C-N    | 5.30  | 127.74      | 122.12   |
| 1   | X     | 23  | HIS  | CA-CB-CG | -5.30 | 108.50      | 113.80   |
| 1   | Z     | 267 | THR  | CA-C-O   | 5.29  | 126.13      | 120.20   |
| 1   | X     | 404 | HIS  | N-CA-C   | 5.29  | 119.81      | 112.45   |
| 1   | X     | 490 | VAL  | N-CA-CB  | 5.29  | 116.18      | 110.62   |
| 1   | Z     | 482 | ARG  | N-CA-C   | -5.28 | 105.53      | 111.28   |
| 1   | X     | 351 | LEU  | N-CA-C   | 5.28  | 122.04      | 110.80   |
| 1   | Y     | 413 | VAL  | N-CA-CB  | 5.27  | 119.67      | 110.65   |
| 1   | X     | 5   | TYR  | CB-CA-C  | -5.27 | 98.98       | 109.79   |
| 1   | Z     | 228 | ASN  | N-CA-CB  | 5.27  | 119.38      | 110.69   |
| 1   | X     | 90  | GLU  | CB-CA-C  | -5.27 | 102.58      | 110.16   |
| 1   | Y     | 214 | LEU  | N-CA-C   | 5.26  | 116.45      | 109.93   |
| 1   | X     | 4   | LYS  | O-C-N    | 5.26  | 128.60      | 122.24   |
| 1   | Z     | 398 | ASP  | CA-CB-CG | 5.26  | 117.86      | 112.60   |
| 1   | Z     | 135 | TYR  | N-CA-CB  | -5.25 | 102.38      | 110.16   |
| 1   | X     | 462 | GLU  | CB-CA-C  | 5.24  | 119.42      | 110.56   |
| 1   | O     | 48  | ASP  | CA-C-N   | 5.24  | 125.29      | 119.32   |
| 1   | O     | 48  | ASP  | C-N-CA   | 5.24  | 125.29      | 119.32   |
| 1   | Z     | 368 | THR  | N-CA-CB  | 5.24  | 118.91      | 111.05   |
| 1   | Y     | 354 | PRO  | CB-CA-C  | -5.24 | 98.90       | 112.00   |
| 1   | X     | 84  | GLU  | CA-C-O   | 5.24  | 124.71      | 118.79   |
| 1   | X     | 271 | MET  | CA-C-N   | -5.24 | 114.68      | 122.74   |
| 1   | X     | 271 | MET  | C-N-CA   | -5.24 | 114.68      | 122.74   |
| 1   | O     | 496 | TRP  | N-CA-C   | -5.23 | 105.64      | 112.23   |
| 1   | Y     | 271 | MET  | CA-C-O   | 5.23  | 126.01      | 120.36   |
| 1   | Z     | 244 | GLY  | N-CA-C   | -5.23 | 104.42      | 111.54   |
| 1   | X     | 109 | ALA  | N-CA-CB  | -5.23 | 100.83      | 109.72   |
| 1   | Y     | 427 | GLY  | N-CA-C   | -5.23 | 107.03      | 115.08   |
| 1   | Z     | 21  | MET  | N-CA-CB  | -5.22 | 102.15      | 111.08   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | O     | 292 | CYS  | CB-CA-C  | -5.21 | 99.42       | 109.37   |
| 1   | Z     | 474 | ILE  | N-CA-CB  | -5.20 | 102.74      | 112.36   |
| 1   | O     | 64  | LEU  | CA-C-N   | 5.20  | 127.56      | 120.54   |
| 1   | O     | 64  | LEU  | C-N-CA   | 5.20  | 127.56      | 120.54   |
| 1   | Z     | 296 | GLY  | N-CA-C   | -5.20 | 107.94      | 115.27   |
| 1   | Z     | 88  | VAL  | CA-C-N   | -5.20 | 114.09      | 122.82   |
| 1   | Z     | 88  | VAL  | C-N-CA   | -5.20 | 114.09      | 122.82   |
| 1   | O     | 83  | ARG  | N-CA-CB  | 5.20  | 119.78      | 110.32   |
| 1   | Y     | 21  | MET  | N-CA-C   | 5.19  | 117.75      | 109.81   |
| 1   | Y     | 127 | ASN  | CA-CB-CG | -5.19 | 107.41      | 112.60   |
| 1   | X     | 432 | ARG  | CA-C-O   | 5.18  | 123.16      | 119.32   |
| 1   | Y     | 480 | ASN  | CA-C-N   | 5.18  | 127.53      | 120.54   |
| 1   | Y     | 480 | ASN  | C-N-CA   | 5.18  | 127.53      | 120.54   |
| 1   | X     | 494 | MET  | CB-CA-C  | 5.18  | 118.81      | 109.64   |
| 1   | O     | 283 | GLU  | CB-CA-C  | -5.18 | 101.31      | 109.34   |
| 1   | Y     | 166 | ASP  | CA-C-N   | 5.18  | 127.47      | 120.38   |
| 1   | Y     | 166 | ASP  | C-N-CA   | 5.18  | 127.47      | 120.38   |
| 1   | Y     | 398 | ASP  | CA-CB-CG | 5.18  | 117.78      | 112.60   |
| 1   | Z     | 367 | LEU  | CB-CA-C  | -5.17 | 101.40      | 109.84   |
| 1   | O     | 466 | ILE  | N-CA-C   | 5.17  | 115.06      | 107.15   |
| 1   | X     | 314 | GLN  | CB-CA-C  | -5.17 | 102.21      | 110.79   |
| 1   | X     | 307 | PHE  | O-C-N    | -5.17 | 116.17      | 122.11   |
| 1   | Z     | 316 | LEU  | CB-CA-C  | -5.16 | 102.55      | 110.81   |
| 1   | X     | 165 | VAL  | N-CA-C   | 5.16  | 118.35      | 111.44   |
| 1   | X     | 475 | GLU  | N-CA-CB  | -5.16 | 101.05      | 109.56   |
| 1   | Z     | 112 | CYS  | CB-CA-C  | 5.15  | 119.35      | 110.79   |
| 1   | X     | 449 | LEU  | N-CA-C   | -5.15 | 105.36      | 110.97   |
| 1   | Y     | 30  | VAL  | N-CA-C   | 5.15  | 115.15      | 108.35   |
| 1   | O     | 84  | GLU  | N-CA-CB  | 5.14  | 119.18      | 110.49   |
| 1   | Y     | 265 | TYR  | CB-CA-C  | -5.14 | 103.76      | 111.73   |
| 1   | Z     | 27  | ILE  | N-CA-CB  | 5.13  | 117.51      | 111.66   |
| 1   | X     | 178 | VAL  | N-CA-C   | 5.13  | 116.67      | 108.87   |
| 1   | Y     | 129 | GLY  | CA-C-O   | 5.13  | 124.48      | 119.04   |
| 1   | O     | 165 | VAL  | N-CA-C   | 5.12  | 115.73      | 110.36   |
| 1   | Z     | 7   | VAL  | N-CA-C   | 5.12  | 115.34      | 108.17   |
| 1   | Z     | 102 | VAL  | N-CA-C   | 5.12  | 116.00      | 110.21   |
| 1   | X     | 463 | LYS  | CA-C-N   | 5.12  | 129.40      | 121.26   |
| 1   | X     | 463 | LYS  | C-N-CA   | 5.12  | 129.40      | 121.26   |
| 1   | O     | 240 | SER  | N-CA-C   | 5.12  | 119.06      | 112.41   |
| 1   | O     | 58  | SER  | CA-CB-OG | -5.11 | 100.89      | 111.10   |
| 1   | Y     | 338 | ASN  | N-CA-CB  | 5.11  | 118.93      | 110.97   |
| 1   | X     | 61  | VAL  | CB-CA-C  | -5.11 | 105.25      | 112.14   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | O     | 190 | MET  | N-CA-C     | -5.10 | 106.47      | 113.56   |
| 1   | Y     | 196 | THR  | N-CA-CB    | -5.10 | 102.62      | 110.12   |
| 1   | Y     | 340 | ASN  | CA-CB-CG   | -5.10 | 107.50      | 112.60   |
| 1   | Y     | 244 | GLY  | N-CA-C     | -5.10 | 101.10      | 113.18   |
| 1   | Z     | 210 | PRO  | N-CA-CB    | 5.10  | 108.60      | 103.25   |
| 1   | X     | 60  | LEU  | CA-C-N     | -5.10 | 113.48      | 120.46   |
| 1   | X     | 60  | LEU  | C-N-CA     | -5.10 | 113.48      | 120.46   |
| 1   | Z     | 42  | PRO  | O-C-N      | 5.10  | 128.53      | 122.98   |
| 1   | X     | 106 | ARG  | CA-C-O     | 5.10  | 124.75      | 119.14   |
| 1   | Z     | 494 | MET  | N-CA-C     | 5.09  | 118.24      | 110.20   |
| 1   | O     | 214 | LEU  | N-CA-C     | 5.09  | 116.24      | 109.93   |
| 1   | X     | 183 | TYR  | O-C-N      | 5.09  | 127.32      | 122.03   |
| 1   | X     | 300 | TYR  | CA-CB-CG   | -5.08 | 104.75      | 113.90   |
| 1   | X     | 39  | TYR  | O-C-N      | 5.08  | 125.49      | 121.17   |
| 1   | Z     | 414 | ALA  | N-CA-CB    | 5.08  | 118.15      | 110.28   |
| 1   | X     | 454 | TRP  | N-CA-C     | -5.08 | 101.57      | 109.24   |
| 1   | O     | 365 | PHE  | N-CA-C     | 5.07  | 116.90      | 109.24   |
| 1   | X     | 82  | GLN  | N-CA-CB    | 5.07  | 117.40      | 109.85   |
| 1   | O     | 409 | ASP  | N-CA-C     | 5.07  | 115.03      | 107.88   |
| 1   | O     | 160 | LEU  | O-C-N      | 5.07  | 129.77      | 123.19   |
| 1   | X     | 99  | ASN  | CA-C-N     | -5.06 | 114.18      | 121.42   |
| 1   | X     | 99  | ASN  | C-N-CA     | -5.06 | 114.18      | 121.42   |
| 1   | X     | 130 | LEU  | CA-C-N     | 5.06  | 129.63      | 123.10   |
| 1   | X     | 130 | LEU  | C-N-CA     | 5.06  | 129.63      | 123.10   |
| 1   | Y     | 80  | THR  | CA-CB-OG1  | 5.06  | 117.19      | 109.60   |
| 1   | Z     | 336 | VAL  | N-CA-CB    | -5.05 | 102.47      | 111.92   |
| 1   | O     | 207 | LEU  | O-C-N      | 5.05  | 128.56      | 122.35   |
| 1   | X     | 86  | THR  | OG1-CB-CG2 | 5.05  | 119.41      | 109.30   |
| 1   | Z     | 384 | ILE  | CA-CB-CG1  | -5.05 | 101.81      | 110.40   |
| 1   | Y     | 137 | SER  | O-C-N      | 5.05  | 127.27      | 122.07   |
| 1   | O     | 30  | VAL  | N-CA-C     | 5.05  | 114.85      | 107.88   |
| 1   | Z     | 179 | HIS  | CA-CB-CG   | 5.05  | 118.85      | 113.80   |
| 1   | O     | 81  | ASN  | N-CA-CB    | -5.04 | 103.90      | 111.56   |
| 1   | X     | 394 | ALA  | O-C-N      | 5.04  | 127.26      | 122.07   |
| 1   | O     | 297 | GLU  | N-CA-C     | -5.03 | 103.41      | 110.50   |
| 1   | Z     | 19  | VAL  | CB-CA-C    | -5.02 | 103.08      | 110.82   |
| 1   | X     | 62  | GLU  | CB-CA-C    | 5.02  | 119.13      | 110.79   |
| 1   | O     | 27  | ILE  | CA-C-N     | -5.02 | 116.43      | 122.35   |
| 1   | O     | 27  | ILE  | C-N-CA     | -5.02 | 116.43      | 122.35   |
| 1   | O     | 485 | GLY  | N-CA-C     | -5.02 | 106.71      | 112.73   |
| 1   | Z     | 312 | SER  | CA-C-O     | 5.02  | 125.74      | 120.42   |
| 1   | Z     | 162 | PHE  | CA-CB-CG   | -5.01 | 108.78      | 113.80   |

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| Mol | Chain | Res | Type | Atoms  | Z    | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|-----|------|--------|------|------------------------|---------------------|
| 1   | X     | 194 | ILE  | N-CA-C | 5.00 | 119.50                 | 113.00              |

All (3) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 1   | Z     | 149 | GLU  | CA   |
| 1   | X     | 147 | HIS  | CA   |
| 1   | X     | 404 | HIS  | CA   |

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   | O     | 3891  | 0        | 3804     | 466     | 0            |
| 1   | X     | 3896  | 0        | 3811     | 442     | 0            |
| 1   | Y     | 3921  | 0        | 3839     | 416     | 0            |
| 1   | Z     | 3913  | 0        | 3841     | 456     | 0            |
| 2   | O     | 10    | 0        | 0        | 2       | 0            |
| 2   | X     | 5     | 0        | 0        | 0       | 0            |
| 2   | Y     | 5     | 0        | 0        | 0       | 0            |
| 2   | Z     | 10    | 0        | 0        | 2       | 0            |
| 3   | O     | 6     | 0        | 8        | 1       | 0            |
| 3   | X     | 6     | 0        | 8        | 1       | 0            |
| 3   | Y     | 6     | 0        | 8        | 3       | 0            |
| 3   | Z     | 6     | 0        | 8        | 7       | 0            |
| 4   | O     | 29    | 0        | 0        | 3       | 0            |
| 4   | X     | 42    | 0        | 0        | 7       | 0            |
| 4   | Y     | 38    | 0        | 0        | 4       | 0            |
| 4   | Z     | 31    | 0        | 0        | 2       | 0            |
| All | All   | 15815 | 0        | 15327    | 1718    | 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 55.

All (1718) 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:Y:33:ARG:HH22  | 1:Z:58:SER:HB2   | 1.15                     | 1.11              |
| 1:O:287:LEU:HD12 | 1:O:303:GLU:HG2  | 1.31                     | 1.11              |
| 1:Y:456:ASN:ND2  | 1:Y:458:ASP:H    | 1.51                     | 1.08              |
| 1:Z:468:ARG:HH11 | 1:Z:468:ARG:HG3  | 1.19                     | 1.07              |
| 1:O:124:ILE:HD13 | 1:O:203:MET:HE1  | 1.28                     | 1.07              |
| 1:Z:320:MET:HE1  | 1:X:373:ALA:HA   | 1.37                     | 1.06              |
| 1:Z:154:ARG:HB3  | 1:Z:159:GLU:HG3  | 1.32                     | 1.05              |
| 1:O:17:ARG:HG3   | 1:O:32:GLN:HG3   | 1.38                     | 1.05              |
| 1:Z:92:GLU:HG2   | 1:Z:93:THR:HG23  | 1.40                     | 1.04              |
| 1:Z:112:CYS:HB3  | 1:Z:132:ILE:HG22 | 1.35                     | 1.04              |
| 1:O:189:THR:HB   | 1:O:191:LEU:HD12 | 1.37                     | 1.03              |
| 1:O:128:THR:HG21 | 1:O:130:LEU:HD22 | 1.39                     | 1.02              |
| 1:Z:125:ARG:HB2  | 1:Z:125:ARG:HH11 | 1.20                     | 1.02              |
| 1:X:124:ILE:HG12 | 1:X:203:MET:HE1  | 1.35                     | 1.02              |
| 1:O:203:MET:HA   | 1:O:206:VAL:HG23 | 1.41                     | 1.00              |
| 1:O:330:GLU:HG3  | 1:O:415:ASN:HD21 | 1.23                     | 1.00              |
| 1:Y:9:LEU:HB2    | 1:Y:79:ILE:HD12  | 1.42                     | 1.00              |
| 1:Z:460:LEU:HA   | 1:Z:463:LYS:HD2  | 1.44                     | 0.99              |
| 1:Z:83:ARG:HB2   | 1:Z:83:ARG:HH11  | 1.24                     | 0.99              |
| 1:Y:272:LEU:HG   | 1:Y:303:GLU:HB2  | 1.42                     | 0.98              |
| 1:Z:424:ASP:HB3  | 1:Z:474:ILE:HD12 | 1.42                     | 0.98              |
| 1:Y:85:THR:HG23  | 1:Y:102:VAL:HA   | 1.40                     | 0.98              |
| 1:Y:219:ARG:HH22 | 1:Y:295:THR:HG23 | 1.25                     | 0.98              |
| 1:X:17:ARG:HG3   | 1:X:32:GLN:HG2   | 1.40                     | 0.98              |
| 1:O:261:ALA:HB2  | 1:O:273:MET:HB2  | 1.46                     | 0.98              |
| 1:O:460:LEU:HD12 | 1:O:463:LYS:HE3  | 1.44                     | 0.96              |
| 1:Z:415:ASN:HD21 | 1:Z:417:PHE:HB3  | 1.29                     | 0.95              |
| 1:X:237:ILE:HG22 | 1:X:238:PRO:HD2  | 1.48                     | 0.95              |
| 1:Y:33:ARG:NH2   | 1:Z:58:SER:HB2   | 1.84                     | 0.92              |
| 1:Z:145:LEU:HB3  | 1:Z:152:ARG:NH1  | 1.84                     | 0.92              |
| 1:X:475:GLU:HB3  | 1:X:478:GLU:HG2  | 1.49                     | 0.92              |
| 1:Y:415:ASN:HD21 | 1:Y:417:PHE:HB3  | 1.34                     | 0.92              |
| 1:X:396:GLN:HE21 | 1:X:403:LEU:H    | 1.15                     | 0.92              |
| 1:X:111:ILE:HD12 | 1:X:111:ILE:H    | 1.32                     | 0.92              |
| 1:Y:219:ARG:NH2  | 1:Y:295:THR:HG23 | 1.84                     | 0.91              |
| 1:X:108:THR:HA   | 1:X:111:ILE:HD13 | 1.50                     | 0.91              |
| 1:Y:421:PHE:CZ   | 1:Y:425:ILE:HD13 | 2.06                     | 0.91              |
| 1:Z:261:ALA:HB2  | 1:Z:273:MET:HB2  | 1.54                     | 0.90              |
| 1:O:271:MET:HE1  | 1:O:392:LEU:HD12 | 1.52                     | 0.90              |
| 1:Z:174:THR:HG21 | 1:Z:178:VAL:HG13 | 1.53                     | 0.90              |
| 1:Z:154:ARG:CB   | 1:Z:159:GLU:HG3  | 2.02                     | 0.90              |
| 1:O:127:ASN:HD22 | 1:O:193:ASN:ND2  | 1.70                     | 0.89              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:161:LEU:HD22 | 1:O:179:HIS:CE1  | 2.07                     | 0.88              |
| 1:O:460:LEU:HA   | 1:O:463:LYS:HE2  | 1.55                     | 0.88              |
| 1:Z:112:CYS:HB3  | 1:Z:132:ILE:CG2  | 2.01                     | 0.88              |
| 1:X:154:ARG:HB3  | 1:X:159:GLU:HG2  | 1.54                     | 0.88              |
| 1:Y:196:THR:HG22 | 1:Y:198:ASP:N    | 1.88                     | 0.88              |
| 1:O:85:THR:HG23  | 1:O:102:VAL:HA   | 1.55                     | 0.87              |
| 1:Y:468:ARG:HG3  | 1:Y:468:ARG:HH11 | 1.40                     | 0.87              |
| 1:Z:351:LEU:HD22 | 1:Z:360:ALA:CB   | 2.03                     | 0.87              |
| 1:O:271:MET:HE1  | 1:O:392:LEU:CD1  | 2.05                     | 0.86              |
| 1:Z:84:GLU:OE2   | 1:Z:188:ARG:HD2  | 1.74                     | 0.86              |
| 1:Y:424:ASP:HB3  | 1:Y:474:ILE:HG21 | 1.56                     | 0.86              |
| 1:Z:156:ARG:HH11 | 1:Z:156:ARG:HG3  | 1.38                     | 0.86              |
| 1:Z:146:ASP:HB2  | 1:Z:147:HIS:CE1  | 2.10                     | 0.86              |
| 1:O:127:ASN:HD22 | 1:O:193:ASN:HD21 | 1.24                     | 0.86              |
| 1:Y:65:THR:HG21  | 1:Z:54:ALA:HA    | 1.56                     | 0.85              |
| 1:Y:180:VAL:HG23 | 1:Y:216:GLU:HG2  | 1.59                     | 0.85              |
| 1:Y:344:VAL:HG22 | 1:Y:364:ILE:HD12 | 1.57                     | 0.85              |
| 1:Y:475:GLU:HG2  | 1:Y:477:THR:HB   | 1.57                     | 0.85              |
| 1:Z:17:ARG:CG    | 1:Z:32:GLN:HG2   | 2.05                     | 0.85              |
| 1:O:128:THR:HG22 | 1:O:130:LEU:HD13 | 1.58                     | 0.85              |
| 1:Z:152:ARG:O    | 1:Z:156:ARG:HG2  | 1.76                     | 0.85              |
| 1:Y:65:THR:CG2   | 1:Z:54:ALA:HA    | 2.07                     | 0.84              |
| 1:O:105:CYS:SG   | 1:O:107:ARG:HD2  | 2.17                     | 0.84              |
| 1:O:330:GLU:HG3  | 1:O:415:ASN:ND2  | 1.92                     | 0.83              |
| 1:Y:323:ILE:HG22 | 1:Y:332:PHE:CD2  | 2.13                     | 0.83              |
| 1:Y:456:ASN:HD21 | 1:Y:458:ASP:H    | 1.24                     | 0.83              |
| 1:O:457:LEU:HA   | 1:O:460:LEU:HD23 | 1.61                     | 0.83              |
| 1:Z:125:ARG:HH11 | 1:Z:125:ARG:CB   | 1.92                     | 0.83              |
| 1:X:154:ARG:HA   | 1:X:157:ARG:HH11 | 1.41                     | 0.83              |
| 1:O:193:ASN:HB3  | 1:O:196:THR:CG2  | 2.09                     | 0.82              |
| 1:Y:475:GLU:HG2  | 1:Y:478:GLU:H    | 1.43                     | 0.82              |
| 1:Y:344:VAL:HG22 | 1:Y:364:ILE:CD1  | 2.09                     | 0.82              |
| 1:Z:6:ILE:CG2    | 1:Z:21:MET:HB3   | 2.09                     | 0.82              |
| 1:O:155:ALA:HB1  | 1:O:210:PRO:HG2  | 1.61                     | 0.82              |
| 1:Y:396:GLN:HE22 | 1:Y:402:ARG:HD3  | 1.43                     | 0.82              |
| 1:O:54:ALA:HA    | 1:X:65:THR:HG21  | 1.61                     | 0.82              |
| 1:Y:475:GLU:CG   | 1:Y:477:THR:HB   | 2.09                     | 0.82              |
| 1:X:406:LEU:HD13 | 1:X:408:VAL:HG12 | 1.61                     | 0.82              |
| 1:Y:328:ASP:HB3  | 1:Y:332:PHE:CE2  | 2.15                     | 0.81              |
| 1:Y:295:THR:HG22 | 1:Y:297:GLU:CD   | 2.06                     | 0.81              |
| 1:X:237:ILE:CG2  | 1:X:238:PRO:HD2  | 2.10                     | 0.81              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Z:315:TRP:CD1  | 1:Z:319:GLU:HG2  | 2.16                     | 0.81              |
| 1:Z:23:HIS:HA    | 1:Z:453:PHE:CE2  | 2.16                     | 0.81              |
| 1:Z:387:GLN:O    | 1:Z:390:ASP:HB2  | 1.78                     | 0.81              |
| 1:Y:328:ASP:HB3  | 1:Y:332:PHE:HE2  | 1.43                     | 0.81              |
| 1:Z:17:ARG:HG2   | 1:Z:32:GLN:HG2   | 1.63                     | 0.81              |
| 1:X:154:ARG:NE   | 1:X:159:GLU:HG2  | 1.96                     | 0.81              |
| 1:X:459:GLU:C    | 1:X:460:LEU:HD13 | 2.05                     | 0.81              |
| 1:Z:347:ALA:HB2  | 1:Z:351:LEU:HD13 | 1.63                     | 0.81              |
| 1:O:359:TYR:CE1  | 1:O:499:HIS:HB3  | 2.16                     | 0.80              |
| 1:Y:256:VAL:HG11 | 1:Y:294:PRO:CA   | 2.11                     | 0.80              |
| 1:X:111:ILE:CG2  | 1:X:139:THR:HG22 | 2.12                     | 0.80              |
| 1:O:154:ARG:HB3  | 1:O:159:GLU:HB2  | 1.63                     | 0.80              |
| 1:X:112:CYS:HB3  | 1:X:132:ILE:HG22 | 1.62                     | 0.80              |
| 1:X:154:ARG:HB3  | 1:X:159:GLU:CG   | 2.11                     | 0.80              |
| 1:O:387:GLN:O    | 1:O:390:ASP:HB2  | 1.83                     | 0.79              |
| 1:Y:147:HIS:HB3  | 4:Y:539:HOH:O    | 1.81                     | 0.79              |
| 1:Y:422:GLN:O    | 1:Y:426:LEU:HD22 | 1.82                     | 0.79              |
| 1:O:460:LEU:H    | 1:O:460:LEU:HD22 | 1.48                     | 0.79              |
| 1:O:180:VAL:CG2  | 1:O:218:ARG:HG3  | 2.13                     | 0.79              |
| 1:Z:320:MET:CE   | 1:X:376:ILE:HD12 | 2.11                     | 0.79              |
| 1:Z:415:ASN:ND2  | 1:Z:417:PHE:HB3  | 1.96                     | 0.79              |
| 1:Y:161:LEU:HD22 | 1:Y:179:HIS:CE1  | 2.18                     | 0.79              |
| 1:Z:83:ARG:HH11  | 1:Z:83:ARG:CB    | 1.96                     | 0.79              |
| 1:Y:80:THR:CG2   | 1:Y:245:ASP:HA   | 2.12                     | 0.78              |
| 1:X:256:VAL:HG11 | 1:X:294:PRO:HB3  | 1.63                     | 0.78              |
| 1:Z:83:ARG:HB2   | 1:Z:83:ARG:NH1   | 1.98                     | 0.78              |
| 1:Y:323:ILE:HG22 | 1:Y:332:PHE:CE2  | 2.19                     | 0.78              |
| 1:X:83:ARG:HD2   | 1:X:244:GLY:HA3  | 1.65                     | 0.78              |
| 1:Z:203:MET:HA   | 1:Z:206:VAL:HG12 | 1.65                     | 0.78              |
| 1:X:314:GLN:HG3  | 1:X:317:ARG:NH2  | 1.99                     | 0.78              |
| 1:Y:271:MET:HE2  | 1:Y:391:VAL:HG23 | 1.64                     | 0.78              |
| 1:Y:54:ALA:HA    | 1:Z:65:THR:CG2   | 2.14                     | 0.78              |
| 1:Y:491:LYS:HA   | 1:Y:494:MET:HE3  | 1.66                     | 0.78              |
| 1:Z:28:ILE:HG22  | 1:Z:29:SER:HB3   | 1.65                     | 0.78              |
| 1:Z:21:MET:HA    | 1:Z:26:ASN:O     | 1.83                     | 0.77              |
| 1:Z:458:ASP:HA   | 1:Z:461:GLN:HG3  | 1.64                     | 0.77              |
| 1:X:29:SER:HB3   | 1:X:63:VAL:CG2   | 2.13                     | 0.77              |
| 1:Z:115:LEU:HA   | 1:Z:120:LEU:HD12 | 1.66                     | 0.77              |
| 1:O:17:ARG:HG3   | 1:O:32:GLN:CG    | 2.15                     | 0.77              |
| 1:Y:50:MET:HA    | 1:Y:50:MET:HE3   | 1.64                     | 0.77              |
| 1:Y:155:ALA:HB1  | 1:Y:213:MET:CE   | 2.15                     | 0.77              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Y:196:THR:HG22 | 1:Y:198:ASP:H    | 1.49                     | 0.77              |
| 1:Z:174:THR:HG21 | 1:Z:178:VAL:CG1  | 2.15                     | 0.76              |
| 1:X:80:THR:HG21  | 1:X:245:ASP:HA   | 1.65                     | 0.76              |
| 1:O:437:GLU:O    | 1:O:441:LEU:HD23 | 1.85                     | 0.76              |
| 1:O:237:ILE:HG23 | 1:O:238:PRO:HD2  | 1.66                     | 0.76              |
| 1:X:482:ARG:CB   | 1:X:482:ARG:HH11 | 1.97                     | 0.76              |
| 1:Z:320:MET:HE1  | 1:X:376:ILE:HD12 | 1.66                     | 0.76              |
| 1:O:128:THR:HG21 | 1:O:130:LEU:CD2  | 2.14                     | 0.76              |
| 1:Y:406:LEU:HD13 | 1:Y:408:VAL:CG1  | 2.16                     | 0.76              |
| 1:X:159:GLU:O    | 1:X:160:LEU:HD23 | 1.85                     | 0.76              |
| 1:X:240:SER:HB2  | 1:X:450:ALA:HB3  | 1.66                     | 0.76              |
| 1:O:173:MET:HB3  | 1:O:227:THR:HG21 | 1.68                     | 0.76              |
| 1:Y:179:HIS:ND1  | 1:Y:215:PRO:HA   | 2.00                     | 0.76              |
| 1:O:271:MET:HE3  | 1:O:406:LEU:HD11 | 1.67                     | 0.76              |
| 1:X:330:GLU:HG3  | 1:X:415:ASN:HD21 | 1.50                     | 0.76              |
| 1:O:403:LEU:HD23 | 1:O:405:ALA:O    | 1.86                     | 0.76              |
| 1:O:173:MET:HB3  | 1:O:227:THR:CG2  | 2.16                     | 0.76              |
| 1:Y:271:MET:CE   | 1:Y:391:VAL:HG23 | 2.15                     | 0.76              |
| 1:Y:483:TYR:CE2  | 1:Y:487:LYS:HE2  | 2.21                     | 0.76              |
| 1:X:124:ILE:CG1  | 1:X:203:MET:HE1  | 2.15                     | 0.76              |
| 1:O:173:MET:O    | 1:O:227:THR:HG22 | 1.86                     | 0.75              |
| 1:O:250:LEU:CD1  | 1:O:255:CYS:HB2  | 2.16                     | 0.75              |
| 1:Y:48:ASP:HB3   | 1:Y:51:GLU:HB2   | 1.68                     | 0.75              |
| 1:Z:362:GLY:HA3  | 1:X:367:LEU:HB2  | 1.67                     | 0.75              |
| 1:Z:173:MET:O    | 1:Z:227:THR:HG23 | 1.85                     | 0.75              |
| 1:O:460:LEU:HA   | 1:O:463:LYS:CE   | 2.16                     | 0.75              |
| 1:Z:170:ILE:CD1  | 1:Z:242:ILE:HD11 | 2.17                     | 0.75              |
| 1:O:258:GLU:HB2  | 1:O:275:THR:C    | 2.12                     | 0.75              |
| 1:O:313:ILE:HD11 | 1:O:381:LEU:HD23 | 1.69                     | 0.75              |
| 1:Y:121:GLU:O    | 1:Y:125:ARG:HB2  | 1.85                     | 0.75              |
| 1:O:154:ARG:HA   | 1:O:159:GLU:HG3  | 1.68                     | 0.74              |
| 1:O:421:PHE:O    | 1:O:424:ASP:HB2  | 1.86                     | 0.74              |
| 1:Y:54:ALA:HA    | 1:Z:65:THR:HG21  | 1.69                     | 0.74              |
| 1:O:193:ASN:HB3  | 1:O:196:THR:HG22 | 1.68                     | 0.74              |
| 1:O:460:LEU:CD1  | 1:O:463:LYS:HE3  | 2.15                     | 0.74              |
| 1:X:108:THR:CA   | 1:X:111:ILE:HD13 | 2.16                     | 0.74              |
| 1:O:201:ASP:O    | 1:O:205:GLU:HB3  | 1.87                     | 0.74              |
| 1:Y:78:GLY:C     | 1:Y:79:ILE:HD13  | 2.12                     | 0.74              |
| 1:Z:6:ILE:HG22   | 1:Z:21:MET:HB3   | 1.68                     | 0.74              |
| 1:O:54:ALA:HA    | 1:X:65:THR:CG2   | 2.18                     | 0.74              |
| 1:O:203:MET:HA   | 1:O:206:VAL:CG2  | 2.17                     | 0.74              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Z:105:CYS:SG   | 1:Z:107:ARG:HD2  | 2.28                     | 0.74              |
| 1:X:422:GLN:HE21 | 1:X:426:LEU:HD22 | 1.52                     | 0.74              |
| 1:O:130:LEU:HD23 | 1:O:190:MET:HG3  | 1.68                     | 0.74              |
| 1:Y:83:ARG:NH1   | 1:Y:246:GLN:HG2  | 2.02                     | 0.74              |
| 1:Y:256:VAL:HG11 | 1:Y:294:PRO:HA   | 1.70                     | 0.74              |
| 1:Z:320:MET:HE1  | 1:X:373:ALA:CA   | 2.17                     | 0.74              |
| 1:Z:203:MET:HA   | 1:Z:206:VAL:CG1  | 2.17                     | 0.74              |
| 1:Y:155:ALA:HB1  | 1:Y:213:MET:HE2  | 1.70                     | 0.74              |
| 1:Z:193:ASN:HB3  | 1:Z:196:THR:HG22 | 1.70                     | 0.73              |
| 1:O:80:THR:HG21  | 1:O:245:ASP:HA   | 1.69                     | 0.73              |
| 1:O:65:THR:CG2   | 1:X:54:ALA:HA    | 2.18                     | 0.73              |
| 1:Z:424:ASP:O    | 1:Z:479:ARG:NH1  | 2.20                     | 0.73              |
| 1:Y:468:ARG:HG3  | 1:Y:468:ARG:NH1  | 2.01                     | 0.73              |
| 1:Z:378:ARG:O    | 1:Z:382:GLU:HG3  | 1.88                     | 0.73              |
| 1:Z:147:HIS:ND1  | 1:Z:147:HIS:N    | 2.36                     | 0.73              |
| 1:X:486:TRP:CD1  | 1:X:487:LYS:HD2  | 2.24                     | 0.73              |
| 1:O:460:LEU:O    | 1:O:463:LYS:HG2  | 1.89                     | 0.73              |
| 1:Y:19:VAL:HG11  | 1:Y:27:ILE:HD12  | 1.69                     | 0.73              |
| 1:X:21:MET:HA    | 1:X:26:ASN:O     | 1.88                     | 0.73              |
| 1:X:478:GLU:O    | 1:X:481:TYR:HB3  | 1.88                     | 0.73              |
| 1:Y:90:GLU:HB2   | 1:Y:93:THR:OG1   | 1.89                     | 0.73              |
| 1:Z:86:THR:OG1   | 1:Z:137:SER:HB3  | 1.88                     | 0.73              |
| 1:O:188:ARG:HH22 | 1:O:303:GLU:CD   | 1.97                     | 0.72              |
| 1:O:455:GLN:HB3  | 1:O:459:GLU:OE2  | 1.89                     | 0.72              |
| 1:Y:55:THR:O     | 1:Y:59:THR:HG23  | 1.88                     | 0.72              |
| 1:X:189:THR:OG1  | 1:X:191:LEU:HB2  | 1.89                     | 0.72              |
| 1:X:410:GLY:O    | 1:X:413:VAL:HG22 | 1.88                     | 0.72              |
| 1:O:317:ARG:HB2  | 1:O:323:ILE:HD11 | 1.70                     | 0.72              |
| 1:Z:332:PHE:HA   | 1:Z:335:LYS:HD3  | 1.71                     | 0.72              |
| 1:X:3:LYS:N      | 1:X:4:LYS:HZ3    | 1.87                     | 0.72              |
| 1:X:154:ARG:HA   | 1:X:157:ARG:NH1  | 2.05                     | 0.72              |
| 1:X:328:ASP:O    | 1:X:331:TYR:HB3  | 1.88                     | 0.72              |
| 1:Y:180:VAL:CG2  | 1:Y:218:ARG:HG3  | 2.20                     | 0.72              |
| 1:X:483:TYR:O    | 1:X:486:TRP:HB3  | 1.89                     | 0.72              |
| 1:O:203:MET:CA   | 1:O:206:VAL:HG23 | 2.19                     | 0.72              |
| 1:Z:402:ARG:HG3  | 1:Z:402:ARG:HH11 | 1.54                     | 0.72              |
| 1:Z:458:ASP:HA   | 1:Z:461:GLN:CG   | 2.19                     | 0.72              |
| 1:O:308:MET:HE1  | 1:Y:369:ARG:HD2  | 1.71                     | 0.72              |
| 1:X:111:ILE:HG21 | 1:X:139:THR:HG22 | 1.71                     | 0.72              |
| 1:O:128:THR:CG2  | 1:O:130:LEU:HD22 | 2.19                     | 0.71              |
| 1:X:418:LEU:HD13 | 1:X:419:MET:CE   | 2.19                     | 0.71              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:156:ARG:CG   | 1:O:210:PRO:HG3  | 2.20                     | 0.71              |
| 1:Y:112:CYS:HA   | 1:Y:115:LEU:HD23 | 1.70                     | 0.71              |
| 1:Y:434:GLU:HG3  | 1:Y:467:GLU:HB2  | 1.72                     | 0.71              |
| 1:Z:84:GLU:HB2   | 1:Z:103:TRP:HB3  | 1.71                     | 0.71              |
| 1:X:17:ARG:HD3   | 1:X:17:ARG:N     | 2.05                     | 0.71              |
| 1:Z:143:TRP:O    | 1:Z:147:HIS:ND1  | 2.23                     | 0.71              |
| 1:X:267:THR:HG23 | 1:X:311:ALA:HB2  | 1.71                     | 0.71              |
| 1:O:17:ARG:N     | 1:O:17:ARG:HD3   | 2.05                     | 0.71              |
| 1:Y:80:THR:HG22  | 1:Y:245:ASP:HA   | 1.71                     | 0.71              |
| 1:X:295:THR:HG23 | 1:X:297:GLU:OE2  | 1.91                     | 0.71              |
| 1:O:357:ASP:OD2  | 1:O:360:ALA:HB2  | 1.90                     | 0.71              |
| 1:Y:458:ASP:HA   | 1:Y:461:GLN:HE21 | 1.55                     | 0.71              |
| 1:X:202:LYS:O    | 1:X:206:VAL:HG23 | 1.89                     | 0.71              |
| 1:X:434:GLU:HG3  | 1:X:467:GLU:HB2  | 1.71                     | 0.71              |
| 1:X:482:ARG:HH11 | 1:X:482:ARG:CA   | 2.03                     | 0.71              |
| 1:O:80:THR:CG2   | 1:O:245:ASP:HA   | 2.21                     | 0.71              |
| 1:Z:154:ARG:CA   | 1:Z:159:GLU:HG3  | 2.20                     | 0.71              |
| 1:Z:157:ARG:HB3  | 1:Z:157:ARG:HH11 | 1.54                     | 0.71              |
| 1:Z:340:ASN:HD22 | 1:Z:371:VAL:HG23 | 1.56                     | 0.71              |
| 1:O:179:HIS:CD2  | 1:O:215:PRO:HB3  | 2.26                     | 0.71              |
| 1:O:250:LEU:HD11 | 1:O:255:CYS:HB2  | 1.73                     | 0.71              |
| 1:O:255:CYS:HB3  | 1:O:260:MET:HB3  | 1.73                     | 0.71              |
| 1:O:65:THR:HG23  | 1:X:54:ALA:HA    | 1.73                     | 0.71              |
| 1:Z:12:GLY:HA3   | 1:Z:17:ARG:NH1   | 2.06                     | 0.71              |
| 1:Z:17:ARG:HG3   | 1:Z:32:GLN:HG2   | 1.73                     | 0.71              |
| 1:X:120:LEU:O    | 1:X:124:ILE:HG13 | 1.90                     | 0.71              |
| 1:O:254:LEU:O    | 1:O:256:VAL:HG22 | 1.91                     | 0.70              |
| 1:Z:50:MET:HE2   | 1:Z:168:TRP:HH2  | 1.56                     | 0.70              |
| 1:Y:156:ARG:O    | 1:Y:212:GLU:HG2  | 1.91                     | 0.70              |
| 1:Y:483:TYR:CD2  | 1:Y:487:LYS:HE2  | 2.27                     | 0.70              |
| 1:Z:483:TYR:O    | 1:Z:486:TRP:HB3  | 1.91                     | 0.70              |
| 1:X:124:ILE:HG12 | 1:X:203:MET:CE   | 2.16                     | 0.70              |
| 1:Y:469:GLU:HB3  | 1:Y:471:ARG:NH2  | 2.06                     | 0.70              |
| 1:O:458:ASP:O    | 1:O:461:GLN:HG3  | 1.91                     | 0.70              |
| 1:Y:21:MET:HA    | 1:Y:26:ASN:O     | 1.91                     | 0.70              |
| 1:Z:429:ARG:HG2  | 1:Z:471:ARG:HG2  | 1.74                     | 0.70              |
| 1:Z:19:VAL:CG1   | 1:Z:27:ILE:HG23  | 2.22                     | 0.70              |
| 1:X:435:VAL:HG11 | 1:X:441:LEU:HD11 | 1.73                     | 0.70              |
| 1:O:224:TYR:CE2  | 1:O:242:ILE:HG13 | 2.26                     | 0.70              |
| 1:Z:322:LEU:N    | 1:Z:322:LEU:HD23 | 2.07                     | 0.70              |
| 1:X:322:LEU:HD23 | 1:X:322:LEU:H    | 1.56                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:84:GLU:OE2   | 1:O:188:ARG:HD2  | 1.92                     | 0.70              |
| 1:Z:146:ASP:HB2  | 1:Z:147:HIS:ND1  | 2.06                     | 0.70              |
| 1:X:90:GLU:HB2   | 1:X:93:THR:OG1   | 1.92                     | 0.70              |
| 1:O:251:PHE:CE2  | 1:O:446:LEU:HD13 | 2.27                     | 0.70              |
| 1:Z:460:LEU:HA   | 1:Z:463:LYS:CD   | 2.22                     | 0.70              |
| 1:X:3:LYS:HD3    | 1:X:72:ASP:O     | 1.92                     | 0.70              |
| 1:X:210:PRO:O    | 1:X:213:MET:HG3  | 1.92                     | 0.69              |
| 1:X:322:LEU:HD23 | 1:X:322:LEU:N    | 2.06                     | 0.69              |
| 1:Y:475:GLU:HB3  | 1:Y:478:GLU:HB2  | 1.73                     | 0.69              |
| 1:Y:478:GLU:O    | 1:Y:481:TYR:HB3  | 1.92                     | 0.69              |
| 1:Z:267:THR:HG23 | 1:Z:311:ALA:HB2  | 1.73                     | 0.69              |
| 1:X:80:THR:CG2   | 1:X:245:ASP:HA   | 2.22                     | 0.69              |
| 1:X:346:PRO:HA   | 1:X:348:PHE:CE1  | 2.27                     | 0.69              |
| 1:Y:90:GLU:HG3   | 1:Y:95:LYS:O     | 1.92                     | 0.69              |
| 1:O:265:TYR:HB3  | 1:O:412:ALA:HB3  | 1.74                     | 0.69              |
| 1:O:362:GLY:C    | 1:Y:367:LEU:HB2  | 2.17                     | 0.69              |
| 1:O:483:TYR:O    | 1:O:486:TRP:HB3  | 1.91                     | 0.69              |
| 1:Z:313:ILE:HD11 | 1:Z:381:LEU:HD23 | 1.73                     | 0.69              |
| 1:Y:90:GLU:OE2   | 1:Y:93:THR:HG21  | 1.93                     | 0.69              |
| 1:O:196:THR:CG2  | 1:O:198:ASP:H    | 2.06                     | 0.69              |
| 1:X:313:ILE:H    | 1:X:313:ILE:HD12 | 1.57                     | 0.69              |
| 1:Z:80:THR:HG21  | 1:Z:248:ALA:CB   | 2.23                     | 0.69              |
| 1:O:83:ARG:NE    | 3:O:504:GOL:O2   | 2.26                     | 0.69              |
| 1:O:85:THR:HG23  | 1:O:102:VAL:CA   | 2.22                     | 0.69              |
| 1:Z:92:GLU:CG    | 1:Z:93:THR:HG23  | 2.20                     | 0.69              |
| 1:Z:147:HIS:N    | 1:Z:147:HIS:HD1  | 1.91                     | 0.69              |
| 1:X:64:LEU:CD2   | 1:X:69:ILE:HB    | 2.22                     | 0.69              |
| 1:X:64:LEU:HD23  | 1:X:69:ILE:HB    | 1.75                     | 0.69              |
| 1:X:250:LEU:HD12 | 1:X:255:CYS:HB2  | 1.75                     | 0.68              |
| 1:O:128:THR:HG21 | 1:O:130:LEU:HB2  | 1.75                     | 0.68              |
| 1:O:234:GLY:N    | 2:O:502:SO4:O2   | 2.26                     | 0.68              |
| 1:Z:6:ILE:HD13   | 1:Z:7:VAL:N      | 2.08                     | 0.68              |
| 1:Z:403:LEU:H    | 1:Z:403:LEU:HD12 | 1.59                     | 0.68              |
| 1:Y:68:ASP:C     | 1:Y:69:ILE:HD13  | 2.19                     | 0.68              |
| 1:Y:85:THR:CG2   | 1:Y:102:VAL:HA   | 2.22                     | 0.68              |
| 1:Y:399:SER:HB2  | 1:Y:401:ILE:HD12 | 1.74                     | 0.68              |
| 1:X:415:ASN:HD21 | 1:X:417:PHE:HB3  | 1.58                     | 0.68              |
| 1:Z:468:ARG:HG3  | 1:Z:468:ARG:NH1  | 1.96                     | 0.68              |
| 1:Z:328:ASP:O    | 1:Z:331:TYR:HB3  | 1.93                     | 0.68              |
| 1:O:202:LYS:HD3  | 1:O:206:VAL:HG22 | 1.75                     | 0.68              |
| 1:Z:429:ARG:CG   | 1:Z:471:ARG:HG2  | 2.24                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Y:415:ASN:ND2  | 1:Y:417:PHE:HB3  | 2.08                     | 0.68              |
| 1:O:415:ASN:HD21 | 1:O:417:PHE:HB3  | 1.59                     | 0.67              |
| 1:X:227:THR:N    | 1:X:237:ILE:O    | 2.25                     | 0.67              |
| 1:X:351:LEU:HD22 | 1:X:360:ALA:HB3  | 1.75                     | 0.67              |
| 1:O:127:ASN:ND2  | 1:O:193:ASN:HD21 | 1.90                     | 0.67              |
| 1:O:462:GLU:CD   | 1:O:462:GLU:H    | 2.03                     | 0.67              |
| 1:X:287:LEU:O    | 1:X:302:LEU:HD23 | 1.94                     | 0.67              |
| 1:X:347:ALA:HA   | 4:X:523:HOH:O    | 1.94                     | 0.67              |
| 1:X:426:LEU:HB3  | 1:X:428:THR:HB   | 1.76                     | 0.67              |
| 1:O:259:GLY:HA2  | 1:O:273:MET:HE2  | 1.76                     | 0.67              |
| 1:X:415:ASN:ND2  | 1:X:417:PHE:HB3  | 2.09                     | 0.67              |
| 1:Z:147:HIS:HB3  | 4:Z:535:HOH:O    | 1.93                     | 0.67              |
| 1:Z:278:LYS:HE3  | 1:Z:280:VAL:CG2  | 2.25                     | 0.67              |
| 1:X:460:LEU:HD13 | 1:X:460:LEU:N    | 2.09                     | 0.67              |
| 1:O:155:ALA:CB   | 1:O:210:PRO:HG2  | 2.24                     | 0.67              |
| 1:Y:418:LEU:HD13 | 1:Y:419:MET:CE   | 2.25                     | 0.67              |
| 1:Z:237:ILE:HG23 | 1:Z:238:PRO:HD2  | 1.75                     | 0.67              |
| 1:O:23:HIS:HA    | 1:O:453:PHE:CE2  | 2.29                     | 0.67              |
| 1:O:410:GLY:O    | 1:O:413:VAL:HG22 | 1.93                     | 0.67              |
| 1:Z:347:ALA:HB2  | 1:Z:351:LEU:CD1  | 2.25                     | 0.67              |
| 1:X:186:ALA:O    | 1:X:189:THR:HG23 | 1.94                     | 0.67              |
| 1:Z:325:ASP:O    | 1:Z:328:ASP:HB2  | 1.95                     | 0.66              |
| 1:Z:460:LEU:O    | 1:Z:463:LYS:HB2  | 1.95                     | 0.66              |
| 1:O:216:GLU:OE2  | 1:O:218:ARG:HD3  | 1.95                     | 0.66              |
| 1:Z:253:GLN:NE2  | 1:Z:409:ASP:OD2  | 2.27                     | 0.66              |
| 1:Z:313:ILE:HD11 | 1:Z:381:LEU:CD2  | 2.25                     | 0.66              |
| 1:X:29:SER:HB3   | 1:X:63:VAL:HG23  | 1.76                     | 0.66              |
| 1:O:152:ARG:NH2  | 1:O:208:ASP:HB3  | 2.08                     | 0.66              |
| 1:Z:44:TRP:HA    | 1:Z:105:CYS:SG   | 2.36                     | 0.66              |
| 1:Z:496:TRP:CZ3  | 1:X:488:LYS:HD2  | 2.31                     | 0.66              |
| 1:O:86:THR:OG1   | 1:O:137:SER:HB3  | 1.96                     | 0.66              |
| 1:O:141:VAL:HG11 | 1:O:209:ILE:HG12 | 1.76                     | 0.66              |
| 1:O:150:GLY:O    | 1:O:153:GLU:HB2  | 1.95                     | 0.66              |
| 1:Y:201:ASP:OD1  | 1:Y:211:ARG:NH1  | 2.29                     | 0.66              |
| 1:Z:83:ARG:NH1   | 3:Z:504:GOL:O2   | 2.28                     | 0.66              |
| 1:Z:12:GLY:HA3   | 1:Z:17:ARG:HH12  | 1.61                     | 0.66              |
| 1:Z:269:CYS:HB2  | 1:Z:306:VAL:HB   | 1.77                     | 0.66              |
| 1:X:179:HIS:CD2  | 1:X:215:PRO:HB3  | 2.30                     | 0.66              |
| 1:Z:40:PRO:HG2   | 1:Z:44:TRP:HB3   | 1.77                     | 0.66              |
| 1:Y:33:ARG:HH22  | 1:Z:58:SER:CB    | 2.00                     | 0.66              |
| 1:Y:83:ARG:HD3   | 1:Y:245:ASP:OD1  | 1.96                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Z:203:MET:O    | 1:Z:206:VAL:HG12 | 1.96                     | 0.66              |
| 1:Z:203:MET:CA   | 1:Z:206:VAL:HG12 | 2.25                     | 0.66              |
| 1:X:108:THR:HB   | 1:X:139:THR:HB   | 1.78                     | 0.66              |
| 1:Y:19:VAL:CG1   | 1:Y:27:ILE:HD12  | 2.25                     | 0.66              |
| 1:Y:90:GLU:OE2   | 1:Y:95:LYS:HD2   | 1.96                     | 0.66              |
| 1:X:148:VAL:HB   | 1:X:151:SER:OG   | 1.96                     | 0.66              |
| 1:X:438:VAL:HA   | 1:X:441:LEU:HD13 | 1.78                     | 0.66              |
| 1:X:478:GLU:O    | 1:X:482:ARG:HG2  | 1.96                     | 0.66              |
| 1:Z:166:ASP:N    | 1:Z:166:ASP:OD1  | 2.27                     | 0.65              |
| 1:Z:466:ILE:HD13 | 1:Z:466:ILE:N    | 2.10                     | 0.65              |
| 1:Y:123:TYR:CD2  | 1:Y:203:MET:HE3  | 2.32                     | 0.65              |
| 1:O:128:THR:CG2  | 1:O:130:LEU:HB2  | 2.27                     | 0.65              |
| 1:O:468:ARG:HD2  | 1:O:470:PHE:CE1  | 2.31                     | 0.65              |
| 1:Y:174:THR:O    | 1:Y:176:GLY:N    | 2.29                     | 0.65              |
| 1:Y:227:THR:N    | 1:Y:237:ILE:O    | 2.29                     | 0.65              |
| 1:O:15:SER:O     | 1:O:17:ARG:NH1   | 2.30                     | 0.65              |
| 1:O:40:PRO:HG2   | 1:O:44:TRP:HB2   | 1.77                     | 0.65              |
| 1:O:193:ASN:HB3  | 1:O:196:THR:HG21 | 1.78                     | 0.65              |
| 1:Y:196:THR:CG2  | 1:Y:198:ASP:HB3  | 2.26                     | 0.65              |
| 1:X:178:VAL:CG1  | 1:X:180:VAL:HB   | 2.27                     | 0.65              |
| 1:X:214:LEU:N    | 1:X:214:LEU:HD23 | 2.11                     | 0.65              |
| 1:X:219:ARG:NH2  | 1:X:295:THR:O    | 2.29                     | 0.65              |
| 1:Y:40:PRO:HD2   | 1:Y:44:TRP:HB2   | 1.77                     | 0.65              |
| 1:Z:22:ASP:OD1   | 1:Z:24:ASP:N     | 2.28                     | 0.65              |
| 1:Z:157:ARG:HG3  | 1:Z:157:ARG:O    | 1.96                     | 0.65              |
| 1:Z:315:TRP:HD1  | 1:Z:319:GLU:HG2  | 1.57                     | 0.65              |
| 1:O:123:TYR:O    | 1:O:126:SER:N    | 2.30                     | 0.65              |
| 1:O:236:ARG:NH2  | 2:O:502:SO4:O2   | 2.30                     | 0.65              |
| 1:Z:201:ASP:OD2  | 1:Z:211:ARG:NH1  | 2.30                     | 0.65              |
| 1:Z:203:MET:C    | 1:Z:206:VAL:HG12 | 2.21                     | 0.65              |
| 1:X:406:LEU:CD1  | 1:X:408:VAL:HG12 | 2.26                     | 0.65              |
| 1:O:211:ARG:HA   | 1:O:214:LEU:HD13 | 1.78                     | 0.65              |
| 1:X:22:ASP:OD1   | 1:X:24:ASP:N     | 2.29                     | 0.65              |
| 1:O:421:PHE:O    | 1:O:425:ILE:HG22 | 1.96                     | 0.65              |
| 1:Z:240:SER:HB2  | 1:Z:450:ALA:CB   | 2.27                     | 0.65              |
| 1:X:169:LEU:O    | 1:X:173:MET:HG3  | 1.97                     | 0.65              |
| 1:X:193:ASN:HB3  | 1:X:196:THR:CG2  | 2.27                     | 0.65              |
| 1:O:156:ARG:HG2  | 1:O:210:PRO:HG3  | 1.78                     | 0.65              |
| 1:Y:87:ILE:HD12  | 1:Y:168:TRP:CG   | 2.32                     | 0.65              |
| 1:Z:40:PRO:HG2   | 1:Z:44:TRP:CB    | 2.25                     | 0.65              |
| 1:Z:226:GLN:NE2  | 1:Z:236:ARG:HG2  | 2.12                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:202:LYS:HE2  | 1:O:205:GLU:HG2  | 1.78                     | 0.64              |
| 1:O:261:ALA:HB2  | 1:O:273:MET:CB   | 2.26                     | 0.64              |
| 1:O:378:ARG:O    | 1:O:382:GLU:HG3  | 1.96                     | 0.64              |
| 1:Y:226:GLN:HG2  | 1:Y:238:PRO:HA   | 1.79                     | 0.64              |
| 1:Z:212:GLU:OE1  | 1:Z:212:GLU:N    | 2.30                     | 0.64              |
| 1:O:62:GLU:HB3   | 1:X:58:SER:OG    | 1.98                     | 0.64              |
| 1:O:127:ASN:ND2  | 1:O:193:ASN:ND2  | 2.43                     | 0.64              |
| 1:Y:466:ILE:HD13 | 1:Y:466:ILE:O    | 1.97                     | 0.64              |
| 1:O:202:LYS:HD3  | 1:O:202:LYS:C    | 2.23                     | 0.64              |
| 1:O:240:SER:HB2  | 1:O:450:ALA:CB   | 2.27                     | 0.64              |
| 1:O:458:ASP:HA   | 1:O:461:GLN:CD   | 2.23                     | 0.64              |
| 1:Y:280:VAL:CG1  | 1:Y:302:LEU:HD21 | 2.28                     | 0.64              |
| 1:O:283:GLU:HB2  | 1:O:398:ASP:OD1  | 1.97                     | 0.64              |
| 1:Z:49:PRO:HB3   | 1:Z:87:ILE:HD13  | 1.80                     | 0.64              |
| 1:O:237:ILE:CG2  | 1:O:238:PRO:HD2  | 2.28                     | 0.64              |
| 1:Y:428:THR:HG22 | 1:Y:429:ARG:O    | 1.98                     | 0.64              |
| 1:Z:253:GLN:HG2  | 1:Z:438:VAL:HG21 | 1.80                     | 0.64              |
| 1:X:105:CYS:SG   | 1:X:107:ARG:HB3  | 2.36                     | 0.64              |
| 1:Z:365:PHE:CZ   | 1:Z:492:ARG:HB3  | 2.33                     | 0.64              |
| 1:Z:497:GLU:HG2  | 4:Z:529:HOH:O    | 1.98                     | 0.64              |
| 1:X:180:VAL:CG2  | 1:X:218:ARG:HG3  | 2.27                     | 0.64              |
| 1:O:442:GLY:O    | 1:O:445:TYR:HB2  | 1.97                     | 0.64              |
| 1:X:133:ASP:OD2  | 1:X:135:TYR:HB2  | 1.98                     | 0.64              |
| 1:X:240:SER:HB2  | 1:X:450:ALA:CB   | 2.28                     | 0.64              |
| 1:O:458:ASP:HA   | 1:O:461:GLN:CG   | 2.28                     | 0.64              |
| 1:Z:62:GLU:O     | 1:Z:66:LYS:HB2   | 1.98                     | 0.64              |
| 1:X:154:ARG:HB3  | 1:X:159:GLU:CB   | 2.28                     | 0.64              |
| 1:X:154:ARG:O    | 1:X:159:GLU:HB2  | 1.98                     | 0.64              |
| 1:O:85:THR:HG23  | 1:O:101:ILE:C    | 2.23                     | 0.63              |
| 1:Y:3:LYS:CB     | 1:Y:3:LYS:HZ3    | 2.12                     | 0.63              |
| 1:Z:403:LEU:HD12 | 1:Z:403:LEU:N    | 2.13                     | 0.63              |
| 1:O:59:THR:O     | 1:O:63:VAL:HG22  | 1.98                     | 0.63              |
| 1:Y:376:ILE:HD13 | 1:Y:376:ILE:N    | 2.13                     | 0.63              |
| 1:Y:105:CYS:SG   | 1:Y:107:ARG:HD2  | 2.39                     | 0.63              |
| 1:Z:486:TRP:O    | 1:Z:490:VAL:HG23 | 1.99                     | 0.63              |
| 1:X:381:LEU:N    | 1:X:381:LEU:HD23 | 2.11                     | 0.63              |
| 1:O:458:ASP:HA   | 1:O:461:GLN:HG3  | 1.81                     | 0.63              |
| 1:O:211:ARG:HG2  | 1:O:211:ARG:O    | 1.98                     | 0.63              |
| 1:Y:19:VAL:HG12  | 1:Y:27:ILE:HG23  | 1.81                     | 0.63              |
| 1:O:456:ASN:O    | 1:O:459:GLU:HG3  | 1.98                     | 0.63              |
| 1:Z:226:GLN:HA   | 1:Z:237:ILE:O    | 1.98                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:174:THR:HA   | 1:O:177:ARG:NH2  | 2.13                     | 0.63              |
| 1:Z:351:LEU:HD22 | 1:Z:360:ALA:HB2  | 1.81                     | 0.63              |
| 1:O:428:THR:HG22 | 1:O:429:ARG:O    | 1.99                     | 0.63              |
| 1:Y:271:MET:HE2  | 1:Y:391:VAL:CG2  | 2.28                     | 0.63              |
| 1:O:396:GLN:NE2  | 1:O:403:LEU:H    | 1.95                     | 0.63              |
| 1:Z:141:VAL:HG12 | 1:Z:145:LEU:HD22 | 1.80                     | 0.63              |
| 1:Z:152:ARG:O    | 1:Z:155:ALA:HB3  | 1.99                     | 0.63              |
| 1:O:362:GLY:CA   | 1:Y:367:LEU:HB2  | 2.28                     | 0.62              |
| 1:Y:217:VAL:C    | 1:Y:218:ARG:HG2  | 2.24                     | 0.62              |
| 1:Y:415:ASN:ND2  | 1:Y:418:LEU:H    | 1.97                     | 0.62              |
| 1:X:313:ILE:HD12 | 1:X:313:ILE:N    | 2.13                     | 0.62              |
| 1:X:345:VAL:O    | 1:X:362:GLY:HA2  | 1.99                     | 0.62              |
| 1:O:85:THR:HA    | 1:O:101:ILE:O    | 1.99                     | 0.62              |
| 1:X:157:ARG:HH12 | 1:X:159:GLU:CD   | 2.07                     | 0.62              |
| 1:X:108:THR:OG1  | 1:X:134:PRO:HB3  | 1.99                     | 0.62              |
| 1:X:154:ARG:CZ   | 1:X:159:GLU:HG2  | 2.28                     | 0.62              |
| 1:X:471:ARG:NH1  | 1:X:471:ARG:HG3  | 2.12                     | 0.62              |
| 1:X:111:ILE:HD12 | 1:X:111:ILE:N    | 2.12                     | 0.62              |
| 1:X:216:GLU:OE2  | 1:X:218:ARG:NH1  | 2.32                     | 0.62              |
| 1:X:415:ASN:C    | 1:X:415:ASN:HD22 | 2.06                     | 0.62              |
| 1:Y:65:THR:HG22  | 1:Y:66:LYS:N     | 2.15                     | 0.62              |
| 1:Y:325:ASP:O    | 1:Y:328:ASP:HB2  | 1.99                     | 0.62              |
| 1:Z:125:ARG:HB2  | 1:Z:125:ARG:NH1  | 2.05                     | 0.62              |
| 1:Y:9:LEU:HB2    | 1:Y:79:ILE:CD1   | 2.25                     | 0.62              |
| 1:Y:387:GLN:O    | 1:Y:390:ASP:HB2  | 1.99                     | 0.62              |
| 1:Z:83:ARG:NH1   | 3:Z:504:GOL:O1   | 2.27                     | 0.62              |
| 1:Y:93:THR:OG1   | 1:Y:95:LYS:N     | 2.29                     | 0.62              |
| 1:Y:193:ASN:HB2  | 1:Y:200:ASP:OD2  | 2.00                     | 0.62              |
| 1:X:152:ARG:HH11 | 1:X:152:ARG:HG2  | 1.65                     | 0.62              |
| 1:O:496:TRP:CZ3  | 1:Y:488:LYS:HD2  | 2.34                     | 0.62              |
| 1:Y:112:CYS:HB3  | 1:Y:132:ILE:HG22 | 1.81                     | 0.62              |
| 1:Z:169:LEU:O    | 1:Z:173:MET:HG3  | 1.99                     | 0.62              |
| 1:O:313:ILE:HD11 | 1:O:381:LEU:CD2  | 2.29                     | 0.62              |
| 1:Y:50:MET:HA    | 1:Y:50:MET:CE    | 2.30                     | 0.62              |
| 1:Y:281:LYS:NZ   | 1:Y:283:GLU:OE2  | 2.29                     | 0.62              |
| 1:X:21:MET:HE2   | 1:X:27:ILE:HD13  | 1.81                     | 0.62              |
| 1:O:260:MET:O    | 1:O:273:MET:HA   | 2.00                     | 0.61              |
| 1:Y:295:THR:HG22 | 1:Y:297:GLU:OE1  | 2.00                     | 0.61              |
| 1:Z:23:HIS:HA    | 1:Z:453:PHE:CZ   | 2.35                     | 0.61              |
| 1:O:71:SER:HA    | 1:O:74:ILE:HD12  | 1.81                     | 0.61              |
| 1:O:295:THR:OG1  | 1:O:297:GLU:HG2  | 2.00                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Y:432:ARG:O    | 1:Y:467:GLU:N    | 2.34                     | 0.61              |
| 1:Z:275:THR:O    | 1:Z:278:LYS:HG2  | 2.01                     | 0.61              |
| 1:Z:415:ASN:ND2  | 1:Z:418:LEU:H    | 1.98                     | 0.61              |
| 1:X:256:VAL:HG11 | 1:X:294:PRO:CB   | 2.30                     | 0.61              |
| 1:X:180:VAL:HG21 | 1:X:218:ARG:HG3  | 1.80                     | 0.61              |
| 1:O:313:ILE:N    | 1:O:313:ILE:HD13 | 2.16                     | 0.61              |
| 1:O:351:LEU:HD23 | 1:O:494:MET:HE3  | 1.83                     | 0.61              |
| 1:O:415:ASN:ND2  | 1:O:418:LEU:H    | 1.98                     | 0.61              |
| 1:Y:170:ILE:HG22 | 1:Y:171:TRP:N    | 2.14                     | 0.61              |
| 1:Y:280:VAL:HG12 | 1:Y:302:LEU:HD21 | 1.82                     | 0.61              |
| 1:Z:191:LEU:HD11 | 1:Z:209:ILE:HD13 | 1.81                     | 0.61              |
| 1:Z:203:MET:SD   | 1:Z:206:VAL:HG11 | 2.40                     | 0.61              |
| 1:O:65:THR:HG23  | 1:X:54:ALA:CB    | 2.31                     | 0.61              |
| 1:Y:418:LEU:HD13 | 1:Y:419:MET:HE2  | 1.83                     | 0.61              |
| 1:X:84:GLU:HG2   | 1:X:103:TRP:HB3  | 1.83                     | 0.61              |
| 1:X:389:ARG:HG2  | 1:X:483:TYR:CE1  | 2.36                     | 0.61              |
| 1:Y:325:ASP:HB2  | 1:Y:328:ASP:OD1  | 2.00                     | 0.61              |
| 1:Y:476:THR:O    | 1:Y:479:ARG:N    | 2.32                     | 0.61              |
| 1:O:174:THR:C    | 1:O:175:GLN:HG2  | 2.24                     | 0.61              |
| 1:Z:476:THR:HA   | 1:Z:479:ARG:HG2  | 1.82                     | 0.61              |
| 1:O:432:ARG:NE   | 1:O:467:GLU:OE1  | 2.34                     | 0.61              |
| 1:Y:128:THR:OG1  | 1:Y:130:LEU:HB2  | 2.01                     | 0.61              |
| 1:Y:180:VAL:HG21 | 1:Y:218:ARG:HG3  | 1.81                     | 0.61              |
| 1:Y:17:ARG:HG3   | 1:Y:32:GLN:HG3   | 1.81                     | 0.61              |
| 1:Y:115:LEU:HD22 | 1:Y:115:LEU:N    | 2.15                     | 0.61              |
| 1:Z:233:GLY:HA2  | 2:Z:502:SO4:O2   | 2.01                     | 0.61              |
| 1:X:194:ILE:HG22 | 1:X:290:ILE:CD1  | 2.31                     | 0.61              |
| 1:X:437:GLU:C    | 1:X:441:LEU:HD12 | 2.26                     | 0.61              |
| 1:X:486:TRP:HD1  | 1:X:487:LYS:HD2  | 1.63                     | 0.61              |
| 1:X:429:ARG:HA   | 1:X:470:PHE:O    | 2.00                     | 0.60              |
| 1:Z:156:ARG:C    | 1:Z:158:GLY:H    | 2.08                     | 0.60              |
| 1:X:12:GLY:HA3   | 1:X:17:ARG:HH12  | 1.65                     | 0.60              |
| 1:O:328:ASP:O    | 1:O:331:TYR:HB3  | 2.00                     | 0.60              |
| 1:O:396:GLN:HE21 | 1:O:403:LEU:H    | 1.49                     | 0.60              |
| 1:O:415:ASN:ND2  | 1:O:417:PHE:HB3  | 2.16                     | 0.60              |
| 1:Z:336:VAL:HG13 | 1:Z:338:ASN:O    | 2.01                     | 0.60              |
| 1:X:152:ARG:HH11 | 1:X:152:ARG:CG   | 2.14                     | 0.60              |
| 1:Y:351:LEU:HD22 | 1:Y:360:ALA:CB   | 2.31                     | 0.60              |
| 1:X:111:ILE:HG22 | 1:X:139:THR:HG22 | 1.83                     | 0.60              |
| 1:X:194:ILE:HG22 | 1:X:290:ILE:HD12 | 1.82                     | 0.60              |
| 1:X:258:GLU:HA   | 1:X:274:ASN:O    | 2.02                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:214:LEU:N    | 1:O:214:LEU:HD12 | 2.16                     | 0.60              |
| 1:Z:194:ILE:HD12 | 1:Z:300:TYR:CE2  | 2.37                     | 0.60              |
| 1:X:386:TYR:HE1  | 1:X:425:ILE:CD1  | 2.14                     | 0.60              |
| 1:O:458:ASP:N    | 1:O:458:ASP:OD1  | 2.29                     | 0.60              |
| 1:Y:48:ASP:OD1   | 1:Y:49:PRO:HD2   | 2.01                     | 0.60              |
| 1:Z:138:GLY:N    | 1:Z:189:THR:O    | 2.33                     | 0.60              |
| 1:O:362:GLY:HA3  | 1:Y:367:LEU:HB2  | 1.83                     | 0.60              |
| 1:O:475:GLU:O    | 1:O:477:THR:N    | 2.35                     | 0.60              |
| 1:Z:456:ASN:HD22 | 1:Z:458:ASP:N    | 1.99                     | 0.60              |
| 1:O:422:GLN:HA   | 1:O:425:ILE:CG2  | 2.32                     | 0.60              |
| 1:Y:458:ASP:HA   | 1:Y:461:GLN:NE2  | 2.16                     | 0.60              |
| 1:Y:316:LEU:HA   | 1:Y:320:MET:HB2  | 1.84                     | 0.60              |
| 1:X:293:GLY:O    | 1:X:295:THR:N    | 2.34                     | 0.60              |
| 1:Z:457:LEU:O    | 1:Z:461:GLN:HG2  | 2.02                     | 0.60              |
| 1:Y:61:VAL:HG21  | 1:Z:61:VAL:HG21  | 1.84                     | 0.59              |
| 1:X:111:ILE:H    | 1:X:111:ILE:CD1  | 2.08                     | 0.59              |
| 1:X:80:THR:HG21  | 1:X:248:ALA:HB3  | 1.84                     | 0.59              |
| 1:X:227:THR:O    | 1:X:237:ILE:N    | 2.31                     | 0.59              |
| 1:X:471:ARG:HG3  | 1:X:471:ARG:HH11 | 1.66                     | 0.59              |
| 1:O:179:HIS:NE2  | 1:O:215:PRO:HB3  | 2.18                     | 0.59              |
| 1:O:200:ASP:OD1  | 1:O:202:LYS:HB3  | 2.02                     | 0.59              |
| 1:O:497:GLU:HG3  | 1:O:498:GLU:N    | 2.17                     | 0.59              |
| 1:Z:237:ILE:CG2  | 1:Z:238:PRO:HD2  | 2.31                     | 0.59              |
| 1:X:122:ASP:O    | 1:X:126:SER:HB2  | 2.02                     | 0.59              |
| 1:Z:403:LEU:H    | 1:Z:403:LEU:CD1  | 2.15                     | 0.59              |
| 1:Z:413:VAL:HG23 | 1:Z:436:ARG:HG2  | 1.85                     | 0.59              |
| 1:X:258:GLU:HB3  | 1:X:276:GLY:N    | 2.17                     | 0.59              |
| 1:O:85:THR:CG2   | 1:O:102:VAL:HA   | 2.28                     | 0.59              |
| 1:O:156:ARG:HG3  | 1:O:210:PRO:HG3  | 1.83                     | 0.59              |
| 1:Y:85:THR:HG23  | 1:Y:102:VAL:CA   | 2.25                     | 0.59              |
| 1:Y:328:ASP:O    | 1:Y:331:TYR:HB3  | 2.01                     | 0.59              |
| 1:O:84:GLU:HB2   | 1:O:103:TRP:HB3  | 1.83                     | 0.59              |
| 1:O:331:TYR:O    | 1:O:335:LYS:HG2  | 2.02                     | 0.59              |
| 1:Z:402:ARG:HG3  | 1:Z:402:ARG:NH1  | 2.15                     | 0.59              |
| 1:X:184:THR:O    | 1:X:187:SER:HB3  | 2.03                     | 0.59              |
| 1:X:396:GLN:HG2  | 1:X:401:ILE:O    | 2.01                     | 0.59              |
| 1:O:153:GLU:HA   | 1:O:153:GLU:OE2  | 1.90                     | 0.59              |
| 1:Y:19:VAL:CG1   | 1:Y:27:ILE:HG23  | 2.32                     | 0.59              |
| 1:Z:152:ARG:C    | 1:Z:156:ARG:HG2  | 2.28                     | 0.59              |
| 1:X:351:LEU:HD22 | 1:X:360:ALA:CB   | 2.32                     | 0.59              |
| 1:Y:406:LEU:HD13 | 1:Y:408:VAL:HG12 | 1.85                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:X:178:VAL:HG12 | 1:X:180:VAL:HB   | 1.85                     | 0.59              |
| 1:O:227:THR:N    | 1:O:237:ILE:O    | 2.34                     | 0.59              |
| 1:X:407:ARG:CZ   | 1:X:466:ILE:HD11 | 2.32                     | 0.59              |
| 1:Y:500:ASP:OD1  | 1:Y:500:ASP:N    | 2.36                     | 0.58              |
| 1:Z:49:PRO:O     | 1:Z:52:ILE:HB    | 2.03                     | 0.58              |
| 1:Z:133:ASP:CG   | 1:Z:134:PRO:HD2  | 2.28                     | 0.58              |
| 1:Z:460:LEU:CA   | 1:Z:463:LYS:HD2  | 2.28                     | 0.58              |
| 1:X:180:VAL:HG23 | 1:X:216:GLU:HG2  | 1.84                     | 0.58              |
| 1:X:213:MET:C    | 1:X:214:LEU:HD23 | 2.28                     | 0.58              |
| 1:O:134:PRO:O    | 1:O:140:LYS:NZ   | 2.34                     | 0.58              |
| 1:Z:424:ASP:OD1  | 1:Z:473:GLY:N    | 2.29                     | 0.58              |
| 1:O:204:LEU:HD22 | 1:O:209:ILE:O    | 2.03                     | 0.58              |
| 1:O:316:LEU:HA   | 1:O:320:MET:HB2  | 1.86                     | 0.58              |
| 1:Y:256:VAL:HG11 | 1:Y:294:PRO:CB   | 2.34                     | 0.58              |
| 1:Z:36:GLU:HG3   | 1:Z:37:GLN:N     | 2.19                     | 0.58              |
| 1:Z:219:ARG:HG3  | 1:Z:222:GLU:OE1  | 2.03                     | 0.58              |
| 1:X:193:ASN:HB3  | 1:X:196:THR:HG21 | 1.85                     | 0.58              |
| 1:X:313:ILE:H    | 1:X:313:ILE:CD1  | 2.16                     | 0.58              |
| 1:X:438:VAL:HA   | 1:X:441:LEU:CD1  | 2.33                     | 0.58              |
| 1:Y:20:VAL:O     | 1:Y:28:ILE:N     | 2.29                     | 0.58              |
| 1:Y:50:MET:HE3   | 1:Y:50:MET:CA    | 2.33                     | 0.58              |
| 1:Y:475:GLU:OE1  | 1:Y:478:GLU:HB2  | 2.03                     | 0.58              |
| 1:X:286:LEU:HD13 | 1:X:395:MET:CE   | 2.34                     | 0.58              |
| 1:Z:386:TYR:HB3  | 1:Z:486:TRP:CE2  | 2.38                     | 0.58              |
| 1:X:47:HIS:CD2   | 1:X:82:GLN:HE22  | 2.21                     | 0.58              |
| 1:X:130:LEU:HD12 | 1:X:190:MET:CB   | 2.33                     | 0.58              |
| 1:O:196:THR:HG21 | 4:O:514:HOH:O    | 2.03                     | 0.58              |
| 1:O:210:PRO:O    | 1:O:213:MET:HG2  | 2.03                     | 0.58              |
| 1:O:328:ASP:HB3  | 1:O:332:PHE:CE2  | 2.39                     | 0.58              |
| 1:Y:80:THR:HG21  | 1:Y:245:ASP:HA   | 1.84                     | 0.58              |
| 1:Y:429:ARG:HG2  | 1:Y:469:GLU:CD   | 2.28                     | 0.58              |
| 1:Z:157:ARG:HH11 | 1:Z:157:ARG:CB   | 2.17                     | 0.58              |
| 1:Z:499:HIS:CD2  | 1:Z:500:ASP:H    | 2.21                     | 0.58              |
| 1:Z:156:ARG:O    | 1:Z:212:GLU:HG2  | 2.04                     | 0.58              |
| 1:Z:330:GLU:O    | 1:Z:334:THR:HG23 | 2.04                     | 0.58              |
| 1:X:456:ASN:O    | 1:X:459:GLU:HB2  | 2.02                     | 0.58              |
| 1:Y:226:GLN:HA   | 1:Y:237:ILE:O    | 2.04                     | 0.58              |
| 1:Z:106:ARG:HD2  | 1:Z:349:THR:O    | 2.03                     | 0.58              |
| 1:Z:343:TYR:O    | 1:Z:364:ILE:HA   | 2.04                     | 0.58              |
| 1:Z:401:ILE:HG22 | 1:Z:402:ARG:N    | 2.19                     | 0.58              |
| 1:Z:473:GLY:C    | 1:Z:474:ILE:HG13 | 2.28                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:X:90:GLU:HB2   | 1:X:93:THR:HG1   | 1.67                     | 0.58              |
| 1:Z:188:ARG:HH22 | 1:Z:303:GLU:CD   | 2.11                     | 0.57              |
| 1:O:29:SER:OG    | 1:O:63:VAL:HG12  | 2.03                     | 0.57              |
| 1:Z:265:TYR:HB3  | 1:Z:412:ALA:HB3  | 1.86                     | 0.57              |
| 1:X:309:ALA:O    | 1:X:312:SER:HB2  | 2.03                     | 0.57              |
| 1:O:5:TYR:CE2    | 1:O:69:ILE:HG12  | 2.38                     | 0.57              |
| 1:X:84:GLU:OE1   | 1:X:188:ARG:NH1  | 2.37                     | 0.57              |
| 1:Y:33:ARG:HH21  | 1:Z:33:ARG:HH21  | 1.52                     | 0.57              |
| 1:Y:491:LYS:HA   | 1:Y:494:MET:CE   | 2.34                     | 0.57              |
| 1:Z:278:LYS:HE3  | 1:Z:280:VAL:HG23 | 1.85                     | 0.57              |
| 1:X:352:GLY:N    | 4:X:524:HOH:O    | 2.36                     | 0.57              |
| 1:O:261:ALA:HA   | 1:O:272:LEU:O    | 2.05                     | 0.57              |
| 1:Z:131:VAL:HG13 | 1:Z:132:ILE:N    | 2.16                     | 0.57              |
| 1:X:310:GLY:HA2  | 1:X:313:ILE:HD13 | 1.86                     | 0.57              |
| 1:O:251:PHE:HE2  | 1:O:445:TYR:HB3  | 1.70                     | 0.57              |
| 1:Y:54:ALA:HA    | 1:Z:65:THR:HG23  | 1.85                     | 0.57              |
| 1:Y:424:ASP:CB   | 1:Y:474:ILE:HG21 | 2.29                     | 0.57              |
| 1:Y:456:ASN:ND2  | 1:Y:458:ASP:N    | 2.37                     | 0.57              |
| 1:Z:115:LEU:HA   | 1:Z:120:LEU:CD1  | 2.32                     | 0.57              |
| 1:Y:325:ASP:O    | 1:Y:328:ASP:N    | 2.29                     | 0.57              |
| 1:X:423:SER:O    | 1:X:427:GLY:N    | 2.37                     | 0.57              |
| 1:O:325:ASP:O    | 1:O:328:ASP:N    | 2.35                     | 0.57              |
| 1:O:424:ASP:HA   | 1:O:472:PRO:HA   | 1.86                     | 0.57              |
| 1:Y:77:ILE:HG22  | 1:Y:78:GLY:N     | 2.20                     | 0.57              |
| 1:Z:30:VAL:HG12  | 1:Z:31:SER:N     | 2.20                     | 0.57              |
| 1:X:478:GLU:HG3  | 1:X:479:ARG:N    | 2.19                     | 0.57              |
| 1:O:161:LEU:HD22 | 1:O:179:HIS:HE1  | 1.64                     | 0.57              |
| 1:Y:38:ILE:O     | 1:Y:45:VAL:HA    | 2.03                     | 0.57              |
| 1:Y:345:VAL:N    | 1:Y:363:ALA:O    | 2.33                     | 0.57              |
| 1:X:174:THR:C    | 1:X:175:GLN:HG2  | 2.30                     | 0.57              |
| 1:X:457:LEU:O    | 1:X:460:LEU:N    | 2.31                     | 0.57              |
| 1:X:422:GLN:NE2  | 1:X:426:LEU:HD22 | 2.19                     | 0.57              |
| 1:O:70:SER:OG    | 1:O:73:GLN:NE2   | 2.39                     | 0.56              |
| 1:Z:422:GLN:HE21 | 1:Z:426:LEU:HD22 | 1.70                     | 0.56              |
| 1:X:106:ARG:HD2  | 1:X:349:THR:O    | 2.04                     | 0.56              |
| 1:X:342:VAL:HG12 | 1:X:343:TYR:N    | 2.20                     | 0.56              |
| 1:O:30:VAL:HG12  | 1:O:31:SER:N     | 2.19                     | 0.56              |
| 1:Z:122:ASP:O    | 1:Z:126:SER:HB2  | 2.04                     | 0.56              |
| 1:Z:129:GLY:C    | 1:Z:130:LEU:HD23 | 2.30                     | 0.56              |
| 1:Z:156:ARG:HD3  | 1:Z:210:PRO:HG3  | 1.86                     | 0.56              |
| 1:Z:347:ALA:CB   | 1:Z:351:LEU:HD13 | 2.33                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:X:200:ASP:O    | 1:X:204:LEU:HD13 | 2.05                     | 0.56              |
| 1:O:496:TRP:CE3  | 1:Y:488:LYS:HD2  | 2.40                     | 0.56              |
| 1:Z:461:GLN:C    | 1:Z:463:LYS:H    | 2.12                     | 0.56              |
| 1:X:241:GLY:C    | 1:X:242:ILE:HG13 | 2.31                     | 0.56              |
| 1:X:249:ALA:HB2  | 1:X:439:THR:OG1  | 2.05                     | 0.56              |
| 1:X:250:LEU:CD1  | 1:X:255:CYS:HB2  | 2.36                     | 0.56              |
| 1:X:482:ARG:HH11 | 1:X:482:ARG:HB3  | 1.70                     | 0.56              |
| 1:O:128:THR:HB   | 1:O:130:LEU:H    | 1.70                     | 0.56              |
| 1:O:143:TRP:O    | 1:O:147:HIS:ND1  | 2.31                     | 0.56              |
| 1:O:271:MET:CE   | 1:O:392:LEU:HD12 | 2.32                     | 0.56              |
| 1:Y:120:LEU:O    | 1:Y:124:ILE:HG13 | 2.05                     | 0.56              |
| 1:X:157:ARG:HB2  | 1:X:157:ARG:CZ   | 2.35                     | 0.56              |
| 1:X:401:ILE:HG22 | 1:X:403:LEU:HD12 | 1.87                     | 0.56              |
| 1:X:418:LEU:HD13 | 1:X:419:MET:HE1  | 1.86                     | 0.56              |
| 1:Y:2:GLU:O      | 1:Y:73:GLN:HA    | 2.06                     | 0.56              |
| 1:Y:13:THR:O     | 1:Y:13:THR:HG22  | 2.06                     | 0.56              |
| 1:Y:60:LEU:O     | 1:Y:63:VAL:HG23  | 2.06                     | 0.56              |
| 1:Y:455:GLN:H    | 1:Y:459:GLU:CD   | 2.12                     | 0.56              |
| 1:Z:62:GLU:HA    | 1:Z:65:THR:HG22  | 1.87                     | 0.56              |
| 1:Z:157:ARG:HH11 | 1:Z:157:ARG:CG   | 2.19                     | 0.56              |
| 1:Z:293:GLY:O    | 1:Z:295:THR:N    | 2.38                     | 0.56              |
| 1:X:47:HIS:HD2   | 1:X:82:GLN:HE22  | 1.54                     | 0.56              |
| 1:X:251:PHE:CE2  | 1:X:446:LEU:HD11 | 2.40                     | 0.56              |
| 1:X:294:PRO:HD2  | 1:X:297:GLU:OE2  | 2.05                     | 0.56              |
| 1:X:386:TYR:HE1  | 1:X:425:ILE:HD13 | 1.71                     | 0.56              |
| 1:O:137:SER:OG   | 1:O:189:THR:HA   | 2.04                     | 0.56              |
| 1:O:430:VAL:O    | 1:O:469:GLU:HA   | 2.05                     | 0.56              |
| 1:Y:202:LYS:O    | 1:Y:206:VAL:N    | 2.29                     | 0.56              |
| 1:Z:253:GLN:CG   | 1:Z:438:VAL:HG21 | 2.35                     | 0.56              |
| 1:Z:467:GLU:OE1  | 1:Z:468:ARG:HB2  | 2.06                     | 0.56              |
| 1:Y:9:LEU:HD13   | 1:Y:77:ILE:CG2   | 2.36                     | 0.56              |
| 1:Z:271:MET:HE1  | 1:Z:392:LEU:HB2  | 1.88                     | 0.56              |
| 1:Z:295:THR:HB   | 1:Z:297:GLU:HG2  | 1.86                     | 0.56              |
| 1:O:196:THR:HG23 | 1:O:198:ASP:N    | 2.21                     | 0.56              |
| 1:O:204:LEU:CD2  | 1:O:209:ILE:HG22 | 2.36                     | 0.56              |
| 1:Y:240:SER:O    | 1:Y:447:ALA:HA   | 2.05                     | 0.56              |
| 1:Y:474:ILE:HG12 | 1:Y:475:GLU:N    | 2.21                     | 0.56              |
| 1:Z:191:LEU:O    | 1:Z:199:TRP:HE3  | 1.89                     | 0.56              |
| 1:O:40:PRO:HG2   | 1:O:44:TRP:CB    | 2.35                     | 0.56              |
| 1:O:317:ARG:HB2  | 1:O:323:ILE:CD1  | 2.35                     | 0.56              |
| 1:Y:123:TYR:HD2  | 1:Y:203:MET:HE3  | 1.70                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Z:50:MET:HE2   | 1:Z:168:TRP:CH2  | 2.40                     | 0.56              |
| 1:Z:125:ARG:HH11 | 1:Z:125:ARG:CG   | 2.19                     | 0.56              |
| 1:O:189:THR:CB   | 1:O:191:LEU:HD12 | 2.23                     | 0.56              |
| 1:O:394:ALA:O    | 1:O:397:ALA:HB3  | 2.05                     | 0.56              |
| 1:Y:483:TYR:O    | 1:Y:486:TRP:HB3  | 2.06                     | 0.56              |
| 1:Z:108:THR:HB   | 1:Z:139:THR:HB   | 1.89                     | 0.56              |
| 1:X:456:ASN:HD22 | 1:X:458:ASP:HB2  | 1.71                     | 0.56              |
| 1:O:65:THR:HG21  | 1:X:54:ALA:HA    | 1.88                     | 0.55              |
| 1:O:124:ILE:HG23 | 1:O:203:MET:CE   | 2.36                     | 0.55              |
| 1:O:422:GLN:HA   | 1:O:425:ILE:HG22 | 1.88                     | 0.55              |
| 1:Y:269:CYS:HB2  | 1:Y:306:VAL:HB   | 1.89                     | 0.55              |
| 1:Z:320:MET:O    | 1:Z:322:LEU:HD23 | 2.05                     | 0.55              |
| 1:Z:394:ALA:O    | 1:Z:397:ALA:HB3  | 2.06                     | 0.55              |
| 1:O:104:GLN:HB3  | 1:O:349:THR:HG21 | 1.87                     | 0.55              |
| 1:Y:346:PRO:HG3  | 4:Y:512:HOH:O    | 2.06                     | 0.55              |
| 1:O:15:SER:OG    | 1:O:17:ARG:NH1   | 2.39                     | 0.55              |
| 1:O:23:HIS:HA    | 1:O:453:PHE:HE2  | 1.71                     | 0.55              |
| 1:Y:28:ILE:N     | 1:Y:28:ILE:HD13  | 2.20                     | 0.55              |
| 1:Y:346:PRO:HA   | 1:Y:348:PHE:CE1  | 2.41                     | 0.55              |
| 1:Z:48:ASP:O     | 1:Z:52:ILE:HG13  | 2.07                     | 0.55              |
| 1:Z:351:LEU:HD22 | 1:Z:360:ALA:HB1  | 1.88                     | 0.55              |
| 1:X:286:LEU:HD13 | 1:X:395:MET:HE3  | 1.88                     | 0.55              |
| 1:X:351:LEU:HB2  | 1:X:357:ASP:HB3  | 1.88                     | 0.55              |
| 1:O:22:ASP:OD1   | 1:O:24:ASP:N     | 2.39                     | 0.55              |
| 1:O:401:ILE:HG13 | 1:O:402:ARG:N    | 2.22                     | 0.55              |
| 1:Z:318:ASP:O    | 1:Z:321:LYS:HE2  | 2.07                     | 0.55              |
| 1:O:164:THR:O    | 1:O:167:THR:HB   | 2.07                     | 0.55              |
| 1:O:308:MET:HE3  | 1:O:349:THR:HG23 | 1.87                     | 0.55              |
| 1:O:422:GLN:O    | 1:O:426:LEU:HD22 | 2.07                     | 0.55              |
| 1:Y:108:THR:HB   | 1:Y:139:THR:HB   | 1.88                     | 0.55              |
| 1:X:251:PHE:CD2  | 1:X:446:LEU:HD11 | 2.42                     | 0.55              |
| 1:X:378:ARG:O    | 1:X:382:GLU:HG3  | 2.06                     | 0.55              |
| 1:X:482:ARG:HH11 | 1:X:482:ARG:HA   | 1.70                     | 0.55              |
| 1:O:16:SER:C     | 1:O:17:ARG:HD3   | 2.32                     | 0.55              |
| 1:O:202:LYS:O    | 1:O:205:GLU:HG2  | 2.06                     | 0.55              |
| 1:Z:86:THR:HG23  | 1:Z:162:PHE:HE1  | 1.71                     | 0.55              |
| 1:X:477:THR:O    | 1:X:481:TYR:HB2  | 2.06                     | 0.55              |
| 1:O:269:CYS:HB2  | 1:O:306:VAL:HB   | 1.88                     | 0.55              |
| 1:X:123:TYR:CE2  | 1:X:203:MET:HE2  | 2.42                     | 0.55              |
| 1:O:32:GLN:O     | 1:O:33:ARG:HD3   | 2.07                     | 0.55              |
| 1:O:124:ILE:HG21 | 1:O:190:MET:SD   | 2.47                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:331:TYR:CZ   | 1:O:335:LYS:HE3  | 2.42                     | 0.55              |
| 1:O:458:ASP:C    | 1:O:461:GLN:HG3  | 2.32                     | 0.55              |
| 1:Y:102:VAL:HG12 | 1:Y:103:TRP:N    | 2.21                     | 0.55              |
| 1:Z:210:PRO:O    | 1:Z:213:MET:HG2  | 2.07                     | 0.55              |
| 1:X:174:THR:O    | 1:X:175:GLN:HG2  | 2.07                     | 0.55              |
| 1:O:415:ASN:C    | 1:O:415:ASN:HD22 | 2.15                     | 0.55              |
| 1:Y:82:GLN:HG3   | 1:Y:82:GLN:O     | 2.07                     | 0.55              |
| 1:Z:170:ILE:HD11 | 1:Z:242:ILE:HD11 | 1.88                     | 0.55              |
| 1:O:70:SER:H     | 1:O:73:GLN:HE22  | 1.55                     | 0.55              |
| 1:Y:389:ARG:HH12 | 1:Y:479:ARG:HG3  | 1.72                     | 0.55              |
| 1:X:15:SER:O     | 1:X:17:ARG:NH1   | 2.39                     | 0.55              |
| 1:X:83:ARG:NH1   | 3:X:503:GOL:O1   | 2.39                     | 0.55              |
| 1:X:254:LEU:O    | 1:X:256:VAL:N    | 2.40                     | 0.55              |
| 1:O:460:LEU:CA   | 1:O:463:LYS:HE2  | 2.34                     | 0.54              |
| 1:X:79:ILE:HD11  | 1:X:173:MET:HE2  | 1.88                     | 0.54              |
| 1:X:196:THR:HG22 | 1:X:198:ASP:H    | 1.72                     | 0.54              |
| 1:X:312:SER:O    | 1:X:315:TRP:HB3  | 2.07                     | 0.54              |
| 1:X:316:LEU:HA   | 1:X:320:MET:HB2  | 1.88                     | 0.54              |
| 1:O:64:LEU:CD2   | 1:O:74:ILE:HD11  | 2.37                     | 0.54              |
| 1:O:460:LEU:O    | 1:O:463:LYS:HE2  | 2.06                     | 0.54              |
| 1:Y:222:GLU:O    | 1:Y:240:SER:HA   | 2.07                     | 0.54              |
| 1:Z:316:LEU:HA   | 1:Z:320:MET:HB2  | 1.88                     | 0.54              |
| 1:Z:363:ALA:HA   | 1:X:364:ILE:O    | 2.08                     | 0.54              |
| 1:X:110:GLU:O    | 1:X:113:GLU:N    | 2.40                     | 0.54              |
| 1:O:149:GLU:CD   | 1:O:149:GLU:H    | 2.16                     | 0.54              |
| 1:Y:191:LEU:CD2  | 1:Y:207:LEU:HD12 | 2.37                     | 0.54              |
| 1:Y:312:SER:O    | 1:Y:315:TRP:HB3  | 2.07                     | 0.54              |
| 1:Z:130:LEU:HD23 | 1:Z:130:LEU:N    | 2.16                     | 0.54              |
| 1:X:159:GLU:HB3  | 1:X:160:LEU:HG   | 1.88                     | 0.54              |
| 1:X:320:MET:O    | 1:X:322:LEU:HD23 | 2.07                     | 0.54              |
| 1:X:475:GLU:HG2  | 1:X:477:THR:OG1  | 2.07                     | 0.54              |
| 1:X:3:LYS:N      | 1:X:4:LYS:NZ     | 2.54                     | 0.54              |
| 1:X:84:GLU:HG2   | 1:X:103:TRP:CB   | 2.37                     | 0.54              |
| 1:X:317:ARG:HB2  | 1:X:323:ILE:HG13 | 1.89                     | 0.54              |
| 1:X:386:TYR:HB3  | 1:X:486:TRP:CE2  | 2.42                     | 0.54              |
| 1:X:497:GLU:HG3  | 1:X:498:GLU:N    | 2.22                     | 0.54              |
| 1:O:196:THR:HG22 | 1:O:198:ASP:H    | 1.72                     | 0.54              |
| 1:Z:106:ARG:NH1  | 1:Z:307:PHE:HE2  | 2.04                     | 0.54              |
| 1:Z:317:ARG:O    | 1:Z:321:LYS:HA   | 2.08                     | 0.54              |
| 1:Z:399:SER:HB2  | 1:Z:401:ILE:HD12 | 1.90                     | 0.54              |
| 1:Y:78:GLY:O     | 1:Y:79:ILE:HD13  | 2.06                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:X:202:LYS:O    | 1:X:205:GLU:HB3  | 2.08                     | 0.54              |
| 1:O:332:PHE:HA   | 1:O:374:ASN:HD21 | 1.73                     | 0.54              |
| 1:Y:392:LEU:HG   | 1:Y:392:LEU:O    | 2.08                     | 0.54              |
| 1:Z:240:SER:O    | 1:Z:447:ALA:HA   | 2.08                     | 0.54              |
| 1:Z:392:LEU:HD23 | 1:Z:392:LEU:C    | 2.33                     | 0.54              |
| 1:O:31:SER:HB3   | 1:O:62:GLU:OE2   | 2.07                     | 0.54              |
| 1:Z:171:TRP:CE3  | 1:Z:172:LYS:HD2  | 2.43                     | 0.54              |
| 1:Z:194:ILE:HD12 | 1:Z:300:TYR:HE2  | 1.72                     | 0.54              |
| 1:Z:200:ASP:HB3  | 1:Z:203:MET:HB2  | 1.90                     | 0.54              |
| 1:X:44:TRP:CE2   | 1:X:107:ARG:HB2  | 2.43                     | 0.54              |
| 1:X:180:VAL:HG22 | 1:X:218:ARG:CG   | 2.38                     | 0.54              |
| 1:O:322:LEU:CD2  | 1:Y:322:LEU:HD21 | 2.37                     | 0.53              |
| 1:Y:468:ARG:HH11 | 1:Y:468:ARG:CG   | 2.15                     | 0.53              |
| 1:Z:289:THR:O    | 1:Z:301:ALA:N    | 2.40                     | 0.53              |
| 1:X:445:TYR:N    | 1:X:445:TYR:CD1  | 2.75                     | 0.53              |
| 1:O:92:GLU:HB3   | 1:O:93:THR:HG23  | 1.89                     | 0.53              |
| 1:O:130:LEU:O    | 1:O:131:VAL:HG23 | 2.08                     | 0.53              |
| 1:O:402:ARG:HH21 | 1:O:404:HIS:CD2  | 2.26                     | 0.53              |
| 1:Z:423:SER:O    | 1:Z:427:GLY:N    | 2.35                     | 0.53              |
| 1:O:406:LEU:HD22 | 1:O:407:ARG:N    | 2.23                     | 0.53              |
| 1:O:457:LEU:O    | 1:O:460:LEU:HB2  | 2.08                     | 0.53              |
| 1:Y:174:THR:HG21 | 1:Y:178:VAL:HG13 | 1.90                     | 0.53              |
| 1:Y:180:VAL:HG22 | 1:Y:218:ARG:HG3  | 1.90                     | 0.53              |
| 1:Z:40:PRO:HG2   | 1:Z:44:TRP:HE3   | 1.72                     | 0.53              |
| 1:Z:362:GLY:CA   | 1:X:367:LEU:HB2  | 2.36                     | 0.53              |
| 1:Z:422:GLN:NE2  | 1:Z:426:LEU:HD22 | 2.23                     | 0.53              |
| 1:X:37:GLN:OE1   | 1:X:47:HIS:HE1   | 1.91                     | 0.53              |
| 1:Y:40:PRO:HG2   | 1:Y:44:TRP:HE3   | 1.73                     | 0.53              |
| 1:X:70:SER:O     | 1:X:73:GLN:OE1   | 2.26                     | 0.53              |
| 1:X:85:THR:HG23  | 1:X:102:VAL:HA   | 1.91                     | 0.53              |
| 1:O:70:SER:H     | 1:O:73:GLN:NE2   | 2.06                     | 0.53              |
| 1:Y:115:LEU:HD22 | 1:Y:115:LEU:H    | 1.72                     | 0.53              |
| 1:Y:406:LEU:HD13 | 1:Y:408:VAL:HG13 | 1.90                     | 0.53              |
| 1:Z:92:GLU:HG2   | 1:Z:93:THR:N     | 2.23                     | 0.53              |
| 1:X:166:ASP:OD1  | 1:X:166:ASP:N    | 2.41                     | 0.53              |
| 1:O:128:THR:HG22 | 1:O:128:THR:O    | 2.09                     | 0.53              |
| 1:O:234:GLY:H    | 1:O:236:ARG:NH2  | 2.06                     | 0.53              |
| 1:X:144:ILE:O    | 1:X:148:VAL:HG23 | 2.08                     | 0.53              |
| 1:Y:127:ASN:HD22 | 1:Y:193:ASN:HD21 | 1.56                     | 0.53              |
| 1:Y:169:LEU:O    | 1:Y:173:MET:HG3  | 2.09                     | 0.53              |
| 1:Y:182:ASP:OD2  | 1:Y:184:THR:HG23 | 2.09                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Z:183:TYR:CE1  | 1:Z:217:VAL:HG12 | 2.43                     | 0.53              |
| 1:Z:352:GLY:O    | 1:Z:355:TYR:N    | 2.37                     | 0.53              |
| 1:Z:401:ILE:HG22 | 1:Z:402:ARG:H    | 1.72                     | 0.53              |
| 1:X:9:LEU:HD12   | 1:X:9:LEU:N      | 2.24                     | 0.53              |
| 1:X:253:GLN:O    | 1:X:254:LEU:HB2  | 2.09                     | 0.53              |
| 1:X:469:GLU:HG2  | 1:X:471:ARG:CZ   | 2.38                     | 0.53              |
| 1:O:51:GLU:O     | 1:O:55:THR:HG23  | 2.09                     | 0.53              |
| 1:O:65:THR:HG23  | 1:X:54:ALA:CA    | 2.38                     | 0.53              |
| 1:O:152:ARG:HH21 | 1:O:208:ASP:HB3  | 1.71                     | 0.53              |
| 1:O:152:ARG:O    | 1:O:156:ARG:HG3  | 2.08                     | 0.53              |
| 1:Y:330:GLU:O    | 1:Y:334:THR:HG23 | 2.09                     | 0.53              |
| 1:Y:456:ASN:O    | 1:Y:459:GLU:HB2  | 2.08                     | 0.53              |
| 1:Z:19:VAL:HG12  | 1:Z:20:VAL:N     | 2.23                     | 0.53              |
| 1:Z:173:MET:HB3  | 1:Z:227:THR:HG21 | 1.90                     | 0.53              |
| 1:X:123:TYR:CD2  | 1:X:203:MET:HE2  | 2.43                     | 0.53              |
| 1:O:156:ARG:HA   | 1:O:212:GLU:OE1  | 2.09                     | 0.53              |
| 1:Y:272:LEU:CG   | 1:Y:303:GLU:HB2  | 2.28                     | 0.53              |
| 1:Z:5:TYR:CE2    | 1:Z:69:ILE:HD13  | 2.43                     | 0.53              |
| 1:X:216:GLU:OE2  | 1:X:218:ARG:HD3  | 2.08                     | 0.53              |
| 1:O:142:LYS:O    | 1:O:146:ASP:OD1  | 2.26                     | 0.53              |
| 1:Y:44:TRP:N     | 1:Y:44:TRP:CD1   | 2.75                     | 0.53              |
| 1:Z:162:PHE:CD1  | 1:Z:163:GLY:N    | 2.77                     | 0.53              |
| 1:X:19:VAL:HG11  | 1:X:27:ILE:CD1   | 2.39                     | 0.53              |
| 1:Y:415:ASN:HD22 | 1:Y:418:LEU:H    | 1.55                     | 0.52              |
| 1:Z:389:ARG:O    | 1:Z:393:GLU:HG2  | 2.09                     | 0.52              |
| 1:X:65:THR:CG2   | 1:X:66:LYS:N     | 2.72                     | 0.52              |
| 1:X:320:MET:CA   | 1:X:320:MET:HE3  | 2.38                     | 0.52              |
| 1:X:476:THR:O    | 1:X:479:ARG:N    | 2.42                     | 0.52              |
| 1:Y:297:GLU:OE1  | 1:Y:297:GLU:N    | 2.33                     | 0.52              |
| 1:Y:456:ASN:ND2  | 1:Y:458:ASP:OD1  | 2.42                     | 0.52              |
| 1:Z:83:ARG:HH12  | 3:Z:504:GOL:C1   | 2.23                     | 0.52              |
| 1:Z:499:HIS:CG   | 1:Z:500:ASP:N    | 2.77                     | 0.52              |
| 1:X:44:TRP:N     | 1:X:44:TRP:CD1   | 2.75                     | 0.52              |
| 1:X:191:LEU:HD22 | 1:X:204:LEU:HD12 | 1.91                     | 0.52              |
| 1:Y:9:LEU:HD13   | 1:Y:77:ILE:HG21  | 1.91                     | 0.52              |
| 1:Z:83:ARG:NH1   | 3:Z:504:GOL:C2   | 2.72                     | 0.52              |
| 1:Z:123:TYR:CE2  | 1:Z:202:LYS:HG2  | 2.45                     | 0.52              |
| 1:O:253:GLN:NE2  | 1:O:407:ARG:HG3  | 2.24                     | 0.52              |
| 1:Y:20:VAL:O     | 1:Y:27:ILE:HA    | 2.10                     | 0.52              |
| 1:Z:311:ALA:HA   | 1:Z:314:GLN:HG2  | 1.92                     | 0.52              |
| 1:O:44:TRP:N     | 1:O:44:TRP:CD1   | 2.75                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:62:GLU:HA    | 1:O:65:THR:HG22  | 1.90                     | 0.52              |
| 1:O:101:ILE:CG2  | 1:O:140:LYS:HG2  | 2.40                     | 0.52              |
| 1:Y:49:PRO:HB3   | 1:Y:87:ILE:HD13  | 1.90                     | 0.52              |
| 1:O:82:GLN:NE2   | 1:O:85:THR:OG1   | 2.42                     | 0.52              |
| 1:Y:98:TYR:CD2   | 1:Y:99:ASN:N     | 2.78                     | 0.52              |
| 1:Z:174:THR:CG2  | 1:Z:178:VAL:HG13 | 2.32                     | 0.52              |
| 1:X:80:THR:HG22  | 1:X:245:ASP:N    | 2.24                     | 0.52              |
| 1:X:106:ARG:NH1  | 1:X:307:PHE:CE2  | 2.78                     | 0.52              |
| 1:O:204:LEU:HD23 | 1:O:209:ILE:HB   | 1.92                     | 0.52              |
| 1:O:259:GLY:CA   | 1:O:273:MET:HE2  | 2.39                     | 0.52              |
| 1:Y:137:SER:O    | 1:Y:141:VAL:HG23 | 2.09                     | 0.52              |
| 1:Y:430:VAL:O    | 1:Y:469:GLU:HA   | 2.09                     | 0.52              |
| 1:Z:41:LYS:O     | 1:Z:44:TRP:HB2   | 2.10                     | 0.52              |
| 1:Z:115:LEU:N    | 1:Z:115:LEU:HD12 | 2.25                     | 0.52              |
| 1:X:19:VAL:HG11  | 1:X:27:ILE:HD12  | 1.92                     | 0.52              |
| 1:X:154:ARG:NH1  | 1:X:160:LEU:HD21 | 2.24                     | 0.52              |
| 1:Z:6:ILE:HD13   | 1:Z:6:ILE:C      | 2.34                     | 0.52              |
| 1:Z:357:ASP:OD2  | 1:Z:360:ALA:HB2  | 2.10                     | 0.52              |
| 1:X:125:ARG:N    | 4:X:534:HOH:O    | 2.43                     | 0.52              |
| 1:O:123:TYR:CZ   | 1:O:202:LYS:HG3  | 2.45                     | 0.51              |
| 1:O:196:THR:HG23 | 1:O:198:ASP:H    | 1.75                     | 0.51              |
| 1:O:317:ARG:O    | 1:O:321:LYS:HA   | 2.10                     | 0.51              |
| 1:O:317:ARG:HA   | 1:O:323:ILE:CG1  | 2.40                     | 0.51              |
| 1:Y:103:TRP:CE3  | 1:Y:104:GLN:HG3  | 2.45                     | 0.51              |
| 1:Y:396:GLN:NE2  | 1:Y:402:ARG:HA   | 2.25                     | 0.51              |
| 1:X:180:VAL:CG2  | 1:X:216:GLU:HG2  | 2.39                     | 0.51              |
| 1:O:209:ILE:O    | 1:O:209:ILE:HG22 | 2.10                     | 0.51              |
| 1:Z:293:GLY:C    | 1:Z:295:THR:H    | 2.18                     | 0.51              |
| 1:Z:386:TYR:HB3  | 1:Z:486:TRP:CD2  | 2.44                     | 0.51              |
| 1:Z:436:ARG:N    | 1:Z:436:ARG:HD2  | 2.25                     | 0.51              |
| 1:O:221:SER:O    | 1:O:222:GLU:HB2  | 2.10                     | 0.51              |
| 1:O:226:GLN:HA   | 1:O:237:ILE:O    | 2.11                     | 0.51              |
| 1:Y:59:THR:O     | 1:Y:63:VAL:HG22  | 2.10                     | 0.51              |
| 1:Y:61:VAL:O     | 1:Y:65:THR:HB    | 2.10                     | 0.51              |
| 1:Y:161:LEU:HD13 | 1:Y:179:HIS:CD2  | 2.45                     | 0.51              |
| 1:Z:37:GLN:OE1   | 1:Z:47:HIS:HE1   | 1.93                     | 0.51              |
| 1:Z:147:HIS:HD1  | 1:Z:147:HIS:H    | 1.56                     | 0.51              |
| 1:Z:156:ARG:HG3  | 1:Z:156:ARG:NH1  | 2.14                     | 0.51              |
| 1:X:98:TYR:CD2   | 1:X:99:ASN:N     | 2.78                     | 0.51              |
| 1:X:85:THR:HA    | 1:X:101:ILE:O    | 2.10                     | 0.51              |
| 1:X:259:GLY:N    | 1:X:274:ASN:O    | 2.41                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:154:ARG:CA   | 1:O:159:GLU:HG3  | 2.40                     | 0.51              |
| 1:Y:351:LEU:HD22 | 1:Y:360:ALA:HB1  | 1.92                     | 0.51              |
| 1:Y:428:THR:CG2  | 1:Y:429:ARG:N    | 2.74                     | 0.51              |
| 1:Z:415:ASN:O    | 1:Z:419:MET:HG2  | 2.10                     | 0.51              |
| 1:X:35:PHE:HE2   | 1:X:47:HIS:CD2   | 2.29                     | 0.51              |
| 1:O:280:VAL:O    | 1:O:288:THR:HG21 | 2.11                     | 0.51              |
| 1:Z:179:HIS:ND1  | 1:Z:215:PRO:HA   | 2.26                     | 0.51              |
| 1:X:48:ASP:O     | 1:X:51:GLU:N     | 2.43                     | 0.51              |
| 1:O:85:THR:HG23  | 1:O:101:ILE:O    | 2.11                     | 0.51              |
| 1:O:157:ARG:HB2  | 1:O:159:GLU:HG3  | 1.93                     | 0.51              |
| 1:O:224:TYR:CZ   | 1:O:242:ILE:HG13 | 2.46                     | 0.51              |
| 1:O:308:MET:HE1  | 1:Y:369:ARG:CD   | 2.39                     | 0.51              |
| 1:Y:455:GLN:N    | 1:Y:459:GLU:OE1  | 2.41                     | 0.51              |
| 1:Z:40:PRO:CG    | 1:Z:44:TRP:HB3   | 2.40                     | 0.51              |
| 1:Z:298:VAL:O    | 1:Z:299:ASN:OD1  | 2.28                     | 0.51              |
| 1:X:153:GLU:O    | 1:X:156:ARG:N    | 2.42                     | 0.51              |
| 1:Y:191:LEU:HD21 | 1:Y:207:LEU:CD1  | 2.41                     | 0.51              |
| 1:Y:193:ASN:HB3  | 1:Y:196:THR:HB   | 1.92                     | 0.51              |
| 1:Y:441:LEU:HD13 | 1:Y:445:TYR:OH   | 2.11                     | 0.51              |
| 1:Z:49:PRO:HG2   | 1:Z:96:PRO:CG    | 2.40                     | 0.51              |
| 1:Z:120:LEU:O    | 1:Z:124:ILE:HD12 | 2.10                     | 0.51              |
| 1:Z:180:VAL:HG21 | 1:Z:218:ARG:HG3  | 1.91                     | 0.51              |
| 1:O:166:ASP:N    | 1:O:166:ASP:OD1  | 2.44                     | 0.51              |
| 1:Y:219:ARG:HH22 | 1:Y:295:THR:CG2  | 2.09                     | 0.51              |
| 1:Y:486:TRP:O    | 1:Y:490:VAL:N    | 2.37                     | 0.51              |
| 1:Z:135:TYR:OH   | 3:Z:504:GOL:O1   | 2.24                     | 0.51              |
| 1:X:21:MET:HE2   | 1:X:27:ILE:CD1   | 2.41                     | 0.51              |
| 1:O:282:SER:OG   | 1:O:398:ASP:OD2  | 2.28                     | 0.51              |
| 1:Y:98:TYR:HD2   | 1:Y:99:ASN:O     | 1.94                     | 0.51              |
| 1:Z:428:THR:HG23 | 1:Z:429:ARG:O    | 2.11                     | 0.51              |
| 1:X:7:VAL:CG2    | 1:X:74:ILE:HG23  | 2.40                     | 0.51              |
| 1:O:114:HIS:ND1  | 1:O:114:HIS:N    | 2.56                     | 0.50              |
| 1:Y:80:THR:HG22  | 1:Y:245:ASP:CA   | 2.37                     | 0.50              |
| 1:Y:456:ASN:HD21 | 1:Y:458:ASP:CB   | 2.23                     | 0.50              |
| 1:Z:83:ARG:HH11  | 1:Z:83:ARG:CG    | 2.24                     | 0.50              |
| 1:O:57:SER:O     | 1:O:60:LEU:HB3   | 2.12                     | 0.50              |
| 1:O:121:GLU:HA   | 1:O:132:ILE:HD11 | 1.93                     | 0.50              |
| 1:O:250:LEU:HD11 | 1:O:255:CYS:CB   | 2.40                     | 0.50              |
| 1:Y:141:VAL:HG12 | 1:Y:145:LEU:HD22 | 1.92                     | 0.50              |
| 1:Y:179:HIS:CE1  | 1:Y:215:PRO:HA   | 2.46                     | 0.50              |
| 1:Y:295:THR:N    | 1:Y:297:GLU:OE1  | 2.38                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Z:115:LEU:N    | 1:Z:115:LEU:CD1  | 2.74                     | 0.50              |
| 1:Z:415:ASN:HB3  | 1:Z:418:LEU:HB2  | 1.93                     | 0.50              |
| 1:X:7:VAL:HA     | 1:X:19:VAL:O     | 2.12                     | 0.50              |
| 1:X:251:PHE:HE1  | 1:X:293:GLY:O    | 1.95                     | 0.50              |
| 1:O:68:ASP:HB2   | 1:X:50:MET:CE    | 2.41                     | 0.50              |
| 1:Y:441:LEU:HD13 | 1:Y:445:TYR:CZ   | 2.46                     | 0.50              |
| 1:Z:48:ASP:HB3   | 1:Z:51:GLU:HB2   | 1.94                     | 0.50              |
| 1:Z:51:GLU:O     | 1:Z:55:THR:HG23  | 2.11                     | 0.50              |
| 1:Z:271:MET:C    | 1:Z:272:LEU:HD12 | 2.37                     | 0.50              |
| 1:Z:348:PHE:CE2  | 1:X:367:LEU:HB3  | 2.46                     | 0.50              |
| 1:O:98:TYR:CE2   | 1:O:101:ILE:HD11 | 2.47                     | 0.50              |
| 1:O:233:GLY:C    | 1:O:235:THR:H    | 2.17                     | 0.50              |
| 1:Z:180:VAL:HG22 | 1:Z:181:THR:H    | 1.77                     | 0.50              |
| 1:Z:206:VAL:HG13 | 1:Z:207:LEU:N    | 2.26                     | 0.50              |
| 1:O:384:ILE:HG22 | 1:O:385:ALA:N    | 2.24                     | 0.50              |
| 1:Y:345:VAL:O    | 1:Y:362:GLY:HA2  | 2.12                     | 0.50              |
| 1:Y:369:ARG:HB2  | 4:Y:525:HOH:O    | 2.11                     | 0.50              |
| 1:Y:456:ASN:HD21 | 1:Y:458:ASP:N    | 2.00                     | 0.50              |
| 1:Z:80:THR:CG2   | 1:Z:248:ALA:HB2  | 2.41                     | 0.50              |
| 1:Z:89:TRP:N     | 1:Z:89:TRP:CE3   | 2.80                     | 0.50              |
| 1:X:342:VAL:HG13 | 1:X:365:PHE:O    | 2.11                     | 0.50              |
| 1:O:108:THR:OG1  | 1:O:134:PRO:HB3  | 2.12                     | 0.50              |
| 1:X:232:LYS:O    | 1:X:233:GLY:O    | 2.30                     | 0.50              |
| 1:X:326:ALA:O    | 1:X:329:SER:OG   | 2.28                     | 0.50              |
| 1:Z:120:LEU:C    | 1:Z:124:ILE:HD12 | 2.37                     | 0.50              |
| 1:Z:225:GLY:O    | 1:Z:238:PRO:HA   | 2.12                     | 0.50              |
| 1:X:225:GLY:O    | 1:X:238:PRO:HA   | 2.11                     | 0.50              |
| 1:O:332:PHE:O    | 1:O:374:ASN:ND2  | 2.39                     | 0.50              |
| 1:O:345:VAL:O    | 1:O:362:GLY:HA2  | 2.12                     | 0.50              |
| 1:O:368:THR:O    | 1:O:371:VAL:HB   | 2.12                     | 0.50              |
| 1:Y:127:ASN:HD22 | 1:Y:193:ASN:ND2  | 2.10                     | 0.50              |
| 1:Y:202:LYS:HG3  | 1:Y:206:VAL:HG23 | 1.93                     | 0.50              |
| 1:Y:355:TYR:OH   | 1:Y:390:ASP:OD2  | 2.29                     | 0.50              |
| 1:Z:142:LYS:O    | 1:Z:145:LEU:HB2  | 2.12                     | 0.50              |
| 1:O:12:GLY:HA3   | 1:O:17:ARG:HH12  | 1.77                     | 0.50              |
| 1:Y:317:ARG:NH1  | 1:Y:326:ALA:HB2  | 2.26                     | 0.50              |
| 1:Z:294:PRO:HD2  | 1:Z:297:GLU:OE2  | 2.11                     | 0.50              |
| 1:O:4:LYS:N      | 1:O:73:GLN:O     | 2.45                     | 0.49              |
| 1:O:128:THR:HG21 | 1:O:130:LEU:CB   | 2.41                     | 0.49              |
| 1:X:320:MET:HB3  | 1:X:322:LEU:HG   | 1.94                     | 0.49              |
| 1:X:330:GLU:HG3  | 1:X:415:ASN:ND2  | 2.24                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:85:THR:HG22  | 1:O:100:ALA:HB1  | 1.94                     | 0.49              |
| 1:O:187:SER:HB3  | 1:O:289:THR:HG22 | 1.92                     | 0.49              |
| 1:O:234:GLY:N    | 1:O:236:ARG:HH21 | 2.10                     | 0.49              |
| 1:O:250:LEU:HD12 | 1:O:255:CYS:HB2  | 1.92                     | 0.49              |
| 1:Z:19:VAL:HG13  | 1:Z:27:ILE:HG23  | 1.94                     | 0.49              |
| 1:X:295:THR:O    | 1:X:295:THR:OG1  | 2.29                     | 0.49              |
| 1:O:85:THR:HG23  | 1:O:102:VAL:N    | 2.27                     | 0.49              |
| 1:Z:140:LYS:O    | 1:Z:144:ILE:HG13 | 2.12                     | 0.49              |
| 1:Z:415:ASN:HD22 | 1:Z:417:PHE:N    | 2.10                     | 0.49              |
| 1:O:154:ARG:HB3  | 1:O:159:GLU:CB   | 2.41                     | 0.49              |
| 1:Y:93:THR:OG1   | 1:Y:95:LYS:HB3   | 2.12                     | 0.49              |
| 1:Y:226:GLN:HB3  | 1:Y:236:ARG:HB3  | 1.94                     | 0.49              |
| 1:Y:330:GLU:HG3  | 1:Y:415:ASN:ND2  | 2.27                     | 0.49              |
| 1:O:28:ILE:N     | 1:O:28:ILE:CD1   | 2.76                     | 0.49              |
| 1:O:48:ASP:OD1   | 1:O:49:PRO:HD2   | 2.12                     | 0.49              |
| 1:O:444:ALA:O    | 1:O:447:ALA:N    | 2.45                     | 0.49              |
| 1:Y:84:GLU:OE2   | 1:Y:188:ARG:NH1  | 2.45                     | 0.49              |
| 1:Z:174:THR:O    | 1:Z:177:ARG:N    | 2.29                     | 0.49              |
| 1:X:351:LEU:HB3  | 1:X:355:TYR:HB2  | 1.95                     | 0.49              |
| 1:O:153:GLU:O    | 1:O:156:ARG:N    | 2.45                     | 0.49              |
| 1:Y:269:CYS:CB   | 1:Y:306:VAL:HB   | 2.42                     | 0.49              |
| 1:Y:284:ASN:OD1  | 1:Y:398:ASP:OD1  | 2.30                     | 0.49              |
| 1:Y:338:ASN:CB   | 1:Y:482:ARG:HH22 | 2.25                     | 0.49              |
| 1:Z:246:GLN:O    | 1:Z:249:ALA:HB3  | 2.12                     | 0.49              |
| 1:Z:455:GLN:N    | 1:Z:459:GLU:OE2  | 2.27                     | 0.49              |
| 1:Y:475:GLU:CD   | 1:Y:477:THR:HB   | 2.37                     | 0.49              |
| 1:Z:432:ARG:HD2  | 1:Z:467:GLU:OE1  | 2.11                     | 0.49              |
| 1:X:162:PHE:CG   | 1:X:163:GLY:N    | 2.79                     | 0.49              |
| 1:X:435:VAL:O    | 1:X:435:VAL:HG12 | 2.13                     | 0.49              |
| 1:O:130:LEU:HD22 | 1:O:190:MET:HA   | 1.94                     | 0.49              |
| 1:O:251:PHE:CE2  | 1:O:446:LEU:CD1  | 2.95                     | 0.49              |
| 1:Z:401:ILE:CG2  | 1:Z:402:ARG:H    | 2.26                     | 0.49              |
| 1:Z:475:GLU:HG3  | 1:Z:478:GLU:OE1  | 2.12                     | 0.49              |
| 1:Z:489:ALA:O    | 1:Z:492:ARG:N    | 2.46                     | 0.49              |
| 1:X:258:GLU:HB3  | 1:X:276:GLY:CA   | 2.42                     | 0.49              |
| 1:O:369:ARG:HD2  | 1:Y:308:MET:HE1  | 1.94                     | 0.49              |
| 1:Y:80:THR:HG23  | 1:Y:248:ALA:HB2  | 1.95                     | 0.49              |
| 1:Y:342:VAL:HG12 | 1:Y:343:TYR:N    | 2.27                     | 0.49              |
| 1:X:3:LYS:HA     | 1:X:73:GLN:O     | 2.13                     | 0.49              |
| 1:X:126:SER:O    | 1:X:195:HIS:HE1  | 1.95                     | 0.49              |
| 1:X:164:THR:OG1  | 1:X:166:ASP:OD1  | 2.30                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:X:343:TYR:OH   | 1:X:485:GLY:HA3  | 2.12                     | 0.49              |
| 1:Y:33:ARG:NH2   | 1:Z:33:ARG:HH21  | 2.11                     | 0.49              |
| 1:Y:85:THR:HG23  | 1:Y:101:ILE:O    | 2.12                     | 0.49              |
| 1:Y:210:PRO:HB2  | 1:Y:213:MET:HE2  | 1.93                     | 0.49              |
| 1:Z:331:TYR:CE2  | 1:Z:335:LYS:NZ   | 2.79                     | 0.49              |
| 1:X:196:THR:HG22 | 1:X:197:LEU:N    | 2.28                     | 0.49              |
| 1:X:263:ASN:HB2  | 1:X:406:LEU:HD11 | 1.95                     | 0.49              |
| 1:X:396:GLN:NE2  | 1:X:403:LEU:H    | 1.95                     | 0.49              |
| 1:X:465:VAL:HG12 | 1:X:466:ILE:N    | 2.28                     | 0.49              |
| 1:X:482:ARG:HG2  | 1:X:482:ARG:H    | 1.41                     | 0.49              |
| 1:O:320:MET:HB3  | 1:O:322:LEU:HG   | 1.94                     | 0.48              |
| 1:O:332:PHE:HA   | 1:O:374:ASN:ND2  | 2.27                     | 0.48              |
| 1:Y:154:ARG:HB3  | 1:Y:159:GLU:HB2  | 1.95                     | 0.48              |
| 1:Y:221:SER:OG   | 1:Y:446:LEU:O    | 2.27                     | 0.48              |
| 1:Y:344:VAL:C    | 1:Y:345:VAL:HG23 | 2.37                     | 0.48              |
| 1:Z:194:ILE:HG13 | 1:Z:195:HIS:CE1  | 2.48                     | 0.48              |
| 1:X:64:LEU:HD22  | 1:X:69:ILE:HB    | 1.94                     | 0.48              |
| 1:X:320:MET:CE   | 1:X:320:MET:HA   | 2.37                     | 0.48              |
| 1:X:331:TYR:O    | 1:X:335:LYS:HG3  | 2.13                     | 0.48              |
| 1:O:124:ILE:HD13 | 1:O:203:MET:CE   | 2.20                     | 0.48              |
| 1:O:202:LYS:O    | 1:O:206:VAL:HG22 | 2.13                     | 0.48              |
| 1:O:372:ASN:O    | 1:O:375:HIS:HB2  | 2.13                     | 0.48              |
| 1:Z:284:ASN:OD1  | 1:Z:398:ASP:OD1  | 2.31                     | 0.48              |
| 1:O:155:ALA:HB1  | 1:O:213:MET:CE   | 2.43                     | 0.48              |
| 1:O:180:VAL:HG21 | 1:O:218:ARG:HG3  | 1.95                     | 0.48              |
| 1:O:422:GLN:CA   | 1:O:425:ILE:HG22 | 2.43                     | 0.48              |
| 1:O:478:GLU:O    | 1:O:481:TYR:N    | 2.47                     | 0.48              |
| 1:Y:303:GLU:HG3  | 1:Y:304:GLY:N    | 2.27                     | 0.48              |
| 1:Z:223:VAL:HG22 | 1:Z:240:SER:HB3  | 1.95                     | 0.48              |
| 1:X:6:ILE:HG21   | 1:X:444:ALA:HB1  | 1.94                     | 0.48              |
| 1:O:68:ASP:HB2   | 1:X:50:MET:HE2   | 1.95                     | 0.48              |
| 1:O:142:LYS:CD   | 1:O:207:LEU:HD22 | 2.43                     | 0.48              |
| 1:O:245:ASP:O    | 1:O:249:ALA:N    | 2.45                     | 0.48              |
| 1:O:422:GLN:NE2  | 1:O:426:LEU:HD22 | 2.27                     | 0.48              |
| 1:Z:289:THR:O    | 1:Z:300:TYR:HA   | 2.14                     | 0.48              |
| 1:Z:346:PRO:HG3  | 1:Z:383:SER:HB2  | 1.94                     | 0.48              |
| 1:X:103:TRP:CD1  | 1:X:103:TRP:H    | 2.31                     | 0.48              |
| 1:X:106:ARG:O    | 1:X:108:THR:N    | 2.46                     | 0.48              |
| 1:X:180:VAL:HG22 | 1:X:218:ARG:HG2  | 1.95                     | 0.48              |
| 1:O:147:HIS:HB3  | 4:O:533:HOH:O    | 2.12                     | 0.48              |
| 1:O:309:ALA:O    | 1:O:312:SER:HB2  | 2.13                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:322:LEU:HD21 | 1:Y:322:LEU:HD21 | 1.95                     | 0.48              |
| 1:O:3:LYS:HA     | 1:O:73:GLN:C     | 2.38                     | 0.48              |
| 1:Y:69:ILE:HD13  | 1:Y:69:ILE:N     | 2.27                     | 0.48              |
| 1:Z:40:PRO:HG2   | 1:Z:44:TRP:CE3   | 2.49                     | 0.48              |
| 1:Z:95:LYS:HE3   | 1:Z:96:PRO:O     | 2.13                     | 0.48              |
| 1:Z:203:MET:HA   | 1:Z:206:VAL:HG11 | 1.94                     | 0.48              |
| 1:Z:382:GLU:OE2  | 1:Z:482:ARG:NH2  | 2.47                     | 0.48              |
| 1:X:130:LEU:HD12 | 1:X:190:MET:HA   | 1.94                     | 0.48              |
| 1:X:130:LEU:CD1  | 1:X:190:MET:HB2  | 2.44                     | 0.48              |
| 1:X:409:ASP:HB2  | 1:X:438:VAL:HG21 | 1.95                     | 0.48              |
| 1:O:456:ASN:HD22 | 1:O:458:ASP:N    | 2.11                     | 0.48              |
| 1:O:468:ARG:HD2  | 1:O:470:PHE:CZ   | 2.49                     | 0.48              |
| 1:X:217:VAL:HG12 | 1:X:218:ARG:N    | 2.28                     | 0.48              |
| 1:O:47:HIS:O     | 1:O:99:ASN:HB3   | 2.14                     | 0.48              |
| 1:O:61:VAL:O     | 1:O:65:THR:HB    | 2.13                     | 0.48              |
| 1:O:138:GLY:O    | 1:O:141:VAL:HB   | 2.13                     | 0.48              |
| 1:O:250:LEU:HD13 | 1:O:262:LYS:HG2  | 1.96                     | 0.48              |
| 1:O:340:ASN:HB2  | 1:O:375:HIS:CD2  | 2.49                     | 0.48              |
| 1:O:459:GLU:O    | 1:O:462:GLU:OE1  | 2.32                     | 0.48              |
| 1:Y:338:ASN:HB3  | 1:Y:482:ARG:NH2  | 2.28                     | 0.48              |
| 1:Y:451:VAL:HG23 | 1:Y:451:VAL:O    | 2.14                     | 0.48              |
| 1:Z:474:ILE:HG23 | 1:Z:478:GLU:HB2  | 1.94                     | 0.48              |
| 1:X:457:LEU:HD23 | 1:X:457:LEU:HA   | 1.63                     | 0.48              |
| 1:O:346:PRO:HA   | 1:O:348:PHE:CE1  | 2.49                     | 0.48              |
| 1:Y:19:VAL:HG11  | 1:Y:27:ILE:CD1   | 2.42                     | 0.48              |
| 1:Y:156:ARG:C    | 1:Y:158:GLY:H    | 2.19                     | 0.48              |
| 1:Y:254:LEU:HD12 | 1:Y:254:LEU:HA   | 1.73                     | 0.48              |
| 1:Z:44:TRP:N     | 1:Z:44:TRP:CD1   | 2.78                     | 0.48              |
| 1:Z:48:ASP:OD1   | 1:Z:49:PRO:HD2   | 2.14                     | 0.48              |
| 1:O:128:THR:HG21 | 1:O:130:LEU:CG   | 2.43                     | 0.48              |
| 1:O:436:ARG:C    | 1:O:438:VAL:H    | 2.22                     | 0.48              |
| 1:O:475:GLU:C    | 1:O:477:THR:H    | 2.20                     | 0.48              |
| 1:Y:281:LYS:O    | 1:Y:281:LYS:HD2  | 2.13                     | 0.48              |
| 1:X:346:PRO:HA   | 1:X:348:PHE:HE1  | 1.77                     | 0.48              |
| 1:O:24:ASP:O     | 1:O:25:ALA:HB3   | 2.14                     | 0.47              |
| 1:Y:456:ASN:HD21 | 1:Y:458:ASP:CG   | 2.22                     | 0.47              |
| 1:Z:89:TRP:HB2   | 1:Z:95:LYS:O     | 2.13                     | 0.47              |
| 1:Z:456:ASN:HD22 | 1:Z:456:ASN:C    | 2.22                     | 0.47              |
| 1:O:28:ILE:HG22  | 1:O:29:SER:HB3   | 1.95                     | 0.47              |
| 1:O:89:TRP:HA    | 1:O:96:PRO:HA    | 1.96                     | 0.47              |
| 1:O:130:LEU:CD2  | 1:O:190:MET:HG3  | 2.41                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:131:VAL:CG1  | 1:O:132:ILE:N    | 2.77                     | 0.47              |
| 1:O:342:VAL:HG12 | 1:O:343:TYR:N    | 2.29                     | 0.47              |
| 1:Y:33:ARG:NE    | 1:Z:33:ARG:CZ    | 2.77                     | 0.47              |
| 1:Y:396:GLN:CD   | 1:Y:402:ARG:HA   | 2.39                     | 0.47              |
| 1:O:258:GLU:HA   | 1:O:274:ASN:O    | 2.14                     | 0.47              |
| 1:O:259:GLY:C    | 1:O:273:MET:HE2  | 2.38                     | 0.47              |
| 1:O:351:LEU:HB3  | 1:O:355:TYR:HB2  | 1.97                     | 0.47              |
| 1:Y:204:LEU:N    | 1:Y:204:LEU:HD23 | 2.29                     | 0.47              |
| 1:Z:365:PHE:CE1  | 1:Z:492:ARG:HB3  | 2.49                     | 0.47              |
| 1:Z:381:LEU:O    | 1:Z:384:ILE:HB   | 2.14                     | 0.47              |
| 1:Z:481:TYR:O    | 1:Z:484:ALA:HB3  | 2.13                     | 0.47              |
| 1:X:153:GLU:O    | 1:X:156:ARG:HB2  | 2.14                     | 0.47              |
| 1:X:229:ILE:N    | 4:X:525:HOH:O    | 2.36                     | 0.47              |
| 1:X:418:LEU:HD13 | 1:X:419:MET:HE2  | 1.96                     | 0.47              |
| 1:O:64:LEU:HD22  | 1:O:74:ILE:HD11  | 1.96                     | 0.47              |
| 1:O:259:GLY:N    | 1:O:274:ASN:O    | 2.40                     | 0.47              |
| 1:O:352:GLY:O    | 1:O:355:TYR:N    | 2.40                     | 0.47              |
| 1:O:461:GLN:H    | 1:O:461:GLN:HG2  | 1.32                     | 0.47              |
| 1:Y:293:GLY:HA3  | 1:Y:297:GLU:CD   | 2.40                     | 0.47              |
| 1:Z:6:ILE:HG23   | 1:Z:21:MET:HB3   | 1.94                     | 0.47              |
| 1:Z:124:ILE:HG13 | 1:Z:203:MET:CE   | 2.44                     | 0.47              |
| 1:X:264:THR:HG22 | 1:X:265:TYR:N    | 2.28                     | 0.47              |
| 1:X:289:THR:O    | 1:X:301:ALA:N    | 2.41                     | 0.47              |
| 1:O:447:ALA:O    | 1:O:450:ALA:HB3  | 2.15                     | 0.47              |
| 1:Y:83:ARG:NH1   | 3:Y:503:GOL:C2   | 2.78                     | 0.47              |
| 1:Z:346:PRO:HA   | 1:Z:348:PHE:CE1  | 2.50                     | 0.47              |
| 1:X:103:TRP:CZ3  | 1:X:104:GLN:HG3  | 2.49                     | 0.47              |
| 1:X:114:HIS:CD2  | 1:X:114:HIS:N    | 2.81                     | 0.47              |
| 1:Y:102:VAL:CG1  | 1:Y:103:TRP:N    | 2.77                     | 0.47              |
| 1:Y:339:THR:HG22 | 1:Y:378:ARG:HG2  | 1.97                     | 0.47              |
| 1:Z:154:ARG:HA   | 1:Z:157:ARG:HG2  | 1.95                     | 0.47              |
| 1:X:154:ARG:C    | 1:X:159:GLU:HB2  | 2.40                     | 0.47              |
| 1:X:386:TYR:CE1  | 1:X:425:ILE:HD13 | 2.48                     | 0.47              |
| 1:O:80:THR:HG23  | 1:O:248:ALA:HB2  | 1.96                     | 0.47              |
| 1:O:125:ARG:O    | 1:O:125:ARG:HG3  | 2.13                     | 0.47              |
| 1:O:142:LYS:HD3  | 1:O:207:LEU:HD22 | 1.97                     | 0.47              |
| 1:O:174:THR:CA   | 1:O:177:ARG:NH2  | 2.78                     | 0.47              |
| 1:O:193:ASN:C    | 1:O:195:HIS:H    | 2.21                     | 0.47              |
| 1:O:242:ILE:HG22 | 1:O:243:ALA:N    | 2.30                     | 0.47              |
| 1:O:456:ASN:ND2  | 1:O:458:ASP:HB2  | 2.30                     | 0.47              |
| 1:O:460:LEU:HD22 | 1:O:460:LEU:N    | 2.22                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:461:GLN:O    | 1:O:463:LYS:N    | 2.48                     | 0.47              |
| 1:Y:101:ILE:HG22 | 1:Y:140:LYS:HD3  | 1.96                     | 0.47              |
| 1:Y:249:ALA:HB2  | 1:Y:439:THR:OG1  | 2.15                     | 0.47              |
| 1:Z:153:GLU:CD   | 1:Z:153:GLU:H    | 2.21                     | 0.47              |
| 1:Z:499:HIS:CG   | 1:Z:500:ASP:H    | 2.32                     | 0.47              |
| 1:X:474:ILE:HG23 | 1:X:478:GLU:HG3  | 1.96                     | 0.47              |
| 1:Y:24:ASP:O     | 1:Y:25:ALA:HB3   | 2.14                     | 0.47              |
| 1:Z:114:HIS:ND1  | 1:Z:114:HIS:N    | 2.59                     | 0.47              |
| 1:Z:342:VAL:CG2  | 1:Z:371:VAL:HG21 | 2.45                     | 0.47              |
| 1:X:74:ILE:HD13  | 1:X:74:ILE:N     | 2.29                     | 0.47              |
| 1:X:254:LEU:HD12 | 1:X:254:LEU:HA   | 1.73                     | 0.47              |
| 1:O:31:SER:CB    | 1:O:62:GLU:HG3   | 2.44                     | 0.47              |
| 1:O:33:ARG:HH12  | 1:O:62:GLU:CD    | 2.23                     | 0.47              |
| 1:O:492:ARG:HD3  | 1:Y:496:TRP:HZ3  | 1.80                     | 0.47              |
| 1:O:492:ARG:HG2  | 1:O:492:ARG:HH11 | 1.78                     | 0.47              |
| 1:Z:28:ILE:N     | 1:Z:28:ILE:HD12  | 2.30                     | 0.47              |
| 1:X:46:GLU:HA    | 1:X:100:ALA:O    | 2.14                     | 0.47              |
| 1:X:302:LEU:HD23 | 1:X:302:LEU:HA   | 1.77                     | 0.47              |
| 1:O:415:ASN:HD22 | 1:O:417:PHE:N    | 2.13                     | 0.47              |
| 1:Y:114:HIS:N    | 1:Y:114:HIS:CD2  | 2.81                     | 0.47              |
| 1:Y:130:LEU:HD13 | 1:Y:136:PHE:CD2  | 2.50                     | 0.47              |
| 1:Y:415:ASN:ND2  | 1:Y:417:PHE:H    | 2.13                     | 0.47              |
| 1:Z:115:LEU:CA   | 1:Z:120:LEU:HD12 | 2.42                     | 0.47              |
| 1:Z:234:GLY:H    | 1:Z:236:ARG:NH2  | 2.13                     | 0.47              |
| 1:Z:392:LEU:O    | 1:Z:395:MET:HB3  | 2.15                     | 0.47              |
| 1:Z:396:GLN:HG2  | 1:Z:401:ILE:O    | 2.14                     | 0.47              |
| 1:Z:408:VAL:HG22 | 1:Z:431:GLU:O    | 2.14                     | 0.47              |
| 1:X:6:ILE:HD12   | 1:X:453:PHE:CD2  | 2.50                     | 0.47              |
| 1:X:478:GLU:HA   | 1:X:481:TYR:CB   | 2.44                     | 0.47              |
| 1:O:54:ALA:HB2   | 1:X:65:THR:HG23  | 1.96                     | 0.46              |
| 1:O:155:ALA:HB1  | 1:O:213:MET:HE3  | 1.97                     | 0.46              |
| 1:Y:3:LYS:HZ3    | 1:Y:3:LYS:HB3    | 1.78                     | 0.46              |
| 1:Y:174:THR:C    | 1:Y:176:GLY:H    | 2.22                     | 0.46              |
| 1:Y:271:MET:HE1  | 1:Y:391:VAL:HG23 | 1.94                     | 0.46              |
| 1:Y:376:ILE:HD12 | 1:Y:376:ILE:HA   | 1.69                     | 0.46              |
| 1:Z:13:THR:OG1   | 2:Z:503:SO4:O1   | 2.29                     | 0.46              |
| 1:X:241:GLY:O    | 1:X:242:ILE:HG13 | 2.15                     | 0.46              |
| 1:O:317:ARG:HA   | 1:O:323:ILE:HG12 | 1.97                     | 0.46              |
| 1:Y:270:PHE:HE1  | 4:Y:527:HOH:O    | 1.98                     | 0.46              |
| 1:Y:389:ARG:O    | 1:Y:393:GLU:HG3  | 2.15                     | 0.46              |
| 1:Z:80:THR:CG2   | 1:Z:248:ALA:CB   | 2.93                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Z:124:ILE:CG1  | 1:Z:203:MET:HE1  | 2.45                     | 0.46              |
| 1:Z:214:LEU:HB3  | 1:Z:215:PRO:HD2  | 1.98                     | 0.46              |
| 1:Z:227:THR:N    | 1:Z:237:ILE:O    | 2.43                     | 0.46              |
| 1:O:54:ALA:CB    | 1:X:65:THR:HG23  | 2.46                     | 0.46              |
| 1:Y:41:LYS:HD3   | 1:Y:44:TRP:CZ2   | 2.50                     | 0.46              |
| 1:Y:90:GLU:HB2   | 1:Y:93:THR:HG1   | 1.78                     | 0.46              |
| 1:Y:202:LYS:O    | 1:Y:205:GLU:N    | 2.49                     | 0.46              |
| 1:Z:5:TYR:CE2    | 1:Z:69:ILE:CD1   | 2.99                     | 0.46              |
| 1:Z:60:LEU:C     | 1:Z:60:LEU:HD12  | 2.39                     | 0.46              |
| 1:Z:373:ALA:O    | 1:Z:377:ILE:N    | 2.44                     | 0.46              |
| 1:X:180:VAL:CG2  | 1:X:218:ARG:CG   | 2.92                     | 0.46              |
| 1:X:286:LEU:CD1  | 1:X:395:MET:CE   | 2.94                     | 0.46              |
| 1:Y:108:THR:HG21 | 1:Y:139:THR:C    | 2.41                     | 0.46              |
| 1:Y:112:CYS:SG   | 1:Y:139:THR:HG21 | 2.55                     | 0.46              |
| 1:Y:438:VAL:O    | 1:Y:441:LEU:HB2  | 2.16                     | 0.46              |
| 1:Z:12:GLY:O     | 1:Z:35:PHE:HZ    | 1.98                     | 0.46              |
| 1:Z:85:THR:HG23  | 1:Z:102:VAL:HA   | 1.97                     | 0.46              |
| 1:X:196:THR:CG2  | 1:X:198:ASP:N    | 2.78                     | 0.46              |
| 1:X:346:PRO:CA   | 1:X:348:PHE:CE1  | 2.97                     | 0.46              |
| 1:O:214:LEU:N    | 1:O:214:LEU:CD1  | 2.79                     | 0.46              |
| 1:O:351:LEU:HD22 | 1:O:360:ALA:CB   | 2.46                     | 0.46              |
| 1:Y:98:TYR:CG    | 1:Y:99:ASN:N     | 2.83                     | 0.46              |
| 1:Y:179:HIS:CE1  | 1:Y:215:PRO:CA   | 2.98                     | 0.46              |
| 1:Y:415:ASN:HD22 | 1:Y:417:PHE:N    | 2.14                     | 0.46              |
| 1:Z:157:ARG:CG   | 1:Z:157:ARG:NH1  | 2.78                     | 0.46              |
| 1:Z:179:HIS:CE1  | 1:Z:215:PRO:HA   | 2.50                     | 0.46              |
| 1:Z:456:ASN:ND2  | 1:Z:459:GLU:N    | 2.63                     | 0.46              |
| 1:Z:494:MET:O    | 1:Z:495:ALA:HB3  | 2.16                     | 0.46              |
| 1:X:204:LEU:N    | 1:X:204:LEU:CD1  | 2.79                     | 0.46              |
| 1:X:263:ASN:CB   | 1:X:406:LEU:HD11 | 2.45                     | 0.46              |
| 1:X:459:GLU:HB3  | 1:X:460:LEU:HD13 | 1.97                     | 0.46              |
| 1:O:234:GLY:H    | 1:O:236:ARG:HH21 | 1.63                     | 0.46              |
| 1:O:340:ASN:HD22 | 1:O:371:VAL:HG23 | 1.81                     | 0.46              |
| 1:Y:429:ARG:HG2  | 1:Y:469:GLU:OE2  | 2.15                     | 0.46              |
| 1:X:179:HIS:NE2  | 1:X:215:PRO:HB3  | 2.31                     | 0.46              |
| 1:X:196:THR:CG2  | 1:X:198:ASP:H    | 2.29                     | 0.46              |
| 1:X:348:PHE:N    | 1:X:348:PHE:CD1  | 2.83                     | 0.46              |
| 1:X:456:ASN:ND2  | 1:X:458:ASP:HB2  | 2.31                     | 0.46              |
| 1:Y:256:VAL:HG12 | 1:Y:294:PRO:HG3  | 1.98                     | 0.46              |
| 1:Z:143:TRP:CE3  | 1:Z:144:ILE:HA   | 2.51                     | 0.46              |
| 1:Z:146:ASP:HB2  | 1:Z:147:HIS:HD1  | 1.77                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Z:332:PHE:O    | 1:Z:335:LYS:HB2  | 2.16                     | 0.46              |
| 1:X:286:LEU:CD1  | 1:X:395:MET:HE3  | 2.46                     | 0.46              |
| 1:Y:36:GLU:HG3   | 1:Y:37:GLN:N     | 2.30                     | 0.46              |
| 1:Y:136:PHE:O    | 1:Y:140:LYS:HG3  | 2.16                     | 0.46              |
| 1:Z:9:LEU:HD12   | 1:Z:9:LEU:HA     | 1.61                     | 0.46              |
| 1:Z:19:VAL:HG13  | 1:Z:27:ILE:CG2   | 2.46                     | 0.46              |
| 1:X:270:PHE:N    | 1:X:270:PHE:CD1  | 2.84                     | 0.46              |
| 1:X:389:ARG:HG2  | 1:X:483:TYR:CZ   | 2.50                     | 0.46              |
| 1:O:26:ASN:O     | 1:O:28:ILE:HD13  | 2.14                     | 0.46              |
| 1:O:91:LYS:HB2   | 1:O:161:LEU:HG   | 1.96                     | 0.46              |
| 1:O:389:ARG:HB2  | 1:O:426:LEU:HD13 | 1.98                     | 0.46              |
| 1:O:407:ARG:HD3  | 1:O:407:ARG:HA   | 1.53                     | 0.46              |
| 1:O:471:ARG:HA   | 1:O:472:PRO:HD3  | 1.84                     | 0.46              |
| 1:Y:54:ALA:CA    | 1:Z:65:THR:HG23  | 2.46                     | 0.46              |
| 1:Y:71:SER:HA    | 1:Y:74:ILE:HD12  | 1.98                     | 0.46              |
| 1:Y:161:LEU:HD22 | 1:Y:179:HIS:NE2  | 2.29                     | 0.46              |
| 1:X:24:ASP:N     | 1:X:24:ASP:OD1   | 2.48                     | 0.46              |
| 1:X:154:ARG:CB   | 1:X:159:GLU:CB   | 2.93                     | 0.46              |
| 1:X:263:ASN:O    | 1:X:408:VAL:HA   | 2.16                     | 0.46              |
| 1:O:496:TRP:CZ3  | 1:Y:488:LYS:HG2  | 2.51                     | 0.46              |
| 1:Z:23:HIS:CA    | 1:Z:453:PHE:CZ   | 2.99                     | 0.46              |
| 1:Z:115:LEU:HG   | 1:Z:120:LEU:HD13 | 1.98                     | 0.46              |
| 1:Z:410:GLY:O    | 1:Z:413:VAL:HG22 | 2.16                     | 0.46              |
| 1:Z:456:ASN:HD22 | 1:Z:459:GLU:H    | 1.63                     | 0.46              |
| 1:X:41:LYS:HB2   | 1:X:42:PRO:CD    | 2.46                     | 0.46              |
| 1:X:90:GLU:CB    | 1:X:93:THR:HG1   | 2.28                     | 0.46              |
| 1:X:154:ARG:NH2  | 1:X:159:GLU:CG   | 2.79                     | 0.46              |
| 1:X:438:VAL:N    | 1:X:441:LEU:HD12 | 2.31                     | 0.46              |
| 1:O:332:PHE:CA   | 1:O:374:ASN:ND2  | 2.79                     | 0.45              |
| 1:O:406:LEU:HD23 | 1:O:406:LEU:HA   | 1.61                     | 0.45              |
| 1:Y:486:TRP:CE2  | 1:Y:490:VAL:CG2  | 2.99                     | 0.45              |
| 1:Z:83:ARG:HH12  | 3:Z:504:GOL:C2   | 2.29                     | 0.45              |
| 1:Z:118:ASP:HB2  | 1:Z:120:LEU:CD1  | 2.45                     | 0.45              |
| 1:Z:157:ARG:HG2  | 1:Z:157:ARG:NH1  | 2.30                     | 0.45              |
| 1:Z:166:ASP:CG   | 1:Z:167:THR:H    | 2.23                     | 0.45              |
| 1:X:130:LEU:HD12 | 1:X:190:MET:CA   | 2.47                     | 0.45              |
| 1:O:460:LEU:H    | 1:O:460:LEU:CD2  | 2.25                     | 0.45              |
| 1:Y:33:ARG:HH12  | 1:Y:62:GLU:CD    | 2.24                     | 0.45              |
| 1:Y:271:MET:HE2  | 1:Y:271:MET:HB3  | 1.72                     | 0.45              |
| 1:Y:280:VAL:HG11 | 1:Y:302:LEU:HD21 | 1.97                     | 0.45              |
| 1:Z:101:ILE:HG23 | 1:Z:107:ARG:NH1  | 2.31                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:X:4:LYS:H      | 1:X:4:LYS:HG2    | 1.51                     | 0.45              |
| 1:Y:20:VAL:O     | 1:Y:28:ILE:HG12  | 2.15                     | 0.45              |
| 1:Y:433:PRO:O    | 1:Y:467:GLU:HB3  | 2.16                     | 0.45              |
| 1:Z:54:ALA:O     | 1:Z:58:SER:OG    | 2.29                     | 0.45              |
| 1:Z:371:VAL:O    | 1:Z:371:VAL:HG12 | 2.14                     | 0.45              |
| 1:X:251:PHE:CE2  | 1:X:446:LEU:CD1  | 2.98                     | 0.45              |
| 1:X:277:GLU:O    | 1:X:300:TYR:HD2  | 1.99                     | 0.45              |
| 1:X:478:GLU:HB2  | 4:X:545:HOH:O    | 2.16                     | 0.45              |
| 1:O:27:ILE:HD13  | 1:O:27:ILE:N     | 2.31                     | 0.45              |
| 1:O:27:ILE:HG22  | 1:O:28:ILE:N     | 2.30                     | 0.45              |
| 1:Y:165:VAL:O    | 1:Y:169:LEU:HG   | 2.16                     | 0.45              |
| 1:Z:162:PHE:CG   | 1:Z:163:GLY:N    | 2.81                     | 0.45              |
| 1:Z:272:LEU:HG   | 1:Z:303:GLU:HB2  | 1.97                     | 0.45              |
| 1:Z:474:ILE:O    | 1:Z:479:ARG:NH2  | 2.49                     | 0.45              |
| 1:O:406:LEU:CD2  | 1:O:407:ARG:N    | 2.79                     | 0.45              |
| 1:O:468:ARG:HD3  | 1:O:469:GLU:N    | 2.31                     | 0.45              |
| 1:Y:110:GLU:O    | 1:Y:113:GLU:HB2  | 2.17                     | 0.45              |
| 1:Y:145:LEU:HD12 | 1:Y:145:LEU:HA   | 1.58                     | 0.45              |
| 1:Y:280:VAL:HG13 | 1:Y:281:LYS:N    | 2.30                     | 0.45              |
| 1:Y:364:ILE:HG22 | 1:Y:365:PHE:N    | 2.31                     | 0.45              |
| 1:Y:474:ILE:HG21 | 1:Y:474:ILE:HD12 | 1.72                     | 0.45              |
| 1:Z:124:ILE:O    | 1:Z:128:THR:OG1  | 2.27                     | 0.45              |
| 1:Z:191:LEU:HD23 | 1:Z:191:LEU:HA   | 1.54                     | 0.45              |
| 1:Z:436:ARG:N    | 1:Z:436:ARG:CD   | 2.79                     | 0.45              |
| 1:Z:456:ASN:HD22 | 1:Z:458:ASP:H    | 1.65                     | 0.45              |
| 1:X:39:TYR:HA    | 1:X:40:PRO:HD2   | 1.63                     | 0.45              |
| 1:O:402:ARG:NH2  | 1:O:404:HIS:HA   | 2.31                     | 0.45              |
| 1:O:457:LEU:HA   | 1:O:457:LEU:HD22 | 1.73                     | 0.45              |
| 1:Y:331:TYR:CE1  | 1:Y:335:LYS:HD3  | 2.52                     | 0.45              |
| 1:Y:344:VAL:HG22 | 1:Y:364:ILE:HD13 | 1.94                     | 0.45              |
| 1:Z:28:ILE:N     | 1:Z:28:ILE:CD1   | 2.79                     | 0.45              |
| 1:Z:401:ILE:CG2  | 1:Z:402:ARG:N    | 2.79                     | 0.45              |
| 1:Z:427:GLY:C    | 1:Z:472:PRO:HG3  | 2.42                     | 0.45              |
| 1:X:130:LEU:HD12 | 1:X:190:MET:CG   | 2.47                     | 0.45              |
| 1:X:154:ARG:NH2  | 1:X:159:GLU:HG3  | 2.31                     | 0.45              |
| 1:X:261:ALA:HA   | 1:X:272:LEU:O    | 2.17                     | 0.45              |
| 1:X:428:THR:CG2  | 1:X:429:ARG:N    | 2.79                     | 0.45              |
| 1:O:44:TRP:N     | 1:O:44:TRP:HD1   | 2.14                     | 0.45              |
| 1:O:219:ARG:CG   | 1:O:220:SER:N    | 2.80                     | 0.45              |
| 1:O:240:SER:HB2  | 1:O:450:ALA:HB3  | 1.96                     | 0.45              |
| 1:O:246:GLN:OE1  | 1:O:246:GLN:HA   | 2.16                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:457:LEU:O    | 1:O:460:LEU:N    | 2.50                     | 0.45              |
| 1:Y:21:MET:HG2   | 1:Y:25:ALA:C     | 2.41                     | 0.45              |
| 1:X:83:ARG:HH11  | 1:X:83:ARG:HB2   | 1.82                     | 0.45              |
| 1:X:154:ARG:HE   | 1:X:159:GLU:HG2  | 1.77                     | 0.45              |
| 1:X:269:CYS:HB3  | 1:X:306:VAL:HB   | 1.98                     | 0.45              |
| 1:X:342:VAL:CG1  | 1:X:343:TYR:N    | 2.79                     | 0.45              |
| 1:O:27:ILE:N     | 1:O:27:ILE:CD1   | 2.80                     | 0.45              |
| 1:O:80:THR:HG21  | 1:O:248:ALA:CB   | 2.46                     | 0.45              |
| 1:Y:83:ARG:CZ    | 1:Y:246:GLN:HG2  | 2.46                     | 0.45              |
| 1:Y:103:TRP:CZ3  | 1:Y:104:GLN:HG2  | 2.51                     | 0.45              |
| 1:Y:381:LEU:HD12 | 1:Y:417:PHE:CD2  | 2.52                     | 0.45              |
| 1:Z:460:LEU:C    | 1:Z:463:LYS:HB2  | 2.41                     | 0.45              |
| 1:O:353:ALA:CB   | 1:O:354:PRO:HA   | 2.40                     | 0.45              |
| 1:Y:415:ASN:HD22 | 1:Y:417:PHE:H    | 1.64                     | 0.45              |
| 1:Z:15:SER:OG    | 1:Z:17:ARG:HD2   | 2.16                     | 0.45              |
| 1:Z:240:SER:HB2  | 1:Z:450:ALA:HB3  | 1.98                     | 0.45              |
| 1:Z:335:LYS:HB3  | 1:Z:374:ASN:ND2  | 2.32                     | 0.45              |
| 1:X:320:MET:O    | 1:X:320:MET:HE3  | 2.17                     | 0.45              |
| 1:O:93:THR:OG1   | 1:O:94:GLY:N     | 2.50                     | 0.45              |
| 1:O:347:ALA:HB2  | 1:O:351:LEU:HD13 | 1.99                     | 0.45              |
| 1:O:357:ASP:HA   | 1:O:358:PRO:HD2  | 1.83                     | 0.45              |
| 1:Y:403:LEU:HD13 | 1:Y:403:LEU:N    | 2.32                     | 0.45              |
| 1:Z:390:ASP:O    | 1:Z:393:GLU:HB2  | 2.17                     | 0.45              |
| 1:Z:473:GLY:O    | 1:Z:474:ILE:HG13 | 2.17                     | 0.45              |
| 1:Z:475:GLU:HG3  | 1:Z:475:GLU:H    | 1.64                     | 0.45              |
| 1:O:410:GLY:O    | 1:O:413:VAL:HG13 | 2.18                     | 0.44              |
| 1:Y:19:VAL:CG1   | 1:Y:27:ILE:CG2   | 2.95                     | 0.44              |
| 1:Y:69:ILE:HD12  | 1:Y:69:ILE:HA    | 1.79                     | 0.44              |
| 1:Y:202:LYS:O    | 1:Y:206:VAL:HB   | 2.17                     | 0.44              |
| 1:Y:293:GLY:N    | 1:Y:297:GLU:O    | 2.28                     | 0.44              |
| 1:Y:357:ASP:OD2  | 1:Y:494:MET:HB3  | 2.17                     | 0.44              |
| 1:Z:5:TYR:O      | 1:Z:75:ALA:N     | 2.45                     | 0.44              |
| 1:Z:124:ILE:HD13 | 1:Z:132:ILE:CG1  | 2.48                     | 0.44              |
| 1:X:418:LEU:HD23 | 1:X:418:LEU:HA   | 1.67                     | 0.44              |
| 1:O:83:ARG:HE    | 1:O:83:ARG:HB2   | 1.66                     | 0.44              |
| 1:O:422:GLN:NE2  | 1:O:426:LEU:CD2  | 2.80                     | 0.44              |
| 1:Y:274:ASN:HD21 | 1:Y:299:ASN:HD22 | 1.63                     | 0.44              |
| 1:Z:323:ILE:HG22 | 1:Z:332:PHE:CE2  | 2.51                     | 0.44              |
| 1:X:192:PHE:HB2  | 1:X:199:TRP:CZ3  | 2.52                     | 0.44              |
| 1:X:351:LEU:HA   | 1:X:351:LEU:HD13 | 1.41                     | 0.44              |
| 1:X:390:ASP:OD1  | 1:X:483:TYR:OH   | 2.30                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:44:TRP:C     | 1:O:45:VAL:HG23  | 2.41                     | 0.44              |
| 1:O:50:MET:O     | 1:O:53:TRP:HB3   | 2.17                     | 0.44              |
| 1:Y:328:ASP:O    | 1:Y:331:TYR:N    | 2.51                     | 0.44              |
| 1:Z:286:LEU:N    | 1:Z:286:LEU:HD23 | 2.32                     | 0.44              |
| 1:Z:293:GLY:C    | 1:Z:295:THR:N    | 2.75                     | 0.44              |
| 1:X:6:ILE:CG2    | 1:X:7:VAL:N      | 2.79                     | 0.44              |
| 1:X:262:LYS:HD2  | 1:X:262:LYS:C    | 2.42                     | 0.44              |
| 1:X:297:GLU:H    | 1:X:297:GLU:HG3  | 1.24                     | 0.44              |
| 1:X:344:VAL:HG23 | 1:X:379:ALA:CB   | 2.48                     | 0.44              |
| 1:O:21:MET:HE1   | 1:O:444:ALA:HB2  | 1.99                     | 0.44              |
| 1:O:78:GLY:HA2   | 1:O:447:ALA:HB2  | 1.99                     | 0.44              |
| 1:O:359:TYR:CZ   | 1:O:499:HIS:HB3  | 2.52                     | 0.44              |
| 1:O:362:GLY:O    | 1:Y:367:LEU:HB2  | 2.16                     | 0.44              |
| 1:Y:338:ASN:CB   | 1:Y:482:ARG:NH2  | 2.81                     | 0.44              |
| 1:Y:486:TRP:CD1  | 1:Y:487:LYS:HG3  | 2.52                     | 0.44              |
| 1:Z:266:GLY:N    | 1:Z:268:GLY:O    | 2.50                     | 0.44              |
| 1:Z:351:LEU:N    | 1:Z:357:ASP:O    | 2.51                     | 0.44              |
| 1:Z:403:LEU:N    | 1:Z:403:LEU:CD1  | 2.78                     | 0.44              |
| 1:Z:438:VAL:HA   | 1:Z:441:LEU:HD12 | 2.00                     | 0.44              |
| 1:X:483:TYR:O    | 1:X:487:LYS:HG2  | 2.18                     | 0.44              |
| 1:O:122:ASP:O    | 1:O:126:SER:OG   | 2.27                     | 0.44              |
| 1:Z:40:PRO:CG    | 1:Z:44:TRP:HE3   | 2.30                     | 0.44              |
| 1:Z:348:PHE:CD1  | 1:Z:348:PHE:N    | 2.78                     | 0.44              |
| 1:Z:430:VAL:O    | 1:Z:469:GLU:HA   | 2.17                     | 0.44              |
| 1:X:322:LEU:N    | 1:X:322:LEU:CD2  | 2.80                     | 0.44              |
| 1:O:251:PHE:CZ   | 1:O:446:LEU:CD1  | 3.01                     | 0.44              |
| 1:O:298:VAL:CG1  | 1:O:299:ASN:N    | 2.79                     | 0.44              |
| 1:O:457:LEU:O    | 1:O:461:GLN:HG2  | 2.17                     | 0.44              |
| 1:Y:44:TRP:N     | 1:Y:44:TRP:HD1   | 2.14                     | 0.44              |
| 1:Z:81:ASN:N     | 1:Z:81:ASN:ND2   | 2.66                     | 0.44              |
| 1:Z:357:ASP:C    | 1:Z:359:TYR:H    | 2.26                     | 0.44              |
| 1:O:163:GLY:HA2  | 4:O:529:HOH:O    | 2.17                     | 0.44              |
| 1:Y:83:ARG:HH11  | 3:Y:503:GOL:C2   | 2.31                     | 0.44              |
| 1:Y:109:ALA:HA   | 1:Y:134:PRO:HG3  | 2.00                     | 0.44              |
| 1:Y:196:THR:O    | 1:Y:197:LEU:HB2  | 2.18                     | 0.44              |
| 1:X:109:ALA:HA   | 1:X:134:PRO:HG3  | 2.00                     | 0.44              |
| 1:X:125:ARG:HB2  | 4:X:534:HOH:O    | 2.18                     | 0.44              |
| 1:X:293:GLY:C    | 1:X:295:THR:N    | 2.75                     | 0.44              |
| 1:X:295:THR:HG23 | 1:X:297:GLU:CD   | 2.42                     | 0.44              |
| 1:X:317:ARG:NE   | 1:X:326:ALA:HB2  | 2.33                     | 0.44              |
| 1:X:469:GLU:HG2  | 1:X:471:ARG:NH2  | 2.33                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:23:HIS:HE1   | 1:O:453:PHE:O    | 2.00                     | 0.44              |
| 1:O:330:GLU:O    | 1:O:334:THR:OG1  | 2.28                     | 0.44              |
| 1:Z:106:ARG:NH1  | 1:Z:307:PHE:CE2  | 2.85                     | 0.44              |
| 1:Z:171:TRP:HE3  | 1:Z:172:LYS:HD2  | 1.82                     | 0.44              |
| 1:Z:320:MET:HE3  | 1:X:373:ALA:HB2  | 2.00                     | 0.44              |
| 1:X:124:ILE:CD1  | 1:X:203:MET:HE1  | 2.48                     | 0.44              |
| 1:X:182:ASP:OD2  | 1:X:220:SER:OG   | 2.25                     | 0.44              |
| 1:X:436:ARG:HE   | 1:X:436:ARG:HB2  | 1.41                     | 0.44              |
| 1:X:471:ARG:HH11 | 1:X:471:ARG:CG   | 2.31                     | 0.44              |
| 1:O:53:TRP:HA    | 1:O:53:TRP:HE3   | 1.83                     | 0.44              |
| 1:Y:196:THR:HG23 | 1:Y:198:ASP:HB3  | 1.98                     | 0.44              |
| 1:Y:225:GLY:O    | 1:Y:238:PRO:HA   | 2.18                     | 0.44              |
| 1:Y:486:TRP:HD1  | 1:Y:487:LYS:HG3  | 1.83                     | 0.44              |
| 1:Z:170:ILE:HD13 | 1:Z:242:ILE:HD11 | 1.97                     | 0.44              |
| 1:Z:188:ARG:HA   | 1:Z:188:ARG:HD3  | 1.61                     | 0.44              |
| 1:Z:193:ASN:OD1  | 1:Z:196:THR:HB   | 2.18                     | 0.44              |
| 1:X:273:MET:HE1  | 1:X:403:LEU:HD11 | 1.99                     | 0.44              |
| 1:X:314:GLN:HG3  | 1:X:317:ARG:HH21 | 1.79                     | 0.44              |
| 1:O:441:LEU:N    | 1:O:441:LEU:CD2  | 2.80                     | 0.43              |
| 1:Y:84:GLU:HB2   | 1:Y:103:TRP:HB3  | 1.99                     | 0.43              |
| 1:Y:338:ASN:HD22 | 1:Y:338:ASN:N    | 2.16                     | 0.43              |
| 1:Y:396:GLN:OE1  | 1:Y:402:ARG:HB2  | 2.18                     | 0.43              |
| 1:Z:37:GLN:NE2   | 1:Z:47:HIS:CE1   | 2.86                     | 0.43              |
| 1:Z:337:GLN:H    | 1:Z:337:GLN:HG2  | 1.34                     | 0.43              |
| 1:X:156:ARG:HH11 | 1:X:156:ARG:HD2  | 1.59                     | 0.43              |
| 1:X:193:ASN:CG   | 1:X:196:THR:HB   | 2.43                     | 0.43              |
| 1:X:426:LEU:HD12 | 1:X:426:LEU:HA   | 1.85                     | 0.43              |
| 1:O:75:ALA:O     | 1:O:76:ALA:HB2   | 2.18                     | 0.43              |
| 1:O:232:LYS:O    | 1:O:233:GLY:O    | 2.36                     | 0.43              |
| 1:O:475:GLU:C    | 1:O:477:THR:N    | 2.76                     | 0.43              |
| 1:Y:21:MET:HB2   | 1:Y:21:MET:HE3   | 1.56                     | 0.43              |
| 1:Y:54:ALA:CB    | 1:Z:65:THR:HG23  | 2.48                     | 0.43              |
| 1:Y:184:THR:HG23 | 1:Y:184:THR:H    | 1.44                     | 0.43              |
| 1:O:317:ARG:HA   | 1:O:323:ILE:HG13 | 2.00                     | 0.43              |
| 1:O:332:PHE:C    | 1:O:374:ASN:HD22 | 2.23                     | 0.43              |
| 1:Y:280:VAL:HG12 | 1:Y:280:VAL:O    | 2.15                     | 0.43              |
| 1:Y:441:LEU:O    | 1:Y:444:ALA:HB3  | 2.18                     | 0.43              |
| 1:Y:454:TRP:CD1  | 1:Y:460:LEU:HD21 | 2.53                     | 0.43              |
| 1:Y:344:VAL:HG13 | 1:Y:364:ILE:HD13 | 1.99                     | 0.43              |
| 1:Z:24:ASP:O     | 1:Z:25:ALA:HB3   | 2.18                     | 0.43              |
| 1:Z:37:GLN:HE22  | 1:Z:47:HIS:CE1   | 2.37                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Z:80:THR:HG22  | 1:Z:243:ALA:O    | 2.19                     | 0.43              |
| 1:Z:271:MET:HE1  | 1:Z:392:LEU:CB   | 2.48                     | 0.43              |
| 1:X:103:TRP:CE3  | 1:X:104:GLN:HG3  | 2.53                     | 0.43              |
| 1:X:152:ARG:HG2  | 1:X:152:ARG:NH1  | 2.33                     | 0.43              |
| 1:X:487:LYS:HE3  | 1:X:487:LYS:HB3  | 1.69                     | 0.43              |
| 1:O:446:LEU:HA   | 1:O:446:LEU:HD12 | 1.58                     | 0.43              |
| 1:Y:57:SER:O     | 1:Y:60:LEU:HB3   | 2.17                     | 0.43              |
| 1:Y:271:MET:O    | 1:Y:303:GLU:HA   | 2.18                     | 0.43              |
| 1:Z:17:ARG:HG3   | 1:Z:32:GLN:HA    | 2.00                     | 0.43              |
| 1:Z:182:ASP:HA   | 1:Z:218:ARG:O    | 2.18                     | 0.43              |
| 1:Z:474:ILE:HG23 | 1:Z:478:GLU:CB   | 2.48                     | 0.43              |
| 1:X:17:ARG:HG3   | 1:X:32:GLN:CG    | 2.29                     | 0.43              |
| 1:O:36:GLU:HG3   | 1:O:37:GLN:N     | 2.31                     | 0.43              |
| 1:O:128:THR:CG2  | 1:O:130:LEU:CB   | 2.97                     | 0.43              |
| 1:O:128:THR:CG2  | 1:O:130:LEU:HD13 | 2.39                     | 0.43              |
| 1:O:255:CYS:HB3  | 1:O:260:MET:CB   | 2.45                     | 0.43              |
| 1:X:216:GLU:CD   | 1:X:218:ARG:HH11 | 2.26                     | 0.43              |
| 1:X:293:GLY:C    | 1:X:295:THR:H    | 2.26                     | 0.43              |
| 1:X:377:ILE:HG21 | 1:X:377:ILE:HD13 | 1.56                     | 0.43              |
| 1:X:460:LEU:H    | 1:X:460:LEU:HD22 | 1.83                     | 0.43              |
| 1:O:458:ASP:CA   | 1:O:461:GLN:HG3  | 2.47                     | 0.43              |
| 1:Y:490:VAL:HG12 | 1:Y:494:MET:HE2  | 2.01                     | 0.43              |
| 1:Z:154:ARG:HB3  | 1:Z:159:GLU:CG   | 2.24                     | 0.43              |
| 1:Z:372:ASN:H    | 1:Z:375:HIS:CE1  | 2.36                     | 0.43              |
| 1:Z:456:ASN:ND2  | 1:Z:459:GLU:H    | 2.16                     | 0.43              |
| 1:X:65:THR:HG23  | 1:X:66:LYS:N     | 2.31                     | 0.43              |
| 1:O:101:ILE:HG22 | 1:O:140:LYS:HG2  | 2.01                     | 0.43              |
| 1:O:344:VAL:HG22 | 1:O:364:ILE:HG12 | 2.01                     | 0.43              |
| 1:Y:93:THR:CB    | 1:Y:95:LYS:HB3   | 2.48                     | 0.43              |
| 1:Y:104:GLN:HB3  | 1:Y:349:THR:HG21 | 2.00                     | 0.43              |
| 1:Y:250:LEU:CD1  | 1:Y:255:CYS:HB2  | 2.49                     | 0.43              |
| 1:Y:280:VAL:O    | 1:Y:288:THR:OG1  | 2.32                     | 0.43              |
| 1:Y:335:LYS:HE3  | 1:Y:374:ASN:HD21 | 1.84                     | 0.43              |
| 1:Y:421:PHE:CE2  | 1:Y:425:ILE:HD13 | 2.53                     | 0.43              |
| 1:Y:462:GLU:OE1  | 1:Y:462:GLU:HA   | 2.16                     | 0.43              |
| 1:Z:95:LYS:HA    | 1:Z:96:PRO:HD3   | 1.66                     | 0.43              |
| 1:Z:402:ARG:HD2  | 1:Z:404:HIS:CE1  | 2.54                     | 0.43              |
| 1:X:6:ILE:CD1    | 1:X:453:PHE:CD2  | 3.01                     | 0.43              |
| 1:X:402:ARG:HE   | 1:X:402:ARG:HB2  | 1.43                     | 0.43              |
| 1:X:474:ILE:HG23 | 1:X:478:GLU:CG   | 2.48                     | 0.43              |
| 1:O:80:THR:HG21  | 1:O:248:ALA:HB3  | 2.01                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:124:ILE:H    | 1:O:124:ILE:HG12 | 1.24                     | 0.43              |
| 1:O:168:TRP:O    | 1:O:172:LYS:HG2  | 2.19                     | 0.43              |
| 1:Y:164:THR:HB   | 1:Y:166:ASP:OD1  | 2.19                     | 0.43              |
| 1:Z:152:ARG:O    | 1:Z:156:ARG:N    | 2.35                     | 0.43              |
| 1:X:320:MET:HE3  | 1:X:320:MET:HA   | 2.00                     | 0.43              |
| 1:X:422:GLN:O    | 1:X:426:LEU:HD22 | 2.19                     | 0.43              |
| 1:X:482:ARG:HA   | 1:X:482:ARG:NH1  | 2.33                     | 0.43              |
| 1:O:192:PHE:HB2  | 1:O:199:TRP:CZ3  | 2.54                     | 0.43              |
| 1:Y:253:GLN:O    | 1:Y:254:LEU:HB2  | 2.18                     | 0.43              |
| 1:Z:115:LEU:CD1  | 1:Z:115:LEU:H    | 2.32                     | 0.43              |
| 1:X:90:GLU:HA    | 1:X:160:LEU:CD2  | 2.49                     | 0.43              |
| 1:X:191:LEU:HD21 | 1:X:207:LEU:CD1  | 2.49                     | 0.43              |
| 1:X:282:SER:HA   | 1:X:398:ASP:OD2  | 2.18                     | 0.43              |
| 1:X:432:ARG:HA   | 1:X:433:PRO:HD2  | 1.87                     | 0.43              |
| 1:O:88:VAL:HA    | 1:O:161:LEU:O    | 2.18                     | 0.42              |
| 1:Y:30:VAL:O     | 1:Y:66:LYS:NZ    | 2.31                     | 0.42              |
| 1:Y:155:ALA:HB1  | 1:Y:213:MET:HE1  | 1.98                     | 0.42              |
| 1:Y:194:ILE:HG22 | 1:Y:290:ILE:HD11 | 1.99                     | 0.42              |
| 1:Y:256:VAL:CG1  | 1:Y:294:PRO:CG   | 2.97                     | 0.42              |
| 1:Z:66:LYS:HB3   | 1:Z:66:LYS:HE3   | 1.80                     | 0.42              |
| 1:Z:168:TRP:CZ3  | 1:Z:172:LYS:HD3  | 2.54                     | 0.42              |
| 1:X:6:ILE:CD1    | 1:X:453:PHE:CG   | 3.02                     | 0.42              |
| 1:X:421:PHE:O    | 1:X:424:ASP:HB2  | 2.19                     | 0.42              |
| 1:O:80:THR:CG2   | 1:O:248:ALA:CB   | 2.97                     | 0.42              |
| 1:O:202:LYS:HD3  | 1:O:206:VAL:CG2  | 2.47                     | 0.42              |
| 1:O:382:GLU:HB3  | 1:O:421:PHE:CE2  | 2.54                     | 0.42              |
| 1:Y:15:SER:OG    | 1:Y:17:ARG:NH1   | 2.52                     | 0.42              |
| 1:Y:85:THR:HG23  | 1:Y:101:ILE:C    | 2.44                     | 0.42              |
| 1:Y:115:LEU:HD13 | 1:Y:115:LEU:HA   | 1.62                     | 0.42              |
| 1:Y:351:LEU:CD2  | 1:Y:360:ALA:CB   | 2.97                     | 0.42              |
| 1:Z:137:SER:OG   | 1:Z:189:THR:HA   | 2.19                     | 0.42              |
| 1:O:67:ALA:CB    | 1:O:69:ILE:HD12  | 2.49                     | 0.42              |
| 1:O:142:LYS:HD3  | 1:O:207:LEU:CD2  | 2.49                     | 0.42              |
| 1:O:184:THR:H    | 1:O:184:THR:HG23 | 1.47                     | 0.42              |
| 1:O:211:ARG:CA   | 1:O:214:LEU:HD13 | 2.48                     | 0.42              |
| 1:O:264:THR:CG2  | 1:O:265:TYR:N    | 2.81                     | 0.42              |
| 1:O:422:GLN:HE21 | 1:O:426:LEU:HD22 | 1.83                     | 0.42              |
| 1:Y:28:ILE:HG23  | 1:Y:28:ILE:HD12  | 1.80                     | 0.42              |
| 1:Y:237:ILE:HG23 | 1:Y:238:PRO:HD2  | 2.01                     | 0.42              |
| 1:Y:409:ASP:CB   | 1:Y:438:VAL:HG21 | 2.49                     | 0.42              |
| 1:Y:488:LYS:HB3  | 1:Y:488:LYS:HE3  | 1.82                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Y:494:MET:O    | 1:Y:495:ALA:HB3  | 2.19                     | 0.42              |
| 1:Z:456:ASN:C    | 1:Z:456:ASN:ND2  | 2.77                     | 0.42              |
| 1:X:190:MET:N    | 4:X:518:HOH:O    | 2.51                     | 0.42              |
| 1:O:155:ALA:CB   | 1:O:213:MET:HE1  | 2.50                     | 0.42              |
| 1:O:335:LYS:HB2  | 1:O:374:ASN:ND2  | 2.33                     | 0.42              |
| 1:Y:130:LEU:N    | 1:Y:130:LEU:HD23 | 2.33                     | 0.42              |
| 1:Y:180:VAL:HG22 | 1:Y:216:GLU:O    | 2.20                     | 0.42              |
| 1:Y:466:ILE:HD13 | 1:Y:466:ILE:C    | 2.43                     | 0.42              |
| 1:Y:491:LYS:HA   | 1:Y:494:MET:HG3  | 2.01                     | 0.42              |
| 1:Z:183:TYR:CD2  | 1:Z:298:VAL:CG2  | 3.03                     | 0.42              |
| 1:Z:496:TRP:CZ3  | 1:X:488:LYS:CD   | 3.01                     | 0.42              |
| 1:X:8:ALA:C      | 1:X:9:LEU:HD12   | 2.45                     | 0.42              |
| 1:X:104:GLN:HB3  | 1:X:349:THR:HG21 | 2.01                     | 0.42              |
| 1:X:264:THR:O    | 1:X:269:CYS:HA   | 2.20                     | 0.42              |
| 1:X:432:ARG:NH2  | 1:X:468:ARG:HD3  | 2.35                     | 0.42              |
| 1:O:19:VAL:HG12  | 1:O:20:VAL:N     | 2.34                     | 0.42              |
| 1:O:82:GLN:HA    | 1:O:245:ASP:OD2  | 2.20                     | 0.42              |
| 1:O:396:GLN:HE21 | 1:O:403:LEU:HB2  | 1.85                     | 0.42              |
| 1:Z:103:TRP:HB2  | 1:Z:135:TYR:CE1  | 2.54                     | 0.42              |
| 1:Z:219:ARG:O    | 1:Z:224:TYR:OH   | 2.28                     | 0.42              |
| 1:Z:458:ASP:CA   | 1:Z:461:GLN:HG3  | 2.44                     | 0.42              |
| 1:X:180:VAL:HG11 | 1:X:224:TYR:HB3  | 2.02                     | 0.42              |
| 1:X:409:ASP:CG   | 1:X:438:VAL:HG21 | 2.44                     | 0.42              |
| 1:X:460:LEU:N    | 1:X:460:LEU:HD22 | 2.35                     | 0.42              |
| 1:O:128:THR:C    | 1:O:130:LEU:N    | 2.76                     | 0.42              |
| 1:O:130:LEU:HD12 | 1:O:130:LEU:HA   | 1.60                     | 0.42              |
| 1:O:207:LEU:HD23 | 1:O:207:LEU:HA   | 1.91                     | 0.42              |
| 1:O:307:PHE:HD2  | 1:O:349:THR:O    | 2.02                     | 0.42              |
| 1:O:425:ILE:O    | 1:O:425:ILE:HG13 | 2.18                     | 0.42              |
| 1:O:471:ARG:CB   | 1:O:472:PRO:HD2  | 2.48                     | 0.42              |
| 1:Y:47:HIS:CE1   | 1:Y:102:VAL:HG21 | 2.55                     | 0.42              |
| 1:Z:135:TYR:O    | 1:Z:140:LYS:NZ   | 2.49                     | 0.42              |
| 1:Z:391:VAL:CG2  | 1:Z:392:LEU:N    | 2.76                     | 0.42              |
| 1:Z:453:PHE:CE2  | 1:Z:454:TRP:CZ2  | 3.08                     | 0.42              |
| 1:X:254:LEU:HD11 | 1:X:457:LEU:HD22 | 1.99                     | 0.42              |
| 1:O:108:THR:HG22 | 1:O:143:TRP:HB2  | 2.01                     | 0.42              |
| 1:O:359:TYR:O    | 1:O:497:GLU:N    | 2.40                     | 0.42              |
| 1:O:415:ASN:CG   | 1:O:418:LEU:HB2  | 2.44                     | 0.42              |
| 1:O:435:VAL:HG23 | 1:O:437:GLU:OE1  | 2.19                     | 0.42              |
| 1:Y:145:LEU:HD12 | 1:Y:151:SER:OG   | 2.19                     | 0.42              |
| 1:Y:191:LEU:HD21 | 1:Y:207:LEU:HD13 | 2.01                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Z:117:ARG:C    | 1:Z:119:GLY:H    | 2.28                     | 0.42              |
| 1:Z:457:LEU:HD23 | 1:Z:457:LEU:HA   | 1.47                     | 0.42              |
| 1:X:47:HIS:O     | 1:X:99:ASN:HB3   | 2.20                     | 0.42              |
| 1:O:80:THR:HG22  | 1:O:245:ASP:N    | 2.34                     | 0.42              |
| 1:Y:33:ARG:NH2   | 1:Z:33:ARG:NH2   | 2.68                     | 0.42              |
| 1:Y:486:TRP:CE2  | 1:Y:490:VAL:HG21 | 2.55                     | 0.42              |
| 1:Z:89:TRP:HB2   | 1:Z:95:LYS:C     | 2.44                     | 0.42              |
| 1:Z:156:ARG:HG2  | 1:Z:156:ARG:H    | 1.66                     | 0.42              |
| 1:Z:492:ARG:NH1  | 1:X:492:ARG:O    | 2.53                     | 0.42              |
| 1:X:171:TRP:CE2  | 1:X:176:GLY:HA2  | 2.54                     | 0.42              |
| 1:X:271:MET:HE1  | 1:X:392:LEU:HD12 | 2.00                     | 0.42              |
| 1:X:320:MET:CA   | 1:X:320:MET:CE   | 2.97                     | 0.42              |
| 1:X:363:ALA:C    | 1:X:364:ILE:HG13 | 2.44                     | 0.42              |
| 1:X:381:LEU:O    | 1:X:384:ILE:HB   | 2.20                     | 0.42              |
| 1:X:386:TYR:HE1  | 1:X:425:ILE:HD11 | 1.84                     | 0.42              |
| 1:X:431:GLU:O    | 1:X:433:PRO:HD3  | 2.19                     | 0.42              |
| 1:X:446:LEU:HD12 | 1:X:446:LEU:HA   | 1.84                     | 0.42              |
| 1:O:38:ILE:HB    | 1:O:46:GLU:O     | 2.20                     | 0.42              |
| 1:O:192:PHE:CD1  | 1:O:192:PHE:C    | 2.97                     | 0.42              |
| 1:O:245:ASP:O    | 1:O:248:ALA:HB3  | 2.19                     | 0.42              |
| 1:Y:133:ASP:OD1  | 1:Y:135:TYR:HB2  | 2.20                     | 0.42              |
| 1:Y:439:THR:HG22 | 1:Y:440:ALA:N    | 2.32                     | 0.42              |
| 1:X:152:ARG:CG   | 1:X:152:ARG:NH1  | 2.79                     | 0.42              |
| 1:X:191:LEU:CD2  | 1:X:207:LEU:HD12 | 2.50                     | 0.42              |
| 1:X:433:PRO:O    | 1:X:467:GLU:HB3  | 2.20                     | 0.42              |
| 1:O:213:MET:HE3  | 1:O:213:MET:HB3  | 1.79                     | 0.42              |
| 1:Z:137:SER:HA   | 1:Z:140:LYS:HD2  | 2.02                     | 0.42              |
| 1:Z:179:HIS:CE1  | 1:Z:215:PRO:CA   | 3.03                     | 0.42              |
| 1:Z:206:VAL:CG1  | 1:Z:207:LEU:N    | 2.83                     | 0.42              |
| 1:Z:270:PHE:CD1  | 1:Z:270:PHE:N    | 2.87                     | 0.42              |
| 1:Z:456:ASN:ND2  | 1:Z:459:GLU:HG3  | 2.35                     | 0.42              |
| 1:X:249:ALA:O    | 1:X:253:GLN:N    | 2.53                     | 0.42              |
| 1:X:409:ASP:CB   | 1:X:438:VAL:HG21 | 2.49                     | 0.42              |
| 1:O:9:LEU:HD12   | 1:O:9:LEU:HA     | 1.60                     | 0.41              |
| 1:O:25:ALA:HB3   | 1:O:463:LYS:CD   | 2.50                     | 0.41              |
| 1:O:289:THR:HB   | 1:O:290:ILE:H    | 1.48                     | 0.41              |
| 1:Y:9:LEU:HD23   | 1:Y:56:GLN:CG    | 2.50                     | 0.41              |
| 1:Y:87:ILE:HD13  | 1:Y:87:ILE:HG21  | 1.86                     | 0.41              |
| 1:Z:142:LYS:HG3  | 1:Z:146:ASP:OD2  | 2.20                     | 0.41              |
| 1:X:83:ARG:NH1   | 1:X:246:GLN:HG2  | 2.35                     | 0.41              |
| 1:X:130:LEU:HD12 | 1:X:190:MET:HG3  | 2.02                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:X:355:TYR:HB3  | 1:X:494:MET:HE3  | 2.02                     | 0.41              |
| 1:X:420:GLN:OE1  | 1:X:471:ARG:O    | 2.37                     | 0.41              |
| 1:O:103:TRP:CZ3  | 1:O:104:GLN:HG3  | 2.56                     | 0.41              |
| 1:O:325:ASP:O    | 1:O:328:ASP:HB2  | 2.20                     | 0.41              |
| 1:O:340:ASN:HB2  | 1:O:375:HIS:NE2  | 2.35                     | 0.41              |
| 1:O:353:ALA:HB1  | 1:O:354:PRO:HA   | 2.01                     | 0.41              |
| 1:O:360:ALA:O    | 1:O:361:ARG:HD3  | 2.19                     | 0.41              |
| 1:Y:263:ASN:O    | 1:Y:408:VAL:HA   | 2.19                     | 0.41              |
| 1:Y:342:VAL:HG21 | 1:Y:371:VAL:HG11 | 2.01                     | 0.41              |
| 1:Y:475:GLU:CB   | 1:Y:478:GLU:HB2  | 2.48                     | 0.41              |
| 1:Z:71:SER:O     | 1:Z:74:ILE:HD12  | 2.21                     | 0.41              |
| 1:Z:103:TRP:CD2  | 3:Z:504:GOL:H11  | 2.55                     | 0.41              |
| 1:Z:351:LEU:HB3  | 1:Z:355:TYR:HB2  | 2.02                     | 0.41              |
| 1:Z:426:LEU:HD12 | 1:Z:426:LEU:HA   | 1.77                     | 0.41              |
| 1:X:196:THR:O    | 1:X:196:THR:HG23 | 2.10                     | 0.41              |
| 1:X:323:ILE:HD12 | 1:X:326:ALA:HA   | 2.01                     | 0.41              |
| 1:X:415:ASN:HD22 | 1:X:416:ASN:N    | 2.19                     | 0.41              |
| 1:O:38:ILE:O     | 1:O:40:PRO:HD3   | 2.19                     | 0.41              |
| 1:O:353:ALA:HA   | 1:O:354:PRO:HA   | 1.67                     | 0.41              |
| 1:O:466:ILE:O    | 1:O:466:ILE:HG22 | 2.17                     | 0.41              |
| 1:Y:33:ARG:HB2   | 1:Y:59:THR:CG2   | 2.50                     | 0.41              |
| 1:Y:33:ARG:NH1   | 1:Y:62:GLU:CD    | 2.79                     | 0.41              |
| 1:Y:50:MET:O     | 1:Y:53:TRP:HB3   | 2.20                     | 0.41              |
| 1:Y:226:GLN:HG2  | 1:Y:238:PRO:CA   | 2.47                     | 0.41              |
| 1:Y:323:ILE:HD12 | 1:Y:326:ALA:HA   | 2.02                     | 0.41              |
| 1:Y:429:ARG:NH1  | 1:Y:469:GLU:OE2  | 2.54                     | 0.41              |
| 1:Y:433:PRO:HA   | 1:Y:466:ILE:HA   | 2.01                     | 0.41              |
| 1:Z:124:ILE:HD13 | 1:Z:132:ILE:HG12 | 2.01                     | 0.41              |
| 1:Z:315:TRP:O    | 1:Z:319:GLU:HB2  | 2.19                     | 0.41              |
| 1:Z:397:ALA:HB3  | 1:Z:398:ASP:H    | 1.58                     | 0.41              |
| 1:X:217:VAL:CG1  | 1:X:218:ARG:N    | 2.83                     | 0.41              |
| 1:X:248:ALA:O    | 1:X:442:GLY:HA3  | 2.20                     | 0.41              |
| 1:O:128:THR:CB   | 1:O:130:LEU:HB2  | 2.51                     | 0.41              |
| 1:Y:95:LYS:HB3   | 1:Y:95:LYS:HE2   | 1.81                     | 0.41              |
| 1:Y:294:PRO:HD2  | 1:Y:297:GLU:OE2  | 2.21                     | 0.41              |
| 1:Y:316:LEU:HD11 | 1:Y:380:THR:HG21 | 2.02                     | 0.41              |
| 1:Y:352:GLY:O    | 1:Y:353:ALA:HB2  | 2.20                     | 0.41              |
| 1:Z:81:ASN:HB2   | 1:Z:165:VAL:CG1  | 2.50                     | 0.41              |
| 1:Z:191:LEU:HD22 | 1:Z:204:LEU:HD13 | 2.03                     | 0.41              |
| 1:X:156:ARG:HG3  | 1:X:210:PRO:HG3  | 2.02                     | 0.41              |
| 1:X:179:HIS:CE1  | 1:X:215:PRO:HA   | 2.56                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:X:344:VAL:HG23 | 1:X:379:ALA:HB3  | 2.02                     | 0.41              |
| 1:O:53:TRP:HA    | 1:O:53:TRP:CE3   | 2.55                     | 0.41              |
| 1:O:345:VAL:HA   | 1:O:346:PRO:HD3  | 1.50                     | 0.41              |
| 1:O:381:LEU:HD12 | 1:O:417:PHE:CD2  | 2.56                     | 0.41              |
| 1:O:415:ASN:ND2  | 1:O:415:ASN:C    | 2.77                     | 0.41              |
| 1:Y:97:ILE:HD12  | 1:Y:148:VAL:HG21 | 2.01                     | 0.41              |
| 1:Y:267:THR:HG23 | 1:Y:311:ALA:HB2  | 2.02                     | 0.41              |
| 1:Y:289:THR:HG23 | 1:Y:301:ALA:HB3  | 2.02                     | 0.41              |
| 1:Y:294:PRO:O    | 1:Y:457:LEU:HD12 | 2.20                     | 0.41              |
| 1:Y:469:GLU:O    | 1:Y:471:ARG:NH1  | 2.54                     | 0.41              |
| 1:X:179:HIS:CE1  | 1:X:215:PRO:CA   | 3.04                     | 0.41              |
| 1:Z:113:GLU:O    | 1:Z:117:ARG:HG2  | 2.20                     | 0.41              |
| 1:X:108:THR:CB   | 1:X:139:THR:HB   | 2.47                     | 0.41              |
| 1:X:433:PRO:HA   | 1:X:465:VAL:O    | 2.20                     | 0.41              |
| 1:O:128:THR:HB   | 1:O:130:LEU:HB2  | 2.03                     | 0.41              |
| 1:O:205:GLU:CG   | 1:O:206:VAL:N    | 2.82                     | 0.41              |
| 1:Y:33:ARG:HH21  | 1:Z:33:ARG:NH2   | 2.16                     | 0.41              |
| 1:Y:156:ARG:C    | 1:Y:158:GLY:N    | 2.79                     | 0.41              |
| 1:Y:256:VAL:CG1  | 1:Y:294:PRO:CD   | 2.99                     | 0.41              |
| 1:Z:80:THR:HG21  | 1:Z:248:ALA:HB3  | 2.02                     | 0.41              |
| 1:Z:86:THR:HG23  | 1:Z:162:PHE:CE1  | 2.52                     | 0.41              |
| 1:X:11:GLN:CD    | 1:X:52:ILE:HG23  | 2.46                     | 0.41              |
| 1:X:64:LEU:HD22  | 1:X:69:ILE:CG2   | 2.50                     | 0.41              |
| 1:X:90:GLU:HA    | 1:X:160:LEU:HD23 | 2.03                     | 0.41              |
| 1:O:64:LEU:HD21  | 1:O:74:ILE:HD11  | 2.02                     | 0.41              |
| 1:O:153:GLU:N    | 1:O:153:GLU:OE1  | 2.53                     | 0.41              |
| 1:O:153:GLU:C    | 1:O:155:ALA:N    | 2.77                     | 0.41              |
| 1:O:486:TRP:O    | 1:O:490:VAL:HG23 | 2.21                     | 0.41              |
| 1:Y:305:ALA:O    | 1:Y:353:ALA:HB3  | 2.21                     | 0.41              |
| 1:Y:317:ARG:NH1  | 1:Y:326:ALA:CB   | 2.83                     | 0.41              |
| 1:Y:331:TYR:O    | 1:Y:335:LYS:HG3  | 2.20                     | 0.41              |
| 1:Z:153:GLU:HB2  | 1:Z:154:ARG:H    | 1.31                     | 0.41              |
| 1:Z:345:VAL:HG11 | 1:Z:493:ALA:HB3  | 2.03                     | 0.41              |
| 1:Z:461:GLN:HE21 | 1:Z:461:GLN:HB3  | 1.35                     | 0.41              |
| 1:X:249:ALA:O    | 1:X:253:GLN:HB2  | 2.20                     | 0.41              |
| 1:X:438:VAL:CA   | 1:X:441:LEU:CD1  | 2.99                     | 0.41              |
| 1:O:155:ALA:CB   | 1:O:213:MET:CE   | 2.99                     | 0.41              |
| 1:O:340:ASN:ND2  | 1:O:371:VAL:HG23 | 2.36                     | 0.41              |
| 1:Y:33:ARG:HE    | 1:Z:33:ARG:NH2   | 2.19                     | 0.41              |
| 1:Y:68:ASP:O     | 1:Y:69:ILE:HD13  | 2.20                     | 0.41              |
| 1:Y:188:ARG:HA   | 1:Y:188:ARG:HD2  | 1.63                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Y:230:GLY:HA3  | 1:Z:228:ASN:O    | 2.21                     | 0.41              |
| 1:Y:338:ASN:HB3  | 1:Y:482:ARG:HH22 | 1.84                     | 0.41              |
| 1:Y:476:THR:HG22 | 1:Y:477:THR:N    | 2.35                     | 0.41              |
| 1:Z:49:PRO:HB2   | 1:Z:168:TRP:CZ2  | 2.55                     | 0.41              |
| 1:Z:87:ILE:O     | 1:Z:163:GLY:N    | 2.54                     | 0.41              |
| 1:Z:103:TRP:CD1  | 1:Z:103:TRP:H    | 2.39                     | 0.41              |
| 1:Z:117:ARG:HG2  | 1:Z:117:ARG:H    | 1.63                     | 0.41              |
| 1:Z:125:ARG:NH1  | 1:Z:125:ARG:CG   | 2.78                     | 0.41              |
| 1:Z:131:VAL:O    | 1:Z:131:VAL:HG12 | 2.18                     | 0.41              |
| 1:Z:205:GLU:CG   | 1:Z:206:VAL:N    | 2.81                     | 0.41              |
| 1:Z:396:GLN:O    | 1:Z:400:GLY:N    | 2.44                     | 0.41              |
| 1:Z:492:ARG:HD2  | 1:X:496:TRP:HZ3  | 1.86                     | 0.41              |
| 1:Z:496:TRP:CH2  | 1:X:488:LYS:HD2  | 2.56                     | 0.41              |
| 1:X:174:THR:HB   | 1:X:177:ARG:NH1  | 2.36                     | 0.41              |
| 1:X:288:THR:HG22 | 1:X:289:THR:N    | 2.31                     | 0.41              |
| 1:X:435:VAL:CG1  | 1:X:441:LEU:HD11 | 2.47                     | 0.41              |
| 1:X:438:VAL:N    | 1:X:441:LEU:CD1  | 2.84                     | 0.41              |
| 1:O:171:TRP:CE2  | 1:O:176:GLY:HA2  | 2.56                     | 0.41              |
| 1:O:340:ASN:HD22 | 1:O:371:VAL:CG2  | 2.34                     | 0.41              |
| 1:O:369:ARG:NH1  | 1:Y:104:GLN:OE1  | 2.54                     | 0.41              |
| 1:Y:33:ARG:NE    | 1:Z:33:ARG:NH2   | 2.69                     | 0.41              |
| 1:Y:62:GLU:HB2   | 1:Z:58:SER:HB3   | 2.02                     | 0.41              |
| 1:Y:172:LYS:HA   | 1:Y:172:LYS:HD2  | 1.93                     | 0.41              |
| 1:Y:424:ASP:CB   | 1:Y:474:ILE:CG2  | 2.99                     | 0.41              |
| 1:X:169:LEU:HA   | 1:X:169:LEU:HD23 | 1.90                     | 0.41              |
| 1:X:222:GLU:O    | 1:X:240:SER:HA   | 2.21                     | 0.41              |
| 1:O:254:LEU:HA   | 1:O:254:LEU:HD12 | 1.80                     | 0.40              |
| 1:Y:175:GLN:CA   | 1:Y:175:GLN:NE2  | 2.82                     | 0.40              |
| 1:Y:483:TYR:CE2  | 1:Y:487:LYS:CE   | 2.98                     | 0.40              |
| 1:X:29:SER:CB    | 1:X:63:VAL:HG23  | 2.48                     | 0.40              |
| 1:X:328:ASP:HB3  | 1:X:332:PHE:CE2  | 2.56                     | 0.40              |
| 1:X:414:ALA:HB2  | 1:X:436:ARG:NH1  | 2.36                     | 0.40              |
| 1:O:62:GLU:HA    | 1:O:65:THR:CG2   | 2.50                     | 0.40              |
| 1:O:193:ASN:OD1  | 1:O:195:HIS:HB2  | 2.20                     | 0.40              |
| 1:Y:83:ARG:NH1   | 3:Y:503:GOL:H2   | 2.37                     | 0.40              |
| 1:Y:457:LEU:HA   | 1:Y:457:LEU:HD23 | 1.66                     | 0.40              |
| 1:Z:111:ILE:O    | 1:Z:115:LEU:HD13 | 2.21                     | 0.40              |
| 1:X:95:LYS:HA    | 1:X:96:PRO:HD3   | 1.90                     | 0.40              |
| 1:X:223:VAL:O    | 1:X:223:VAL:HG12 | 2.21                     | 0.40              |
| 1:Y:30:VAL:HG12  | 1:Y:31:SER:N     | 2.36                     | 0.40              |
| 1:Y:210:PRO:C    | 1:Y:212:GLU:N    | 2.78                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Y:486:TRP:CZ2  | 1:Y:490:VAL:CG2  | 3.04                     | 0.40              |
| 1:Z:154:ARG:HB3  | 1:Z:154:ARG:HE   | 1.42                     | 0.40              |
| 1:Z:253:GLN:O    | 1:Z:254:LEU:HB2  | 2.21                     | 0.40              |
| 1:Z:475:GLU:O    | 1:Z:478:GLU:N    | 2.50                     | 0.40              |
| 1:X:194:ILE:HG22 | 1:X:290:ILE:HD11 | 2.03                     | 0.40              |
| 1:X:384:ILE:O    | 1:X:387:GLN:HB2  | 2.21                     | 0.40              |
| 1:X:478:GLU:HA   | 1:X:481:TYR:HB2  | 2.02                     | 0.40              |
| 1:X:499:HIS:H    | 1:X:499:HIS:CD2  | 2.39                     | 0.40              |
| 1:O:11:GLN:CD    | 1:O:52:ILE:HG23  | 2.46                     | 0.40              |
| 1:O:48:ASP:HA    | 1:O:49:PRO:HD3   | 1.91                     | 0.40              |
| 1:O:112:CYS:SG   | 1:O:134:PRO:HD3  | 2.62                     | 0.40              |
| 1:O:151:SER:C    | 1:O:153:GLU:N    | 2.79                     | 0.40              |
| 1:O:192:PHE:HB2  | 1:O:199:TRP:CE3  | 2.56                     | 0.40              |
| 1:O:286:LEU:N    | 1:O:286:LEU:HD23 | 2.37                     | 0.40              |
| 1:O:488:LYS:HD3  | 1:Y:496:TRP:CZ3  | 2.55                     | 0.40              |
| 1:Y:418:LEU:CD1  | 1:Y:419:MET:CE   | 2.98                     | 0.40              |
| 1:Z:98:TYR:OH    | 1:Z:107:ARG:NH2  | 2.55                     | 0.40              |
| 1:Z:314:GLN:NE2  | 1:X:369:ARG:HH22 | 2.19                     | 0.40              |
| 1:Z:316:LEU:HA   | 1:Z:316:LEU:HD23 | 1.79                     | 0.40              |
| 1:Z:413:VAL:HG23 | 1:Z:436:ARG:CG   | 2.50                     | 0.40              |
| 1:X:145:LEU:HA   | 1:X:145:LEU:HD12 | 1.61                     | 0.40              |
| 1:X:347:ALA:O    | 1:X:361:ARG:HA   | 2.21                     | 0.40              |
| 1:X:407:ARG:NH1  | 1:X:466:ILE:HD11 | 2.37                     | 0.40              |
| 1:X:478:GLU:HA   | 1:X:481:TYR:HB3  | 2.03                     | 0.40              |
| 1:O:80:THR:HG22  | 1:O:245:ASP:HA   | 1.97                     | 0.40              |
| 1:O:204:LEU:CD2  | 1:O:209:ILE:CG2  | 2.99                     | 0.40              |
| 1:Y:123:TYR:CE2  | 1:Y:203:MET:HE3  | 2.55                     | 0.40              |
| 1:Z:81:ASN:N     | 1:Z:81:ASN:HD22  | 2.19                     | 0.40              |
| 1:Z:124:ILE:CG1  | 1:Z:203:MET:CE   | 2.98                     | 0.40              |
| 1:Z:183:TYR:HB3  | 1:Z:290:ILE:HD13 | 2.03                     | 0.40              |
| 1:Z:281:LYS:NZ   | 1:Z:281:LYS:HB3  | 2.36                     | 0.40              |
| 1:Z:337:GLN:HE21 | 1:Z:337:GLN:HB3  | 1.40                     | 0.40              |
| 1:Z:346:PRO:CG   | 1:Z:383:SER:HB2  | 2.51                     | 0.40              |
| 1:Z:456:ASN:O    | 1:Z:459:GLU:HB2  | 2.22                     | 0.40              |
| 1:X:159:GLU:C    | 1:X:160:LEU:HD23 | 2.46                     | 0.40              |
| 1:X:482:ARG:CA   | 1:X:482:ARG:NH1  | 2.79                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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   | O     | 484/501 (97%)   | 409 (84%)  | 58 (12%) | 17 (4%)  | 3           | 2 |
| 1   | X     | 496/501 (99%)   | 436 (88%)  | 42 (8%)  | 18 (4%)  | 2           | 2 |
| 1   | Y     | 497/501 (99%)   | 442 (89%)  | 46 (9%)  | 9 (2%)   | 6           | 8 |
| 1   | Z     | 496/501 (99%)   | 448 (90%)  | 39 (8%)  | 9 (2%)   | 6           | 8 |
| All | All   | 1973/2004 (98%) | 1735 (88%) | 185 (9%) | 53 (3%)  | 4           | 3 |

All (53) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | O     | 149 | GLU  |
| 1   | O     | 232 | LYS  |
| 1   | O     | 233 | GLY  |
| 1   | O     | 461 | GLN  |
| 1   | Y     | 175 | GLN  |
| 1   | Z     | 149 | GLU  |
| 1   | Z     | 476 | THR  |
| 1   | X     | 107 | ARG  |
| 1   | X     | 159 | GLU  |
| 1   | X     | 233 | GLY  |
| 1   | X     | 322 | LEU  |
| 1   | X     | 438 | VAL  |
| 1   | O     | 326 | ALA  |
| 1   | O     | 462 | GLU  |
| 1   | O     | 464 | ALA  |
| 1   | O     | 476 | THR  |
| 1   | Y     | 325 | ASP  |
| 1   | Y     | 453 | PHE  |
| 1   | Z     | 153 | GLU  |
| 1   | Z     | 284 | ASN  |
| 1   | X     | 149 | GLU  |
| 1   | X     | 326 | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | X     | 450 | ALA  |
| 1   | X     | 477 | THR  |
| 1   | O     | 71  | SER  |
| 1   | Y     | 138 | GLY  |
| 1   | Z     | 232 | LYS  |
| 1   | Z     | 233 | GLY  |
| 1   | Z     | 294 | PRO  |
| 1   | X     | 153 | GLU  |
| 1   | X     | 223 | VAL  |
| 1   | O     | 92  | GLU  |
| 1   | O     | 99  | ASN  |
| 1   | O     | 309 | ALA  |
| 1   | Y     | 92  | GLU  |
| 1   | X     | 294 | PRO  |
| 1   | X     | 458 | ASP  |
| 1   | X     | 463 | LYS  |
| 1   | X     | 476 | THR  |
| 1   | O     | 222 | GLU  |
| 1   | Y     | 177 | ARG  |
| 1   | Y     | 353 | ALA  |
| 1   | Y     | 477 | THR  |
| 1   | Z     | 397 | ALA  |
| 1   | Z     | 398 | ASP  |
| 1   | O     | 294 | PRO  |
| 1   | Y     | 438 | VAL  |
| 1   | X     | 157 | ARG  |
| 1   | X     | 138 | GLY  |
| 1   | X     | 206 | VAL  |
| 1   | O     | 442 | GLY  |
| 1   | O     | 472 | PRO  |
| 1   | O     | 194 | ILE  |

### 5.3.2 Protein sidechains ⓘ

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

10 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 2   | SO4  | Y     | 502 | -    | 4,4,4        | 1.58 | 1 (25%)     | 6,6,6       | 0.51 | 0           |
| 2   | SO4  | O     | 503 | -    | 4,4,4        | 1.76 | 1 (25%)     | 6,6,6       | 0.43 | 0           |
| 3   | GOL  | X     | 503 | -    | 5,5,5        | 0.33 | 0           | 5,5,5       | 0.79 | 0           |
| 3   | GOL  | O     | 504 | -    | 5,5,5        | 0.92 | 0           | 5,5,5       | 0.78 | 0           |
| 2   | SO4  | X     | 502 | -    | 4,4,4        | 1.76 | 1 (25%)     | 6,6,6       | 0.24 | 0           |
| 3   | GOL  | Z     | 504 | -    | 5,5,5        | 0.20 | 0           | 5,5,5       | 0.85 | 0           |
| 3   | GOL  | Y     | 503 | -    | 5,5,5        | 0.36 | 0           | 5,5,5       | 0.33 | 0           |
| 2   | SO4  | O     | 502 | -    | 4,4,4        | 1.17 | 1 (25%)     | 6,6,6       | 0.38 | 0           |
| 2   | SO4  | Z     | 503 | -    | 4,4,4        | 1.74 | 1 (25%)     | 6,6,6       | 0.38 | 0           |
| 2   | SO4  | Z     | 502 | -    | 4,4,4        | 1.09 | 0           | 6,6,6       | 0.27 | 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 |
|-----|------|-------|-----|------|---------|----------|-------|
| 3   | GOL  | O     | 504 | -    | -       | 0/4/4/4  | -     |
| 3   | GOL  | Z     | 504 | -    | -       | 1/4/4/4  | -     |
| 3   | GOL  | Y     | 503 | -    | -       | 2/4/4/4  | -     |
| 3   | GOL  | X     | 503 | -    | -       | 0/4/4/4  | -     |

All (5) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 2   | X     | 502 | SO4  | O1-S  | 2.93  | 1.62        | 1.44     |
| 2   | O     | 503 | SO4  | O3-S  | 2.79  | 1.71        | 1.48     |
| 2   | Y     | 502 | SO4  | O3-S  | 2.70  | 1.70        | 1.48     |
| 2   | Z     | 503 | SO4  | O2-S  | 2.31  | 1.58        | 1.44     |
| 2   | O     | 502 | SO4  | O1-S  | -2.12 | 1.32        | 1.44     |

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 3   | Z     | 504 | GOL  | O1-C1-C2-C3 |
| 3   | Y     | 503 | GOL  | O1-C1-C2-C3 |
| 3   | Y     | 503 | GOL  | O1-C1-C2-O2 |

There are no ring outliers.

7 monomers are involved in 16 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3   | X     | 503 | GOL  | 1       | 0            |
| 3   | O     | 504 | GOL  | 1       | 0            |
| 3   | Z     | 504 | GOL  | 7       | 0            |
| 3   | Y     | 503 | GOL  | 3       | 0            |
| 2   | O     | 502 | SO4  | 2       | 0            |
| 2   | Z     | 503 | SO4  | 1       | 0            |
| 2   | Z     | 502 | SO4  | 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2      | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|--------------|-----------------------|-------|
| 1   | O     | 497/501 (99%)   | -0.49  | 1 (0%) 91 90 | 10, 36, 67, 75        | 0     |
| 1   | X     | 498/501 (99%)   | -0.51  | 1 (0%) 91 90 | 13, 34, 67, 75        | 0     |
| 1   | Y     | 499/501 (99%)   | -0.61  | 1 (0%) 91 90 | 13, 34, 65, 75        | 0     |
| 1   | Z     | 498/501 (99%)   | -0.64  | 0 100 100    | 12, 33, 62, 75        | 0     |
| All | All   | 1992/2004 (99%) | -0.56  | 3 (0%) 91 90 | 10, 34, 65, 75        | 0     |

All (3) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | Y     | 327 | TYR  | 2.3  |
| 1   | O     | 326 | ALA  | 2.3  |
| 1   | X     | 465 | VAL  | 2.2  |

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

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

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 2   | SO4  | O     | 503 | 5/5   | 0.93 | 0.09 | 37,48,75,75                 | 0     |
| 2   | SO4  | Y     | 502 | 5/5   | 0.94 | 0.12 | 36,67,75,75                 | 0     |
| 2   | SO4  | Z     | 503 | 5/5   | 0.94 | 0.08 | 51,60,75,75                 | 0     |
| 2   | SO4  | X     | 502 | 5/5   | 0.94 | 0.09 | 30,75,75,75                 | 0     |
| 3   | GOL  | O     | 504 | 6/6   | 0.96 | 0.07 | 12,23,29,40                 | 0     |
| 2   | SO4  | O     | 502 | 5/5   | 0.98 | 0.07 | 11,36,68,75                 | 0     |
| 3   | GOL  | Y     | 503 | 6/6   | 0.98 | 0.06 | 11,18,30,63                 | 0     |
| 3   | GOL  | Z     | 504 | 6/6   | 0.98 | 0.04 | 5,16,20,54                  | 0     |
| 3   | GOL  | X     | 503 | 6/6   | 0.98 | 0.05 | 5,20,29,35                  | 0     |
| 2   | SO4  | Z     | 502 | 5/5   | 0.99 | 0.06 | 27,48,75,75                 | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.