



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 09:49 AM UTC

PDB ID : 1IVO / pdb\_00001ivo  
Title : Crystal Structure of the Complex of Human Epidermal Growth Factor and Receptor Extracellular Domains.  
Authors : Ogiso, H.; Ishitani, R.; Nureki, O.; Fukai, S.; Yamanaka, M.; Kim, J.H.; Saito, K.; Shirouzu, M.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)  
Deposited on : 2002-03-28  
Resolution : 3.30 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)

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

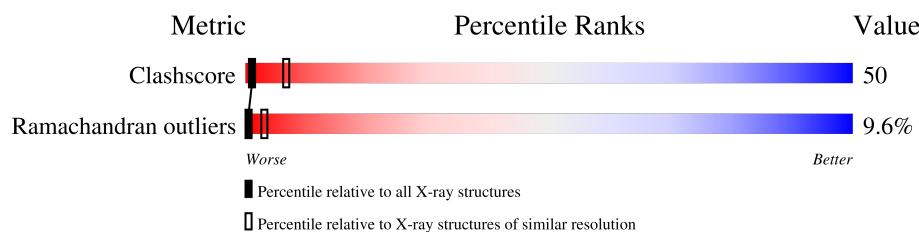
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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                      | 1209 (3.32-3.28)                                      |
| Ramachandran outliers | 187476                      | 1188 (3.32-3.28)                                      |

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

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 622    | 31% 44% 7% 18%   |
| 1   | B     | 622    | 29% 48% 5% 18%   |
| 2   | C     | 53     | 34% 51% • 11%    |
| 2   | D     | 53     | 34% 51% • 11%    |
| 3   | E     | 2      | 50% 50%          |

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 |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 4   | NAG  | A     | 1328 | -         | -        | X       | -                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 4   | NAG  | B     | 1328 | -         | -        | X       | -                |

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8892 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 Epidermal Growth Factor Receptor.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 511      | Total | C    | N   | O   | S  | 111     | 0       | 0     |
|     |       |          | 3956  | 2446 | 706 | 760 | 44 |         |         |       |
| 1   | B     | 510      | Total | C    | N   | O   | S  | 62      | 0       | 0     |
|     |       |          | 3947  | 2441 | 705 | 757 | 44 |         |         |       |

- Molecule 2 is a protein called Epidermal growth factor.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 2   | C     | 47       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 385   | 244 | 63 | 71 | 7 |         |         |       |
| 2   | D     | 47       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 385   | 244 | 63 | 71 | 7 |         |         |       |

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



| Mol | Chain | Residues | Atoms |    |   |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|---------|-------|
| 3   | E     | 2        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |         |       |

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).

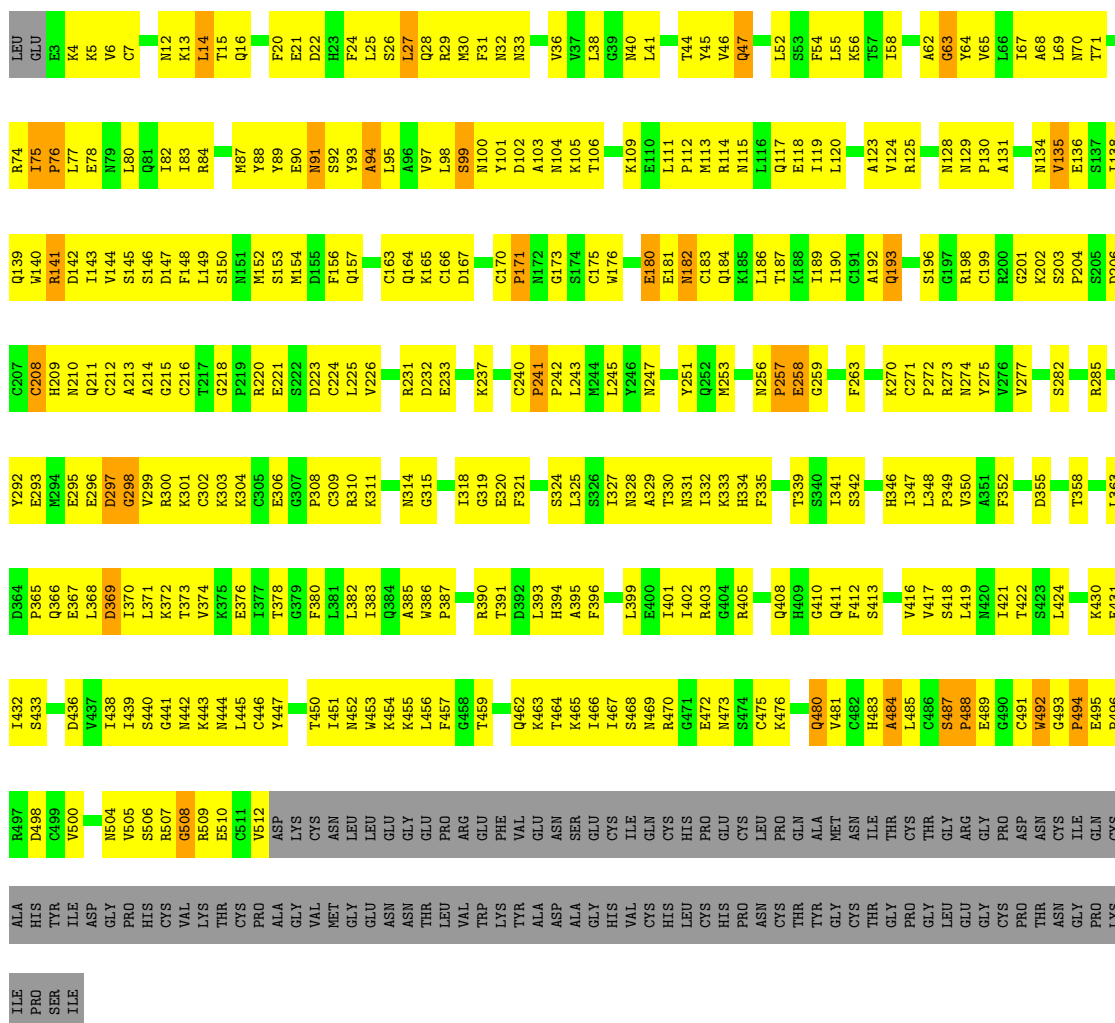


| Mol | Chain | Residues | Atoms |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 4   | A     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 4   | A     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 4   | A     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 4   | A     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 4   | A     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 4   | B     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 4   | B     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 4   | B     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |

- Molecule 5 is water.

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 5   | A     | 35       | Total | O  | 0       | 0       |
|     |       |          | 35    | 35 |         |         |
| 5   | B     | 32       | Total | O  | 0       | 0       |
|     |       |          | 32    | 32 |         |         |
| 5   | C     | 6        | Total | O  | 0       | 0       |
|     |       |          | 6     | 6  |         |         |
| 5   | D     | 6        | Total | O  | 0       | 0       |
|     |       |          | 6     | 6  |         |         |





- Molecule 2: Epidermal growth factor



- Molecule 2: Epidermal growth factor



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





## 4 Data and refinement statistics

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

| Property                                                 | Value                                                       | Source    |
|----------------------------------------------------------|-------------------------------------------------------------|-----------|
| Space group                                              | P 31 2 1                                                    | Depositor |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$ | 220.16 Å   220.16 Å   113.12 Å<br>90.00°   90.00°   120.00° | Depositor |
| Resolution (Å)                                           | 10.00 – 3.30                                                | Depositor |
| % Data completeness<br>(in resolution range)             | 98.0 (10.00-3.30)                                           | Depositor |
| $R_{merge}$                                              | 0.07                                                        | Depositor |
| $R_{sym}$                                                | 0.07                                                        | Depositor |
| Refinement program                                       | CNS 1.0                                                     | Depositor |
| R, $R_{free}$                                            | 0.255 , 0.326                                               | Depositor |
| Estimated twinning fraction                              | No twinning to report.                                      | Xtriage   |
| Total number of atoms                                    | 8892                                                        | wwPDB-VP  |
| Average B, all atoms (Å <sup>2</sup> )                   | 82.0                                                        | wwPDB-VP  |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

| Mol | Chain | Bond lengths |             | Bond angles |                 |
|-----|-------|--------------|-------------|-------------|-----------------|
|     |       | RMSZ         | $\# Z  > 5$ | RMSZ        | $\# Z  > 5$     |
| 1   | A     | 0.43         | 0/4027      | 1.06        | 26/5438 (0.5%)  |
| 1   | B     | 0.41         | 0/4018      | 1.03        | 19/5426 (0.4%)  |
| 2   | C     | 0.43         | 0/396       | 1.03        | 2/536 (0.4%)    |
| 2   | D     | 0.41         | 0/396       | 1.01        | 3/536 (0.6%)    |
| All | All   | 0.42         | 0/8837      | 1.04        | 50/11936 (0.4%) |

There are no bond length outliers.

All (50) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | B     | 258 | GLU  | N-CA-C | -9.15 | 99.16       | 110.88   |
| 1   | A     | 75  | ILE  | CA-C-N | 8.68  | 130.68      | 119.84   |
| 1   | A     | 75  | ILE  | C-N-CA | 8.68  | 130.68      | 119.84   |
| 1   | A     | 405 | ARG  | N-CA-C | -8.44 | 102.76      | 113.23   |
| 1   | B     | 47  | GLN  | N-CA-C | 8.29  | 121.22      | 110.53   |
| 2   | D     | 8   | LEU  | N-CA-C | -8.09 | 102.50      | 112.38   |
| 1   | B     | 369 | ASP  | N-CA-C | -7.79 | 103.75      | 113.18   |
| 1   | A     | 332 | ILE  | N-CA-C | -7.55 | 101.71      | 112.35   |
| 1   | B     | 298 | GLY  | N-CA-C | -7.38 | 106.05      | 115.42   |
| 1   | B     | 75  | ILE  | CA-C-N | 7.23  | 128.88      | 119.84   |
| 1   | B     | 75  | ILE  | C-N-CA | 7.23  | 128.88      | 119.84   |
| 1   | A     | 47  | GLN  | N-CA-C | 7.13  | 121.42      | 110.36   |
| 1   | A     | 212 | CYS  | N-CA-C | 6.98  | 120.56      | 108.76   |
| 1   | A     | 200 | ARG  | N-CA-C | -6.95 | 105.07      | 113.97   |
| 2   | C     | 45  | ARG  | N-CA-C | -6.84 | 100.35      | 110.48   |
| 1   | A     | 208 | CYS  | N-CA-C | 6.82  | 119.53      | 110.53   |
| 1   | A     | 339 | THR  | N-CA-C | -6.71 | 104.79      | 114.12   |
| 1   | B     | 492 | TRP  | N-CA-C | -6.48 | 105.67      | 112.93   |
| 1   | A     | 500 | VAL  | N-CA-C | -6.30 | 105.59      | 111.45   |
| 1   | A     | 401 | ILE  | N-CA-C | 6.21  | 116.55      | 108.35   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | B     | 332 | ILE  | N-CA-C  | -6.18 | 103.95      | 113.16   |
| 1   | B     | 164 | GLN  | N-CA-C  | 6.08  | 118.14      | 110.24   |
| 1   | A     | 111 | LEU  | CA-C-N  | 6.03  | 127.38      | 119.84   |
| 1   | A     | 111 | LEU  | C-N-CA  | 6.03  | 127.38      | 119.84   |
| 1   | A     | 240 | CYS  | CA-C-N  | 6.02  | 126.58      | 120.38   |
| 1   | A     | 240 | CYS  | C-N-CA  | 6.02  | 126.58      | 120.38   |
| 1   | B     | 212 | CYS  | N-CA-C  | 5.91  | 118.16      | 109.24   |
| 2   | D     | 32  | ASN  | N-CA-C  | -5.86 | 100.80      | 109.11   |
| 1   | B     | 208 | CYS  | N-CA-C  | 5.80  | 117.39      | 110.19   |
| 1   | A     | 314 | ASN  | N-CA-C  | 5.75  | 117.35      | 111.14   |
| 1   | B     | 301 | LYS  | N-CA-C  | -5.73 | 100.83      | 109.60   |
| 1   | A     | 6   | VAL  | N-CA-C  | 5.64  | 118.06      | 108.86   |
| 1   | A     | 451 | ILE  | N-CA-C  | 5.51  | 120.56      | 113.07   |
| 1   | A     | 98  | LEU  | N-CA-C  | 5.45  | 118.11      | 109.50   |
| 1   | B     | 480 | GLN  | CB-CA-C | -5.42 | 110.34      | 116.63   |
| 1   | A     | 394 | HIS  | N-CA-C  | 5.39  | 116.85      | 110.97   |
| 1   | B     | 94  | ALA  | N-CA-C  | -5.38 | 106.85      | 113.41   |
| 1   | A     | 247 | ASN  | CA-C-N  | 5.31  | 125.12      | 119.28   |
| 1   | A     | 247 | ASN  | C-N-CA  | 5.31  | 125.12      | 119.28   |
| 1   | B     | 170 | CYS  | CA-C-N  | 5.30  | 126.46      | 119.84   |
| 1   | B     | 170 | CYS  | C-N-CA  | 5.30  | 126.46      | 119.84   |
| 1   | A     | 291 | SER  | N-CA-C  | 5.28  | 116.02      | 108.74   |
| 1   | B     | 508 | GLY  | N-CA-C  | -5.26 | 100.72      | 113.18   |
| 1   | A     | 240 | CYS  | N-CA-C  | 5.24  | 117.55      | 110.31   |
| 1   | A     | 412 | PHE  | N-CA-C  | 5.14  | 117.62      | 109.24   |
| 1   | A     | 103 | ALA  | N-CA-C  | -5.12 | 106.13      | 112.38   |
| 2   | C     | 32  | ASN  | N-CA-C  | -5.10 | 102.52      | 109.71   |
| 1   | B     | 233 | GLU  | CB-CA-C | -5.08 | 110.33      | 117.23   |
| 2   | D     | 18  | GLY  | N-CA-C  | -5.04 | 106.14      | 111.93   |
| 1   | B     | 224 | CYS  | N-CA-C  | 5.02  | 117.58      | 109.40   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 3956  | 0        | 3843     | 371     | 0            |
| 1   | B     | 3947  | 0        | 3843     | 429     | 0            |
| 2   | C     | 385   | 0        | 344      | 28      | 0            |
| 2   | D     | 385   | 0        | 344      | 43      | 0            |
| 3   | E     | 28    | 0        | 25       | 4       | 0            |
| 4   | A     | 70    | 0        | 65       | 10      | 0            |
| 4   | B     | 42    | 0        | 39       | 22      | 0            |
| 5   | A     | 35    | 0        | 0        | 2       | 0            |
| 5   | B     | 32    | 0        | 0        | 5       | 0            |
| 5   | C     | 6     | 0        | 0        | 1       | 0            |
| 5   | D     | 6     | 0        | 0        | 2       | 0            |
| All | All   | 8892  | 0        | 8503     | 852     | 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 50.

All (852) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:243:LEU:HA   | 1:B:256:ASN:HB3  | 1.34                     | 1.09              |
| 1:A:174:SER:HB3  | 1:A:184:GLN:HB3  | 1.39                     | 1.02              |
| 1:A:481:VAL:HG12 | 1:A:482:CYS:H    | 1.24                     | 0.99              |
| 1:B:328:ASN:H    | 4:B:1328:NAG:H82 | 1.27                     | 0.97              |
| 1:A:331:ASN:HB2  | 4:A:1328:NAG:HN2 | 1.29                     | 0.96              |
| 1:A:439:ILE:HB   | 1:A:466:ILE:HG22 | 1.48                     | 0.94              |
| 1:B:328:ASN:H    | 4:B:1328:NAG:C8  | 1.81                     | 0.93              |
| 1:B:416:VAL:HG23 | 1:B:439:ILE:HG23 | 1.50                     | 0.93              |
| 1:B:442:ASN:HB2  | 1:B:469:ASN:HD22 | 1.35                     | 0.92              |
| 1:B:7:CYS:HB2    | 1:B:30:MET:HE2   | 1.51                     | 0.91              |
| 1:B:295:GLU:HB3  | 1:B:300:ARG:HD2  | 1.50                     | 0.91              |
| 1:B:366:GLN:HA   | 1:B:366:GLN:HE21 | 1.34                     | 0.91              |
| 1:B:349:PRO:HG3  | 1:B:385:ALA:HB2  | 1.53                     | 0.90              |
| 1:B:327:ILE:HA   | 4:B:1328:NAG:H83 | 1.53                     | 0.90              |
| 1:A:190:ILE:HD13 | 1:A:202:LYS:HA   | 1.52                     | 0.90              |
| 1:B:391:THR:HB   | 1:B:422:THR:HG22 | 1.54                     | 0.89              |
| 1:B:6:VAL:HG12   | 1:B:36:VAL:HB    | 1.54                     | 0.89              |
| 1:B:243:LEU:CA   | 1:B:256:ASN:HB3  | 2.02                     | 0.89              |
| 1:B:4:LYS:HD3    | 1:B:4:LYS:H      | 1.36                     | 0.88              |
| 1:B:485:LEU:HD12 | 1:B:485:LEU:H    | 1.37                     | 0.88              |
| 1:A:46:VAL:HG11  | 1:A:52:LEU:HD11  | 1.56                     | 0.88              |
| 1:B:390:ARG:HH11 | 1:B:390:ARG:HB2  | 1.36                     | 0.88              |
| 1:A:186:LEU:HD12 | 1:A:186:LEU:H    | 1.39                     | 0.87              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:99:SER:HA    | 1:B:128:ASN:O    | 1.76                     | 0.86              |
| 1:B:123:ALA:HB1  | 1:B:152:MET:HB3  | 1.59                     | 0.85              |
| 1:B:432:ILE:HB   | 1:B:457:PHE:HB3  | 1.57                     | 0.85              |
| 1:B:196:SER:HB3  | 1:B:210:ASN:HB3  | 1.56                     | 0.84              |
| 1:B:78:GLU:HA    | 1:B:112:PRO:O    | 1.76                     | 0.84              |
| 1:B:78:GLU:HG2   | 1:B:112:PRO:HB2  | 1.60                     | 0.83              |
| 1:B:303:LYS:HA   | 1:B:303:LYS:HE2  | 1.62                     | 0.81              |
| 1:A:123:ALA:HB1  | 1:A:152:MET:HB3  | 1.63                     | 0.81              |
| 1:A:139:GLN:H    | 1:A:184:GLN:HE22 | 1.26                     | 0.79              |
| 1:B:390:ARG:HB2  | 1:B:390:ARG:NH1  | 1.96                     | 0.79              |
| 1:B:439:ILE:HB   | 1:B:466:ILE:HG23 | 1.64                     | 0.79              |
| 1:A:245:LEU:HD13 | 1:A:256:ASN:HB2  | 1.64                     | 0.79              |
| 1:B:442:ASN:HB2  | 1:B:469:ASN:ND2  | 1.97                     | 0.79              |
| 1:B:47:GLN:HA    | 1:B:47:GLN:HE21  | 1.48                     | 0.78              |
| 1:B:480:GLN:HG3  | 1:B:481:VAL:H    | 1.48                     | 0.78              |
| 1:A:84:ARG:HD3   | 1:A:120:LEU:HD12 | 1.64                     | 0.78              |
| 1:A:148:PHE:C    | 1:A:150:SER:H    | 1.93                     | 0.77              |
| 2:D:15:LEU:HD21  | 2:D:41:ARG:NH2   | 1.99                     | 0.77              |
| 1:A:450:THR:O    | 1:A:490:GLY:HA3  | 1.83                     | 0.76              |
| 1:A:475:CYS:SG   | 1:A:480:GLN:HB2  | 2.24                     | 0.76              |
| 1:B:366:GLN:HA   | 1:B:366:GLN:NE2  | 2.00                     | 0.76              |
| 1:B:371:LEU:HB2  | 1:B:395:ALA:HB1  | 1.67                     | 0.76              |
| 1:B:135:VAL:HA   | 1:B:138:ILE:HD13 | 1.67                     | 0.76              |
| 1:B:328:ASN:OD1  | 4:B:1328:NAG:H2  | 1.86                     | 0.76              |
| 1:A:139:GLN:N    | 1:A:184:GLN:HE22 | 1.83                     | 0.76              |
| 1:B:510:GLU:OE1  | 1:B:512:VAL:HG13 | 1.86                     | 0.76              |
| 1:A:401:ILE:HG12 | 1:A:431:GLU:HB3  | 1.68                     | 0.76              |
| 1:A:215:GLY:H    | 1:A:225:LEU:HD12 | 1.50                     | 0.75              |
| 1:B:218:GLY:H    | 1:B:223:ASP:HB3  | 1.51                     | 0.75              |
| 1:A:203:SER:H    | 1:A:204:PRO:HD2  | 1.51                     | 0.75              |
| 1:A:215:GLY:N    | 1:A:225:LEU:HD12 | 2.01                     | 0.75              |
| 1:A:82:ILE:HD11  | 1:A:120:LEU:HG   | 1.68                     | 0.75              |
| 1:A:115:ASN:O    | 1:A:117:GLN:HG3  | 1.87                     | 0.75              |
| 1:B:101:TYR:HB3  | 1:B:130:PRO:HD2  | 1.69                     | 0.75              |
| 1:A:485:LEU:H    | 1:A:485:LEU:CD2  | 2.00                     | 0.74              |
| 1:A:485:LEU:H    | 1:A:485:LEU:HD23 | 1.52                     | 0.73              |
| 1:B:297:ASP:HB2  | 1:B:299:VAL:HG22 | 1.70                     | 0.73              |
| 1:B:88:TYR:HD2   | 1:B:92:SER:H     | 1.34                     | 0.73              |
| 1:A:300:ARG:HH21 | 1:A:403:ARG:NH2  | 1.87                     | 0.73              |
| 1:B:69:LEU:HD11  | 2:D:26:LEU:HD11  | 1.69                     | 0.73              |
| 1:B:4:LYS:HD3    | 1:B:4:LYS:N      | 2.03                     | 0.73              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:295:GLU:HB3  | 1:A:300:ARG:HG2  | 1.71                     | 0.73              |
| 2:D:19:VAL:HG22  | 2:D:32:ASN:HB3   | 1.70                     | 0.73              |
| 1:B:271:CYS:SG   | 1:B:277:VAL:HG22 | 2.29                     | 0.72              |
| 1:A:53:SER:O     | 1:A:56:LYS:HG3   | 1.89                     | 0.72              |
| 1:A:275:TYR:CD2  | 1:A:405:ARG:HD3  | 2.25                     | 0.72              |
| 1:A:470:ARG:HG2  | 1:A:470:ARG:HH11 | 1.55                     | 0.72              |
| 1:A:16:GLN:HB2   | 1:A:45:TYR:CE1   | 2.24                     | 0.72              |
| 1:A:46:VAL:HG12  | 1:A:72:VAL:HB    | 1.70                     | 0.72              |
| 1:A:408:GLN:HE21 | 1:A:408:GLN:HA   | 1.55                     | 0.72              |
| 1:A:446:CYS:C    | 1:A:447:TYR:HD1  | 1.97                     | 0.71              |
| 1:A:331:ASN:HB2  | 4:A:1328:NAG:N2  | 2.02                     | 0.71              |
| 1:A:432:ILE:HB   | 1:A:457:PHE:HB3  | 1.71                     | 0.71              |
| 1:A:138:ILE:HG12 | 1:A:176:TRP:CE2  | 2.26                     | 0.71              |
| 1:B:16:GLN:HB2   | 1:B:45:TYR:CE1   | 2.26                     | 0.71              |
| 1:A:201:GLY:HA3  | 1:A:204:PRO:HG2  | 1.72                     | 0.71              |
| 1:B:245:LEU:HG   | 1:B:257:PRO:HD3  | 1.73                     | 0.71              |
| 1:A:203:SER:N    | 1:A:204:PRO:HD2  | 2.06                     | 0.70              |
| 1:B:62:ALA:O     | 1:B:84:ARG:HB2   | 1.90                     | 0.70              |
| 1:B:463:LYS:NZ   | 1:B:463:LYS:HB3  | 2.05                     | 0.70              |
| 1:B:318:ILE:HD12 | 1:B:319:GLY:H    | 1.56                     | 0.70              |
| 1:A:330:THR:HB   | 4:A:1328:NAG:H2  | 1.73                     | 0.70              |
| 1:B:41:LEU:HD23  | 1:B:65:VAL:HG22  | 1.73                     | 0.70              |
| 1:A:201:GLY:C    | 1:A:203:SER:H    | 2.00                     | 0.70              |
| 1:B:349:PRO:CG   | 1:B:385:ALA:HB2  | 2.21                     | 0.70              |
| 1:B:436:ASP:CG   | 1:B:463:LYS:HG2  | 2.17                     | 0.70              |
| 1:A:25:LEU:O     | 1:A:29:ARG:HG3   | 1.92                     | 0.70              |
| 1:A:446:CYS:C    | 1:A:447:TYR:CD1  | 2.70                     | 0.70              |
| 1:B:109:LYS:HA   | 1:B:131:ALA:O    | 1.90                     | 0.70              |
| 1:B:257:PRO:HG2  | 1:B:258:GLU:H    | 1.57                     | 0.70              |
| 1:B:505:VAL:O    | 1:B:507:ARG:HG3  | 1.91                     | 0.70              |
| 2:C:8:LEU:O      | 2:C:11:ASP:HB3   | 1.92                     | 0.69              |
| 1:A:403:ARG:HG3  | 1:A:403:ARG:HH11 | 1.58                     | 0.69              |
| 1:A:478:THR:HB   | 1:A:480:GLN:HG3  | 1.75                     | 0.69              |
| 1:B:123:ALA:HB1  | 1:B:152:MET:CB   | 2.23                     | 0.69              |
| 1:B:442:ASN:HD22 | 1:B:469:ASN:HD21 | 1.40                     | 0.69              |
| 1:A:62:ALA:O     | 1:A:84:ARG:HB2   | 1.93                     | 0.69              |
| 2:D:49:TRP:HA    | 2:D:49:TRP:CE3   | 2.27                     | 0.69              |
| 1:B:243:LEU:HA   | 1:B:256:ASN:CB   | 2.20                     | 0.68              |
| 1:B:408:GLN:C    | 1:B:410:GLY:H    | 2.00                     | 0.68              |
| 1:A:47:GLN:HB2   | 1:A:50:TYR:CE1   | 2.29                     | 0.68              |
| 1:A:102:ASP:HB2  | 1:A:106:THR:O    | 1.94                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:93:TYR:HA    | 1:A:123:ALA:O    | 1.93                     | 0.68              |
| 1:A:165:LYS:HG3  | 1:A:166:CYS:H    | 1.59                     | 0.68              |
| 1:B:459:THR:HB   | 1:B:462:GLN:HE21 | 1.59                     | 0.67              |
| 1:B:46:VAL:HG11  | 1:B:52:LEU:HD21  | 1.74                     | 0.67              |
| 1:B:134:ASN:HB3  | 1:B:175:CYS:O    | 1.92                     | 0.67              |
| 1:B:454:LYS:H    | 1:B:454:LYS:HD3  | 1.60                     | 0.67              |
| 1:A:391:THR:HB   | 1:A:422:THR:HG22 | 1.76                     | 0.67              |
| 3:E:1:NAG:H4     | 3:E:2:NAG:N2     | 2.09                     | 0.67              |
| 1:A:111:LEU:HG   | 1:A:113:MET:HE2  | 1.76                     | 0.66              |
| 2:C:21:MET:HE3   | 2:C:23:ILE:HD11  | 1.77                     | 0.66              |
| 1:B:124:VAL:H    | 1:B:152:MET:HE3  | 1.59                     | 0.66              |
| 1:B:347:ILE:HB   | 1:B:383:ILE:HG23 | 1.76                     | 0.66              |
| 1:A:447:TYR:OH   | 1:A:494:PRO:HG3  | 1.95                     | 0.66              |
| 1:A:99:SER:HA    | 1:A:128:ASN:O    | 1.95                     | 0.66              |
| 1:A:89:TYR:CE2   | 1:A:90:GLU:HG2   | 2.31                     | 0.66              |
| 1:A:142:ASP:OD2  | 1:A:188:LYS:HB3  | 1.96                     | 0.66              |
| 1:B:32:ASN:O     | 1:B:33:ASN:HB2   | 1.94                     | 0.66              |
| 1:B:115:ASN:O    | 1:B:117:GLN:HG3  | 1.96                     | 0.66              |
| 1:A:412:PHE:HE1  | 2:C:48:LYS:HB3   | 1.61                     | 0.65              |
| 1:A:506:SER:HB2  | 1:A:511:CYS:SG   | 2.36                     | 0.65              |
| 1:A:472:GLU:C    | 1:A:474:SER:H    | 2.05                     | 0.65              |
| 1:B:403:ARG:O    | 1:B:433:SER:HB2  | 1.95                     | 0.65              |
| 1:B:485:LEU:HD22 | 1:B:496:PRO:HG3  | 1.79                     | 0.65              |
| 2:D:49:TRP:HA    | 2:D:49:TRP:HE3   | 1.59                     | 0.65              |
| 1:A:125:ARG:HG2  | 1:A:125:ARG:HH11 | 1.61                     | 0.65              |
| 1:A:235:THR:OG1  | 1:A:237:LYS:HE2  | 1.97                     | 0.65              |
| 1:A:489:GLU:OE2  | 1:A:501:SER:HB2  | 1.97                     | 0.65              |
| 1:B:84:ARG:HG3   | 1:B:84:ARG:HH11  | 1.62                     | 0.65              |
| 1:A:111:LEU:CD2  | 1:A:113:MET:HE2  | 2.27                     | 0.65              |
| 1:A:216:CYS:SG   | 1:A:218:GLY:O    | 2.55                     | 0.65              |
| 1:A:310:ARG:C    | 1:A:311:LYS:HD3  | 2.23                     | 0.64              |
| 1:B:45:TYR:HE2   | 1:B:69:LEU:HD23  | 1.62                     | 0.64              |
| 1:B:4:LYS:H      | 1:B:4:LYS:CD     | 2.07                     | 0.64              |
| 1:B:232:ASP:CB   | 1:B:237:LYS:HD2  | 2.27                     | 0.64              |
| 1:A:75:ILE:O     | 1:A:112:PRO:HD2  | 1.97                     | 0.64              |
| 1:A:423:SER:HA   | 1:A:445:LEU:CD1  | 2.27                     | 0.64              |
| 1:A:78:GLU:HA    | 1:A:112:PRO:O    | 1.98                     | 0.64              |
| 1:A:174:SER:CB   | 1:A:184:GLN:HB3  | 2.22                     | 0.64              |
| 1:B:444:ASN:H    | 1:B:444:ASN:ND2  | 1.96                     | 0.63              |
| 1:A:152:MET:HE3  | 1:A:154:MET:SD   | 2.39                     | 0.63              |
| 1:A:386:TRP:CZ2  | 1:A:393:LEU:HA   | 2.34                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:76:PRO:O     | 1:A:78:GLU:N     | 2.29                     | 0.63              |
| 1:B:40:ASN:ND2   | 1:B:64:TYR:H     | 1.96                     | 0.63              |
| 1:B:459:THR:HB   | 1:B:462:GLN:NE2  | 2.13                     | 0.63              |
| 2:C:7:PRO:HD3    | 2:C:29:TYR:CE2   | 2.34                     | 0.63              |
| 1:B:14:LEU:HD21  | 2:D:26:LEU:CD1   | 2.29                     | 0.63              |
| 1:A:189:ILE:C    | 1:A:191:CYS:H    | 2.04                     | 0.63              |
| 1:B:331:ASN:HB2  | 4:B:1328:NAG:O3  | 1.98                     | 0.63              |
| 1:A:76:PRO:C     | 1:A:78:GLU:H     | 2.07                     | 0.62              |
| 1:A:349:PRO:HD2  | 5:C:57:HOH:O     | 1.98                     | 0.62              |
| 1:A:47:GLN:HA    | 1:A:71:THR:OG1   | 1.99                     | 0.62              |
| 1:A:84:ARG:HD3   | 1:A:120:LEU:CD1  | 2.30                     | 0.62              |
| 1:A:138:ILE:HG23 | 1:A:184:GLN:NE2  | 2.15                     | 0.62              |
| 1:B:431:GLU:HA   | 1:B:456:LEU:O    | 1.99                     | 0.62              |
| 1:B:480:GLN:HG3  | 1:B:481:VAL:N    | 2.14                     | 0.62              |
| 1:A:481:VAL:HG12 | 1:A:482:CYS:N    | 2.05                     | 0.62              |
| 1:B:218:GLY:N    | 1:B:223:ASP:HB3  | 2.15                     | 0.62              |
| 1:A:112:PRO:O    | 1:A:114:ARG:HD2  | 1.99                     | 0.62              |
| 1:B:93:TYR:HA    | 1:B:123:ALA:O    | 2.00                     | 0.62              |
| 1:A:174:SER:HB3  | 1:A:184:GLN:HE21 | 1.65                     | 0.62              |
| 1:A:364:ASP:HB3  | 1:A:367:GLU:HG2  | 1.82                     | 0.61              |
| 1:B:152:MET:O    | 1:B:152:MET:HG3  | 1.98                     | 0.61              |
| 1:B:339:THR:HG22 | 1:B:373:THR:O    | 1.99                     | 0.61              |
| 1:B:190:ILE:HG22 | 1:B:190:ILE:O    | 2.00                     | 0.61              |
| 1:A:444:ASN:HA   | 1:A:470:ARG:HD3  | 1.81                     | 0.61              |
| 1:A:371:LEU:C    | 1:A:373:THR:H    | 2.09                     | 0.61              |
| 1:A:453:TRP:C    | 1:A:455:LYS:H    | 2.08                     | 0.61              |
| 1:A:360:THR:HG21 | 4:A:1328:NAG:H62 | 1.82                     | 0.60              |
| 1:B:303:LYS:HD3  | 1:B:304:LYS:H    | 1.65                     | 0.60              |
| 1:B:328:ASN:N    | 4:B:1328:NAG:H82 | 2.09                     | 0.60              |
| 1:A:149:LEU:HA   | 1:A:152:MET:HG2  | 1.84                     | 0.60              |
| 1:B:331:ASN:HB2  | 4:B:1328:NAG:O7  | 2.00                     | 0.60              |
| 1:A:438:ILE:HD13 | 2:C:47:LEU:HD22  | 1.82                     | 0.60              |
| 1:B:29:ARG:HD2   | 2:D:49:TRP:CZ2   | 2.35                     | 0.60              |
| 1:B:368:LEU:O    | 1:B:395:ALA:HB2  | 2.01                     | 0.60              |
| 1:B:421:ILE:HG13 | 1:B:445:LEU:HD13 | 1.83                     | 0.60              |
| 1:A:316:ILE:HD11 | 1:A:327:ILE:HG13 | 1.83                     | 0.60              |
| 1:B:296:GLU:C    | 1:B:298:GLY:H    | 2.09                     | 0.60              |
| 1:A:16:GLN:HB2   | 1:A:45:TYR:HE1   | 1.62                     | 0.60              |
| 2:D:23:ILE:HG22  | 2:D:23:ILE:O     | 2.01                     | 0.60              |
| 1:B:328:ASN:O    | 4:B:1328:NAG:H82 | 2.00                     | 0.60              |
| 1:B:243:LEU:C    | 1:B:256:ASN:HB3  | 2.27                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:47:GLN:HA    | 1:B:47:GLN:NE2   | 2.16                     | 0.59              |
| 1:B:187:THR:HB   | 1:B:199:CYS:O    | 2.02                     | 0.59              |
| 1:A:138:ILE:HG12 | 1:A:176:TRP:NE1  | 2.16                     | 0.59              |
| 1:A:198:ARG:O    | 1:A:208:CYS:HB2  | 2.02                     | 0.59              |
| 1:B:130:PRO:O    | 1:B:131:ALA:HB3  | 2.01                     | 0.59              |
| 1:B:186:LEU:H    | 1:B:186:LEU:CD2  | 2.15                     | 0.59              |
| 1:A:275:TYR:HD2  | 1:A:405:ARG:HD3  | 1.68                     | 0.59              |
| 1:B:209:HIS:CE1  | 1:B:211:GLN:HB2  | 2.37                     | 0.59              |
| 1:A:352:PHE:HE2  | 1:A:387:PRO:HG3  | 1.66                     | 0.59              |
| 1:A:355:ASP:OD2  | 1:A:358:THR:HG23 | 2.01                     | 0.59              |
| 1:A:380:PHE:CD1  | 1:A:380:PHE:C    | 2.80                     | 0.59              |
| 1:A:455:LYS:HD3  | 1:A:456:LEU:N    | 2.17                     | 0.59              |
| 1:A:466:ILE:HD12 | 1:A:466:ILE:O    | 2.02                     | 0.59              |
| 1:B:352:PHE:HE2  | 1:B:363:LEU:HD23 | 1.67                     | 0.59              |
| 1:A:118:GLU:HG2  | 1:A:213:ALA:HB1  | 1.83                     | 0.59              |
| 2:C:26:LEU:O     | 2:C:28:LYS:HG2   | 2.01                     | 0.59              |
| 1:A:187:THR:HA   | 1:A:190:ILE:HD11 | 1.85                     | 0.59              |
| 1:A:457:PHE:HD2  | 1:A:457:PHE:O    | 1.86                     | 0.59              |
| 1:A:403:ARG:HH11 | 1:A:403:ARG:CG   | 2.15                     | 0.59              |
| 1:A:371:LEU:O    | 1:A:373:THR:N    | 2.36                     | 0.59              |
| 1:A:398:ASN:HD22 | 1:A:398:ASN:N    | 2.01                     | 0.59              |
| 1:B:56:LYS:HE3   | 1:B:78:GLU:OE1   | 2.03                     | 0.59              |
| 1:B:292:TYR:O    | 1:B:302:CYS:HB2  | 2.02                     | 0.59              |
| 1:B:125:ARG:HA   | 1:B:153:SER:O    | 2.03                     | 0.59              |
| 2:D:48:LYS:O     | 2:D:49:TRP:CD2   | 2.55                     | 0.59              |
| 1:A:216:CYS:HB2  | 1:A:223:ASP:O    | 2.03                     | 0.58              |
| 1:B:140:TRP:C    | 1:B:142:ASP:N    | 2.60                     | 0.58              |
| 1:B:139:GLN:HG3  | 1:B:184:GLN:HE22 | 1.68                     | 0.58              |
| 1:A:186:LEU:H    | 1:A:186:LEU:CD1  | 2.14                     | 0.58              |
| 1:A:253:MET:HE1  | 1:B:282:SER:OG   | 2.03                     | 0.58              |
| 1:A:293:GLU:OE1  | 1:A:300:ARG:HD3  | 2.04                     | 0.58              |
| 1:A:446:CYS:SG   | 1:A:470:ARG:HG2  | 2.42                     | 0.58              |
| 1:B:93:TYR:CE2   | 1:B:125:ARG:HB2  | 2.38                     | 0.58              |
| 1:A:414:LEU:HD23 | 1:A:415:ALA:N    | 2.19                     | 0.58              |
| 1:B:4:LYS:HE3    | 1:B:231:ARG:NH1  | 2.19                     | 0.58              |
| 1:A:44:THR:HG22  | 1:A:68:ALA:O     | 2.03                     | 0.58              |
| 1:A:507:ARG:HD2  | 1:A:507:ARG:C    | 2.28                     | 0.58              |
| 1:B:14:LEU:HD21  | 2:D:26:LEU:HD12  | 1.85                     | 0.58              |
| 1:A:139:GLN:HE22 | 1:A:172:ASN:HB2  | 1.68                     | 0.58              |
| 1:B:47:GLN:HE21  | 1:B:47:GLN:CA    | 2.17                     | 0.58              |
| 1:B:444:ASN:H    | 1:B:444:ASN:HD22 | 1.52                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:70:ASN:HB3   | 1:A:72:VAL:HG12  | 1.84                     | 0.58              |
| 1:A:290:ASP:HA   | 1:A:309:CYS:SG   | 2.43                     | 0.58              |
| 1:B:270:LYS:HG2  | 1:B:271:CYS:N    | 2.17                     | 0.58              |
| 1:B:422:THR:HA   | 1:B:444:ASN:O    | 2.04                     | 0.58              |
| 1:B:180:GLU:HB2  | 1:B:182:ASN:OD1  | 2.03                     | 0.58              |
| 1:B:341:ILE:O    | 1:B:378:THR:HG23 | 2.04                     | 0.58              |
| 1:B:25:LEU:O     | 1:B:29:ARG:HG3   | 2.04                     | 0.57              |
| 1:B:28:GLN:HG3   | 1:B:54:PHE:CE2   | 2.39                     | 0.57              |
| 1:B:295:GLU:HB3  | 1:B:300:ARG:HA   | 1.85                     | 0.57              |
| 1:B:463:LYS:HB3  | 1:B:463:LYS:HZ3  | 1.69                     | 0.57              |
| 1:A:130:PRO:HA   | 1:A:157:GLN:NE2  | 2.19                     | 0.57              |
| 1:B:144:VAL:HG12 | 1:B:145:SER:N    | 2.19                     | 0.57              |
| 1:B:438:ILE:HG13 | 1:B:465:LYS:O    | 2.04                     | 0.57              |
| 2:D:45:ARG:O     | 2:D:47:LEU:N     | 2.37                     | 0.57              |
| 1:B:421:ILE:HG13 | 1:B:445:LEU:CD1  | 2.34                     | 0.57              |
| 1:B:472:GLU:N    | 5:B:1339:HOH:O   | 2.36                     | 0.57              |
| 1:A:6:VAL:HG12   | 1:A:36:VAL:HB    | 1.86                     | 0.57              |
| 1:A:97:VAL:O     | 1:A:98:LEU:HD23  | 2.04                     | 0.57              |
| 1:B:216:CYS:HA   | 1:B:225:LEU:HD13 | 1.86                     | 0.57              |
| 1:B:295:GLU:CB   | 1:B:300:ARG:HA   | 2.33                     | 0.57              |
| 1:B:16:GLN:HB2   | 1:B:45:TYR:CD1   | 2.40                     | 0.57              |
| 1:B:74:ARG:NH1   | 1:B:112:PRO:HG2  | 2.20                     | 0.57              |
| 1:B:215:GLY:CA   | 1:B:225:LEU:HD22 | 2.34                     | 0.57              |
| 1:B:119:ILE:HG22 | 1:B:119:ILE:O    | 2.05                     | 0.57              |
| 1:B:69:LEU:CD1   | 2:D:26:LEU:HD11  | 2.35                     | 0.57              |
| 1:B:367:GLU:O    | 1:B:370:ILE:HB   | 2.04                     | 0.57              |
| 1:A:453:TRP:O    | 1:A:455:LYS:N    | 2.38                     | 0.57              |
| 1:A:509:ARG:HD2  | 1:A:509:ARG:N    | 2.20                     | 0.57              |
| 1:B:41:LEU:HB3   | 1:B:65:VAL:HG22  | 1.85                     | 0.57              |
| 1:B:225:LEU:O    | 1:B:226:VAL:HG13 | 2.05                     | 0.57              |
| 1:A:82:ILE:HD11  | 1:A:120:LEU:CG   | 2.36                     | 0.56              |
| 1:A:68:ALA:HA    | 1:A:98:LEU:O     | 2.05                     | 0.56              |
| 1:B:44:THR:HG22  | 1:B:68:ALA:O     | 2.05                     | 0.56              |
| 1:A:190:ILE:HD12 | 1:A:199:CYS:SG   | 2.45                     | 0.56              |
| 1:A:335:PHE:HA   | 1:A:338:CYS:SG   | 2.46                     | 0.56              |
| 1:B:47:GLN:HA    | 1:B:71:THR:OG1   | 2.04                     | 0.56              |
| 1:A:97:VAL:C     | 1:A:98:LEU:HD23  | 2.30                     | 0.56              |
| 1:A:148:PHE:O    | 1:A:150:SER:N    | 2.38                     | 0.56              |
| 1:A:295:GLU:HA   | 1:A:300:ARG:HA   | 1.87                     | 0.56              |
| 1:B:216:CYS:HB2  | 1:B:223:ASP:O    | 2.04                     | 0.56              |
| 1:A:426:LEU:O    | 1:A:428:SER:N    | 2.37                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:443:LYS:HG3  | 1:B:444:ASN:H    | 1.70                     | 0.56              |
| 1:A:144:VAL:HG12 | 1:A:145:SER:N    | 2.21                     | 0.56              |
| 1:A:251:TYR:C    | 1:A:252:GLN:HE21 | 2.14                     | 0.56              |
| 1:B:401:ILE:HG13 | 1:B:431:GLU:HB3  | 1.87                     | 0.56              |
| 1:B:408:GLN:C    | 1:B:410:GLY:N    | 2.63                     | 0.56              |
| 1:B:198:ARG:O    | 1:B:208:CYS:HB2  | 2.06                     | 0.56              |
| 1:B:393:LEU:HB2  | 1:B:424:LEU:O    | 2.06                     | 0.56              |
| 1:A:84:ARG:HH11  | 1:A:84:ARG:HG3   | 1.72                     | 0.55              |
| 1:A:124:VAL:HG13 | 1:A:154:MET:SD   | 2.46                     | 0.55              |
| 1:B:140:TRP:O    | 1:B:142:ASP:N    | 2.39                     | 0.55              |
| 1:B:483:HIS:O    | 1:B:484:ALA:HB2  | 2.05                     | 0.55              |
| 1:B:436:ASP:OD2  | 1:B:463:LYS:HG2  | 2.06                     | 0.55              |
| 1:B:484:ALA:HB3  | 1:B:485:LEU:HD12 | 1.88                     | 0.55              |
| 1:A:310:ARG:HD2  | 1:A:310:ARG:N    | 2.22                     | 0.55              |
| 1:B:113:MET:HE3  | 1:B:176:TRP:CZ3  | 2.42                     | 0.55              |
| 1:A:46:VAL:HG11  | 1:A:52:LEU:CD1   | 2.32                     | 0.55              |
| 1:A:408:GLN:C    | 1:A:410:GLY:N    | 2.62                     | 0.55              |
| 1:A:35:GLU:HG2   | 1:A:57:THR:HG22  | 1.89                     | 0.55              |
| 1:B:181:GLU:C    | 1:B:183:CYS:H    | 2.14                     | 0.55              |
| 1:B:352:PHE:CZ   | 1:B:387:PRO:HD3  | 2.41                     | 0.55              |
| 1:B:453:TRP:CD1  | 1:B:453:TRP:H    | 2.24                     | 0.55              |
| 1:A:331:ASN:CB   | 4:A:1328:NAG:HN2 | 2.13                     | 0.55              |
| 2:D:45:ARG:HG3   | 2:D:45:ARG:HH11  | 1.71                     | 0.55              |
| 1:A:175:CYS:HA   | 1:A:183:CYS:HA   | 1.88                     | 0.55              |
| 1:A:429:LEU:HD21 | 1:A:432:ILE:HD11 | 1.88                     | 0.55              |
| 1:A:487:SER:HB2  | 1:A:488:PRO:CD   | 2.36                     | 0.55              |
| 1:A:487:SER:HB2  | 1:A:488:PRO:HD2  | 1.88                     | 0.55              |
| 1:B:459:THR:N    | 1:B:462:GLN:HE21 | 2.04                     | 0.55              |
| 1:A:417:VAL:HG11 | 2:C:47:LEU:CD2   | 2.37                     | 0.55              |
| 1:A:444:ASN:HA   | 1:A:470:ARG:CD   | 2.37                     | 0.55              |
| 1:B:386:TRP:HB3  | 1:B:419:LEU:HD12 | 1.89                     | 0.55              |
| 1:B:416:VAL:CG2  | 1:B:439:ILE:HG23 | 2.31                     | 0.55              |
| 1:A:111:LEU:CG   | 1:A:113:MET:HE2  | 2.36                     | 0.54              |
| 1:A:186:LEU:HD12 | 1:A:186:LEU:N    | 2.15                     | 0.54              |
| 1:B:196:SER:HB3  | 1:B:210:ASN:CB   | 2.35                     | 0.54              |
| 1:A:350:VAL:CG2  | 1:A:355:ASP:HB2  | 2.37                     | 0.54              |
| 1:B:29:ARG:NH1   | 2:D:49:TRP:NE1   | 2.54                     | 0.54              |
| 1:B:442:ASN:HB3  | 1:B:445:LEU:HB2  | 1.89                     | 0.54              |
| 1:B:297:ASP:C    | 1:B:299:VAL:H    | 2.15                     | 0.54              |
| 1:B:319:GLY:C    | 1:B:321:PHE:H    | 2.14                     | 0.54              |
| 1:B:442:ASN:HD22 | 1:B:469:ASN:ND2  | 2.05                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:36:VAL:HG22  | 1:A:60:GLU:CG    | 2.37                     | 0.54              |
| 1:A:329:ALA:O    | 1:A:330:THR:C    | 2.51                     | 0.54              |
| 1:A:76:PRO:O     | 1:A:78:GLU:HG2   | 2.07                     | 0.54              |
| 1:B:140:TRP:O    | 1:B:143:ILE:N    | 2.41                     | 0.54              |
| 1:B:247:ASN:C    | 1:B:247:ASN:HD22 | 2.14                     | 0.54              |
| 1:B:451:ILE:O    | 1:B:452:ASN:C    | 2.50                     | 0.54              |
| 1:A:280:HIS:CG   | 1:B:253:MET:HE1  | 2.42                     | 0.54              |
| 1:A:300:ARG:NH2  | 1:A:403:ARG:NH2  | 2.55                     | 0.54              |
| 1:B:114:ARG:HA   | 1:B:176:TRP:CD1  | 2.43                     | 0.54              |
| 1:A:371:LEU:HB2  | 1:A:395:ALA:HB1  | 1.89                     | 0.54              |
| 1:A:446:CYS:O    | 1:A:447:TYR:HD1  | 1.91                     | 0.54              |
| 2:D:9:SER:C      | 2:D:11:ASP:H     | 2.15                     | 0.54              |
| 1:A:251:TYR:O    | 1:A:252:GLN:NE2  | 2.41                     | 0.54              |
| 1:A:454:LYS:O    | 1:A:454:LYS:HD3  | 2.07                     | 0.54              |
| 1:B:432:ILE:O    | 1:B:457:PHE:HB2  | 2.08                     | 0.54              |
| 1:B:464:THR:HG23 | 1:B:464:THR:O    | 2.08                     | 0.54              |
| 1:B:95:LEU:HB3   | 1:B:124:VAL:HG13 | 1.90                     | 0.54              |
| 1:B:138:ILE:HD11 | 1:B:175:CYS:C    | 2.33                     | 0.53              |
| 1:B:295:GLU:HB2  | 1:B:299:VAL:O    | 2.07                     | 0.53              |
| 2:D:7:PRO:C      | 2:D:9:SER:N      | 2.63                     | 0.53              |
| 1:B:74:ARG:HH12  | 1:B:112:PRO:HG2  | 1.74                     | 0.53              |
| 1:B:124:VAL:HB   | 1:B:154:MET:CE   | 2.37                     | 0.53              |
| 2:D:8:LEU:HA     | 2:D:11:ASP:OD2   | 2.08                     | 0.53              |
| 2:D:9:SER:O      | 2:D:11:ASP:N     | 2.41                     | 0.53              |
| 1:A:423:SER:HA   | 1:A:445:LEU:HD13 | 1.91                     | 0.53              |
| 1:B:480:GLN:O    | 1:B:481:VAL:O    | 2.26                     | 0.53              |
| 1:A:181:GLU:C    | 1:A:183:CYS:H    | 2.17                     | 0.53              |
| 1:B:417:VAL:O    | 1:B:419:LEU:HD22 | 2.08                     | 0.53              |
| 1:A:473:ASN:N    | 1:A:473:ASN:HD22 | 2.05                     | 0.53              |
| 1:B:507:ARG:HA   | 1:B:510:GLU:O    | 2.09                     | 0.53              |
| 1:A:280:HIS:CD2  | 1:B:253:MET:HE1  | 2.43                     | 0.53              |
| 1:A:394:HIS:O    | 1:A:397:GLU:HG3  | 2.08                     | 0.53              |
| 1:B:15:THR:HG23  | 2:D:31:CYS:O     | 2.09                     | 0.53              |
| 1:B:242:PRO:O    | 1:B:257:PRO:HD2  | 2.08                     | 0.53              |
| 1:A:92:SER:O     | 1:A:123:ALA:HB3  | 2.08                     | 0.53              |
| 1:B:329:ALA:HB2  | 1:B:363:LEU:HA   | 1.90                     | 0.53              |
| 1:B:352:PHE:CE1  | 1:B:387:PRO:HD3  | 2.44                     | 0.53              |
| 1:B:385:ALA:O    | 1:B:386:TRP:HB2  | 2.09                     | 0.53              |
| 1:A:125:ARG:HG2  | 1:A:125:ARG:NH1  | 2.21                     | 0.52              |
| 1:B:47:GLN:NE2   | 1:B:71:THR:OG1   | 2.42                     | 0.52              |
| 1:B:352:PHE:CE2  | 1:B:363:LEU:HD23 | 2.44                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:110:GLU:OE1  | 1:A:110:GLU:HA   | 2.08                     | 0.52              |
| 1:A:142:ASP:CG   | 1:A:188:LYS:HB3  | 2.34                     | 0.52              |
| 1:A:104:ASN:O    | 1:A:105:LYS:HB2  | 2.08                     | 0.52              |
| 1:B:446:CYS:C    | 1:B:447:TYR:CD1  | 2.87                     | 0.52              |
| 1:B:453:TRP:O    | 1:B:455:LYS:N    | 2.43                     | 0.52              |
| 1:A:508:GLY:C    | 1:A:510:GLU:H    | 2.17                     | 0.52              |
| 1:B:26:SER:O     | 1:B:28:GLN:N     | 2.43                     | 0.52              |
| 1:B:140:TRP:C    | 1:B:142:ASP:H    | 2.18                     | 0.52              |
| 1:B:432:ILE:O    | 1:B:457:PHE:CB   | 2.58                     | 0.52              |
| 1:B:232:ASP:OD2  | 1:B:237:LYS:HD2  | 2.08                     | 0.52              |
| 1:A:45:TYR:CE2   | 1:A:69:LEU:HD12  | 2.45                     | 0.52              |
| 1:B:12:ASN:C     | 1:B:12:ASN:HD22  | 2.17                     | 0.52              |
| 1:B:114:ARG:HH11 | 1:B:182:ASN:ND2  | 2.08                     | 0.52              |
| 1:B:358:THR:HG21 | 4:B:1328:NAG:O6  | 2.09                     | 0.52              |
| 1:B:510:GLU:CD   | 1:B:512:VAL:HG13 | 2.35                     | 0.52              |
| 1:B:190:ILE:O    | 1:B:199:CYS:SG   | 2.68                     | 0.52              |
| 1:A:352:PHE:CE2  | 1:A:387:PRO:HG3  | 2.45                     | 0.52              |
| 1:B:186:LEU:HG   | 1:B:190:ILE:HG13 | 1.92                     | 0.52              |
| 1:B:311:LYS:HD2  | 1:B:311:LYS:O    | 2.10                     | 0.52              |
| 1:B:491:CYS:HA   | 1:B:500:VAL:HG23 | 1.92                     | 0.52              |
| 1:A:89:TYR:O     | 1:A:91:ASN:N     | 2.44                     | 0.51              |
| 1:A:397:GLU:C    | 1:A:398:ASN:HD22 | 2.18                     | 0.51              |
| 1:B:30:MET:HG2   | 1:B:31:PHE:CE1   | 2.44                     | 0.51              |
| 1:B:215:GLY:N    | 1:B:225:LEU:HD22 | 2.25                     | 0.51              |
| 1:B:443:LYS:O    | 1:B:470:ARG:HA   | 2.10                     | 0.51              |
| 1:B:504:ASN:C    | 1:B:506:SER:H    | 2.19                     | 0.51              |
| 1:A:101:TYR:HB3  | 1:A:130:PRO:HD2  | 1.91                     | 0.51              |
| 1:A:409:HIS:CE1  | 2:C:38:ILE:HD11  | 2.45                     | 0.51              |
| 1:B:45:TYR:CE2   | 1:B:69:LEU:HD23  | 2.43                     | 0.51              |
| 1:B:293:GLU:HA   | 1:B:302:CYS:CB   | 2.40                     | 0.51              |
| 2:C:19:VAL:HG22  | 2:C:32:ASN:HB3   | 1.91                     | 0.51              |
| 1:A:489:GLU:O    | 1:A:490:GLY:O    | 2.29                     | 0.51              |
| 1:B:91:ASN:O     | 1:B:92:SER:OG    | 2.20                     | 0.51              |
| 1:A:311:LYS:HD3  | 1:A:311:LYS:N    | 2.25                     | 0.51              |
| 1:A:371:LEU:C    | 1:A:373:THR:N    | 2.67                     | 0.51              |
| 1:B:186:LEU:H    | 1:B:186:LEU:HD23 | 1.76                     | 0.51              |
| 2:C:50:TRP:CD1   | 2:C:50:TRP:H     | 2.28                     | 0.51              |
| 1:B:4:LYS:HE3    | 1:B:231:ARG:HH12 | 1.74                     | 0.51              |
| 1:A:472:GLU:C    | 1:A:474:SER:N    | 2.68                     | 0.51              |
| 1:B:324:SER:HA   | 4:B:1328:NAG:H5  | 1.92                     | 0.51              |
| 1:B:508:GLY:O    | 1:B:509:ARG:HB2  | 2.10                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:333:LYS:HE3  | 1:B:334:HIS:HE1  | 1.74                     | 0.51              |
| 1:B:508:GLY:O    | 1:B:509:ARG:HD2  | 2.11                     | 0.51              |
| 1:B:75:ILE:HG22  | 1:B:77:LEU:HG    | 1.91                     | 0.51              |
| 1:B:202:LYS:HD3  | 1:B:202:LYS:C    | 2.35                     | 0.51              |
| 1:A:201:GLY:O    | 1:A:203:SER:N    | 2.44                     | 0.51              |
| 1:B:232:ASP:HB2  | 1:B:237:LYS:HD2  | 1.92                     | 0.51              |
| 2:C:9:SER:C      | 2:C:11:ASP:H     | 2.18                     | 0.51              |
| 1:A:213:ALA:O    | 1:A:214:ALA:HB3  | 2.10                     | 0.50              |
| 1:B:138:ILE:HG23 | 1:B:184:GLN:OE1  | 2.11                     | 0.50              |
| 1:A:130:PRO:O    | 1:A:131:ALA:HB3  | 2.10                     | 0.50              |
| 1:A:497:ARG:HG3  | 1:A:498:ASP:OD2  | 2.11                     | 0.50              |
| 1:B:220:ARG:HG3  | 1:B:221:GLU:H    | 1.76                     | 0.50              |
| 1:B:453:TRP:C    | 1:B:455:LYS:N    | 2.68                     | 0.50              |
| 1:B:4:LYS:HG3    | 1:B:36:VAL:HG21  | 1.93                     | 0.50              |
| 1:B:41:LEU:HD23  | 1:B:65:VAL:CG2   | 2.40                     | 0.50              |
| 1:B:417:VAL:HA   | 1:B:440:SER:O    | 2.10                     | 0.50              |
| 2:D:6:CYS:SG     | 2:D:29:TYR:HD2   | 2.35                     | 0.50              |
| 1:A:333:LYS:HG2  | 5:A:2441:HOH:O   | 2.10                     | 0.50              |
| 1:A:408:GLN:C    | 1:A:410:GLY:H    | 2.19                     | 0.50              |
| 1:A:76:PRO:C     | 1:A:78:GLU:N     | 2.69                     | 0.50              |
| 1:B:28:GLN:HA    | 1:B:54:PHE:CZ    | 2.46                     | 0.50              |
| 1:B:485:LEU:HD12 | 1:B:485:LEU:N    | 2.16                     | 0.50              |
| 2:C:24:GLU:N     | 2:C:24:GLU:CD    | 2.70                     | 0.50              |
| 1:A:65:VAL:HB    | 1:A:95:LEU:HD13  | 1.92                     | 0.50              |
| 1:A:187:THR:HB   | 1:A:199:CYS:O    | 2.11                     | 0.50              |
| 1:A:403:ARG:CG   | 1:A:403:ARG:NH1  | 2.73                     | 0.50              |
| 1:B:28:GLN:O     | 1:B:32:ASN:HB2   | 2.12                     | 0.50              |
| 1:A:451:ILE:HG22 | 1:A:451:ILE:O    | 2.11                     | 0.50              |
| 1:B:311:LYS:HD2  | 1:B:311:LYS:C    | 2.36                     | 0.50              |
| 1:A:109:LYS:NZ   | 1:A:163:CYS:HB3  | 2.26                     | 0.50              |
| 1:A:114:ARG:CD   | 1:A:114:ARG:H    | 2.25                     | 0.50              |
| 1:A:394:HIS:HA   | 1:A:397:GLU:HG3  | 1.93                     | 0.50              |
| 1:A:426:LEU:C    | 1:A:428:SER:H    | 2.20                     | 0.50              |
| 1:B:241:PRO:CB   | 1:B:259:GLY:HA2  | 2.41                     | 0.50              |
| 2:C:45:ARG:HG2   | 2:C:45:ARG:HH11  | 1.77                     | 0.50              |
| 3:E:1:NAG:H4     | 3:E:2:NAG:HN2    | 1.77                     | 0.50              |
| 1:A:192:ALA:O    | 1:A:193:GLN:C    | 2.55                     | 0.50              |
| 1:A:220:ARG:HH11 | 1:A:220:ARG:HG3  | 1.77                     | 0.50              |
| 1:A:326:SER:OG   | 1:A:351:ALA:HB2  | 2.12                     | 0.50              |
| 1:B:417:VAL:HG12 | 1:B:440:SER:H    | 1.77                     | 0.50              |
| 1:B:459:THR:CB   | 1:B:462:GLN:HE21 | 2.23                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:494:PRO:HG2  | 1:B:495:GLU:H    | 1.77                     | 0.50              |
| 2:D:22:TYR:OH    | 2:D:27:ASP:HA    | 2.11                     | 0.50              |
| 1:B:111:LEU:HG   | 1:B:113:MET:HG3  | 1.94                     | 0.49              |
| 2:D:15:LEU:HD21  | 2:D:41:ARG:HH21  | 1.76                     | 0.49              |
| 2:C:49:TRP:HA    | 2:C:49:TRP:CE3   | 2.47                     | 0.49              |
| 1:A:485:LEU:HB2  | 5:A:2443:HOH:O   | 2.12                     | 0.49              |
| 1:B:399:LEU:HD21 | 1:B:402:ILE:HD11 | 1.95                     | 0.49              |
| 1:A:134:ASN:HB3  | 1:A:175:CYS:O    | 2.12                     | 0.49              |
| 1:A:481:VAL:HG12 | 1:A:483:HIS:H    | 1.78                     | 0.49              |
| 1:B:129:ASN:C    | 1:B:157:GLN:HE22 | 2.20                     | 0.49              |
| 1:B:92:SER:O     | 1:B:123:ALA:HB3  | 2.13                     | 0.49              |
| 1:B:134:ASN:O    | 1:B:136:GLU:N    | 2.45                     | 0.49              |
| 1:B:333:LYS:C    | 1:B:335:PHE:H    | 2.19                     | 0.49              |
| 1:B:485:LEU:H    | 1:B:485:LEU:CD1  | 2.05                     | 0.49              |
| 1:A:153:SER:O    | 1:A:154:MET:HB3  | 2.12                     | 0.49              |
| 1:A:327:ILE:HA   | 4:A:1328:NAG:H81 | 1.95                     | 0.49              |
| 1:B:256:ASN:HB2  | 1:B:259:GLY:HA3  | 1.94                     | 0.49              |
| 1:B:325:LEU:O    | 1:B:348:LEU:HD12 | 2.12                     | 0.49              |
| 1:B:339:THR:HA   | 1:B:374:VAL:HA   | 1.95                     | 0.49              |
| 1:B:350:VAL:CG2  | 1:B:355:ASP:HB2  | 2.42                     | 0.49              |
| 1:A:189:ILE:C    | 1:A:191:CYS:N    | 2.70                     | 0.49              |
| 1:A:504:ASN:O    | 1:A:505:VAL:C    | 2.55                     | 0.49              |
| 1:B:149:LEU:HD12 | 1:B:150:SER:H    | 1.77                     | 0.49              |
| 1:A:73:GLU:HA    | 1:A:107:GLY:O    | 2.13                     | 0.49              |
| 1:B:46:VAL:HG23  | 1:B:70:ASN:OD1   | 2.12                     | 0.49              |
| 1:A:203:SER:N    | 1:A:204:PRO:CD   | 2.76                     | 0.49              |
| 1:A:485:LEU:HD23 | 1:A:485:LEU:N    | 2.25                     | 0.49              |
| 1:A:13:LYS:HB3   | 1:A:42:GLU:OE2   | 2.12                     | 0.49              |
| 1:A:16:GLN:HE22  | 1:A:20:PHE:HE2   | 1.61                     | 0.49              |
| 1:B:243:LEU:O    | 1:B:256:ASN:N    | 2.45                     | 0.49              |
| 2:D:6:CYS:HB3    | 2:D:10:HIS:HB2   | 1.95                     | 0.49              |
| 1:A:71:THR:O     | 1:A:72:VAL:C     | 2.56                     | 0.48              |
| 1:A:300:ARG:HH21 | 1:A:403:ARG:HH21 | 1.59                     | 0.48              |
| 1:B:84:ARG:HH11  | 1:B:84:ARG:CG    | 2.26                     | 0.48              |
| 1:B:444:ASN:HD22 | 1:B:444:ASN:N    | 2.09                     | 0.48              |
| 2:D:7:PRO:HB2    | 2:D:9:SER:HB3    | 1.95                     | 0.48              |
| 1:A:296:GLU:O    | 1:A:298:GLY:N    | 2.42                     | 0.48              |
| 1:A:453:TRP:C    | 1:A:455:LYS:N    | 2.70                     | 0.48              |
| 1:B:20:PHE:HD1   | 1:B:20:PHE:H     | 1.61                     | 0.48              |
| 2:D:6:CYS:SG     | 2:D:29:TYR:CD2   | 3.06                     | 0.48              |
| 1:A:253:MET:HE1  | 1:B:282:SER:CB   | 2.43                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:102:ASP:O    | 1:B:105:LYS:N    | 2.45                     | 0.48              |
| 1:B:368:LEU:O    | 1:B:395:ALA:CB   | 2.61                     | 0.48              |
| 1:B:453:TRP:CD1  | 1:B:453:TRP:N    | 2.81                     | 0.48              |
| 1:B:67:ILE:O     | 1:B:97:VAL:HA    | 2.13                     | 0.48              |
| 1:B:293:GLU:HA   | 1:B:302:CYS:HB3  | 1.96                     | 0.48              |
| 1:B:485:LEU:CD2  | 1:B:496:PRO:HG3  | 2.42                     | 0.48              |
| 1:B:199:CYS:SG   | 1:B:201:GLY:O    | 2.72                     | 0.48              |
| 1:B:203:SER:HB3  | 1:B:206:ASP:CG   | 2.39                     | 0.48              |
| 1:B:328:ASN:N    | 4:B:1328:NAG:C8  | 2.65                     | 0.48              |
| 1:B:371:LEU:O    | 1:B:395:ALA:O    | 2.31                     | 0.48              |
| 2:C:46:ASP:CG    | 2:C:49:TRP:CD1   | 2.92                     | 0.48              |
| 2:D:48:LYS:O     | 2:D:49:TRP:CG    | 2.66                     | 0.48              |
| 1:A:151:ASN:OD1  | 1:A:151:ASN:O    | 2.31                     | 0.48              |
| 1:A:394:HIS:O    | 1:A:396:PHE:N    | 2.47                     | 0.48              |
| 1:B:69:LEU:CD1   | 1:B:69:LEU:N     | 2.77                     | 0.48              |
| 1:B:180:GLU:O    | 1:B:181:GLU:C    | 2.56                     | 0.48              |
| 2:D:49:TRP:CB    | 5:D:57:HOH:O     | 2.62                     | 0.48              |
| 1:A:28:GLN:HA    | 1:A:54:PHE:CZ    | 2.49                     | 0.48              |
| 1:B:380:PHE:CB   | 1:B:413:SER:HA   | 2.44                     | 0.48              |
| 1:B:439:ILE:O    | 1:B:466:ILE:HA   | 2.14                     | 0.48              |
| 1:B:467:ILE:HG22 | 1:B:468:SER:N    | 2.28                     | 0.48              |
| 1:B:510:GLU:HG3  | 1:B:512:VAL:HG22 | 1.95                     | 0.48              |
| 1:A:3:GLU:OE1    | 1:A:3:GLU:HA     | 2.13                     | 0.48              |
| 1:A:67:ILE:O     | 1:A:67:ILE:HG22  | 2.14                     | 0.48              |
| 1:B:209:HIS:ND1  | 1:B:211:GLN:HB2  | 2.28                     | 0.48              |
| 1:B:390:ARG:HH11 | 1:B:390:ARG:CB   | 2.17                     | 0.48              |
| 1:B:447:TYR:CE2  | 1:B:480:GLN:O    | 2.66                     | 0.48              |
| 1:B:453:TRP:HA   | 1:B:456:LEU:HD23 | 1.96                     | 0.48              |
| 1:A:19:THR:O     | 1:A:20:PHE:C     | 2.57                     | 0.48              |
| 1:A:62:ALA:HA    | 1:A:84:ARG:HB2   | 1.96                     | 0.48              |
| 1:A:72:VAL:HG22  | 1:A:73:GLU:N     | 2.28                     | 0.48              |
| 1:A:508:GLY:C    | 1:A:510:GLU:N    | 2.71                     | 0.48              |
| 2:C:15:LEU:HD23  | 2:C:15:LEU:N     | 2.28                     | 0.48              |
| 1:A:242:PRO:O    | 1:A:256:ASN:HB3  | 2.14                     | 0.47              |
| 1:B:346:HIS:HE2  | 1:B:380:PHE:HZ   | 1.61                     | 0.47              |
| 1:A:478:THR:C    | 1:A:480:GLN:H    | 2.21                     | 0.47              |
| 1:B:38:LEU:O     | 1:B:62:ALA:HB3   | 2.14                     | 0.47              |
| 1:A:47:GLN:HB2   | 1:A:50:TYR:CD1   | 2.48                     | 0.47              |
| 1:B:69:LEU:HD11  | 2:D:26:LEU:CD1   | 2.43                     | 0.47              |
| 1:B:453:TRP:O    | 1:B:456:LEU:N    | 2.47                     | 0.47              |
| 2:C:46:ASP:CG    | 2:C:49:TRP:HD1   | 2.23                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:62:ALA:O     | 1:A:85:GLY:N     | 2.47                     | 0.47              |
| 1:A:473:ASN:N    | 1:A:473:ASN:ND2  | 2.62                     | 0.47              |
| 1:B:394:HIS:ND1  | 1:B:395:ALA:N    | 2.62                     | 0.47              |
| 1:B:78:GLU:O     | 1:B:115:ASN:HB2  | 2.14                     | 0.47              |
| 1:B:324:SER:HB3  | 4:B:1328:NAG:H3  | 1.96                     | 0.47              |
| 1:B:386:TRP:CZ2  | 1:B:393:LEU:HA   | 2.49                     | 0.47              |
| 1:A:138:ILE:HA   | 1:A:184:GLN:NE2  | 2.30                     | 0.47              |
| 1:A:243:LEU:N    | 1:A:243:LEU:CD1  | 2.77                     | 0.47              |
| 1:A:403:ARG:O    | 1:A:433:SER:HB2  | 2.14                     | 0.47              |
| 1:B:296:GLU:C    | 1:B:298:GLY:N    | 2.73                     | 0.47              |
| 1:A:56:LYS:HG2   | 1:A:76:PRO:HB3   | 1.97                     | 0.47              |
| 1:A:140:TRP:C    | 1:A:142:ASP:N    | 2.70                     | 0.47              |
| 1:A:199:CYS:HA   | 1:A:208:CYS:H    | 1.79                     | 0.47              |
| 1:A:483:HIS:O    | 1:A:484:ALA:HB2  | 2.14                     | 0.47              |
| 1:B:26:SER:C     | 1:B:28:GLN:N     | 2.72                     | 0.47              |
| 1:B:58:ILE:HG22  | 1:B:80:LEU:HD13  | 1.97                     | 0.47              |
| 1:B:64:TYR:HB2   | 1:B:94:ALA:O     | 2.14                     | 0.47              |
| 1:B:296:GLU:O    | 1:B:298:GLY:N    | 2.45                     | 0.47              |
| 1:B:330:THR:HG22 | 1:B:331:ASN:ND2  | 2.30                     | 0.47              |
| 1:A:420:ASN:OD1  | 3:E:1:NAG:H2     | 2.15                     | 0.47              |
| 1:A:425:GLY:C    | 1:A:427:ARG:H    | 2.23                     | 0.47              |
| 1:B:87:MET:C     | 1:B:88:TYR:HD1   | 2.22                     | 0.47              |
| 1:A:114:ARG:HG3  | 1:A:182:ASN:OD1  | 2.15                     | 0.47              |
| 1:A:432:ILE:HG22 | 1:A:432:ILE:O    | 2.15                     | 0.47              |
| 1:A:450:THR:O    | 1:A:490:GLY:CA   | 2.61                     | 0.47              |
| 1:B:303:LYS:CD   | 1:B:304:LYS:H    | 2.28                     | 0.47              |
| 1:B:412:PHE:HA   | 1:B:436:ASP:O    | 2.14                     | 0.47              |
| 1:B:416:VAL:O    | 1:B:439:ILE:HA   | 2.15                     | 0.47              |
| 1:A:45:TYR:HE2   | 1:A:69:LEU:HD12  | 1.79                     | 0.47              |
| 1:B:134:ASN:C    | 1:B:136:GLU:N    | 2.71                     | 0.47              |
| 1:B:443:LYS:HG3  | 1:B:444:ASN:N    | 2.29                     | 0.47              |
| 1:A:252:GLN:HE21 | 1:A:252:GLN:CA   | 2.28                     | 0.46              |
| 1:A:347:ILE:HD11 | 1:A:396:PHE:HZ   | 1.80                     | 0.46              |
| 1:A:422:THR:HA   | 1:A:444:ASN:O    | 2.14                     | 0.46              |
| 1:A:451:ILE:O    | 1:A:451:ILE:CG2  | 2.62                     | 0.46              |
| 1:A:102:ASP:C    | 1:A:104:ASN:N    | 2.71                     | 0.46              |
| 1:B:124:VAL:HB   | 1:B:154:MET:HE1  | 1.96                     | 0.46              |
| 1:B:315:GLY:O    | 1:B:318:ILE:HG22 | 2.15                     | 0.46              |
| 1:B:432:ILE:N    | 1:B:456:LEU:O    | 2.48                     | 0.46              |
| 2:D:22:TYR:CE2   | 2:D:24:GLU:HA    | 2.50                     | 0.46              |
| 1:A:174:SER:HB3  | 1:A:184:GLN:NE2  | 2.30                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:482:CYS:O    | 1:A:485:LEU:HD23 | 2.15                     | 0.46              |
| 1:B:310:ARG:HG2  | 1:B:310:ARG:HH11 | 1.80                     | 0.46              |
| 4:B:1032:NAG:H83 | 4:B:1032:NAG:O3  | 2.16                     | 0.46              |
| 2:D:38:ILE:HG12  | 2:D:39:GLY:N     | 2.31                     | 0.46              |
| 1:A:82:ILE:HA    | 1:A:118:GLU:O    | 2.15                     | 0.46              |
| 1:A:87:MET:O     | 1:A:88:TYR:HD2   | 1.98                     | 0.46              |
| 1:A:213:ALA:HB3  | 1:A:226:VAL:HG23 | 1.97                     | 0.46              |
| 1:B:7:CYS:HB2    | 1:B:30:MET:CE    | 2.34                     | 0.46              |
| 1:A:113:MET:HE3  | 1:A:176:TRP:CZ3  | 2.49                     | 0.46              |
| 1:A:65:VAL:HB    | 1:A:95:LEU:CD1   | 2.46                     | 0.46              |
| 1:A:138:ILE:HD11 | 1:A:175:CYS:C    | 2.40                     | 0.46              |
| 1:A:350:VAL:HG21 | 1:A:355:ASP:HB2  | 1.96                     | 0.46              |
| 1:A:389:ASN:O    | 1:A:390:ARG:HD3  | 2.15                     | 0.46              |
| 1:A:466:ILE:O    | 1:A:466:ILE:CD1  | 2.61                     | 0.46              |
| 1:B:189:ILE:HG13 | 1:B:190:ILE:HG12 | 1.97                     | 0.46              |
| 1:B:213:ALA:O    | 1:B:214:ALA:HB3  | 2.15                     | 0.46              |
| 1:B:215:GLY:C    | 1:B:225:LEU:HD22 | 2.40                     | 0.46              |
| 1:B:303:LYS:HE2  | 1:B:303:LYS:CA   | 2.40                     | 0.46              |
| 1:B:324:SER:CB   | 4:B:1328:NAG:H3  | 2.46                     | 0.46              |
| 2:C:13:TYR:CE2   | 2:C:41:ARG:HG2   | 2.51                     | 0.46              |
| 1:B:464:THR:HG22 | 5:B:1346:HOH:O   | 2.15                     | 0.46              |
| 1:A:12:ASN:O     | 1:A:15:THR:HB    | 2.16                     | 0.46              |
| 1:A:125:ARG:HA   | 1:A:153:SER:O    | 2.16                     | 0.46              |
| 1:A:174:SER:HB3  | 1:A:184:GLN:CB   | 2.27                     | 0.46              |
| 1:B:209:HIS:C    | 1:B:211:GLN:H    | 2.24                     | 0.46              |
| 1:B:328:ASN:H    | 4:B:1328:NAG:H83 | 1.72                     | 0.46              |
| 2:D:7:PRO:HD3    | 2:D:29:TYR:CZ    | 2.51                     | 0.46              |
| 1:A:201:GLY:C    | 1:A:203:SER:N    | 2.66                     | 0.46              |
| 1:A:478:THR:CB   | 1:A:480:GLN:HG3  | 2.44                     | 0.46              |
| 1:B:346:HIS:HD2  | 1:B:382:LEU:HB3  | 1.80                     | 0.46              |
| 1:B:363:LEU:O    | 1:B:365:PRO:HD3  | 2.16                     | 0.46              |
| 1:A:379:GLY:CA   | 1:A:406:THR:HG23 | 2.45                     | 0.46              |
| 1:B:12:ASN:OD1   | 2:D:38:ILE:HG13  | 2.16                     | 0.46              |
| 1:B:104:ASN:O    | 1:B:106:THR:HG23 | 2.16                     | 0.46              |
| 1:B:213:ALA:HB3  | 1:B:226:VAL:HG23 | 1.98                     | 0.46              |
| 1:B:319:GLY:C    | 1:B:321:PHE:N    | 2.72                     | 0.46              |
| 1:A:171:PRO:C    | 1:A:173:GLY:H    | 2.23                     | 0.45              |
| 1:B:82:ILE:HG12  | 1:B:83:ILE:N     | 2.29                     | 0.45              |
| 2:C:50:TRP:CD1   | 2:C:50:TRP:N     | 2.84                     | 0.45              |
| 1:A:148:PHE:C    | 1:A:150:SER:N    | 2.61                     | 0.45              |
| 1:A:324:SER:HB3  | 4:A:1328:NAG:H5  | 1.98                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:247:ASN:C    | 1:B:247:ASN:ND2  | 2.74                     | 0.45              |
| 1:B:318:ILE:CD1  | 1:B:319:GLY:H    | 2.27                     | 0.45              |
| 1:A:28:GLN:O     | 1:A:32:ASN:HB2   | 2.17                     | 0.45              |
| 1:A:285:ARG:NH2  | 1:B:251:TYR:CE2  | 2.84                     | 0.45              |
| 1:A:310:ARG:HD2  | 1:A:310:ARG:H    | 1.82                     | 0.45              |
| 1:B:69:LEU:N     | 1:B:69:LEU:HD12  | 2.32                     | 0.45              |
| 1:B:339:THR:HA   | 1:B:373:THR:O    | 2.17                     | 0.45              |
| 1:A:89:TYR:O     | 1:A:90:GLU:C     | 2.59                     | 0.45              |
| 1:A:391:THR:HB   | 1:A:422:THR:H    | 1.82                     | 0.45              |
| 1:A:478:THR:C    | 1:A:480:GLN:N    | 2.74                     | 0.45              |
| 1:B:149:LEU:HD12 | 1:B:150:SER:N    | 2.31                     | 0.45              |
| 1:B:285:ARG:HD3  | 1:B:405:ARG:HB3  | 1.97                     | 0.45              |
| 1:B:295:GLU:CB   | 1:B:300:ARG:HD2  | 2.36                     | 0.45              |
| 1:A:431:GLU:HA   | 1:A:456:LEU:O    | 2.16                     | 0.45              |
| 1:B:129:ASN:C    | 1:B:157:GLN:NE2  | 2.75                     | 0.45              |
| 1:B:272:PRO:O    | 1:B:274:ASN:N    | 2.49                     | 0.45              |
| 1:B:453:TRP:C    | 1:B:455:LYS:H    | 2.25                     | 0.45              |
| 1:A:195:CYS:O    | 1:A:196:SER:C    | 2.59                     | 0.45              |
| 1:A:443:LYS:O    | 1:A:470:ARG:HA   | 2.17                     | 0.45              |
| 1:B:124:VAL:HB   | 1:B:152:MET:CE   | 2.47                     | 0.45              |
| 1:A:10:THR:O     | 1:A:40:ASN:HB2   | 2.17                     | 0.45              |
| 1:A:451:ILE:O    | 1:A:452:ASN:C    | 2.60                     | 0.45              |
| 1:A:497:ARG:HB3  | 1:A:510:GLU:HB3  | 1.99                     | 0.45              |
| 1:B:40:ASN:ND2   | 1:B:63:GLY:HA3   | 2.32                     | 0.45              |
| 1:B:55:LEU:HB3   | 1:B:77:LEU:CD2   | 2.47                     | 0.45              |
| 1:B:494:PRO:HG2  | 1:B:495:GLU:N    | 2.32                     | 0.45              |
| 1:B:117:GLN:HA   | 1:B:143:ILE:HD12 | 1.99                     | 0.45              |
| 1:B:446:CYS:SG   | 1:B:470:ARG:HG2  | 2.57                     | 0.45              |
| 1:B:473:ASN:O    | 1:B:476:LYS:HD3  | 2.17                     | 0.45              |
| 1:A:85:GLY:C     | 1:A:87:MET:H     | 2.23                     | 0.45              |
| 1:A:394:HIS:C    | 1:A:396:PHE:N    | 2.74                     | 0.45              |
| 1:B:333:LYS:HE3  | 1:B:334:HIS:CE1  | 2.51                     | 0.45              |
| 1:A:379:GLY:HA2  | 1:A:406:THR:HG23 | 1.98                     | 0.45              |
| 1:A:432:ILE:O    | 1:A:457:PHE:HB2  | 2.17                     | 0.45              |
| 1:A:451:ILE:HB   | 1:A:453:TRP:CE2  | 2.52                     | 0.44              |
| 1:B:29:ARG:NH1   | 2:D:49:TRP:HE1   | 2.14                     | 0.44              |
| 1:B:327:ILE:CA   | 4:B:1328:NAG:H83 | 2.36                     | 0.44              |
| 1:B:376:GLU:HB2  | 1:B:401:ILE:CG2  | 2.48                     | 0.44              |
| 1:B:149:LEU:O    | 1:B:152:MET:HG2  | 2.17                     | 0.44              |
| 1:B:192:ALA:O    | 1:B:193:GLN:C    | 2.60                     | 0.44              |
| 1:B:454:LYS:HD3  | 1:B:454:LYS:N    | 2.31                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:9:SER:C      | 2:C:11:ASP:N     | 2.76                     | 0.44              |
| 1:B:140:TRP:O    | 1:B:141:ARG:C    | 2.58                     | 0.44              |
| 1:B:324:SER:OG   | 4:B:1328:NAG:H3  | 2.18                     | 0.44              |
| 1:B:352:PHE:HE1  | 1:B:386:TRP:HA   | 1.83                     | 0.44              |
| 1:A:12:ASN:HB3   | 2:C:39:GLY:HA2   | 1.99                     | 0.44              |
| 1:A:135:VAL:C    | 1:A:137:SER:H    | 2.26                     | 0.44              |
| 1:A:381:LEU:HD11 | 1:A:383:ILE:HD11 | 1.98                     | 0.44              |
| 1:A:391:THR:O    | 1:A:392:ASP:HB2  | 2.16                     | 0.44              |
| 1:A:455:LYS:HD3  | 1:A:455:LYS:C    | 2.42                     | 0.44              |
| 1:B:232:ASP:CG   | 1:B:237:LYS:HD2  | 2.42                     | 0.44              |
| 1:B:240:CYS:O    | 1:B:241:PRO:C    | 2.60                     | 0.44              |
| 1:A:36:VAL:HG22  | 1:A:60:GLU:HG3   | 1.99                     | 0.44              |
| 1:A:477:ALA:C    | 1:A:479:GLY:H    | 2.23                     | 0.44              |
| 1:B:21:GLU:HG2   | 1:B:25:LEU:HD23  | 2.00                     | 0.44              |
| 1:B:271:CYS:O    | 1:B:272:PRO:C    | 2.60                     | 0.44              |
| 1:B:331:ASN:C    | 4:B:1328:NAG:H81 | 2.42                     | 0.44              |
| 1:B:507:ARG:HB2  | 1:B:508:GLY:H    | 1.52                     | 0.44              |
| 2:C:26:LEU:O     | 2:C:27:ASP:C     | 2.59                     | 0.44              |
| 1:A:145:SER:O    | 1:A:147:ASP:N    | 2.51                     | 0.44              |
| 1:A:364:ASP:O    | 1:A:365:PRO:C    | 2.61                     | 0.44              |
| 1:B:24:PHE:O     | 1:B:25:LEU:C     | 2.60                     | 0.44              |
| 1:B:295:GLU:O    | 1:B:295:GLU:HG3  | 2.17                     | 0.44              |
| 1:B:310:ARG:HD2  | 1:B:310:ARG:N    | 2.32                     | 0.44              |
| 1:B:487:SER:HB3  | 1:B:488:PRO:HD2  | 1.99                     | 0.44              |
| 2:D:39:GLY:HA3   | 2:D:43:GLN:OE1   | 2.18                     | 0.44              |
| 1:A:126:PHE:H    | 1:A:154:MET:HB3  | 1.83                     | 0.44              |
| 1:B:98:LEU:O     | 1:B:99:SER:C     | 2.61                     | 0.44              |
| 1:B:109:LYS:NZ   | 1:B:163:CYS:HB3  | 2.32                     | 0.44              |
| 1:A:200:ARG:HD3  | 1:A:216:CYS:O    | 2.18                     | 0.44              |
| 1:B:152:MET:HE3  | 1:B:152:MET:HB2  | 1.89                     | 0.44              |
| 1:B:181:GLU:O    | 1:B:183:CYS:N    | 2.50                     | 0.44              |
| 1:B:257:PRO:CG   | 1:B:258:GLU:H    | 2.21                     | 0.44              |
| 1:B:391:THR:HB   | 1:B:422:THR:CG2  | 2.37                     | 0.44              |
| 1:B:444:ASN:ND2  | 1:B:444:ASN:N    | 2.59                     | 0.44              |
| 2:C:50:TRP:O     | 2:C:51:GLU:C     | 2.61                     | 0.44              |
| 1:A:263:PHE:HE1  | 1:A:275:TYR:CE1  | 2.36                     | 0.43              |
| 1:A:324:SER:HB3  | 4:A:1328:NAG:H3  | 2.00                     | 0.43              |
| 1:B:125:ARG:HH11 | 1:B:125:ARG:HG3  | 1.83                     | 0.43              |
| 1:B:438:ILE:O    | 1:B:438:ILE:HG23 | 2.17                     | 0.43              |
| 1:A:35:GLU:HA    | 1:A:57:THR:O     | 2.18                     | 0.43              |
| 1:A:52:LEU:O     | 1:A:76:PRO:HG2   | 2.18                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:124:VAL:N    | 1:B:152:MET:HE3  | 2.31                     | 0.43              |
| 2:C:16:HIS:HD2   | 2:C:42:CYS:O     | 2.01                     | 0.43              |
| 1:A:430:LYS:O    | 1:A:430:LYS:CG   | 2.65                     | 0.43              |
| 1:B:41:LEU:HD13  | 1:B:58:ILE:CD1   | 2.48                     | 0.43              |
| 1:B:90:GLU:O     | 1:B:91:ASN:HB2   | 2.17                     | 0.43              |
| 1:B:475:CYS:O    | 1:B:476:LYS:C    | 2.61                     | 0.43              |
| 1:A:45:TYR:HE2   | 1:A:69:LEU:CD1   | 2.31                     | 0.43              |
| 1:A:134:ASN:ND2  | 1:A:177:GLY:HA2  | 2.33                     | 0.43              |
| 1:A:408:GLN:HA   | 1:A:408:GLN:NE2  | 2.28                     | 0.43              |
| 1:B:4:LYS:HB3    | 5:B:1332:HOH:O   | 2.18                     | 0.43              |
| 1:A:209:HIS:CD2  | 1:A:221:GLU:HB2  | 2.53                     | 0.43              |
| 1:A:216:CYS:SG   | 1:A:216:CYS:O    | 2.76                     | 0.43              |
| 1:A:438:ILE:HG23 | 1:A:438:ILE:O    | 2.18                     | 0.43              |
| 1:B:78:GLU:HG2   | 1:B:112:PRO:CB   | 2.41                     | 0.43              |
| 1:A:391:THR:CB   | 1:A:422:THR:HG22 | 2.46                     | 0.43              |
| 1:B:411:GLN:OE1  | 2:D:48:LYS:HE3   | 2.19                     | 0.43              |
| 1:B:487:SER:C    | 1:B:489:GLU:H    | 2.26                     | 0.43              |
| 1:B:15:THR:CG2   | 1:B:16:GLN:N     | 2.81                     | 0.43              |
| 1:B:25:LEU:H     | 1:B:25:LEU:HD22  | 1.84                     | 0.43              |
| 1:A:37:VAL:CG2   | 1:A:61:VAL:HG22  | 2.49                     | 0.43              |
| 1:A:503:ARG:O    | 1:A:504:ASN:HB2  | 2.19                     | 0.43              |
| 1:A:246:TYR:HA   | 1:A:253:MET:SD   | 2.58                     | 0.43              |
| 1:A:470:ARG:HH11 | 1:A:470:ARG:CG   | 2.26                     | 0.43              |
| 1:B:89:TYR:C     | 1:B:91:ASN:N     | 2.76                     | 0.43              |
| 1:B:439:ILE:HG22 | 1:B:442:ASN:ND2  | 2.34                     | 0.43              |
| 2:D:43:GLN:OE1   | 2:D:43:GLN:N     | 2.45                     | 0.43              |
| 1:A:67:ILE:O     | 1:A:97:VAL:HA    | 2.19                     | 0.43              |
| 1:A:97:VAL:HG21  | 1:A:126:PHE:CE2  | 2.53                     | 0.43              |
| 1:A:314:ASN:HB3  | 1:A:318:ILE:CG2  | 2.49                     | 0.43              |
| 1:B:29:ARG:HB3   | 2:D:49:TRP:CH2   | 2.54                     | 0.43              |
| 1:B:331:ASN:O    | 4:B:1328:NAG:H81 | 2.18                     | 0.43              |
| 1:B:424:LEU:HD13 | 1:B:492:TRP:CZ3  | 2.54                     | 0.43              |
| 1:A:385:ALA:O    | 1:A:386:TRP:HB2  | 2.17                     | 0.42              |
| 1:B:21:GLU:O     | 1:B:22:ASP:C     | 2.62                     | 0.42              |
| 1:B:487:SER:HB3  | 1:B:488:PRO:CD   | 2.49                     | 0.42              |
| 1:A:241:PRO:CB   | 1:A:258:GLU:O    | 2.67                     | 0.42              |
| 1:B:102:ASP:O    | 1:B:103:ALA:C    | 2.63                     | 0.42              |
| 1:B:380:PHE:HB2  | 1:B:413:SER:HA   | 2.00                     | 0.42              |
| 1:B:438:ILE:HG21 | 2:D:47:LEU:HD22  | 2.00                     | 0.42              |
| 1:A:478:THR:HG21 | 1:A:480:GLN:HE21 | 1.84                     | 0.42              |
| 4:A:1337:NAG:O3  | 4:A:1337:NAG:C7  | 2.66                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:201:GLY:HA3  | 1:B:206:ASP:HB3  | 2.00                     | 0.42              |
| 2:C:43:GLN:OE1   | 2:C:43:GLN:N     | 2.46                     | 0.42              |
| 2:D:50:TRP:O     | 2:D:51:GLU:C     | 2.62                     | 0.42              |
| 1:A:71:THR:C     | 1:A:72:VAL:O     | 2.60                     | 0.42              |
| 1:A:457:PHE:C    | 1:A:457:PHE:CD2  | 2.97                     | 0.42              |
| 1:B:118:GLU:HG3  | 1:B:119:ILE:N    | 2.34                     | 0.42              |
| 1:B:146:SER:C    | 1:B:148:PHE:H    | 2.27                     | 0.42              |
| 1:B:328:ASN:OD1  | 4:B:1328:NAG:C2  | 2.60                     | 0.42              |
| 1:A:101:TYR:O    | 1:A:101:TYR:HD1  | 2.03                     | 0.42              |
| 1:A:218:GLY:H    | 1:A:223:ASP:HB2  | 1.85                     | 0.42              |
| 1:B:32:ASN:O     | 1:B:33:ASN:CB    | 2.65                     | 0.42              |
| 1:A:126:PHE:HB2  | 1:A:154:MET:HB2  | 2.01                     | 0.42              |
| 1:B:442:ASN:CB   | 1:B:469:ASN:HD22 | 2.19                     | 0.42              |
| 1:A:315:GLY:O    | 1:A:316:ILE:C    | 2.62                     | 0.42              |
| 1:A:333:LYS:H    | 1:A:333:LYS:HG3  | 1.67                     | 0.42              |
| 1:A:495:GLU:HA   | 1:A:496:PRO:HD3  | 1.84                     | 0.42              |
| 1:B:167:ASP:OD2  | 1:B:167:ASP:C    | 2.62                     | 0.42              |
| 1:B:124:VAL:HG21 | 1:B:140:TRP:CE3  | 2.55                     | 0.42              |
| 1:A:62:ALA:HA    | 1:A:84:ARG:HG3   | 2.02                     | 0.42              |
| 1:A:78:GLU:HB3   | 1:A:112:PRO:HB2  | 2.02                     | 0.42              |
| 1:A:194:GLN:O    | 1:A:194:GLN:HG3  | 2.20                     | 0.42              |
| 1:A:243:LEU:N    | 1:A:243:LEU:HD12 | 2.35                     | 0.42              |
| 1:A:489:GLU:HB3  | 1:A:500:VAL:CG1  | 2.50                     | 0.42              |
| 1:B:152:MET:O    | 1:B:152:MET:CG   | 2.67                     | 0.42              |
| 1:B:274:ASN:OD1  | 1:B:275:TYR:HD2  | 2.03                     | 0.42              |
| 1:A:109:LYS:HG3  | 1:A:131:ALA:O    | 2.19                     | 0.42              |
| 1:A:110:GLU:C    | 1:A:112:PRO:HD3  | 2.45                     | 0.42              |
| 1:A:114:ARG:HD2  | 1:A:114:ARG:H    | 1.84                     | 0.42              |
| 1:A:448:ALA:C    | 1:A:450:THR:H    | 2.27                     | 0.42              |
| 1:A:478:THR:HG22 | 1:A:478:THR:O    | 2.20                     | 0.42              |
| 1:B:82:ILE:HD11  | 1:B:120:LEU:HD12 | 2.00                     | 0.42              |
| 1:B:130:PRO:O    | 1:B:131:ALA:CB   | 2.66                     | 0.42              |
| 1:B:171:PRO:C    | 1:B:173:GLY:H    | 2.27                     | 0.42              |
| 1:B:463:LYS:NZ   | 1:B:463:LYS:CB   | 2.79                     | 0.42              |
| 4:B:1151:NAG:H3  | 4:B:1151:NAG:H82 | 2.02                     | 0.42              |
| 1:A:55:LEU:HB3   | 1:A:77:LEU:HD23  | 2.01                     | 0.41              |
| 1:A:89:TYR:C     | 1:A:91:ASN:N     | 2.76                     | 0.41              |
| 1:B:5:LYS:HD3    | 5:B:1341:HOH:O   | 2.20                     | 0.41              |
| 1:B:181:GLU:C    | 1:B:183:CYS:N    | 2.78                     | 0.41              |
| 1:B:331:ASN:CB   | 4:B:1328:NAG:O7  | 2.67                     | 0.41              |
| 1:B:430:LYS:HE3  | 5:B:1338:HOH:O   | 2.20                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:13:LYS:C     | 1:A:15:THR:H     | 2.28                     | 0.41              |
| 1:A:29:ARG:HB3   | 2:C:49:TRP:CZ2   | 2.55                     | 0.41              |
| 1:A:487:SER:OG   | 1:A:501:SER:HB3  | 2.20                     | 0.41              |
| 1:A:497:ARG:HA   | 1:A:510:GLU:HA   | 2.01                     | 0.41              |
| 1:B:82:ILE:HD12  | 1:B:213:ALA:CB   | 2.49                     | 0.41              |
| 1:B:192:ALA:CB   | 1:B:204:PRO:HA   | 2.50                     | 0.41              |
| 2:D:34:VAL:HG12  | 2:D:35:VAL:N     | 2.35                     | 0.41              |
| 1:A:434:ASP:OD2  | 1:A:435:GLY:N    | 2.46                     | 0.41              |
| 1:B:470:ARG:HG2  | 1:B:470:ARG:HH11 | 1.85                     | 0.41              |
| 1:A:48:ARG:HG2   | 1:A:48:ARG:HH11  | 1.85                     | 0.41              |
| 1:A:247:ASN:HB2  | 1:A:254:ASP:OD2  | 2.20                     | 0.41              |
| 1:A:457:PHE:HD2  | 1:A:457:PHE:C    | 2.28                     | 0.41              |
| 1:B:97:VAL:HG12  | 1:B:100:ASN:HD22 | 1.85                     | 0.41              |
| 1:B:418:SER:HA   | 1:B:441:GLY:O    | 2.21                     | 0.41              |
| 1:B:432:ILE:O    | 1:B:433:SER:C    | 2.62                     | 0.41              |
| 1:B:475:CYS:HB3  | 1:B:480:GLN:HB2  | 2.02                     | 0.41              |
| 1:A:139:GLN:HG2  | 1:A:174:SER:OG   | 2.21                     | 0.41              |
| 1:A:272:PRO:O    | 1:A:274:ASN:N    | 2.53                     | 0.41              |
| 1:A:312:VAL:HG23 | 1:A:312:VAL:O    | 2.20                     | 0.41              |
| 1:A:376:GLU:OE1  | 1:A:403:ARG:NH1  | 2.50                     | 0.41              |
| 1:A:472:GLU:O    | 1:A:474:SER:N    | 2.54                     | 0.41              |
| 1:A:478:THR:CG2  | 1:A:480:GLN:HG3  | 2.50                     | 0.41              |
| 1:B:314:ASN:O    | 1:B:342:SER:O    | 2.38                     | 0.41              |
| 1:B:369:ASP:O    | 1:B:372:LYS:HB2  | 2.20                     | 0.41              |
| 1:B:393:LEU:HD12 | 1:B:424:LEU:HA   | 2.02                     | 0.41              |
| 2:C:37:TYR:CD2   | 2:C:45:ARG:HA    | 2.55                     | 0.41              |
| 1:A:13:LYS:O     | 1:A:15:THR:N     | 2.54                     | 0.41              |
| 1:A:19:THR:H     | 1:A:22:ASP:HB2   | 1.85                     | 0.41              |
| 1:A:46:VAL:CG1   | 1:A:72:VAL:HB    | 2.46                     | 0.41              |
| 1:A:144:VAL:CG1  | 1:A:145:SER:N    | 2.84                     | 0.41              |
| 1:B:82:ILE:HD11  | 1:B:120:LEU:CD1  | 2.51                     | 0.41              |
| 1:B:134:ASN:O    | 1:B:135:VAL:C    | 2.64                     | 0.41              |
| 2:D:49:TRP:HB2   | 5:D:57:HOH:O     | 2.19                     | 0.41              |
| 3:E:1:NAG:C4     | 3:E:2:NAG:N2     | 2.81                     | 0.41              |
| 1:A:446:CYS:O    | 1:A:447:TYR:CD1  | 2.73                     | 0.41              |
| 1:B:144:VAL:CG1  | 1:B:145:SER:N    | 2.83                     | 0.41              |
| 1:B:349:PRO:CD   | 1:B:385:ALA:HB2  | 2.50                     | 0.41              |
| 1:A:44:THR:O     | 1:A:45:TYR:HB2   | 2.21                     | 0.41              |
| 1:A:141:ARG:HG3  | 1:A:141:ARG:HH11 | 1.86                     | 0.41              |
| 1:A:380:PHE:HB3  | 1:A:406:THR:O    | 2.20                     | 0.41              |
| 1:A:457:PHE:HB2  | 1:A:462:GLN:HE22 | 1.85                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:128:ASN:C    | 1:B:130:PRO:HD3  | 2.46                     | 0.41              |
| 1:B:319:GLY:O    | 1:B:321:PHE:N    | 2.54                     | 0.41              |
| 1:B:376:GLU:CB   | 1:B:401:ILE:HG22 | 2.50                     | 0.41              |
| 1:B:447:TYR:HE2  | 1:B:480:GLN:O    | 2.03                     | 0.41              |
| 1:A:46:VAL:HG21  | 1:A:52:LEU:HD11  | 2.03                     | 0.41              |
| 1:A:68:ALA:O     | 1:A:69:LEU:HB2   | 2.21                     | 0.41              |
| 1:A:173:GLY:O    | 1:A:174:SER:C    | 2.64                     | 0.41              |
| 1:A:331:ASN:C    | 4:A:1328:NAG:O7  | 2.64                     | 0.41              |
| 1:A:442:ASN:O    | 1:A:443:LYS:C    | 2.63                     | 0.41              |
| 1:A:453:TRP:CE3  | 1:A:456:LEU:HD23 | 2.56                     | 0.41              |
| 1:A:454:LYS:HA   | 1:A:454:LYS:HE3  | 2.02                     | 0.41              |
| 1:B:26:SER:O     | 1:B:27:LEU:C     | 2.63                     | 0.41              |
| 1:B:394:HIS:C    | 1:B:396:PHE:N    | 2.79                     | 0.41              |
| 1:A:140:TRP:C    | 1:A:142:ASP:H    | 2.27                     | 0.41              |
| 1:B:124:VAL:HB   | 1:B:154:MET:HE3  | 2.03                     | 0.41              |
| 1:A:430:LYS:O    | 1:A:430:LYS:HG3  | 2.21                     | 0.40              |
| 1:B:21:GLU:O     | 1:B:24:PHE:N     | 2.53                     | 0.40              |
| 1:B:75:ILE:HA    | 1:B:76:PRO:HD3   | 1.83                     | 0.40              |
| 1:B:102:ASP:HB2  | 1:B:106:THR:O    | 2.21                     | 0.40              |
| 1:B:135:VAL:HG12 | 1:B:156:PHE:CE2  | 2.56                     | 0.40              |
| 1:B:366:GLN:HE21 | 1:B:366:GLN:CA   | 2.18                     | 0.40              |
| 1:B:394:HIS:O    | 1:B:395:ALA:C    | 2.64                     | 0.40              |
| 1:B:459:THR:N    | 1:B:462:GLN:NE2  | 2.68                     | 0.40              |
| 1:B:480:GLN:O    | 1:B:481:VAL:C    | 2.63                     | 0.40              |
| 1:B:74:ARG:O     | 1:B:76:PRO:HD3   | 2.21                     | 0.40              |
| 1:B:138:ILE:HG12 | 1:B:176:TRP:CE2  | 2.55                     | 0.40              |
| 1:B:257:PRO:HG2  | 1:B:258:GLU:N    | 2.32                     | 0.40              |
| 1:B:493:GLY:HA3  | 1:B:498:ASP:OD1  | 2.21                     | 0.40              |
| 1:A:102:ASP:C    | 1:A:104:ASN:H    | 2.29                     | 0.40              |
| 1:A:261:TYR:HB2  | 1:A:268:VAL:HG23 | 2.02                     | 0.40              |
| 1:A:427:ARG:HA   | 1:A:492:TRP:CD1  | 2.57                     | 0.40              |
| 1:B:55:LEU:HB3   | 1:B:77:LEU:HD23  | 2.03                     | 0.40              |
| 1:B:166:CYS:O    | 1:B:167:ASP:C    | 2.64                     | 0.40              |
| 1:B:380:PHE:CE1  | 1:B:408:GLN:HG2  | 2.56                     | 0.40              |
| 1:B:447:TYR:O    | 1:B:450:THR:OG1  | 2.35                     | 0.40              |
| 2:D:45:ARG:HG3   | 2:D:45:ARG:NH1   | 2.36                     | 0.40              |
| 1:A:54:PHE:CD1   | 1:A:54:PHE:C     | 2.99                     | 0.40              |
| 1:A:414:LEU:C    | 1:A:414:LEU:CD2  | 2.95                     | 0.40              |
| 1:B:310:ARG:HB3  | 1:B:311:LYS:H    | 1.71                     | 0.40              |
| 1:B:386:TRP:O    | 1:B:387:PRO:C    | 2.64                     | 0.40              |
| 1:B:451:ILE:O    | 1:B:451:ILE:HG22 | 2.20                     | 0.40              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:B:483:HIS:O   | 1:B:484:ALA:CB  | 2.68                     | 0.40              |
| 2:C:24:GLU:CD   | 2:C:24:GLU:H    | 2.29                     | 0.40              |
| 1:A:20:PHE:CD1  | 1:A:47:GLN:CD   | 3.00                     | 0.40              |
| 1:A:65:VAL:O    | 1:A:95:LEU:HD12 | 2.21                     | 0.40              |
| 1:A:394:HIS:O   | 1:A:397:GLU:N   | 2.55                     | 0.40              |
| 1:B:68:ALA:HB1  | 1:B:69:LEU:HD13 | 2.04                     | 0.40              |
| 1:B:69:LEU:HD21 | 2:D:23:ILE:HG21 | 2.03                     | 0.40              |
| 1:B:263:PHE:CE1 | 1:B:272:PRO:HG2 | 2.56                     | 0.40              |
| 1:B:318:ILE:CG1 | 1:B:319:GLY:N   | 2.84                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed       | Favoured  | Allowed   | Outliers | Percentiles |   |
|-----|-------|----------------|-----------|-----------|----------|-------------|---|
| 1   | A     | 378/622 (61%)  | 270 (71%) | 69 (18%)  | 39 (10%) | 0           | 2 |
| 1   | B     | 307/622 (49%)  | 225 (73%) | 55 (18%)  | 27 (9%)  | 0           | 4 |
| All | All   | 685/1244 (55%) | 495 (72%) | 124 (18%) | 66 (10%) | 0           | 3 |

All (66) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 171 | PRO  |
| 1   | A     | 203 | SER  |
| 1   | A     | 310 | ARG  |
| 1   | A     | 311 | LYS  |
| 1   | A     | 427 | ARG  |
| 1   | A     | 433 | SER  |
| 1   | A     | 490 | GLY  |
| 1   | B     | 13  | LYS  |
| 1   | B     | 14  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 171 | PRO  |
| 1   | B     | 273 | ARG  |
| 1   | B     | 309 | CYS  |
| 1   | B     | 484 | ALA  |
| 1   | A     | 193 | GLN  |
| 1   | A     | 196 | SER  |
| 1   | A     | 202 | LYS  |
| 1   | A     | 273 | ARG  |
| 1   | A     | 288 | GLY  |
| 1   | A     | 372 | LYS  |
| 1   | A     | 389 | ASN  |
| 1   | A     | 443 | LYS  |
| 1   | A     | 454 | LYS  |
| 1   | A     | 484 | ALA  |
| 1   | A     | 505 | VAL  |
| 1   | B     | 27  | LEU  |
| 1   | B     | 180 | GLU  |
| 1   | B     | 257 | PRO  |
| 1   | A     | 77  | LEU  |
| 1   | A     | 174 | SER  |
| 1   | A     | 241 | PRO  |
| 1   | A     | 297 | ASP  |
| 1   | A     | 316 | ILE  |
| 1   | A     | 330 | THR  |
| 1   | A     | 395 | ALA  |
| 1   | A     | 486 | CYS  |
| 1   | B     | 99  | SER  |
| 1   | B     | 135 | VAL  |
| 1   | B     | 141 | ARG  |
| 1   | B     | 182 | ASN  |
| 1   | B     | 241 | PRO  |
| 1   | B     | 297 | ASP  |
| 1   | B     | 306 | GLU  |
| 1   | B     | 320 | GLU  |
| 1   | A     | 154 | MET  |
| 1   | A     | 322 | LYS  |
| 1   | A     | 449 | ASN  |
| 1   | A     | 473 | ASN  |
| 1   | A     | 482 | CYS  |
| 1   | A     | 483 | HIS  |
| 1   | B     | 91  | ASN  |
| 1   | B     | 147 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 165 | LYS  |
| 1   | B     | 193 | GLN  |
| 1   | B     | 488 | PRO  |
| 1   | A     | 76  | PRO  |
| 1   | A     | 168 | PRO  |
| 1   | A     | 179 | GLY  |
| 1   | A     | 190 | ILE  |
| 1   | A     | 481 | VAL  |
| 1   | A     | 494 | PRO  |
| 1   | B     | 494 | PRO  |
| 1   | A     | 319 | GLY  |
| 1   | B     | 487 | SER  |
| 1   | B     | 76  | PRO  |
| 1   | B     | 308 | PRO  |
| 1   | B     | 63  | GLY  |

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

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

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

2 monosaccharides 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 |
| 3   | NAG  | E     | 1   | 3,1  | 14,14,15     | 0.65 | 0        | 17,19,21    | 1.11 | 1 (5%)   |
| 3   | NAG  | E     | 2   | 3    | 14,14,15     | 0.70 | 0        | 17,19,21    | 0.67 | 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   | NAG  | E     | 1   | 3,1  | -       | 4/6/23/26 | 0/1/1/1 |
| 3   | NAG  | E     | 2   | 3    | -       | 5/6/23/26 | 0/1/1/1 |

There are no bond length outliers.

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 3   | E     | 1   | NAG  | C4-C3-C2 | 3.13 | 115.60      | 111.02   |

There are no chirality outliers.

All (9) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 3   | E     | 1   | NAG  | C8-C7-N2-C2 |
| 3   | E     | 1   | NAG  | O7-C7-N2-C2 |
| 3   | E     | 2   | NAG  | C8-C7-N2-C2 |
| 3   | E     | 2   | NAG  | O7-C7-N2-C2 |
| 3   | E     | 1   | NAG  | O5-C5-C6-O6 |
| 3   | E     | 2   | NAG  | O5-C5-C6-O6 |
| 3   | E     | 1   | NAG  | C4-C5-C6-O6 |
| 3   | E     | 2   | NAG  | C4-C5-C6-O6 |
| 3   | E     | 2   | NAG  | C3-C2-N2-C7 |

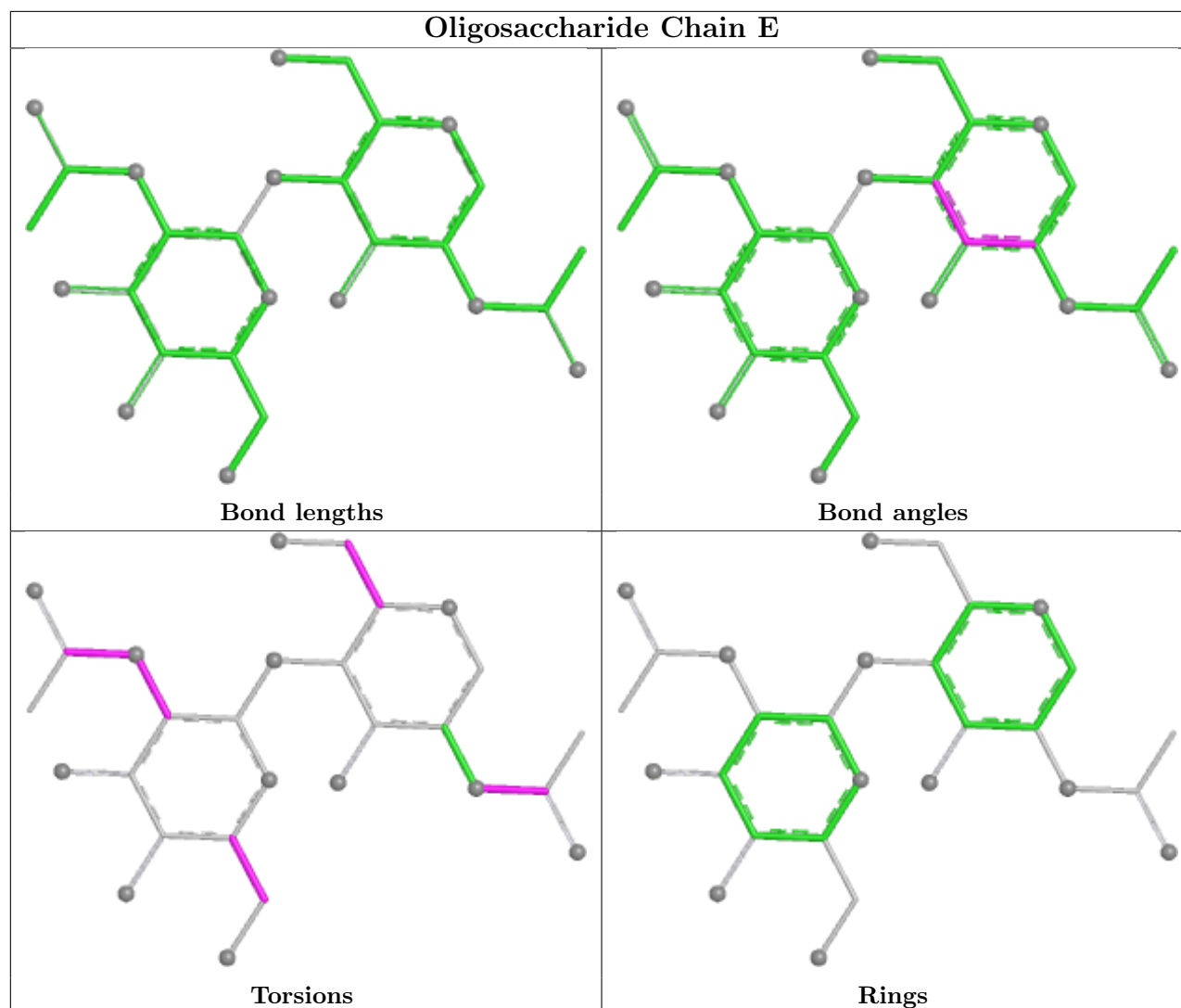
There are no ring outliers.

2 monomers are involved in 4 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3   | E     | 1   | NAG  | 4       | 0            |
| 3   | E     | 2   | NAG  | 3       | 0            |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for oligosaccharide.



## 5.6 Ligand geometry [i](#)

8 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 | $\# Z  > 2$ |
| 4   | NAG  | A     | 1032 | 1    | 14,14,15     | 0.60 | 0           | 17,19,21    | 0.66 | 0           |
| 4   | NAG  | A     | 1337 | 1    | 14,14,15     | 0.56 | 0           | 17,19,21    | 0.56 | 0           |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 4   | NAG  | B     | 1151 | 1    | 14,14,15     | 0.64 | 0        | 17,19,21    | 0.59 | 0        |
| 4   | NAG  | A     | 1328 | 1    | 14,14,15     | 0.84 | 1 (7%)   | 17,19,21    | 0.96 | 1 (5%)   |
| 4   | NAG  | A     | 1151 | 1    | 14,14,15     | 0.62 | 0        | 17,19,21    | 0.83 | 1 (5%)   |
| 4   | NAG  | B     | 1032 | 1    | 14,14,15     | 0.50 | 0        | 17,19,21    | 0.82 | 1 (5%)   |
| 4   | NAG  | A     | 1172 | 1    | 14,14,15     | 0.62 | 0        | 17,19,21    | 0.68 | 0        |
| 4   | NAG  | B     | 1328 | 1    | 14,14,15     | 0.76 | 0        | 17,19,21    | 0.99 | 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   |
|-----|------|-------|------|------|---------|-----------|---------|
| 4   | NAG  | A     | 1032 | 1    | -       | 4/6/23/26 | 0/1/1/1 |
| 4   | NAG  | A     | 1337 | 1    | -       | 3/6/23/26 | 0/1/1/1 |
| 4   | NAG  | B     | 1151 | 1    | -       | 5/6/23/26 | 0/1/1/1 |
| 4   | NAG  | A     | 1328 | 1    | -       | 4/6/23/26 | 0/1/1/1 |
| 4   | NAG  | A     | 1151 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 4   | NAG  | B     | 1032 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 4   | NAG  | A     | 1172 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 4   | NAG  | B     | 1328 | 1    | -       | 2/6/23/26 | 0/1/1/1 |

All (1) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 4   | A     | 1328 | NAG  | C1-C2 | 2.59 | 1.55        | 1.52     |

All (3) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 4   | A     | 1328 | NAG  | C3-C4-C5 | -2.61 | 105.51      | 110.23   |
| 4   | B     | 1032 | NAG  | C2-N2-C7 | -2.39 | 119.70      | 122.90   |
| 4   | A     | 1151 | NAG  | C2-N2-C7 | -2.02 | 120.19      | 122.90   |

There are no chirality outliers.

All (24) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       |
|-----|-------|------|------|-------------|
| 4   | A     | 1032 | NAG  | C3-C2-N2-C7 |

*Continued on next page...*

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| Mol | Chain | Res  | Type | Atoms       |
|-----|-------|------|------|-------------|
| 4   | A     | 1032 | NAG  | C8-C7-N2-C2 |
| 4   | A     | 1032 | NAG  | O7-C7-N2-C2 |
| 4   | A     | 1151 | NAG  | C8-C7-N2-C2 |
| 4   | A     | 1151 | NAG  | O7-C7-N2-C2 |
| 4   | A     | 1172 | NAG  | C8-C7-N2-C2 |
| 4   | A     | 1172 | NAG  | O7-C7-N2-C2 |
| 4   | A     | 1328 | NAG  | C1-C2-N2-C7 |
| 4   | A     | 1328 | NAG  | C8-C7-N2-C2 |
| 4   | A     | 1328 | NAG  | O7-C7-N2-C2 |
| 4   | A     | 1337 | NAG  | C3-C2-N2-C7 |
| 4   | A     | 1337 | NAG  | C8-C7-N2-C2 |
| 4   | A     | 1337 | NAG  | O7-C7-N2-C2 |
| 4   | B     | 1032 | NAG  | C8-C7-N2-C2 |
| 4   | B     | 1032 | NAG  | O7-C7-N2-C2 |
| 4   | B     | 1151 | NAG  | C8-C7-N2-C2 |
| 4   | B     | 1151 | NAG  | O7-C7-N2-C2 |
| 4   | B     | 1328 | NAG  | C8-C7-N2-C2 |
| 4   | B     | 1328 | NAG  | O7-C7-N2-C2 |
| 4   | B     | 1151 | NAG  | C4-C5-C6-O6 |
| 4   | B     | 1151 | NAG  | O5-C5-C6-O6 |
| 4   | A     | 1032 | NAG  | O5-C5-C6-O6 |
| 4   | B     | 1151 | NAG  | C3-C2-N2-C7 |
| 4   | A     | 1328 | NAG  | O5-C5-C6-O6 |

There are no ring outliers.

5 monomers are involved in 32 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 4   | A     | 1337 | NAG  | 1       | 0            |
| 4   | B     | 1151 | NAG  | 1       | 0            |
| 4   | A     | 1328 | NAG  | 9       | 0            |
| 4   | B     | 1032 | NAG  | 1       | 0            |
| 4   | B     | 1328 | NAG  | 20      | 0            |

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.