



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 09:29 PM UTC

PDB ID : 3PTO / pdb\_00003pto  
Title : Crystal Structure of an empty Vesicular Stomatitis Virus Nucleocapsid Protein Complex  
Authors : Luo, M.; Green, T.J.; Rowse, M.  
Deposited on : 2010-12-03  
Resolution : 3.01 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

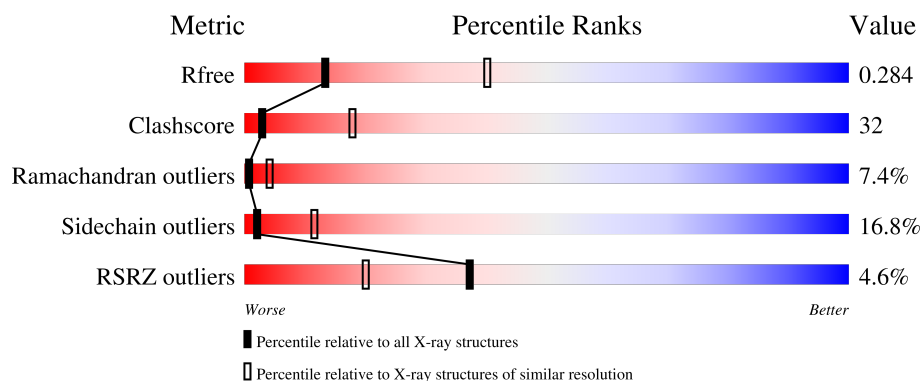
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.01 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)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 2672 (3.00-3.00)                                      |
| Clashscore            | 190562                      | 2977 (3.00-3.00)                                      |
| Ramachandran outliers | 187476                      | 2877 (3.00-3.00)                                      |
| Sidechain outliers    | 187428                      | 2880 (3.00-3.00)                                      |
| RSRZ outliers         | 180081                      | 2671 (3.00-3.00)                                      |

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

| Mol | Chain | Length | Quality of chain                                                                                   |
|-----|-------|--------|----------------------------------------------------------------------------------------------------|
| 1   | A     | 421    | <div> <div>4%</div> <div> <div>48%</div> <div>36%</div> <div>12%</div> <div>..</div> </div> </div> |
| 1   | B     | 421    | <div> <div>5%</div> <div> <div>47%</div> <div>37%</div> <div>13%</div> <div>..</div> </div> </div> |
| 1   | C     | 421    | <div> <div>5%</div> <div> <div>48%</div> <div>36%</div> <div>12%</div> <div>..</div> </div> </div> |
| 1   | D     | 421    | <div> <div>6%</div> <div> <div>48%</div> <div>38%</div> <div>11%</div> <div>..</div> </div> </div> |
| 1   | E     | 421    | <div> <div>2%</div> <div> <div>47%</div> <div>37%</div> <div>12%</div> <div>..</div> </div> </div> |

## 2 Entry composition [i](#)

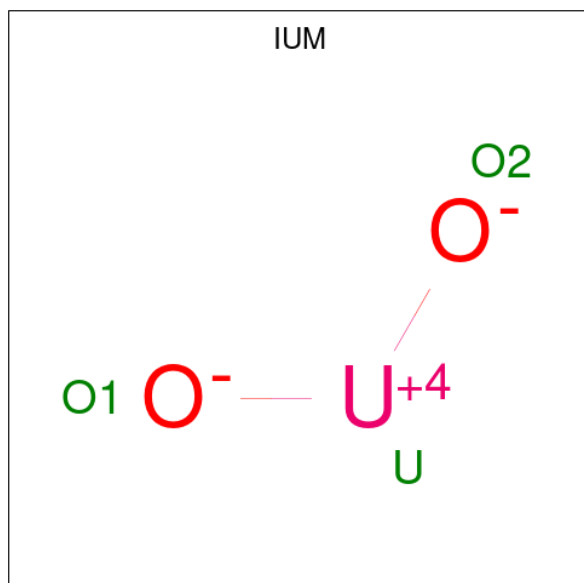
There are 2 unique types of molecules in this entry. The entry contains 16467 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Nucleoprotein.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 416      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3298  | 2101 | 553 | 626 | 18 |         |         |       |
| 1   | B     | 415      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3290  | 2097 | 552 | 623 | 18 |         |         |       |
| 1   | C     | 413      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3275  | 2089 | 550 | 618 | 18 |         |         |       |
| 1   | D     | 416      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3298  | 2103 | 553 | 624 | 18 |         |         |       |
| 1   | E     | 415      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3291  | 2097 | 552 | 624 | 18 |         |         |       |

- Molecule 2 is URANYL (VI) ION (CCD ID: IUM) (formula: O<sub>2</sub>U).



| Mol | Chain | Residues | Atoms |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 2   | A     | 1        | Total | U | 0       | 0       |
|     |       |          | 1     | 1 |         |         |

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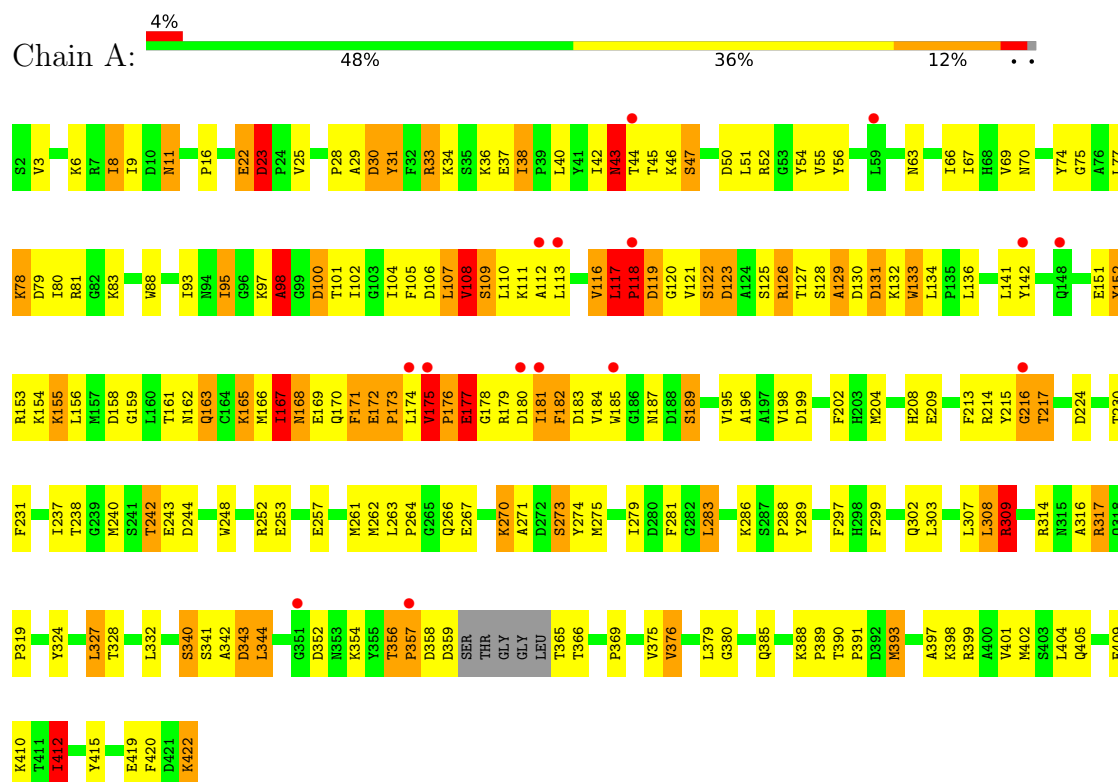
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| Mol | Chain | Residues | Atoms |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 2   | A     | 1        | Total | U | 0       | 0       |
|     |       |          | 1     | 1 |         |         |
| 2   | A     | 1        | Total | U | 0       | 0       |
|     |       |          | 1     | 1 |         |         |
| 2   | A     | 1        | Total | U | 0       | 0       |
|     |       |          | 1     | 1 |         |         |
| 2   | B     | 1        | Total | U | 0       | 0       |
|     |       |          | 1     | 1 |         |         |
| 2   | B     | 1        | Total | U | 0       | 0       |
|     |       |          | 1     | 1 |         |         |
| 2   | B     | 1        | Total | U | 0       | 0       |
|     |       |          | 1     | 1 |         |         |
| 2   | C     | 1        | Total | U | 0       | 0       |
|     |       |          | 1     | 1 |         |         |
| 2   | C     | 1        | Total | U | 0       | 0       |
|     |       |          | 1     | 1 |         |         |
| 2   | C     | 1        | Total | U | 0       | 0       |
|     |       |          | 1     | 1 |         |         |
| 2   | D     | 1        | Total | U | 0       | 0       |
|     |       |          | 1     | 1 |         |         |
| 2   | D     | 1        | Total | U | 0       | 0       |
|     |       |          | 1     | 1 |         |         |
| 2   | D     | 1        | Total | U | 0       | 0       |
|     |       |          | 1     | 1 |         |         |
| 2   | E     | 1        | Total | U | 0       | 0       |
|     |       |          | 1     | 1 |         |         |
| 2   | E     | 1        | Total | U | 0       | 0       |
|     |       |          | 1     | 1 |         |         |

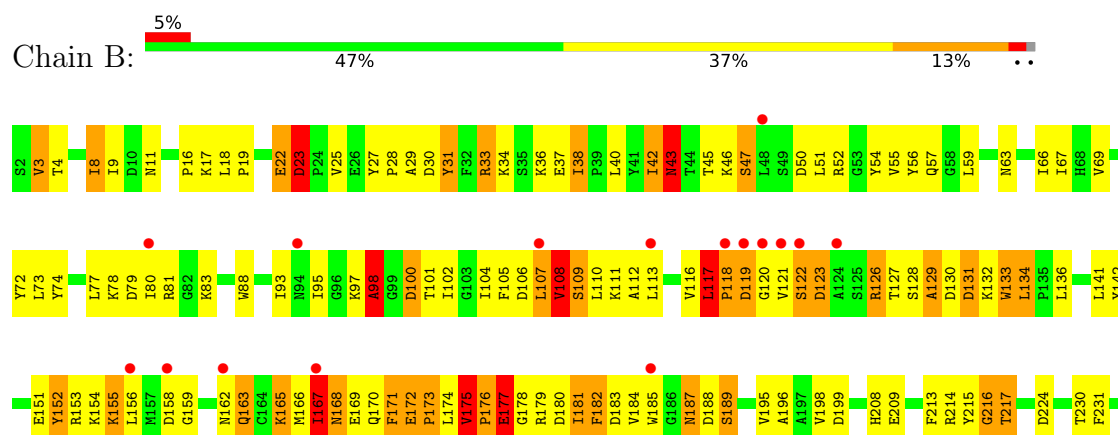
### 3 Residue-property plots [i](#)

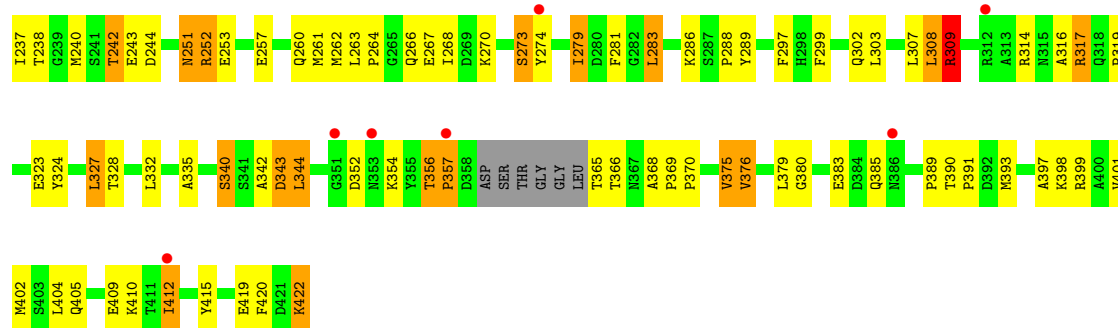
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

#### • Molecule 1: Nucleoprotein

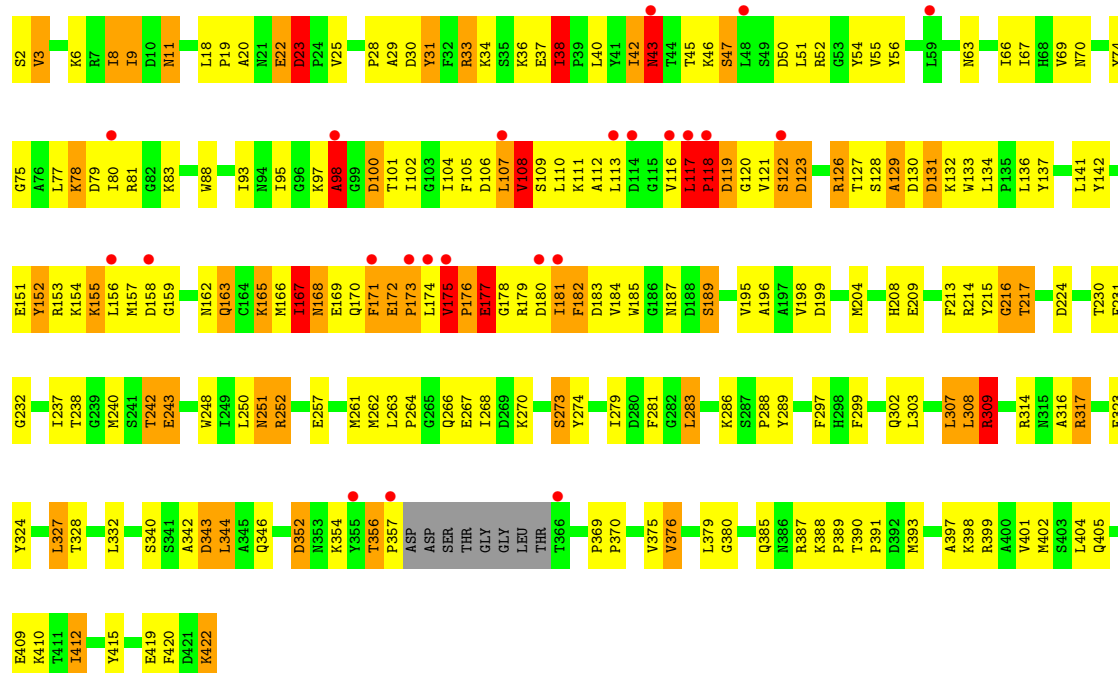


#### • Molecule 1: Nucleoprotein

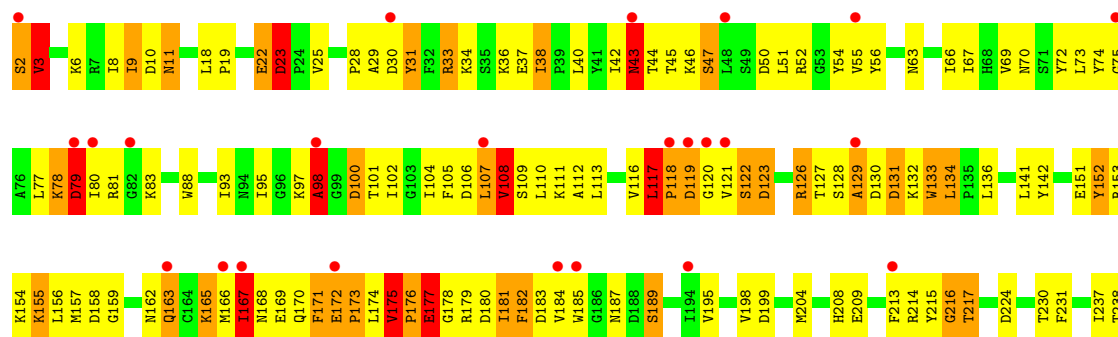


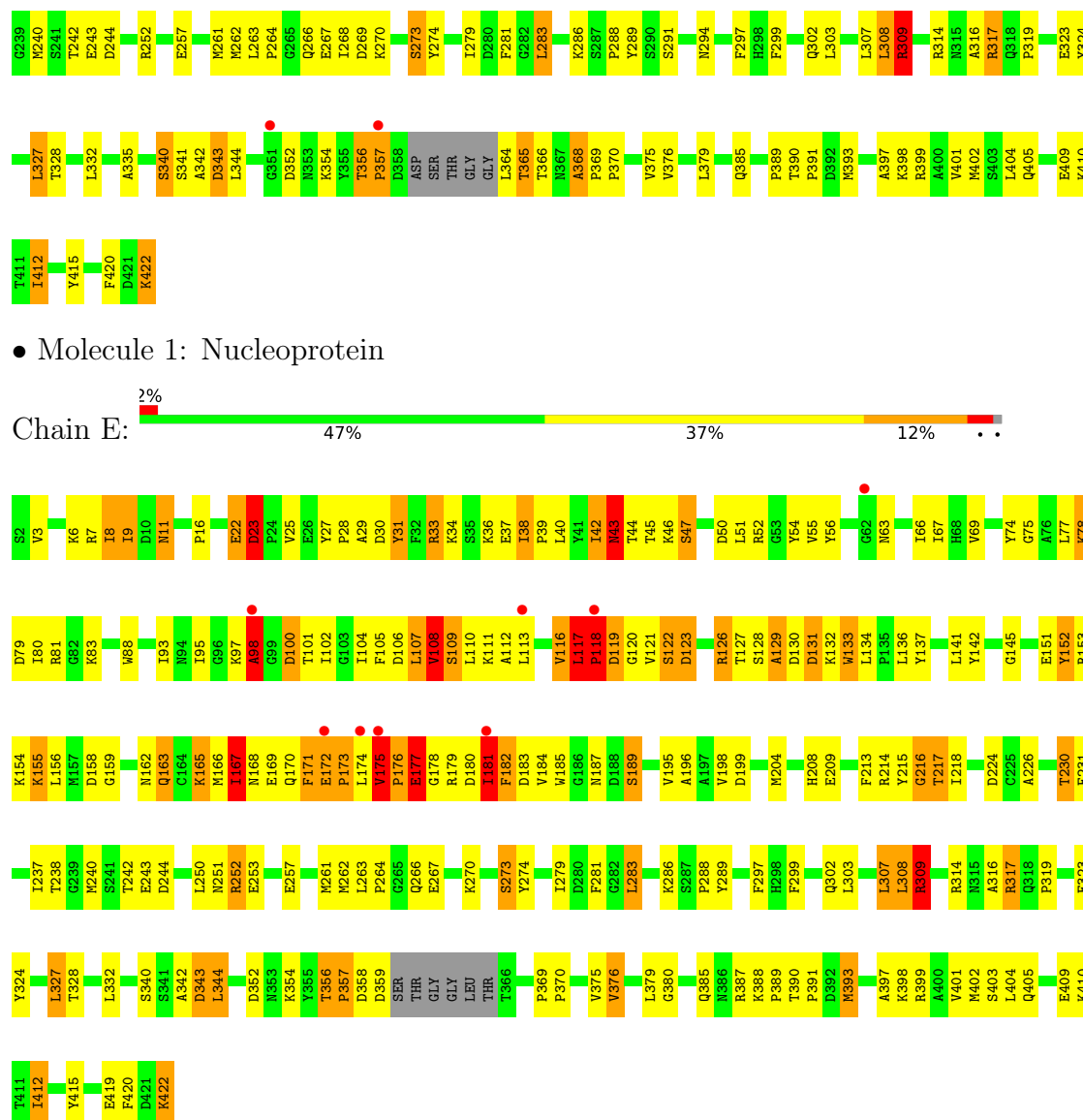


• Molecule 1: Nucleoprotein



• Molecule 1: Nucleoprotein





• Molecule 1: Nucleoprotein

## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 21 21 2                                                   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 165.64Å 234.06Å 75.97Å<br>90.00° 90.00° 90.00°              | Depositor        |
| Resolution (Å)                                                          | 38.76 – 3.01<br>38.76 – 3.01                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 82.3 (38.76-3.01)<br>82.3 (38.76-3.01)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.07                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 3.10 (at 3.01Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX 1.6.1 _357                                           | Depositor        |
| R, $R_{free}$                                                           | 0.258 , 0.291<br>0.250 , 0.284                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 2000 reflections (3.88%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 80.7                                                        | Xtriage          |
| Anisotropy                                                              | 0.555                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.30 , 58.2                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.91                                                        | EDS              |
| Total number of atoms                                                   | 16467                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 100.0                                                       | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.69% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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

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     | 0.67         | 2/3373 (0.1%)  | 1.00        | 14/4565 (0.3%)  |
| 1   | B     | 0.68         | 0/3365         | 1.02        | 20/4554 (0.4%)  |
| 1   | C     | 0.70         | 0/3350         | 1.00        | 16/4533 (0.4%)  |
| 1   | D     | 0.67         | 0/3373         | 1.02        | 18/4565 (0.4%)  |
| 1   | E     | 0.65         | 0/3366         | 1.00        | 15/4555 (0.3%)  |
| All | All   | 0.67         | 2/16827 (0.0%) | 1.01        | 83/22772 (0.4%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 2                   |
| 1   | B     | 0                   | 2                   |
| 1   | C     | 0                   | 3                   |
| 1   | D     | 0                   | 3                   |
| 1   | E     | 0                   | 2                   |
| All | All   | 0                   | 12                  |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 1   | A     | 412 | ILE  | CA-CB | 5.28 | 1.61        | 1.54     |
| 1   | A     | 30  | ASP  | CB-CG | 5.00 | 1.64        | 1.52     |

All (83) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1   | E     | 175 | VAL  | CA-C-N | 8.89 | 130.96      | 119.84   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | E     | 175 | VAL  | C-N-CA | 8.89  | 130.96      | 119.84   |
| 1   | A     | 175 | VAL  | CA-C-N | 8.84  | 130.89      | 119.84   |
| 1   | A     | 175 | VAL  | C-N-CA | 8.84  | 130.89      | 119.84   |
| 1   | C     | 177 | GLU  | N-CA-C | -8.78 | 92.11       | 110.80   |
| 1   | C     | 175 | VAL  | CA-C-N | 8.75  | 130.78      | 119.84   |
| 1   | C     | 175 | VAL  | C-N-CA | 8.75  | 130.78      | 119.84   |
| 1   | D     | 177 | GLU  | N-CA-C | -8.62 | 92.45       | 110.80   |
| 1   | B     | 175 | VAL  | CA-C-N | 8.58  | 130.56      | 119.84   |
| 1   | B     | 175 | VAL  | C-N-CA | 8.58  | 130.56      | 119.84   |
| 1   | E     | 177 | GLU  | N-CA-C | -8.50 | 92.69       | 110.80   |
| 1   | B     | 177 | GLU  | N-CA-C | -8.48 | 92.75       | 110.80   |
| 1   | D     | 175 | VAL  | CA-C-N | 8.38  | 130.31      | 119.84   |
| 1   | D     | 175 | VAL  | C-N-CA | 8.38  | 130.31      | 119.84   |
| 1   | A     | 177 | GLU  | N-CA-C | -8.02 | 93.72       | 110.80   |
| 1   | A     | 108 | VAL  | N-CA-C | 7.04  | 123.98      | 109.34   |
| 1   | B     | 108 | VAL  | N-CA-C | 6.93  | 123.76      | 109.34   |
| 1   | D     | 368 | ALA  | CA-C-N | 6.86  | 124.60      | 119.66   |
| 1   | D     | 368 | ALA  | C-N-CA | 6.86  | 124.60      | 119.66   |
| 1   | A     | 129 | ALA  | N-CA-C | -6.82 | 103.53      | 110.97   |
| 1   | D     | 108 | VAL  | N-CA-C | 6.71  | 123.30      | 109.34   |
| 1   | B     | 23  | ASP  | CA-C-N | 6.69  | 126.60      | 119.85   |
| 1   | B     | 23  | ASP  | C-N-CA | 6.69  | 126.60      | 119.85   |
| 1   | C     | 108 | VAL  | N-CA-C | 6.64  | 123.16      | 109.34   |
| 1   | E     | 369 | PRO  | CA-C-N | 6.61  | 128.10      | 119.84   |
| 1   | E     | 369 | PRO  | C-N-CA | 6.61  | 128.10      | 119.84   |
| 1   | E     | 108 | VAL  | N-CA-C | 6.60  | 123.06      | 109.34   |
| 1   | B     | 129 | ALA  | N-CA-C | -6.42 | 103.97      | 110.97   |
| 1   | A     | 119 | ASP  | N-CA-C | 6.33  | 119.84      | 110.48   |
| 1   | D     | 184 | VAL  | N-CA-C | -6.22 | 105.56      | 113.22   |
| 1   | E     | 129 | ALA  | N-CA-C | -6.14 | 104.28      | 110.97   |
| 1   | C     | 119 | ASP  | N-CA-C | 6.11  | 119.52      | 110.48   |
| 1   | D     | 23  | ASP  | CA-C-N | 6.11  | 126.02      | 119.85   |
| 1   | D     | 23  | ASP  | C-N-CA | 6.11  | 126.02      | 119.85   |
| 1   | E     | 119 | ASP  | N-CA-C | 6.09  | 119.49      | 110.48   |
| 1   | D     | 369 | PRO  | O-C-N  | 6.06  | 124.00      | 121.15   |
| 1   | E     | 23  | ASP  | CA-C-N | 6.06  | 125.97      | 119.85   |
| 1   | E     | 23  | ASP  | C-N-CA | 6.06  | 125.97      | 119.85   |
| 1   | B     | 369 | PRO  | O-C-N  | 6.05  | 124.00      | 121.15   |
| 1   | A     | 369 | PRO  | CA-C-N | 5.95  | 127.28      | 119.84   |
| 1   | A     | 369 | PRO  | C-N-CA | 5.95  | 127.28      | 119.84   |
| 1   | B     | 369 | PRO  | CA-C-N | 5.93  | 127.25      | 119.84   |
| 1   | B     | 369 | PRO  | C-N-CA | 5.93  | 127.25      | 119.84   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | C     | 129 | ALA  | N-CA-C  | -5.92 | 104.52      | 110.97   |
| 1   | D     | 369 | PRO  | CA-C-N  | 5.87  | 127.18      | 119.84   |
| 1   | D     | 369 | PRO  | C-N-CA  | 5.87  | 127.18      | 119.84   |
| 1   | D     | 119 | ASP  | N-CA-C  | 5.83  | 119.11      | 110.48   |
| 1   | A     | 23  | ASP  | CA-C-N  | 5.79  | 125.74      | 119.78   |
| 1   | A     | 23  | ASP  | C-N-CA  | 5.79  | 125.74      | 119.78   |
| 1   | C     | 369 | PRO  | CA-C-N  | 5.76  | 127.04      | 119.84   |
| 1   | C     | 369 | PRO  | C-N-CA  | 5.76  | 127.04      | 119.84   |
| 1   | D     | 3   | VAL  | N-CA-C  | 5.75  | 121.30      | 109.34   |
| 1   | C     | 38  | ILE  | CA-C-N  | 5.75  | 126.65      | 119.98   |
| 1   | C     | 38  | ILE  | C-N-CA  | 5.75  | 126.65      | 119.98   |
| 1   | D     | 177 | GLU  | CA-C-N  | 5.69  | 130.16      | 121.51   |
| 1   | D     | 177 | GLU  | C-N-CA  | 5.69  | 130.16      | 121.51   |
| 1   | B     | 368 | ALA  | CA-C-N  | 5.66  | 123.74      | 119.66   |
| 1   | B     | 368 | ALA  | C-N-CA  | 5.66  | 123.74      | 119.66   |
| 1   | B     | 119 | ASP  | N-CA-C  | 5.61  | 119.06      | 110.20   |
| 1   | C     | 23  | ASP  | CA-C-N  | 5.57  | 125.51      | 119.78   |
| 1   | C     | 23  | ASP  | C-N-CA  | 5.57  | 125.51      | 119.78   |
| 1   | C     | 177 | GLU  | CA-C-N  | 5.55  | 129.94      | 121.51   |
| 1   | C     | 177 | GLU  | C-N-CA  | 5.55  | 129.94      | 121.51   |
| 1   | D     | 129 | ALA  | N-CA-C  | -5.52 | 104.95      | 110.97   |
| 1   | B     | 177 | GLU  | CA-C-N  | 5.45  | 129.79      | 121.51   |
| 1   | B     | 177 | GLU  | C-N-CA  | 5.45  | 129.79      | 121.51   |
| 1   | B     | 184 | VAL  | N-CA-C  | -5.38 | 106.60      | 113.22   |
| 1   | E     | 109 | SER  | N-CA-C  | 5.35  | 117.44      | 109.25   |
| 1   | A     | 109 | SER  | N-CA-C  | 5.29  | 117.35      | 109.25   |
| 1   | A     | 369 | PRO  | O-C-N   | 5.27  | 123.63      | 121.15   |
| 1   | E     | 177 | GLU  | CA-C-N  | 5.26  | 129.51      | 121.51   |
| 1   | E     | 177 | GLU  | C-N-CA  | 5.26  | 129.51      | 121.51   |
| 1   | B     | 109 | SER  | N-CA-C  | 5.15  | 117.14      | 109.25   |
| 1   | A     | 184 | VAL  | N-CA-C  | -5.15 | 106.89      | 113.22   |
| 1   | C     | 369 | PRO  | O-C-N   | 5.11  | 123.55      | 121.15   |
| 1   | E     | 184 | VAL  | N-CA-C  | -5.09 | 106.96      | 113.22   |
| 1   | B     | 375 | VAL  | CB-CA-C | -5.09 | 105.37      | 111.88   |
| 1   | A     | 168 | ASN  | N-CA-C  | 5.08  | 121.63      | 110.80   |
| 1   | E     | 369 | PRO  | O-C-N   | 5.07  | 123.53      | 121.15   |
| 1   | B     | 168 | ASN  | N-CA-C  | 5.05  | 121.57      | 110.80   |
| 1   | C     | 168 | ASN  | N-CA-C  | 5.01  | 121.48      | 110.80   |
| 1   | D     | 291 | SER  | N-CA-C  | -5.00 | 107.12      | 113.18   |
| 1   | B     | 279 | ILE  | N-CA-C  | 5.00  | 115.67      | 110.82   |

There are no chirality outliers.

All (12) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | A     | 107 | LEU  | Peptide |
| 1   | A     | 98  | ALA  | Peptide |
| 1   | B     | 107 | LEU  | Peptide |
| 1   | B     | 98  | ALA  | Peptide |
| 1   | C     | 107 | LEU  | Peptide |
| 1   | C     | 2   | SER  | Peptide |
| 1   | C     | 98  | ALA  | Peptide |
| 1   | D     | 107 | LEU  | Peptide |
| 1   | D     | 2   | SER  | Peptide |
| 1   | D     | 98  | ALA  | Peptide |
| 1   | E     | 107 | LEU  | Peptide |
| 1   | E     | 98  | ALA  | Peptide |

## 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     | 3298  | 0        | 3257     | 214     | 0            |
| 1   | B     | 3290  | 0        | 3253     | 235     | 0            |
| 1   | C     | 3275  | 0        | 3242     | 226     | 0            |
| 1   | D     | 3298  | 0        | 3264     | 218     | 0            |
| 1   | E     | 3291  | 0        | 3250     | 211     | 0            |
| 2   | A     | 4     | 0        | 0        | 0       | 0            |
| 2   | B     | 3     | 0        | 0        | 0       | 0            |
| 2   | C     | 3     | 0        | 0        | 0       | 0            |
| 2   | D     | 3     | 0        | 0        | 0       | 0            |
| 2   | E     | 2     | 0        | 0        | 0       | 0            |
| All | All   | 16467 | 0        | 16266    | 1053    | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 32.

All (1053) 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:C:376:VAL:HG13 | 1:D:354:LYS:HB2 | 1.26                     | 1.14              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:317:ARG:H    | 1:B:317:ARG:HD2  | 1.10                     | 1.13              |
| 1:D:117:LEU:HB3  | 1:D:118:PRO:HD2  | 1.29                     | 1.12              |
| 1:C:117:LEU:HB3  | 1:C:118:PRO:HD2  | 1.27                     | 1.12              |
| 1:D:2:SER:N      | 1:D:3:VAL:HG23   | 1.63                     | 1.12              |
| 1:C:317:ARG:H    | 1:C:317:ARG:HD2  | 1.13                     | 1.11              |
| 1:E:117:LEU:HB3  | 1:E:118:PRO:HD2  | 1.28                     | 1.11              |
| 1:D:317:ARG:H    | 1:D:317:ARG:HD2  | 1.07                     | 1.09              |
| 1:E:317:ARG:H    | 1:E:317:ARG:HD2  | 1.05                     | 1.09              |
| 1:A:117:LEU:HB3  | 1:A:118:PRO:HD2  | 1.28                     | 1.09              |
| 1:A:376:VAL:HG13 | 1:B:354:LYS:HB2  | 1.33                     | 1.08              |
| 1:B:117:LEU:HB3  | 1:B:118:PRO:HD2  | 1.29                     | 1.08              |
| 1:A:317:ARG:H    | 1:A:317:ARG:HD2  | 1.07                     | 1.07              |
| 1:A:354:LYS:HB2  | 1:E:376:VAL:HG13 | 1.34                     | 1.05              |
| 1:E:214:ARG:HA   | 1:E:217:THR:HG22 | 1.34                     | 1.05              |
| 1:C:214:ARG:HA   | 1:C:217:THR:HG22 | 1.35                     | 1.03              |
| 1:A:214:ARG:HA   | 1:A:217:THR:HG22 | 1.33                     | 1.03              |
| 1:D:214:ARG:HA   | 1:D:217:THR:HG22 | 1.38                     | 1.03              |
| 1:B:214:ARG:HA   | 1:B:217:THR:HG22 | 1.36                     | 1.02              |
| 1:B:380:GLY:HA2  | 1:C:354:LYS:NZ   | 1.80                     | 0.96              |
| 1:B:356:THR:HG23 | 1:B:357:PRO:HD3  | 1.46                     | 0.96              |
| 1:D:129:ALA:HB1  | 1:D:133:TRP:HE1  | 1.30                     | 0.95              |
| 1:C:117:LEU:HB3  | 1:C:118:PRO:CD   | 1.97                     | 0.95              |
| 1:B:117:LEU:HB3  | 1:B:118:PRO:CD   | 1.97                     | 0.95              |
| 1:D:317:ARG:HD2  | 1:D:317:ARG:N    | 1.81                     | 0.94              |
| 1:A:117:LEU:HB3  | 1:A:118:PRO:CD   | 1.98                     | 0.94              |
| 1:D:356:THR:HG23 | 1:D:357:PRO:HD3  | 1.48                     | 0.94              |
| 1:E:117:LEU:HB3  | 1:E:118:PRO:CD   | 1.98                     | 0.94              |
| 1:A:356:THR:HG23 | 1:A:357:PRO:HD3  | 1.46                     | 0.94              |
| 1:D:117:LEU:HB3  | 1:D:118:PRO:CD   | 1.98                     | 0.94              |
| 1:C:129:ALA:HB1  | 1:C:133:TRP:HE1  | 1.33                     | 0.93              |
| 1:B:129:ALA:HB1  | 1:B:133:TRP:HE1  | 1.32                     | 0.93              |
| 1:E:37:GLU:HB2   | 1:E:108:VAL:HG11 | 1.50                     | 0.93              |
| 1:A:129:ALA:HB1  | 1:A:133:TRP:HE1  | 1.34                     | 0.92              |
| 1:E:317:ARG:HD2  | 1:E:317:ARG:N    | 1.85                     | 0.92              |
| 1:B:365:THR:HG23 | 1:B:366:THR:H    | 1.34                     | 0.92              |
| 1:A:37:GLU:HB2   | 1:A:108:VAL:HG11 | 1.52                     | 0.91              |
| 1:E:356:THR:HG23 | 1:E:357:PRO:HD3  | 1.48                     | 0.91              |
| 1:D:317:ARG:H    | 1:D:317:ARG:CD   | 1.82                     | 0.91              |
| 1:C:356:THR:HG23 | 1:C:357:PRO:HD3  | 1.50                     | 0.91              |
| 1:E:129:ALA:HB1  | 1:E:133:TRP:HE1  | 1.34                     | 0.91              |
| 1:A:324:TYR:O    | 1:A:328:THR:HG23 | 1.70                     | 0.91              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:181:ILE:H    | 1:C:181:ILE:HD12 | 1.33                     | 0.91              |
| 1:C:324:TYR:O    | 1:C:328:THR:HG23 | 1.69                     | 0.90              |
| 1:B:317:ARG:HD2  | 1:B:317:ARG:N    | 1.86                     | 0.89              |
| 1:A:317:ARG:H    | 1:A:317:ARG:CD   | 1.85                     | 0.88              |
| 1:B:317:ARG:H    | 1:B:317:ARG:CD   | 1.86                     | 0.88              |
| 1:B:37:GLU:HB2   | 1:B:108:VAL:HG11 | 1.56                     | 0.88              |
| 1:A:317:ARG:HD2  | 1:A:317:ARG:N    | 1.86                     | 0.88              |
| 1:A:365:THR:HG23 | 1:A:366:THR:H    | 1.36                     | 0.88              |
| 1:B:181:ILE:HD12 | 1:B:181:ILE:H    | 1.37                     | 0.88              |
| 1:D:181:ILE:HD12 | 1:D:181:ILE:H    | 1.37                     | 0.87              |
| 1:E:181:ILE:H    | 1:E:181:ILE:HD12 | 1.39                     | 0.87              |
| 1:D:324:TYR:O    | 1:D:328:THR:HG23 | 1.73                     | 0.87              |
| 1:E:317:ARG:H    | 1:E:317:ARG:CD   | 1.87                     | 0.87              |
| 1:B:187:ASN:ND2  | 1:C:165:LYS:HD3  | 1.89                     | 0.86              |
| 1:B:141:LEU:HD13 | 1:B:182:PHE:HD2  | 1.40                     | 0.86              |
| 1:C:385:GLN:HG2  | 1:C:390:THR:HG22 | 1.58                     | 0.86              |
| 1:A:385:GLN:HG2  | 1:A:390:THR:HG22 | 1.57                     | 0.85              |
| 1:E:385:GLN:HG2  | 1:E:390:THR:HG22 | 1.57                     | 0.85              |
| 1:A:181:ILE:HD12 | 1:A:181:ILE:H    | 1.38                     | 0.85              |
| 1:C:152:TYR:HE1  | 1:C:153:ARG:HH11 | 1.25                     | 0.85              |
| 1:B:385:GLN:HG2  | 1:B:390:THR:HG22 | 1.57                     | 0.84              |
| 1:B:324:TYR:O    | 1:B:328:THR:HG23 | 1.76                     | 0.84              |
| 1:D:37:GLU:HB2   | 1:D:108:VAL:HG11 | 1.56                     | 0.84              |
| 1:C:37:GLU:HB2   | 1:C:108:VAL:HG11 | 1.57                     | 0.84              |
| 1:D:141:LEU:HD13 | 1:D:182:PHE:HD2  | 1.42                     | 0.84              |
| 1:E:88:TRP:CD2   | 1:E:95:ILE:HD11  | 2.13                     | 0.83              |
| 1:A:88:TRP:CD2   | 1:A:95:ILE:HD11  | 2.14                     | 0.83              |
| 1:D:365:THR:HG23 | 1:D:366:THR:H    | 1.44                     | 0.82              |
| 1:C:317:ARG:H    | 1:C:317:ARG:CD   | 1.91                     | 0.82              |
| 1:A:214:ARG:HA   | 1:A:217:THR:CG2  | 2.09                     | 0.82              |
| 1:D:385:GLN:HG2  | 1:D:390:THR:HG22 | 1.60                     | 0.82              |
| 1:C:141:LEU:HD13 | 1:C:182:PHE:HD2  | 1.42                     | 0.82              |
| 1:E:141:LEU:HD13 | 1:E:182:PHE:HD2  | 1.43                     | 0.81              |
| 1:B:88:TRP:CD2   | 1:B:95:ILE:HD11  | 2.16                     | 0.81              |
| 1:C:317:ARG:HD2  | 1:C:317:ARG:N    | 1.93                     | 0.80              |
| 1:D:126:ARG:HD3  | 1:D:127:THR:H    | 1.46                     | 0.80              |
| 1:A:152:TYR:HE1  | 1:A:153:ARG:HH11 | 1.29                     | 0.80              |
| 1:E:152:TYR:HE1  | 1:E:153:ARG:HH11 | 1.30                     | 0.80              |
| 1:A:141:LEU:HD13 | 1:A:182:PHE:HD2  | 1.45                     | 0.80              |
| 1:C:88:TRP:CD2   | 1:C:95:ILE:HD11  | 2.17                     | 0.80              |
| 1:C:155:LYS:O    | 1:C:158:ASP:HB3  | 1.83                     | 0.79              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:214:ARG:HA   | 1:E:217:THR:CG2  | 2.12                     | 0.79              |
| 1:B:3:VAL:HG22   | 1:B:4:THR:H      | 1.48                     | 0.78              |
| 1:B:376:VAL:HG13 | 1:C:354:LYS:HB2  | 1.65                     | 0.78              |
| 1:B:106:ASP:C    | 1:B:107:LEU:HG   | 2.09                     | 0.78              |
| 1:B:152:TYR:HE1  | 1:B:153:ARG:HH11 | 1.32                     | 0.78              |
| 1:A:126:ARG:HD3  | 1:A:127:THR:H    | 1.49                     | 0.78              |
| 1:A:155:LYS:O    | 1:A:158:ASP:HB3  | 1.83                     | 0.77              |
| 1:C:152:TYR:CZ   | 1:C:153:ARG:HD3  | 2.18                     | 0.77              |
| 1:C:126:ARG:HD3  | 1:C:127:THR:H    | 1.49                     | 0.77              |
| 1:C:152:TYR:CE1  | 1:C:153:ARG:NH1  | 2.52                     | 0.77              |
| 1:B:126:ARG:HD3  | 1:B:127:THR:H    | 1.48                     | 0.77              |
| 1:B:214:ARG:HA   | 1:B:217:THR:CG2  | 2.13                     | 0.76              |
| 1:D:43:ASN:HA    | 1:D:112:ALA:H    | 1.50                     | 0.76              |
| 1:D:152:TYR:HE1  | 1:D:153:ARG:HH11 | 1.34                     | 0.76              |
| 1:D:364:LEU:O    | 1:D:365:THR:HG22 | 1.86                     | 0.75              |
| 1:B:155:LYS:O    | 1:B:158:ASP:HB3  | 1.86                     | 0.75              |
| 1:A:152:TYR:CZ   | 1:A:153:ARG:HD3  | 2.20                     | 0.75              |
| 1:C:184:VAL:HG11 | 1:D:165:LYS:HA   | 1.69                     | 0.75              |
| 1:E:155:LYS:O    | 1:E:158:ASP:HB3  | 1.85                     | 0.75              |
| 1:E:324:TYR:O    | 1:E:328:THR:HG23 | 1.86                     | 0.75              |
| 1:E:399:ARG:HA   | 1:E:402:MET:HE3  | 1.69                     | 0.75              |
| 1:D:106:ASP:C    | 1:D:107:LEU:HG   | 2.12                     | 0.74              |
| 1:A:43:ASN:HA    | 1:A:112:ALA:H    | 1.51                     | 0.74              |
| 1:C:214:ARG:HA   | 1:C:217:THR:CG2  | 2.14                     | 0.74              |
| 1:E:126:ARG:HD3  | 1:E:127:THR:H    | 1.51                     | 0.74              |
| 1:A:314:ARG:HD2  | 1:A:404:LEU:HD22 | 1.69                     | 0.74              |
| 1:B:152:TYR:CZ   | 1:B:153:ARG:HD3  | 2.22                     | 0.74              |
| 1:D:172:GLU:HB3  | 1:D:173:PRO:HD3  | 1.70                     | 0.74              |
| 1:D:214:ARG:HA   | 1:D:217:THR:CG2  | 2.16                     | 0.74              |
| 1:A:106:ASP:C    | 1:A:107:LEU:HG   | 2.13                     | 0.74              |
| 1:C:172:GLU:HB3  | 1:C:173:PRO:HD3  | 1.70                     | 0.74              |
| 1:D:88:TRP:CD2   | 1:D:95:ILE:HD11  | 2.22                     | 0.74              |
| 1:E:47:SER:HB2   | 1:E:50:ASP:HB2   | 1.68                     | 0.74              |
| 1:E:43:ASN:HA    | 1:E:112:ALA:H    | 1.52                     | 0.74              |
| 1:D:155:LYS:O    | 1:D:158:ASP:HB3  | 1.88                     | 0.74              |
| 1:E:152:TYR:CZ   | 1:E:153:ARG:HD3  | 2.21                     | 0.73              |
| 1:D:152:TYR:CZ   | 1:D:153:ARG:HD3  | 2.23                     | 0.73              |
| 1:A:398:LYS:HG2  | 1:A:402:MET:HE2  | 1.69                     | 0.73              |
| 1:B:47:SER:HB2   | 1:B:50:ASP:HB2   | 1.70                     | 0.73              |
| 1:C:47:SER:HB2   | 1:C:50:ASP:HB2   | 1.69                     | 0.73              |
| 1:A:152:TYR:CE1  | 1:A:153:ARG:NH1  | 2.57                     | 0.73              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:380:GLY:HA2 | 1:B:354:LYS:NZ   | 2.04                     | 0.73              |
| 1:D:314:ARG:HD2 | 1:D:404:LEU:HD22 | 1.70                     | 0.73              |
| 1:C:152:TYR:HE1 | 1:C:153:ARG:NH1  | 1.87                     | 0.73              |
| 1:B:18:LEU:HD22 | 1:C:232:GLY:HA2  | 1.70                     | 0.72              |
| 1:C:106:ASP:C   | 1:C:107:LEU:HG   | 2.13                     | 0.72              |
| 1:E:398:LYS:HG2 | 1:E:402:MET:HE2  | 1.70                     | 0.72              |
| 1:D:81:ARG:HB3  | 1:D:208:HIS:HE2  | 1.54                     | 0.72              |
| 1:C:179:ARG:HA  | 1:C:183:ASP:CG   | 2.13                     | 0.72              |
| 1:E:106:ASP:C   | 1:E:107:LEU:HG   | 2.12                     | 0.72              |
| 1:A:47:SER:HB2  | 1:A:50:ASP:HB2   | 1.70                     | 0.72              |
| 1:B:152:TYR:CE1 | 1:B:153:ARG:NH1  | 2.57                     | 0.72              |
| 1:D:47:SER:HB2  | 1:D:50:ASP:HB2   | 1.72                     | 0.72              |
| 1:E:179:ARG:HA  | 1:E:183:ASP:CG   | 2.13                     | 0.72              |
| 1:C:43:ASN:HA   | 1:C:112:ALA:H    | 1.55                     | 0.72              |
| 1:E:172:GLU:HB3 | 1:E:173:PRO:HD3  | 1.70                     | 0.72              |
| 1:A:172:GLU:HB3 | 1:A:173:PRO:HD3  | 1.70                     | 0.72              |
| 1:A:388:LYS:HE2 | 1:B:340:SER:HB2  | 1.72                     | 0.72              |
| 1:C:399:ARG:HA  | 1:C:402:MET:HE3  | 1.71                     | 0.72              |
| 1:B:172:GLU:HB3 | 1:B:173:PRO:HD3  | 1.71                     | 0.71              |
| 1:E:152:TYR:CE1 | 1:E:153:ARG:NH1  | 2.57                     | 0.71              |
| 1:A:399:ARG:HA  | 1:A:402:MET:HE3  | 1.71                     | 0.71              |
| 1:E:199:ASP:HB2 | 1:E:217:THR:HG23 | 1.73                     | 0.71              |
| 1:A:299:PHE:HE1 | 1:A:328:THR:HG22 | 1.56                     | 0.71              |
| 1:A:299:PHE:CE1 | 1:A:328:THR:HG22 | 2.26                     | 0.70              |
| 1:B:43:ASN:HA   | 1:B:112:ALA:H    | 1.53                     | 0.70              |
| 1:D:398:LYS:HG2 | 1:D:402:MET:HE2  | 1.73                     | 0.70              |
| 1:B:399:ARG:HA  | 1:B:402:MET:HE3  | 1.72                     | 0.70              |
| 1:A:179:ARG:HA  | 1:A:183:ASP:CG   | 2.15                     | 0.70              |
| 1:D:179:ARG:HA  | 1:D:183:ASP:CG   | 2.17                     | 0.70              |
| 1:E:314:ARG:HD2 | 1:E:404:LEU:HD22 | 1.74                     | 0.70              |
| 1:A:422:LYS:HA  | 1:A:422:LYS:NZ   | 2.06                     | 0.70              |
| 1:C:29:ALA:H    | 1:C:266:GLN:HE22 | 1.40                     | 0.70              |
| 1:E:88:TRP:CE2  | 1:E:95:ILE:HD11  | 2.27                     | 0.70              |
| 1:C:314:ARG:HD2 | 1:C:404:LEU:HD22 | 1.73                     | 0.70              |
| 1:B:177:GLU:HG2 | 1:B:183:ASP:OD1  | 1.91                     | 0.69              |
| 1:D:399:ARG:HA  | 1:D:402:MET:HE3  | 1.73                     | 0.69              |
| 1:B:34:LYS:HD2  | 1:B:34:LYS:N     | 2.08                     | 0.69              |
| 1:C:105:PHE:C   | 1:C:107:LEU:H    | 2.01                     | 0.69              |
| 1:C:34:LYS:HD2  | 1:C:34:LYS:N     | 2.07                     | 0.69              |
| 1:B:422:LYS:NZ  | 1:B:422:LYS:HA   | 2.08                     | 0.69              |
| 1:C:177:GLU:HG2 | 1:C:183:ASP:OD1  | 1.92                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:105:PHE:C    | 1:A:107:LEU:H    | 2.00                     | 0.68              |
| 1:C:308:LEU:O    | 1:C:309:ARG:HB2  | 1.92                     | 0.68              |
| 1:B:105:PHE:C    | 1:B:107:LEU:H    | 2.01                     | 0.68              |
| 1:C:398:LYS:HG2  | 1:C:402:MET:HE2  | 1.73                     | 0.68              |
| 1:A:88:TRP:CE2   | 1:A:95:ILE:HD11  | 2.28                     | 0.68              |
| 1:A:376:VAL:CG1  | 1:B:354:LYS:HB2  | 2.19                     | 0.68              |
| 1:B:179:ARG:HA   | 1:B:183:ASP:CG   | 2.18                     | 0.68              |
| 1:B:97:LYS:O     | 1:B:98:ALA:C     | 2.37                     | 0.68              |
| 1:B:380:GLY:HA2  | 1:C:354:LYS:HZ3  | 1.56                     | 0.68              |
| 1:D:2:SER:CA     | 1:D:3:VAL:HG23   | 2.23                     | 0.67              |
| 1:E:177:GLU:HG2  | 1:E:183:ASP:OD1  | 1.94                     | 0.67              |
| 1:A:177:GLU:HG2  | 1:A:183:ASP:OD1  | 1.94                     | 0.67              |
| 1:D:117:LEU:CB   | 1:D:118:PRO:HD2  | 2.18                     | 0.67              |
| 1:B:88:TRP:CE2   | 1:B:95:ILE:HD11  | 2.29                     | 0.67              |
| 1:A:152:TYR:HE1  | 1:A:153:ARG:NH1  | 1.91                     | 0.67              |
| 1:C:199:ASP:HB2  | 1:C:217:THR:HG23 | 1.76                     | 0.67              |
| 1:D:299:PHE:CE1  | 1:D:328:THR:HG22 | 2.29                     | 0.67              |
| 1:E:385:GLN:HG2  | 1:E:390:THR:CG2  | 2.25                     | 0.67              |
| 1:C:388:LYS:HE2  | 1:D:340:SER:HB2  | 1.77                     | 0.67              |
| 1:D:34:LYS:HD2   | 1:D:34:LYS:N     | 2.10                     | 0.67              |
| 1:D:51:LEU:O     | 1:D:55:VAL:HG22  | 1.95                     | 0.67              |
| 1:B:314:ARG:HD2  | 1:B:404:LEU:HD22 | 1.75                     | 0.67              |
| 1:D:97:LYS:O     | 1:D:98:ALA:C     | 2.37                     | 0.67              |
| 1:D:152:TYR:CE1  | 1:D:153:ARG:NH1  | 2.61                     | 0.67              |
| 1:D:105:PHE:C    | 1:D:107:LEU:H    | 2.03                     | 0.67              |
| 1:C:45:THR:C     | 1:C:46:LYS:HD2   | 2.19                     | 0.66              |
| 1:D:299:PHE:HE1  | 1:D:328:THR:HG22 | 1.58                     | 0.66              |
| 1:B:117:LEU:CB   | 1:B:118:PRO:HD2  | 2.18                     | 0.66              |
| 1:B:141:LEU:HD13 | 1:B:182:PHE:CD2  | 2.28                     | 0.66              |
| 1:B:398:LYS:HG2  | 1:B:402:MET:HE2  | 1.75                     | 0.66              |
| 1:C:141:LEU:HD13 | 1:C:182:PHE:CD2  | 2.29                     | 0.66              |
| 1:B:299:PHE:HE1  | 1:B:328:THR:HG22 | 1.60                     | 0.66              |
| 1:B:299:PHE:CE1  | 1:B:328:THR:HG22 | 2.30                     | 0.66              |
| 1:E:299:PHE:CE1  | 1:E:328:THR:HG22 | 2.30                     | 0.66              |
| 1:E:152:TYR:HE1  | 1:E:153:ARG:NH1  | 1.91                     | 0.66              |
| 1:E:34:LYS:N     | 1:E:34:LYS:HD2   | 2.10                     | 0.66              |
| 1:E:105:PHE:C    | 1:E:107:LEU:H    | 2.03                     | 0.66              |
| 1:C:181:ILE:HD12 | 1:C:181:ILE:N    | 2.08                     | 0.66              |
| 1:C:376:VAL:CG1  | 1:D:354:LYS:HB2  | 2.17                     | 0.66              |
| 1:B:152:TYR:HE1  | 1:B:153:ARG:NH1  | 1.92                     | 0.66              |
| 1:A:81:ARG:HB3   | 1:A:208:HIS:HE2  | 1.60                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:267:GLU:OE2  | 1:C:273:SER:HB2  | 1.95                     | 0.65              |
| 1:D:81:ARG:CB    | 1:D:208:HIS:HE2  | 2.08                     | 0.65              |
| 1:D:83:LYS:HE2   | 1:D:101:THR:HG22 | 1.79                     | 0.65              |
| 1:B:81:ARG:CB    | 1:B:208:HIS:HE2  | 2.10                     | 0.65              |
| 1:C:299:PHE:HE1  | 1:C:328:THR:HG22 | 1.62                     | 0.65              |
| 1:D:2:SER:N      | 1:D:3:VAL:CG2    | 2.53                     | 0.65              |
| 1:C:97:LYS:O     | 1:C:98:ALA:C     | 2.39                     | 0.65              |
| 1:A:288:PRO:HG2  | 1:A:289:TYR:CE2  | 2.32                     | 0.65              |
| 1:D:126:ARG:HD3  | 1:D:127:THR:N    | 2.12                     | 0.65              |
| 1:C:299:PHE:CE1  | 1:C:328:THR:HG22 | 2.32                     | 0.65              |
| 1:D:385:GLN:HG2  | 1:D:390:THR:CG2  | 2.26                     | 0.65              |
| 1:D:422:LYS:NZ   | 1:D:422:LYS:HA   | 2.12                     | 0.65              |
| 1:E:45:THR:C     | 1:E:46:LYS:HD2   | 2.22                     | 0.65              |
| 1:A:29:ALA:H     | 1:A:266:GLN:HE22 | 1.44                     | 0.65              |
| 1:A:79:ASP:O     | 1:A:79:ASP:OD2   | 2.15                     | 0.65              |
| 1:A:34:LYS:HD2   | 1:A:34:LYS:N     | 2.11                     | 0.65              |
| 1:A:267:GLU:OE2  | 1:A:273:SER:HB2  | 1.97                     | 0.65              |
| 1:C:184:VAL:CG1  | 1:D:165:LYS:HA   | 2.27                     | 0.65              |
| 1:D:136:LEU:HD23 | 1:D:136:LEU:O    | 1.96                     | 0.65              |
| 1:E:267:GLU:OE2  | 1:E:273:SER:HB2  | 1.96                     | 0.64              |
| 1:B:51:LEU:O     | 1:B:55:VAL:HG22  | 1.96                     | 0.64              |
| 1:D:50:ASP:OD1   | 1:D:121:VAL:HA   | 1.97                     | 0.64              |
| 1:D:141:LEU:HD13 | 1:D:182:PHE:CD2  | 2.31                     | 0.64              |
| 1:A:385:GLN:HG2  | 1:A:390:THR:CG2  | 2.26                     | 0.64              |
| 1:A:81:ARG:CB    | 1:A:208:HIS:HE2  | 2.09                     | 0.64              |
| 1:C:88:TRP:CE2   | 1:C:95:ILE:HD11  | 2.32                     | 0.64              |
| 1:D:79:ASP:O     | 1:D:79:ASP:OD2   | 2.16                     | 0.64              |
| 1:E:97:LYS:O     | 1:E:98:ALA:C     | 2.40                     | 0.64              |
| 1:B:238:THR:HG22 | 1:B:308:LEU:HD23 | 1.78                     | 0.64              |
| 1:D:177:GLU:HG2  | 1:D:183:ASP:OD1  | 1.98                     | 0.64              |
| 1:A:97:LYS:O     | 1:A:98:ALA:C     | 2.40                     | 0.64              |
| 1:E:81:ARG:CB    | 1:E:208:HIS:HE2  | 2.10                     | 0.64              |
| 1:B:181:ILE:HD12 | 1:B:181:ILE:N    | 2.13                     | 0.64              |
| 1:E:81:ARG:HB3   | 1:E:208:HIS:HE2  | 1.63                     | 0.64              |
| 1:E:117:LEU:CB   | 1:E:118:PRO:HD2  | 2.18                     | 0.64              |
| 1:B:79:ASP:O     | 1:B:79:ASP:OD2   | 2.16                     | 0.63              |
| 1:C:81:ARG:HB3   | 1:C:208:HIS:HE2  | 1.62                     | 0.63              |
| 1:C:422:LYS:HA   | 1:C:422:LYS:NZ   | 2.12                     | 0.63              |
| 1:A:182:PHE:HD1  | 1:A:183:ASP:N    | 1.95                     | 0.63              |
| 1:A:340:SER:HB2  | 1:E:388:LYS:HE2  | 1.78                     | 0.63              |
| 1:B:308:LEU:O    | 1:B:309:ARG:HB2  | 1.98                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:385:GLN:HG2  | 1:C:390:THR:CG2  | 2.28                     | 0.63              |
| 1:D:152:TYR:HE1  | 1:D:153:ARG:NH1  | 1.96                     | 0.63              |
| 1:E:354:LYS:HE3  | 1:E:356:THR:HA   | 1.80                     | 0.63              |
| 1:C:81:ARG:CB    | 1:C:208:HIS:HE2  | 2.10                     | 0.63              |
| 1:B:385:GLN:HG2  | 1:B:390:THR:CG2  | 2.26                     | 0.63              |
| 1:E:159:GLY:O    | 1:E:163:GLN:NE2  | 2.31                     | 0.63              |
| 1:B:29:ALA:C     | 1:B:31:TYR:H     | 2.06                     | 0.63              |
| 1:B:81:ARG:HB3   | 1:B:208:HIS:HE2  | 1.63                     | 0.63              |
| 1:C:354:LYS:HE3  | 1:C:356:THR:HA   | 1.81                     | 0.63              |
| 1:B:267:GLU:OE2  | 1:B:273:SER:HB2  | 1.97                     | 0.63              |
| 1:C:79:ASP:O     | 1:C:79:ASP:OD2   | 2.16                     | 0.63              |
| 1:A:199:ASP:HB2  | 1:A:217:THR:HG23 | 1.80                     | 0.63              |
| 1:A:308:LEU:O    | 1:A:309:ARG:HB2  | 1.98                     | 0.63              |
| 1:C:238:THR:HG22 | 1:C:308:LEU:HD23 | 1.81                     | 0.62              |
| 1:D:267:GLU:OE2  | 1:D:273:SER:HB2  | 1.99                     | 0.62              |
| 1:D:152:TYR:CE1  | 1:D:177:GLU:HB2  | 2.34                     | 0.62              |
| 1:D:328:THR:HG21 | 1:D:415:TYR:OH   | 1.99                     | 0.62              |
| 1:A:141:LEU:HD13 | 1:A:182:PHE:CD2  | 2.32                     | 0.62              |
| 1:D:29:ALA:C     | 1:D:31:TYR:H     | 2.07                     | 0.62              |
| 1:D:159:GLY:O    | 1:D:163:GLN:NE2  | 2.32                     | 0.62              |
| 1:A:181:ILE:HD12 | 1:A:181:ILE:N    | 2.13                     | 0.62              |
| 1:B:45:THR:C     | 1:B:46:LYS:HD2   | 2.24                     | 0.62              |
| 1:B:66:ILE:HD12  | 1:B:69:VAL:CG2   | 2.29                     | 0.62              |
| 1:E:422:LYS:NZ   | 1:E:422:LYS:HA   | 2.15                     | 0.62              |
| 1:E:141:LEU:HD13 | 1:E:182:PHE:CD2  | 2.30                     | 0.62              |
| 1:A:238:THR:HG22 | 1:A:308:LEU:HD23 | 1.81                     | 0.62              |
| 1:A:354:LYS:HE3  | 1:A:356:THR:HA   | 1.82                     | 0.62              |
| 1:C:159:GLY:O    | 1:C:163:GLN:NE2  | 2.32                     | 0.62              |
| 1:D:29:ALA:H     | 1:D:266:GLN:HE22 | 1.48                     | 0.62              |
| 1:A:45:THR:C     | 1:A:46:LYS:HD2   | 2.24                     | 0.62              |
| 1:D:181:ILE:HD12 | 1:D:181:ILE:N    | 2.14                     | 0.62              |
| 1:E:29:ALA:C     | 1:E:31:TYR:H     | 2.08                     | 0.62              |
| 1:E:299:PHE:HE1  | 1:E:328:THR:HG22 | 1.64                     | 0.62              |
| 1:B:288:PRO:HG2  | 1:B:289:TYR:CE2  | 2.34                     | 0.61              |
| 1:C:51:LEU:O     | 1:C:55:VAL:HG22  | 2.00                     | 0.61              |
| 1:C:83:LYS:HE2   | 1:C:101:THR:HG22 | 1.82                     | 0.61              |
| 1:E:83:LYS:HE2   | 1:E:101:THR:HG22 | 1.82                     | 0.61              |
| 1:B:50:ASP:OD1   | 1:B:121:VAL:HA   | 1.99                     | 0.61              |
| 1:B:126:ARG:HD3  | 1:B:127:THR:N    | 2.16                     | 0.61              |
| 1:B:152:TYR:CE1  | 1:B:177:GLU:HB2  | 2.35                     | 0.61              |
| 1:C:172:GLU:HB3  | 1:C:173:PRO:CD   | 2.29                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:261:MET:HE1  | 1:C:297:PHE:CD2  | 2.35                     | 0.61              |
| 1:B:354:LYS:HE3  | 1:B:356:THR:HA   | 1.83                     | 0.61              |
| 1:B:380:GLY:HA2  | 1:C:354:LYS:HZ2  | 1.64                     | 0.61              |
| 1:D:199:ASP:HB2  | 1:D:217:THR:HG23 | 1.83                     | 0.61              |
| 1:D:389:PRO:HA   | 1:D:393:MET:HE2  | 1.83                     | 0.61              |
| 1:E:29:ALA:H     | 1:E:266:GLN:HE22 | 1.47                     | 0.61              |
| 1:E:281:PHE:HB3  | 1:E:283:LEU:HD21 | 1.83                     | 0.61              |
| 1:B:136:LEU:HD23 | 1:B:136:LEU:O    | 2.01                     | 0.61              |
| 1:E:182:PHE:HD1  | 1:E:183:ASP:N    | 1.99                     | 0.61              |
| 1:E:42:ILE:HD12  | 1:E:74:TYR:HB2   | 1.82                     | 0.61              |
| 1:A:117:LEU:CB   | 1:A:118:PRO:HD2  | 2.18                     | 0.61              |
| 1:C:182:PHE:HD1  | 1:C:183:ASP:N    | 1.99                     | 0.61              |
| 1:D:172:GLU:HB3  | 1:D:173:PRO:CD   | 2.31                     | 0.61              |
| 1:C:376:VAL:HG13 | 1:D:354:LYS:CB   | 2.18                     | 0.60              |
| 1:D:401:VAL:HG21 | 1:D:420:PHE:HB2  | 1.82                     | 0.60              |
| 1:E:66:ILE:HD12  | 1:E:69:VAL:CG2   | 2.31                     | 0.60              |
| 1:E:136:LEU:O    | 1:E:136:LEU:HD23 | 2.01                     | 0.60              |
| 1:E:172:GLU:HB3  | 1:E:173:PRO:CD   | 2.30                     | 0.60              |
| 1:C:389:PRO:HA   | 1:C:393:MET:HE2  | 1.83                     | 0.60              |
| 1:B:38:ILE:O     | 1:B:108:VAL:HB   | 2.00                     | 0.60              |
| 1:C:117:LEU:CB   | 1:C:118:PRO:HD2  | 2.17                     | 0.60              |
| 1:D:33:ARG:NH1   | 1:D:33:ARG:HG2   | 2.15                     | 0.60              |
| 1:E:166:MET:O    | 1:E:167:ILE:HG23 | 2.01                     | 0.60              |
| 1:A:29:ALA:C     | 1:A:31:TYR:H     | 2.09                     | 0.60              |
| 1:B:159:GLY:O    | 1:B:163:GLN:NE2  | 2.35                     | 0.60              |
| 1:C:42:ILE:HD12  | 1:C:74:TYR:HB2   | 1.83                     | 0.60              |
| 1:A:83:LYS:HE2   | 1:A:101:THR:HG22 | 1.84                     | 0.60              |
| 1:E:79:ASP:O     | 1:E:79:ASP:OD2   | 2.19                     | 0.60              |
| 1:E:303:LEU:HA   | 1:E:412:ILE:HD13 | 1.83                     | 0.60              |
| 1:A:172:GLU:HB3  | 1:A:173:PRO:CD   | 2.30                     | 0.60              |
| 1:C:66:ILE:HD12  | 1:C:69:VAL:CG2   | 2.30                     | 0.60              |
| 1:E:181:ILE:HD12 | 1:E:181:ILE:N    | 2.15                     | 0.60              |
| 1:E:33:ARG:NH1   | 1:E:33:ARG:HG2   | 2.16                     | 0.60              |
| 1:B:172:GLU:HB3  | 1:B:173:PRO:CD   | 2.32                     | 0.60              |
| 1:E:288:PRO:HG2  | 1:E:289:TYR:CE2  | 2.37                     | 0.60              |
| 1:A:51:LEU:O     | 1:A:55:VAL:HG22  | 2.01                     | 0.59              |
| 1:B:199:ASP:HB2  | 1:B:217:THR:HG23 | 1.82                     | 0.59              |
| 1:A:136:LEU:HD23 | 1:A:136:LEU:O    | 2.02                     | 0.59              |
| 1:A:303:LEU:HA   | 1:A:412:ILE:HD13 | 1.83                     | 0.59              |
| 1:B:375:VAL:HG12 | 1:B:379:LEU:HD12 | 1.84                     | 0.59              |
| 1:D:45:THR:C     | 1:D:46:LYS:HD2   | 2.26                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:308:LEU:O    | 1:D:309:ARG:HB2  | 2.01                     | 0.59              |
| 1:E:126:ARG:HD3  | 1:E:127:THR:N    | 2.17                     | 0.59              |
| 1:B:401:VAL:HG21 | 1:B:420:PHE:HB2  | 1.85                     | 0.59              |
| 1:C:136:LEU:O    | 1:C:136:LEU:HD23 | 2.02                     | 0.59              |
| 1:D:33:ARG:HG2   | 1:D:33:ARG:HH11  | 1.66                     | 0.59              |
| 1:B:129:ALA:HB1  | 1:B:133:TRP:NE1  | 2.12                     | 0.59              |
| 1:B:141:LEU:HD22 | 1:B:182:PHE:CE2  | 2.37                     | 0.59              |
| 1:C:166:MET:O    | 1:C:167:ILE:HG23 | 2.02                     | 0.59              |
| 1:E:152:TYR:CE1  | 1:E:177:GLU:HB2  | 2.37                     | 0.59              |
| 1:E:328:THR:HG21 | 1:E:415:TYR:OH   | 2.03                     | 0.59              |
| 1:A:152:TYR:CE1  | 1:A:177:GLU:HB2  | 2.37                     | 0.59              |
| 1:B:166:MET:O    | 1:B:167:ILE:HG23 | 2.02                     | 0.59              |
| 1:D:365:THR:HG23 | 1:D:366:THR:N    | 2.16                     | 0.59              |
| 1:A:328:THR:HG21 | 1:A:415:TYR:OH   | 2.03                     | 0.59              |
| 1:C:152:TYR:CE1  | 1:C:177:GLU:HB2  | 2.38                     | 0.59              |
| 1:A:129:ALA:HB1  | 1:A:133:TRP:NE1  | 2.13                     | 0.59              |
| 1:C:288:PRO:HG2  | 1:C:289:TYR:CE2  | 2.38                     | 0.59              |
| 1:C:328:THR:HG21 | 1:C:415:TYR:OH   | 2.03                     | 0.59              |
| 1:D:31:TYR:C     | 1:D:31:TYR:CD1   | 2.80                     | 0.59              |
| 1:D:129:ALA:HB1  | 1:D:133:TRP:NE1  | 2.10                     | 0.59              |
| 1:B:83:LYS:HE2   | 1:B:101:THR:HG22 | 1.85                     | 0.59              |
| 1:D:354:LYS:HE3  | 1:D:356:THR:HA   | 1.85                     | 0.59              |
| 1:A:375:VAL:HG12 | 1:A:379:LEU:HD12 | 1.85                     | 0.58              |
| 1:B:17:LYS:HG3   | 1:C:268:ILE:HD11 | 1.85                     | 0.58              |
| 1:C:126:ARG:HD3  | 1:C:127:THR:N    | 2.16                     | 0.58              |
| 1:A:159:GLY:O    | 1:A:163:GLN:NE2  | 2.36                     | 0.58              |
| 1:C:42:ILE:HD12  | 1:C:74:TYR:CD2   | 2.38                     | 0.58              |
| 1:D:281:PHE:HB3  | 1:D:283:LEU:HD21 | 1.85                     | 0.58              |
| 1:E:51:LEU:O     | 1:E:55:VAL:HG22  | 2.03                     | 0.58              |
| 1:E:261:MET:HE1  | 1:E:297:PHE:CD2  | 2.38                     | 0.58              |
| 1:B:182:PHE:HD1  | 1:B:183:ASP:N    | 2.01                     | 0.58              |
| 1:D:42:ILE:HD12  | 1:D:74:TYR:HB2   | 1.85                     | 0.58              |
| 1:D:288:PRO:HG2  | 1:D:289:TYR:CE2  | 2.39                     | 0.58              |
| 1:A:214:ARG:CA   | 1:A:217:THR:HG22 | 2.22                     | 0.58              |
| 1:D:238:THR:HG22 | 1:D:308:LEU:HD23 | 1.83                     | 0.58              |
| 1:A:126:ARG:HD3  | 1:A:127:THR:N    | 2.16                     | 0.58              |
| 1:A:422:LYS:HA   | 1:A:422:LYS:CE   | 2.33                     | 0.58              |
| 1:E:31:TYR:CD1   | 1:E:31:TYR:C     | 2.81                     | 0.58              |
| 1:A:66:ILE:HD12  | 1:A:69:VAL:CG2   | 2.33                     | 0.58              |
| 1:B:31:TYR:CD1   | 1:B:31:TYR:C     | 2.81                     | 0.58              |
| 1:C:33:ARG:NH1   | 1:C:33:ARG:HG2   | 2.18                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:238:THR:HG22 | 1:E:308:LEU:HD23 | 1.85                     | 0.58              |
| 1:A:33:ARG:NH1   | 1:A:33:ARG:HG2   | 2.18                     | 0.57              |
| 1:B:356:THR:CG2  | 1:B:357:PRO:HD3  | 2.28                     | 0.57              |
| 1:D:182:PHE:HD1  | 1:D:183:ASP:N    | 2.01                     | 0.57              |
| 1:A:356:THR:CG2  | 1:A:357:PRO:HD3  | 2.28                     | 0.57              |
| 1:B:389:PRO:HA   | 1:B:393:MET:HE2  | 1.85                     | 0.57              |
| 1:A:281:PHE:HB3  | 1:A:283:LEU:HD21 | 1.87                     | 0.57              |
| 1:B:281:PHE:HB3  | 1:B:283:LEU:HD21 | 1.86                     | 0.57              |
| 1:A:50:ASP:OD1   | 1:A:121:VAL:HA   | 2.04                     | 0.57              |
| 1:C:42:ILE:CD1   | 1:C:74:TYR:HB2   | 2.35                     | 0.57              |
| 1:A:261:MET:HE1  | 1:A:297:PHE:CD2  | 2.39                     | 0.57              |
| 1:D:88:TRP:CE2   | 1:D:95:ILE:HD11  | 2.40                     | 0.57              |
| 1:B:33:ARG:HG2   | 1:B:33:ARG:HH11  | 1.70                     | 0.57              |
| 1:C:141:LEU:HD22 | 1:C:182:PHE:CE2  | 2.39                     | 0.57              |
| 1:D:141:LEU:HD22 | 1:D:182:PHE:CE2  | 2.40                     | 0.57              |
| 1:E:38:ILE:O     | 1:E:108:VAL:HB   | 2.05                     | 0.57              |
| 1:E:308:LEU:O    | 1:E:309:ARG:HB2  | 2.05                     | 0.56              |
| 1:C:303:LEU:HA   | 1:C:412:ILE:HD13 | 1.85                     | 0.56              |
| 1:D:240:MET:HE2  | 1:D:244:ASP:HB3  | 1.87                     | 0.56              |
| 1:A:33:ARG:HG2   | 1:A:33:ARG:HH11  | 1.70                     | 0.56              |
| 1:B:42:ILE:HD12  | 1:B:74:TYR:HB2   | 1.85                     | 0.56              |
| 1:B:188:ASP:HA   | 1:C:166:MET:HE1  | 1.87                     | 0.56              |
| 1:C:33:ARG:HG2   | 1:C:33:ARG:HH11  | 1.70                     | 0.56              |
| 1:C:29:ALA:C     | 1:C:31:TYR:H     | 2.14                     | 0.56              |
| 1:D:66:ILE:HD12  | 1:D:69:VAL:CG2   | 2.35                     | 0.56              |
| 1:E:50:ASP:OD1   | 1:E:121:VAL:HA   | 2.05                     | 0.56              |
| 1:E:214:ARG:CA   | 1:E:217:THR:HG22 | 2.24                     | 0.56              |
| 1:B:33:ARG:HG2   | 1:B:33:ARG:NH1   | 2.19                     | 0.56              |
| 1:D:422:LYS:HA   | 1:D:422:LYS:CE   | 2.36                     | 0.56              |
| 1:A:42:ILE:HD12  | 1:A:74:TYR:HB2   | 1.86                     | 0.56              |
| 1:B:422:LYS:HA   | 1:B:422:LYS:CE   | 2.35                     | 0.56              |
| 1:A:376:VAL:HG13 | 1:B:354:LYS:CB   | 2.21                     | 0.56              |
| 1:B:29:ALA:H     | 1:B:266:GLN:HE22 | 1.52                     | 0.56              |
| 1:B:342:ALA:HB1  | 1:B:344:LEU:HD23 | 1.87                     | 0.56              |
| 1:C:31:TYR:CD1   | 1:C:31:TYR:C     | 2.84                     | 0.56              |
| 1:D:356:THR:CG2  | 1:D:357:PRO:HD3  | 2.29                     | 0.56              |
| 1:E:422:LYS:HA   | 1:E:422:LYS:CE   | 2.36                     | 0.56              |
| 1:A:31:TYR:CD1   | 1:A:31:TYR:C     | 2.84                     | 0.55              |
| 1:A:166:MET:O    | 1:A:167:ILE:HG23 | 2.06                     | 0.55              |
| 1:C:422:LYS:HA   | 1:C:422:LYS:CE   | 2.36                     | 0.55              |
| 1:A:43:ASN:HB3   | 1:A:112:ALA:O    | 2.06                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:328:THR:HG21 | 1:B:415:TYR:OH   | 2.06                     | 0.55              |
| 1:D:153:ARG:HH21 | 1:D:171:PHE:HZ   | 1.55                     | 0.55              |
| 1:E:33:ARG:HG2   | 1:E:33:ARG:HH11  | 1.69                     | 0.55              |
| 1:D:166:MET:O    | 1:D:167:ILE:HG23 | 2.06                     | 0.55              |
| 1:B:365:THR:HG23 | 1:B:366:THR:N    | 2.14                     | 0.55              |
| 1:C:38:ILE:O     | 1:C:108:VAL:HB   | 2.04                     | 0.55              |
| 1:A:38:ILE:O     | 1:A:108:VAL:HB   | 2.06                     | 0.55              |
| 1:D:38:ILE:O     | 1:D:108:VAL:HB   | 2.06                     | 0.55              |
| 1:D:257:GLU:O    | 1:D:261:MET:HG3  | 2.07                     | 0.55              |
| 1:E:42:ILE:CD1   | 1:E:74:TYR:HB2   | 2.36                     | 0.55              |
| 1:A:409:GLU:O    | 1:A:410:LYS:HB2  | 2.06                     | 0.55              |
| 1:E:141:LEU:HD22 | 1:E:182:PHE:CE2  | 2.42                     | 0.55              |
| 1:C:409:GLU:O    | 1:C:410:LYS:HB2  | 2.07                     | 0.55              |
| 1:A:401:VAL:HG21 | 1:A:420:PHE:HB2  | 1.90                     | 0.54              |
| 1:A:380:GLY:HA2  | 1:B:354:LYS:HZ3  | 1.71                     | 0.54              |
| 1:A:389:PRO:HB3  | 1:A:393:MET:HE2  | 1.89                     | 0.54              |
| 1:B:43:ASN:CA    | 1:B:112:ALA:H    | 2.20                     | 0.54              |
| 1:A:342:ALA:HB1  | 1:A:344:LEU:HD23 | 1.89                     | 0.54              |
| 1:C:302:GLN:HG2  | 1:C:316:ALA:CB   | 2.36                     | 0.54              |
| 1:C:342:ALA:HB1  | 1:C:344:LEU:HD23 | 1.89                     | 0.54              |
| 1:E:104:ILE:HD13 | 1:E:198:VAL:HG22 | 1.89                     | 0.54              |
| 1:B:188:ASP:OD1  | 1:C:166:MET:HE3  | 2.07                     | 0.54              |
| 1:B:383:GLU:HG3  | 1:C:354:LYS:HE2  | 1.89                     | 0.54              |
| 1:C:50:ASP:OD1   | 1:C:121:VAL:HA   | 2.07                     | 0.54              |
| 1:D:153:ARG:NH2  | 1:D:171:PHE:HZ   | 2.05                     | 0.54              |
| 1:E:409:GLU:O    | 1:E:410:LYS:HB2  | 2.07                     | 0.54              |
| 1:B:42:ILE:CD1   | 1:B:74:TYR:HB2   | 2.38                     | 0.54              |
| 1:B:66:ILE:HD12  | 1:B:69:VAL:HG21  | 1.88                     | 0.54              |
| 1:C:175:VAL:HG13 | 1:C:181:ILE:HG12 | 1.88                     | 0.54              |
| 1:E:302:GLN:HG2  | 1:E:316:ALA:CB   | 2.38                     | 0.54              |
| 1:E:43:ASN:CA    | 1:E:112:ALA:H    | 2.20                     | 0.53              |
| 1:B:18:LEU:HD22  | 1:C:232:GLY:CA   | 2.38                     | 0.53              |
| 1:E:401:VAL:HG21 | 1:E:420:PHE:HB2  | 1.91                     | 0.53              |
| 1:C:129:ALA:HB1  | 1:C:133:TRP:NE1  | 2.14                     | 0.53              |
| 1:C:401:VAL:HG21 | 1:C:420:PHE:HB2  | 1.89                     | 0.53              |
| 1:D:107:LEU:CD2  | 1:D:274:TYR:OH   | 2.57                     | 0.53              |
| 1:B:240:MET:HE2  | 1:B:244:ASP:HB3  | 1.91                     | 0.53              |
| 1:C:257:GLU:O    | 1:C:261:MET:HG3  | 2.09                     | 0.53              |
| 1:D:29:ALA:O     | 1:D:31:TYR:N     | 2.42                     | 0.53              |
| 1:D:214:ARG:CA   | 1:D:217:THR:HG22 | 2.27                     | 0.53              |
| 1:D:261:MET:HE1  | 1:D:297:PHE:CD2  | 2.42                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:199:ASP:CB   | 1:E:217:THR:HG23 | 2.39                     | 0.53              |
| 1:B:303:LEU:HA   | 1:B:412:ILE:HD13 | 1.89                     | 0.53              |
| 1:C:123:ASP:N    | 1:C:123:ASP:OD1  | 2.42                     | 0.53              |
| 1:C:163:GLN:O    | 1:C:167:ILE:HG13 | 2.09                     | 0.53              |
| 1:C:375:VAL:HG12 | 1:C:379:LEU:HD12 | 1.91                     | 0.53              |
| 1:E:356:THR:CG2  | 1:E:357:PRO:HD3  | 2.30                     | 0.53              |
| 1:D:42:ILE:CD1   | 1:D:74:TYR:HB2   | 2.39                     | 0.53              |
| 1:D:342:ALA:HB1  | 1:D:344:LEU:HD23 | 1.91                     | 0.53              |
| 1:B:153:ARG:NH2  | 1:B:171:PHE:HZ   | 2.07                     | 0.53              |
| 1:A:365:THR:HG23 | 1:A:366:THR:N    | 2.15                     | 0.52              |
| 1:D:308:LEU:HD13 | 1:D:335:ALA:HB1  | 1.91                     | 0.52              |
| 1:A:344:LEU:CD1  | 1:E:250:LEU:HD13 | 2.40                     | 0.52              |
| 1:C:153:ARG:HH21 | 1:C:171:PHE:HZ   | 1.57                     | 0.52              |
| 1:D:163:GLN:O    | 1:D:167:ILE:HG13 | 2.09                     | 0.52              |
| 1:A:43:ASN:CA    | 1:A:112:ALA:H    | 2.20                     | 0.52              |
| 1:B:29:ALA:O     | 1:B:31:TYR:N     | 2.42                     | 0.52              |
| 1:B:42:ILE:HD12  | 1:B:74:TYR:CD2   | 2.44                     | 0.52              |
| 1:C:356:THR:CG2  | 1:C:357:PRO:HD3  | 2.32                     | 0.52              |
| 1:E:75:GLY:HA2   | 1:E:78:LYS:HD2   | 1.91                     | 0.52              |
| 1:E:129:ALA:HB1  | 1:E:133:TRP:NE1  | 2.14                     | 0.52              |
| 1:E:175:VAL:HG13 | 1:E:181:ILE:HG12 | 1.90                     | 0.52              |
| 1:A:175:VAL:HG13 | 1:A:181:ILE:HG12 | 1.91                     | 0.52              |
| 1:A:240:MET:HE2  | 1:A:244:ASP:HB3  | 1.92                     | 0.52              |
| 1:B:56:TYR:CE1   | 1:B:126:ARG:CZ   | 2.92                     | 0.52              |
| 1:E:163:GLN:O    | 1:E:167:ILE:HG13 | 2.09                     | 0.52              |
| 1:E:169:GLU:O    | 1:E:170:GLN:HG2  | 2.08                     | 0.52              |
| 1:A:52:ARG:HD3   | 1:A:127:THR:O    | 2.09                     | 0.52              |
| 1:A:163:GLN:O    | 1:A:167:ILE:HG13 | 2.10                     | 0.52              |
| 1:A:354:LYS:HB2  | 1:E:376:VAL:CG1  | 2.24                     | 0.52              |
| 1:B:106:ASP:O    | 1:B:107:LEU:HG   | 2.09                     | 0.52              |
| 1:C:43:ASN:OD1   | 1:C:112:ALA:HB3  | 2.09                     | 0.52              |
| 1:D:175:VAL:HG13 | 1:D:181:ILE:HG12 | 1.91                     | 0.52              |
| 1:E:109:SER:O    | 1:E:110:LEU:HD23 | 2.09                     | 0.52              |
| 1:A:354:LYS:NZ   | 1:E:380:GLY:HA2  | 2.24                     | 0.52              |
| 1:B:52:ARG:HD3   | 1:B:127:THR:O    | 2.09                     | 0.52              |
| 1:B:153:ARG:HH21 | 1:B:171:PHE:HZ   | 1.57                     | 0.52              |
| 1:D:52:ARG:HD3   | 1:D:127:THR:O    | 2.10                     | 0.52              |
| 1:D:56:TYR:CE1   | 1:D:126:ARG:CZ   | 2.93                     | 0.52              |
| 1:E:375:VAL:HG12 | 1:E:379:LEU:HD12 | 1.92                     | 0.52              |
| 1:E:33:ARG:HH11  | 1:E:33:ARG:CG    | 2.23                     | 0.52              |
| 1:E:317:ARG:O    | 1:E:319:PRO:HD3  | 2.10                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:141:LEU:HD22 | 1:A:182:PHE:CE2  | 2.45                     | 0.51              |
| 1:B:178:GLY:O    | 1:B:179:ARG:HB2  | 2.09                     | 0.51              |
| 1:B:302:GLN:HG2  | 1:B:316:ALA:CB   | 2.40                     | 0.51              |
| 1:C:281:PHE:HB3  | 1:C:283:LEU:HD21 | 1.92                     | 0.51              |
| 1:A:42:ILE:CD1   | 1:A:74:TYR:HB2   | 2.39                     | 0.51              |
| 1:A:66:ILE:HD12  | 1:A:69:VAL:HG21  | 1.91                     | 0.51              |
| 1:A:105:PHE:C    | 1:A:107:LEU:N    | 2.68                     | 0.51              |
| 1:A:107:LEU:CD2  | 1:A:274:TYR:OH   | 2.58                     | 0.51              |
| 1:A:302:GLN:HG2  | 1:A:316:ALA:CB   | 2.39                     | 0.51              |
| 1:C:42:ILE:O     | 1:C:42:ILE:HG22  | 2.09                     | 0.51              |
| 1:D:66:ILE:HD12  | 1:D:69:VAL:HG21  | 1.92                     | 0.51              |
| 1:D:178:GLY:O    | 1:D:179:ARG:HB2  | 2.11                     | 0.51              |
| 1:A:169:GLU:O    | 1:A:170:GLN:HG2  | 2.10                     | 0.51              |
| 1:C:66:ILE:HD12  | 1:C:69:VAL:HG21  | 1.90                     | 0.51              |
| 1:E:42:ILE:O     | 1:E:42:ILE:HG22  | 2.09                     | 0.51              |
| 1:E:52:ARG:HD3   | 1:E:127:THR:O    | 2.10                     | 0.51              |
| 1:E:240:MET:HE2  | 1:E:244:ASP:HB3  | 1.91                     | 0.51              |
| 1:C:52:ARG:HD3   | 1:C:127:THR:O    | 2.10                     | 0.51              |
| 1:C:419:GLU:O    | 1:C:419:GLU:HG3  | 2.11                     | 0.51              |
| 1:D:303:LEU:HA   | 1:D:412:ILE:HD13 | 1.91                     | 0.51              |
| 1:E:342:ALA:HB1  | 1:E:344:LEU:HD23 | 1.92                     | 0.51              |
| 1:C:56:TYR:CE1   | 1:C:126:ARG:CZ   | 2.93                     | 0.51              |
| 1:A:106:ASP:O    | 1:A:107:LEU:HG   | 2.10                     | 0.51              |
| 1:D:33:ARG:HH11  | 1:D:33:ARG:CG    | 2.23                     | 0.51              |
| 1:D:302:GLN:HG2  | 1:D:316:ALA:CB   | 2.40                     | 0.51              |
| 1:E:390:THR:HB   | 1:E:391:PRO:HD2  | 1.93                     | 0.51              |
| 1:C:169:GLU:O    | 1:C:170:GLN:HG2  | 2.10                     | 0.51              |
| 1:D:43:ASN:CA    | 1:D:112:ALA:H    | 2.22                     | 0.51              |
| 1:E:42:ILE:HD12  | 1:E:74:TYR:CD2   | 2.45                     | 0.51              |
| 1:E:43:ASN:OD1   | 1:E:112:ALA:HB3  | 2.11                     | 0.51              |
| 1:A:42:ILE:HD12  | 1:A:74:TYR:CD2   | 2.45                     | 0.51              |
| 1:A:182:PHE:HD1  | 1:A:183:ASP:H    | 1.59                     | 0.51              |
| 1:C:107:LEU:CD2  | 1:C:274:TYR:OH   | 2.59                     | 0.51              |
| 1:D:43:ASN:HB3   | 1:D:112:ALA:O    | 2.11                     | 0.51              |
| 1:D:176:PRO:O    | 1:D:177:GLU:HB2  | 2.11                     | 0.51              |
| 1:E:106:ASP:O    | 1:E:107:LEU:HG   | 2.10                     | 0.51              |
| 1:C:397:ALA:O    | 1:C:401:VAL:HG22 | 2.11                     | 0.51              |
| 1:D:123:ASP:OD1  | 1:D:123:ASP:N    | 2.44                     | 0.51              |
| 1:C:109:SER:O    | 1:C:110:LEU:HD23 | 2.11                     | 0.50              |
| 1:B:169:GLU:O    | 1:B:170:GLN:HG2  | 2.11                     | 0.50              |
| 1:D:375:VAL:HG12 | 1:D:379:LEU:HD12 | 1.92                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:166:MET:C    | 1:A:167:ILE:HG12 | 2.36                     | 0.50              |
| 1:A:257:GLU:O    | 1:A:261:MET:HG3  | 2.12                     | 0.50              |
| 1:A:342:ALA:CB   | 1:A:344:LEU:HD23 | 2.40                     | 0.50              |
| 1:D:79:ASP:C     | 1:D:81:ARG:H     | 2.20                     | 0.50              |
| 1:B:130:ASP:CG   | 1:B:131:ASP:H    | 2.18                     | 0.50              |
| 1:B:166:MET:C    | 1:B:167:ILE:HG12 | 2.34                     | 0.50              |
| 1:B:342:ALA:CB   | 1:B:344:LEU:HD23 | 2.41                     | 0.50              |
| 1:C:43:ASN:CA    | 1:C:112:ALA:H    | 2.23                     | 0.50              |
| 1:E:107:LEU:CD2  | 1:E:274:TYR:OH   | 2.59                     | 0.50              |
| 1:A:43:ASN:HB3   | 1:A:112:ALA:C    | 2.37                     | 0.50              |
| 1:A:161:THR:HG22 | 1:E:179:ARG:O    | 2.12                     | 0.50              |
| 1:A:389:PRO:HA   | 1:A:393:MET:HE2  | 1.93                     | 0.50              |
| 1:B:175:VAL:HG13 | 1:B:181:ILE:HG12 | 1.92                     | 0.50              |
| 1:B:261:MET:HE1  | 1:B:297:PHE:CD2  | 2.46                     | 0.50              |
| 1:C:196:ALA:HB3  | 1:C:281:PHE:CE1  | 2.47                     | 0.50              |
| 1:E:123:ASP:OD1  | 1:E:123:ASP:N    | 2.43                     | 0.50              |
| 1:A:42:ILE:HG22  | 1:A:42:ILE:O     | 2.11                     | 0.50              |
| 1:A:79:ASP:C     | 1:A:81:ARG:H     | 2.20                     | 0.50              |
| 1:E:389:PRO:HA   | 1:E:393:MET:HE2  | 1.92                     | 0.50              |
| 1:C:130:ASP:CG   | 1:C:131:ASP:H    | 2.19                     | 0.50              |
| 1:E:153:ARG:NH2  | 1:E:171:PHE:HZ   | 2.10                     | 0.50              |
| 1:B:105:PHE:C    | 1:B:107:LEU:N    | 2.70                     | 0.50              |
| 1:B:42:ILE:HG22  | 1:B:42:ILE:O     | 2.12                     | 0.50              |
| 1:B:163:GLN:O    | 1:B:167:ILE:HG13 | 2.11                     | 0.50              |
| 1:C:342:ALA:CB   | 1:C:344:LEU:HD23 | 2.42                     | 0.50              |
| 1:E:142:TYR:CD1  | 1:E:195:VAL:HG11 | 2.46                     | 0.50              |
| 1:E:166:MET:C    | 1:E:167:ILE:HG12 | 2.35                     | 0.50              |
| 1:A:75:GLY:HA2   | 1:A:78:LYS:HD2   | 1.93                     | 0.49              |
| 1:B:376:VAL:HG21 | 1:C:352:ASP:OD1  | 2.11                     | 0.49              |
| 1:C:75:GLY:HA2   | 1:C:78:LYS:HD2   | 1.94                     | 0.49              |
| 1:C:415:TYR:C    | 1:C:415:TYR:CD1  | 2.89                     | 0.49              |
| 1:A:123:ASP:N    | 1:A:123:ASP:OD1  | 2.44                     | 0.49              |
| 1:D:25:VAL:HG21  | 1:D:288:PRO:HB3  | 1.93                     | 0.49              |
| 1:E:257:GLU:O    | 1:E:261:MET:HG3  | 2.12                     | 0.49              |
| 1:A:283:LEU:N    | 1:A:283:LEU:HD23 | 2.28                     | 0.49              |
| 1:B:176:PRO:O    | 1:B:177:GLU:HB2  | 2.11                     | 0.49              |
| 1:B:397:ALA:O    | 1:B:401:VAL:HG22 | 2.12                     | 0.49              |
| 1:D:43:ASN:OD1   | 1:D:112:ALA:HB3  | 2.12                     | 0.49              |
| 1:D:126:ARG:CD   | 1:D:127:THR:N    | 2.75                     | 0.49              |
| 1:D:151:GLU:O    | 1:D:154:LYS:HB3  | 2.13                     | 0.49              |
| 1:A:130:ASP:CG   | 1:A:131:ASP:H    | 2.19                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:22:GLU:O     | 1:B:23:ASP:C     | 2.56                     | 0.49              |
| 1:C:42:ILE:O     | 1:C:43:ASN:C     | 2.55                     | 0.49              |
| 1:A:33:ARG:HH11  | 1:A:33:ARG:CG    | 2.25                     | 0.49              |
| 1:A:199:ASP:OD1  | 1:A:217:THR:HG23 | 2.11                     | 0.49              |
| 1:C:153:ARG:NH2  | 1:C:171:PHE:HZ   | 2.10                     | 0.49              |
| 1:E:153:ARG:HH21 | 1:E:171:PHE:HZ   | 1.60                     | 0.49              |
| 1:A:93:ILE:HG22  | 1:A:95:ILE:HG22  | 1.95                     | 0.49              |
| 1:C:43:ASN:HB3   | 1:C:112:ALA:O    | 2.13                     | 0.49              |
| 1:D:42:ILE:HG22  | 1:D:42:ILE:O     | 2.11                     | 0.49              |
| 1:D:397:ALA:O    | 1:D:401:VAL:HG22 | 2.13                     | 0.49              |
| 1:E:151:GLU:O    | 1:E:151:GLU:HG2  | 2.12                     | 0.49              |
| 1:A:153:ARG:NH2  | 1:A:171:PHE:HZ   | 2.11                     | 0.49              |
| 1:B:79:ASP:C     | 1:B:81:ARG:H     | 2.21                     | 0.49              |
| 1:B:151:GLU:HG2  | 1:B:151:GLU:O    | 2.12                     | 0.49              |
| 1:D:169:GLU:O    | 1:D:170:GLN:HG2  | 2.12                     | 0.49              |
| 1:E:43:ASN:HB3   | 1:E:112:ALA:O    | 2.13                     | 0.49              |
| 1:C:33:ARG:HH11  | 1:C:33:ARG:CG    | 2.25                     | 0.49              |
| 1:E:66:ILE:HD12  | 1:E:69:VAL:HG21  | 1.94                     | 0.49              |
| 1:E:23:ASP:HB2   | 1:E:286:LYS:HE3  | 1.95                     | 0.49              |
| 1:E:130:ASP:CG   | 1:E:131:ASP:H    | 2.20                     | 0.49              |
| 1:A:77:LEU:C     | 1:A:79:ASP:H     | 2.21                     | 0.48              |
| 1:A:153:ARG:HH21 | 1:A:171:PHE:HZ   | 1.60                     | 0.48              |
| 1:B:33:ARG:HH11  | 1:B:33:ARG:CG    | 2.25                     | 0.48              |
| 1:B:43:ASN:HB3   | 1:B:112:ALA:O    | 2.12                     | 0.48              |
| 1:B:123:ASP:OD1  | 1:B:123:ASP:N    | 2.46                     | 0.48              |
| 1:C:29:ALA:H     | 1:C:266:GLN:NE2  | 2.08                     | 0.48              |
| 1:D:231:PHE:CE2  | 1:D:262:MET:HE3  | 2.47                     | 0.48              |
| 1:E:56:TYR:CE1   | 1:E:126:ARG:CZ   | 2.95                     | 0.48              |
| 1:B:104:ILE:HD13 | 1:B:198:VAL:HG22 | 1.94                     | 0.48              |
| 1:B:213:PHE:C    | 1:B:215:TYR:H    | 2.21                     | 0.48              |
| 1:D:106:ASP:O    | 1:D:107:LEU:HG   | 2.12                     | 0.48              |
| 1:C:199:ASP:CB   | 1:C:217:THR:HG23 | 2.43                     | 0.48              |
| 1:D:81:ARG:O     | 1:D:102:ILE:O    | 2.31                     | 0.48              |
| 1:E:126:ARG:HA   | 1:E:126:ARG:HH11 | 1.78                     | 0.48              |
| 1:C:250:LEU:HD13 | 1:D:344:LEU:CD1  | 2.43                     | 0.48              |
| 1:B:257:GLU:O    | 1:B:261:MET:HG3  | 2.13                     | 0.48              |
| 1:B:383:GLU:HG3  | 1:C:354:LYS:NZ   | 2.29                     | 0.48              |
| 1:D:77:LEU:C     | 1:D:79:ASP:H     | 2.22                     | 0.48              |
| 1:E:213:PHE:C    | 1:E:215:TYR:H    | 2.22                     | 0.48              |
| 1:A:133:TRP:HB3  | 1:A:167:ILE:HD12 | 1.95                     | 0.48              |
| 1:B:97:LYS:NZ    | 1:B:97:LYS:HB2   | 2.29                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:107:LEU:CD2  | 1:B:274:TYR:OH   | 2.62                     | 0.48              |
| 1:D:43:ASN:HA    | 1:D:111:LYS:HB3  | 1.96                     | 0.48              |
| 1:E:22:GLU:O     | 1:E:23:ASP:C     | 2.56                     | 0.48              |
| 1:E:28:PRO:HD2   | 1:E:266:GLN:NE2  | 2.29                     | 0.48              |
| 1:E:176:PRO:O    | 1:E:177:GLU:HB2  | 2.12                     | 0.48              |
| 1:A:317:ARG:O    | 1:A:319:PRO:HD3  | 2.14                     | 0.48              |
| 1:C:77:LEU:C     | 1:C:79:ASP:H     | 2.22                     | 0.48              |
| 1:C:105:PHE:C    | 1:C:107:LEU:N    | 2.70                     | 0.48              |
| 1:D:133:TRP:HB3  | 1:D:167:ILE:HD12 | 1.95                     | 0.48              |
| 1:A:56:TYR:CE1   | 1:A:126:ARG:CZ   | 2.96                     | 0.48              |
| 1:A:199:ASP:CB   | 1:A:217:THR:HG23 | 2.43                     | 0.48              |
| 1:B:214:ARG:CA   | 1:B:217:THR:HG22 | 2.25                     | 0.48              |
| 1:E:77:LEU:C     | 1:E:79:ASP:H     | 2.22                     | 0.48              |
| 1:E:79:ASP:C     | 1:E:81:ARG:H     | 2.22                     | 0.48              |
| 1:E:342:ALA:CB   | 1:E:344:LEU:HD23 | 2.43                     | 0.48              |
| 1:A:109:SER:O    | 1:A:110:LEU:HD23 | 2.14                     | 0.48              |
| 1:A:273:SER:OG   | 1:A:274:TYR:N    | 2.46                     | 0.48              |
| 1:B:18:LEU:CD2   | 1:C:232:GLY:HA2  | 2.42                     | 0.48              |
| 1:B:42:ILE:O     | 1:B:43:ASN:C     | 2.57                     | 0.48              |
| 1:B:43:ASN:OD1   | 1:B:112:ALA:HB3  | 2.13                     | 0.48              |
| 1:D:213:PHE:C    | 1:D:215:TYR:H    | 2.20                     | 0.48              |
| 1:E:196:ALA:HB3  | 1:E:281:PHE:CE1  | 2.49                     | 0.48              |
| 1:A:270:LYS:HD2  | 1:A:271:ALA:H    | 1.79                     | 0.48              |
| 1:B:409:GLU:O    | 1:B:410:LYS:HB2  | 2.12                     | 0.48              |
| 1:E:43:ASN:HB3   | 1:E:112:ALA:C    | 2.39                     | 0.48              |
| 1:E:358:ASP:O    | 1:E:359:ASP:CB   | 2.61                     | 0.48              |
| 1:A:142:TYR:CD1  | 1:A:195:VAL:HG11 | 2.49                     | 0.47              |
| 1:A:151:GLU:O    | 1:A:151:GLU:HG2  | 2.13                     | 0.47              |
| 1:C:182:PHE:HD1  | 1:C:183:ASP:H    | 1.62                     | 0.47              |
| 1:E:93:ILE:HG22  | 1:E:95:ILE:HG22  | 1.96                     | 0.47              |
| 1:E:263:LEU:HA   | 1:E:264:PRO:HD3  | 1.64                     | 0.47              |
| 1:B:376:VAL:HG21 | 1:C:352:ASP:CG   | 2.38                     | 0.47              |
| 1:C:93:ILE:HG22  | 1:C:95:ILE:HG22  | 1.95                     | 0.47              |
| 1:C:213:PHE:C    | 1:C:215:TYR:H    | 2.23                     | 0.47              |
| 1:E:29:ALA:O     | 1:E:31:TYR:N     | 2.45                     | 0.47              |
| 1:E:177:GLU:HA   | 1:E:181:ILE:CD1  | 2.45                     | 0.47              |
| 1:E:358:ASP:O    | 1:E:359:ASP:HB2  | 2.13                     | 0.47              |
| 1:B:3:VAL:CG2    | 1:B:4:THR:H      | 2.23                     | 0.47              |
| 1:D:28:PRO:HD2   | 1:D:266:GLN:NE2  | 2.29                     | 0.47              |
| 1:D:182:PHE:N    | 1:D:182:PHE:CD1  | 2.80                     | 0.47              |
| 1:D:342:ALA:CB   | 1:D:344:LEU:HD23 | 2.45                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:25:VAL:HG21  | 1:E:288:PRO:HB3  | 1.95                     | 0.47              |
| 1:C:126:ARG:HA   | 1:C:126:ARG:HH11 | 1.79                     | 0.47              |
| 1:D:42:ILE:HD12  | 1:D:74:TYR:CD2   | 2.50                     | 0.47              |
| 1:D:126:ARG:HH11 | 1:D:126:ARG:HA   | 1.79                     | 0.47              |
| 1:D:317:ARG:N    | 1:D:317:ARG:CD   | 2.55                     | 0.47              |
| 1:E:136:LEU:HB2  | 1:E:213:PHE:CE2  | 2.50                     | 0.47              |
| 1:A:42:ILE:O     | 1:A:43:ASN:C     | 2.58                     | 0.47              |
| 1:A:136:LEU:HB2  | 1:A:213:PHE:HE2  | 1.79                     | 0.47              |
| 1:A:136:LEU:HB2  | 1:A:213:PHE:CE2  | 2.49                     | 0.47              |
| 1:B:43:ASN:HB3   | 1:B:112:ALA:C    | 2.39                     | 0.47              |
| 1:C:43:ASN:HA    | 1:C:111:LYS:HB3  | 1.97                     | 0.47              |
| 1:C:56:TYR:HE1   | 1:C:126:ARG:NH1  | 2.13                     | 0.47              |
| 1:C:169:GLU:CG   | 1:C:170:GLN:H    | 2.28                     | 0.47              |
| 1:C:224:ASP:HB2  | 1:C:279:ILE:HG13 | 1.97                     | 0.47              |
| 1:D:23:ASP:HB2   | 1:D:286:LYS:HE3  | 1.96                     | 0.47              |
| 1:B:343:ASP:HB2  | 1:B:344:LEU:H    | 1.48                     | 0.47              |
| 1:C:23:ASP:HB2   | 1:C:286:LYS:HE3  | 1.97                     | 0.47              |
| 1:D:104:ILE:HD13 | 1:D:198:VAL:HG22 | 1.95                     | 0.47              |
| 1:D:177:GLU:HA   | 1:D:181:ILE:CD1  | 2.45                     | 0.47              |
| 1:A:22:GLU:O     | 1:A:23:ASP:C     | 2.57                     | 0.47              |
| 1:A:126:ARG:HA   | 1:A:126:ARG:HH11 | 1.80                     | 0.47              |
| 1:A:327:LEU:HD12 | 1:A:327:LEU:HA   | 1.78                     | 0.47              |
| 1:C:43:ASN:HB3   | 1:C:112:ALA:C    | 2.40                     | 0.47              |
| 1:C:175:VAL:O    | 1:C:181:ILE:HG12 | 2.15                     | 0.47              |
| 1:D:29:ALA:C     | 1:D:31:TYR:N     | 2.73                     | 0.47              |
| 1:D:66:ILE:HD13  | 1:D:185:TRP:CD1  | 2.50                     | 0.47              |
| 1:D:130:ASP:CG   | 1:D:131:ASP:H    | 2.23                     | 0.47              |
| 1:D:182:PHE:HD1  | 1:D:183:ASP:H    | 1.61                     | 0.47              |
| 1:D:166:MET:C    | 1:D:167:ILE:HG12 | 2.39                     | 0.47              |
| 1:A:43:ASN:HA    | 1:A:111:LYS:HB3  | 1.97                     | 0.47              |
| 1:A:175:VAL:O    | 1:A:181:ILE:HG12 | 2.15                     | 0.47              |
| 1:B:23:ASP:HB2   | 1:B:286:LYS:HE3  | 1.97                     | 0.47              |
| 1:B:29:ALA:C     | 1:B:31:TYR:N     | 2.73                     | 0.47              |
| 1:C:166:MET:C    | 1:C:167:ILE:HG12 | 2.37                     | 0.47              |
| 1:E:178:GLY:O    | 1:E:179:ARG:HB2  | 2.15                     | 0.47              |
| 1:A:66:ILE:HD13  | 1:A:185:TRP:CD1  | 2.49                     | 0.47              |
| 1:B:28:PRO:HD2   | 1:B:266:GLN:NE2  | 2.30                     | 0.47              |
| 1:B:383:GLU:HG3  | 1:C:354:LYS:CE   | 2.44                     | 0.47              |
| 1:D:364:LEU:O    | 1:D:365:THR:CG2  | 2.62                     | 0.47              |
| 1:E:107:LEU:C    | 1:E:108:VAL:HG23 | 2.40                     | 0.47              |
| 1:E:253:GLU:O    | 1:E:257:GLU:HG3  | 2.15                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:56:TYR:HE1   | 1:A:126:ARG:NH1  | 2.13                     | 0.46              |
| 1:A:151:GLU:O    | 1:A:154:LYS:HB3  | 2.14                     | 0.46              |
| 1:B:188:ASP:HA   | 1:C:166:MET:CE   | 2.45                     | 0.46              |
| 1:C:106:ASP:O    | 1:C:107:LEU:HG   | 2.15                     | 0.46              |
| 1:C:380:GLY:HA2  | 1:D:354:LYS:NZ   | 2.30                     | 0.46              |
| 1:D:136:LEU:HB2  | 1:D:213:PHE:CE2  | 2.50                     | 0.46              |
| 1:A:415:TYR:CD1  | 1:A:415:TYR:C    | 2.93                     | 0.46              |
| 1:C:142:TYR:CD1  | 1:C:195:VAL:HG11 | 2.51                     | 0.46              |
| 1:D:42:ILE:O     | 1:D:43:ASN:C     | 2.58                     | 0.46              |
| 1:D:56:TYR:HE1   | 1:D:126:ARG:NH1  | 2.13                     | 0.46              |
| 1:D:97:LYS:NZ    | 1:D:97:LYS:HB2   | 2.27                     | 0.46              |
| 1:D:390:THR:HB   | 1:D:391:PRO:HD2  | 1.96                     | 0.46              |
| 1:D:409:GLU:O    | 1:D:410:LYS:HB2  | 2.15                     | 0.46              |
| 1:A:29:ALA:H     | 1:A:266:GLN:NE2  | 2.12                     | 0.46              |
| 1:A:176:PRO:O    | 1:A:177:GLU:HB2  | 2.13                     | 0.46              |
| 1:B:16:PRO:HB2   | 1:C:242:THR:OG1  | 2.16                     | 0.46              |
| 1:B:100:ASP:OD1  | 1:B:100:ASP:N    | 2.48                     | 0.46              |
| 1:B:182:PHE:HD1  | 1:B:183:ASP:H    | 1.62                     | 0.46              |
| 1:C:127:THR:OG1  | 1:C:128:SER:N    | 2.46                     | 0.46              |
| 1:A:231:PHE:CE2  | 1:A:262:MET:HE3  | 2.51                     | 0.46              |
| 1:B:379:LEU:CD1  | 1:C:346:GLN:HB2  | 2.46                     | 0.46              |
| 1:C:104:ILE:HD13 | 1:C:198:VAL:HG22 | 1.97                     | 0.46              |
| 1:D:199:ASP:CB   | 1:D:217:THR:HG23 | 2.46                     | 0.46              |
| 1:E:42:ILE:O     | 1:E:43:ASN:C     | 2.59                     | 0.46              |
| 1:A:43:ASN:OD1   | 1:A:112:ALA:HB3  | 2.16                     | 0.46              |
| 1:A:275:MET:SD   | 1:A:275:MET:C    | 2.98                     | 0.46              |
| 1:A:344:LEU:HD12 | 1:E:250:LEU:HD13 | 1.97                     | 0.46              |
| 1:B:181:ILE:H    | 1:B:181:ILE:CD1  | 2.16                     | 0.46              |
| 1:D:43:ASN:HB3   | 1:D:112:ALA:C    | 2.40                     | 0.46              |
| 1:D:263:LEU:HA   | 1:D:264:PRO:HD3  | 1.61                     | 0.46              |
| 1:E:28:PRO:HD2   | 1:E:266:GLN:HE21 | 1.81                     | 0.46              |
| 1:E:182:PHE:HD1  | 1:E:183:ASP:H    | 1.62                     | 0.46              |
| 1:B:231:PHE:CE2  | 1:B:262:MET:HE3  | 2.51                     | 0.46              |
| 1:C:308:LEU:O    | 1:C:309:ARG:CB   | 2.64                     | 0.46              |
| 1:A:182:PHE:CD1  | 1:A:183:ASP:N    | 2.81                     | 0.46              |
| 1:E:6:LYS:NZ     | 1:E:11:ASN:HD21  | 2.14                     | 0.46              |
| 1:E:181:ILE:H    | 1:E:181:ILE:CD1  | 2.18                     | 0.46              |
| 1:A:177:GLU:HA   | 1:A:181:ILE:CD1  | 2.46                     | 0.46              |
| 1:B:56:TYR:HE1   | 1:B:126:ARG:NH1  | 2.13                     | 0.46              |
| 1:B:126:ARG:HH11 | 1:B:126:ARG:HA   | 1.81                     | 0.46              |
| 1:B:422:LYS:HA   | 1:B:422:LYS:HZ3  | 1.80                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:177:GLU:HA   | 1:C:181:ILE:CD1  | 2.46                     | 0.46              |
| 1:E:156:LEU:HD23 | 1:E:156:LEU:O    | 2.16                     | 0.46              |
| 1:D:224:ASP:HB2  | 1:D:279:ILE:HG13 | 1.98                     | 0.46              |
| 1:E:397:ALA:O    | 1:E:401:VAL:HG22 | 2.15                     | 0.46              |
| 1:C:28:PRO:HG2   | 1:C:266:GLN:HE21 | 1.81                     | 0.46              |
| 1:C:79:ASP:C     | 1:C:81:ARG:H     | 2.24                     | 0.46              |
| 1:C:283:LEU:HD23 | 1:C:283:LEU:N    | 2.31                     | 0.46              |
| 1:E:151:GLU:O    | 1:E:154:LYS:HB3  | 2.15                     | 0.46              |
| 1:A:97:LYS:NZ    | 1:A:97:LYS:HB2   | 2.31                     | 0.45              |
| 1:B:317:ARG:O    | 1:B:319:PRO:HD3  | 2.17                     | 0.45              |
| 1:C:151:GLU:O    | 1:C:154:LYS:HB3  | 2.16                     | 0.45              |
| 1:A:127:THR:OG1  | 1:A:128:SER:N    | 2.49                     | 0.45              |
| 1:B:127:THR:OG1  | 1:B:128:SER:N    | 2.49                     | 0.45              |
| 1:D:136:LEU:HB2  | 1:D:213:PHE:HE2  | 1.82                     | 0.45              |
| 1:E:83:LYS:HE3   | 1:E:83:LYS:HB2   | 1.62                     | 0.45              |
| 1:B:43:ASN:HA    | 1:B:111:LYS:HB3  | 1.99                     | 0.45              |
| 1:B:177:GLU:HA   | 1:B:181:ILE:CD1  | 2.46                     | 0.45              |
| 1:B:199:ASP:CB   | 1:B:217:THR:HG23 | 2.47                     | 0.45              |
| 1:B:263:LEU:HA   | 1:B:264:PRO:HD3  | 1.63                     | 0.45              |
| 1:C:151:GLU:O    | 1:C:151:GLU:HG2  | 2.17                     | 0.45              |
| 1:B:126:ARG:CD   | 1:B:127:THR:N    | 2.80                     | 0.45              |
| 1:C:327:LEU:HD12 | 1:C:327:LEU:HA   | 1.74                     | 0.45              |
| 1:C:390:THR:HB   | 1:C:391:PRO:HD2  | 1.98                     | 0.45              |
| 1:D:75:GLY:HA2   | 1:D:78:LYS:HD2   | 1.99                     | 0.45              |
| 1:E:43:ASN:HA    | 1:E:111:LYS:HB3  | 1.98                     | 0.45              |
| 1:C:178:GLY:O    | 1:C:179:ARG:HB2  | 2.17                     | 0.45              |
| 1:C:389:PRO:HB3  | 1:C:393:MET:HE2  | 1.98                     | 0.45              |
| 1:D:109:SER:O    | 1:D:110:LEU:HD23 | 2.16                     | 0.45              |
| 1:E:81:ARG:O     | 1:E:102:ILE:O    | 2.35                     | 0.45              |
| 1:A:344:LEU:HD13 | 1:E:250:LEU:HB3  | 1.99                     | 0.45              |
| 1:A:419:GLU:OE2  | 1:B:309:ARG:HD3  | 2.17                     | 0.45              |
| 1:B:77:LEU:C     | 1:B:79:ASP:H     | 2.24                     | 0.45              |
| 1:C:6:LYS:NZ     | 1:C:11:ASN:HD21  | 2.15                     | 0.45              |
| 1:D:18:LEU:HB2   | 1:D:19:PRO:HD2   | 1.98                     | 0.45              |
| 1:D:122:SER:OG   | 1:D:123:ASP:OD1  | 2.35                     | 0.45              |
| 1:E:412:ILE:HD12 | 1:E:412:ILE:O    | 2.16                     | 0.45              |
| 1:A:23:ASP:HB2   | 1:A:286:LYS:HE3  | 1.99                     | 0.45              |
| 1:A:81:ARG:O     | 1:A:102:ILE:O    | 2.34                     | 0.45              |
| 1:A:240:MET:HE1  | 1:A:248:TRP:CD1  | 2.52                     | 0.45              |
| 1:B:136:LEU:HB2  | 1:B:213:PHE:CE2  | 2.51                     | 0.45              |
| 1:C:182:PHE:CD1  | 1:C:182:PHE:N    | 2.80                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:343:ASP:HB2  | 1:C:344:LEU:H    | 1.49                     | 0.45              |
| 1:D:22:GLU:O     | 1:D:23:ASP:C     | 2.59                     | 0.45              |
| 1:D:105:PHE:C    | 1:D:107:LEU:N    | 2.71                     | 0.45              |
| 1:D:181:ILE:H    | 1:D:181:ILE:CD1  | 2.16                     | 0.45              |
| 1:E:8:ILE:O      | 1:E:9:ILE:C      | 2.59                     | 0.45              |
| 1:E:136:LEU:HB2  | 1:E:213:PHE:HE2  | 1.82                     | 0.45              |
| 1:A:213:PHE:C    | 1:A:215:TYR:H    | 2.25                     | 0.45              |
| 1:B:66:ILE:HD13  | 1:B:185:TRP:CD1  | 2.52                     | 0.45              |
| 1:D:126:ARG:CD   | 1:D:127:THR:H    | 2.24                     | 0.45              |
| 1:E:28:PRO:O     | 1:E:31:TYR:HB3   | 2.17                     | 0.45              |
| 1:A:169:GLU:CG   | 1:A:170:GLN:H    | 2.30                     | 0.45              |
| 1:B:109:SER:O    | 1:B:110:LEU:HD23 | 2.17                     | 0.45              |
| 1:D:93:ILE:HG22  | 1:D:95:ILE:HG22  | 1.98                     | 0.45              |
| 1:E:66:ILE:HD13  | 1:E:185:TRP:CD1  | 2.51                     | 0.45              |
| 1:E:224:ASP:HB2  | 1:E:279:ILE:HG13 | 1.99                     | 0.45              |
| 1:A:25:VAL:HG21  | 1:A:288:PRO:HB3  | 1.98                     | 0.45              |
| 1:A:178:GLY:O    | 1:A:179:ARG:HB2  | 2.17                     | 0.45              |
| 1:B:93:ILE:HD12  | 1:B:93:ILE:N     | 2.32                     | 0.45              |
| 1:C:136:LEU:HB2  | 1:C:213:PHE:HE2  | 1.83                     | 0.45              |
| 1:C:214:ARG:CA   | 1:C:217:THR:HG22 | 2.26                     | 0.45              |
| 1:C:307:LEU:HD12 | 1:C:307:LEU:HA   | 1.81                     | 0.45              |
| 1:E:93:ILE:N     | 1:E:93:ILE:HD12  | 2.32                     | 0.45              |
| 1:E:105:PHE:C    | 1:E:107:LEU:N    | 2.71                     | 0.45              |
| 1:E:175:VAL:O    | 1:E:181:ILE:HG12 | 2.17                     | 0.45              |
| 1:A:29:ALA:O     | 1:A:31:TYR:N     | 2.50                     | 0.44              |
| 1:A:397:ALA:O    | 1:A:401:VAL:HG22 | 2.17                     | 0.44              |
| 1:B:308:LEU:HD12 | 1:B:308:LEU:HA   | 1.74                     | 0.44              |
| 1:C:100:ASP:N    | 1:C:100:ASP:OD1  | 2.50                     | 0.44              |
| 1:D:142:TYR:CD1  | 1:D:195:VAL:HG11 | 2.52                     | 0.44              |
| 1:E:97:LYS:NZ    | 1:E:97:LYS:HB2   | 2.31                     | 0.44              |
| 1:E:127:THR:OG1  | 1:E:128:SER:N    | 2.50                     | 0.44              |
| 1:E:169:GLU:CG   | 1:E:170:GLN:H    | 2.29                     | 0.44              |
| 1:A:8:ILE:O      | 1:A:9:ILE:C      | 2.59                     | 0.44              |
| 1:B:56:TYR:CE1   | 1:B:126:ARG:NH2  | 2.85                     | 0.44              |
| 1:B:163:GLN:C    | 1:B:165:LYS:N    | 2.74                     | 0.44              |
| 1:C:18:LEU:HB2   | 1:C:19:PRO:HD2   | 1.99                     | 0.44              |
| 1:D:33:ARG:NH1   | 1:D:33:ARG:CG    | 2.81                     | 0.44              |
| 1:E:38:ILE:HA    | 1:E:39:PRO:HD2   | 1.81                     | 0.44              |
| 1:A:182:PHE:CD1  | 1:A:182:PHE:N    | 2.82                     | 0.44              |
| 1:B:83:LYS:HE3   | 1:B:83:LYS:HB2   | 1.59                     | 0.44              |
| 1:B:151:GLU:O    | 1:B:154:LYS:HB3  | 2.17                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:136:LEU:HB2  | 1:C:213:PHE:CE2  | 2.51                     | 0.44              |
| 1:C:170:GLN:HB3  | 1:C:171:PHE:H    | 1.62                     | 0.44              |
| 1:E:327:LEU:HD12 | 1:E:327:LEU:HA   | 1.71                     | 0.44              |
| 1:A:196:ALA:HB3  | 1:A:281:PHE:CE1  | 2.52                     | 0.44              |
| 1:B:224:ASP:HB2  | 1:B:279:ILE:HG13 | 2.00                     | 0.44              |
| 1:B:389:PRO:HB3  | 1:B:393:MET:HE2  | 1.99                     | 0.44              |
| 1:B:415:TYR:CD1  | 1:B:415:TYR:C    | 2.95                     | 0.44              |
| 1:C:42:ILE:HD12  | 1:C:74:TYR:HD2   | 1.81                     | 0.44              |
| 1:C:176:PRO:O    | 1:C:177:GLU:HB2  | 2.17                     | 0.44              |
| 1:D:83:LYS:HB2   | 1:D:83:LYS:HE3   | 1.61                     | 0.44              |
| 1:E:415:TYR:CD1  | 1:E:415:TYR:C    | 2.94                     | 0.44              |
| 1:A:263:LEU:HA   | 1:A:264:PRO:HD3  | 1.68                     | 0.44              |
| 1:D:151:GLU:O    | 1:D:151:GLU:HG2  | 2.18                     | 0.44              |
| 1:D:343:ASP:HB2  | 1:D:344:LEU:H    | 1.48                     | 0.44              |
| 1:E:389:PRO:HB3  | 1:E:393:MET:HE2  | 1.99                     | 0.44              |
| 1:A:390:THR:HB   | 1:A:391:PRO:HD2  | 1.99                     | 0.44              |
| 1:D:231:PHE:HE2  | 1:D:262:MET:HE3  | 1.83                     | 0.44              |
| 1:E:88:TRP:CD2   | 1:E:204:MET:HE2  | 2.53                     | 0.44              |
| 1:B:28:PRO:HG2   | 1:B:266:GLN:HE21 | 1.83                     | 0.44              |
| 1:C:169:GLU:HG3  | 1:C:170:GLN:H    | 1.83                     | 0.44              |
| 1:D:127:THR:OG1  | 1:D:128:SER:N    | 2.47                     | 0.44              |
| 1:D:156:LEU:O    | 1:D:156:LEU:HD23 | 2.17                     | 0.44              |
| 1:E:199:ASP:OD1  | 1:E:218:ILE:HA   | 2.18                     | 0.44              |
| 1:A:28:PRO:HG2   | 1:A:266:GLN:HE21 | 1.83                     | 0.44              |
| 1:B:170:GLN:HB3  | 1:B:171:PHE:H    | 1.62                     | 0.44              |
| 1:E:283:LEU:HD23 | 1:E:283:LEU:N    | 2.33                     | 0.44              |
| 1:A:224:ASP:HB2  | 1:A:279:ILE:HG13 | 2.00                     | 0.44              |
| 1:B:25:VAL:HG21  | 1:B:288:PRO:HB3  | 1.99                     | 0.44              |
| 1:B:136:LEU:HB2  | 1:B:213:PHE:HE2  | 1.83                     | 0.44              |
| 1:D:54:TYR:CZ    | 1:D:122:SER:HB2  | 2.53                     | 0.44              |
| 1:E:182:PHE:N    | 1:E:182:PHE:CD1  | 2.82                     | 0.44              |
| 1:A:126:ARG:CD   | 1:A:127:THR:N    | 2.81                     | 0.43              |
| 1:A:170:GLN:HB3  | 1:A:171:PHE:H    | 1.62                     | 0.43              |
| 1:A:242:THR:OG1  | 1:E:16:PRO:HB2   | 2.18                     | 0.43              |
| 1:C:156:LEU:HD23 | 1:C:156:LEU:O    | 2.17                     | 0.43              |
| 1:C:389:PRO:CA   | 1:C:393:MET:HE2  | 2.48                     | 0.43              |
| 1:D:364:LEU:C    | 1:D:365:THR:HG22 | 2.42                     | 0.43              |
| 1:E:231:PHE:CE2  | 1:E:262:MET:HE3  | 2.53                     | 0.43              |
| 1:A:6:LYS:NZ     | 1:A:11:ASN:HD21  | 2.15                     | 0.43              |
| 1:C:22:GLU:O     | 1:C:23:ASP:C     | 2.61                     | 0.43              |
| 1:C:182:PHE:CD1  | 1:C:183:ASP:N    | 2.84                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:28:PRO:HD2   | 1:D:266:GLN:HE21 | 1.83                     | 0.43              |
| 1:D:182:PHE:CD1  | 1:D:183:ASP:N    | 2.86                     | 0.43              |
| 1:D:389:PRO:CA   | 1:D:393:MET:HE2  | 2.48                     | 0.43              |
| 1:C:56:TYR:CE1   | 1:C:126:ARG:NH2  | 2.87                     | 0.43              |
| 1:C:133:TRP:HB3  | 1:C:167:ILE:HD12 | 1.99                     | 0.43              |
| 1:D:50:ASP:CG    | 1:D:121:VAL:HA   | 2.43                     | 0.43              |
| 1:E:343:ASP:HB2  | 1:E:344:LEU:H    | 1.47                     | 0.43              |
| 1:B:156:LEU:HD23 | 1:B:156:LEU:O    | 2.18                     | 0.43              |
| 1:B:182:PHE:N    | 1:B:182:PHE:CD1  | 2.81                     | 0.43              |
| 1:D:56:TYR:CE1   | 1:D:126:ARG:NH2  | 2.87                     | 0.43              |
| 1:D:88:TRP:CD2   | 1:D:204:MET:HE2  | 2.54                     | 0.43              |
| 1:D:163:GLN:C    | 1:D:165:LYS:N    | 2.77                     | 0.43              |
| 1:D:364:LEU:HB3  | 1:D:368:ALA:HB2  | 2.00                     | 0.43              |
| 1:B:8:ILE:O      | 1:B:9:ILE:C      | 2.61                     | 0.43              |
| 1:B:73:LEU:O     | 1:B:74:TYR:C     | 2.62                     | 0.43              |
| 1:C:263:LEU:HA   | 1:C:264:PRO:HD3  | 1.64                     | 0.43              |
| 1:D:175:VAL:HA   | 1:D:176:PRO:HD2  | 1.71                     | 0.43              |
| 1:E:273:SER:OG   | 1:E:274:TYR:N    | 2.52                     | 0.43              |
| 1:A:214:ARG:C    | 1:A:216:GLY:H    | 2.27                     | 0.43              |
| 1:A:354:LYS:HZ3  | 1:E:380:GLY:HA2  | 1.83                     | 0.43              |
| 1:B:17:LYS:O     | 1:C:262:MET:HE1  | 2.18                     | 0.43              |
| 1:B:268:ILE:HG21 | 1:B:268:ILE:HD13 | 1.71                     | 0.43              |
| 1:D:6:LYS:NZ     | 1:D:11:ASN:HD21  | 2.17                     | 0.43              |
| 1:E:402:MET:O    | 1:E:403:SER:OG   | 2.28                     | 0.43              |
| 1:C:122:SER:OG   | 1:C:123:ASP:OD1  | 2.33                     | 0.43              |
| 1:D:199:ASP:OD1  | 1:D:214:ARG:NE   | 2.44                     | 0.43              |
| 1:E:100:ASP:OD1  | 1:E:100:ASP:N    | 2.51                     | 0.43              |
| 1:E:199:ASP:OD1  | 1:E:217:THR:HG23 | 2.18                     | 0.43              |
| 1:A:341:SER:HB2  | 1:E:387:ARG:NH2  | 2.34                     | 0.43              |
| 1:B:28:PRO:HD2   | 1:B:266:GLN:HE21 | 1.84                     | 0.43              |
| 1:B:72:TYR:CE1   | 1:B:134:LEU:CD1  | 3.02                     | 0.43              |
| 1:B:175:VAL:O    | 1:B:181:ILE:HG12 | 2.18                     | 0.43              |
| 1:C:308:LEU:HA   | 1:C:308:LEU:HD12 | 1.76                     | 0.43              |
| 1:D:153:ARG:O    | 1:D:157:MET:HG3  | 2.18                     | 0.43              |
| 1:A:22:GLU:HB3   | 1:A:23:ASP:H     | 1.69                     | 0.43              |
| 1:B:18:LEU:HB2   | 1:B:19:PRO:HD2   | 2.00                     | 0.43              |
| 1:B:390:THR:HB   | 1:B:391:PRO:HD2  | 2.00                     | 0.43              |
| 1:C:66:ILE:HD13  | 1:C:185:TRP:CD1  | 2.54                     | 0.43              |
| 1:E:213:PHE:C    | 1:E:215:TYR:N    | 2.77                     | 0.43              |
| 1:A:163:GLN:C    | 1:A:165:LYS:N    | 2.77                     | 0.43              |
| 1:B:81:ARG:O     | 1:B:102:ILE:O    | 2.37                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:327:LEU:HD12 | 1:B:327:LEU:HA   | 1.78                     | 0.42              |
| 1:D:43:ASN:HB2   | 1:D:44:THR:H     | 1.67                     | 0.42              |
| 1:A:104:ILE:HD13 | 1:A:198:VAL:HG22 | 2.01                     | 0.42              |
| 1:C:97:LYS:HB2   | 1:C:97:LYS:NZ    | 2.30                     | 0.42              |
| 1:D:117:LEU:O    | 1:D:118:PRO:O    | 2.37                     | 0.42              |
| 1:D:283:LEU:N    | 1:D:283:LEU:HD23 | 2.34                     | 0.42              |
| 1:B:93:ILE:HG22  | 1:B:95:ILE:HG22  | 2.01                     | 0.42              |
| 1:B:107:LEU:C    | 1:B:108:VAL:HG23 | 2.44                     | 0.42              |
| 1:B:142:TYR:CD1  | 1:B:195:VAL:HG11 | 2.54                     | 0.42              |
| 1:D:28:PRO:O     | 1:D:31:TYR:HB3   | 2.19                     | 0.42              |
| 1:E:169:GLU:HG3  | 1:E:170:GLN:H    | 1.83                     | 0.42              |
| 1:B:257:GLU:O    | 1:B:260:GLN:HB3  | 2.19                     | 0.42              |
| 1:C:8:ILE:O      | 1:C:9:ILE:C      | 2.63                     | 0.42              |
| 1:E:28:PRO:HG2   | 1:E:266:GLN:HE21 | 1.85                     | 0.42              |
| 1:A:309:ARG:HD3  | 1:E:419:GLU:OE2  | 2.19                     | 0.42              |
| 1:C:54:TYR:HE1   | 1:C:118:PRO:HB2  | 1.85                     | 0.42              |
| 1:A:93:ILE:N     | 1:A:93:ILE:HD12  | 2.34                     | 0.42              |
| 1:A:422:LYS:HA   | 1:A:422:LYS:HZ2  | 1.83                     | 0.42              |
| 1:B:308:LEU:HD13 | 1:B:335:ALA:HB1  | 2.01                     | 0.42              |
| 1:C:88:TRP:CD2   | 1:C:204:MET:HE2  | 2.54                     | 0.42              |
| 1:E:54:TYR:CZ    | 1:E:122:SER:HB2  | 2.54                     | 0.42              |
| 1:A:28:PRO:HD2   | 1:A:266:GLN:NE2  | 2.35                     | 0.42              |
| 1:A:83:LYS:HB2   | 1:A:83:LYS:HE3   | 1.63                     | 0.42              |
| 1:B:54:TYR:CZ    | 1:B:122:SER:HB2  | 2.55                     | 0.42              |
| 1:C:56:TYR:CE1   | 1:C:126:ARG:NH1  | 2.87                     | 0.42              |
| 1:C:213:PHE:C    | 1:C:215:TYR:N    | 2.78                     | 0.42              |
| 1:D:72:TYR:CE1   | 1:D:134:LEU:CD1  | 3.03                     | 0.42              |
| 1:E:307:LEU:HD12 | 1:E:307:LEU:HA   | 1.77                     | 0.42              |
| 1:A:54:TYR:CZ    | 1:A:122:SER:HB2  | 2.54                     | 0.42              |
| 1:B:163:GLN:C    | 1:B:165:LYS:H    | 2.28                     | 0.42              |
| 1:B:308:LEU:O    | 1:B:309:ARG:CB   | 2.64                     | 0.42              |
| 1:D:56:TYR:CE1   | 1:D:126:ARG:NH1  | 2.88                     | 0.42              |
| 1:D:107:LEU:HD22 | 1:D:274:TYR:OH   | 2.19                     | 0.42              |
| 1:E:56:TYR:HE1   | 1:E:126:ARG:NH1  | 2.18                     | 0.42              |
| 1:A:43:ASN:HB2   | 1:A:44:THR:H     | 1.71                     | 0.42              |
| 1:B:117:LEU:CB   | 1:B:118:PRO:CD   | 2.79                     | 0.42              |
| 1:B:141:LEU:HD22 | 1:B:182:PHE:CD2  | 2.55                     | 0.42              |
| 1:B:389:PRO:CA   | 1:B:393:MET:HE2  | 2.50                     | 0.42              |
| 1:B:419:GLU:O    | 1:B:419:GLU:HG3  | 2.20                     | 0.42              |
| 1:D:175:VAL:O    | 1:D:181:ILE:HG12 | 2.20                     | 0.42              |
| 1:D:323:GLU:O    | 1:D:327:LEU:HB2  | 2.20                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:389:PRO:HB3  | 1:D:393:MET:HE2  | 2.02                     | 0.42              |
| 1:A:88:TRP:CD2   | 1:A:204:MET:HE2  | 2.55                     | 0.42              |
| 1:A:343:ASP:HB2  | 1:A:344:LEU:H    | 1.47                     | 0.42              |
| 1:B:133:TRP:HB3  | 1:B:167:ILE:HD12 | 2.00                     | 0.42              |
| 1:B:283:LEU:N    | 1:B:283:LEU:HD23 | 2.35                     | 0.42              |
| 1:E:145:GLY:HA2  | 1:E:183:ASP:HB3  | 2.02                     | 0.42              |
| 1:E:251:ASN:O    | 1:E:252:ARG:C    | 2.61                     | 0.42              |
| 1:C:137:TYR:O    | 1:C:141:LEU:HG   | 2.20                     | 0.41              |
| 1:C:181:ILE:HB   | 1:C:182:PHE:H    | 1.66                     | 0.41              |
| 1:E:226:ALA:O    | 1:E:230:THR:HG23 | 2.20                     | 0.41              |
| 1:E:390:THR:O    | 1:E:393:MET:HG2  | 2.20                     | 0.41              |
| 1:A:100:ASP:N    | 1:A:100:ASP:OD1  | 2.52                     | 0.41              |
| 1:B:253:GLU:OE2  | 1:B:253:GLU:N    | 2.53                     | 0.41              |
| 1:D:73:LEU:O     | 1:D:74:TYR:C     | 2.63                     | 0.41              |
| 1:E:27:TYR:HB3   | 1:E:266:GLN:NE2  | 2.35                     | 0.41              |
| 1:E:181:ILE:HB   | 1:E:182:PHE:H    | 1.64                     | 0.41              |
| 1:B:213:PHE:C    | 1:B:215:TYR:N    | 2.76                     | 0.41              |
| 1:C:251:ASN:O    | 1:C:252:ARG:C    | 2.61                     | 0.41              |
| 1:C:323:GLU:O    | 1:C:327:LEU:HB2  | 2.19                     | 0.41              |
| 1:D:29:ALA:H     | 1:D:266:GLN:NE2  | 2.15                     | 0.41              |
| 1:D:69:VAL:HG23  | 1:D:70:ASN:N     | 2.35                     | 0.41              |
| 1:D:415:TYR:CD1  | 1:D:415:TYR:C    | 2.98                     | 0.41              |
| 1:E:214:ARG:C    | 1:E:216:GLY:H    | 2.28                     | 0.41              |
| 1:B:323:GLU:O    | 1:B:327:LEU:HB2  | 2.20                     | 0.41              |
| 1:C:126:ARG:CD   | 1:C:127:THR:N    | 2.82                     | 0.41              |
| 1:D:54:TYR:CE2   | 1:D:122:SER:HB2  | 2.56                     | 0.41              |
| 1:D:56:TYR:C     | 1:D:56:TYR:CD2   | 2.98                     | 0.41              |
| 1:A:107:LEU:HD22 | 1:A:274:TYR:OH   | 2.21                     | 0.41              |
| 1:A:122:SER:OG   | 1:A:123:ASP:OD1  | 2.34                     | 0.41              |
| 1:A:288:PRO:HG2  | 1:A:289:TYR:CD2  | 2.55                     | 0.41              |
| 1:B:57:GLN:C     | 1:B:59:LEU:N     | 2.78                     | 0.41              |
| 1:B:176:PRO:HB2  | 1:B:177:GLU:H    | 1.70                     | 0.41              |
| 1:C:20:ALA:HB2   | 1:D:269:ASP:O    | 2.20                     | 0.41              |
| 1:C:231:PHE:CE2  | 1:C:262:MET:HE3  | 2.55                     | 0.41              |
| 1:D:422:LYS:HA   | 1:D:422:LYS:HZ3  | 1.84                     | 0.41              |
| 1:A:117:LEU:O    | 1:A:118:PRO:O    | 2.38                     | 0.41              |
| 1:A:156:LEU:O    | 1:A:156:LEU:HD23 | 2.20                     | 0.41              |
| 1:A:253:GLU:O    | 1:A:257:GLU:HG3  | 2.21                     | 0.41              |
| 1:B:27:TYR:HB3   | 1:B:266:GLN:NE2  | 2.36                     | 0.41              |
| 1:B:251:ASN:O    | 1:B:252:ARG:C    | 2.63                     | 0.41              |
| 1:C:130:ASP:O    | 1:C:131:ASP:C    | 2.63                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:169:GLU:CG   | 1:D:170:GLN:H    | 2.32                     | 0.41              |
| 1:E:29:ALA:H     | 1:E:266:GLN:NE2  | 2.14                     | 0.41              |
| 1:A:56:TYR:CE1   | 1:A:126:ARG:NH1  | 2.88                     | 0.41              |
| 1:A:213:PHE:C    | 1:A:215:TYR:N    | 2.78                     | 0.41              |
| 1:B:54:TYR:HE1   | 1:B:118:PRO:HB2  | 1.85                     | 0.41              |
| 1:B:57:GLN:C     | 1:B:59:LEU:H     | 2.29                     | 0.41              |
| 1:B:117:LEU:O    | 1:B:118:PRO:O    | 2.38                     | 0.41              |
| 1:C:25:VAL:HG21  | 1:C:288:PRO:HB3  | 2.02                     | 0.41              |
| 1:C:81:ARG:O     | 1:C:102:ILE:O    | 2.39                     | 0.41              |
| 1:C:93:ILE:N     | 1:C:93:ILE:HD12  | 2.36                     | 0.41              |
| 1:D:213:PHE:C    | 1:D:215:TYR:N    | 2.76                     | 0.41              |
| 1:A:54:TYR:HE1   | 1:A:118:PRO:HB2  | 1.86                     | 0.41              |
| 1:B:169:GLU:CG   | 1:B:170:GLN:H    | 2.33                     | 0.41              |
| 1:C:163:GLN:C    | 1:C:165:LYS:H    | 2.29                     | 0.41              |
| 1:C:181:ILE:H    | 1:C:181:ILE:CD1  | 2.14                     | 0.41              |
| 1:E:163:GLN:C    | 1:E:165:LYS:N    | 2.78                     | 0.41              |
| 1:A:16:PRO:HB2   | 1:B:242:THR:OG1  | 2.20                     | 0.41              |
| 1:A:44:THR:HG21  | 1:A:116:VAL:HG22 | 2.03                     | 0.41              |
| 1:A:69:VAL:HG23  | 1:A:70:ASN:N     | 2.36                     | 0.41              |
| 1:B:29:ALA:H     | 1:B:266:GLN:NE2  | 2.18                     | 0.41              |
| 1:B:56:TYR:CE1   | 1:B:126:ARG:NH1  | 2.89                     | 0.41              |
| 1:B:286:LYS:HB2  | 1:B:286:LYS:HE2  | 1.91                     | 0.41              |
| 1:C:163:GLN:C    | 1:C:165:LYS:N    | 2.76                     | 0.41              |
| 1:D:9:ILE:HG23   | 1:D:10:ASP:N     | 2.36                     | 0.41              |
| 1:D:93:ILE:HD12  | 1:D:93:ILE:N     | 2.36                     | 0.41              |
| 1:D:364:LEU:CB   | 1:D:368:ALA:HB2  | 2.51                     | 0.41              |
| 1:E:122:SER:OG   | 1:E:123:ASP:OD1  | 2.36                     | 0.41              |
| 1:E:137:TYR:O    | 1:E:141:LEU:HG   | 2.21                     | 0.41              |
| 1:E:142:TYR:CE1  | 1:E:195:VAL:HG11 | 2.56                     | 0.41              |
| 1:E:182:PHE:CD1  | 1:E:183:ASP:N    | 2.84                     | 0.41              |
| 1:E:354:LYS:CE   | 1:E:356:THR:HA   | 2.50                     | 0.41              |
| 1:B:365:THR:CG2  | 1:B:366:THR:H    | 2.14                     | 0.41              |
| 1:B:376:VAL:CG1  | 1:C:354:LYS:HB2  | 2.44                     | 0.41              |
| 1:C:199:ASP:OD1  | 1:C:217:THR:HG23 | 2.20                     | 0.41              |
| 1:C:387:ARG:NH2  | 1:D:341:SER:HB2  | 2.35                     | 0.41              |
| 1:D:100:ASP:OD1  | 1:D:100:ASP:N    | 2.52                     | 0.41              |
| 1:D:268:ILE:HG21 | 1:D:268:ILE:HD13 | 1.71                     | 0.41              |
| 1:E:44:THR:HG21  | 1:E:116:VAL:HG22 | 2.03                     | 0.41              |
| 1:E:126:ARG:CD   | 1:E:127:THR:N    | 2.83                     | 0.41              |
| 1:E:133:TRP:HB3  | 1:E:167:ILE:HD12 | 2.03                     | 0.41              |
| 1:C:28:PRO:O     | 1:C:31:TYR:HB3   | 2.21                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:29:ALA:O     | 1:C:31:TYR:N     | 2.54                     | 0.40              |
| 1:C:107:LEU:HD22 | 1:C:274:TYR:OH   | 2.21                     | 0.40              |
| 1:C:214:ARG:C    | 1:C:216:GLY:H    | 2.30                     | 0.40              |
| 1:B:54:TYR:CE1   | 1:B:118:PRO:HB2  | 2.56                     | 0.40              |
| 1:B:199:ASP:OD1  | 1:B:217:THR:HG23 | 2.21                     | 0.40              |
| 1:C:240:MET:HE1  | 1:C:248:TRP:CD1  | 2.57                     | 0.40              |
| 1:D:317:ARG:O    | 1:D:319:PRO:HD3  | 2.21                     | 0.40              |
| 1:E:323:GLU:O    | 1:E:327:LEU:HB2  | 2.21                     | 0.40              |
| 1:A:202:PHE:HB2  | 1:A:214:ARG:HD3  | 2.04                     | 0.40              |
| 1:B:196:ALA:HB3  | 1:B:281:PHE:CE1  | 2.56                     | 0.40              |
| 1:C:54:TYR:CE1   | 1:C:118:PRO:HB2  | 2.56                     | 0.40              |
| 1:D:257:GLU:HB3  | 1:D:294:ASN:OD1  | 2.21                     | 0.40              |
| 1:A:50:ASP:HB3   | 1:A:54:TYR:HE2   | 1.87                     | 0.40              |
| 1:A:54:TYR:CE2   | 1:A:122:SER:HB2  | 2.57                     | 0.40              |
| 1:B:81:ARG:HB2   | 1:B:208:HIS:HE2  | 1.84                     | 0.40              |
| 1:B:214:ARG:C    | 1:B:216:GLY:H    | 2.29                     | 0.40              |
| 1:C:69:VAL:HG23  | 1:C:70:ASN:N     | 2.36                     | 0.40              |
| 1:C:153:ARG:O    | 1:C:157:MET:HG3  | 2.21                     | 0.40              |
| 1:D:199:ASP:OD1  | 1:D:217:THR:HG23 | 2.20                     | 0.40              |
| 1:D:214:ARG:C    | 1:D:216:GLY:H    | 2.29                     | 0.40              |
| 1:E:22:GLU:HB3   | 1:E:23:ASP:H     | 1.70                     | 0.40              |
| 1:A:175:VAL:HA   | 1:A:176:PRO:HD2  | 1.72                     | 0.40              |
| 1:B:317:ARG:N    | 1:B:317:ARG:CD   | 2.60                     | 0.40              |
| 1:C:22:GLU:HB3   | 1:C:23:ASP:H     | 1.68                     | 0.40              |
| 1:C:107:LEU:C    | 1:C:108:VAL:HG23 | 2.46                     | 0.40              |
| 1:C:243:GLU:H    | 1:C:243:GLU:HG2  | 1.65                     | 0.40              |
| 1:E:29:ALA:C     | 1:E:31:TYR:N     | 2.74                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |   |
|-----|-------|-----------------|------------|-----------|----------|-------------|---|
| 1   | A     | 412/421 (98%)   | 329 (80%)  | 54 (13%)  | 29 (7%)  | 1           | 4 |
| 1   | B     | 411/421 (98%)   | 327 (80%)  | 54 (13%)  | 30 (7%)  | 1           | 4 |
| 1   | C     | 409/421 (97%)   | 325 (80%)  | 55 (13%)  | 29 (7%)  | 1           | 4 |
| 1   | D     | 412/421 (98%)   | 328 (80%)  | 51 (12%)  | 33 (8%)  | 1           | 3 |
| 1   | E     | 411/421 (98%)   | 324 (79%)  | 56 (14%)  | 31 (8%)  | 1           | 4 |
| All | All   | 2055/2105 (98%) | 1633 (80%) | 270 (13%) | 152 (7%) | 1           | 4 |

All (152) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 43  | ASN  |
| 1   | A     | 118 | PRO  |
| 1   | A     | 122 | SER  |
| 1   | A     | 168 | ASN  |
| 1   | A     | 171 | PHE  |
| 1   | A     | 176 | PRO  |
| 1   | A     | 177 | GLU  |
| 1   | A     | 343 | ASP  |
| 1   | B     | 43  | ASN  |
| 1   | B     | 118 | PRO  |
| 1   | B     | 168 | ASN  |
| 1   | B     | 171 | PHE  |
| 1   | B     | 176 | PRO  |
| 1   | B     | 177 | GLU  |
| 1   | B     | 343 | ASP  |
| 1   | C     | 43  | ASN  |
| 1   | C     | 108 | VAL  |
| 1   | C     | 118 | PRO  |
| 1   | C     | 122 | SER  |
| 1   | C     | 168 | ASN  |
| 1   | C     | 171 | PHE  |
| 1   | C     | 176 | PRO  |
| 1   | C     | 177 | GLU  |
| 1   | C     | 343 | ASP  |
| 1   | D     | 43  | ASN  |
| 1   | D     | 118 | PRO  |
| 1   | D     | 122 | SER  |
| 1   | D     | 168 | ASN  |
| 1   | D     | 171 | PHE  |
| 1   | D     | 176 | PRO  |
| 1   | D     | 177 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 343 | ASP  |
| 1   | E     | 43  | ASN  |
| 1   | E     | 118 | PRO  |
| 1   | E     | 122 | SER  |
| 1   | E     | 168 | ASN  |
| 1   | E     | 171 | PHE  |
| 1   | E     | 176 | PRO  |
| 1   | E     | 177 | GLU  |
| 1   | E     | 343 | ASP  |
| 1   | A     | 63  | ASN  |
| 1   | A     | 108 | VAL  |
| 1   | A     | 113 | LEU  |
| 1   | A     | 165 | LYS  |
| 1   | A     | 167 | ILE  |
| 1   | A     | 172 | GLU  |
| 1   | B     | 30  | ASP  |
| 1   | B     | 63  | ASN  |
| 1   | B     | 98  | ALA  |
| 1   | B     | 108 | VAL  |
| 1   | B     | 122 | SER  |
| 1   | B     | 165 | LYS  |
| 1   | B     | 167 | ILE  |
| 1   | B     | 172 | GLU  |
| 1   | B     | 189 | SER  |
| 1   | C     | 63  | ASN  |
| 1   | C     | 165 | LYS  |
| 1   | C     | 167 | ILE  |
| 1   | C     | 172 | GLU  |
| 1   | D     | 30  | ASP  |
| 1   | D     | 63  | ASN  |
| 1   | D     | 98  | ALA  |
| 1   | D     | 108 | VAL  |
| 1   | D     | 165 | LYS  |
| 1   | D     | 167 | ILE  |
| 1   | D     | 172 | GLU  |
| 1   | E     | 30  | ASP  |
| 1   | E     | 63  | ASN  |
| 1   | E     | 108 | VAL  |
| 1   | E     | 165 | LYS  |
| 1   | E     | 167 | ILE  |
| 1   | E     | 172 | GLU  |
| 1   | A     | 98  | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 113 | LEU  |
| 1   | B     | 132 | LYS  |
| 1   | C     | 30  | ASP  |
| 1   | C     | 98  | ALA  |
| 1   | C     | 113 | LEU  |
| 1   | C     | 120 | GLY  |
| 1   | D     | 80  | ILE  |
| 1   | D     | 113 | LEU  |
| 1   | D     | 120 | GLY  |
| 1   | D     | 189 | SER  |
| 1   | E     | 98  | ALA  |
| 1   | E     | 113 | LEU  |
| 1   | A     | 30  | ASP  |
| 1   | A     | 80  | ILE  |
| 1   | A     | 120 | GLY  |
| 1   | A     | 189 | SER  |
| 1   | A     | 309 | ARG  |
| 1   | B     | 47  | SER  |
| 1   | B     | 80  | ILE  |
| 1   | B     | 120 | GLY  |
| 1   | B     | 131 | ASP  |
| 1   | B     | 309 | ARG  |
| 1   | C     | 80  | ILE  |
| 1   | C     | 189 | SER  |
| 1   | C     | 216 | GLY  |
| 1   | C     | 309 | ARG  |
| 1   | D     | 3   | VAL  |
| 1   | D     | 47  | SER  |
| 1   | D     | 117 | LEU  |
| 1   | D     | 309 | ARG  |
| 1   | D     | 357 | PRO  |
| 1   | D     | 365 | THR  |
| 1   | E     | 47  | SER  |
| 1   | E     | 80  | ILE  |
| 1   | E     | 120 | GLY  |
| 1   | E     | 132 | LYS  |
| 1   | E     | 189 | SER  |
| 1   | A     | 23  | ASP  |
| 1   | A     | 47  | SER  |
| 1   | A     | 117 | LEU  |
| 1   | A     | 132 | LYS  |
| 1   | A     | 357 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 23  | ASP  |
| 1   | B     | 117 | LEU  |
| 1   | B     | 133 | TRP  |
| 1   | B     | 357 | PRO  |
| 1   | C     | 23  | ASP  |
| 1   | C     | 47  | SER  |
| 1   | C     | 117 | LEU  |
| 1   | C     | 131 | ASP  |
| 1   | C     | 173 | PRO  |
| 1   | D     | 23  | ASP  |
| 1   | D     | 79  | ASP  |
| 1   | D     | 132 | LYS  |
| 1   | D     | 133 | TRP  |
| 1   | E     | 23  | ASP  |
| 1   | E     | 117 | LEU  |
| 1   | E     | 131 | ASP  |
| 1   | E     | 133 | TRP  |
| 1   | E     | 309 | ARG  |
| 1   | E     | 357 | PRO  |
| 1   | A     | 131 | ASP  |
| 1   | A     | 133 | TRP  |
| 1   | A     | 173 | PRO  |
| 1   | A     | 216 | GLY  |
| 1   | B     | 216 | GLY  |
| 1   | C     | 132 | LYS  |
| 1   | D     | 131 | ASP  |
| 1   | D     | 173 | PRO  |
| 1   | D     | 216 | GLY  |
| 1   | D     | 370 | PRO  |
| 1   | E     | 173 | PRO  |
| 1   | E     | 216 | GLY  |
| 1   | E     | 370 | PRO  |
| 1   | B     | 173 | PRO  |
| 1   | C     | 370 | PRO  |
| 1   | B     | 370 | PRO  |
| 1   | C     | 3   | VAL  |
| 1   | E     | 181 | ILE  |

### 5.3.2 Protein sidechains ⓘ

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

resolution.

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

| Mol | Chain | Analysed        | Rotameric  | Outliers  | Percentiles |    |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 1   | A     | 359/362 (99%)   | 297 (83%)  | 62 (17%)  | 2           | 10 |
| 1   | B     | 358/362 (99%)   | 299 (84%)  | 59 (16%)  | 2           | 12 |
| 1   | C     | 356/362 (98%)   | 296 (83%)  | 60 (17%)  | 2           | 11 |
| 1   | D     | 359/362 (99%)   | 302 (84%)  | 57 (16%)  | 2           | 13 |
| 1   | E     | 358/362 (99%)   | 296 (83%)  | 62 (17%)  | 2           | 10 |
| All | All   | 1790/1810 (99%) | 1490 (83%) | 300 (17%) | 2           | 11 |

All (300) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 3   | VAL  |
| 1   | A     | 8   | ILE  |
| 1   | A     | 11  | ASN  |
| 1   | A     | 22  | GLU  |
| 1   | A     | 31  | TYR  |
| 1   | A     | 33  | ARG  |
| 1   | A     | 36  | LYS  |
| 1   | A     | 38  | ILE  |
| 1   | A     | 40  | LEU  |
| 1   | A     | 43  | ASN  |
| 1   | A     | 67  | ILE  |
| 1   | A     | 78  | LYS  |
| 1   | A     | 95  | ILE  |
| 1   | A     | 100 | ASP  |
| 1   | A     | 116 | VAL  |
| 1   | A     | 117 | LEU  |
| 1   | A     | 118 | PRO  |
| 1   | A     | 119 | ASP  |
| 1   | A     | 123 | ASP  |
| 1   | A     | 125 | SER  |
| 1   | A     | 126 | ARG  |
| 1   | A     | 134 | LEU  |
| 1   | A     | 152 | TYR  |
| 1   | A     | 155 | LYS  |
| 1   | A     | 162 | ASN  |
| 1   | A     | 163 | GLN  |
| 1   | A     | 167 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 174 | LEU  |
| 1   | A     | 175 | VAL  |
| 1   | A     | 177 | GLU  |
| 1   | A     | 180 | ASP  |
| 1   | A     | 181 | ILE  |
| 1   | A     | 182 | PHE  |
| 1   | A     | 187 | ASN  |
| 1   | A     | 189 | SER  |
| 1   | A     | 209 | GLU  |
| 1   | A     | 217 | THR  |
| 1   | A     | 230 | THR  |
| 1   | A     | 237 | ILE  |
| 1   | A     | 242 | THR  |
| 1   | A     | 243 | GLU  |
| 1   | A     | 252 | ARG  |
| 1   | A     | 270 | LYS  |
| 1   | A     | 273 | SER  |
| 1   | A     | 283 | LEU  |
| 1   | A     | 307 | LEU  |
| 1   | A     | 308 | LEU  |
| 1   | A     | 309 | ARG  |
| 1   | A     | 317 | ARG  |
| 1   | A     | 327 | LEU  |
| 1   | A     | 332 | LEU  |
| 1   | A     | 340 | SER  |
| 1   | A     | 344 | LEU  |
| 1   | A     | 352 | ASP  |
| 1   | A     | 356 | THR  |
| 1   | A     | 358 | ASP  |
| 1   | A     | 359 | ASP  |
| 1   | A     | 376 | VAL  |
| 1   | A     | 393 | MET  |
| 1   | A     | 405 | GLN  |
| 1   | A     | 412 | ILE  |
| 1   | A     | 422 | LYS  |
| 1   | B     | 3   | VAL  |
| 1   | B     | 8   | ILE  |
| 1   | B     | 11  | ASN  |
| 1   | B     | 22  | GLU  |
| 1   | B     | 31  | TYR  |
| 1   | B     | 33  | ARG  |
| 1   | B     | 36  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 38  | ILE  |
| 1   | B     | 40  | LEU  |
| 1   | B     | 42  | ILE  |
| 1   | B     | 43  | ASN  |
| 1   | B     | 67  | ILE  |
| 1   | B     | 78  | LYS  |
| 1   | B     | 100 | ASP  |
| 1   | B     | 108 | VAL  |
| 1   | B     | 116 | VAL  |
| 1   | B     | 117 | LEU  |
| 1   | B     | 119 | ASP  |
| 1   | B     | 123 | ASP  |
| 1   | B     | 126 | ARG  |
| 1   | B     | 134 | LEU  |
| 1   | B     | 152 | TYR  |
| 1   | B     | 155 | LYS  |
| 1   | B     | 162 | ASN  |
| 1   | B     | 163 | GLN  |
| 1   | B     | 167 | ILE  |
| 1   | B     | 174 | LEU  |
| 1   | B     | 175 | VAL  |
| 1   | B     | 177 | GLU  |
| 1   | B     | 180 | ASP  |
| 1   | B     | 181 | ILE  |
| 1   | B     | 182 | PHE  |
| 1   | B     | 187 | ASN  |
| 1   | B     | 189 | SER  |
| 1   | B     | 209 | GLU  |
| 1   | B     | 217 | THR  |
| 1   | B     | 230 | THR  |
| 1   | B     | 237 | ILE  |
| 1   | B     | 242 | THR  |
| 1   | B     | 243 | GLU  |
| 1   | B     | 251 | ASN  |
| 1   | B     | 252 | ARG  |
| 1   | B     | 270 | LYS  |
| 1   | B     | 273 | SER  |
| 1   | B     | 283 | LEU  |
| 1   | B     | 307 | LEU  |
| 1   | B     | 308 | LEU  |
| 1   | B     | 309 | ARG  |
| 1   | B     | 317 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 327 | LEU  |
| 1   | B     | 332 | LEU  |
| 1   | B     | 340 | SER  |
| 1   | B     | 344 | LEU  |
| 1   | B     | 352 | ASP  |
| 1   | B     | 356 | THR  |
| 1   | B     | 376 | VAL  |
| 1   | B     | 405 | GLN  |
| 1   | B     | 412 | ILE  |
| 1   | B     | 422 | LYS  |
| 1   | C     | 3   | VAL  |
| 1   | C     | 8   | ILE  |
| 1   | C     | 9   | ILE  |
| 1   | C     | 11  | ASN  |
| 1   | C     | 22  | GLU  |
| 1   | C     | 31  | TYR  |
| 1   | C     | 33  | ARG  |
| 1   | C     | 36  | LYS  |
| 1   | C     | 38  | ILE  |
| 1   | C     | 40  | LEU  |
| 1   | C     | 42  | ILE  |
| 1   | C     | 43  | ASN  |
| 1   | C     | 67  | ILE  |
| 1   | C     | 78  | LYS  |
| 1   | C     | 100 | ASP  |
| 1   | C     | 116 | VAL  |
| 1   | C     | 117 | LEU  |
| 1   | C     | 118 | PRO  |
| 1   | C     | 119 | ASP  |
| 1   | C     | 123 | ASP  |
| 1   | C     | 126 | ARG  |
| 1   | C     | 134 | LEU  |
| 1   | C     | 152 | TYR  |
| 1   | C     | 155 | LYS  |
| 1   | C     | 162 | ASN  |
| 1   | C     | 163 | GLN  |
| 1   | C     | 167 | ILE  |
| 1   | C     | 174 | LEU  |
| 1   | C     | 175 | VAL  |
| 1   | C     | 177 | GLU  |
| 1   | C     | 180 | ASP  |
| 1   | C     | 181 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 182 | PHE  |
| 1   | C     | 187 | ASN  |
| 1   | C     | 189 | SER  |
| 1   | C     | 209 | GLU  |
| 1   | C     | 217 | THR  |
| 1   | C     | 230 | THR  |
| 1   | C     | 237 | ILE  |
| 1   | C     | 242 | THR  |
| 1   | C     | 243 | GLU  |
| 1   | C     | 251 | ASN  |
| 1   | C     | 252 | ARG  |
| 1   | C     | 270 | LYS  |
| 1   | C     | 273 | SER  |
| 1   | C     | 283 | LEU  |
| 1   | C     | 307 | LEU  |
| 1   | C     | 308 | LEU  |
| 1   | C     | 309 | ARG  |
| 1   | C     | 317 | ARG  |
| 1   | C     | 327 | LEU  |
| 1   | C     | 332 | LEU  |
| 1   | C     | 340 | SER  |
| 1   | C     | 344 | LEU  |
| 1   | C     | 352 | ASP  |
| 1   | C     | 356 | THR  |
| 1   | C     | 376 | VAL  |
| 1   | C     | 405 | GLN  |
| 1   | C     | 412 | ILE  |
| 1   | C     | 422 | LYS  |
| 1   | D     | 3   | VAL  |
| 1   | D     | 8   | ILE  |
| 1   | D     | 9   | ILE  |
| 1   | D     | 11  | ASN  |
| 1   | D     | 22  | GLU  |
| 1   | D     | 31  | TYR  |
| 1   | D     | 33  | ARG  |
| 1   | D     | 36  | LYS  |
| 1   | D     | 38  | ILE  |
| 1   | D     | 40  | LEU  |
| 1   | D     | 43  | ASN  |
| 1   | D     | 67  | ILE  |
| 1   | D     | 78  | LYS  |
| 1   | D     | 79  | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 100 | ASP  |
| 1   | D     | 116 | VAL  |
| 1   | D     | 117 | LEU  |
| 1   | D     | 119 | ASP  |
| 1   | D     | 123 | ASP  |
| 1   | D     | 126 | ARG  |
| 1   | D     | 134 | LEU  |
| 1   | D     | 152 | TYR  |
| 1   | D     | 155 | LYS  |
| 1   | D     | 162 | ASN  |
| 1   | D     | 163 | GLN  |
| 1   | D     | 167 | ILE  |
| 1   | D     | 174 | LEU  |
| 1   | D     | 175 | VAL  |
| 1   | D     | 177 | GLU  |
| 1   | D     | 180 | ASP  |
| 1   | D     | 181 | ILE  |
| 1   | D     | 182 | PHE  |
| 1   | D     | 187 | ASN  |
| 1   | D     | 189 | SER  |
| 1   | D     | 209 | GLU  |
| 1   | D     | 217 | THR  |
| 1   | D     | 230 | THR  |
| 1   | D     | 237 | ILE  |
| 1   | D     | 242 | THR  |
| 1   | D     | 243 | GLU  |
| 1   | D     | 252 | ARG  |
| 1   | D     | 270 | LYS  |
| 1   | D     | 273 | SER  |
| 1   | D     | 283 | LEU  |
| 1   | D     | 307 | LEU  |
| 1   | D     | 308 | LEU  |
| 1   | D     | 309 | ARG  |
| 1   | D     | 317 | ARG  |
| 1   | D     | 327 | LEU  |
| 1   | D     | 332 | LEU  |
| 1   | D     | 340 | SER  |
| 1   | D     | 352 | ASP  |
| 1   | D     | 356 | THR  |
| 1   | D     | 376 | VAL  |
| 1   | D     | 405 | GLN  |
| 1   | D     | 412 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 422 | LYS  |
| 1   | E     | 3   | VAL  |
| 1   | E     | 7   | ARG  |
| 1   | E     | 8   | ILE  |
| 1   | E     | 9   | ILE  |
| 1   | E     | 11  | ASN  |
| 1   | E     | 22  | GLU  |
| 1   | E     | 31  | TYR  |
| 1   | E     | 33  | ARG  |
| 1   | E     | 36  | LYS  |
| 1   | E     | 38  | ILE  |
| 1   | E     | 40  | LEU  |
| 1   | E     | 42  | ILE  |
| 1   | E     | 43  | ASN  |
| 1   | E     | 67  | ILE  |
| 1   | E     | 78  | LYS  |
| 1   | E     | 100 | ASP  |
| 1   | E     | 108 | VAL  |
| 1   | E     | 116 | VAL  |
| 1   | E     | 117 | LEU  |
| 1   | E     | 118 | PRO  |
| 1   | E     | 119 | ASP  |
| 1   | E     | 123 | ASP  |
| 1   | E     | 126 | ARG  |
| 1   | E     | 134 | LEU  |
| 1   | E     | 152 | TYR  |
| 1   | E     | 155 | LYS  |
| 1   | E     | 162 | ASN  |
| 1   | E     | 163 | GLN  |
| 1   | E     | 167 | ILE  |
| 1   | E     | 174 | LEU  |
| 1   | E     | 175 | VAL  |
| 1   | E     | 177 | GLU  |
| 1   | E     | 180 | ASP  |
| 1   | E     | 181 | ILE  |
| 1   | E     | 182 | PHE  |
| 1   | E     | 187 | ASN  |
| 1   | E     | 189 | SER  |
| 1   | E     | 209 | GLU  |
| 1   | E     | 217 | THR  |
| 1   | E     | 230 | THR  |
| 1   | E     | 237 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 242 | THR  |
| 1   | E     | 243 | GLU  |
| 1   | E     | 252 | ARG  |
| 1   | E     | 270 | LYS  |
| 1   | E     | 273 | SER  |
| 1   | E     | 283 | LEU  |
| 1   | E     | 307 | LEU  |
| 1   | E     | 308 | LEU  |
| 1   | E     | 309 | ARG  |
| 1   | E     | 317 | ARG  |
| 1   | E     | 327 | LEU  |
| 1   | E     | 332 | LEU  |
| 1   | E     | 340 | SER  |
| 1   | E     | 344 | LEU  |
| 1   | E     | 352 | ASP  |
| 1   | E     | 356 | THR  |
| 1   | E     | 376 | VAL  |
| 1   | E     | 393 | MET  |
| 1   | E     | 405 | GLN  |
| 1   | E     | 412 | ILE  |
| 1   | E     | 422 | LYS  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 11  | ASN  |
| 1   | A     | 57  | GLN  |
| 1   | A     | 68  | HIS  |
| 1   | A     | 70  | ASN  |
| 1   | A     | 163 | GLN  |
| 1   | A     | 266 | GLN  |
| 1   | A     | 347 | GLN  |
| 1   | B     | 11  | ASN  |
| 1   | B     | 68  | HIS  |
| 1   | B     | 70  | ASN  |
| 1   | B     | 163 | GLN  |
| 1   | B     | 187 | ASN  |
| 1   | B     | 266 | GLN  |
| 1   | B     | 346 | GLN  |
| 1   | B     | 347 | GLN  |
| 1   | C     | 11  | ASN  |
| 1   | C     | 68  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 70  | ASN  |
| 1   | C     | 163 | GLN  |
| 1   | C     | 203 | HIS  |
| 1   | C     | 266 | GLN  |
| 1   | C     | 347 | GLN  |
| 1   | C     | 395 | GLN  |
| 1   | D     | 11  | ASN  |
| 1   | D     | 57  | GLN  |
| 1   | D     | 68  | HIS  |
| 1   | D     | 70  | ASN  |
| 1   | D     | 163 | GLN  |
| 1   | D     | 203 | HIS  |
| 1   | D     | 266 | GLN  |
| 1   | D     | 346 | GLN  |
| 1   | D     | 347 | GLN  |
| 1   | E     | 11  | ASN  |
| 1   | E     | 70  | ASN  |
| 1   | E     | 163 | GLN  |
| 1   | E     | 190 | ASN  |
| 1   | E     | 266 | GLN  |
| 1   | E     | 347 | GLN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 15 are modelled with single atom - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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 ⓘ

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ > 2 |       | OWAB(Å <sup>2</sup> ) | Q < 0.9 |
|-----|-------|-----------------|--------|-----------|-------|-----------------------|---------|
| 1   | A     | 416/421 (98%)   | 0.28   | 15 (3%)   | 46 26 | 62, 93, 152, 180      | 0       |
| 1   | B     | 415/421 (98%)   | 0.32   | 23 (5%)   | 30 15 | 63, 93, 151, 164      | 0       |
| 1   | C     | 413/421 (98%)   | 0.39   | 23 (5%)   | 30 15 | 62, 93, 150, 164      | 0       |
| 1   | D     | 416/421 (98%)   | 0.53   | 26 (6%)   | 26 13 | 63, 93, 152, 164      | 0       |
| 1   | E     | 415/421 (98%)   | 0.25   | 8 (1%)    | 66 43 | 62, 94, 152, 175      | 0       |
| All | All   | 2075/2105 (98%) | 0.35   | 95 (4%)   | 37 20 | 62, 93, 152, 180      | 0       |

All (95) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 118 | PRO  | 3.8  |
| 1   | D     | 2   | SER  | 3.7  |
| 1   | B     | 185 | TRP  | 3.7  |
| 1   | C     | 181 | ILE  | 3.6  |
| 1   | D     | 351 | GLY  | 3.6  |
| 1   | B     | 351 | GLY  | 3.5  |
| 1   | C     | 158 | ASP  | 3.5  |
| 1   | C     | 122 | SER  | 3.3  |
| 1   | B     | 357 | PRO  | 3.3  |
| 1   | D     | 43  | ASN  | 3.3  |
| 1   | C     | 180 | ASP  | 3.3  |
| 1   | C     | 175 | VAL  | 3.3  |
| 1   | A     | 351 | GLY  | 3.3  |
| 1   | E     | 118 | PRO  | 3.1  |
| 1   | D     | 75  | GLY  | 3.1  |
| 1   | B     | 48  | LEU  | 3.0  |
| 1   | D     | 118 | PRO  | 3.0  |
| 1   | B     | 120 | GLY  | 2.9  |
| 1   | A     | 142 | TYR  | 2.9  |
| 1   | C     | 107 | LEU  | 2.9  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 118 | PRO  | 2.9  |
| 1   | D     | 48  | LEU  | 2.8  |
| 1   | D     | 98  | ALA  | 2.8  |
| 1   | D     | 121 | VAL  | 2.8  |
| 1   | E     | 174 | LEU  | 2.8  |
| 1   | C     | 357 | PRO  | 2.7  |
| 1   | C     | 48  | LEU  | 2.7  |
| 1   | B     | 386 | ASN  | 2.7  |
| 1   | B     | 162 | ASN  | 2.7  |
| 1   | A     | 216 | GLY  | 2.7  |
| 1   | B     | 119 | ASP  | 2.7  |
| 1   | D     | 357 | PRO  | 2.6  |
| 1   | D     | 166 | MET  | 2.6  |
| 1   | D     | 82  | GLY  | 2.6  |
| 1   | A     | 118 | PRO  | 2.6  |
| 1   | B     | 158 | ASP  | 2.5  |
| 1   | E     | 175 | VAL  | 2.5  |
| 1   | D     | 163 | GLN  | 2.5  |
| 1   | D     | 172 | GLU  | 2.5  |
| 1   | E     | 98  | ALA  | 2.5  |
| 1   | B     | 412 | ILE  | 2.5  |
| 1   | B     | 124 | ALA  | 2.5  |
| 1   | A     | 113 | LEU  | 2.5  |
| 1   | C     | 59  | LEU  | 2.5  |
| 1   | C     | 116 | VAL  | 2.5  |
| 1   | A     | 175 | VAL  | 2.4  |
| 1   | A     | 181 | ILE  | 2.4  |
| 1   | D     | 167 | ILE  | 2.4  |
| 1   | B     | 107 | LEU  | 2.4  |
| 1   | A     | 59  | LEU  | 2.4  |
| 1   | D     | 80  | ILE  | 2.4  |
| 1   | C     | 174 | LEU  | 2.4  |
| 1   | D     | 55  | VAL  | 2.4  |
| 1   | E     | 62  | GLY  | 2.3  |
| 1   | B     | 80  | ILE  | 2.3  |
| 1   | D     | 129 | ALA  | 2.3  |
| 1   | D     | 185 | TRP  | 2.3  |
| 1   | C     | 114 | ASP  | 2.3  |
| 1   | C     | 355 | TYR  | 2.3  |
| 1   | C     | 171 | PHE  | 2.3  |
| 1   | C     | 113 | LEU  | 2.3  |
| 1   | C     | 117 | LEU  | 2.3  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 312 | ARG  | 2.3  |
| 1   | D     | 79  | ASP  | 2.3  |
| 1   | E     | 172 | GLU  | 2.2  |
| 1   | E     | 181 | ILE  | 2.2  |
| 1   | A     | 185 | TRP  | 2.2  |
| 1   | D     | 194 | ILE  | 2.2  |
| 1   | D     | 120 | GLY  | 2.2  |
| 1   | B     | 122 | SER  | 2.2  |
| 1   | D     | 30  | ASP  | 2.2  |
| 1   | C     | 366 | THR  | 2.2  |
| 1   | C     | 43  | ASN  | 2.2  |
| 1   | C     | 156 | LEU  | 2.2  |
| 1   | A     | 112 | ALA  | 2.2  |
| 1   | A     | 180 | ASP  | 2.1  |
| 1   | B     | 156 | LEU  | 2.1  |
| 1   | D     | 107 | LEU  | 2.1  |
| 1   | E     | 113 | LEU  | 2.1  |
| 1   | B     | 353 | ASN  | 2.1  |
| 1   | A     | 174 | LEU  | 2.1  |
| 1   | D     | 184 | VAL  | 2.1  |
| 1   | B     | 94  | ASN  | 2.1  |
| 1   | D     | 119 | ASP  | 2.1  |
| 1   | A     | 44  | THR  | 2.1  |
| 1   | B     | 274 | TYR  | 2.1  |
| 1   | A     | 357 | PRO  | 2.1  |
| 1   | C     | 173 | PRO  | 2.1  |
| 1   | D     | 213 | PHE  | 2.1  |
| 1   | B     | 167 | ILE  | 2.0  |
| 1   | A     | 148 | GLN  | 2.0  |
| 1   | B     | 113 | LEU  | 2.0  |
| 1   | C     | 98  | ALA  | 2.0  |
| 1   | B     | 121 | VAL  | 2.0  |
| 1   | C     | 80  | ILE  | 2.0  |

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

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

## 6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 2   | IUM  | B     | 423 | 1/3   | 0.83 | 0.19 | 225,225,225,225            | 0     |
| 2   | IUM  | D     | 423 | 1/3   | 0.86 | 0.17 | 224,224,224,224            | 0     |
| 2   | IUM  | E     | 424 | 1/3   | 0.93 | 0.21 | 232,232,232,232            | 0     |
| 2   | IUM  | E     | 423 | 1/3   | 0.94 | 0.11 | 197,197,197,197            | 0     |
| 2   | IUM  | B     | 425 | 1/3   | 0.94 | 0.18 | 229,229,229,229            | 0     |
| 2   | IUM  | A     | 1   | 1/3   | 0.95 | 0.08 | 212,212,212,212            | 0     |
| 2   | IUM  | C     | 425 | 1/3   | 0.96 | 0.11 | 177,177,177,177            | 0     |
| 2   | IUM  | A     | 424 | 1/3   | 0.97 | 0.08 | 204,204,204,204            | 0     |
| 2   | IUM  | C     | 423 | 1/3   | 0.97 | 0.09 | 170,170,170,170            | 0     |
| 2   | IUM  | A     | 425 | 1/3   | 0.98 | 0.10 | 192,192,192,192            | 0     |
| 2   | IUM  | D     | 424 | 1/3   | 0.99 | 0.02 | 117,117,117,117            | 0     |
| 2   | IUM  | C     | 424 | 1/3   | 1.00 | 0.02 | 110,110,110,110            | 0     |
| 2   | IUM  | D     | 425 | 1/3   | 1.00 | 0.03 | 111,111,111,111            | 0     |
| 2   | IUM  | A     | 423 | 1/3   | 1.00 | 0.05 | 116,116,116,116            | 0     |
| 2   | IUM  | B     | 424 | 1/3   | 1.00 | 0.03 | 116,116,116,116            | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.