



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:36 PM UTC

PDB ID : 6ZC5 / pdb\_00006zc5  
Title : Human Adenovirus serotype D10 FiberKnob protein  
Authors : Baker, A.T.; Mundy, R.M.; Rizkallah, P.J.; Parker, A.L.  
Deposited on : 2020-06-09  
Resolution : 2.50 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                                                             |

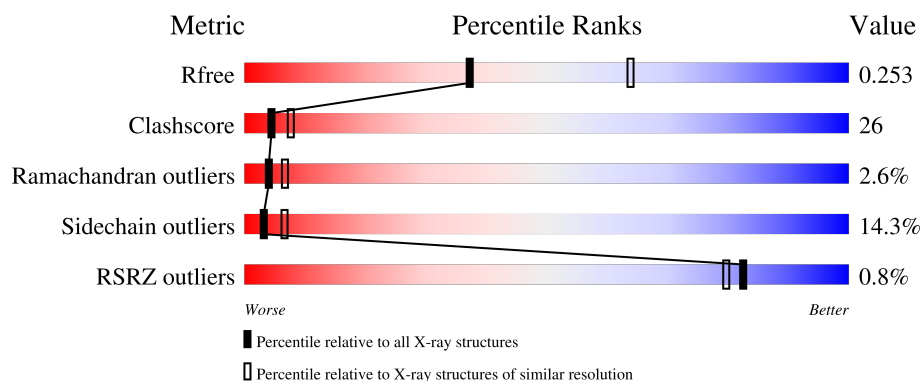
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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                      | 5829 (2.50-2.50)                                      |
| Clashscore            | 190562                      | 6492 (2.50-2.50)                                      |
| Ramachandran outliers | 187476                      | 6378 (2.50-2.50)                                      |
| Sidechain outliers    | 187428                      | 6380 (2.50-2.50)                                      |
| RSRZ outliers         | 180081                      | 5833 (2.50-2.50)                                      |

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     | 189    | <br>52% 39% 6% 2% 1%  |
| 1   | B     | 189    | <br>62% 29% 5% 2% 1%  |
| 1   | C     | 189    | <br>54% 37% 5% 2% 1%  |
| 1   | D     | 189    | <br>41% 39% 15% 2% 1% |
| 1   | E     | 189    | <br>44% 40% 12% 2% 1% |

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| Mol | Chain | Length | Quality of chain                                                                        |
|-----|-------|--------|-----------------------------------------------------------------------------------------|
| 1   | F     | 189    | <div><div></div><div>2%</div><div>52%</div><div>39%</div><div>8%</div><div></div></div> |
| 1   | G     | 189    | <div><div></div><div>%</div><div>53%</div><div>34%</div><div>12%</div><div></div></div> |
| 1   | H     | 189    | <div><div></div><div>41%</div><div>40%</div><div>15%</div><div></div></div>             |
| 1   | I     | 189    | <div><div></div><div>%</div><div>45%</div><div>39%</div><div>12%</div><div></div></div> |
| 1   | J     | 189    | <div><div></div><div>%</div><div>54%</div><div>37%</div><div>5%</div><div></div></div>  |
| 1   | K     | 189    | <div><div></div><div>%</div><div>44%</div><div>35%</div><div>14%</div><div></div></div> |
| 1   | L     | 189    | <div><div></div><div>%</div><div>53%</div><div>33%</div><div>11%</div><div></div></div> |

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 17536 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.

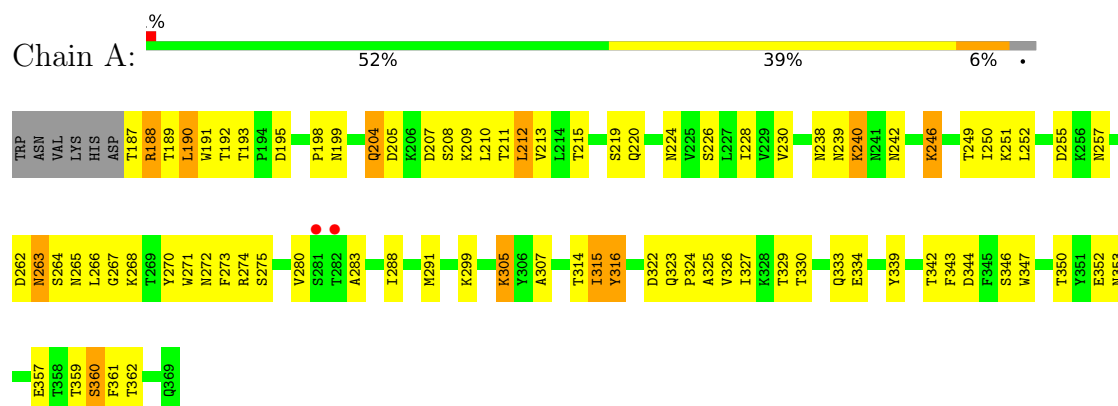
- Molecule 1 is a protein called Fiber.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | A     | 183      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1450  | 929 | 234 | 283 | 4 |         |         |       |
| 1   | B     | 183      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1450  | 929 | 234 | 283 | 4 |         |         |       |
| 1   | C     | 183      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1450  | 929 | 234 | 283 | 4 |         |         |       |
| 1   | D     | 184      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1458  | 933 | 235 | 286 | 4 |         |         |       |
| 1   | E     | 186      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1477  | 945 | 240 | 288 | 4 |         |         |       |
| 1   | F     | 186      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1477  | 945 | 240 | 288 | 4 |         |         |       |
| 1   | G     | 189      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1506  | 965 | 245 | 292 | 4 |         |         |       |
| 1   | H     | 183      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1450  | 929 | 234 | 283 | 4 |         |         |       |
| 1   | I     | 183      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1450  | 929 | 234 | 283 | 4 |         |         |       |
| 1   | J     | 183      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1450  | 929 | 234 | 283 | 4 |         |         |       |
| 1   | K     | 185      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1468  | 939 | 238 | 287 | 4 |         |         |       |
| 1   | L     | 183      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1450  | 929 | 234 | 283 | 4 |         |         |       |

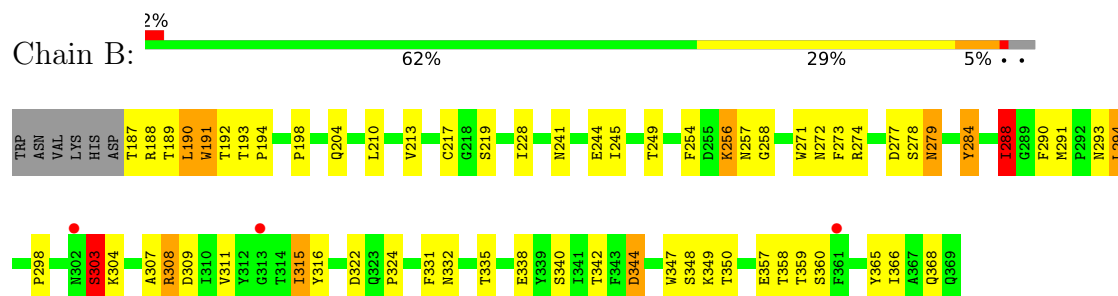
### 3 Residue-property plots [i](#)

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.

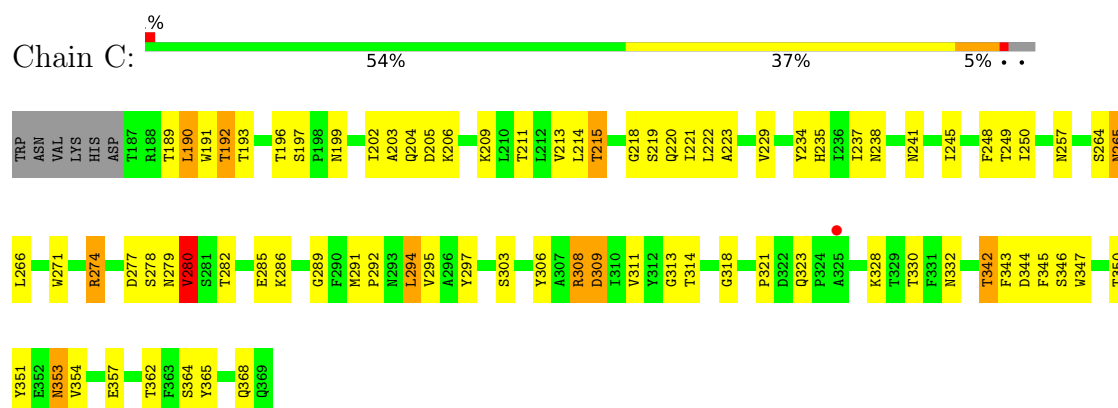
#### • Molecule 1: Fiber



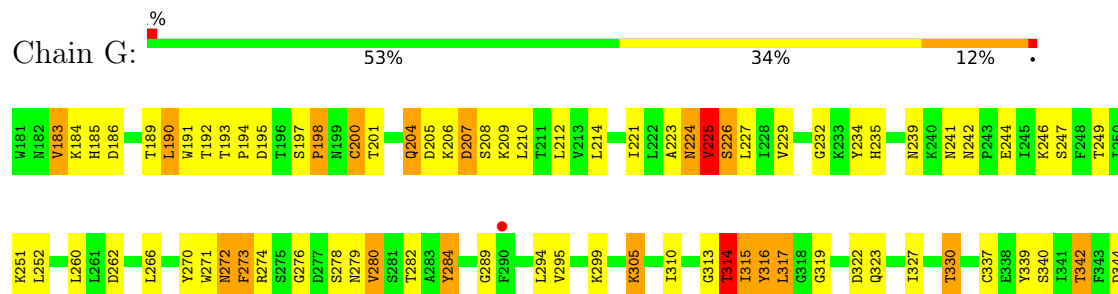
#### • Molecule 1: Fiber



#### • Molecule 1: Fiber



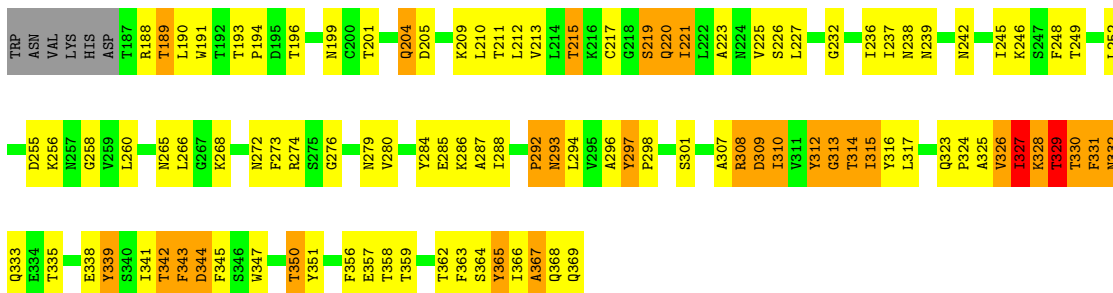
#### • Molecule 1: Fiber





• Molecule 1: Fiber

Chain H: 41% 40% 15% ..



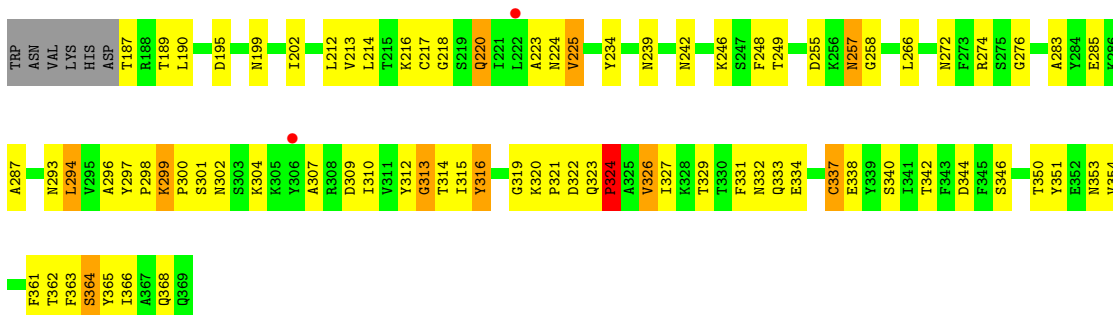
• Molecule 1: Fiber

Chain I: 45% 39% 12% ..



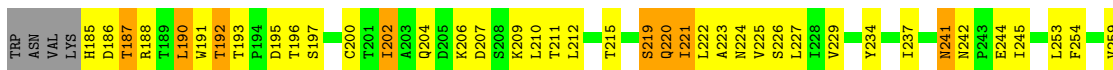
• Molecule 1: Fiber

Chain J: 54% 37% 5% ..



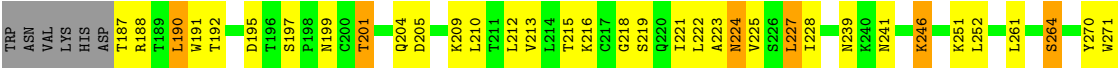
• Molecule 1: Fiber

Chain K: 44% 35% 14% ..





● Molecule 1: Fiber



## 4 Data and refinement statistics

| Property                                                                | Value                                                                                | Source           |
|-------------------------------------------------------------------------|--------------------------------------------------------------------------------------|------------------|
| Space group                                                             | P 31                                                                                 | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 101.36Å 101.36Å 326.72Å<br>90.00° 90.00° 120.00°                                     | Depositor        |
| Resolution (Å)                                                          | 108.91 – 2.50<br>108.91 – 2.50                                                       | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 98.6 (108.91-2.50)<br>98.6 (108.91-2.50)                                             | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.15                                                                                 | Depositor        |
| $R_{sym}$                                                               | (Not available)                                                                      | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.64 (at 2.52Å)                                                                      | Xtriage          |
| Refinement program                                                      | REFMAC 5.8.0258                                                                      | Depositor        |
| R, $R_{free}$                                                           | 0.219 , 0.251<br>0.220 , 0.253                                                       | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 6341 reflections (4.88%)                                                             | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 54.6                                                                                 | Xtriage          |
| Anisotropy                                                              | 0.859                                                                                | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.29 , 86.6                                                                          | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.24$                          | Xtriage          |
| Estimated twinning fraction                                             | 0.467 for -h,-k,l<br>0.477 for h,-h-k,-l<br>0.467 for -k,-h,-l                       | Xtriage          |
| Reported twinning fraction                                              | 0.253 for H, K, L<br>0.254 for K, H, -L<br>0.245 for -h,-k,l<br>0.248 for -K, -H, -L | Depositor        |
| Outliers                                                                | 0 of 128203 reflections                                                              | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.95                                                                                 | EDS              |
| Total number of atoms                                                   | 17536                                                                                | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 86.0                                                                                 | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.91% 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

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

| Mol | Chain | Bond lengths |                  | Bond angles |                 |
|-----|-------|--------------|------------------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5          | RMSZ        | # Z  >5         |
| 1   | A     | 1.23         | 4/1484 (0.3%)    | 1.42        | 2/2016 (0.1%)   |
| 1   | B     | 1.10         | 0/1484           | 1.36        | 0/2016          |
| 1   | C     | 1.07         | 0/1484           | 1.29        | 0/2016          |
| 1   | D     | 1.57         | 20/1492 (1.3%)   | 1.62        | 17/2027 (0.8%)  |
| 1   | E     | 1.41         | 12/1512 (0.8%)   | 1.45        | 6/2053 (0.3%)   |
| 1   | F     | 1.24         | 6/1512 (0.4%)    | 1.37        | 2/2053 (0.1%)   |
| 1   | G     | 1.29         | 9/1543 (0.6%)    | 1.38        | 7/2097 (0.3%)   |
| 1   | H     | 1.72         | 35/1484 (2.4%)   | 1.54        | 5/2016 (0.2%)   |
| 1   | I     | 1.27         | 4/1484 (0.3%)    | 1.43        | 2/2016 (0.1%)   |
| 1   | J     | 1.19         | 3/1484 (0.2%)    | 1.40        | 1/2016 (0.0%)   |
| 1   | K     | 1.60         | 25/1503 (1.7%)   | 1.48        | 9/2042 (0.4%)   |
| 1   | L     | 1.15         | 2/1484 (0.1%)    | 1.38        | 3/2016 (0.1%)   |
| All | All   | 1.33         | 120/17950 (0.7%) | 1.43        | 54/24384 (0.2%) |

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                   | 1                   |
| 1   | D     | 0                   | 2                   |
| 1   | E     | 0                   | 4                   |
| 1   | G     | 0                   | 2                   |
| 1   | I     | 0                   | 2                   |
| 1   | J     | 0                   | 3                   |
| 1   | K     | 0                   | 3                   |
| All | All   | 0                   | 17                  |

All (120) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 1   | H     | 292 | PRO  | C-O   | -14.66 | 1.09        | 1.23     |

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| Mol | Chain | Res | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1   | K     | 327 | ILE  | C-O     | -11.91 | 1.09        | 1.24     |
| 1   | D     | 361 | PHE  | C-O     | -11.37 | 1.09        | 1.23     |
| 1   | H     | 309 | ASP  | CG-OD1  | -9.38  | 1.07        | 1.25     |
| 1   | G     | 316 | TYR  | C-O     | 9.16   | 1.35        | 1.23     |
| 1   | H     | 366 | ILE  | C-O     | -8.96  | 1.14        | 1.24     |
| 1   | E     | 363 | PHE  | C-O     | -8.94  | 1.12        | 1.24     |
| 1   | D     | 225 | VAL  | C-O     | -8.89  | 1.14        | 1.24     |
| 1   | D     | 361 | PHE  | CG-CD1  | -8.89  | 1.20        | 1.38     |
| 1   | K     | 292 | PRO  | N-CD    | -8.85  | 1.35        | 1.47     |
| 1   | H     | 328 | LYS  | C-N     | -8.77  | 1.20        | 1.33     |
| 1   | H     | 327 | ILE  | CA-C    | 8.64   | 1.63        | 1.52     |
| 1   | E     | 309 | ASP  | C-O     | 8.62   | 1.34        | 1.24     |
| 1   | K     | 185 | HIS  | CE1-NE2 | 8.61   | 1.41        | 1.32     |
| 1   | D     | 343 | PHE  | N-CA    | 8.54   | 1.56        | 1.46     |
| 1   | D     | 342 | THR  | C-N     | -8.46  | 1.21        | 1.33     |
| 1   | E     | 308 | ARG  | C-O     | 8.38   | 1.33        | 1.24     |
| 1   | D     | 330 | THR  | C-O     | 8.30   | 1.34        | 1.23     |
| 1   | G     | 226 | SER  | C-O     | 8.22   | 1.34        | 1.24     |
| 1   | K     | 328 | LYS  | N-CA    | 8.20   | 1.58        | 1.46     |
| 1   | H     | 313 | GLY  | C-N     | -7.91  | 1.23        | 1.33     |
| 1   | J     | 316 | TYR  | C-O     | 7.88   | 1.33        | 1.23     |
| 1   | F     | 313 | GLY  | C-O     | 7.80   | 1.31        | 1.23     |
| 1   | H     | 327 | ILE  | C-O     | -7.79  | 1.14        | 1.24     |
| 1   | H     | 292 | PRO  | CA-C    | 7.76   | 1.59        | 1.52     |
| 1   | L     | 362 | THR  | C-O     | 7.73   | 1.33        | 1.23     |
| 1   | H     | 326 | VAL  | C-N     | -7.49  | 1.23        | 1.33     |
| 1   | D     | 213 | VAL  | C-O     | -7.40  | 1.16        | 1.24     |
| 1   | D     | 224 | ASN  | CG-ND2  | -7.37  | 1.17        | 1.33     |
| 1   | H     | 292 | PRO  | N-CD    | -7.29  | 1.37        | 1.47     |
| 1   | E     | 364 | SER  | C-O     | 7.22   | 1.33        | 1.24     |
| 1   | K     | 342 | THR  | C-O     | 7.19   | 1.32        | 1.23     |
| 1   | H     | 328 | LYS  | N-CA    | 7.06   | 1.56        | 1.46     |
| 1   | E     | 222 | LEU  | C-O     | 7.04   | 1.32        | 1.24     |
| 1   | K     | 366 | ILE  | C-O     | 7.04   | 1.32        | 1.24     |
| 1   | G     | 314 | THR  | C-O     | 6.98   | 1.32        | 1.23     |
| 1   | H     | 328 | LYS  | CA-CB   | 6.92   | 1.61        | 1.53     |
| 1   | H     | 327 | ILE  | N-CA    | 6.87   | 1.54        | 1.46     |
| 1   | I     | 330 | THR  | C-O     | 6.85   | 1.32        | 1.23     |
| 1   | F     | 326 | VAL  | C-O     | 6.84   | 1.32        | 1.24     |
| 1   | H     | 329 | THR  | N-CA    | 6.77   | 1.54        | 1.46     |
| 1   | K     | 327 | ILE  | N-CA    | 6.75   | 1.56        | 1.46     |
| 1   | H     | 328 | LYS  | C-O     | -6.74  | 1.15        | 1.23     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | K     | 292 | PRO  | CA-C   | 6.73  | 1.61        | 1.52     |
| 1   | A     | 212 | LEU  | C-O    | -6.72 | 1.15        | 1.23     |
| 1   | J     | 321 | PRO  | C-O    | -6.67 | 1.15        | 1.24     |
| 1   | H     | 313 | GLY  | C-O    | 6.64  | 1.31        | 1.24     |
| 1   | H     | 313 | GLY  | N-CA   | 6.59  | 1.53        | 1.45     |
| 1   | K     | 362 | THR  | C-O    | 6.59  | 1.31        | 1.23     |
| 1   | D     | 315 | ILE  | CA-C   | 6.57  | 1.61        | 1.52     |
| 1   | K     | 327 | ILE  | C-N    | -6.57 | 1.25        | 1.33     |
| 1   | H     | 221 | ILE  | C-O    | 6.52  | 1.31        | 1.24     |
| 1   | K     | 293 | ASN  | C-O    | 6.47  | 1.31        | 1.24     |
| 1   | E     | 311 | VAL  | C-O    | 6.43  | 1.30        | 1.24     |
| 1   | K     | 327 | ILE  | CA-C   | 6.39  | 1.60        | 1.52     |
| 1   | D     | 342 | THR  | N-CA   | 6.38  | 1.53        | 1.46     |
| 1   | D     | 316 | TYR  | CA-C   | -6.37 | 1.44        | 1.52     |
| 1   | D     | 328 | LYS  | C-O    | -6.34 | 1.16        | 1.23     |
| 1   | K     | 313 | GLY  | C-O    | 6.33  | 1.30        | 1.23     |
| 1   | A     | 265 | ASN  | C-O    | -6.27 | 1.16        | 1.24     |
| 1   | I     | 360 | SER  | C-O    | 6.22  | 1.31        | 1.23     |
| 1   | G     | 359 | THR  | CA-C   | -6.21 | 1.44        | 1.52     |
| 1   | G     | 360 | SER  | N-CA   | 6.20  | 1.53        | 1.46     |
| 1   | K     | 329 | THR  | N-CA   | 6.18  | 1.54        | 1.46     |
| 1   | H     | 292 | PRO  | C-N    | -6.16 | 1.24        | 1.33     |
| 1   | I     | 310 | ILE  | C-O    | 6.15  | 1.30        | 1.24     |
| 1   | D     | 330 | THR  | N-CA   | 6.14  | 1.53        | 1.45     |
| 1   | E     | 308 | ARG  | N-CA   | 6.10  | 1.53        | 1.46     |
| 1   | G     | 226 | SER  | CA-CB  | -6.09 | 1.43        | 1.53     |
| 1   | D     | 362 | THR  | C-O    | 6.08  | 1.31        | 1.23     |
| 1   | D     | 363 | PHE  | CG-CD1 | -6.07 | 1.26        | 1.38     |
| 1   | K     | 328 | LYS  | C-N    | -6.07 | 1.25        | 1.33     |
| 1   | L     | 360 | SER  | C-O    | 6.07  | 1.31        | 1.24     |
| 1   | H     | 312 | TYR  | C-O    | 6.02  | 1.31        | 1.23     |
| 1   | K     | 309 | ASP  | CG-OD1 | -6.02 | 1.14        | 1.25     |
| 1   | H     | 344 | ASP  | N-CA   | 6.01  | 1.53        | 1.46     |
| 1   | H     | 327 | ILE  | CB-CG2 | -6.01 | 1.32        | 1.52     |
| 1   | K     | 295 | VAL  | C-O    | 6.00  | 1.29        | 1.23     |
| 1   | G     | 361 | PHE  | C-O    | -5.99 | 1.17        | 1.24     |
| 1   | H     | 297 | TYR  | CZ-OH  | 5.96  | 1.50        | 1.38     |
| 1   | E     | 308 | ARG  | NE-CZ  | -5.96 | 1.26        | 1.33     |
| 1   | H     | 314 | THR  | N-CA   | 5.92  | 1.53        | 1.46     |
| 1   | E     | 331 | PHE  | CG-CD1 | -5.90 | 1.26        | 1.38     |
| 1   | E     | 361 | PHE  | C-O    | 5.85  | 1.30        | 1.23     |
| 1   | A     | 360 | SER  | C-O    | 5.84  | 1.30        | 1.23     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | F     | 319 | GLY  | C-O    | 5.84  | 1.32        | 1.24     |
| 1   | H     | 342 | THR  | C-O    | 5.83  | 1.31        | 1.23     |
| 1   | F     | 314 | THR  | C-O    | 5.75  | 1.31        | 1.24     |
| 1   | H     | 314 | THR  | C-N    | -5.74 | 1.27        | 1.33     |
| 1   | G     | 363 | PHE  | C-O    | 5.64  | 1.30        | 1.23     |
| 1   | H     | 293 | ASN  | C-O    | 5.61  | 1.30        | 1.24     |
| 1   | H     | 248 | PHE  | N-CA   | 5.58  | 1.53        | 1.45     |
| 1   | D     | 360 | SER  | C-O    | 5.58  | 1.30        | 1.23     |
| 1   | K     | 326 | VAL  | N-CA   | 5.55  | 1.52        | 1.46     |
| 1   | D     | 343 | PHE  | C-N    | -5.53 | 1.24        | 1.33     |
| 1   | K     | 327 | ILE  | CB-CG2 | -5.50 | 1.34        | 1.52     |
| 1   | F     | 313 | GLY  | N-CA   | 5.46  | 1.51        | 1.45     |
| 1   | K     | 345 | PHE  | N-CA   | 5.44  | 1.52        | 1.46     |
| 1   | E     | 310 | ILE  | N-CA   | 5.44  | 1.52        | 1.46     |
| 1   | H     | 345 | PHE  | N-CA   | 5.40  | 1.52        | 1.46     |
| 1   | K     | 313 | GLY  | C-N    | -5.38 | 1.26        | 1.33     |
| 1   | H     | 293 | ASN  | N-CA   | 5.37  | 1.53        | 1.46     |
| 1   | I     | 342 | THR  | N-CA   | 5.35  | 1.52        | 1.46     |
| 1   | J     | 225 | VAL  | N-CA   | 5.31  | 1.52        | 1.46     |
| 1   | A     | 362 | THR  | C-O    | 5.25  | 1.29        | 1.23     |
| 1   | K     | 185 | HIS  | N-CA   | 5.22  | 1.56        | 1.46     |
| 1   | K     | 326 | VAL  | C-N    | -5.22 | 1.25        | 1.33     |
| 1   | K     | 313 | GLY  | N-CA   | 5.19  | 1.51        | 1.45     |
| 1   | H     | 326 | VAL  | N-CA   | 5.18  | 1.52        | 1.46     |
| 1   | F     | 363 | PHE  | C-O    | 5.17  | 1.29        | 1.23     |
| 1   | G     | 224 | ASN  | C-O    | 5.17  | 1.30        | 1.24     |
| 1   | E     | 364 | SER  | CA-CB  | 5.16  | 1.62        | 1.53     |
| 1   | H     | 367 | ALA  | N-CA   | 5.16  | 1.52        | 1.46     |
| 1   | D     | 324 | PRO  | CA-CB  | -5.08 | 1.46        | 1.53     |
| 1   | H     | 362 | THR  | C-O    | 5.07  | 1.30        | 1.24     |
| 1   | H     | 343 | PHE  | CG-CD1 | -5.07 | 1.28        | 1.38     |
| 1   | H     | 310 | ILE  | C-O    | -5.06 | 1.18        | 1.24     |
| 1   | D     | 344 | ASP  | CG-OD2 | -5.04 | 1.15        | 1.25     |
| 1   | D     | 311 | VAL  | C-O    | -5.04 | 1.18        | 1.24     |
| 1   | K     | 343 | PHE  | CG-CD2 | -5.03 | 1.28        | 1.38     |

All (54) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | D     | 358 | THR  | CA-C-N | 8.82  | 135.18      | 123.00   |
| 1   | D     | 358 | THR  | C-N-CA | 8.82  | 135.18      | 123.00   |
| 1   | D     | 316 | TYR  | CA-C-O | -8.08 | 110.28      | 120.14   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | D     | 361 | PHE  | CA-C-O    | -8.03 | 112.52      | 121.51   |
| 1   | D     | 359 | THR  | CA-CB-OG1 | -7.90 | 97.76       | 109.60   |
| 1   | H     | 327 | ILE  | CA-C-O    | -7.62 | 111.25      | 120.78   |
| 1   | D     | 358 | THR  | CA-CB-OG1 | -7.55 | 98.27       | 109.60   |
| 1   | H     | 292 | PRO  | CB-CA-C   | 7.46  | 118.19      | 111.40   |
| 1   | D     | 316 | TYR  | O-C-N     | 7.45  | 131.91      | 123.42   |
| 1   | J     | 313 | GLY  | CA-C-O    | -7.35 | 114.64      | 121.63   |
| 1   | G     | 361 | PHE  | CA-C-O    | -7.34 | 112.46      | 120.24   |
| 1   | K     | 328 | LYS  | CB-CA-C   | -7.01 | 100.86      | 111.73   |
| 1   | D     | 359 | THR  | CB-CA-C   | -6.93 | 97.73       | 109.72   |
| 1   | D     | 224 | ASN  | CB-CA-C   | -6.79 | 101.45      | 111.77   |
| 1   | E     | 308 | ARG  | CB-CA-C   | 6.51  | 121.11      | 110.88   |
| 1   | K     | 326 | VAL  | CA-C-N    | -6.44 | 114.35      | 123.10   |
| 1   | K     | 326 | VAL  | C-N-CA    | -6.44 | 114.35      | 123.10   |
| 1   | G     | 363 | PHE  | CA-C-O    | -6.30 | 114.71      | 121.45   |
| 1   | D     | 357 | GLU  | CA-C-O    | -6.19 | 114.10      | 120.54   |
| 1   | D     | 329 | THR  | CA-CB-OG1 | -6.10 | 100.44      | 109.60   |
| 1   | G     | 359 | THR  | CA-CB-OG1 | -6.09 | 100.46      | 109.60   |
| 1   | K     | 343 | PHE  | CA-C-O    | -6.06 | 113.41      | 120.62   |
| 1   | D     | 266 | LEU  | CA-C-N    | 6.05  | 127.55      | 120.71   |
| 1   | D     | 266 | LEU  | C-N-CA    | 6.05  | 127.55      | 120.71   |
| 1   | G     | 359 | THR  | CB-CA-C   | -5.90 | 100.29      | 109.61   |
| 1   | E     | 309 | ASP  | CA-CB-CG  | -5.87 | 106.73      | 112.60   |
| 1   | H     | 298 | PRO  | N-CA-C    | 5.86  | 119.71      | 111.33   |
| 1   | L     | 295 | VAL  | CA-C-N    | 5.67  | 127.88      | 120.28   |
| 1   | L     | 295 | VAL  | C-N-CA    | 5.67  | 127.88      | 120.28   |
| 1   | I     | 312 | TYR  | CA-C-N    | 5.63  | 128.10      | 122.30   |
| 1   | I     | 312 | TYR  | C-N-CA    | 5.63  | 128.10      | 122.30   |
| 1   | D     | 358 | THR  | CA-C-O    | -5.62 | 115.02      | 121.82   |
| 1   | A     | 316 | TYR  | CA-C-O    | -5.61 | 113.64      | 120.54   |
| 1   | K     | 329 | THR  | CA-C-O    | -5.61 | 114.92      | 120.98   |
| 1   | A     | 212 | LEU  | CA-C-O    | -5.60 | 114.89      | 121.16   |
| 1   | E     | 294 | LEU  | N-CA-C    | -5.57 | 104.73      | 112.30   |
| 1   | K     | 367 | ALA  | CA-C-N    | 5.56  | 127.67      | 120.44   |
| 1   | K     | 367 | ALA  | C-N-CA    | 5.56  | 127.67      | 120.44   |
| 1   | H     | 329 | THR  | CA-C-O    | -5.42 | 114.56      | 120.36   |
| 1   | L     | 222 | LEU  | CA-C-O    | -5.40 | 115.68      | 121.56   |
| 1   | D     | 363 | PHE  | CA-C-O    | -5.39 | 115.68      | 121.45   |
| 1   | H     | 332 | ASN  | CB-CA-C   | -5.29 | 99.88       | 110.42   |
| 1   | G     | 359 | THR  | CA-C-O    | -5.26 | 115.39      | 121.07   |
| 1   | D     | 360 | SER  | N-CA-C    | -5.23 | 103.44      | 110.24   |
| 1   | K     | 292 | PRO  | N-CA-C    | -5.21 | 101.73      | 112.47   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | F     | 232 | GLY  | CA-C-N  | 5.20  | 127.50      | 120.38   |
| 1   | F     | 232 | GLY  | C-N-CA  | 5.20  | 127.50      | 120.38   |
| 1   | E     | 364 | SER  | CA-C-N  | 5.20  | 131.55      | 122.82   |
| 1   | E     | 364 | SER  | C-N-CA  | 5.20  | 131.55      | 122.82   |
| 1   | G     | 317 | LEU  | CB-CA-C | -5.13 | 104.21      | 111.76   |
| 1   | K     | 328 | LYS  | CA-C-O  | -5.13 | 115.22      | 121.58   |
| 1   | D     | 225 | VAL  | N-CA-CB | 5.11  | 117.18      | 111.21   |
| 1   | G     | 225 | VAL  | CA-C-O  | -5.04 | 115.10      | 120.39   |
| 1   | E     | 311 | VAL  | O-C-N   | 5.03  | 127.50      | 122.97   |

There are no chirality outliers.

All (17) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | A     | 283 | ALA  | Peptide   |
| 1   | D     | 190 | LEU  | Peptide   |
| 1   | D     | 363 | PHE  | Mainchain |
| 1   | E     | 185 | HIS  | Peptide   |
| 1   | E     | 186 | ASP  | Peptide   |
| 1   | E     | 222 | LEU  | Peptide   |
| 1   | E     | 310 | ILE  | Mainchain |
| 1   | G     | 225 | VAL  | Peptide   |
| 1   | G     | 319 | GLY  | Peptide   |
| 1   | I     | 191 | TRP  | Peptide   |
| 1   | I     | 347 | TRP  | Peptide   |
| 1   | J     | 313 | GLY  | Mainchain |
| 1   | J     | 319 | GLY  | Peptide   |
| 1   | J     | 337 | CYS  | Peptide   |
| 1   | K     | 291 | MET  | Mainchain |
| 1   | K     | 313 | GLY  | Peptide   |
| 1   | K     | 328 | LYS  | Mainchain |

## 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     | 1450  | 0        | 1430     | 72      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | B     | 1450  | 0        | 1430     | 72      | 0            |
| 1   | C     | 1450  | 0        | 1430     | 58      | 1            |
| 1   | D     | 1458  | 0        | 1434     | 109     | 0            |
| 1   | E     | 1477  | 0        | 1454     | 113     | 0            |
| 1   | F     | 1477  | 0        | 1454     | 86      | 0            |
| 1   | G     | 1506  | 0        | 1478     | 87      | 0            |
| 1   | H     | 1450  | 0        | 1429     | 130     | 0            |
| 1   | I     | 1450  | 0        | 1430     | 79      | 0            |
| 1   | J     | 1450  | 0        | 1430     | 49      | 0            |
| 1   | K     | 1468  | 0        | 1441     | 106     | 1            |
| 1   | L     | 1450  | 0        | 1430     | 72      | 0            |
| All | All   | 17536 | 0        | 17270    | 919     | 1            |

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 26.

All (919) 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:H:315:ILE:HD13 | 1:H:358:THR:OG1  | 1.15                     | 1.27              |
| 1:E:222:LEU:O    | 1:F:220:GLN:NE2  | 1.66                     | 1.26              |
| 1:D:364:SER:OG   | 1:F:362:THR:HG21 | 1.33                     | 1.23              |
| 1:H:313:GLY:O    | 1:H:327:ILE:N    | 1.68                     | 1.22              |
| 1:K:309:ASP:OD2  | 1:K:333:GLN:NE2  | 1.74                     | 1.20              |
| 1:G:226:SER:OG   | 1:G:358:THR:O    | 1.62                     | 1.18              |
| 1:G:273:PHE:O    | 1:G:279:ASN:ND2  | 1.75                     | 1.17              |
| 1:B:191:TRP:CZ2  | 1:B:274:ARG:HD2  | 1.80                     | 1.16              |
| 1:D:299:LYS:NZ   | 1:D:337:CYS:O    | 1.77                     | 1.16              |
| 1:K:313:GLY:O    | 1:K:327:ILE:N    | 1.76                     | 1.16              |
| 1:F:249:THR:OG1  | 1:F:344:ASP:OD1  | 1.63                     | 1.16              |
| 1:B:191:TRP:CE2  | 1:B:274:ARG:HD2  | 1.79                     | 1.16              |
| 1:I:249:THR:OG1  | 1:I:344:ASP:OD1  | 1.59                     | 1.14              |
| 1:A:213:VAL:HG21 | 1:B:366:ILE:HD11 | 1.27                     | 1.14              |
| 1:D:201:THR:O    | 1:D:265:ASN:ND2  | 1.81                     | 1.12              |
| 1:F:221:ILE:HG21 | 1:F:365:TYR:CE1  | 1.86                     | 1.10              |
| 1:H:315:ILE:CD1  | 1:H:358:THR:OG1  | 2.04                     | 1.05              |
| 1:H:249:THR:OG1  | 1:H:344:ASP:OD1  | 1.75                     | 1.04              |
| 1:K:330:THR:O    | 1:K:342:THR:HG23 | 1.59                     | 1.03              |
| 1:E:330:THR:CG2  | 1:E:333:GLN:HB2  | 1.89                     | 1.02              |
| 1:I:236:ILE:HG22 | 1:I:355:GLU:HA   | 1.38                     | 1.02              |
| 1:E:291:MET:HE2  | 1:E:291:MET:HA   | 1.42                     | 1.01              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:221:ILE:HG21 | 1:F:365:TYR:CZ   | 1.94                     | 1.01              |
| 1:H:309:ASP:O    | 1:H:330:THR:HG22 | 1.60                     | 1.01              |
| 1:E:330:THR:HG22 | 1:E:333:GLN:HB2  | 1.42                     | 1.01              |
| 1:E:315:ILE:HD12 | 1:E:315:ILE:O    | 1.58                     | 1.01              |
| 1:D:198:PRO:O    | 1:I:270:TYR:OH   | 1.80                     | 0.98              |
| 1:K:331:PHE:CE2  | 1:K:365:TYR:HB3  | 1.98                     | 0.98              |
| 1:E:222:LEU:C    | 1:F:220:GLN:NE2  | 2.21                     | 0.97              |
| 1:H:293:ASN:HB2  | 1:H:368:GLN:HA   | 1.47                     | 0.96              |
| 1:I:246:LYS:HB3  | 1:I:347:TRP:CZ2  | 2.00                     | 0.95              |
| 1:D:312:TYR:OH   | 1:F:319:GLY:O    | 1.84                     | 0.94              |
| 1:I:224:ASN:ND2  | 1:I:362:THR:OG1  | 2.00                     | 0.94              |
| 1:B:191:TRP:CE2  | 1:B:274:ARG:CD   | 2.50                     | 0.93              |
| 1:E:200:CYS:SG   | 1:E:208:SER:OG   | 2.27                     | 0.92              |
| 1:A:195:ASP:OD2  | 1:L:195:ASP:OD2  | 1.88                     | 0.91              |
| 1:D:223:ALA:O    | 1:D:362:THR:HA   | 1.72                     | 0.90              |
| 1:A:357:GLU:OE1  | 1:B:307:ALA:N    | 2.05                     | 0.90              |
| 1:B:191:TRP:CH2  | 1:B:194:PRO:HD3  | 2.07                     | 0.90              |
| 1:K:227:LEU:H    | 1:K:358:THR:HG22 | 1.37                     | 0.89              |
| 1:L:187:THR:N    | 1:L:216:LYS:O    | 2.06                     | 0.89              |
| 1:E:315:ILE:O    | 1:E:315:ILE:CD1  | 2.21                     | 0.88              |
| 1:G:223:ALA:HB1  | 1:G:363:PHE:CZ   | 2.08                     | 0.88              |
| 1:H:315:ILE:HD13 | 1:H:358:THR:HG1  | 0.89                     | 0.88              |
| 1:G:223:ALA:CB   | 1:G:363:PHE:CZ   | 2.57                     | 0.87              |
| 1:I:193:THR:O    | 1:I:209:LYS:NZ   | 2.07                     | 0.87              |
| 1:I:238:ASN:O    | 1:I:239:ASN:ND2  | 2.08                     | 0.86              |
| 1:L:224:ASN:ND2  | 1:L:362:THR:OG1  | 2.08                     | 0.86              |
| 1:D:315:ILE:HG22 | 1:D:359:THR:O    | 1.74                     | 0.86              |
| 1:K:331:PHE:CE2  | 1:K:365:TYR:CB   | 2.58                     | 0.86              |
| 1:E:222:LEU:C    | 1:F:220:GLN:HE22 | 1.84                     | 0.85              |
| 1:E:362:THR:HG21 | 1:F:364:SER:OG   | 1.74                     | 0.85              |
| 1:K:365:TYR:HD1  | 1:K:365:TYR:O    | 1.60                     | 0.85              |
| 1:B:274:ARG:NH1  | 1:C:219:SER:OG   | 2.10                     | 0.85              |
| 1:H:258:GLY:O    | 1:H:287:ALA:HB3  | 1.77                     | 0.84              |
| 1:C:193:THR:HG23 | 1:C:279:ASN:HD21 | 1.39                     | 0.84              |
| 1:B:191:TRP:CD2  | 1:B:274:ARG:HD3  | 2.12                     | 0.84              |
| 1:H:365:TYR:HD1  | 1:H:365:TYR:O    | 1.59                     | 0.84              |
| 1:E:215:THR:OG1  | 1:F:220:GLN:CG   | 2.27                     | 0.83              |
| 1:B:303:SER:OG   | 1:L:278:SER:N    | 2.12                     | 0.83              |
| 1:D:206:LYS:O    | 1:I:269:THR:HG21 | 1.78                     | 0.83              |
| 1:K:315:ILE:HD13 | 1:K:358:THR:OG1  | 1.80                     | 0.82              |
| 1:A:299:LYS:NZ   | 1:A:334:GLU:O    | 2.12                     | 0.81              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:365:TYR:O    | 1:K:365:TYR:CD1  | 2.34                     | 0.81              |
| 1:E:215:THR:OG1  | 1:F:220:GLN:HG2  | 1.80                     | 0.80              |
| 1:D:271:TRP:CD1  | 1:D:284:TYR:HH   | 2.00                     | 0.80              |
| 1:C:189:THR:HG22 | 1:C:215:THR:HG23 | 1.62                     | 0.80              |
| 1:J:324:PRO:HD2  | 1:J:351:TYR:OH   | 1.81                     | 0.80              |
| 1:B:191:TRP:CD2  | 1:B:274:ARG:CD   | 2.65                     | 0.80              |
| 1:G:190:LEU:HD21 | 1:G:273:PHE:CE1  | 2.17                     | 0.80              |
| 1:G:204:GLN:OE1  | 1:G:232:GLY:HA2  | 1.82                     | 0.79              |
| 1:H:293:ASN:CB   | 1:H:368:GLN:HA   | 2.12                     | 0.79              |
| 1:E:306:TYR:HB2  | 1:E:308:ARG:NH1  | 1.97                     | 0.79              |
| 1:H:329:THR:HG23 | 1:H:343:PHE:CD1  | 2.16                     | 0.79              |
| 1:L:239:ASN:HD21 | 1:L:347:TRP:HH2  | 1.28                     | 0.78              |
| 1:H:365:TYR:O    | 1:H:365:TYR:CD1  | 2.37                     | 0.78              |
| 1:H:315:ILE:CD1  | 1:H:358:THR:HG1  | 1.85                     | 0.77              |
| 1:I:236:ILE:CG2  | 1:I:355:GLU:HA   | 2.14                     | 0.77              |
| 1:B:274:ARG:HB3  | 1:B:277:ASP:HA   | 1.67                     | 0.77              |
| 1:H:333:GLN:NE2  | 1:H:333:GLN:O    | 2.17                     | 0.77              |
| 1:D:213:VAL:HG12 | 1:E:220:GLN:HE21 | 1.49                     | 0.77              |
| 1:D:223:ALA:HB3  | 1:D:363:PHE:O    | 1.85                     | 0.76              |
| 1:A:193:THR:O    | 1:A:209:LYS:NZ   | 2.18                     | 0.76              |
| 1:G:226:SER:OG   | 1:G:358:THR:OG1  | 2.03                     | 0.76              |
| 1:H:293:ASN:O    | 1:H:296:ALA:HB3  | 1.85                     | 0.76              |
| 1:D:316:TYR:CE1  | 1:D:324:PRO:HB3  | 2.20                     | 0.76              |
| 1:F:217:CYS:HB2  | 1:F:220:GLN:HB2  | 1.67                     | 0.76              |
| 1:G:189:THR:OG1  | 1:H:219:SER:OG   | 2.03                     | 0.75              |
| 1:A:316:TYR:CE1  | 1:A:324:PRO:HB3  | 2.21                     | 0.75              |
| 1:B:245:ILE:CG2  | 1:B:347:TRP:HB3  | 2.16                     | 0.75              |
| 1:F:221:ILE:O    | 1:F:364:SER:HB2  | 1.86                     | 0.75              |
| 1:K:196:THR:HA   | 1:K:209:LYS:HG2  | 1.67                     | 0.75              |
| 1:K:311:VAL:HG12 | 1:K:311:VAL:O    | 1.85                     | 0.75              |
| 1:A:213:VAL:CG2  | 1:B:366:ILE:HD11 | 2.14                     | 0.74              |
| 1:F:260:LEU:O    | 1:F:268:LYS:NZ   | 2.19                     | 0.74              |
| 1:G:204:GLN:OE1  | 1:G:232:GLY:CA   | 2.35                     | 0.74              |
| 1:D:270:TYR:OH   | 1:I:198:PRO:O    | 2.05                     | 0.74              |
| 1:I:236:ILE:HG22 | 1:I:355:GLU:CA   | 2.16                     | 0.73              |
| 1:A:249:THR:OG1  | 1:A:344:ASP:OD1  | 2.06                     | 0.73              |
| 1:K:193:THR:O    | 1:K:209:LYS:NZ   | 2.21                     | 0.73              |
| 1:K:365:TYR:CD1  | 1:K:365:TYR:C    | 2.65                     | 0.73              |
| 1:D:359:THR:HG22 | 1:E:310:ILE:HB   | 1.71                     | 0.72              |
| 1:B:191:TRP:CZ2  | 1:B:193:THR:HA   | 2.24                     | 0.72              |
| 1:C:193:THR:CG2  | 1:C:279:ASN:HD21 | 2.02                     | 0.72              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:238:ASN:ND2  | 1:A:353:ASN:OD1  | 2.22                     | 0.72              |
| 1:E:330:THR:HG21 | 1:E:333:GLN:HB2  | 1.71                     | 0.72              |
| 1:L:297:TYR:OH   | 1:L:366:ILE:N    | 2.23                     | 0.72              |
| 1:K:365:TYR:HD1  | 1:K:365:TYR:C    | 1.98                     | 0.72              |
| 1:F:199:ASN:O    | 1:F:266:LEU:HD12 | 1.90                     | 0.72              |
| 1:G:327:ILE:HG21 | 1:G:361:PHE:CD2  | 2.25                     | 0.72              |
| 1:L:219:SER:O    | 1:L:367:ALA:HB3  | 1.90                     | 0.72              |
| 1:F:313:GLY:HA3  | 1:F:361:PHE:CZ   | 2.25                     | 0.71              |
| 1:E:330:THR:CG2  | 1:E:333:GLN:CB   | 2.68                     | 0.71              |
| 1:K:210:LEU:HD13 | 1:K:227:LEU:HD13 | 1.73                     | 0.70              |
| 1:J:315:ILE:HD12 | 1:J:315:ILE:O    | 1.90                     | 0.70              |
| 1:B:291:MET:HE2  | 1:B:291:MET:HA   | 1.73                     | 0.70              |
| 1:H:210:LEU:HD12 | 1:H:226:SER:O    | 1.92                     | 0.70              |
| 1:L:286:LYS:O    | 1:L:286:LYS:HG3  | 1.90                     | 0.70              |
| 1:K:305:LYS:C    | 1:K:305:LYS:HD2  | 2.16                     | 0.70              |
| 1:A:315:ILE:HG22 | 1:A:359:THR:O    | 1.91                     | 0.70              |
| 1:B:274:ARG:CZ   | 1:C:219:SER:OG   | 2.39                     | 0.70              |
| 1:C:193:THR:O    | 1:C:209:LYS:NZ   | 2.24                     | 0.70              |
| 1:D:255:ASP:C    | 1:D:255:ASP:OD1  | 2.35                     | 0.70              |
| 1:F:195:ASP:O    | 1:F:209:LYS:NZ   | 2.24                     | 0.70              |
| 1:G:223:ALA:HB3  | 1:G:363:PHE:CZ   | 2.26                     | 0.69              |
| 1:E:331:PHE:CE1  | 1:E:365:TYR:HD2  | 2.10                     | 0.69              |
| 1:H:293:ASN:HB2  | 1:H:368:GLN:CA   | 2.20                     | 0.69              |
| 1:I:239:ASN:HB3  | 1:I:353:ASN:ND2  | 2.08                     | 0.69              |
| 1:D:215:THR:OG1  | 1:E:220:GLN:NE2  | 2.26                     | 0.69              |
| 1:K:331:PHE:HE2  | 1:K:365:TYR:CB   | 2.04                     | 0.69              |
| 1:A:224:ASN:OD1  | 1:B:308:ARG:NH2  | 2.19                     | 0.68              |
| 1:L:216:LYS:NZ   | 1:L:218:GLY:O    | 2.26                     | 0.68              |
| 1:F:339:TYR:HE1  | 1:F:368:GLN:HE21 | 1.40                     | 0.68              |
| 1:E:331:PHE:CZ   | 1:E:365:TYR:HB3  | 2.29                     | 0.68              |
| 1:D:322:ASP:OD1  | 1:D:322:ASP:N    | 2.25                     | 0.68              |
| 1:F:221:ILE:CG2  | 1:F:365:TYR:CE1  | 2.74                     | 0.68              |
| 1:E:215:THR:CB   | 1:F:220:GLN:HG3  | 2.24                     | 0.68              |
| 1:I:238:ASN:C    | 1:I:239:ASN:HD22 | 2.02                     | 0.68              |
| 1:A:220:GLN:OE1  | 1:C:222:LEU:CD2  | 2.41                     | 0.67              |
| 1:H:333:GLN:O    | 1:H:333:GLN:HG3  | 1.93                     | 0.67              |
| 1:F:207:ASP:HB2  | 1:F:231:ALA:O    | 1.94                     | 0.67              |
| 1:A:190:LEU:HD22 | 1:A:271:TRP:CE2  | 2.29                     | 0.67              |
| 1:H:317:LEU:HD22 | 1:H:356:PHE:HA   | 1.77                     | 0.67              |
| 1:F:255:ASP:OD1  | 1:F:259:VAL:HG22 | 1.93                     | 0.66              |
| 1:K:241:ASN:OD1  | 1:K:241:ASN:N    | 2.29                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:189:THR:HB   | 1:H:215:THR:HA   | 1.77                     | 0.66              |
| 1:G:260:LEU:HD22 | 1:G:266:LEU:HD23 | 1.78                     | 0.65              |
| 1:D:213:VAL:CG1  | 1:E:220:GLN:HE21 | 2.10                     | 0.65              |
| 1:E:221:ILE:O    | 1:E:364:SER:HB2  | 1.96                     | 0.65              |
| 1:E:291:MET:HA   | 1:E:291:MET:CE   | 2.23                     | 0.65              |
| 1:G:316:TYR:HE2  | 1:H:312:TYR:HB3  | 1.60                     | 0.65              |
| 1:L:299:LYS:HB3  | 1:L:332:ASN:O    | 1.97                     | 0.65              |
| 1:B:191:TRP:CE3  | 1:B:274:ARG:HD3  | 2.31                     | 0.65              |
| 1:A:192:THR:HG22 | 1:A:212:LEU:O    | 1.96                     | 0.65              |
| 1:K:315:ILE:HD12 | 1:K:315:ILE:O    | 1.96                     | 0.65              |
| 1:D:215:THR:HG21 | 1:E:217:CYS:O    | 1.97                     | 0.65              |
| 1:D:223:ALA:O    | 1:D:362:THR:CA   | 2.45                     | 0.65              |
| 1:E:224:ASN:ND2  | 1:E:361:PHE:O    | 2.29                     | 0.65              |
| 1:G:224:ASN:OD1  | 1:H:308:ARG:NH2  | 2.30                     | 0.65              |
| 1:J:320:LYS:O    | 1:J:323:GLN:O    | 2.16                     | 0.64              |
| 1:A:192:THR:HG21 | 1:A:210:LEU:O    | 1.97                     | 0.64              |
| 1:A:213:VAL:HG21 | 1:B:366:ILE:CD1  | 2.18                     | 0.64              |
| 1:I:255:ASP:OD1  | 1:I:255:ASP:C    | 2.40                     | 0.64              |
| 1:G:223:ALA:HB3  | 1:G:363:PHE:CE2  | 2.31                     | 0.64              |
| 1:J:293:ASN:HB3  | 1:J:296:ALA:HB3  | 1.79                     | 0.64              |
| 1:L:291:MET:HE2  | 1:L:291:MET:HA   | 1.78                     | 0.64              |
| 1:A:255:ASP:OD1  | 1:A:257:ASN:N    | 2.31                     | 0.64              |
| 1:K:308:ARG:O    | 1:K:308:ARG:HG2  | 1.98                     | 0.64              |
| 1:B:191:TRP:CH2  | 1:B:194:PRO:CD   | 2.81                     | 0.64              |
| 1:I:272:ASN:HB3  | 1:I:279:ASN:HB3  | 1.80                     | 0.64              |
| 1:D:197:SER:OG   | 1:I:197:SER:CB   | 2.46                     | 0.64              |
| 1:H:294:LEU:HD23 | 1:H:339:TYR:CE2  | 2.32                     | 0.64              |
| 1:C:343:PHE:HB3  | 1:C:345:PHE:CE2  | 2.33                     | 0.63              |
| 1:H:338:GLU:HB3  | 1:H:339:TYR:CE1  | 2.33                     | 0.63              |
| 1:E:257:ASN:O    | 1:E:287:ALA:HB3  | 1.99                     | 0.63              |
| 1:E:193:THR:O    | 1:E:209:LYS:NZ   | 2.30                     | 0.63              |
| 1:B:344:ASP:N    | 1:B:344:ASP:OD1  | 2.32                     | 0.63              |
| 1:B:245:ILE:HG22 | 1:B:347:TRP:HB3  | 1.81                     | 0.62              |
| 1:E:215:THR:OG1  | 1:F:220:GLN:HG3  | 1.99                     | 0.62              |
| 1:D:212:LEU:HD13 | 1:D:225:VAL:HG23 | 1.81                     | 0.62              |
| 1:D:189:THR:HG21 | 1:E:219:SER:OG   | 1.99                     | 0.62              |
| 1:D:191:TRP:CD1  | 1:D:191:TRP:O    | 2.52                     | 0.62              |
| 1:F:313:GLY:HA3  | 1:F:361:PHE:CE2  | 2.35                     | 0.62              |
| 1:G:273:PHE:HB2  | 1:G:280:VAL:HG13 | 1.81                     | 0.62              |
| 1:H:365:TYR:CD1  | 1:H:365:TYR:C    | 2.77                     | 0.62              |
| 1:C:220:GLN:NE2  | 1:C:364:SER:HB2  | 2.15                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:191:TRP:CD1  | 1:G:279:ASN:HD21 | 2.18                     | 0.62              |
| 1:K:331:PHE:CZ   | 1:K:365:TYR:HB3  | 2.34                     | 0.62              |
| 1:L:300:PRO:HB2  | 1:L:304:LYS:HD3  | 1.81                     | 0.62              |
| 1:B:191:TRP:CD1  | 1:B:191:TRP:C    | 2.78                     | 0.62              |
| 1:D:311:VAL:HG11 | 1:D:363:PHE:HB2  | 1.81                     | 0.62              |
| 1:J:224:ASN:HB2  | 1:K:220:GLN:CD   | 2.25                     | 0.62              |
| 1:F:316:TYR:N    | 1:F:316:TYR:CD1  | 2.67                     | 0.62              |
| 1:H:333:GLN:O    | 1:H:333:GLN:CG   | 2.48                     | 0.62              |
| 1:B:316:TYR:CE2  | 1:B:324:PRO:HB3  | 2.35                     | 0.62              |
| 1:E:362:THR:CG2  | 1:F:364:SER:OG   | 2.47                     | 0.62              |
| 1:H:272:ASN:OD1  | 1:H:284:TYR:HB3  | 2.00                     | 0.62              |
| 1:K:211:THR:HG22 | 1:K:211:THR:O    | 2.00                     | 0.62              |
| 1:H:331:PHE:CE2  | 1:H:365:TYR:CB   | 2.83                     | 0.61              |
| 1:K:227:LEU:N    | 1:K:358:THR:HG22 | 2.13                     | 0.61              |
| 1:D:200:CYS:O    | 1:D:208:SER:OG   | 2.14                     | 0.61              |
| 1:K:212:LEU:HD13 | 1:K:225:VAL:HB   | 1.82                     | 0.61              |
| 1:K:331:PHE:O    | 1:K:333:GLN:HG2  | 2.00                     | 0.61              |
| 1:A:316:TYR:O    | 1:A:359:THR:HG23 | 1.99                     | 0.61              |
| 1:E:332:ASN:ND2  | 1:E:339:TYR:HA   | 2.16                     | 0.61              |
| 1:G:226:SER:HB3  | 1:H:308:ARG:HD2  | 1.82                     | 0.61              |
| 1:H:329:THR:HG23 | 1:H:343:PHE:CE1  | 2.35                     | 0.61              |
| 1:K:329:THR:HG23 | 1:K:343:PHE:CE2  | 2.36                     | 0.61              |
| 1:H:256:LYS:HA   | 1:H:338:GLU:HG3  | 1.82                     | 0.61              |
| 1:H:331:PHE:CE2  | 1:H:365:TYR:HB2  | 2.35                     | 0.61              |
| 1:E:252:LEU:N    | 1:E:252:LEU:CD1  | 2.63                     | 0.61              |
| 1:F:221:ILE:CG2  | 1:F:365:TYR:CZ   | 2.78                     | 0.61              |
| 1:G:225:VAL:O    | 1:G:225:VAL:HG13 | 2.00                     | 0.61              |
| 1:K:294:LEU:HD12 | 1:K:297:TYR:O    | 2.01                     | 0.61              |
| 1:K:187:THR:O    | 1:K:273:PHE:CE1  | 2.53                     | 0.61              |
| 1:G:190:LEU:HD21 | 1:G:273:PHE:CD1  | 2.36                     | 0.61              |
| 1:C:202:ILE:HD11 | 1:C:250:ILE:HD11 | 1.82                     | 0.61              |
| 1:L:225:VAL:HG21 | 1:L:343:PHE:CE2  | 2.35                     | 0.61              |
| 1:D:360:SER:HB2  | 1:E:311:VAL:HG22 | 1.82                     | 0.61              |
| 1:K:237:ILE:CG2  | 1:K:347:TRP:CH2  | 2.83                     | 0.61              |
| 1:K:368:GLN:OE1  | 1:K:368:GLN:O    | 2.19                     | 0.61              |
| 1:L:275:SER:HB3  | 1:L:280:VAL:HB   | 1.82                     | 0.61              |
| 1:F:291:MET:HA   | 1:F:291:MET:HE2  | 1.83                     | 0.60              |
| 1:K:331:PHE:O    | 1:K:332:ASN:C    | 2.44                     | 0.60              |
| 1:L:190:LEU:HD22 | 1:L:271:TRP:CE2  | 2.35                     | 0.60              |
| 1:L:292:PRO:HB3  | 1:L:297:TYR:CE1  | 2.36                     | 0.60              |
| 1:G:357:GLU:OE1  | 1:H:307:ALA:N    | 2.33                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:235:HIS:CD2  | 1:I:236:ILE:HG23 | 2.36                     | 0.60              |
| 1:I:329:THR:OG1  | 1:I:343:PHE:CD1  | 2.54                     | 0.60              |
| 1:J:249:THR:HG23 | 1:J:344:ASP:OD1  | 2.02                     | 0.60              |
| 1:D:225:VAL:HG11 | 1:D:327:ILE:HD13 | 1.84                     | 0.60              |
| 1:E:192:THR:HG21 | 1:E:211:THR:HA   | 1.84                     | 0.60              |
| 1:F:314:THR:HG22 | 1:F:316:TYR:CE1  | 2.37                     | 0.60              |
| 1:A:322:ASP:OD1  | 1:A:323:GLN:NE2  | 2.31                     | 0.60              |
| 1:H:274:ARG:NH2  | 1:I:369:GLN:O    | 2.34                     | 0.60              |
| 1:D:321:PRO:O    | 1:D:324:PRO:HD3  | 2.01                     | 0.60              |
| 1:I:192:THR:HG21 | 1:I:210:LEU:O    | 2.02                     | 0.60              |
| 1:E:331:PHE:CE2  | 1:E:365:TYR:HB3  | 2.36                     | 0.59              |
| 1:I:187:THR:O    | 1:I:187:THR:HG22 | 2.01                     | 0.59              |
| 1:K:311:VAL:O    | 1:K:311:VAL:CG1  | 2.49                     | 0.59              |
| 1:C:203:ALA:HB2  | 1:C:234:TYR:CE2  | 2.37                     | 0.59              |
| 1:G:316:TYR:HE2  | 1:H:312:TYR:CB   | 2.15                     | 0.59              |
| 1:J:299:LYS:HG2  | 1:J:300:PRO:HD2  | 1.84                     | 0.59              |
| 1:H:286:LYS:HD2  | 1:H:286:LYS:N    | 2.16                     | 0.59              |
| 1:K:202:ILE:O    | 1:K:207:ASP:CG   | 2.46                     | 0.59              |
| 1:K:331:PHE:CE2  | 1:K:365:TYR:HB2  | 2.37                     | 0.59              |
| 1:B:190:LEU:HD13 | 1:B:271:TRP:CZ2  | 2.38                     | 0.59              |
| 1:H:317:LEU:O    | 1:H:323:GLN:OE1  | 2.20                     | 0.59              |
| 1:J:220:GLN:NE2  | 1:L:215:THR:OG1  | 2.35                     | 0.59              |
| 1:C:309:ASP:OD1  | 1:C:309:ASP:N    | 2.32                     | 0.59              |
| 1:E:279:ASN:O    | 1:E:280:VAL:HG22 | 2.03                     | 0.59              |
| 1:K:224:ASN:ND2  | 1:L:364:SER:O    | 2.36                     | 0.59              |
| 1:K:312:TYR:CE2  | 1:K:328:LYS:HG3  | 2.37                     | 0.59              |
| 1:A:246:LYS:HA   | 1:A:347:TRP:CE2  | 2.38                     | 0.59              |
| 1:E:332:ASN:HD22 | 1:E:339:TYR:HA   | 1.68                     | 0.59              |
| 1:H:221:ILE:HG12 | 1:H:367:ALA:HB2  | 1.85                     | 0.59              |
| 1:H:284:TYR:CE1  | 1:H:287:ALA:HB2  | 2.37                     | 0.59              |
| 1:J:224:ASN:HB2  | 1:K:220:GLN:OE1  | 2.02                     | 0.59              |
| 1:A:191:TRP:CZ2  | 1:A:274:ARG:HG3  | 2.38                     | 0.59              |
| 1:H:284:TYR:HE1  | 1:H:287:ALA:HB2  | 1.68                     | 0.59              |
| 1:I:250:ILE:N    | 1:I:343:PHE:O    | 2.32                     | 0.59              |
| 1:L:195:ASP:OD1  | 1:L:209:LYS:NZ   | 2.34                     | 0.59              |
| 1:L:261:LEU:O    | 1:L:264:SER:OG   | 2.20                     | 0.59              |
| 1:H:309:ASP:O    | 1:H:330:THR:CG2  | 2.44                     | 0.58              |
| 1:G:209:LYS:O    | 1:G:227:LEU:HD12 | 2.03                     | 0.58              |
| 1:H:293:ASN:C    | 1:H:293:ASN:OD1  | 2.45                     | 0.58              |
| 1:H:296:ALA:C    | 1:H:297:TYR:CD2  | 2.81                     | 0.58              |
| 1:I:191:TRP:CZ2  | 1:I:274:ARG:HG3  | 2.38                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:239:ASN:HB3  | 1:I:353:ASN:HD21 | 1.67                     | 0.58              |
| 1:J:239:ASN:HB3  | 1:J:350:THR:HG23 | 1.85                     | 0.58              |
| 1:K:315:ILE:CD1  | 1:K:358:THR:OG1  | 2.50                     | 0.58              |
| 1:K:294:LEU:HD13 | 1:K:332:ASN:CG   | 2.29                     | 0.58              |
| 1:K:331:PHE:CD1  | 1:K:331:PHE:N    | 2.69                     | 0.58              |
| 1:C:289:GLY:C    | 1:C:291:MET:H    | 2.11                     | 0.58              |
| 1:G:316:TYR:CE2  | 1:H:312:TYR:CB   | 2.87                     | 0.58              |
| 1:H:365:TYR:HD1  | 1:H:365:TYR:C    | 2.10                     | 0.58              |
| 1:E:254:PHE:HB3  | 1:E:258:GLY:HA2  | 1.85                     | 0.58              |
| 1:G:315:ILE:HD12 | 1:G:315:ILE:O    | 2.03                     | 0.58              |
| 1:J:224:ASN:ND2  | 1:K:364:SER:OG   | 2.37                     | 0.58              |
| 1:D:315:ILE:CG2  | 1:D:359:THR:O    | 2.49                     | 0.58              |
| 1:I:290:PHE:O    | 1:I:365:TYR:OH   | 2.18                     | 0.58              |
| 1:G:337:CYS:SG   | 1:G:339:TYR:O    | 2.62                     | 0.58              |
| 1:L:219:SER:O    | 1:L:367:ALA:CB   | 2.51                     | 0.58              |
| 1:H:258:GLY:O    | 1:H:287:ALA:CB   | 2.51                     | 0.57              |
| 1:G:200:CYS:SG   | 1:G:208:SER:OG   | 2.37                     | 0.57              |
| 1:H:331:PHE:N    | 1:H:331:PHE:CD1  | 2.71                     | 0.57              |
| 1:D:322:ASP:O    | 1:D:324:PRO:HD2  | 2.04                     | 0.57              |
| 1:K:226:SER:OG   | 1:K:358:THR:CG2  | 2.52                     | 0.57              |
| 1:L:252:LEU:HD12 | 1:L:252:LEU:N    | 2.18                     | 0.57              |
| 1:F:315:ILE:O    | 1:F:315:ILE:HD12 | 2.04                     | 0.57              |
| 1:B:348:SER:OG   | 1:B:349:LYS:N    | 2.38                     | 0.57              |
| 1:A:224:ASN:ND2  | 1:A:361:PHE:O    | 2.37                     | 0.57              |
| 1:F:195:ASP:OD1  | 1:F:197:SER:OG   | 2.22                     | 0.57              |
| 1:H:227:LEU:H    | 1:H:358:THR:HG22 | 1.68                     | 0.57              |
| 1:H:274:ARG:NE   | 1:H:276:GLY:O    | 2.38                     | 0.57              |
| 1:K:227:LEU:H    | 1:K:358:THR:CG2  | 2.15                     | 0.57              |
| 1:E:252:LEU:N    | 1:E:252:LEU:HD12 | 2.20                     | 0.56              |
| 1:I:239:ASN:CB   | 1:I:353:ASN:ND2  | 2.68                     | 0.56              |
| 1:D:356:PHE:O    | 1:D:356:PHE:CD1  | 2.59                     | 0.56              |
| 1:F:217:CYS:O    | 1:F:220:GLN:N    | 2.39                     | 0.56              |
| 1:H:227:LEU:N    | 1:H:358:THR:HG22 | 2.21                     | 0.56              |
| 1:F:332:ASN:ND2  | 1:F:339:TYR:HA   | 2.21                     | 0.56              |
| 1:K:315:ILE:HD12 | 1:K:315:ILE:C    | 2.30                     | 0.56              |
| 1:D:299:LYS:O    | 1:D:299:LYS:HG3  | 2.06                     | 0.56              |
| 1:H:245:ILE:O    | 1:H:347:TRP:CH2  | 2.58                     | 0.56              |
| 1:I:223:ALA:O    | 1:I:362:THR:HA   | 2.04                     | 0.56              |
| 1:J:368:GLN:O    | 1:L:274:ARG:NH2  | 2.37                     | 0.56              |
| 1:K:279:ASN:O    | 1:K:280:VAL:HG22 | 2.06                     | 0.56              |
| 1:B:190:LEU:HD23 | 1:B:273:PHE:HD1  | 1.69                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:191:TRP:CH2  | 1:B:274:ARG:HD2  | 2.34                     | 0.56              |
| 1:E:224:ASN:ND2  | 1:E:362:THR:OG1  | 2.38                     | 0.56              |
| 1:E:306:TYR:HB2  | 1:E:308:ARG:HH11 | 1.69                     | 0.56              |
| 1:I:239:ASN:HA   | 1:I:352:GLU:HA   | 1.88                     | 0.56              |
| 1:F:316:TYR:CE2  | 1:F:324:PRO:HB3  | 2.41                     | 0.56              |
| 1:G:315:ILE:HG23 | 1:G:361:PHE:HB2  | 1.87                     | 0.56              |
| 1:K:331:PHE:HE2  | 1:K:365:TYR:HB3  | 1.57                     | 0.56              |
| 1:D:213:VAL:HG21 | 1:E:366:ILE:CD1  | 2.36                     | 0.56              |
| 1:G:223:ALA:CB   | 1:G:363:PHE:CE2  | 2.89                     | 0.56              |
| 1:D:358:THR:O    | 1:E:307:ALA:HB3  | 2.05                     | 0.55              |
| 1:A:228:ILE:HG22 | 1:A:230:VAL:HG13 | 1.88                     | 0.55              |
| 1:A:252:LEU:N    | 1:A:252:LEU:HD12 | 2.22                     | 0.55              |
| 1:A:291:MET:HA   | 1:A:291:MET:HE2  | 1.88                     | 0.55              |
| 1:L:285:GLU:O    | 1:L:286:LYS:C    | 2.49                     | 0.55              |
| 1:B:245:ILE:HG22 | 1:B:347:TRP:CB   | 2.36                     | 0.55              |
| 1:D:357:GLU:O    | 1:D:357:GLU:HG3  | 2.06                     | 0.55              |
| 1:H:294:LEU:HD23 | 1:H:339:TYR:CD2  | 2.41                     | 0.55              |
| 1:K:254:PHE:CD2  | 1:K:291:MET:HE1  | 2.40                     | 0.55              |
| 1:J:223:ALA:HB1  | 1:J:363:PHE:CZ   | 2.41                     | 0.55              |
| 1:H:331:PHE:CZ   | 1:H:365:TYR:HB3  | 2.42                     | 0.55              |
| 1:H:221:ILE:O    | 1:H:364:SER:HA   | 2.07                     | 0.55              |
| 1:K:226:SER:OG   | 1:K:358:THR:HG22 | 2.07                     | 0.55              |
| 1:K:363:PHE:CD1  | 1:K:363:PHE:C    | 2.84                     | 0.55              |
| 1:F:237:ILE:HG23 | 1:F:347:TRP:CH2  | 2.41                     | 0.55              |
| 1:H:191:TRP:CH2  | 1:H:194:PRO:HD3  | 2.42                     | 0.55              |
| 1:I:190:LEU:HD22 | 1:I:271:TRP:CE2  | 2.42                     | 0.55              |
| 1:J:332:ASN:HD22 | 1:J:340:SER:H    | 1.55                     | 0.55              |
| 1:D:212:LEU:HD13 | 1:D:225:VAL:CG2  | 2.36                     | 0.55              |
| 1:G:358:THR:O    | 1:G:358:THR:OG1  | 2.26                     | 0.54              |
| 1:I:195:ASP:OD1  | 1:I:209:LYS:NZ   | 2.40                     | 0.54              |
| 1:C:223:ALA:O    | 1:C:362:THR:HA   | 2.08                     | 0.54              |
| 1:D:271:TRP:HD1  | 1:D:284:TYR:HH   | 1.54                     | 0.54              |
| 1:C:313:GLY:O    | 1:C:314:THR:OG1  | 2.23                     | 0.54              |
| 1:E:293:ASN:O    | 1:E:297:TYR:HB2  | 2.07                     | 0.54              |
| 1:E:297:TYR:HB3  | 1:E:309:ASP:OD1  | 2.08                     | 0.54              |
| 1:F:200:CYS:HB3  | 1:F:208:SER:OG   | 2.08                     | 0.54              |
| 1:G:327:ILE:CG2  | 1:G:361:PHE:CD2  | 2.90                     | 0.54              |
| 1:H:225:VAL:HG11 | 1:H:327:ILE:HD11 | 1.89                     | 0.54              |
| 1:H:296:ALA:HB1  | 1:H:297:TYR:CE2  | 2.42                     | 0.54              |
| 1:K:312:TYR:CE1  | 1:K:328:LYS:HB2  | 2.43                     | 0.54              |
| 1:H:191:TRP:HB2  | 1:H:213:VAL:HG13 | 1.89                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:307:ALA:HB3  | 1:L:358:THR:O    | 2.08                     | 0.54              |
| 1:D:191:TRP:CD1  | 1:D:191:TRP:C    | 2.85                     | 0.54              |
| 1:K:316:TYR:O    | 1:K:359:THR:HG23 | 2.07                     | 0.54              |
| 1:L:192:THR:CG2  | 1:L:212:LEU:H    | 2.21                     | 0.54              |
| 1:L:352:GLU:O    | 1:L:352:GLU:HG3  | 2.04                     | 0.54              |
| 1:A:272:ASN:OD1  | 1:A:273:PHE:N    | 2.37                     | 0.53              |
| 1:H:312:TYR:CE1  | 1:H:328:LYS:HB2  | 2.43                     | 0.53              |
| 1:A:226:SER:CB   | 1:B:308:ARG:HD2  | 2.38                     | 0.53              |
| 1:K:329:THR:HG23 | 1:K:343:PHE:CD2  | 2.42                     | 0.53              |
| 1:L:192:THR:HG21 | 1:L:210:LEU:O    | 2.08                     | 0.53              |
| 1:F:315:ILE:HG13 | 1:F:327:ILE:HG22 | 1.91                     | 0.53              |
| 1:G:225:VAL:O    | 1:G:225:VAL:CG1  | 2.56                     | 0.53              |
| 1:K:237:ILE:HG23 | 1:K:347:TRP:CH2  | 2.43                     | 0.53              |
| 1:A:305:LYS:HD3  | 1:A:305:LYS:C    | 2.33                     | 0.53              |
| 1:A:316:TYR:HE1  | 1:A:324:PRO:HB3  | 1.73                     | 0.53              |
| 1:H:294:LEU:CD2  | 1:H:339:TYR:CD2  | 2.92                     | 0.53              |
| 1:B:274:ARG:NH2  | 1:C:219:SER:OG   | 2.40                     | 0.53              |
| 1:B:288:ILE:HG13 | 1:B:290:PHE:HB2  | 1.91                     | 0.53              |
| 1:F:330:THR:O    | 1:F:342:THR:HG23 | 2.09                     | 0.53              |
| 1:K:293:ASN:HA   | 1:K:368:GLN:HA   | 1.91                     | 0.53              |
| 1:D:224:ASN:HA   | 1:D:361:PHE:O    | 2.09                     | 0.53              |
| 1:D:300:PRO:HD2  | 1:D:333:GLN:HE22 | 1.72                     | 0.53              |
| 1:E:260:LEU:HD11 | 1:E:264:SER:CB   | 2.38                     | 0.53              |
| 1:G:191:TRP:CE2  | 1:G:274:ARG:HB2  | 2.44                     | 0.53              |
| 1:D:200:CYS:HB3  | 1:D:208:SER:O    | 2.08                     | 0.53              |
| 1:L:352:GLU:O    | 1:L:352:GLU:CG   | 2.55                     | 0.53              |
| 1:E:274:ARG:HG2  | 1:E:275:SER:N    | 2.23                     | 0.53              |
| 1:K:312:TYR:CZ   | 1:K:328:LYS:HG3  | 2.44                     | 0.53              |
| 1:G:224:ASN:HB2  | 1:H:220:GLN:CD   | 2.34                     | 0.53              |
| 1:G:310:ILE:HG12 | 1:G:330:THR:HG23 | 1.90                     | 0.53              |
| 1:C:203:ALA:HB2  | 1:C:234:TYR:HE2  | 1.74                     | 0.53              |
| 1:D:249:THR:OG1  | 1:D:344:ASP:OD1  | 2.16                     | 0.53              |
| 1:E:215:THR:HB   | 1:F:220:GLN:HG3  | 1.88                     | 0.53              |
| 1:H:296:ALA:C    | 1:H:297:TYR:CG   | 2.87                     | 0.53              |
| 1:A:199:ASN:HB3  | 1:A:270:TYR:CD2  | 2.45                     | 0.52              |
| 1:I:246:LYS:HB3  | 1:I:347:TRP:CH2  | 2.42                     | 0.52              |
| 1:B:332:ASN:HD22 | 1:B:340:SER:H    | 1.58                     | 0.52              |
| 1:L:191:TRP:CZ2  | 1:L:274:ARG:HG3  | 2.44                     | 0.52              |
| 1:L:201:THR:OG1  | 1:L:205:ASP:HA   | 2.09                     | 0.52              |
| 1:G:190:LEU:HD12 | 1:G:271:TRP:CE2  | 2.44                     | 0.52              |
| 1:B:294:LEU:O    | 1:B:298:PRO:HA   | 2.10                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:264:SER:O    | 1:C:266:LEU:N    | 2.43                     | 0.52              |
| 1:D:189:THR:HG21 | 1:E:219:SER:CB   | 2.39                     | 0.52              |
| 1:E:357:GLU:OE1  | 1:F:306:TYR:HA   | 2.10                     | 0.52              |
| 1:F:297:TYR:OH   | 1:F:366:ILE:HG13 | 2.09                     | 0.52              |
| 1:G:364:SER:CB   | 1:I:362:THR:HG21 | 2.40                     | 0.52              |
| 1:H:215:THR:HG21 | 1:I:217:CYS:O    | 2.09                     | 0.52              |
| 1:I:237:ILE:O    | 1:I:238:ASN:C    | 2.53                     | 0.52              |
| 1:A:224:ASN:HA   | 1:A:361:PHE:O    | 2.10                     | 0.52              |
| 1:B:190:LEU:HD23 | 1:B:273:PHE:CD1  | 2.45                     | 0.52              |
| 1:B:303:SER:CB   | 1:L:278:SER:HB2  | 2.39                     | 0.52              |
| 1:K:245:ILE:O    | 1:K:347:TRP:CH2  | 2.63                     | 0.52              |
| 1:G:190:LEU:HB3  | 1:G:271:TRP:CZ2  | 2.44                     | 0.52              |
| 1:H:317:LEU:HD21 | 1:H:356:PHE:CD1  | 2.45                     | 0.52              |
| 1:I:226:SER:HB2  | 1:I:360:SER:HA   | 1.92                     | 0.52              |
| 1:I:263:ASN:OD1  | 1:I:263:ASN:N    | 2.42                     | 0.52              |
| 1:K:313:GLY:O    | 1:K:327:ILE:HG22 | 2.09                     | 0.52              |
| 1:K:253:LEU:HD22 | 1:K:337:CYS:SG   | 2.50                     | 0.52              |
| 1:A:246:LYS:HA   | 1:A:347:TRP:CZ2  | 2.44                     | 0.52              |
| 1:D:198:PRO:HG3  | 1:D:230:VAL:HG21 | 1.92                     | 0.52              |
| 1:H:308:ARG:O    | 1:H:308:ARG:HG3  | 2.08                     | 0.52              |
| 1:E:330:THR:HG21 | 1:E:333:GLN:CB   | 2.35                     | 0.52              |
| 1:G:194:PRO:HA   | 1:G:209:LYS:HZ1  | 1.75                     | 0.52              |
| 1:H:191:TRP:CZ2  | 1:H:274:ARG:HD2  | 2.45                     | 0.52              |
| 1:I:242:ASN:N    | 1:I:242:ASN:OD1  | 2.43                     | 0.52              |
| 1:H:223:ALA:HB3  | 1:H:363:PHE:CE1  | 2.45                     | 0.51              |
| 1:H:309:ASP:C    | 1:H:330:THR:HG22 | 2.34                     | 0.51              |
| 1:I:293:ASN:HA   | 1:I:368:GLN:HA   | 1.92                     | 0.51              |
| 1:B:358:THR:O    | 1:C:308:ARG:HB2  | 2.11                     | 0.51              |
| 1:C:280:VAL:O    | 1:C:280:VAL:HG13 | 2.10                     | 0.51              |
| 1:H:256:LYS:CA   | 1:H:338:GLU:HG3  | 2.39                     | 0.51              |
| 1:H:329:THR:CG2  | 1:H:343:PHE:CE1  | 2.93                     | 0.51              |
| 1:J:361:PHE:CG   | 1:J:362:THR:N    | 2.78                     | 0.51              |
| 1:K:212:LEU:HD22 | 1:K:343:PHE:CZ   | 2.45                     | 0.51              |
| 1:B:191:TRP:CZ3  | 1:B:194:PRO:HD3  | 2.45                     | 0.51              |
| 1:G:239:ASN:HB3  | 1:G:350:THR:HG23 | 1.92                     | 0.51              |
| 1:H:239:ASN:O    | 1:H:350:THR:HG22 | 2.11                     | 0.51              |
| 1:K:229:VAL:HG11 | 1:K:234:TYR:O    | 2.11                     | 0.51              |
| 1:F:317:LEU:HD23 | 1:F:358:THR:HG22 | 1.91                     | 0.51              |
| 1:G:204:GLN:HG3  | 1:G:207:ASP:HB3  | 1.93                     | 0.51              |
| 1:H:260:LEU:O    | 1:H:268:LYS:NZ   | 2.43                     | 0.51              |
| 1:E:330:THR:HB   | 1:E:342:THR:HG23 | 1.92                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:272:ASN:OD1  | 1:I:273:PHE:N    | 2.43                     | 0.51              |
| 1:K:312:TYR:OH   | 1:K:328:LYS:HD2  | 2.10                     | 0.51              |
| 1:D:271:TRP:HD1  | 1:D:284:TYR:OH   | 1.93                     | 0.51              |
| 1:D:332:ASN:HD22 | 1:D:340:SER:H    | 1.58                     | 0.51              |
| 1:H:191:TRP:CZ3  | 1:H:194:PRO:HD3  | 2.46                     | 0.51              |
| 1:H:223:ALA:CB   | 1:H:363:PHE:CE1  | 2.94                     | 0.51              |
| 1:B:192:THR:HG21 | 1:B:210:LEU:O    | 2.11                     | 0.51              |
| 1:D:299:LYS:CB   | 1:D:332:ASN:O    | 2.59                     | 0.51              |
| 1:E:338:GLU:HB3  | 1:E:339:TYR:CD1  | 2.46                     | 0.51              |
| 1:F:225:VAL:HG11 | 1:F:327:ILE:HD11 | 1.93                     | 0.51              |
| 1:I:204:GLN:OE1  | 1:I:232:GLY:HA2  | 2.10                     | 0.51              |
| 1:A:255:ASP:OD1  | 1:A:255:ASP:C    | 2.53                     | 0.51              |
| 1:A:329:THR:HG1  | 1:A:343:PHE:HE1  | 1.52                     | 0.51              |
| 1:E:234:TYR:CZ   | 1:E:248:PHE:HB3  | 2.46                     | 0.51              |
| 1:G:190:LEU:HD12 | 1:G:271:TRP:CZ2  | 2.46                     | 0.51              |
| 1:G:364:SER:HB2  | 1:I:362:THR:HG21 | 1.93                     | 0.51              |
| 1:H:191:TRP:CH2  | 1:H:274:ARG:HD2  | 2.46                     | 0.51              |
| 1:B:257:ASN:O    | 1:B:288:ILE:CG2  | 2.59                     | 0.50              |
| 1:E:186:ASP:HB2  | 1:E:188:ARG:NE   | 2.25                     | 0.50              |
| 1:E:216:LYS:HD2  | 1:E:289:GLY:O    | 2.10                     | 0.50              |
| 1:H:338:GLU:HB3  | 1:H:339:TYR:CD1  | 2.45                     | 0.50              |
| 1:C:229:VAL:O    | 1:C:235:HIS:CD2  | 2.64                     | 0.50              |
| 1:E:368:GLN:HE21 | 1:E:368:GLN:HA   | 1.75                     | 0.50              |
| 1:J:316:TYR:HA   | 1:J:324:PRO:HA   | 1.93                     | 0.50              |
| 1:K:210:LEU:HD12 | 1:K:226:SER:O    | 2.11                     | 0.50              |
| 1:K:296:ALA:O    | 1:K:308:ARG:HD2  | 2.11                     | 0.50              |
| 1:L:225:VAL:O    | 1:L:225:VAL:HG13 | 2.12                     | 0.50              |
| 1:H:196:THR:HA   | 1:H:209:LYS:HG2  | 1.93                     | 0.50              |
| 1:J:225:VAL:HG13 | 1:J:225:VAL:O    | 2.10                     | 0.50              |
| 1:D:272:ASN:OD1  | 1:D:284:TYR:HB3  | 2.10                     | 0.50              |
| 1:E:330:THR:HG22 | 1:E:333:GLN:CB   | 2.29                     | 0.50              |
| 1:K:192:THR:HG23 | 1:K:212:LEU:O    | 2.11                     | 0.50              |
| 1:D:225:VAL:CG1  | 1:D:327:ILE:HD13 | 2.41                     | 0.50              |
| 1:I:280:VAL:HG12 | 1:I:280:VAL:O    | 2.12                     | 0.50              |
| 1:D:192:THR:HG21 | 1:D:210:LEU:O    | 2.11                     | 0.50              |
| 1:D:274:ARG:HD3  | 1:D:276:GLY:O    | 2.11                     | 0.50              |
| 1:E:272:ASN:ND2  | 1:E:282:THR:O    | 2.44                     | 0.50              |
| 1:K:221:ILE:HG13 | 1:K:365:TYR:HE1  | 1.77                     | 0.50              |
| 1:K:259:VAL:HG22 | 1:K:285:GLU:HA   | 1.94                     | 0.50              |
| 1:K:317:LEU:HD22 | 1:K:356:PHE:HA   | 1.94                     | 0.50              |
| 1:D:301:SER:OG   | 1:D:302:ASN:N    | 2.45                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:239:ASN:ND2  | 1:J:242:ASN:O    | 2.45                     | 0.50              |
| 1:D:271:TRP:CD1  | 1:D:284:TYR:OH   | 2.62                     | 0.50              |
| 1:G:327:ILE:HG12 | 1:G:327:ILE:O    | 2.12                     | 0.50              |
| 1:F:237:ILE:CG2  | 1:F:347:TRP:CH2  | 2.95                     | 0.49              |
| 1:I:329:THR:OG1  | 1:I:343:PHE:CE1  | 2.64                     | 0.49              |
| 1:I:244:GLU:CD   | 1:I:244:GLU:H    | 2.20                     | 0.49              |
| 1:B:315:ILE:HG21 | 1:B:359:THR:O    | 2.12                     | 0.49              |
| 1:F:340:SER:O    | 1:F:340:SER:OG   | 2.27                     | 0.49              |
| 1:H:272:ASN:HD21 | 1:H:280:VAL:HB   | 1.77                     | 0.49              |
| 1:D:238:ASN:HA   | 1:D:351:TYR:O    | 2.12                     | 0.49              |
| 1:G:224:ASN:HB2  | 1:H:220:GLN:OE1  | 2.11                     | 0.49              |
| 1:G:274:ARG:HD3  | 1:G:274:ARG:C    | 2.37                     | 0.49              |
| 1:H:292:PRO:CB   | 1:H:331:PHE:HB3  | 2.42                     | 0.49              |
| 1:J:324:PRO:HD2  | 1:J:351:TYR:HH   | 1.73                     | 0.49              |
| 1:C:330:THR:HB   | 1:C:342:THR:HG23 | 1.94                     | 0.49              |
| 1:D:351:TYR:HB3  | 1:D:354:VAL:HG21 | 1.95                     | 0.49              |
| 1:E:191:TRP:CZ2  | 1:E:274:ARG:HD2  | 2.48                     | 0.49              |
| 1:A:189:THR:O    | 1:A:273:PHE:HA   | 2.12                     | 0.49              |
| 1:E:238:ASN:CG   | 1:E:241:ASN:ND2  | 2.71                     | 0.49              |
| 1:F:255:ASP:CG   | 1:F:259:VAL:HG22 | 2.38                     | 0.49              |
| 1:L:246:LYS:HA   | 1:L:347:TRP:CZ2  | 2.47                     | 0.49              |
| 1:L:302:ASN:OD1  | 1:L:302:ASN:N    | 2.40                     | 0.49              |
| 1:D:235:HIS:O    | 1:D:355:GLU:HA   | 2.12                     | 0.49              |
| 1:E:223:ALA:N    | 1:F:220:GLN:HE22 | 2.10                     | 0.49              |
| 1:G:347:TRP:CZ3  | 1:G:356:PHE:HE2  | 2.30                     | 0.49              |
| 1:H:226:SER:OG   | 1:H:227:LEU:N    | 2.45                     | 0.49              |
| 1:C:308:ARG:HD3  | 1:C:308:ARG:N    | 2.28                     | 0.49              |
| 1:C:328:LYS:HB3  | 1:C:344:ASP:O    | 2.12                     | 0.49              |
| 1:D:249:THR:HG23 | 1:D:344:ASP:OD1  | 2.12                     | 0.49              |
| 1:G:270:TYR:O    | 1:G:279:ASN:OD1  | 2.31                     | 0.49              |
| 1:H:201:THR:O    | 1:H:265:ASN:HB3  | 2.12                     | 0.49              |
| 1:H:317:LEU:CD2  | 1:H:356:PHE:HA   | 2.42                     | 0.49              |
| 1:B:274:ARG:HH21 | 1:B:277:ASP:HB2  | 1.78                     | 0.49              |
| 1:H:193:THR:O    | 1:H:209:LYS:NZ   | 2.43                     | 0.49              |
| 1:B:322:ASP:C    | 1:B:324:PRO:HD3  | 2.38                     | 0.49              |
| 1:D:364:SER:O    | 1:F:224:ASN:ND2  | 2.45                     | 0.49              |
| 1:H:284:TYR:CD1  | 1:H:284:TYR:C    | 2.91                     | 0.49              |
| 1:K:202:ILE:O    | 1:K:204:GLN:N    | 2.44                     | 0.49              |
| 1:K:227:LEU:N    | 1:K:358:THR:CG2  | 2.75                     | 0.49              |
| 1:A:190:LEU:O    | 1:A:271:TRP:CH2  | 2.66                     | 0.48              |
| 1:A:215:THR:HG21 | 1:B:217:CYS:O    | 2.13                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:216:LYS:HE3  | 1:J:218:GLY:O    | 2.12                     | 0.48              |
| 1:E:212:LEU:HD11 | 1:E:214:LEU:HD21 | 1.95                     | 0.48              |
| 1:E:248:PHE:O    | 1:E:249:THR:OG1  | 2.26                     | 0.48              |
| 1:E:293:ASN:HB2  | 1:E:366:ILE:O    | 2.13                     | 0.48              |
| 1:E:347:TRP:O    | 1:E:347:TRP:CE3  | 2.66                     | 0.48              |
| 1:G:274:ARG:NE   | 1:G:276:GLY:O    | 2.45                     | 0.48              |
| 1:J:223:ALA:CB   | 1:J:363:PHE:CZ   | 2.96                     | 0.48              |
| 1:L:221:ILE:HD11 | 1:L:289:GLY:O    | 2.13                     | 0.48              |
| 1:F:210:LEU:HD12 | 1:F:226:SER:O    | 2.14                     | 0.48              |
| 1:F:332:ASN:HD22 | 1:F:340:SER:H    | 1.59                     | 0.48              |
| 1:G:251:LYS:C    | 1:G:252:LEU:HD12 | 2.37                     | 0.48              |
| 1:A:263:ASN:OD1  | 1:A:263:ASN:N    | 2.46                     | 0.48              |
| 1:B:256:LYS:HA   | 1:B:338:GLU:HG2  | 1.96                     | 0.48              |
| 1:D:279:ASN:O    | 1:D:280:VAL:HG22 | 2.13                     | 0.48              |
| 1:D:363:PHE:HE2  | 1:D:365:TYR:HD2  | 1.62                     | 0.48              |
| 1:J:274:ARG:NE   | 1:J:276:GLY:O    | 2.47                     | 0.48              |
| 1:J:361:PHE:CE1  | 1:J:362:THR:O    | 2.66                     | 0.48              |
| 1:K:229:VAL:HG11 | 1:K:234:TYR:C    | 2.38                     | 0.48              |
| 1:D:356:PHE:O    | 1:D:356:PHE:HD1  | 1.95                     | 0.48              |
| 1:K:202:ILE:O    | 1:K:207:ASP:OD1  | 2.30                     | 0.48              |
| 1:K:322:ASP:N    | 1:K:322:ASP:OD1  | 2.47                     | 0.48              |
| 1:F:225:VAL:HG12 | 1:F:361:PHE:O    | 2.13                     | 0.48              |
| 1:G:226:SER:OG   | 1:G:227:LEU:N    | 2.46                     | 0.48              |
| 1:A:325:ALA:HB1  | 1:A:346:SER:O    | 2.13                     | 0.48              |
| 1:F:324:PRO:O    | 1:F:351:TYR:OH   | 2.30                     | 0.48              |
| 1:I:348:SER:O    | 1:I:349:LYS:HE2  | 2.14                     | 0.48              |
| 1:K:307:ALA:O    | 1:K:309:ASP:N    | 2.47                     | 0.48              |
| 1:L:223:ALA:HB3  | 1:L:363:PHE:CZ   | 2.49                     | 0.48              |
| 1:A:262:ASP:C    | 1:A:264:SER:H    | 2.22                     | 0.48              |
| 1:B:360:SER:HB2  | 1:C:311:VAL:HG22 | 1.96                     | 0.48              |
| 1:D:220:GLN:HG3  | 1:F:215:THR:OG1  | 2.14                     | 0.48              |
| 1:K:223:ALA:HB3  | 1:K:363:PHE:CZ   | 2.49                     | 0.48              |
| 1:L:293:ASN:N    | 1:L:297:TYR:HE1  | 2.12                     | 0.48              |
| 1:L:315:ILE:HD12 | 1:L:315:ILE:O    | 2.14                     | 0.48              |
| 1:A:220:GLN:OE1  | 1:C:222:LEU:HD23 | 2.13                     | 0.47              |
| 1:E:255:ASP:O    | 1:E:258:GLY:N    | 2.40                     | 0.47              |
| 1:F:253:LEU:CD2  | 1:F:340:SER:HB2  | 2.44                     | 0.47              |
| 1:L:317:LEU:O    | 1:L:323:GLN:NE2  | 2.47                     | 0.47              |
| 1:B:191:TRP:HB2  | 1:B:213:VAL:HG22 | 1.95                     | 0.47              |
| 1:H:331:PHE:CE2  | 1:H:365:TYR:HB3  | 2.49                     | 0.47              |
| 1:J:331:PHE:CE2  | 1:J:365:TYR:CB   | 2.97                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:307:ALA:C    | 1:K:309:ASP:H    | 2.22                     | 0.47              |
| 1:C:190:LEU:HD22 | 1:C:271:TRP:CE2  | 2.49                     | 0.47              |
| 1:E:187:THR:OG1  | 1:E:216:LYS:O    | 2.25                     | 0.47              |
| 1:H:223:ALA:CB   | 1:H:363:PHE:CZ   | 2.97                     | 0.47              |
| 1:I:261:LEU:O    | 1:I:264:SER:OG   | 2.27                     | 0.47              |
| 1:I:329:THR:OG1  | 1:I:343:PHE:HD1  | 1.97                     | 0.47              |
| 1:E:221:ILE:HB   | 1:E:365:TYR:CE1  | 2.50                     | 0.47              |
| 1:J:361:PHE:CZ   | 1:J:362:THR:O    | 2.68                     | 0.47              |
| 1:C:221:ILE:O    | 1:C:364:SER:HA   | 2.14                     | 0.47              |
| 1:F:315:ILE:HD12 | 1:F:325:ALA:O    | 2.15                     | 0.47              |
| 1:A:189:THR:HG1  | 1:B:219:SER:CB   | 2.18                     | 0.47              |
| 1:B:189:THR:HG21 | 1:C:219:SER:HB2  | 1.97                     | 0.47              |
| 1:D:319:GLY:O    | 1:E:312:TYR:CE1  | 2.67                     | 0.47              |
| 1:H:310:ILE:HA   | 1:H:330:THR:HG23 | 1.96                     | 0.47              |
| 1:I:228:ILE:N    | 1:I:228:ILE:HD12 | 2.29                     | 0.47              |
| 1:I:252:LEU:O    | 1:I:340:SER:HA   | 2.15                     | 0.47              |
| 1:I:255:ASP:OD1  | 1:I:256:LYS:N    | 2.47                     | 0.47              |
| 1:D:321:PRO:HG3  | 1:E:312:TYR:OH   | 2.15                     | 0.47              |
| 1:I:199:ASN:HB3  | 1:I:270:TYR:CD2  | 2.49                     | 0.47              |
| 1:L:291:MET:HE2  | 1:L:291:MET:CA   | 2.45                     | 0.47              |
| 1:D:190:LEU:HA   | 1:D:273:PHE:HA   | 1.95                     | 0.47              |
| 1:J:189:THR:HG21 | 1:J:213:VAL:HG13 | 1.97                     | 0.47              |
| 1:A:266:LEU:HD12 | 1:A:267:GLY:H    | 1.80                     | 0.47              |
| 1:C:294:LEU:HD23 | 1:C:368:GLN:HE21 | 1.80                     | 0.47              |
| 1:D:272:ASN:O    | 1:D:279:ASN:ND2  | 2.47                     | 0.47              |
| 1:H:297:TYR:CD2  | 1:H:331:PHE:HD2  | 2.33                     | 0.47              |
| 1:H:312:TYR:OH   | 1:H:328:LYS:HD2  | 2.14                     | 0.47              |
| 1:H:331:PHE:CZ   | 1:H:365:TYR:HD2  | 2.32                     | 0.47              |
| 1:L:300:PRO:O    | 1:L:302:ASN:O    | 2.32                     | 0.47              |
| 1:B:303:SER:HB3  | 1:L:278:SER:HB2  | 1.97                     | 0.46              |
| 1:D:299:LYS:HB2  | 1:D:332:ASN:O    | 2.15                     | 0.46              |
| 1:E:330:THR:HB   | 1:E:342:THR:CG2  | 2.45                     | 0.46              |
| 1:F:324:PRO:HD2  | 1:F:351:TYR:OH   | 2.15                     | 0.46              |
| 1:H:204:GLN:OE1  | 1:H:232:GLY:HA3  | 2.15                     | 0.46              |
| 1:H:292:PRO:HD2  | 1:H:339:TYR:HB3  | 1.97                     | 0.46              |
| 1:J:310:ILE:HB   | 1:L:359:THR:HG22 | 1.97                     | 0.46              |
| 1:A:220:GLN:OE1  | 1:C:222:LEU:HD21 | 2.13                     | 0.46              |
| 1:G:212:LEU:HD11 | 1:G:214:LEU:HD21 | 1.97                     | 0.46              |
| 1:H:293:ASN:O    | 1:H:296:ALA:CB   | 2.61                     | 0.46              |
| 1:H:313:GLY:O    | 1:H:327:ILE:HG22 | 2.15                     | 0.46              |
| 1:D:313:GLY:O    | 1:D:326:VAL:HG12 | 2.15                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:307:ALA:O    | 1:J:309:ASP:N    | 2.48                     | 0.46              |
| 1:J:364:SER:OG   | 1:J:365:TYR:N    | 2.48                     | 0.46              |
| 1:E:244:GLU:HG2  | 1:E:245:ILE:HD13 | 1.97                     | 0.46              |
| 1:E:260:LEU:HD11 | 1:E:264:SER:HB2  | 1.97                     | 0.46              |
| 1:F:221:ILE:O    | 1:F:364:SER:CB   | 2.60                     | 0.46              |
| 1:G:310:ILE:HB   | 1:I:359:THR:HG22 | 1.97                     | 0.46              |
| 1:F:223:ALA:O    | 1:F:362:THR:CG2  | 2.63                     | 0.46              |
| 1:I:227:LEU:H    | 1:I:358:THR:HG1  | 1.60                     | 0.46              |
| 1:B:274:ARG:HB3  | 1:B:277:ASP:CA   | 2.43                     | 0.46              |
| 1:H:292:PRO:HB2  | 1:H:331:PHE:HB3  | 1.98                     | 0.46              |
| 1:I:229:VAL:CG2  | 1:I:356:PHE:HB3  | 2.46                     | 0.46              |
| 1:J:258:GLY:HA3  | 1:J:287:ALA:O    | 2.15                     | 0.46              |
| 1:D:196:THR:HG21 | 1:E:308:ARG:NH2  | 2.31                     | 0.46              |
| 1:D:227:LEU:HD23 | 1:D:356:PHE:CE1  | 2.51                     | 0.46              |
| 1:E:334:GLU:HB2  | 1:E:340:SER:CB   | 2.45                     | 0.46              |
| 1:G:191:TRP:NE1  | 1:G:274:ARG:HB2  | 2.31                     | 0.46              |
| 1:L:334:GLU:HB2  | 1:L:340:SER:CB   | 2.46                     | 0.46              |
| 1:B:278:SER:O    | 1:B:279:ASN:ND2  | 2.43                     | 0.46              |
| 1:F:317:LEU:HD11 | 1:F:325:ALA:HB2  | 1.96                     | 0.46              |
| 1:A:249:THR:HG21 | 1:A:251:LYS:HE2  | 1.98                     | 0.46              |
| 1:A:360:SER:HB2  | 1:B:311:VAL:HG22 | 1.97                     | 0.46              |
| 1:H:217:CYS:O    | 1:H:220:GLN:O    | 2.34                     | 0.45              |
| 1:H:242:ASN:O    | 1:H:245:ILE:HG12 | 2.16                     | 0.45              |
| 1:H:314:THR:HA   | 1:H:325:ALA:O    | 2.16                     | 0.45              |
| 1:J:255:ASP:OD2  | 1:J:257:ASN:ND2  | 2.49                     | 0.45              |
| 1:K:192:THR:O    | 1:K:192:THR:OG1  | 2.27                     | 0.45              |
| 1:K:357:GLU:OE1  | 1:L:307:ALA:N    | 2.50                     | 0.45              |
| 1:C:328:LYS:O    | 1:C:344:ASP:N    | 2.27                     | 0.45              |
| 1:H:327:ILE:HG23 | 1:H:327:ILE:O    | 2.15                     | 0.45              |
| 1:I:213:VAL:O    | 1:I:214:LEU:HD23 | 2.16                     | 0.45              |
| 1:A:192:THR:CG2  | 1:A:211:THR:HA   | 2.47                     | 0.45              |
| 1:C:249:THR:HA   | 1:C:343:PHE:O    | 2.17                     | 0.45              |
| 1:E:365:TYR:C    | 1:E:365:TYR:CD1  | 2.95                     | 0.45              |
| 1:E:368:GLN:HE21 | 1:E:368:GLN:CA   | 2.30                     | 0.45              |
| 1:H:312:TYR:CE2  | 1:H:328:LYS:HG3  | 2.50                     | 0.45              |
| 1:K:293:ASN:HB2  | 1:K:368:GLN:HA   | 1.98                     | 0.45              |
| 1:A:204:GLN:HG3  | 1:A:207:ASP:HB3  | 1.99                     | 0.45              |
| 1:D:312:TYR:CZ   | 1:F:319:GLY:O    | 2.69                     | 0.45              |
| 1:E:328:LYS:HB3  | 1:E:344:ASP:HB2  | 1.99                     | 0.45              |
| 1:L:311:VAL:O    | 1:L:311:VAL:HG12 | 2.16                     | 0.45              |
| 1:B:284:TYR:CD1  | 1:B:284:TYR:O    | 2.70                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:237:ILE:HG23 | 1:C:347:TRP:CH2  | 2.51                     | 0.45              |
| 1:H:324:PRO:HD2  | 1:H:351:TYR:OH   | 2.17                     | 0.45              |
| 1:I:326:VAL:O    | 1:I:345:PHE:HA   | 2.16                     | 0.45              |
| 1:B:228:ILE:HD11 | 1:C:308:ARG:HH21 | 1.81                     | 0.45              |
| 1:D:261:LEU:O    | 1:D:264:SER:OG   | 2.27                     | 0.45              |
| 1:D:316:TYR:CD1  | 1:D:324:PRO:HB3  | 2.51                     | 0.45              |
| 1:E:315:ILE:CD1  | 1:E:325:ALA:HB3  | 2.47                     | 0.45              |
| 1:F:190:LEU:HD22 | 1:F:273:PHE:CD1  | 2.51                     | 0.45              |
| 1:H:190:LEU:HA   | 1:H:273:PHE:HA   | 1.98                     | 0.45              |
| 1:A:199:ASN:CB   | 1:A:270:TYR:CD2  | 3.00                     | 0.45              |
| 1:G:271:TRP:CD1  | 1:G:271:TRP:C    | 2.95                     | 0.45              |
| 1:J:302:ASN:C    | 1:J:302:ASN:OD1  | 2.59                     | 0.45              |
| 1:D:291:MET:HB3  | 1:D:339:TYR:CD2  | 2.52                     | 0.45              |
| 1:E:255:ASP:C    | 1:E:257:ASN:H    | 2.25                     | 0.45              |
| 1:G:191:TRP:HE1  | 1:G:279:ASN:ND2  | 2.15                     | 0.45              |
| 1:I:239:ASN:CB   | 1:I:353:ASN:HD21 | 2.28                     | 0.45              |
| 1:B:274:ARG:NE   | 1:B:277:ASP:HA   | 2.32                     | 0.45              |
| 1:F:250:ILE:HG23 | 1:F:265:ASN:HB2  | 1.99                     | 0.45              |
| 1:H:317:LEU:HD21 | 1:H:356:PHE:CG   | 2.52                     | 0.45              |
| 1:J:331:PHE:CE2  | 1:J:365:TYR:HB3  | 2.51                     | 0.45              |
| 1:K:306:TYR:O    | 1:K:308:ARG:N    | 2.50                     | 0.45              |
| 1:K:368:GLN:OE1  | 1:K:368:GLN:HA   | 2.17                     | 0.45              |
| 1:A:315:ILE:HD11 | 1:A:325:ALA:HB3  | 1.99                     | 0.45              |
| 1:D:187:THR:O    | 1:D:187:THR:OG1  | 2.30                     | 0.45              |
| 1:F:197:SER:O    | 1:F:198:PRO:C    | 2.58                     | 0.45              |
| 1:H:212:LEU:HA   | 1:H:225:VAL:HA   | 1.99                     | 0.45              |
| 1:I:224:ASN:ND2  | 1:I:362:THR:HG1  | 2.13                     | 0.45              |
| 1:I:316:TYR:CE2  | 1:I:324:PRO:HB3  | 2.52                     | 0.45              |
| 1:I:353:ASN:N    | 1:I:353:ASN:HD22 | 2.15                     | 0.45              |
| 1:A:220:GLN:HE21 | 1:C:213:VAL:HG12 | 1.82                     | 0.44              |
| 1:H:293:ASN:CA   | 1:H:368:GLN:HA   | 2.47                     | 0.44              |
| 1:J:212:LEU:HD11 | 1:J:214:LEU:HD21 | 2.00                     | 0.44              |
| 1:L:212:LEU:HD13 | 1:L:225:VAL:CG2  | 2.46                     | 0.44              |
| 1:L:300:PRO:HB2  | 1:L:304:LYS:CD   | 2.47                     | 0.44              |
| 1:C:214:LEU:HD13 | 1:C:365:TYR:OH   | 2.17                     | 0.44              |
| 1:C:297:TYR:CD1  | 1:C:309:ASP:HB3  | 2.52                     | 0.44              |
| 1:D:307:ALA:O    | 1:F:359:THR:HA   | 2.16                     | 0.44              |
| 1:D:321:PRO:HG3  | 1:E:312:TYR:CE2  | 2.52                     | 0.44              |
| 1:E:258:GLY:O    | 1:E:287:ALA:CB   | 2.66                     | 0.44              |
| 1:G:246:LYS:HA   | 1:G:347:TRP:CE2  | 2.53                     | 0.44              |
| 1:L:241:ASN:N    | 1:L:241:ASN:HD22 | 2.14                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:226:SER:HB3  | 1:B:308:ARG:HD2  | 2.00                     | 0.44              |
| 1:D:221:ILE:C    | 1:D:222:LEU:O    | 2.58                     | 0.44              |
| 1:E:259:VAL:O    | 1:E:260:LEU:C    | 2.60                     | 0.44              |
| 1:J:199:ASN:ND2  | 1:J:266:LEU:HD11 | 2.32                     | 0.44              |
| 1:B:190:LEU:CD1  | 1:B:271:TRP:CZ2  | 3.00                     | 0.44              |
| 1:J:234:TYR:CZ   | 1:J:248:PHE:HB3  | 2.53                     | 0.44              |
| 1:L:300:PRO:O    | 1:L:301:SER:C    | 2.60                     | 0.44              |
| 1:G:191:TRP:CD1  | 1:G:279:ASN:ND2  | 2.84                     | 0.44              |
| 1:H:293:ASN:HA   | 1:H:368:GLN:HB2  | 1.99                     | 0.44              |
| 1:I:297:TYR:OH   | 1:I:366:ILE:HG12 | 2.18                     | 0.44              |
| 1:I:317:LEU:HD22 | 1:I:356:PHE:HA   | 2.00                     | 0.44              |
| 1:J:190:LEU:HD12 | 1:J:272:ASN:C    | 2.42                     | 0.44              |
| 1:A:198:PRO:O    | 1:L:270:TYR:OH   | 2.26                     | 0.44              |
| 1:B:288:ILE:CG1  | 1:B:290:PHE:HB2  | 2.48                     | 0.44              |
| 1:D:197:SER:CB   | 1:I:197:SER:OG   | 2.66                     | 0.44              |
| 1:D:249:THR:CB   | 1:D:344:ASP:OD1  | 2.66                     | 0.44              |
| 1:I:305:LYS:C    | 1:I:305:LYS:HD2  | 2.42                     | 0.44              |
| 1:C:191:TRP:CZ2  | 1:C:277:ASP:O    | 2.71                     | 0.44              |
| 1:G:201:THR:HG23 | 1:G:205:ASP:HA   | 2.00                     | 0.44              |
| 1:H:293:ASN:O    | 1:H:296:ALA:N    | 2.48                     | 0.44              |
| 1:I:223:ALA:O    | 1:I:363:PHE:N    | 2.49                     | 0.44              |
| 1:J:307:ALA:C    | 1:J:309:ASP:H    | 2.26                     | 0.44              |
| 1:L:192:THR:HG22 | 1:L:212:LEU:H    | 1.82                     | 0.44              |
| 1:A:272:ASN:CG   | 1:A:273:PHE:N    | 2.76                     | 0.44              |
| 1:C:191:TRP:CE2  | 1:C:274:ARG:HG3  | 2.52                     | 0.44              |
| 1:C:237:ILE:CG2  | 1:C:347:TRP:CH2  | 3.00                     | 0.44              |
| 1:E:274:ARG:CG   | 1:E:275:SER:N    | 2.81                     | 0.44              |
| 1:E:358:THR:HG23 | 1:E:359:THR:O    | 2.18                     | 0.44              |
| 1:I:296:ALA:O    | 1:I:308:ARG:NE   | 2.50                     | 0.44              |
| 1:K:307:ALA:C    | 1:K:309:ASP:N    | 2.76                     | 0.44              |
| 1:L:348:SER:O    | 1:L:349:LYS:HB2  | 2.18                     | 0.44              |
| 1:C:192:THR:O    | 1:C:193:THR:C    | 2.61                     | 0.43              |
| 1:E:306:TYR:HD2  | 1:E:308:ARG:NH1  | 2.16                     | 0.43              |
| 1:E:365:TYR:C    | 1:E:365:TYR:HD1  | 2.26                     | 0.43              |
| 1:F:316:TYR:N    | 1:F:316:TYR:HD1  | 2.12                     | 0.43              |
| 1:J:187:THR:O    | 1:J:187:THR:HG22 | 2.17                     | 0.43              |
| 1:K:200:CYS:HA   | 1:K:265:ASN:O    | 2.18                     | 0.43              |
| 1:B:191:TRP:CG   | 1:B:192:THR:N    | 2.83                     | 0.43              |
| 1:C:205:ASP:OD1  | 1:C:206:LYS:HG2  | 2.18                     | 0.43              |
| 1:C:353:ASN:ND2  | 1:D:299:LYS:O    | 2.51                     | 0.43              |
| 1:G:224:ASN:HB2  | 1:H:220:GLN:NE2  | 2.33                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:297:TYR:HD1  | 1:H:309:ASP:HA   | 1.83                     | 0.43              |
| 1:K:362:THR:OG1  | 1:L:364:SER:N    | 2.50                     | 0.43              |
| 1:D:191:TRP:CE2  | 1:D:274:ARG:HG3  | 2.53                     | 0.43              |
| 1:D:317:LEU:HD21 | 1:D:356:PHE:CZ   | 2.53                     | 0.43              |
| 1:A:357:GLU:OE1  | 1:B:307:ALA:HB2  | 2.18                     | 0.43              |
| 1:D:298:PRO:C    | 1:D:300:PRO:HD3  | 2.44                     | 0.43              |
| 1:E:222:LEU:HD23 | 1:F:220:GLN:CB   | 2.48                     | 0.43              |
| 1:E:331:PHE:CE1  | 1:E:365:TYR:CD2  | 2.98                     | 0.43              |
| 1:F:316:TYR:O    | 1:F:359:THR:HG23 | 2.18                     | 0.43              |
| 1:F:317:LEU:CD1  | 1:F:325:ALA:HB2  | 2.48                     | 0.43              |
| 1:H:316:TYR:O    | 1:H:359:THR:HG23 | 2.18                     | 0.43              |
| 1:K:273:PHE:O    | 1:K:279:ASN:OD1  | 2.37                     | 0.43              |
| 1:L:239:ASN:ND2  | 1:L:347:TRP:HH2  | 2.05                     | 0.43              |
| 1:D:326:VAL:O    | 1:D:345:PHE:HA   | 2.18                     | 0.43              |
| 1:J:314:THR:HA   | 1:J:326:VAL:HA   | 2.00                     | 0.43              |
| 1:K:299:LYS:NZ   | 1:K:337:CYS:O    | 2.40                     | 0.43              |
| 1:A:307:ALA:HB2  | 1:C:318:GLY:C    | 2.44                     | 0.43              |
| 1:C:238:ASN:ND2  | 1:C:241:ASN:OD1  | 2.51                     | 0.43              |
| 1:G:229:VAL:HG11 | 1:G:234:TYR:C    | 2.44                     | 0.43              |
| 1:H:191:TRP:CD1  | 1:H:274:ARG:HB2  | 2.53                     | 0.43              |
| 1:K:368:GLN:OE1  | 1:K:368:GLN:CA   | 2.66                     | 0.43              |
| 1:L:197:SER:O    | 1:L:197:SER:OG   | 2.37                     | 0.43              |
| 1:L:286:LYS:O    | 1:L:286:LYS:CG   | 2.62                     | 0.43              |
| 1:A:188:ARG:O    | 1:A:215:THR:HG23 | 2.18                     | 0.43              |
| 1:B:191:TRP:NE1  | 1:B:274:ARG:HG2  | 2.34                     | 0.43              |
| 1:D:360:SER:HB2  | 1:E:311:VAL:CG2  | 2.46                     | 0.43              |
| 1:G:271:TRP:C    | 1:G:272:ASN:CG   | 2.87                     | 0.43              |
| 1:J:297:TYR:OH   | 1:J:366:ILE:HG13 | 2.19                     | 0.43              |
| 1:A:219:SER:H    | 1:C:189:THR:HG21 | 1.84                     | 0.43              |
| 1:A:238:ASN:ND2  | 1:A:352:GLU:HG3  | 2.34                     | 0.43              |
| 1:C:343:PHE:HB3  | 1:C:345:PHE:CZ   | 2.54                     | 0.43              |
| 1:D:366:ILE:CD1  | 1:F:213:VAL:HG21 | 2.48                     | 0.43              |
| 1:G:192:THR:HG21 | 1:G:210:LEU:O    | 2.19                     | 0.43              |
| 1:L:227:LEU:HD23 | 1:L:356:PHE:CE1  | 2.54                     | 0.43              |
| 1:B:254:PHE:HB3  | 1:B:258:GLY:HA2  | 2.00                     | 0.43              |
| 1:F:357:GLU:O    | 1:F:357:GLU:HG3  | 2.19                     | 0.43              |
| 1:D:197:SER:OG   | 1:I:197:SER:HB2  | 2.19                     | 0.43              |
| 1:D:351:TYR:HB3  | 1:D:354:VAL:CG2  | 2.48                     | 0.43              |
| 1:G:249:THR:OG1  | 1:G:344:ASP:OD1  | 2.25                     | 0.43              |
| 1:G:342:THR:O    | 1:G:342:THR:OG1  | 2.36                     | 0.43              |
| 1:K:305:LYS:HG2  | 1:K:333:GLN:HE22 | 1.84                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:226:SER:HB2  | 1:B:308:ARG:CZ   | 2.49                     | 0.42              |
| 1:B:316:TYR:O    | 1:B:359:THR:HG23 | 2.19                     | 0.42              |
| 1:C:202:ILE:HD13 | 1:C:248:PHE:CE1  | 2.53                     | 0.42              |
| 1:C:292:PRO:HG2  | 1:C:332:ASN:ND2  | 2.34                     | 0.42              |
| 1:E:273:PHE:CE2  | 1:E:285:GLU:HB2  | 2.54                     | 0.42              |
| 1:F:195:ASP:CG   | 1:F:197:SER:HG   | 2.25                     | 0.42              |
| 1:G:359:THR:HB   | 1:H:310:ILE:O    | 2.19                     | 0.42              |
| 1:H:237:ILE:CG2  | 1:H:347:TRP:CH2  | 3.02                     | 0.42              |
| 1:J:334:GLU:O    | 1:J:337:CYS:SG   | 2.62                     | 0.42              |
| 1:K:306:TYR:C    | 1:K:308:ARG:N    | 2.77                     | 0.42              |
| 1:A:239:ASN:O    | 1:A:240:LYS:C    | 2.61                     | 0.42              |
| 1:C:257:ASN:HD21 | 1:C:286:LYS:H    | 1.67                     | 0.42              |
| 1:D:213:VAL:HG21 | 1:E:366:ILE:HD13 | 2.00                     | 0.42              |
| 1:E:316:TYR:N    | 1:E:359:THR:OG1  | 2.52                     | 0.42              |
| 1:K:191:TRP:CD1  | 1:K:191:TRP:C    | 2.97                     | 0.42              |
| 1:A:315:ILE:C    | 1:A:315:ILE:HD12 | 2.44                     | 0.42              |
| 1:C:297:TYR:CE1  | 1:C:309:ASP:HA   | 2.54                     | 0.42              |
| 1:D:321:PRO:HG3  | 1:E:312:TYR:CZ   | 2.54                     | 0.42              |
| 1:H:236:ILE:HB   | 1:L:301:SER:HB2  | 2.00                     | 0.42              |
| 1:H:237:ILE:HG21 | 1:H:347:TRP:CZ3  | 2.54                     | 0.42              |
| 1:I:324:PRO:O    | 1:I:351:TYR:OH   | 2.36                     | 0.42              |
| 1:K:305:LYS:C    | 1:K:305:LYS:CD   | 2.89                     | 0.42              |
| 1:L:299:LYS:N    | 1:L:300:PRO:CD   | 2.82                     | 0.42              |
| 1:D:197:SER:OG   | 1:I:197:SER:HB3  | 2.20                     | 0.42              |
| 1:E:315:ILE:CD1  | 1:E:315:ILE:C    | 2.90                     | 0.42              |
| 1:F:190:LEU:HD13 | 1:F:272:ASN:C    | 2.44                     | 0.42              |
| 1:G:327:ILE:O    | 1:G:327:ILE:CG1  | 2.68                     | 0.42              |
| 1:I:304:LYS:HG3  | 1:L:251:LYS:HZ1  | 1.84                     | 0.42              |
| 1:J:332:ASN:N    | 1:J:332:ASN:ND2  | 2.68                     | 0.42              |
| 1:K:320:LYS:HB3  | 1:K:322:ASP:OD1  | 2.19                     | 0.42              |
| 1:D:255:ASP:OD1  | 1:D:256:LYS:N    | 2.53                     | 0.42              |
| 1:D:366:ILE:HD13 | 1:F:213:VAL:HG21 | 2.01                     | 0.42              |
| 1:E:283:ALA:O    | 1:E:285:GLU:N    | 2.53                     | 0.42              |
| 1:H:272:ASN:HB3  | 1:H:279:ASN:HB3  | 2.01                     | 0.42              |
| 1:I:187:THR:O    | 1:I:187:THR:CG2  | 2.66                     | 0.42              |
| 1:L:294:LEU:O    | 1:L:298:PRO:HB3  | 2.20                     | 0.42              |
| 1:E:192:THR:HG22 | 1:E:212:LEU:O    | 2.19                     | 0.42              |
| 1:E:354:VAL:HG12 | 1:E:355:GLU:O    | 2.19                     | 0.42              |
| 1:G:314:THR:CG2  | 1:G:315:ILE:N    | 2.82                     | 0.42              |
| 1:K:195:ASP:C    | 1:K:197:SER:H    | 2.28                     | 0.42              |
| 1:K:293:ASN:C    | 1:K:293:ASN:OD1  | 2.62                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:310:ILE:HG21 | 1:L:312:TYR:CE1  | 2.55                     | 0.42              |
| 1:D:310:ILE:HA   | 1:D:329:THR:O    | 2.20                     | 0.42              |
| 1:G:274:ARG:HH21 | 1:H:369:GLN:HA   | 1.84                     | 0.42              |
| 1:K:219:SER:HA   | 1:K:367:ALA:HB3  | 2.01                     | 0.42              |
| 1:L:292:PRO:CB   | 1:L:297:TYR:CE1  | 3.03                     | 0.42              |
| 1:E:191:TRP:CD1  | 1:E:191:TRP:C    | 2.97                     | 0.42              |
| 1:E:191:TRP:CH2  | 1:E:274:ARG:HD2  | 2.54                     | 0.42              |
| 1:E:323:GLN:HA   | 1:E:351:TYR:CE1  | 2.55                     | 0.42              |
| 1:F:311:VAL:HG11 | 1:F:363:PHE:HB2  | 2.01                     | 0.42              |
| 1:G:313:GLY:HA3  | 1:G:361:PHE:CZ   | 2.55                     | 0.42              |
| 1:E:291:MET:O    | 1:E:367:ALA:HA   | 2.20                     | 0.42              |
| 1:F:327:ILE:O    | 1:F:327:ILE:HG12 | 2.19                     | 0.42              |
| 1:G:197:SER:O    | 1:G:198:PRO:C    | 2.62                     | 0.42              |
| 1:G:271:TRP:O    | 1:G:272:ASN:CG   | 2.62                     | 0.42              |
| 1:G:305:LYS:HD2  | 1:G:305:LYS:C    | 2.45                     | 0.42              |
| 1:I:241:ASN:ND2  | 1:I:242:ASN:OD1  | 2.52                     | 0.42              |
| 1:A:239:ASN:O    | 1:A:242:ASN:N    | 2.53                     | 0.42              |
| 1:C:202:ILE:CD1  | 1:C:248:PHE:CE1  | 3.03                     | 0.42              |
| 1:E:294:LEU:HD13 | 1:E:294:LEU:HA   | 1.91                     | 0.42              |
| 1:I:347:TRP:CD1  | 1:I:347:TRP:N    | 2.87                     | 0.42              |
| 1:K:254:PHE:CG   | 1:K:291:MET:HE1  | 2.55                     | 0.42              |
| 1:E:217:CYS:O    | 1:E:220:GLN:O    | 2.37                     | 0.41              |
| 1:I:273:PHE:O    | 1:I:279:ASN:HA   | 2.20                     | 0.41              |
| 1:C:321:PRO:C    | 1:C:323:GLN:H    | 2.28                     | 0.41              |
| 1:D:227:LEU:HD23 | 1:D:356:PHE:HE1  | 1.85                     | 0.41              |
| 1:D:364:SER:OG   | 1:F:362:THR:CG2  | 2.29                     | 0.41              |
| 1:H:191:TRP:CB   | 1:H:213:VAL:HG13 | 2.50                     | 0.41              |
| 1:J:217:CYS:O    | 1:L:215:THR:HG21 | 2.20                     | 0.41              |
| 1:K:279:ASN:C    | 1:K:281:SER:H    | 2.28                     | 0.41              |
| 1:F:315:ILE:O    | 1:F:315:ILE:CD1  | 2.68                     | 0.41              |
| 1:F:317:LEU:HD22 | 1:F:356:PHE:HA   | 2.02                     | 0.41              |
| 1:F:329:THR:HG1  | 1:F:343:PHE:HD1  | 1.67                     | 0.41              |
| 1:K:192:THR:O    | 1:K:193:THR:C    | 2.63                     | 0.41              |
| 1:A:339:TYR:CD1  | 1:A:339:TYR:N    | 2.87                     | 0.41              |
| 1:G:205:ASP:CG   | 1:G:206:LYS:HG2  | 2.45                     | 0.41              |
| 1:H:297:TYR:O    | 1:H:332:ASN:ND2  | 2.36                     | 0.41              |
| 1:I:313:GLY:HA3  | 1:I:361:PHE:CE2  | 2.56                     | 0.41              |
| 1:L:297:TYR:OH   | 1:L:366:ILE:O    | 2.38                     | 0.41              |
| 1:A:252:LEU:N    | 1:A:252:LEU:CD1  | 2.83                     | 0.41              |
| 1:B:294:LEU:HD13 | 1:B:294:LEU:HA   | 1.80                     | 0.41              |
| 1:E:189:THR:OG1  | 1:F:219:SER:HB2  | 2.20                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:293:ASN:OD1  | 1:F:294:LEU:N    | 2.54                     | 0.41              |
| 1:G:191:TRP:NE1  | 1:G:279:ASN:ND2  | 2.69                     | 0.41              |
| 1:G:322:ASP:OD1  | 1:G:323:GLN:NE2  | 2.53                     | 0.41              |
| 1:J:234:TYR:CE1  | 1:J:248:PHE:HB3  | 2.55                     | 0.41              |
| 1:K:331:PHE:HE2  | 1:K:365:TYR:HB2  | 1.76                     | 0.41              |
| 1:K:331:PHE:N    | 1:K:331:PHE:HD1  | 2.14                     | 0.41              |
| 1:A:210:LEU:HD13 | 1:A:250:ILE:HD13 | 2.03                     | 0.41              |
| 1:D:228:ILE:HG21 | 1:E:306:TYR:CE1  | 2.56                     | 0.41              |
| 1:G:193:THR:O    | 1:G:195:ASP:N    | 2.53                     | 0.41              |
| 1:G:299:LYS:NZ   | 1:G:337:CYS:SG   | 2.92                     | 0.41              |
| 1:H:199:ASN:O    | 1:H:266:LEU:HD12 | 2.20                     | 0.41              |
| 1:H:255:ASP:C    | 1:H:338:GLU:HB2  | 2.45                     | 0.41              |
| 1:B:294:LEU:H    | 1:B:368:GLN:NE2  | 2.18                     | 0.41              |
| 1:C:250:ILE:HG23 | 1:C:265:ASN:HB2  | 2.03                     | 0.41              |
| 1:D:223:ALA:O    | 1:D:363:PHE:N    | 2.52                     | 0.41              |
| 1:D:225:VAL:HG11 | 1:D:327:ILE:CD1  | 2.49                     | 0.41              |
| 1:G:284:TYR:CD1  | 1:G:284:TYR:N    | 2.88                     | 0.41              |
| 1:G:317:LEU:HD22 | 1:G:356:PHE:HA   | 2.03                     | 0.41              |
| 1:H:236:ILE:HB   | 1:L:301:SER:CB   | 2.51                     | 0.41              |
| 1:A:330:THR:HG22 | 1:A:333:GLN:HG3  | 2.03                     | 0.41              |
| 1:F:216:LYS:HB2  | 1:F:290:PHE:CE2  | 2.56                     | 0.41              |
| 1:F:315:ILE:HG13 | 1:F:327:ILE:CG2  | 2.51                     | 0.41              |
| 1:K:237:ILE:HG21 | 1:K:347:TRP:CH2  | 2.56                     | 0.41              |
| 1:A:187:THR:HA   | 1:A:273:PHE:CD1  | 2.56                     | 0.41              |
| 1:A:212:LEU:HD12 | 1:A:224:ASN:O    | 2.20                     | 0.41              |
| 1:A:315:ILE:CG2  | 1:A:359:THR:O    | 2.65                     | 0.41              |
| 1:D:310:ILE:HG13 | 1:D:330:THR:HG23 | 2.03                     | 0.41              |
| 1:E:190:LEU:C    | 1:E:190:LEU:CD2  | 2.93                     | 0.41              |
| 1:E:191:TRP:HB2  | 1:E:213:VAL:HG22 | 2.03                     | 0.41              |
| 1:G:190:LEU:CD2  | 1:G:273:PHE:CD1  | 3.03                     | 0.41              |
| 1:G:316:TYR:CD2  | 1:H:312:TYR:HB2  | 2.55                     | 0.41              |
| 1:H:190:LEU:HD13 | 1:H:273:PHE:CD1  | 2.56                     | 0.41              |
| 1:H:237:ILE:HG23 | 1:H:347:TRP:CH2  | 2.56                     | 0.41              |
| 1:H:238:ASN:HA   | 1:H:351:TYR:O    | 2.21                     | 0.41              |
| 1:I:330:THR:HB   | 1:I:342:THR:HG23 | 2.03                     | 0.41              |
| 1:J:298:PRO:O    | 1:J:333:GLN:NE2  | 2.54                     | 0.41              |
| 1:J:316:TYR:N    | 1:J:316:TYR:CD1  | 2.89                     | 0.41              |
| 1:K:190:LEU:HD23 | 1:K:272:ASN:C    | 2.46                     | 0.41              |
| 1:C:289:GLY:C    | 1:C:291:MET:N    | 2.78                     | 0.41              |
| 1:C:351:TYR:HB3  | 1:C:354:VAL:CG2  | 2.51                     | 0.41              |
| 1:D:241:ASN:OD1  | 1:D:241:ASN:N    | 2.54                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:190:LEU:HD12 | 1:G:271:TRP:NE1  | 2.36                     | 0.41              |
| 1:H:191:TRP:CD1  | 1:H:191:TRP:C    | 2.99                     | 0.41              |
| 1:D:213:VAL:HG12 | 1:E:220:GLN:NE2  | 2.26                     | 0.40              |
| 1:D:216:LYS:HD2  | 1:D:289:GLY:O    | 2.21                     | 0.40              |
| 1:D:253:LEU:HD23 | 1:D:340:SER:HB2  | 2.03                     | 0.40              |
| 1:D:291:MET:O    | 1:D:292:PRO:C    | 2.64                     | 0.40              |
| 1:I:227:LEU:C    | 1:I:228:ILE:HD12 | 2.47                     | 0.40              |
| 1:K:327:ILE:HD12 | 1:K:327:ILE:HG21 | 1.88                     | 0.40              |
| 1:L:216:LYS:HD2  | 1:L:289:GLY:O    | 2.20                     | 0.40              |
| 1:A:188:ARG:C    | 1:A:189:THR:OG1  | 2.64                     | 0.40              |
| 1:B:331:PHE:CE2  | 1:B:365:TYR:HB3  | 2.56                     | 0.40              |
| 1:H:293:ASN:HA   | 1:H:368:GLN:CB   | 2.51                     | 0.40              |
| 1:K:285:GLU:O    | 1:K:286:LYS:HB2  | 2.20                     | 0.40              |
| 1:L:192:THR:OG1  | 1:L:199:ASN:ND2  | 2.54                     | 0.40              |
| 1:L:280:VAL:O    | 1:L:280:VAL:HG13 | 2.21                     | 0.40              |
| 1:B:191:TRP:CZ2  | 1:B:274:ARG:CD   | 2.74                     | 0.40              |
| 1:B:277:ASP:CG   | 1:B:277:ASP:O    | 2.64                     | 0.40              |
| 1:B:293:ASN:HB2  | 1:B:366:ILE:HG22 | 2.02                     | 0.40              |
| 1:E:255:ASP:C    | 1:E:257:ASN:N    | 2.80                     | 0.40              |
| 1:G:305:LYS:C    | 1:G:305:LYS:CD   | 2.95                     | 0.40              |
| 1:I:366:ILE:N    | 1:I:366:ILE:HD13 | 2.36                     | 0.40              |
| 1:J:294:LEU:HD13 | 1:J:298:PRO:HA   | 2.03                     | 0.40              |
| 1:C:313:GLY:C    | 1:C:314:THR:OG1  | 2.64                     | 0.40              |
| 1:D:308:ARG:NH2  | 1:F:194:PRO:O    | 2.54                     | 0.40              |
| 1:E:187:THR:O    | 1:E:187:THR:CG2  | 2.69                     | 0.40              |
| 1:G:221:ILE:HD11 | 1:G:289:GLY:O    | 2.22                     | 0.40              |
| 1:G:315:ILE:CG2  | 1:G:361:PHE:HB2  | 2.51                     | 0.40              |
| 1:K:227:LEU:HD22 | 1:K:345:PHE:CE2  | 2.56                     | 0.40              |
| 1:K:320:LYS:HA   | 1:K:321:PRO:HD3  | 1.95                     | 0.40              |
| 1:L:332:ASN:HD22 | 1:L:340:SER:H    | 1.67                     | 0.40              |
| 1:A:226:SER:OG   | 1:B:308:ARG:HB2  | 2.22                     | 0.40              |
| 1:D:359:THR:O    | 1:D:360:SER:C    | 2.64                     | 0.40              |
| 1:F:236:ILE:HG22 | 1:F:353:ASN:HA   | 2.04                     | 0.40              |
| 1:F:257:ASN:HA   | 1:F:288:ILE:HD11 | 2.03                     | 0.40              |
| 1:G:183:VAL:O    | 1:G:185:HIS:CD2  | 2.75                     | 0.40              |
| 1:I:229:VAL:HG23 | 1:I:356:PHE:HB3  | 2.03                     | 0.40              |

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1        | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------|----------------------|--------------------------|-------------------|
| 1:C:202:ILE:O | 1:K:336:GLY:O[3_554] | 2.11                     | 0.09              |

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|-----------|----------|-------------|----|
| 1   | A     | 181/189 (96%)   | 158 (87%)  | 19 (10%)  | 4 (2%)   | 5           | 9  |
| 1   | B     | 181/189 (96%)   | 153 (84%)  | 25 (14%)  | 3 (2%)   | 7           | 13 |
| 1   | C     | 181/189 (96%)   | 155 (86%)  | 20 (11%)  | 6 (3%)   | 3           | 4  |
| 1   | D     | 182/189 (96%)   | 150 (82%)  | 27 (15%)  | 5 (3%)   | 4           | 6  |
| 1   | E     | 184/189 (97%)   | 150 (82%)  | 27 (15%)  | 7 (4%)   | 2           | 3  |
| 1   | F     | 184/189 (97%)   | 154 (84%)  | 27 (15%)  | 3 (2%)   | 7           | 14 |
| 1   | G     | 187/189 (99%)   | 153 (82%)  | 27 (14%)  | 7 (4%)   | 2           | 3  |
| 1   | H     | 181/189 (96%)   | 156 (86%)  | 24 (13%)  | 1 (1%)   | 21          | 38 |
| 1   | I     | 181/189 (96%)   | 150 (83%)  | 26 (14%)  | 5 (3%)   | 4           | 6  |
| 1   | J     | 181/189 (96%)   | 152 (84%)  | 25 (14%)  | 4 (2%)   | 5           | 9  |
| 1   | K     | 183/189 (97%)   | 152 (83%)  | 25 (14%)  | 6 (3%)   | 3           | 4  |
| 1   | L     | 181/189 (96%)   | 152 (84%)  | 24 (13%)  | 5 (3%)   | 4           | 6  |
| All | All   | 2187/2268 (96%) | 1835 (84%) | 296 (14%) | 56 (3%)  | 4           | 7  |

All (56) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 280 | VAL  |
| 1   | D     | 280 | VAL  |
| 1   | E     | 280 | VAL  |
| 1   | E     | 284 | TYR  |
| 1   | K     | 280 | VAL  |
| 1   | B     | 288 | ILE  |
| 1   | C     | 303 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 323 | GLN  |
| 1   | E     | 195 | ASP  |
| 1   | E     | 256 | LYS  |
| 1   | E     | 273 | PHE  |
| 1   | E     | 367 | ALA  |
| 1   | G     | 183 | VAL  |
| 1   | I     | 264 | SER  |
| 1   | I     | 280 | VAL  |
| 1   | K     | 307 | ALA  |
| 1   | K     | 308 | ARG  |
| 1   | L     | 280 | VAL  |
| 1   | L     | 286 | LYS  |
| 1   | D     | 303 | SER  |
| 1   | E     | 260 | LEU  |
| 1   | F     | 235 | HIS  |
| 1   | F     | 350 | THR  |
| 1   | K     | 206 | LYS  |
| 1   | A     | 240 | LYS  |
| 1   | C     | 265 | ASN  |
| 1   | D     | 247 | SER  |
| 1   | F     | 218 | GLY  |
| 1   | I     | 243 | PRO  |
| 1   | J     | 353 | ASN  |
| 1   | K     | 286 | LYS  |
| 1   | L     | 301 | SER  |
| 1   | A     | 205 | ASP  |
| 1   | A     | 280 | VAL  |
| 1   | B     | 303 | SER  |
| 1   | G     | 198 | PRO  |
| 1   | G     | 235 | HIS  |
| 1   | G     | 247 | SER  |
| 1   | H     | 246 | LYS  |
| 1   | J     | 283 | ALA  |
| 1   | J     | 324 | PRO  |
| 1   | L     | 298 | PRO  |
| 1   | A     | 263 | ASN  |
| 1   | C     | 199 | ASN  |
| 1   | G     | 184 | LYS  |
| 1   | G     | 273 | PHE  |
| 1   | I     | 206 | LYS  |
| 1   | L     | 246 | LYS  |
| 1   | B     | 198 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | I     | 245 | ILE  |
| 1   | K     | 311 | VAL  |
| 1   | C     | 295 | VAL  |
| 1   | G     | 295 | VAL  |
| 1   | C     | 218 | GLY  |
| 1   | D     | 315 | ILE  |
| 1   | J     | 202 | 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     | 164/170 (96%)   | 149 (91%)  | 15 (9%)   | 9           | 19 |
| 1   | B     | 164/170 (96%)   | 140 (85%)  | 24 (15%)  | 3           | 6  |
| 1   | C     | 164/170 (96%)   | 142 (87%)  | 22 (13%)  | 4           | 8  |
| 1   | D     | 165/170 (97%)   | 141 (86%)  | 24 (14%)  | 3           | 6  |
| 1   | E     | 167/170 (98%)   | 143 (86%)  | 24 (14%)  | 3           | 6  |
| 1   | F     | 167/170 (98%)   | 149 (89%)  | 18 (11%)  | 6           | 13 |
| 1   | G     | 170/170 (100%)  | 147 (86%)  | 23 (14%)  | 4           | 8  |
| 1   | H     | 164/170 (96%)   | 138 (84%)  | 26 (16%)  | 2           | 5  |
| 1   | I     | 164/170 (96%)   | 135 (82%)  | 29 (18%)  | 2           | 3  |
| 1   | J     | 164/170 (96%)   | 144 (88%)  | 20 (12%)  | 5           | 10 |
| 1   | K     | 166/170 (98%)   | 132 (80%)  | 34 (20%)  | 1           | 2  |
| 1   | L     | 164/170 (96%)   | 139 (85%)  | 25 (15%)  | 3           | 5  |
| All | All   | 1983/2040 (97%) | 1699 (86%) | 284 (14%) | 3           | 6  |

All (284) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 188 | ARG  |
| 1   | A     | 190 | LEU  |
| 1   | A     | 204 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 208 | SER  |
| 1   | A     | 246 | LYS  |
| 1   | A     | 268 | LYS  |
| 1   | A     | 275 | SER  |
| 1   | A     | 288 | ILE  |
| 1   | A     | 305 | LYS  |
| 1   | A     | 314 | THR  |
| 1   | A     | 315 | ILE  |
| 1   | A     | 326 | VAL  |
| 1   | A     | 327 | ILE  |
| 1   | A     | 342 | THR  |
| 1   | A     | 350 | THR  |
| 1   | B     | 187 | THR  |
| 1   | B     | 188 | ARG  |
| 1   | B     | 190 | LEU  |
| 1   | B     | 191 | TRP  |
| 1   | B     | 204 | GLN  |
| 1   | B     | 241 | ASN  |
| 1   | B     | 244 | GLU  |
| 1   | B     | 249 | THR  |
| 1   | B     | 256 | LYS  |
| 1   | B     | 272 | ASN  |
| 1   | B     | 279 | ASN  |
| 1   | B     | 284 | TYR  |
| 1   | B     | 288 | ILE  |
| 1   | B     | 294 | LEU  |
| 1   | B     | 303 | SER  |
| 1   | B     | 304 | LYS  |
| 1   | B     | 308 | ARG  |
| 1   | B     | 309 | ASP  |
| 1   | B     | 315 | ILE  |
| 1   | B     | 335 | THR  |
| 1   | B     | 342 | THR  |
| 1   | B     | 344 | ASP  |
| 1   | B     | 350 | THR  |
| 1   | B     | 357 | GLU  |
| 1   | C     | 190 | LEU  |
| 1   | C     | 192 | THR  |
| 1   | C     | 196 | THR  |
| 1   | C     | 197 | SER  |
| 1   | C     | 204 | GLN  |
| 1   | C     | 211 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 215 | THR  |
| 1   | C     | 245 | ILE  |
| 1   | C     | 274 | ARG  |
| 1   | C     | 278 | SER  |
| 1   | C     | 280 | VAL  |
| 1   | C     | 282 | THR  |
| 1   | C     | 285 | GLU  |
| 1   | C     | 294 | LEU  |
| 1   | C     | 306 | TYR  |
| 1   | C     | 308 | ARG  |
| 1   | C     | 309 | ASP  |
| 1   | C     | 342 | THR  |
| 1   | C     | 346 | SER  |
| 1   | C     | 350 | THR  |
| 1   | C     | 353 | ASN  |
| 1   | C     | 357 | GLU  |
| 1   | D     | 191 | TRP  |
| 1   | D     | 192 | THR  |
| 1   | D     | 204 | GLN  |
| 1   | D     | 220 | GLN  |
| 1   | D     | 225 | VAL  |
| 1   | D     | 227 | LEU  |
| 1   | D     | 228 | ILE  |
| 1   | D     | 241 | ASN  |
| 1   | D     | 246 | LYS  |
| 1   | D     | 274 | ARG  |
| 1   | D     | 284 | TYR  |
| 1   | D     | 285 | GLU  |
| 1   | D     | 294 | LEU  |
| 1   | D     | 305 | LYS  |
| 1   | D     | 314 | THR  |
| 1   | D     | 315 | ILE  |
| 1   | D     | 322 | ASP  |
| 1   | D     | 326 | VAL  |
| 1   | D     | 327 | ILE  |
| 1   | D     | 342 | THR  |
| 1   | D     | 343 | PHE  |
| 1   | D     | 347 | TRP  |
| 1   | D     | 350 | THR  |
| 1   | D     | 362 | THR  |
| 1   | E     | 185 | HIS  |
| 1   | E     | 187 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 190 | LEU  |
| 1   | E     | 191 | TRP  |
| 1   | E     | 200 | CYS  |
| 1   | E     | 207 | ASP  |
| 1   | E     | 240 | LYS  |
| 1   | E     | 241 | ASN  |
| 1   | E     | 245 | ILE  |
| 1   | E     | 246 | LYS  |
| 1   | E     | 252 | LEU  |
| 1   | E     | 280 | VAL  |
| 1   | E     | 294 | LEU  |
| 1   | E     | 301 | SER  |
| 1   | E     | 310 | ILE  |
| 1   | E     | 314 | THR  |
| 1   | E     | 315 | ILE  |
| 1   | E     | 322 | ASP  |
| 1   | E     | 326 | VAL  |
| 1   | E     | 342 | THR  |
| 1   | E     | 359 | THR  |
| 1   | E     | 365 | TYR  |
| 1   | E     | 368 | GLN  |
| 1   | E     | 369 | GLN  |
| 1   | F     | 187 | THR  |
| 1   | F     | 190 | LEU  |
| 1   | F     | 221 | ILE  |
| 1   | F     | 228 | ILE  |
| 1   | F     | 246 | LYS  |
| 1   | F     | 257 | ASN  |
| 1   | F     | 263 | ASN  |
| 1   | F     | 294 | LEU  |
| 1   | F     | 301 | SER  |
| 1   | F     | 303 | SER  |
| 1   | F     | 315 | ILE  |
| 1   | F     | 316 | TYR  |
| 1   | F     | 326 | VAL  |
| 1   | F     | 327 | ILE  |
| 1   | F     | 334 | GLU  |
| 1   | F     | 342 | THR  |
| 1   | F     | 350 | THR  |
| 1   | F     | 362 | THR  |
| 1   | G     | 186 | ASP  |
| 1   | G     | 190 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 200 | CYS  |
| 1   | G     | 204 | GLN  |
| 1   | G     | 207 | ASP  |
| 1   | G     | 241 | ASN  |
| 1   | G     | 242 | ASN  |
| 1   | G     | 244 | GLU  |
| 1   | G     | 262 | ASP  |
| 1   | G     | 272 | ASN  |
| 1   | G     | 278 | SER  |
| 1   | G     | 280 | VAL  |
| 1   | G     | 282 | THR  |
| 1   | G     | 284 | TYR  |
| 1   | G     | 294 | LEU  |
| 1   | G     | 305 | LYS  |
| 1   | G     | 314 | THR  |
| 1   | G     | 315 | ILE  |
| 1   | G     | 330 | THR  |
| 1   | G     | 340 | SER  |
| 1   | G     | 342 | THR  |
| 1   | G     | 346 | SER  |
| 1   | G     | 360 | SER  |
| 1   | H     | 188 | ARG  |
| 1   | H     | 189 | THR  |
| 1   | H     | 204 | GLN  |
| 1   | H     | 205 | ASP  |
| 1   | H     | 211 | THR  |
| 1   | H     | 215 | THR  |
| 1   | H     | 219 | SER  |
| 1   | H     | 220 | GLN  |
| 1   | H     | 252 | LEU  |
| 1   | H     | 285 | GLU  |
| 1   | H     | 288 | ILE  |
| 1   | H     | 301 | SER  |
| 1   | H     | 308 | ARG  |
| 1   | H     | 315 | ILE  |
| 1   | H     | 326 | VAL  |
| 1   | H     | 327 | ILE  |
| 1   | H     | 329 | THR  |
| 1   | H     | 330 | THR  |
| 1   | H     | 331 | PHE  |
| 1   | H     | 335 | THR  |
| 1   | H     | 339 | TYR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | H     | 341 | ILE  |
| 1   | H     | 342 | THR  |
| 1   | H     | 350 | THR  |
| 1   | H     | 357 | GLU  |
| 1   | H     | 365 | TYR  |
| 1   | I     | 188 | ARG  |
| 1   | I     | 190 | LEU  |
| 1   | I     | 213 | VAL  |
| 1   | I     | 237 | ILE  |
| 1   | I     | 239 | ASN  |
| 1   | I     | 241 | ASN  |
| 1   | I     | 242 | ASN  |
| 1   | I     | 244 | GLU  |
| 1   | I     | 249 | THR  |
| 1   | I     | 251 | LYS  |
| 1   | I     | 261 | LEU  |
| 1   | I     | 263 | ASN  |
| 1   | I     | 275 | SER  |
| 1   | I     | 279 | ASN  |
| 1   | I     | 281 | SER  |
| 1   | I     | 302 | ASN  |
| 1   | I     | 304 | LYS  |
| 1   | I     | 314 | THR  |
| 1   | I     | 326 | VAL  |
| 1   | I     | 327 | ILE  |
| 1   | I     | 329 | THR  |
| 1   | I     | 338 | GLU  |
| 1   | I     | 342 | THR  |
| 1   | I     | 347 | TRP  |
| 1   | I     | 348 | SER  |
| 1   | I     | 349 | LYS  |
| 1   | I     | 353 | ASN  |
| 1   | I     | 357 | GLU  |
| 1   | I     | 366 | ILE  |
| 1   | J     | 195 | ASP  |
| 1   | J     | 220 | GLN  |
| 1   | J     | 246 | LYS  |
| 1   | J     | 257 | ASN  |
| 1   | J     | 285 | GLU  |
| 1   | J     | 294 | LEU  |
| 1   | J     | 299 | LYS  |
| 1   | J     | 301 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | J     | 304 | LYS  |
| 1   | J     | 312 | TYR  |
| 1   | J     | 322 | ASP  |
| 1   | J     | 324 | PRO  |
| 1   | J     | 326 | VAL  |
| 1   | J     | 327 | ILE  |
| 1   | J     | 329 | THR  |
| 1   | J     | 338 | GLU  |
| 1   | J     | 342 | THR  |
| 1   | J     | 346 | SER  |
| 1   | J     | 354 | VAL  |
| 1   | J     | 364 | SER  |
| 1   | K     | 186 | ASP  |
| 1   | K     | 187 | THR  |
| 1   | K     | 188 | ARG  |
| 1   | K     | 190 | LEU  |
| 1   | K     | 192 | THR  |
| 1   | K     | 202 | ILE  |
| 1   | K     | 215 | THR  |
| 1   | K     | 219 | SER  |
| 1   | K     | 220 | GLN  |
| 1   | K     | 221 | ILE  |
| 1   | K     | 222 | LEU  |
| 1   | K     | 241 | ASN  |
| 1   | K     | 242 | ASN  |
| 1   | K     | 244 | GLU  |
| 1   | K     | 280 | VAL  |
| 1   | K     | 282 | THR  |
| 1   | K     | 285 | GLU  |
| 1   | K     | 288 | ILE  |
| 1   | K     | 294 | LEU  |
| 1   | K     | 311 | VAL  |
| 1   | K     | 322 | ASP  |
| 1   | K     | 326 | VAL  |
| 1   | K     | 327 | ILE  |
| 1   | K     | 329 | THR  |
| 1   | K     | 330 | THR  |
| 1   | K     | 331 | PHE  |
| 1   | K     | 335 | THR  |
| 1   | K     | 341 | ILE  |
| 1   | K     | 342 | THR  |
| 1   | K     | 350 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | K     | 358 | THR  |
| 1   | K     | 365 | TYR  |
| 1   | K     | 368 | GLN  |
| 1   | K     | 369 | GLN  |
| 1   | L     | 188 | ARG  |
| 1   | L     | 190 | LEU  |
| 1   | L     | 201 | THR  |
| 1   | L     | 204 | GLN  |
| 1   | L     | 213 | VAL  |
| 1   | L     | 224 | ASN  |
| 1   | L     | 227 | LEU  |
| 1   | L     | 228 | ILE  |
| 1   | L     | 264 | SER  |
| 1   | L     | 278 | SER  |
| 1   | L     | 279 | ASN  |
| 1   | L     | 280 | VAL  |
| 1   | L     | 285 | GLU  |
| 1   | L     | 294 | LEU  |
| 1   | L     | 297 | TYR  |
| 1   | L     | 299 | LYS  |
| 1   | L     | 302 | ASN  |
| 1   | L     | 304 | LYS  |
| 1   | L     | 305 | LYS  |
| 1   | L     | 309 | ASP  |
| 1   | L     | 311 | VAL  |
| 1   | L     | 330 | THR  |
| 1   | L     | 342 | THR  |
| 1   | L     | 352 | GLU  |
| 1   | L     | 359 | THR  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 238 | ASN  |
| 1   | A     | 302 | ASN  |
| 1   | B     | 241 | ASN  |
| 1   | B     | 332 | ASN  |
| 1   | B     | 368 | GLN  |
| 1   | C     | 220 | GLN  |
| 1   | C     | 235 | HIS  |
| 1   | C     | 238 | ASN  |
| 1   | C     | 241 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 257 | ASN  |
| 1   | C     | 302 | ASN  |
| 1   | C     | 332 | ASN  |
| 1   | C     | 368 | GLN  |
| 1   | C     | 369 | GLN  |
| 1   | D     | 204 | GLN  |
| 1   | D     | 238 | ASN  |
| 1   | D     | 332 | ASN  |
| 1   | D     | 333 | GLN  |
| 1   | E     | 185 | HIS  |
| 1   | E     | 220 | GLN  |
| 1   | E     | 224 | ASN  |
| 1   | E     | 241 | ASN  |
| 1   | E     | 332 | ASN  |
| 1   | E     | 368 | GLN  |
| 1   | F     | 220 | GLN  |
| 1   | F     | 224 | ASN  |
| 1   | F     | 241 | ASN  |
| 1   | F     | 302 | ASN  |
| 1   | F     | 332 | ASN  |
| 1   | F     | 353 | ASN  |
| 1   | F     | 368 | GLN  |
| 1   | G     | 182 | ASN  |
| 1   | G     | 185 | HIS  |
| 1   | G     | 220 | GLN  |
| 1   | G     | 238 | ASN  |
| 1   | G     | 239 | ASN  |
| 1   | G     | 332 | ASN  |
| 1   | H     | 353 | ASN  |
| 1   | H     | 369 | GLN  |
| 1   | I     | 224 | ASN  |
| 1   | I     | 241 | ASN  |
| 1   | I     | 302 | ASN  |
| 1   | I     | 323 | GLN  |
| 1   | I     | 353 | ASN  |
| 1   | I     | 368 | GLN  |
| 1   | J     | 204 | GLN  |
| 1   | J     | 220 | GLN  |
| 1   | J     | 224 | ASN  |
| 1   | J     | 239 | ASN  |
| 1   | J     | 257 | ASN  |
| 1   | J     | 332 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | J     | 333 | GLN  |
| 1   | K     | 239 | ASN  |
| 1   | L     | 199 | ASN  |
| 1   | L     | 204 | GLN  |
| 1   | L     | 224 | ASN  |
| 1   | L     | 239 | ASN  |
| 1   | L     | 241 | ASN  |
| 1   | L     | 323 | GLN  |
| 1   | L     | 332 | ASN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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     | 183/189 (96%)   | -0.78  | 2 (1%) 78 75  | 30, 74, 122, 175      | 0     |
| 1   | B     | 183/189 (96%)   | -0.52  | 3 (1%) 70 67  | 44, 108, 144, 201     | 0     |
| 1   | C     | 183/189 (96%)   | -0.61  | 1 (0%) 87 85  | 67, 100, 140, 174     | 0     |
| 1   | D     | 184/189 (97%)   | -0.89  | 0 100 100     | 8, 70, 105, 147       | 0     |
| 1   | E     | 186/189 (98%)   | -0.67  | 1 (0%) 87 85  | 20, 87, 131, 150      | 0     |
| 1   | F     | 186/189 (98%)   | -0.62  | 3 (1%) 70 67  | 30, 86, 114, 131      | 0     |
| 1   | G     | 189/189 (100%)  | -0.59  | 1 (0%) 87 85  | 30, 100, 139, 172     | 0     |
| 1   | H     | 183/189 (96%)   | -0.87  | 0 100 100     | 9, 73, 112, 134       | 0     |
| 1   | I     | 183/189 (96%)   | -0.71  | 1 (0%) 87 85  | 37, 78, 121, 179      | 0     |
| 1   | J     | 183/189 (96%)   | -0.60  | 2 (1%) 78 75  | 30, 99, 139, 169      | 0     |
| 1   | K     | 185/189 (97%)   | -0.73  | 1 (0%) 87 85  | 8, 82, 113, 136       | 0     |
| 1   | L     | 183/189 (96%)   | -0.62  | 2 (1%) 78 75  | 37, 83, 124, 156      | 0     |
| All | All   | 2211/2268 (97%) | -0.68  | 17 (0%) 82 80 | 8, 87, 134, 201       | 0     |

All (17) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 361 | PHE  | 3.9  |
| 1   | G     | 290 | PHE  | 3.3  |
| 1   | C     | 325 | ALA  | 3.2  |
| 1   | A     | 282 | THR  | 2.8  |
| 1   | I     | 283 | ALA  | 2.8  |
| 1   | L     | 356 | PHE  | 2.6  |
| 1   | E     | 343 | PHE  | 2.5  |
| 1   | K     | 363 | PHE  | 2.5  |
| 1   | L     | 357 | GLU  | 2.4  |
| 1   | F     | 327 | ILE  | 2.3  |
| 1   | B     | 313 | GLY  | 2.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | F     | 363 | PHE  | 2.2  |
| 1   | F     | 364 | SER  | 2.2  |
| 1   | J     | 306 | TYR  | 2.1  |
| 1   | A     | 281 | SER  | 2.1  |
| 1   | B     | 302 | ASN  | 2.1  |
| 1   | J     | 222 | LEU  | 2.1  |

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.