



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:52 AM UTC

PDB ID : 1KLF / pdb\_00001klf  
Title : FIMH ADHESIN-FIMC CHAPERONE COMPLEX WITH D-MANNOSE  
Authors : Hung, C.S.; Bouckaert, J.  
Deposited on : 2001-12-11  
Resolution : 2.79 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

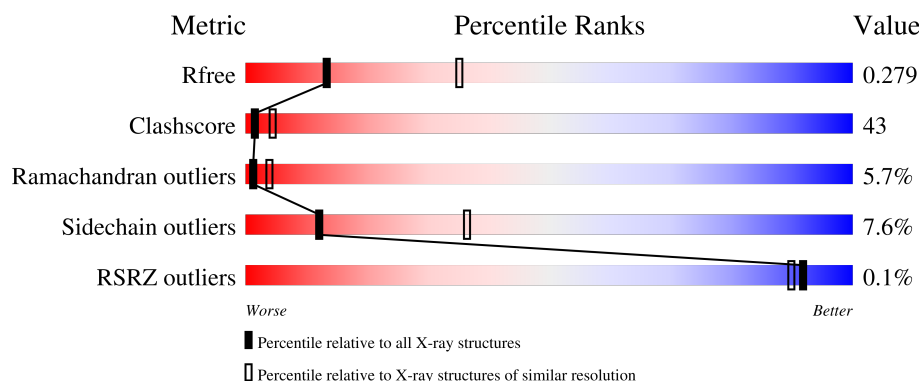
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.79 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.



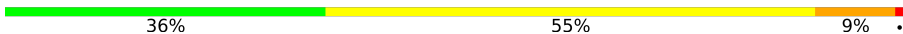
| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 3866 (2.80-2.80)                                      |
| Clashscore            | 190562                      | 4276 (2.80-2.80)                                      |
| Ramachandran outliers | 187476                      | 4196 (2.80-2.80)                                      |
| Sidechain outliers    | 187428                      | 4198 (2.80-2.80)                                      |
| RSRZ outliers         | 180081                      | 3869 (2.80-2.80)                                      |

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     | 205    | <div> <div>40%</div> <div>48%</div> <div>12%</div> </div> |
| 1   | C     | 205    | <div> <div>41%</div> <div>45%</div> <div>14%</div> </div> |
| 1   | E     | 205    | <div> <div>40%</div> <div>46%</div> <div>13%</div> </div> |
| 1   | G     | 205    | <div> <div>39%</div> <div>48%</div> <div>13%</div> </div> |
| 1   | I     | 205    | <div> <div>36%</div> <div>54%</div> <div>9%</div> </div>  |

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| Mol | Chain | Length | Quality of chain                                                                               |
|-----|-------|--------|------------------------------------------------------------------------------------------------|
| 1   | K     | 205    |  37% 54% 9%  |
| 1   | M     | 205    |  36% 55% 9%  |
| 1   | O     | 205    |  36% 54% 9%  |
| 2   | B     | 279    |  53% 37% 10% |
| 2   | D     | 279    |  55% 35% 10% |
| 2   | F     | 279    |  54% 36% 10% |
| 2   | H     | 279    |  53% 37% 10% |
| 2   | J     | 279    |  32% 59% 9%  |
| 2   | L     | 279    |  31% 61% 8%  |
| 2   | N     | 279    |  32% 59% 8%  |
| 2   | P     | 279    |  31% 61% 8%  |

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 29775 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 CHAPERONE PROTEIN FIMC.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | A     | 205      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1596  | 1010 | 276 | 304 | 6 |         |         |       |
| 1   | C     | 205      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1596  | 1010 | 276 | 304 | 6 |         |         |       |
| 1   | E     | 205      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1596  | 1010 | 276 | 304 | 6 |         |         |       |
| 1   | G     | 205      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1596  | 1010 | 276 | 304 | 6 |         |         |       |
| 1   | I     | 205      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1596  | 1010 | 276 | 304 | 6 |         |         |       |
| 1   | K     | 205      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1596  | 1010 | 276 | 304 | 6 |         |         |       |
| 1   | M     | 205      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1596  | 1010 | 276 | 304 | 6 |         |         |       |
| 1   | O     | 205      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1596  | 1010 | 276 | 304 | 6 |         |         |       |

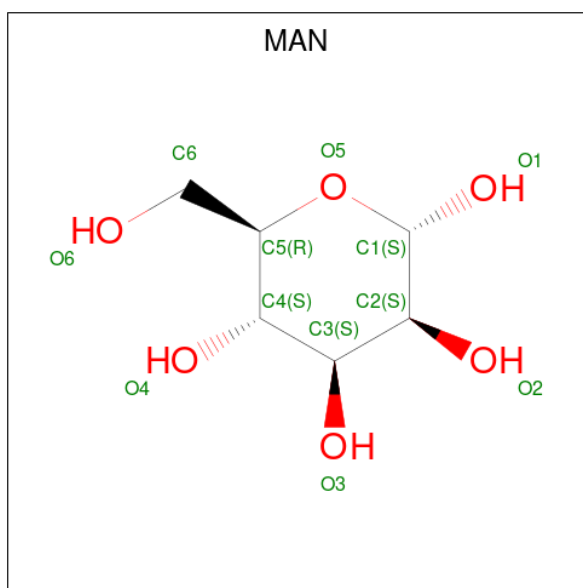
There are 8 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| A     | 18      | VAL      | GLU    | conflict | UNP P31697 |
| C     | 18      | VAL      | GLU    | conflict | UNP P31697 |
| E     | 18      | VAL      | GLU    | conflict | UNP P31697 |
| G     | 18      | VAL      | GLU    | conflict | UNP P31697 |
| I     | 18      | VAL      | GLU    | conflict | UNP P31697 |
| K     | 18      | VAL      | GLU    | conflict | UNP P31697 |
| M     | 18      | VAL      | GLU    | conflict | UNP P31697 |
| O     | 18      | VAL      | GLU    | conflict | UNP P31697 |

- Molecule 2 is a protein called FIMH PROTEIN.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2   | B     | 279      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2052  | 1297 | 342 | 409 | 4 |         |         |       |
| 2   | D     | 279      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2052  | 1297 | 342 | 409 | 4 |         |         |       |
| 2   | F     | 279      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2052  | 1297 | 342 | 409 | 4 |         |         |       |
| 2   | H     | 279      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2052  | 1297 | 342 | 409 | 4 |         |         |       |
| 2   | J     | 279      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2052  | 1297 | 342 | 409 | 4 |         |         |       |
| 2   | L     | 279      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2052  | 1297 | 342 | 409 | 4 |         |         |       |
| 2   | N     | 279      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2052  | 1297 | 342 | 409 | 4 |         |         |       |
| 2   | P     | 279      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2052  | 1297 | 342 | 409 | 4 |         |         |       |

- Molecule 3 is alpha-D-mannopyranose (CCD ID: MAN) (formula:  $C_6H_{12}O_6$ ).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 3   | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 12    | 6 | 6 |         |         |
| 3   | D     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 12    | 6 | 6 |         |         |
| 3   | F     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 12    | 6 | 6 |         |         |
| 3   | H     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 12    | 6 | 6 |         |         |

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| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 3   | J     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 12    | 6 | 6 |         |         |
| 3   | L     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 12    | 6 | 6 |         |         |
| 3   | N     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 12    | 6 | 6 |         |         |
| 3   | P     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 12    | 6 | 6 |         |         |

- Molecule 4 is water.

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 4   | A     | 34       | Total | O  | 0       | 0       |
|     |       |          | 34    | 34 |         |         |
| 4   | B     | 82       | Total | O  | 0       | 0       |
|     |       |          | 82    | 82 |         |         |
| 4   | C     | 37       | Total | O  | 0       | 0       |
|     |       |          | 37    | 37 |         |         |
| 4   | D     | 69       | Total | O  | 0       | 0       |
|     |       |          | 69    | 69 |         |         |
| 4   | E     | 39       | Total | O  | 0       | 0       |
|     |       |          | 39    | 39 |         |         |
| 4   | F     | 78       | Total | O  | 0       | 0       |
|     |       |          | 78    | 78 |         |         |
| 4   | G     | 39       | Total | O  | 0       | 0       |
|     |       |          | 39    | 39 |         |         |
| 4   | H     | 73       | Total | O  | 0       | 0       |
|     |       |          | 73    | 73 |         |         |
| 4   | I     | 2        | Total | O  | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 4   | J     | 9        | Total | O  | 0       | 0       |
|     |       |          | 9     | 9  |         |         |
| 4   | K     | 4        | Total | O  | 0       | 0       |
|     |       |          | 4     | 4  |         |         |
| 4   | L     | 8        | Total | O  | 0       | 0       |
|     |       |          | 8     | 8  |         |         |
| 4   | M     | 2        | Total | O  | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 4   | N     | 8        | Total | O  | 0       | 0       |
|     |       |          | 8     | 8  |         |         |
| 4   | O     | 4        | Total | O  | 0       | 0       |
|     |       |          | 4     | 4  |         |         |

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| Mol | Chain | Residues | Atoms |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 4   | P     | 7        | Total | O | 0       | 0       |
|     |       |          | 7     | 7 |         |         |

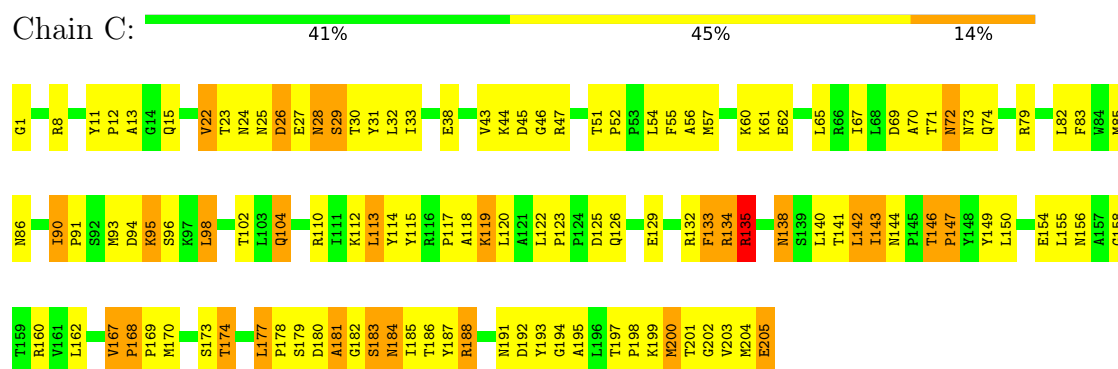
### 3 Residue-property plots

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

#### • Molecule 1: CHAPERONE PROTEIN FIMC



#### • Molecule 1: CHAPERONE PROTEIN FIMC



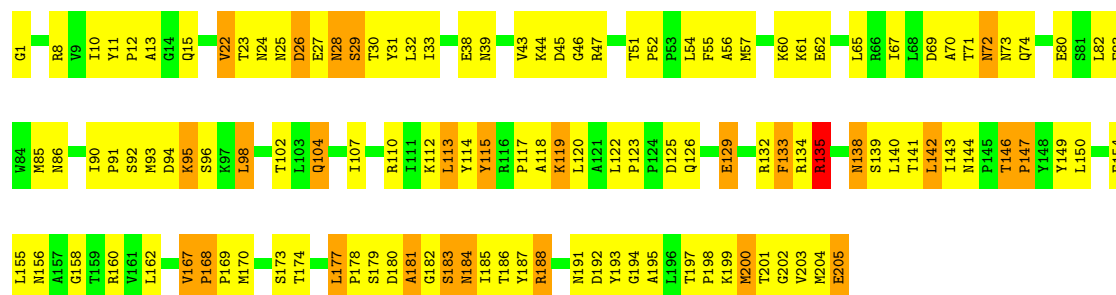
#### • Molecule 1: CHAPERONE PROTEIN FIMC



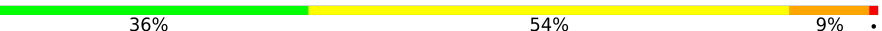


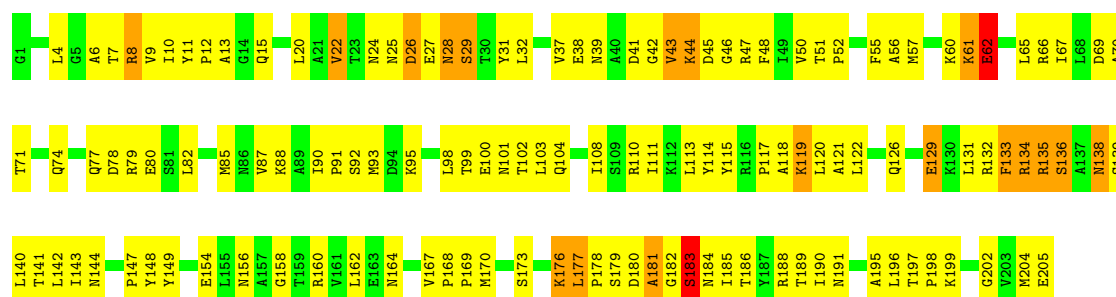
- Molecule 1: CHAPERONE PROTEIN FIMC

Chain G: 



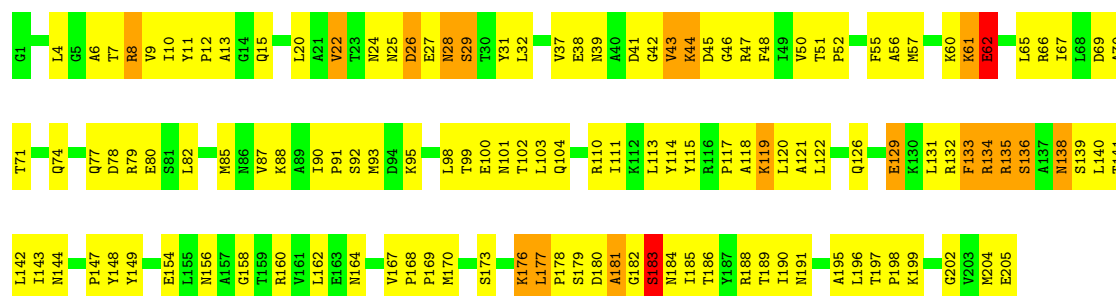
- Molecule 1: CHAPERONE PROTEIN FIMC

Chain I: 



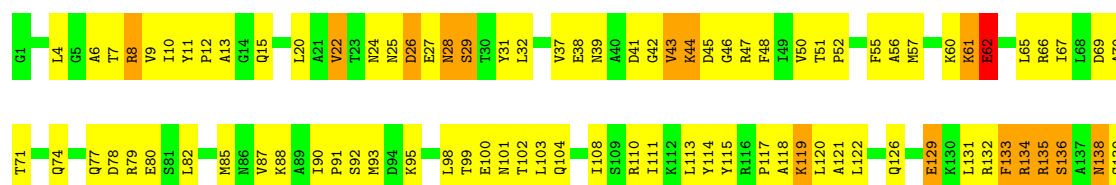
- Molecule 1: CHAPERONE PROTEIN FIMC

Chain K: 



- Molecule 1: CHAPERONE PROTEIN FIMC

Chain M: 





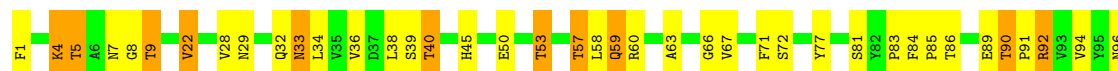
### • Molecule 1: CHAPERONE PROTEIN FIMC



### • Molecule 2: FIMH PROTEIN

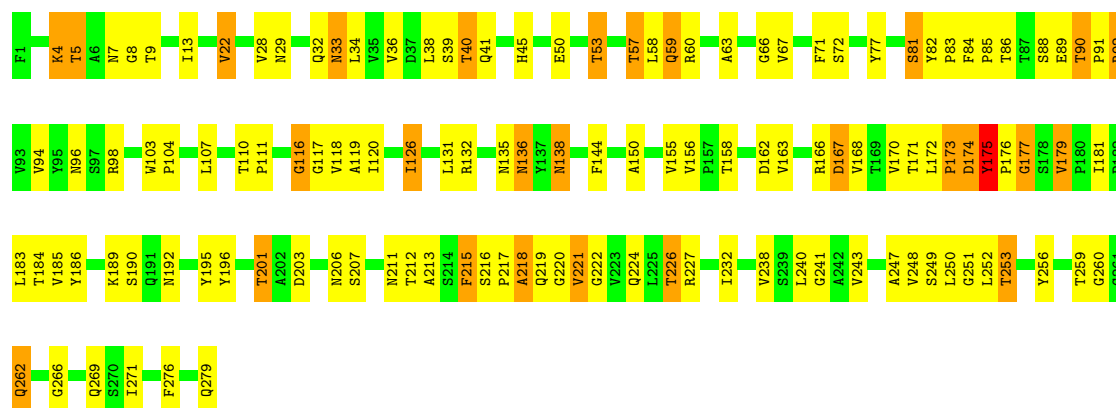


### • Molecule 2: FIMH PROTEIN



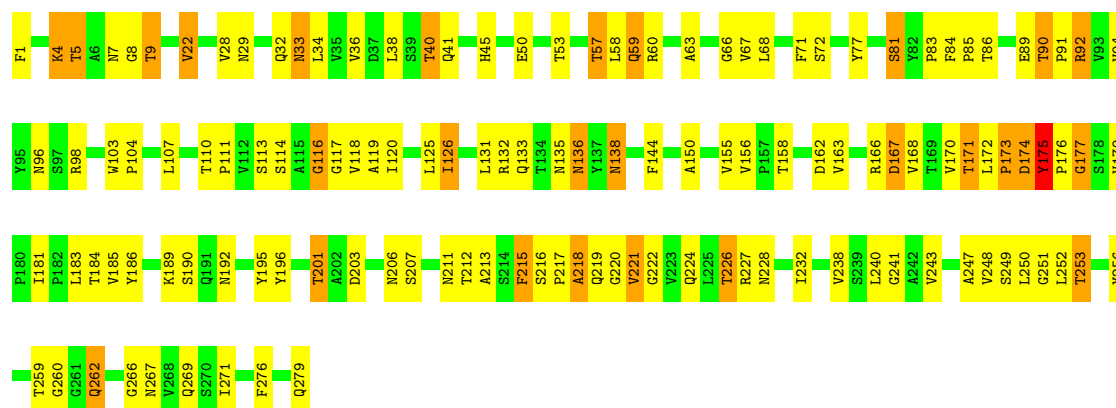
### • Molecule 2: FIMH PROTEIN

Chain F:  54% 36% 10%

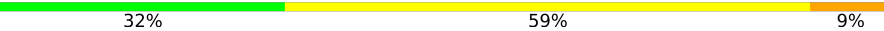


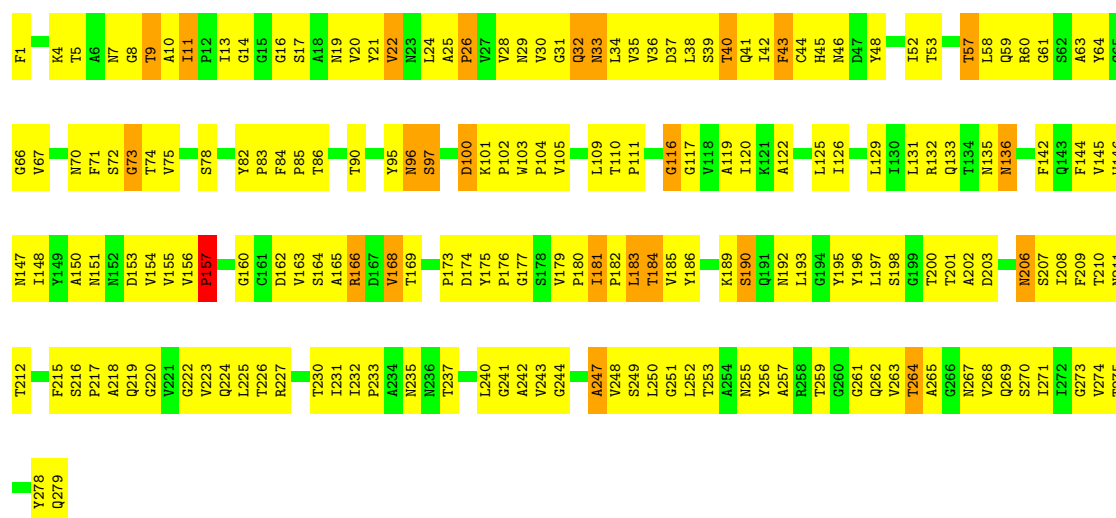
• Molecule 2: FIMH PROTEIN

Chain H:  53% 37% 10%

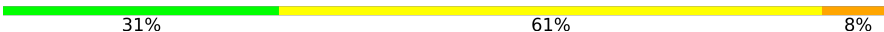


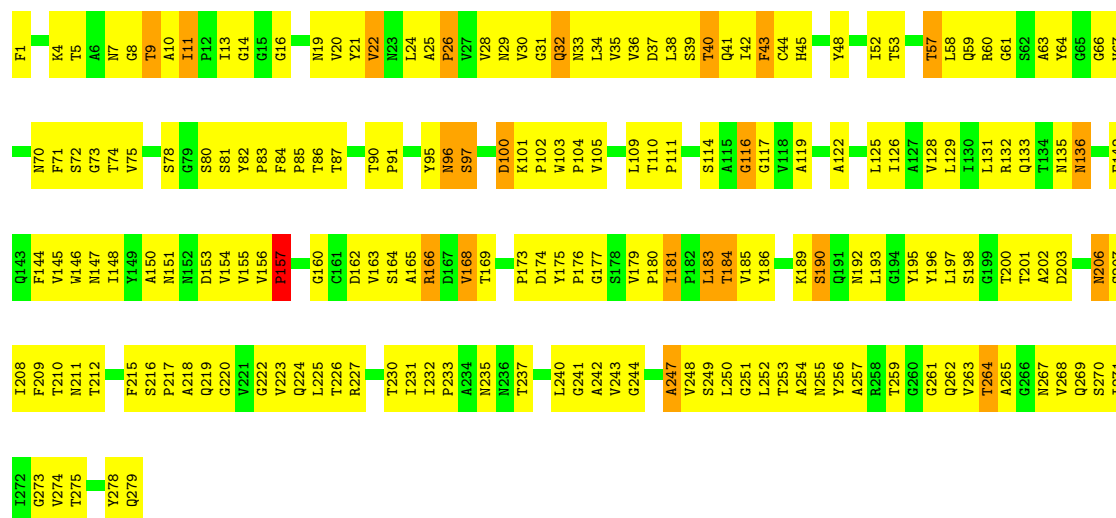
• Molecule 2: FIMH PROTEIN

Chain J:  32% 59% 9%

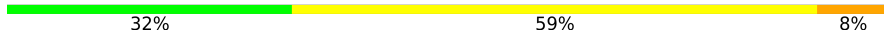


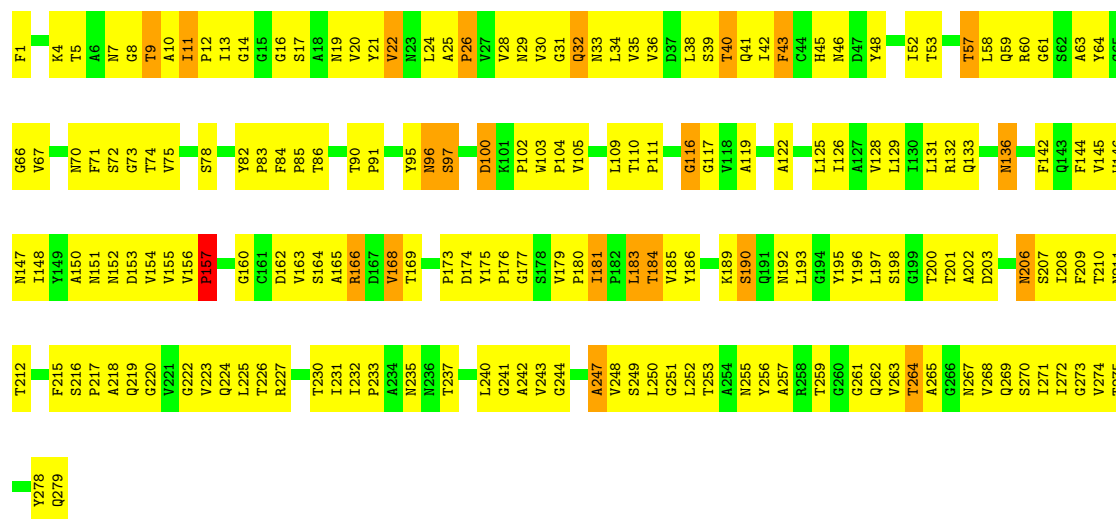
• Molecule 2: FIMH PROTEIN

Chain L: 

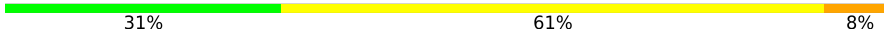


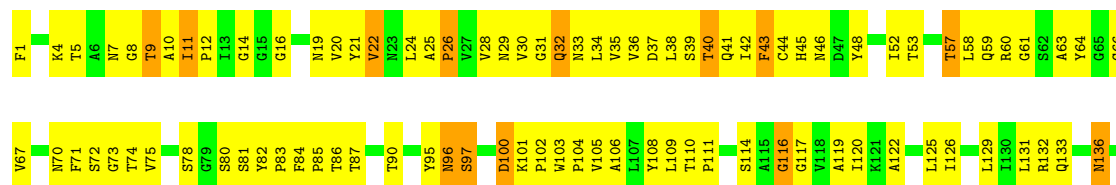
• Molecule 2: FIMH PROTEIN

Chain N: 



• Molecule 2: FIMH PROTEIN

Chain P: 





## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | C 1 2 1                                                     | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 138.08Å 138.13Å 215.35Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 43.68 – 2.79<br>43.68 – 2.79                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 98.9 (43.68-2.79)<br>99.0 (43.68-2.79)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.07                                                        | Depositor        |
| $R_{sym}$                                                               | 0.07                                                        | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.86 (at 2.81Å)                                             | Xtriage          |
| Refinement program                                                      | CNS                                                         | Depositor        |
| R, $R_{free}$                                                           | 0.239 , 0.280<br>0.240 , 0.279                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 9936 reflections (10.02%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 59.1                                                        | Xtriage          |
| Anisotropy                                                              | 0.066                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.32 , 80.8                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$ | Xtriage          |
| Estimated twinning fraction                                             | 0.477 for k,h,-l<br>0.476 for -k,-h,-l<br>0.477 for -h,-k,l | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.96                                                        | EDS              |
| Total number of atoms                                                   | 29775                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 95.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.45% 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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

| Mol | Chain | Bond lengths |         | Bond angles |                  |
|-----|-------|--------------|---------|-------------|------------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5          |
| 1   | A     | 0.54         | 0/1625  | 1.13        | 15/2209 (0.7%)   |
| 1   | C     | 0.54         | 0/1625  | 1.13        | 17/2209 (0.8%)   |
| 1   | E     | 0.54         | 0/1625  | 1.13        | 18/2209 (0.8%)   |
| 1   | G     | 0.54         | 0/1625  | 1.13        | 17/2209 (0.8%)   |
| 1   | I     | 0.37         | 0/1625  | 0.97        | 6/2209 (0.3%)    |
| 1   | K     | 0.37         | 0/1625  | 0.97        | 6/2209 (0.3%)    |
| 1   | M     | 0.37         | 0/1625  | 0.97        | 6/2209 (0.3%)    |
| 1   | O     | 0.38         | 0/1625  | 0.97        | 6/2209 (0.3%)    |
| 2   | B     | 0.60         | 0/2097  | 1.11        | 13/2881 (0.5%)   |
| 2   | D     | 0.61         | 0/2097  | 1.12        | 13/2881 (0.5%)   |
| 2   | F     | 0.60         | 0/2097  | 1.11        | 12/2881 (0.4%)   |
| 2   | H     | 0.60         | 0/2097  | 1.11        | 13/2881 (0.5%)   |
| 2   | J     | 0.36         | 0/2097  | 0.92        | 7/2881 (0.2%)    |
| 2   | L     | 0.36         | 0/2097  | 0.92        | 7/2881 (0.2%)    |
| 2   | N     | 0.36         | 0/2097  | 0.92        | 7/2881 (0.2%)    |
| 2   | P     | 0.36         | 0/2097  | 0.92        | 7/2881 (0.2%)    |
| All | All   | 0.48         | 0/29776 | 1.04        | 170/40720 (0.4%) |

There are no bond length outliers.

All (170) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | E     | 167 | VAL  | CA-C-N | 9.17  | 126.35      | 119.66   |
| 1   | E     | 167 | VAL  | C-N-CA | 9.17  | 126.35      | 119.66   |
| 1   | A     | 167 | VAL  | CA-C-N | 8.98  | 126.21      | 119.66   |
| 1   | A     | 167 | VAL  | C-N-CA | 8.98  | 126.21      | 119.66   |
| 1   | G     | 167 | VAL  | CA-C-N | 8.87  | 126.13      | 119.66   |
| 1   | G     | 167 | VAL  | C-N-CA | 8.87  | 126.13      | 119.66   |
| 1   | M     | 180 | ASP  | N-CA-C | -8.77 | 98.31       | 111.81   |
| 1   | O     | 180 | ASP  | N-CA-C | -8.75 | 98.33       | 111.81   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | K     | 180 | ASP  | N-CA-C | -8.72 | 98.38       | 111.81   |
| 1   | I     | 180 | ASP  | N-CA-C | -8.69 | 98.44       | 111.81   |
| 1   | M     | 177 | LEU  | CA-C-N | 8.50  | 128.23      | 119.56   |
| 1   | M     | 177 | LEU  | C-N-CA | 8.50  | 128.23      | 119.56   |
| 1   | O     | 177 | LEU  | CA-C-N | 8.49  | 128.22      | 119.56   |
| 1   | O     | 177 | LEU  | C-N-CA | 8.49  | 128.22      | 119.56   |
| 1   | I     | 177 | LEU  | CA-C-N | 8.47  | 128.20      | 119.56   |
| 1   | I     | 177 | LEU  | C-N-CA | 8.47  | 128.20      | 119.56   |
| 1   | K     | 177 | LEU  | CA-C-N | 8.47  | 128.20      | 119.56   |
| 1   | K     | 177 | LEU  | C-N-CA | 8.47  | 128.20      | 119.56   |
| 1   | C     | 167 | VAL  | CA-C-N | 8.23  | 125.67      | 119.66   |
| 1   | C     | 167 | VAL  | C-N-CA | 8.23  | 125.67      | 119.66   |
| 2   | H     | 9   | THR  | N-CA-C | 7.65  | 120.76      | 110.35   |
| 2   | F     | 175 | TYR  | CA-C-N | -7.62 | 111.94      | 119.64   |
| 2   | F     | 175 | TYR  | C-N-CA | -7.62 | 111.94      | 119.64   |
| 2   | B     | 177 | GLY  | N-CA-C | 7.61  | 120.70      | 112.33   |
| 2   | F     | 177 | GLY  | N-CA-C | 7.58  | 120.67      | 112.33   |
| 1   | E     | 95  | LYS  | N-CA-C | -7.55 | 104.06      | 113.20   |
| 2   | D     | 22  | VAL  | N-CA-C | 7.54  | 118.66      | 108.11   |
| 2   | D     | 177 | GLY  | N-CA-C | 7.52  | 120.60      | 112.33   |
| 1   | A     | 95  | LYS  | N-CA-C | -7.52 | 104.10      | 113.20   |
| 1   | G     | 95  | LYS  | N-CA-C | -7.52 | 104.10      | 113.20   |
| 2   | H     | 175 | TYR  | CA-C-N | -7.47 | 112.09      | 119.64   |
| 2   | H     | 175 | TYR  | C-N-CA | -7.47 | 112.09      | 119.64   |
| 1   | C     | 95  | LYS  | N-CA-C | -7.46 | 104.17      | 113.20   |
| 2   | H     | 177 | GLY  | N-CA-C | 7.45  | 120.52      | 112.33   |
| 2   | F     | 22  | VAL  | N-CA-C | 7.44  | 118.52      | 108.11   |
| 2   | D     | 175 | TYR  | CA-C-N | -7.26 | 112.31      | 119.64   |
| 2   | D     | 175 | TYR  | C-N-CA | -7.26 | 112.31      | 119.64   |
| 1   | G     | 177 | LEU  | CA-C-N | 7.22  | 126.92      | 119.56   |
| 1   | G     | 177 | LEU  | C-N-CA | 7.22  | 126.92      | 119.56   |
| 2   | D     | 9   | THR  | N-CA-C | 7.21  | 120.68      | 110.23   |
| 2   | B     | 175 | TYR  | CA-C-N | -7.20 | 112.37      | 119.64   |
| 2   | B     | 175 | TYR  | C-N-CA | -7.20 | 112.37      | 119.64   |
| 2   | B     | 9   | THR  | N-CA-C | 7.18  | 120.65      | 110.23   |
| 1   | E     | 177 | LEU  | CA-C-N | 7.16  | 126.86      | 119.56   |
| 1   | E     | 177 | LEU  | C-N-CA | 7.16  | 126.86      | 119.56   |
| 1   | C     | 177 | LEU  | CA-C-N | 7.12  | 126.82      | 119.56   |
| 1   | C     | 177 | LEU  | C-N-CA | 7.12  | 126.82      | 119.56   |
| 1   | A     | 177 | LEU  | CA-C-N | 7.06  | 126.76      | 119.56   |
| 1   | A     | 177 | LEU  | C-N-CA | 7.06  | 126.76      | 119.56   |
| 2   | B     | 22  | VAL  | N-CA-C | 6.99  | 118.55      | 108.48   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | F     | 9   | THR  | N-CA-C | 6.93  | 120.28      | 110.23   |
| 2   | J     | 39  | SER  | N-CA-C | -6.62 | 104.19      | 113.20   |
| 2   | H     | 22  | VAL  | N-CA-C | 6.58  | 117.96      | 108.48   |
| 2   | N     | 39  | SER  | N-CA-C | -6.54 | 104.31      | 113.20   |
| 2   | P     | 39  | SER  | N-CA-C | -6.51 | 104.35      | 113.20   |
| 2   | L     | 39  | SER  | N-CA-C | -6.43 | 104.46      | 113.20   |
| 2   | N     | 72  | SER  | N-CA-C | -6.38 | 99.77       | 109.85   |
| 2   | H     | 34  | LEU  | N-CA-C | -6.38 | 98.84       | 109.24   |
| 2   | F     | 72  | SER  | N-CA-C | -6.36 | 98.62       | 109.24   |
| 2   | F     | 34  | LEU  | N-CA-C | -6.34 | 98.91       | 109.24   |
| 2   | B     | 34  | LEU  | N-CA-C | -6.29 | 98.99       | 109.24   |
| 2   | L     | 72  | SER  | N-CA-C | -6.25 | 99.72       | 109.72   |
| 2   | D     | 34  | LEU  | N-CA-C | -6.22 | 99.10       | 109.24   |
| 2   | D     | 72  | SER  | N-CA-C | -6.21 | 98.88       | 109.24   |
| 2   | J     | 72  | SER  | N-CA-C | -6.14 | 99.90       | 109.72   |
| 2   | P     | 72  | SER  | N-CA-C | -6.14 | 99.90       | 109.72   |
| 1   | C     | 45  | ASP  | N-CA-C | -6.13 | 100.85      | 110.36   |
| 2   | H     | 72  | SER  | N-CA-C | -6.12 | 99.02       | 109.24   |
| 2   | B     | 72  | SER  | N-CA-C | -6.11 | 99.03       | 109.24   |
| 1   | E     | 45  | ASP  | N-CA-C | -6.07 | 100.95      | 110.36   |
| 1   | G     | 167 | VAL  | N-CA-C | 6.07  | 113.56      | 107.55   |
| 1   | G     | 45  | ASP  | N-CA-C | -6.04 | 101.00      | 110.36   |
| 2   | J     | 11  | ILE  | CA-C-N | 6.00  | 126.83      | 120.11   |
| 2   | J     | 11  | ILE  | C-N-CA | 6.00  | 126.83      | 120.11   |
| 1   | E     | 184 | ASN  | N-CA-C | -5.97 | 105.08      | 113.20   |
| 2   | P     | 11  | ILE  | CA-C-N | 5.92  | 126.74      | 120.11   |
| 2   | P     | 11  | ILE  | C-N-CA | 5.92  | 126.74      | 120.11   |
| 1   | A     | 167 | VAL  | N-CA-C | 5.92  | 113.41      | 107.55   |
| 1   | A     | 184 | ASN  | N-CA-C | -5.90 | 105.18      | 113.20   |
| 1   | C     | 167 | VAL  | N-CA-C | 5.86  | 113.35      | 107.55   |
| 1   | G     | 184 | ASN  | N-CA-C | -5.86 | 105.24      | 113.20   |
| 1   | C     | 184 | ASN  | N-CA-C | -5.85 | 105.24      | 113.20   |
| 1   | A     | 45  | ASP  | N-CA-C | -5.83 | 101.33      | 110.36   |
| 2   | H     | 98  | ARG  | N-CA-C | -5.82 | 106.03      | 113.01   |
| 2   | B     | 98  | ARG  | N-CA-C | -5.79 | 106.06      | 113.01   |
| 2   | L     | 11  | ILE  | CA-C-N | 5.77  | 126.57      | 120.11   |
| 2   | L     | 11  | ILE  | C-N-CA | 5.77  | 126.57      | 120.11   |
| 2   | N     | 11  | ILE  | CA-C-N | 5.75  | 126.55      | 120.11   |
| 2   | N     | 11  | ILE  | C-N-CA | 5.75  | 126.55      | 120.11   |
| 2   | D     | 98  | ARG  | N-CA-C | -5.72 | 106.14      | 113.01   |
| 2   | L     | 181 | ILE  | N-CA-C | 5.71  | 113.54      | 108.63   |
| 2   | D     | 103 | TRP  | CA-C-N | 5.68  | 126.94      | 119.84   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | D     | 103 | TRP  | C-N-CA  | 5.68  | 126.94      | 119.84   |
| 1   | G     | 115 | TYR  | N-CA-C  | -5.68 | 99.27       | 108.41   |
| 2   | P     | 181 | ILE  | N-CA-C  | 5.67  | 113.51      | 108.63   |
| 2   | J     | 181 | ILE  | N-CA-C  | 5.66  | 113.50      | 108.63   |
| 2   | B     | 103 | TRP  | CA-C-N  | 5.64  | 126.89      | 119.84   |
| 2   | B     | 103 | TRP  | C-N-CA  | 5.64  | 126.89      | 119.84   |
| 2   | N     | 33  | ASN  | N-CA-C  | 5.63  | 118.04      | 108.02   |
| 2   | D     | 171 | THR  | N-CA-C  | -5.62 | 105.55      | 113.20   |
| 2   | H     | 171 | THR  | N-CA-C  | -5.62 | 105.55      | 113.20   |
| 2   | J     | 33  | ASN  | N-CA-C  | 5.62  | 118.02      | 108.02   |
| 2   | J     | 73  | GLY  | N-CA-C  | 5.61  | 118.95      | 110.75   |
| 2   | B     | 92  | ARG  | N-CA-C  | 5.61  | 118.77      | 109.46   |
| 1   | A     | 115 | TYR  | N-CA-C  | -5.60 | 99.40       | 108.41   |
| 2   | N     | 181 | ILE  | N-CA-C  | 5.60  | 113.44      | 108.63   |
| 1   | E     | 115 | TYR  | N-CA-C  | -5.60 | 99.40       | 108.41   |
| 2   | D     | 92  | ARG  | N-CA-C  | 5.59  | 118.74      | 109.46   |
| 2   | L     | 33  | ASN  | N-CA-C  | 5.57  | 117.94      | 108.02   |
| 2   | B     | 171 | THR  | N-CA-C  | -5.57 | 105.63      | 113.20   |
| 1   | E     | 167 | VAL  | N-CA-C  | 5.56  | 113.05      | 107.55   |
| 1   | C     | 115 | TYR  | N-CA-C  | -5.56 | 99.46       | 108.41   |
| 2   | P     | 33  | ASN  | N-CA-C  | 5.55  | 117.90      | 108.02   |
| 2   | H     | 92  | ARG  | N-CA-C  | 5.54  | 118.65      | 109.46   |
| 2   | H     | 103 | TRP  | CA-C-N  | 5.47  | 126.68      | 119.84   |
| 2   | H     | 103 | TRP  | C-N-CA  | 5.47  | 126.68      | 119.84   |
| 2   | F     | 92  | ARG  | N-CA-C  | 5.47  | 118.53      | 109.46   |
| 2   | L     | 73  | GLY  | N-CA-C  | 5.46  | 118.72      | 110.75   |
| 1   | A     | 133 | PHE  | N-CA-C  | 5.44  | 115.57      | 108.07   |
| 1   | K     | 133 | PHE  | N-CA-C  | 5.43  | 115.56      | 108.07   |
| 2   | P     | 73  | GLY  | N-CA-C  | 5.43  | 118.92      | 110.88   |
| 1   | M     | 133 | PHE  | N-CA-C  | 5.42  | 115.56      | 108.07   |
| 2   | F     | 98  | ARG  | N-CA-C  | -5.40 | 106.53      | 113.01   |
| 1   | M     | 136 | SER  | CB-CA-C | -5.39 | 109.30      | 117.07   |
| 1   | I     | 136 | SER  | CB-CA-C | -5.37 | 109.33      | 117.07   |
| 2   | N     | 73  | GLY  | N-CA-C  | 5.37  | 118.83      | 110.88   |
| 2   | F     | 103 | TRP  | CA-C-N  | 5.37  | 126.55      | 119.84   |
| 2   | F     | 103 | TRP  | C-N-CA  | 5.37  | 126.55      | 119.84   |
| 1   | I     | 133 | PHE  | N-CA-C  | 5.37  | 115.47      | 108.07   |
| 1   | O     | 136 | SER  | CB-CA-C | -5.36 | 109.35      | 117.07   |
| 1   | O     | 133 | PHE  | N-CA-C  | 5.35  | 115.46      | 108.07   |
| 1   | K     | 136 | SER  | CB-CA-C | -5.34 | 109.37      | 117.07   |
| 1   | A     | 135 | ARG  | N-CA-C  | 5.33  | 117.42      | 108.73   |
| 1   | G     | 139 | SER  | N-CA-C  | 5.31  | 117.26      | 108.49   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | F     | 39  | SER  | N-CA-C | -5.31 | 106.50      | 112.87   |
| 1   | G     | 135 | ARG  | N-CA-C | 5.30  | 117.38      | 108.73   |
| 1   | C     | 135 | ARG  | N-CA-C | 5.29  | 117.35      | 108.73   |
| 1   | C     | 98  | LEU  | N-CA-C | 5.27  | 117.71      | 111.33   |
| 1   | G     | 133 | PHE  | N-CA-C | 5.26  | 115.33      | 108.07   |
| 1   | A     | 98  | LEU  | N-CA-C | 5.26  | 117.69      | 111.33   |
| 1   | E     | 133 | PHE  | N-CA-C | 5.25  | 115.31      | 108.07   |
| 1   | C     | 168 | PRO  | CA-C-N | 5.25  | 125.17      | 119.76   |
| 1   | C     | 168 | PRO  | C-N-CA | 5.25  | 125.17      | 119.76   |
| 1   | K     | 136 | SER  | CA-C-O | 5.25  | 120.98      | 117.94   |
| 1   | E     | 135 | ARG  | N-CA-C | 5.24  | 117.27      | 108.73   |
| 1   | C     | 133 | PHE  | N-CA-C | 5.24  | 115.30      | 108.07   |
| 2   | H     | 125 | LEU  | N-CA-C | -5.22 | 101.92      | 109.59   |
| 1   | A     | 139 | SER  | N-CA-C | 5.20  | 117.07      | 108.49   |
| 1   | G     | 168 | PRO  | CA-C-N | 5.17  | 125.08      | 119.76   |
| 1   | G     | 168 | PRO  | C-N-CA | 5.17  | 125.08      | 119.76   |
| 1   | E     | 188 | ARG  | N-CA-C | -5.17 | 101.56      | 109.41   |
| 1   | G     | 188 | ARG  | N-CA-C | -5.17 | 101.56      | 109.41   |
| 1   | I     | 136 | SER  | CA-C-O | 5.16  | 120.93      | 117.94   |
| 1   | O     | 136 | SER  | CA-C-O | 5.15  | 120.92      | 117.94   |
| 1   | E     | 139 | SER  | N-CA-C | 5.14  | 116.97      | 108.49   |
| 2   | B     | 30  | VAL  | N-CA-C | -5.14 | 102.23      | 109.63   |
| 2   | D     | 39  | SER  | N-CA-C | -5.13 | 106.71      | 112.87   |
| 1   | M     | 136 | SER  | CA-C-O | 5.13  | 120.92      | 117.94   |
| 1   | E     | 90  | ILE  | N-CA-C | 5.11  | 112.92      | 107.76   |
| 1   | E     | 98  | LEU  | N-CA-C | 5.10  | 117.51      | 111.33   |
| 1   | G     | 98  | LEU  | N-CA-C | 5.09  | 117.50      | 111.33   |
| 1   | A     | 188 | ARG  | N-CA-C | -5.08 | 101.68      | 109.41   |
| 1   | E     | 180 | ASP  | N-CA-C | -5.08 | 99.97       | 110.80   |
| 1   | G     | 180 | ASP  | N-CA-C | -5.08 | 99.99       | 110.80   |
| 1   | C     | 90  | ILE  | N-CA-C | 5.07  | 112.89      | 107.76   |
| 1   | E     | 168 | PRO  | CA-C-N | 5.07  | 124.98      | 119.76   |
| 1   | E     | 168 | PRO  | C-N-CA | 5.07  | 124.98      | 119.76   |
| 1   | C     | 188 | ARG  | N-CA-C | -5.07 | 101.71      | 109.41   |
| 1   | A     | 180 | ASP  | N-CA-C | -5.06 | 100.02      | 110.80   |
| 1   | C     | 180 | ASP  | N-CA-C | -5.03 | 100.08      | 110.80   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 1596  | 0        | 1639     | 144     | 0            |
| 1   | C     | 1596  | 0        | 1639     | 154     | 0            |
| 1   | E     | 1596  | 0        | 1639     | 137     | 0            |
| 1   | G     | 1596  | 0        | 1639     | 143     | 0            |
| 1   | I     | 1596  | 0        | 1639     | 156     | 0            |
| 1   | K     | 1596  | 0        | 1639     | 156     | 0            |
| 1   | M     | 1596  | 0        | 1639     | 158     | 0            |
| 1   | O     | 1596  | 0        | 1639     | 158     | 0            |
| 2   | B     | 2052  | 0        | 2007     | 146     | 0            |
| 2   | D     | 2052  | 0        | 2007     | 146     | 0            |
| 2   | F     | 2052  | 0        | 2007     | 140     | 0            |
| 2   | H     | 2052  | 0        | 2007     | 146     | 0            |
| 2   | J     | 2052  | 0        | 2007     | 206     | 0            |
| 2   | L     | 2052  | 0        | 2007     | 212     | 0            |
| 2   | N     | 2052  | 0        | 2007     | 211     | 0            |
| 2   | P     | 2052  | 0        | 2007     | 214     | 0            |
| 3   | B     | 12    | 0        | 12       | 0       | 0            |
| 3   | D     | 12    | 0        | 12       | 0       | 0            |
| 3   | F     | 12    | 0        | 12       | 0       | 0            |
| 3   | H     | 12    | 0        | 12       | 0       | 0            |
| 3   | J     | 12    | 0        | 12       | 3       | 0            |
| 3   | L     | 12    | 0        | 12       | 2       | 0            |
| 3   | N     | 12    | 0        | 12       | 1       | 0            |
| 3   | P     | 12    | 0        | 12       | 2       | 0            |
| 4   | A     | 34    | 0        | 0        | 3       | 0            |
| 4   | B     | 82    | 0        | 0        | 3       | 0            |
| 4   | C     | 37    | 0        | 0        | 1       | 0            |
| 4   | D     | 69    | 0        | 0        | 4       | 0            |
| 4   | E     | 39    | 0        | 0        | 0       | 0            |
| 4   | F     | 78    | 0        | 0        | 4       | 0            |
| 4   | G     | 39    | 0        | 0        | 3       | 0            |
| 4   | H     | 73    | 0        | 0        | 4       | 0            |
| 4   | I     | 2     | 0        | 0        | 0       | 0            |
| 4   | J     | 9     | 0        | 0        | 1       | 0            |
| 4   | K     | 4     | 0        | 0        | 0       | 0            |
| 4   | L     | 8     | 0        | 0        | 1       | 0            |
| 4   | M     | 2     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4   | N     | 8     | 0        | 0        | 0       | 0            |
| 4   | O     | 4     | 0        | 0        | 0       | 0            |
| 4   | P     | 7     | 0        | 0        | 0       | 0            |
| All | All   | 29775 | 0        | 29264    | 2522    | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 43.

All (2522) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:134:ARG:HB3  | 1:C:141:THR:HG22 | 1.26                     | 1.14              |
| 2:F:126:ILE:HD12 | 2:F:150:ALA:HB2  | 1.33                     | 1.10              |
| 2:P:224:GLN:HE21 | 2:P:231:ILE:HG21 | 1.16                     | 1.10              |
| 2:H:126:ILE:HD12 | 2:H:150:ALA:HB2  | 1.34                     | 1.09              |
| 2:D:126:ILE:HD12 | 2:D:150:ALA:HB2  | 1.33                     | 1.09              |
| 2:J:224:GLN:HE21 | 2:J:231:ILE:HG21 | 1.17                     | 1.08              |
| 2:B:126:ILE:HD12 | 2:B:150:ALA:HB2  | 1.33                     | 1.07              |
| 2:L:201:THR:HG21 | 2:L:206:ASN:HA   | 1.38                     | 1.06              |
| 2:N:224:GLN:HE21 | 2:N:231:ILE:HG21 | 1.17                     | 1.05              |
| 2:J:196:TYR:HE1  | 2:J:198:SER:HB3  | 1.21                     | 1.05              |
| 2:L:196:TYR:HE1  | 2:L:198:SER:HB3  | 1.22                     | 1.05              |
| 2:L:224:GLN:HE21 | 2:L:231:ILE:HG21 | 1.17                     | 1.04              |
| 2:N:196:TYR:HE1  | 2:N:198:SER:HB3  | 1.22                     | 1.03              |
| 2:N:201:THR:HG21 | 2:N:206:ASN:HA   | 1.37                     | 1.03              |
| 2:J:201:THR:HG21 | 2:J:206:ASN:HA   | 1.38                     | 1.03              |
| 2:B:201:THR:HG21 | 2:B:206:ASN:HA   | 1.44                     | 1.00              |
| 2:P:196:TYR:HE1  | 2:P:198:SER:HB3  | 1.22                     | 1.00              |
| 2:P:201:THR:HG21 | 2:P:206:ASN:HA   | 1.38                     | 1.00              |
| 2:H:201:THR:HG21 | 2:H:206:ASN:HA   | 1.44                     | 1.00              |
| 2:D:201:THR:HG21 | 2:D:206:ASN:HA   | 1.44                     | 0.99              |
| 2:F:201:THR:HG21 | 2:F:206:ASN:HA   | 1.45                     | 0.98              |
| 1:C:134:ARG:HB3  | 1:C:141:THR:CG2  | 1.93                     | 0.98              |
| 1:M:47:ARG:HH22  | 1:M:74:GLN:HE21  | 1.08                     | 0.97              |
| 2:B:170:VAL:HG12 | 2:B:172:LEU:HB2  | 1.47                     | 0.97              |
| 2:D:170:VAL:HG12 | 2:D:172:LEU:HB2  | 1.47                     | 0.96              |
| 1:K:47:ARG:HH22  | 1:K:74:GLN:HE21  | 1.07                     | 0.96              |
| 1:O:47:ARG:HH22  | 1:O:74:GLN:HE21  | 1.07                     | 0.96              |
| 2:F:120:ILE:HG21 | 2:F:126:ILE:HD11 | 1.48                     | 0.96              |
| 2:F:170:VAL:HG12 | 2:F:172:LEU:HB2  | 1.47                     | 0.96              |
| 2:H:170:VAL:HG12 | 2:H:172:LEU:HB2  | 1.47                     | 0.95              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:179:SER:C    | 1:A:181:ALA:H    | 1.74                     | 0.94              |
| 2:H:5:THR:HG21   | 4:H:1644:HOH:O   | 1.68                     | 0.94              |
| 2:N:202:ALA:HB2  | 2:N:210:THR:HG22 | 1.50                     | 0.94              |
| 2:L:57:THR:HG23  | 2:L:132:ARG:HB3  | 1.48                     | 0.94              |
| 2:P:202:ALA:HB2  | 2:P:210:THR:HG22 | 1.50                     | 0.94              |
| 2:D:213:ALA:HB2  | 2:D:269:GLN:HB2  | 1.50                     | 0.93              |
| 2:L:202:ALA:HB2  | 2:L:210:THR:HG22 | 1.50                     | 0.93              |
| 1:C:47:ARG:HH22  | 1:C:74:GLN:HE21  | 0.99                     | 0.93              |
| 2:H:167:ASP:CG   | 2:H:168:VAL:H    | 1.77                     | 0.93              |
| 2:J:202:ALA:HB2  | 2:J:210:THR:HG22 | 1.50                     | 0.93              |
| 1:E:47:ARG:HH22  | 1:E:74:GLN:HE21  | 0.98                     | 0.93              |
| 1:G:135:ARG:HH12 | 1:G:181:ALA:HB1  | 1.34                     | 0.93              |
| 2:B:120:ILE:HG21 | 2:B:126:ILE:HD11 | 1.49                     | 0.92              |
| 2:B:167:ASP:CG   | 2:B:168:VAL:H    | 1.76                     | 0.92              |
| 2:D:120:ILE:HG21 | 2:D:126:ILE:HD11 | 1.49                     | 0.92              |
| 2:J:57:THR:HG23  | 2:J:132:ARG:HB3  | 1.49                     | 0.92              |
| 2:N:57:THR:HG23  | 2:N:132:ARG:HB3  | 1.48                     | 0.92              |
| 1:I:47:ARG:HH22  | 1:I:74:GLN:HE21  | 1.07                     | 0.92              |
| 2:P:57:THR:HG23  | 2:P:132:ARG:HB3  | 1.50                     | 0.92              |
| 1:E:179:SER:C    | 1:E:181:ALA:H    | 1.74                     | 0.92              |
| 1:G:47:ARG:HH22  | 1:G:74:GLN:HE21  | 0.98                     | 0.92              |
| 2:H:120:ILE:HG21 | 2:H:126:ILE:HD11 | 1.49                     | 0.92              |
| 2:F:57:THR:HG22  | 2:F:132:ARG:HB3  | 1.52                     | 0.92              |
| 2:P:264:THR:HG22 | 2:P:265:ALA:H    | 1.35                     | 0.91              |
| 1:C:135:ARG:HH12 | 1:C:181:ALA:HB1  | 1.33                     | 0.91              |
| 2:L:67:VAL:HG21  | 2:L:126:ILE:HG23 | 1.51                     | 0.91              |
| 1:M:39:ASN:HD21  | 1:M:43:VAL:HG13  | 1.35                     | 0.91              |
| 2:H:57:THR:HG22  | 2:H:132:ARG:HB3  | 1.50                     | 0.91              |
| 2:J:264:THR:HG22 | 2:J:265:ALA:H    | 1.35                     | 0.91              |
| 1:K:39:ASN:HD21  | 1:K:43:VAL:HG13  | 1.36                     | 0.91              |
| 2:N:163:VAL:HA   | 2:N:185:VAL:HG22 | 1.53                     | 0.91              |
| 1:A:47:ARG:HH22  | 1:A:74:GLN:HE21  | 0.96                     | 0.91              |
| 2:L:163:VAL:HA   | 2:L:185:VAL:HG22 | 1.52                     | 0.91              |
| 1:A:135:ARG:HH12 | 1:A:181:ALA:HB1  | 1.34                     | 0.91              |
| 1:C:179:SER:C    | 1:C:181:ALA:H    | 1.75                     | 0.91              |
| 2:H:213:ALA:HB2  | 2:H:269:GLN:HB2  | 1.52                     | 0.91              |
| 2:N:67:VAL:HG21  | 2:N:126:ILE:HG23 | 1.52                     | 0.91              |
| 1:E:135:ARG:HH12 | 1:E:181:ALA:HB1  | 1.34                     | 0.90              |
| 2:J:163:VAL:HA   | 2:J:185:VAL:HG22 | 1.53                     | 0.90              |
| 1:G:179:SER:C    | 1:G:181:ALA:H    | 1.74                     | 0.90              |
| 2:P:67:VAL:HG21  | 2:P:126:ILE:HG23 | 1.51                     | 0.90              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:167:ASP:CG   | 2:D:168:VAL:H    | 1.76                     | 0.90              |
| 2:L:264:THR:HG22 | 2:L:265:ALA:H    | 1.35                     | 0.90              |
| 1:I:39:ASN:HD21  | 1:I:43:VAL:HG13  | 1.36                     | 0.90              |
| 2:J:67:VAL:HG21  | 2:J:126:ILE:HG23 | 1.51                     | 0.89              |
| 2:P:163:VAL:HA   | 2:P:185:VAL:HG22 | 1.52                     | 0.89              |
| 2:F:213:ALA:HB2  | 2:F:269:GLN:HB2  | 1.52                     | 0.89              |
| 2:B:57:THR:HG21  | 2:B:89:GLU:OE2   | 1.73                     | 0.89              |
| 2:N:264:THR:HG22 | 2:N:265:ALA:H    | 1.36                     | 0.89              |
| 1:O:39:ASN:HD21  | 1:O:43:VAL:HG13  | 1.36                     | 0.89              |
| 2:B:213:ALA:HB2  | 2:B:269:GLN:HB2  | 1.53                     | 0.89              |
| 2:F:57:THR:HG21  | 2:F:89:GLU:OE2   | 1.72                     | 0.89              |
| 1:A:133:PHE:HD2  | 1:A:140:LEU:HD21 | 1.38                     | 0.88              |
| 2:H:57:THR:HG21  | 2:H:89:GLU:OE2   | 1.73                     | 0.88              |
| 1:M:135:ARG:NH1  | 1:M:181:ALA:HB1  | 1.89                     | 0.88              |
| 2:F:167:ASP:CG   | 2:F:168:VAL:H    | 1.76                     | 0.88              |
| 1:I:176:LYS:HD2  | 1:I:176:LYS:H    | 1.38                     | 0.88              |
| 1:I:27:GLU:HG2   | 1:I:60:LYS:HD2   | 1.55                     | 0.87              |
| 1:O:135:ARG:NH1  | 1:O:181:ALA:HB1  | 1.89                     | 0.87              |
| 2:B:57:THR:HG22  | 2:B:132:ARG:HB3  | 1.57                     | 0.87              |
| 1:C:133:PHE:HD2  | 1:C:140:LEU:HD21 | 1.39                     | 0.87              |
| 1:K:134:ARG:HB3  | 1:K:141:THR:HB   | 1.56                     | 0.87              |
| 1:K:176:LYS:H    | 1:K:176:LYS:HD2  | 1.38                     | 0.87              |
| 1:M:176:LYS:H    | 1:M:176:LYS:HD2  | 1.39                     | 0.87              |
| 1:K:135:ARG:NH1  | 1:K:181:ALA:HB1  | 1.89                     | 0.86              |
| 1:I:134:ARG:HB3  | 1:I:141:THR:HB   | 1.56                     | 0.86              |
| 1:M:27:GLU:HG2   | 1:M:60:LYS:HD2   | 1.55                     | 0.86              |
| 1:E:138:ASN:HA   | 1:E:177:LEU:O    | 1.76                     | 0.86              |
| 2:N:11:ILE:HG23  | 2:N:16:GLY:HA3   | 1.57                     | 0.86              |
| 1:E:133:PHE:HD2  | 1:E:140:LEU:HD21 | 1.38                     | 0.86              |
| 1:I:135:ARG:NH1  | 1:I:181:ALA:HB1  | 1.89                     | 0.86              |
| 1:O:27:GLU:HG2   | 1:O:60:LYS:HD2   | 1.55                     | 0.86              |
| 1:O:134:ARG:HB3  | 1:O:141:THR:HB   | 1.56                     | 0.86              |
| 1:C:138:ASN:HA   | 1:C:177:LEU:O    | 1.76                     | 0.86              |
| 2:D:57:THR:HG21  | 2:D:89:GLU:OE2   | 1.75                     | 0.86              |
| 2:D:57:THR:HG22  | 2:D:132:ARG:HB3  | 1.56                     | 0.86              |
| 1:G:133:PHE:HD2  | 1:G:140:LEU:HD21 | 1.39                     | 0.86              |
| 2:J:58:LEU:H     | 2:J:90:THR:CG2   | 1.89                     | 0.86              |
| 1:K:27:GLU:HG2   | 1:K:60:LYS:HD2   | 1.55                     | 0.86              |
| 2:P:11:ILE:HG23  | 2:P:16:GLY:HA3   | 1.56                     | 0.85              |
| 2:J:11:ILE:HG23  | 2:J:16:GLY:HA3   | 1.56                     | 0.85              |
| 1:O:135:ARG:HH12 | 1:O:181:ALA:CB   | 1.90                     | 0.85              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:92:ARG:HH11  | 2:D:92:ARG:HG3   | 1.41                     | 0.85              |
| 2:F:218:ALA:HB2  | 2:F:266:GLY:C    | 2.02                     | 0.85              |
| 1:G:138:ASN:HA   | 1:G:177:LEU:O    | 1.76                     | 0.85              |
| 1:M:134:ARG:HB3  | 1:M:141:THR:HB   | 1.56                     | 0.85              |
| 2:P:58:LEU:H     | 2:P:90:THR:CG2   | 1.90                     | 0.85              |
| 2:P:58:LEU:H     | 2:P:90:THR:HG22  | 1.42                     | 0.85              |
| 1:A:138:ASN:HA   | 1:A:177:LEU:O    | 1.76                     | 0.84              |
| 2:B:92:ARG:HH11  | 2:B:92:ARG:HG3   | 1.40                     | 0.84              |
| 2:J:5:THR:HG22   | 2:J:7:ASN:H      | 1.42                     | 0.84              |
| 1:O:176:LYS:H    | 1:O:176:LYS:HD2  | 1.38                     | 0.84              |
| 2:L:11:ILE:HG23  | 2:L:16:GLY:HA3   | 1.56                     | 0.84              |
| 2:P:196:TYR:CE1  | 2:P:198:SER:HB3  | 2.11                     | 0.84              |
| 1:C:135:ARG:HH12 | 1:C:181:ALA:CB   | 1.89                     | 0.84              |
| 2:D:218:ALA:HB2  | 2:D:266:GLY:C    | 2.02                     | 0.84              |
| 1:E:135:ARG:HH12 | 1:E:181:ALA:CB   | 1.90                     | 0.84              |
| 2:P:5:THR:HG22   | 2:P:7:ASN:H      | 1.43                     | 0.84              |
| 2:H:218:ALA:HB2  | 2:H:266:GLY:C    | 2.02                     | 0.84              |
| 1:K:135:ARG:HH12 | 1:K:181:ALA:CB   | 1.91                     | 0.84              |
| 1:G:135:ARG:HH12 | 1:G:181:ALA:CB   | 1.90                     | 0.84              |
| 1:M:135:ARG:HH12 | 1:M:181:ALA:CB   | 1.90                     | 0.84              |
| 1:I:135:ARG:HH12 | 1:I:181:ALA:CB   | 1.91                     | 0.84              |
| 2:J:196:TYR:CE1  | 2:J:198:SER:HB3  | 2.11                     | 0.84              |
| 2:N:196:TYR:CE1  | 2:N:198:SER:HB3  | 2.11                     | 0.84              |
| 2:H:59:GLN:HG2   | 2:H:132:ARG:HD2  | 1.60                     | 0.83              |
| 2:L:58:LEU:H     | 2:L:90:THR:HG22  | 1.42                     | 0.83              |
| 1:A:135:ARG:HH12 | 1:A:181:ALA:CB   | 1.90                     | 0.83              |
| 2:L:196:TYR:CE1  | 2:L:198:SER:HB3  | 2.11                     | 0.83              |
| 1:C:135:ARG:NH1  | 1:C:181:ALA:HB1  | 1.93                     | 0.83              |
| 2:N:5:THR:HG22   | 2:N:7:ASN:H      | 1.42                     | 0.83              |
| 2:B:218:ALA:HB2  | 2:B:266:GLY:C    | 2.02                     | 0.83              |
| 2:J:58:LEU:H     | 2:J:90:THR:HG22  | 1.41                     | 0.83              |
| 2:N:58:LEU:H     | 2:N:90:THR:CG2   | 1.91                     | 0.83              |
| 2:L:5:THR:HG22   | 2:L:7:ASN:H      | 1.43                     | 0.83              |
| 2:B:59:GLN:HG2   | 2:B:132:ARG:HD2  | 1.60                     | 0.83              |
| 2:L:58:LEU:H     | 2:L:90:THR:CG2   | 1.90                     | 0.83              |
| 1:G:141:THR:OG1  | 1:G:174:THR:HG22 | 1.78                     | 0.82              |
| 2:D:192:ASN:HD22 | 2:D:279:GLN:HE22 | 1.26                     | 0.82              |
| 1:E:47:ARG:NH2   | 1:E:74:GLN:HE21  | 1.76                     | 0.82              |
| 2:F:92:ARG:HG3   | 2:F:92:ARG:HH11  | 1.44                     | 0.82              |
| 2:L:226:THR:HB   | 2:L:231:ILE:HG12 | 1.62                     | 0.82              |
| 1:A:47:ARG:NH2   | 1:A:74:GLN:HE21  | 1.75                     | 0.82              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:92:ARG:HH11  | 2:H:92:ARG:HG3   | 1.42                     | 0.82              |
| 2:N:58:LEU:H     | 2:N:90:THR:HG22  | 1.42                     | 0.82              |
| 2:P:226:THR:HB   | 2:P:231:ILE:HG12 | 1.62                     | 0.82              |
| 2:N:224:GLN:NE2  | 2:N:231:ILE:HG21 | 1.95                     | 0.82              |
| 2:H:192:ASN:HD22 | 2:H:279:GLN:HE22 | 1.27                     | 0.82              |
| 2:F:59:GLN:HG2   | 2:F:132:ARG:HD2  | 1.60                     | 0.82              |
| 1:G:47:ARG:NH2   | 1:G:74:GLN:HE21  | 1.76                     | 0.82              |
| 2:D:53:THR:H     | 2:D:136:ASN:HD21 | 1.27                     | 0.82              |
| 1:I:177:LEU:HD12 | 1:I:178:PRO:HD2  | 1.61                     | 0.81              |
| 2:N:253:THR:HG22 | 2:N:255:ASN:HD21 | 1.45                     | 0.81              |
| 1:O:177:LEU:HD12 | 1:O:178:PRO:HD2  | 1.61                     | 0.81              |
| 2:B:192:ASN:HD22 | 2:B:279:GLN:HE22 | 1.26                     | 0.81              |
| 2:J:253:THR:HG22 | 2:J:255:ASN:HD21 | 1.44                     | 0.81              |
| 2:P:34:LEU:HD12  | 2:P:35:VAL:H     | 1.44                     | 0.81              |
| 2:N:34:LEU:HD12  | 2:N:35:VAL:H     | 1.45                     | 0.81              |
| 2:D:59:GLN:HG2   | 2:D:132:ARG:HD2  | 1.60                     | 0.81              |
| 1:I:8:ARG:NH2    | 1:I:8:ARG:HB3    | 1.95                     | 0.81              |
| 1:M:8:ARG:NH2    | 1:M:8:ARG:HB3    | 1.95                     | 0.81              |
| 1:E:135:ARG:NH1  | 1:E:181:ALA:HB1  | 1.94                     | 0.81              |
| 2:H:53:THR:H     | 2:H:136:ASN:HD21 | 1.27                     | 0.81              |
| 2:P:224:GLN:NE2  | 2:P:231:ILE:HG21 | 1.94                     | 0.81              |
| 2:P:253:THR:HG22 | 2:P:255:ASN:HD21 | 1.45                     | 0.81              |
| 1:A:135:ARG:NH1  | 1:A:181:ALA:HB1  | 1.94                     | 0.81              |
| 2:F:53:THR:H     | 2:F:136:ASN:HD21 | 1.26                     | 0.81              |
| 2:L:253:THR:HG22 | 2:L:255:ASN:HD21 | 1.45                     | 0.81              |
| 1:M:177:LEU:HD12 | 1:M:178:PRO:HD2  | 1.61                     | 0.81              |
| 2:B:53:THR:H     | 2:B:136:ASN:HD21 | 1.26                     | 0.81              |
| 1:G:135:ARG:NH1  | 1:G:181:ALA:HB1  | 1.94                     | 0.81              |
| 1:K:177:LEU:HD12 | 1:K:178:PRO:HD2  | 1.61                     | 0.81              |
| 2:N:208:ILE:HG23 | 2:N:257:ALA:HB1  | 1.63                     | 0.81              |
| 2:L:34:LEU:HD12  | 2:L:35:VAL:H     | 1.45                     | 0.80              |
| 1:M:39:ASN:ND2   | 1:M:43:VAL:HG13  | 1.95                     | 0.80              |
| 1:I:39:ASN:ND2   | 1:I:43:VAL:HG13  | 1.96                     | 0.80              |
| 2:P:208:ILE:HG23 | 2:P:257:ALA:HB1  | 1.64                     | 0.80              |
| 2:J:226:THR:HB   | 2:J:231:ILE:HG12 | 1.62                     | 0.80              |
| 2:L:208:ILE:HG23 | 2:L:257:ALA:HB1  | 1.63                     | 0.80              |
| 1:M:8:ARG:HB3    | 1:M:8:ARG:HH21   | 1.47                     | 0.80              |
| 1:K:39:ASN:ND2   | 1:K:43:VAL:HG13  | 1.96                     | 0.80              |
| 1:O:8:ARG:NH2    | 1:O:8:ARG:HB3    | 1.95                     | 0.80              |
| 1:O:39:ASN:ND2   | 1:O:43:VAL:HG13  | 1.96                     | 0.80              |
| 1:M:32:LEU:HB2   | 1:M:90:ILE:HB    | 1.64                     | 0.80              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:J:208:ILE:HG23 | 2:J:257:ALA:HB1  | 1.64                     | 0.79              |
| 2:J:224:GLN:NE2  | 2:J:231:ILE:HG21 | 1.95                     | 0.79              |
| 1:K:47:ARG:NH2   | 1:K:74:GLN:HE21  | 1.81                     | 0.79              |
| 2:N:226:THR:HB   | 2:N:231:ILE:HG12 | 1.62                     | 0.79              |
| 1:E:47:ARG:HG3   | 1:E:71:THR:HB    | 1.65                     | 0.79              |
| 1:I:47:ARG:NH2   | 1:I:74:GLN:HE21  | 1.81                     | 0.79              |
| 2:J:34:LEU:HD12  | 2:J:35:VAL:H     | 1.45                     | 0.79              |
| 1:K:8:ARG:HB3    | 1:K:8:ARG:NH2    | 1.96                     | 0.79              |
| 2:F:192:ASN:HD22 | 2:F:279:GLN:HE22 | 1.31                     | 0.79              |
| 1:O:47:ARG:NH2   | 1:O:74:GLN:HE21  | 1.81                     | 0.79              |
| 1:K:32:LEU:HB2   | 1:K:90:ILE:HB    | 1.64                     | 0.79              |
| 2:L:224:GLN:NE2  | 2:L:231:ILE:HG21 | 1.95                     | 0.79              |
| 1:C:47:ARG:NH2   | 1:C:74:GLN:HE21  | 1.78                     | 0.79              |
| 2:H:171:THR:C    | 2:H:173:PRO:HD2  | 2.08                     | 0.78              |
| 1:M:38:GLU:HG2   | 1:M:44:LYS:HG3   | 1.65                     | 0.78              |
| 1:G:52:PRO:HG2   | 1:G:55:PHE:CD2   | 2.18                     | 0.78              |
| 1:I:8:ARG:HB3    | 1:I:8:ARG:HH21   | 1.47                     | 0.78              |
| 2:N:21:TYR:HB3   | 2:N:151:ASN:HD21 | 1.49                     | 0.78              |
| 1:O:32:LEU:HB2   | 1:O:90:ILE:HB    | 1.64                     | 0.78              |
| 1:E:188:ARG:HH11 | 1:E:199:LYS:HB2  | 1.49                     | 0.78              |
| 2:F:171:THR:C    | 2:F:173:PRO:HD2  | 2.08                     | 0.78              |
| 1:G:188:ARG:HH11 | 1:G:199:LYS:HB2  | 1.49                     | 0.78              |
| 2:N:59:GLN:HG3   | 2:N:132:ARG:HB2  | 1.66                     | 0.78              |
| 1:O:8:ARG:HB3    | 1:O:8:ARG:HH21   | 1.47                     | 0.78              |
| 1:A:188:ARG:HH11 | 1:A:199:LYS:HB2  | 1.48                     | 0.78              |
| 1:G:47:ARG:HG3   | 1:G:71:THR:HB    | 1.65                     | 0.78              |
| 2:B:171:THR:C    | 2:B:173:PRO:HD2  | 2.08                     | 0.78              |
| 2:D:192:ASN:HD22 | 2:D:279:GLN:NE2  | 1.82                     | 0.78              |
| 1:A:47:ARG:HG3   | 1:A:71:THR:HB    | 1.64                     | 0.77              |
| 1:C:52:PRO:HG2   | 1:C:55:PHE:CD2   | 2.19                     | 0.77              |
| 1:K:38:GLU:HG2   | 1:K:44:LYS:HG3   | 1.65                     | 0.77              |
| 1:C:134:ARG:HD2  | 1:C:141:THR:CG2  | 2.14                     | 0.77              |
| 1:M:47:ARG:NH2   | 1:M:74:GLN:HE21  | 1.81                     | 0.77              |
| 2:N:226:THR:HG23 | 2:N:253:THR:HB   | 1.66                     | 0.77              |
| 1:O:38:GLU:HG2   | 1:O:44:LYS:HG3   | 1.65                     | 0.77              |
| 2:P:226:THR:HG23 | 2:P:253:THR:HB   | 1.67                     | 0.77              |
| 1:C:47:ARG:HG3   | 1:C:71:THR:HB    | 1.65                     | 0.77              |
| 2:J:226:THR:HG23 | 2:J:253:THR:HB   | 1.66                     | 0.77              |
| 2:P:21:TYR:HB3   | 2:P:151:ASN:HD21 | 1.50                     | 0.77              |
| 2:D:172:LEU:O    | 2:D:174:ASP:N    | 2.18                     | 0.77              |
| 1:I:32:LEU:HB2   | 1:I:90:ILE:HB    | 1.64                     | 0.77              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:192:ASN:HD22 | 2:B:279:GLN:NE2  | 1.83                     | 0.77              |
| 2:J:21:TYR:HB3   | 2:J:151:ASN:HD21 | 1.49                     | 0.77              |
| 2:L:226:THR:HG23 | 2:L:253:THR:HB   | 1.67                     | 0.77              |
| 1:C:134:ARG:HD2  | 1:C:141:THR:HG21 | 1.67                     | 0.76              |
| 1:K:8:ARG:HB3    | 1:K:8:ARG:HH21   | 1.47                     | 0.76              |
| 2:L:21:TYR:HB3   | 2:L:151:ASN:HD21 | 1.50                     | 0.76              |
| 2:L:59:GLN:HG3   | 2:L:132:ARG:HB2  | 1.67                     | 0.76              |
| 2:H:172:LEU:O    | 2:H:174:ASP:N    | 2.18                     | 0.76              |
| 2:J:59:GLN:HG3   | 2:J:132:ARG:HB2  | 1.66                     | 0.76              |
| 1:K:52:PRO:HG2   | 1:K:55:PHE:CD2   | 2.20                     | 0.76              |
| 1:O:176:LYS:HD2  | 1:O:176:LYS:N    | 2.00                     | 0.76              |
| 2:B:172:LEU:O    | 2:B:174:ASP:N    | 2.18                     | 0.76              |
| 2:P:59:GLN:HG3   | 2:P:132:ARG:HB2  | 1.67                     | 0.76              |
| 2:P:197:LEU:HD13 | 2:P:225:LEU:HD12 | 1.67                     | 0.76              |
| 1:O:52:PRO:HG2   | 1:O:55:PHE:CD2   | 2.21                     | 0.76              |
| 1:A:32:LEU:HB2   | 1:A:90:ILE:HB    | 1.68                     | 0.76              |
| 1:C:32:LEU:HB2   | 1:C:90:ILE:HB    | 1.67                     | 0.76              |
| 2:F:172:LEU:O    | 2:F:174:ASP:N    | 2.18                     | 0.76              |
| 1:C:188:ARG:HH11 | 1:C:199:LYS:HB2  | 1.49                     | 0.76              |
| 2:D:171:THR:C    | 2:D:173:PRO:HD2  | 2.10                     | 0.75              |
| 1:E:52:PRO:HG2   | 1:E:55:PHE:CD2   | 2.21                     | 0.75              |
| 1:I:52:PRO:HG2   | 1:I:55:PHE:CD2   | 2.20                     | 0.75              |
| 1:G:112:LYS:HG3  | 4:G:209:HOH:O    | 1.86                     | 0.75              |
| 1:A:52:PRO:HG2   | 1:A:55:PHE:CD2   | 2.21                     | 0.75              |
| 1:I:38:GLU:HG2   | 1:I:44:LYS:HG3   | 1.65                     | 0.75              |
| 1:M:52:PRO:HG2   | 1:M:55:PHE:CD2   | 2.21                     | 0.75              |
| 1:A:47:ARG:HH22  | 1:A:74:GLN:NE2   | 1.80                     | 0.75              |
| 2:B:173:PRO:HG3  | 2:B:179:VAL:HG13 | 1.69                     | 0.75              |
| 2:L:197:LEU:HD13 | 2:L:225:LEU:HD12 | 1.68                     | 0.75              |
| 1:O:185:ILE:HB   | 1:O:202:GLY:HA3  | 1.68                     | 0.75              |
| 1:K:176:LYS:HD2  | 1:K:176:LYS:N    | 2.00                     | 0.75              |
| 2:J:197:LEU:HD13 | 2:J:225:LEU:HD12 | 1.67                     | 0.74              |
| 2:P:180:PRO:HA   | 2:P:253:THR:HA   | 1.70                     | 0.74              |
| 1:G:93:MET:HE1   | 1:G:98:LEU:HD23  | 1.69                     | 0.74              |
| 1:I:185:ILE:HB   | 1:I:202:GLY:HA3  | 1.68                     | 0.74              |
| 2:N:197:LEU:HD13 | 2:N:225:LEU:HD12 | 1.68                     | 0.74              |
| 1:G:32:LEU:HB2   | 1:G:90:ILE:HB    | 1.69                     | 0.74              |
| 1:M:185:ILE:HB   | 1:M:202:GLY:HA3  | 1.68                     | 0.74              |
| 2:H:192:ASN:HD22 | 2:H:279:GLN:NE2  | 1.85                     | 0.74              |
| 2:D:173:PRO:HG3  | 2:D:179:VAL:HG13 | 1.69                     | 0.74              |
| 1:C:134:ARG:CB   | 1:C:141:THR:HG22 | 2.15                     | 0.74              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:N:180:PRO:HA   | 2:N:253:THR:HA   | 1.70                     | 0.74              |
| 1:E:32:LEU:HB2   | 1:E:90:ILE:HB    | 1.70                     | 0.74              |
| 1:K:185:ILE:HB   | 1:K:202:GLY:HA3  | 1.68                     | 0.74              |
| 1:E:47:ARG:HH22  | 1:E:74:GLN:NE2   | 1.82                     | 0.73              |
| 2:H:173:PRO:HG3  | 2:H:179:VAL:HG13 | 1.70                     | 0.73              |
| 2:L:180:PRO:HA   | 2:L:253:THR:HA   | 1.70                     | 0.73              |
| 2:L:180:PRO:HB3  | 2:L:253:THR:HG23 | 1.71                     | 0.73              |
| 1:M:176:LYS:HD2  | 1:M:176:LYS:N    | 2.00                     | 0.73              |
| 2:P:180:PRO:HB3  | 2:P:253:THR:HG23 | 1.71                     | 0.73              |
| 1:A:110:ARG:HD3  | 4:A:222:HOH:O    | 1.87                     | 0.73              |
| 1:G:47:ARG:HH22  | 1:G:74:GLN:NE2   | 1.82                     | 0.73              |
| 2:D:29:ASN:HD22  | 2:D:32:GLN:HE22  | 1.37                     | 0.73              |
| 2:D:226:THR:HG23 | 4:D:1618:HOH:O   | 1.88                     | 0.73              |
| 2:L:186:TYR:HB3  | 2:L:247:ALA:HA   | 1.71                     | 0.73              |
| 2:J:180:PRO:HA   | 2:J:253:THR:HA   | 1.70                     | 0.73              |
| 2:N:180:PRO:HB3  | 2:N:253:THR:HG23 | 1.71                     | 0.73              |
| 2:F:29:ASN:HD22  | 2:F:32:GLN:HE22  | 1.36                     | 0.73              |
| 2:H:29:ASN:HD22  | 2:H:32:GLN:HE22  | 1.36                     | 0.73              |
| 2:N:19:ASN:HD21  | 2:P:219:GLN:NE2  | 1.85                     | 0.73              |
| 1:E:93:MET:HE1   | 1:E:98:LEU:HD23  | 1.72                     | 0.72              |
| 2:J:19:ASN:HD21  | 2:L:219:GLN:NE2  | 1.87                     | 0.72              |
| 1:M:111:ILE:HG22 | 2:N:278:TYR:HB2  | 1.72                     | 0.72              |
| 2:F:173:PRO:HG3  | 2:F:179:VAL:HG13 | 1.70                     | 0.72              |
| 2:N:186:TYR:HB3  | 2:N:247:ALA:HA   | 1.71                     | 0.72              |
| 2:D:201:THR:HG21 | 2:D:206:ASN:HD22 | 1.55                     | 0.72              |
| 2:H:29:ASN:HD22  | 2:H:32:GLN:NE2   | 1.88                     | 0.72              |
| 2:H:57:THR:CG2   | 2:H:132:ARG:HB3  | 2.19                     | 0.72              |
| 2:J:180:PRO:HB3  | 2:J:253:THR:HG23 | 1.72                     | 0.72              |
| 2:B:29:ASN:HD22  | 2:B:32:GLN:HE22  | 1.37                     | 0.72              |
| 1:M:101:ASN:HD22 | 2:N:268:VAL:HG23 | 1.55                     | 0.72              |
| 1:A:112:LYS:HG3  | 4:A:208:HOH:O    | 1.90                     | 0.72              |
| 1:C:93:MET:HE1   | 1:C:98:LEU:HD23  | 1.71                     | 0.72              |
| 1:C:141:THR:HB   | 1:C:174:THR:HG23 | 1.72                     | 0.72              |
| 1:A:93:MET:HE1   | 1:A:98:LEU:HD23  | 1.71                     | 0.71              |
| 1:I:176:LYS:HD2  | 1:I:176:LYS:N    | 2.00                     | 0.71              |
| 2:P:186:TYR:HB3  | 2:P:247:ALA:HA   | 1.71                     | 0.71              |
| 1:O:101:ASN:HD22 | 2:P:268:VAL:HG23 | 1.56                     | 0.71              |
| 2:F:29:ASN:HD22  | 2:F:32:GLN:NE2   | 1.87                     | 0.71              |
| 1:O:111:ILE:HG22 | 2:P:278:TYR:HB2  | 1.72                     | 0.71              |
| 2:F:192:ASN:HD22 | 2:F:279:GLN:NE2  | 1.87                     | 0.71              |
| 1:C:141:THR:HG23 | 1:C:141:THR:O    | 1.90                     | 0.71              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:201:THR:HG21 | 2:F:206:ASN:HD22 | 1.54                     | 0.71              |
| 2:H:84:PHE:HA    | 2:H:85:PRO:C     | 2.15                     | 0.71              |
| 2:J:186:TYR:HB3  | 2:J:247:ALA:HA   | 1.71                     | 0.71              |
| 2:D:29:ASN:HD22  | 2:D:32:GLN:NE2   | 1.89                     | 0.71              |
| 2:H:262:GLN:HA   | 2:H:262:GLN:HE21 | 1.56                     | 0.71              |
| 2:B:201:THR:HG21 | 2:B:206:ASN:HD22 | 1.56                     | 0.71              |
| 1:C:47:ARG:HH22  | 1:C:74:GLN:NE2   | 1.83                     | 0.71              |
| 2:D:32:GLN:O     | 2:D:110:THR:HG23 | 1.91                     | 0.71              |
| 2:F:57:THR:CG2   | 2:F:132:ARG:HB3  | 2.21                     | 0.71              |
| 1:I:111:ILE:HG22 | 2:J:278:TYR:HB2  | 1.72                     | 0.71              |
| 2:J:48:TYR:HB2   | 2:J:52:ILE:HD12  | 1.73                     | 0.71              |
| 2:B:29:ASN:HD22  | 2:B:32:GLN:NE2   | 1.89                     | 0.71              |
| 2:H:32:GLN:O     | 2:H:110:THR:HG23 | 1.90                     | 0.70              |
| 2:P:155:VAL:HG12 | 2:P:157:PRO:HD3  | 1.73                     | 0.70              |
| 2:D:173:PRO:HB2  | 2:D:177:GLY:HA3  | 1.73                     | 0.70              |
| 1:G:24:ASN:HB2   | 1:G:57:MET:HE3   | 1.74                     | 0.70              |
| 2:B:32:GLN:O     | 2:B:110:THR:HG23 | 1.91                     | 0.70              |
| 2:N:155:VAL:HG12 | 2:N:157:PRO:HD3  | 1.73                     | 0.70              |
| 1:K:101:ASN:HD22 | 2:L:268:VAL:HG23 | 1.56                     | 0.70              |
| 1:K:111:ILE:HG22 | 2:L:278:TYR:HB2  | 1.72                     | 0.70              |
| 1:I:101:ASN:HD22 | 2:J:268:VAL:HG23 | 1.56                     | 0.70              |
| 1:E:1:GLY:H1     | 1:E:26:ASP:CG    | 1.99                     | 0.70              |
| 1:M:12:PRO:HB2   | 1:M:15:GLN:HG2   | 1.73                     | 0.70              |
| 2:H:201:THR:HG21 | 2:H:206:ASN:HD22 | 1.55                     | 0.70              |
| 2:L:164:SER:HB2  | 2:L:184:THR:HG23 | 1.74                     | 0.70              |
| 2:B:262:GLN:HE21 | 2:B:262:GLN:HA   | 1.56                     | 0.70              |
| 1:M:182:GLY:O    | 1:M:183:SER:HB2  | 1.92                     | 0.70              |
| 2:P:48:TYR:HB2   | 2:P:52:ILE:HD12  | 1.74                     | 0.70              |
| 2:F:32:GLN:O     | 2:F:110:THR:HG23 | 1.91                     | 0.69              |
| 2:F:262:GLN:HA   | 2:F:262:GLN:HE21 | 1.56                     | 0.69              |
| 2:N:48:TYR:HB2   | 2:N:52:ILE:HD12  | 1.74                     | 0.69              |
| 2:D:57:THR:CG2   | 2:D:132:ARG:HB3  | 2.22                     | 0.69              |
| 1:E:12:PRO:HG2   | 1:E:15:GLN:HE21  | 1.57                     | 0.69              |
| 1:I:12:PRO:HB2   | 1:I:15:GLN:HG2   | 1.73                     | 0.69              |
| 2:B:81:SER:O     | 2:P:114:SER:HB2  | 1.92                     | 0.69              |
| 2:B:173:PRO:HB2  | 2:B:177:GLY:HA3  | 1.74                     | 0.69              |
| 2:D:84:PHE:HA    | 2:D:85:PRO:C     | 2.17                     | 0.69              |
| 2:F:167:ASP:CG   | 2:F:168:VAL:N    | 2.50                     | 0.69              |
| 2:N:164:SER:HB2  | 2:N:184:THR:HG23 | 1.75                     | 0.69              |
| 2:H:58:LEU:H     | 2:H:90:THR:HG22  | 1.57                     | 0.69              |
| 2:J:38:LEU:C     | 2:J:40:THR:H     | 2.00                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:J:84:PHE:HA    | 2:J:85:PRO:C     | 2.18                     | 0.69              |
| 1:K:12:PRO:HB2   | 1:K:15:GLN:HG2   | 1.73                     | 0.69              |
| 1:K:162:LEU:HD21 | 1:K:178:PRO:HD3  | 1.75                     | 0.69              |
| 1:O:12:PRO:HB2   | 1:O:15:GLN:HG2   | 1.73                     | 0.69              |
| 1:O:162:LEU:HD21 | 1:O:178:PRO:HD3  | 1.75                     | 0.69              |
| 1:A:24:ASN:HB2   | 1:A:57:MET:HE3   | 1.74                     | 0.69              |
| 2:F:172:LEU:N    | 2:F:173:PRO:HD2  | 2.07                     | 0.69              |
| 1:G:25:ASN:O     | 1:G:60:LYS:HG2   | 1.93                     | 0.69              |
| 1:I:162:LEU:HD21 | 1:I:178:PRO:HD3  | 1.75                     | 0.69              |
| 2:D:262:GLN:HE21 | 2:D:262:GLN:HA   | 1.57                     | 0.69              |
| 2:L:38:LEU:C     | 2:L:40:THR:H     | 2.01                     | 0.69              |
| 2:L:48:TYR:HB2   | 2:L:52:ILE:HD12  | 1.73                     | 0.69              |
| 2:P:38:LEU:C     | 2:P:40:THR:H     | 2.01                     | 0.69              |
| 1:C:25:ASN:O     | 1:C:60:LYS:HG2   | 1.93                     | 0.69              |
| 2:D:172:LEU:N    | 2:D:173:PRO:HD2  | 2.08                     | 0.69              |
| 1:E:24:ASN:HB2   | 1:E:57:MET:HE3   | 1.74                     | 0.69              |
| 1:E:112:LYS:HG3  | 4:F:1506:HOH:O   | 1.92                     | 0.69              |
| 2:F:84:PHE:HA    | 2:F:85:PRO:C     | 2.17                     | 0.69              |
| 2:H:172:LEU:N    | 2:H:173:PRO:HD2  | 2.06                     | 0.69              |
| 2:H:173:PRO:HB2  | 2:H:177:GLY:HA3  | 1.74                     | 0.69              |
| 1:I:182:GLY:O    | 1:I:183:SER:HB2  | 1.93                     | 0.69              |
| 2:J:155:VAL:HG12 | 2:J:157:PRO:HD3  | 1.73                     | 0.69              |
| 2:L:155:VAL:HG12 | 2:L:157:PRO:HD3  | 1.73                     | 0.69              |
| 1:C:141:THR:CB   | 1:C:174:THR:HG23 | 2.22                     | 0.69              |
| 2:J:264:THR:HG22 | 2:J:265:ALA:N    | 2.08                     | 0.69              |
| 2:B:84:PHE:HA    | 2:B:85:PRO:C     | 2.16                     | 0.69              |
| 1:C:12:PRO:HB2   | 1:C:15:GLN:CG    | 2.23                     | 0.69              |
| 1:I:82:LEU:HD13  | 1:I:114:TYR:CE2  | 2.28                     | 0.69              |
| 1:O:88:LYS:HE2   | 1:O:90:ILE:HG12  | 1.75                     | 0.69              |
| 2:P:164:SER:HB2  | 2:P:184:THR:HG23 | 1.75                     | 0.69              |
| 1:A:12:PRO:HB2   | 1:A:15:GLN:CG    | 2.22                     | 0.68              |
| 2:J:164:SER:HB2  | 2:J:184:THR:HG23 | 1.74                     | 0.68              |
| 2:L:264:THR:HG22 | 2:L:265:ALA:N    | 2.08                     | 0.68              |
| 1:M:88:LYS:HE2   | 1:M:90:ILE:HG12  | 1.75                     | 0.68              |
| 1:M:162:LEU:HD21 | 1:M:178:PRO:HD3  | 1.75                     | 0.68              |
| 2:B:172:LEU:N    | 2:B:173:PRO:HD2  | 2.07                     | 0.68              |
| 1:C:112:LYS:HG3  | 4:D:1605:HOH:O   | 1.94                     | 0.68              |
| 1:C:182:GLY:O    | 1:C:183:SER:HB2  | 1.92                     | 0.68              |
| 2:F:218:ALA:HB2  | 2:F:266:GLY:O    | 1.93                     | 0.68              |
| 2:H:81:SER:O     | 2:L:114:SER:HB2  | 1.93                     | 0.68              |
| 1:A:12:PRO:HG2   | 1:A:15:GLN:HE21  | 1.58                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:182:GLY:O    | 1:A:183:SER:HB2  | 1.92                     | 0.68              |
| 1:G:182:GLY:O    | 1:G:183:SER:HB2  | 1.93                     | 0.68              |
| 2:B:57:THR:CG2   | 2:B:132:ARG:HB3  | 2.24                     | 0.68              |
| 1:E:86:ASN:HD21  | 1:E:110:ARG:HE   | 1.42                     | 0.68              |
| 1:G:86:ASN:HD21  | 1:G:110:ARG:HE   | 1.41                     | 0.68              |
| 1:M:82:LEU:HD13  | 1:M:114:TYR:CE2  | 2.28                     | 0.68              |
| 1:O:82:LEU:HD13  | 1:O:114:TYR:CE2  | 2.28                     | 0.68              |
| 1:C:24:ASN:HB2   | 1:C:57:MET:HE3   | 1.75                     | 0.68              |
| 1:G:12:PRO:HG2   | 1:G:15:GLN:HE21  | 1.59                     | 0.68              |
| 2:H:53:THR:HB    | 2:H:136:ASN:OD1  | 1.93                     | 0.68              |
| 2:L:84:PHE:HA    | 2:L:85:PRO:C     | 2.18                     | 0.68              |
| 2:B:218:ALA:HB2  | 2:B:266:GLY:O    | 1.94                     | 0.68              |
| 1:G:27:GLU:HG3   | 1:G:60:LYS:HD2   | 1.74                     | 0.68              |
| 1:O:135:ARG:NH1  | 1:O:181:ALA:CB   | 2.53                     | 0.68              |
| 1:E:182:GLY:O    | 1:E:183:SER:HB2  | 1.93                     | 0.68              |
| 2:F:173:PRO:HB2  | 2:F:177:GLY:HA3  | 1.74                     | 0.68              |
| 1:K:79:ARG:HB3   | 1:K:170:MET:CE   | 2.24                     | 0.68              |
| 2:B:116:GLY:HA2  | 2:B:189:LYS:HE2  | 1.76                     | 0.68              |
| 1:K:135:ARG:NH1  | 1:K:181:ALA:CB   | 2.53                     | 0.68              |
| 1:M:138:ASN:HA   | 1:M:177:LEU:O    | 1.94                     | 0.68              |
| 2:N:84:PHE:HA    | 2:N:85:PRO:C     | 2.18                     | 0.68              |
| 2:P:84:PHE:HA    | 2:P:85:PRO:C     | 2.17                     | 0.68              |
| 1:A:25:ASN:O     | 1:A:60:LYS:HG2   | 1.93                     | 0.68              |
| 1:C:12:PRO:HG2   | 1:C:15:GLN:HE21  | 1.59                     | 0.68              |
| 1:K:82:LEU:HD13  | 1:K:114:TYR:CE2  | 2.29                     | 0.68              |
| 2:D:53:THR:HB    | 2:D:136:ASN:OD1  | 1.94                     | 0.67              |
| 1:G:12:PRO:HB2   | 1:G:15:GLN:CG    | 2.24                     | 0.67              |
| 1:I:79:ARG:HB3   | 1:I:170:MET:CE   | 2.24                     | 0.67              |
| 1:K:88:LYS:HE2   | 1:K:90:ILE:HG12  | 1.76                     | 0.67              |
| 1:O:79:ARG:HB3   | 1:O:170:MET:CE   | 2.23                     | 0.67              |
| 1:A:86:ASN:HD21  | 1:A:110:ARG:HE   | 1.42                     | 0.67              |
| 1:A:144:ASN:ND2  | 1:A:150:LEU:HG   | 2.10                     | 0.67              |
| 2:B:53:THR:H     | 2:B:136:ASN:ND2  | 1.92                     | 0.67              |
| 2:B:167:ASP:CG   | 2:B:168:VAL:N    | 2.50                     | 0.67              |
| 2:H:167:ASP:CG   | 2:H:168:VAL:N    | 2.50                     | 0.67              |
| 1:K:138:ASN:HA   | 1:K:177:LEU:O    | 1.94                     | 0.67              |
| 2:N:38:LEU:C     | 2:N:40:THR:H     | 2.01                     | 0.67              |
| 2:F:58:LEU:H     | 2:F:90:THR:HG22  | 1.59                     | 0.67              |
| 1:I:138:ASN:HA   | 1:I:177:LEU:O    | 1.94                     | 0.67              |
| 1:K:182:GLY:O    | 1:K:183:SER:HB2  | 1.93                     | 0.67              |
| 2:N:105:VAL:HG11 | 2:N:129:LEU:HD13 | 1.77                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:58:LEU:H     | 2:B:90:THR:HG22  | 1.58                     | 0.67              |
| 2:D:218:ALA:HB2  | 2:D:266:GLY:O    | 1.93                     | 0.67              |
| 1:E:25:ASN:O     | 1:E:60:LYS:HG2   | 1.93                     | 0.67              |
| 2:P:24:LEU:HD22  | 2:P:36:VAL:HG22  | 1.77                     | 0.67              |
| 2:B:217:PRO:O    | 2:B:219:GLN:N    | 2.28                     | 0.67              |
| 2:B:226:THR:HG23 | 4:B:1508:HOH:O   | 1.94                     | 0.67              |
| 2:D:221:VAL:O    | 2:D:259:THR:HG23 | 1.95                     | 0.67              |
| 1:G:188:ARG:NH1  | 1:G:199:LYS:H    | 1.92                     | 0.67              |
| 2:J:186:TYR:HB2  | 2:J:244:GLY:O    | 1.95                     | 0.67              |
| 1:O:12:PRO:HB2   | 1:O:15:GLN:CG    | 2.25                     | 0.67              |
| 1:O:138:ASN:HA   | 1:O:177:LEU:O    | 1.94                     | 0.67              |
| 2:B:53:THR:HB    | 2:B:136:ASN:OD1  | 1.94                     | 0.67              |
| 1:K:79:ARG:HB3   | 1:K:170:MET:HE3  | 1.77                     | 0.67              |
| 2:N:219:GLN:OE1  | 2:N:262:GLN:HG2  | 1.95                     | 0.67              |
| 1:C:86:ASN:HD21  | 1:C:110:ARG:HE   | 1.42                     | 0.67              |
| 2:D:53:THR:H     | 2:D:136:ASN:ND2  | 1.93                     | 0.67              |
| 2:D:116:GLY:HA2  | 2:D:189:LYS:HE2  | 1.77                     | 0.67              |
| 1:E:27:GLU:HG3   | 1:E:60:LYS:HD2   | 1.74                     | 0.67              |
| 2:H:211:ASN:HD22 | 2:H:212:THR:N    | 1.92                     | 0.67              |
| 1:O:182:GLY:O    | 1:O:183:SER:HB2  | 1.93                     | 0.67              |
| 1:A:12:PRO:HB2   | 1:A:15:GLN:HG3   | 1.77                     | 0.67              |
| 2:H:218:ALA:HB2  | 2:H:266:GLY:O    | 1.93                     | 0.67              |
| 1:A:188:ARG:NH1  | 1:A:199:LYS:H    | 1.93                     | 0.67              |
| 1:C:188:ARG:NH1  | 1:C:199:LYS:H    | 1.92                     | 0.67              |
| 1:I:88:LYS:HE2   | 1:I:90:ILE:HG12  | 1.75                     | 0.67              |
| 1:M:79:ARG:HB3   | 1:M:170:MET:CE   | 2.24                     | 0.67              |
| 1:A:27:GLU:HG3   | 1:A:60:LYS:HD2   | 1.76                     | 0.66              |
| 1:C:27:GLU:HG3   | 1:C:60:LYS:HD2   | 1.75                     | 0.66              |
| 1:M:135:ARG:CZ   | 1:M:181:ALA:HB1  | 2.25                     | 0.66              |
| 2:N:24:LEU:HD22  | 2:N:36:VAL:HG22  | 1.77                     | 0.66              |
| 1:C:12:PRO:HB2   | 1:C:15:GLN:HG3   | 1.77                     | 0.66              |
| 1:E:188:ARG:NH1  | 1:E:199:LYS:H    | 1.94                     | 0.66              |
| 2:N:186:TYR:HB2  | 2:N:244:GLY:O    | 1.95                     | 0.66              |
| 2:P:219:GLN:OE1  | 2:P:262:GLN:HG2  | 1.95                     | 0.66              |
| 2:H:217:PRO:O    | 2:H:219:GLN:N    | 2.28                     | 0.66              |
| 1:I:135:ARG:CZ   | 1:I:181:ALA:HB1  | 2.25                     | 0.66              |
| 1:M:126:GLN:HA   | 1:M:129:GLU:OE1  | 1.96                     | 0.66              |
| 1:O:79:ARG:HB3   | 1:O:170:MET:HE3  | 1.77                     | 0.66              |
| 2:P:264:THR:HG22 | 2:P:265:ALA:N    | 2.07                     | 0.66              |
| 1:C:110:ARG:HD3  | 4:C:223:HOH:O    | 1.95                     | 0.66              |
| 1:C:122:LEU:HD11 | 1:C:126:GLN:O    | 1.95                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:77:TYR:CD2   | 2:H:90:THR:HG21  | 2.30                     | 0.66              |
| 1:M:12:PRO:HB2   | 1:M:15:GLN:CG    | 2.25                     | 0.66              |
| 2:L:219:GLN:OE1  | 2:L:262:GLN:HG2  | 1.94                     | 0.66              |
| 2:N:264:THR:HG22 | 2:N:265:ALA:N    | 2.08                     | 0.66              |
| 2:P:186:TYR:HB2  | 2:P:244:GLY:O    | 1.96                     | 0.66              |
| 2:D:217:PRO:O    | 2:D:219:GLN:N    | 2.29                     | 0.66              |
| 2:F:211:ASN:HD22 | 2:F:212:THR:N    | 1.93                     | 0.66              |
| 1:I:102:THR:O    | 2:J:269:GLN:HA   | 1.96                     | 0.66              |
| 2:L:24:LEU:HD22  | 2:L:36:VAL:HG22  | 1.76                     | 0.66              |
| 1:O:135:ARG:CZ   | 1:O:181:ALA:HB1  | 2.25                     | 0.66              |
| 2:B:221:VAL:O    | 2:B:259:THR:HG23 | 1.96                     | 0.66              |
| 1:I:10:ILE:O     | 1:I:12:PRO:HD3   | 1.96                     | 0.66              |
| 2:J:219:GLN:OE1  | 2:J:262:GLN:HG2  | 1.94                     | 0.66              |
| 1:K:103:LEU:HD12 | 2:L:270:SER:O    | 1.96                     | 0.66              |
| 2:F:116:GLY:HA2  | 2:F:189:LYS:HE2  | 1.77                     | 0.66              |
| 1:C:144:ASN:ND2  | 1:C:150:LEU:HG   | 2.10                     | 0.66              |
| 2:D:77:TYR:CD2   | 2:D:90:THR:HG21  | 2.30                     | 0.66              |
| 1:I:12:PRO:HB2   | 1:I:15:GLN:CG    | 2.25                     | 0.66              |
| 1:I:79:ARG:HB3   | 1:I:170:MET:HE3  | 1.77                     | 0.66              |
| 1:K:126:GLN:HA   | 1:K:129:GLU:OE1  | 1.95                     | 0.66              |
| 1:M:135:ARG:NH1  | 1:M:181:ALA:CB   | 2.53                     | 0.66              |
| 2:L:43:PHE:CD2   | 2:L:102:PRO:HB3  | 2.31                     | 0.66              |
| 2:D:58:LEU:H     | 2:D:90:THR:HG22  | 1.60                     | 0.65              |
| 2:H:53:THR:H     | 2:H:136:ASN:ND2  | 1.94                     | 0.65              |
| 2:N:43:PHE:CD2   | 2:N:102:PRO:HB3  | 2.31                     | 0.65              |
| 1:A:122:LEU:HD11 | 1:A:126:GLN:O    | 1.96                     | 0.65              |
| 1:G:12:PRO:HB2   | 1:G:15:GLN:HG3   | 1.78                     | 0.65              |
| 1:I:103:LEU:HD12 | 2:J:270:SER:O    | 1.96                     | 0.65              |
| 1:M:102:THR:O    | 2:N:269:GLN:HA   | 1.96                     | 0.65              |
| 2:P:43:PHE:CD2   | 2:P:102:PRO:HB3  | 2.31                     | 0.65              |
| 2:J:24:LEU:HD22  | 2:J:36:VAL:HG22  | 1.77                     | 0.65              |
| 1:O:126:GLN:HA   | 1:O:129:GLU:OE1  | 1.96                     | 0.65              |
| 1:K:12:PRO:HB2   | 1:K:15:GLN:CG    | 2.25                     | 0.65              |
| 1:K:135:ARG:CZ   | 1:K:181:ALA:HB1  | 2.25                     | 0.65              |
| 1:O:10:ILE:O     | 1:O:12:PRO:HD3   | 1.96                     | 0.65              |
| 1:I:126:GLN:HA   | 1:I:129:GLU:OE1  | 1.95                     | 0.65              |
| 2:L:116:GLY:HA3  | 2:L:189:LYS:HG3  | 1.79                     | 0.65              |
| 2:B:77:TYR:CD2   | 2:B:90:THR:HG21  | 2.31                     | 0.65              |
| 2:F:53:THR:HB    | 2:F:136:ASN:OD1  | 1.95                     | 0.65              |
| 1:G:73:ASN:HA    | 4:G:222:HOH:O    | 1.97                     | 0.65              |
| 1:G:144:ASN:ND2  | 1:G:150:LEU:HG   | 2.12                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:122:LEU:HD11 | 1:E:126:GLN:O    | 1.97                     | 0.65              |
| 2:F:53:THR:H     | 2:F:136:ASN:ND2  | 1.93                     | 0.65              |
| 2:L:105:VAL:HG11 | 2:L:129:LEU:HD13 | 1.77                     | 0.65              |
| 2:N:116:GLY:HA3  | 2:N:189:LYS:HG3  | 1.79                     | 0.65              |
| 1:O:102:THR:O    | 2:P:269:GLN:HA   | 1.96                     | 0.65              |
| 2:B:211:ASN:HD22 | 2:B:212:THR:N    | 1.94                     | 0.65              |
| 2:F:217:PRO:O    | 2:F:219:GLN:N    | 2.30                     | 0.65              |
| 1:G:122:LEU:HD11 | 1:G:126:GLN:O    | 1.96                     | 0.65              |
| 2:J:105:VAL:HG11 | 2:J:129:LEU:HD13 | 1.77                     | 0.65              |
| 1:E:12:PRO:HB2   | 1:E:15:GLN:CG    | 2.26                     | 0.65              |
| 1:E:144:ASN:ND2  | 1:E:150:LEU:HG   | 2.11                     | 0.65              |
| 2:F:221:VAL:O    | 2:F:259:THR:HG23 | 1.96                     | 0.65              |
| 2:L:186:TYR:HB2  | 2:L:244:GLY:O    | 1.95                     | 0.65              |
| 1:M:103:LEU:HD12 | 2:N:270:SER:O    | 1.96                     | 0.65              |
| 1:O:103:LEU:HD12 | 2:P:270:SER:O    | 1.96                     | 0.65              |
| 2:J:58:LEU:N     | 2:J:90:THR:HG22  | 2.12                     | 0.65              |
| 1:K:10:ILE:O     | 1:K:12:PRO:HD3   | 1.96                     | 0.65              |
| 1:K:102:THR:O    | 2:L:269:GLN:HA   | 1.96                     | 0.65              |
| 2:B:90:THR:HG23  | 2:B:91:PRO:O     | 1.96                     | 0.64              |
| 2:P:95:TYR:OH    | 2:P:103:TRP:HA   | 1.97                     | 0.64              |
| 2:P:105:VAL:HG11 | 2:P:129:LEU:HD13 | 1.78                     | 0.64              |
| 2:F:77:TYR:CD2   | 2:F:90:THR:HG21  | 2.31                     | 0.64              |
| 2:P:116:GLY:HA3  | 2:P:189:LYS:HG3  | 1.79                     | 0.64              |
| 2:D:90:THR:HG23  | 2:D:91:PRO:O     | 1.97                     | 0.64              |
| 2:D:211:ASN:HD22 | 2:D:212:THR:N    | 1.94                     | 0.64              |
| 2:J:43:PHE:CD2   | 2:J:102:PRO:HB3  | 2.32                     | 0.64              |
| 2:J:116:GLY:HA3  | 2:J:189:LYS:HG3  | 1.79                     | 0.64              |
| 1:M:10:ILE:O     | 1:M:12:PRO:HD3   | 1.96                     | 0.64              |
| 2:B:192:ASN:ND2  | 2:B:279:GLN:HE22 | 1.95                     | 0.64              |
| 2:H:221:VAL:O    | 2:H:259:THR:HG23 | 1.97                     | 0.64              |
| 2:J:43:PHE:HA    | 2:J:102:PRO:HA   | 1.80                     | 0.64              |
| 2:P:58:LEU:N     | 2:P:90:THR:HG22  | 2.12                     | 0.64              |
| 2:H:116:GLY:HA2  | 2:H:189:LYS:HE2  | 1.79                     | 0.64              |
| 2:J:95:TYR:OH    | 2:J:103:TRP:HA   | 1.97                     | 0.64              |
| 1:M:27:GLU:HA    | 1:M:60:LYS:HG3   | 1.79                     | 0.64              |
| 1:C:134:ARG:CD   | 1:C:141:THR:HG21 | 2.28                     | 0.64              |
| 1:M:79:ARG:HB3   | 1:M:170:MET:HE3  | 1.78                     | 0.64              |
| 1:O:24:ASN:HB2   | 1:O:57:MET:HE3   | 1.80                     | 0.64              |
| 2:L:43:PHE:HA    | 2:L:102:PRO:HA   | 1.79                     | 0.64              |
| 2:N:95:TYR:OH    | 2:N:103:TRP:HA   | 1.97                     | 0.64              |
| 1:A:97:LYS:HE3   | 4:B:1573:HOH:O   | 1.96                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:102:THR:CA   | 2:F:171:THR:HG22 | 2.28                     | 0.64              |
| 2:N:43:PHE:HA    | 2:N:102:PRO:HA   | 1.80                     | 0.64              |
| 1:O:156:ASN:C    | 1:O:158:GLY:H    | 2.06                     | 0.64              |
| 1:I:156:ASN:C    | 1:I:158:GLY:H    | 2.07                     | 0.63              |
| 2:L:67:VAL:HG13  | 2:L:109:LEU:HD13 | 1.80                     | 0.63              |
| 1:A:156:ASN:HB2  | 1:A:186:THR:OG1  | 1.99                     | 0.63              |
| 1:G:102:THR:CA   | 2:H:171:THR:HG22 | 2.28                     | 0.63              |
| 1:K:27:GLU:HA    | 1:K:60:LYS:HG3   | 1.80                     | 0.63              |
| 2:L:95:TYR:OH    | 2:L:103:TRP:HA   | 1.98                     | 0.63              |
| 1:M:4:LEU:HD21   | 1:M:87:VAL:HG21  | 1.80                     | 0.63              |
| 1:O:135:ARG:NH1  | 1:O:177:LEU:HD11 | 2.13                     | 0.63              |
| 1:M:24:ASN:HB2   | 1:M:57:MET:HE3   | 1.81                     | 0.63              |
| 2:N:67:VAL:HG13  | 2:N:109:LEU:HD13 | 1.79                     | 0.63              |
| 1:C:102:THR:CA   | 2:D:171:THR:HG22 | 2.27                     | 0.63              |
| 2:D:92:ARG:HG3   | 2:D:92:ARG:NH1   | 2.10                     | 0.63              |
| 1:M:162:LEU:HD21 | 1:M:178:PRO:CD   | 2.29                     | 0.63              |
| 2:B:92:ARG:HG3   | 2:B:92:ARG:NH1   | 2.09                     | 0.63              |
| 1:G:140:LEU:HD23 | 1:G:141:THR:N    | 2.14                     | 0.63              |
| 1:I:24:ASN:HB2   | 1:I:57:MET:HE3   | 1.80                     | 0.63              |
| 2:N:58:LEU:N     | 2:N:90:THR:HG22  | 2.13                     | 0.63              |
| 1:A:138:ASN:C    | 1:A:177:LEU:HB3  | 2.24                     | 0.63              |
| 1:G:104:GLN:HG3  | 2:H:168:VAL:HG23 | 1.81                     | 0.63              |
| 1:K:135:ARG:NH1  | 1:K:177:LEU:HD11 | 2.13                     | 0.63              |
| 2:L:58:LEU:N     | 2:L:90:THR:HG22  | 2.13                     | 0.63              |
| 1:C:11:TYR:HB2   | 1:C:113:LEU:HD11 | 1.81                     | 0.63              |
| 1:C:134:ARG:CZ   | 1:C:141:THR:HG21 | 2.29                     | 0.63              |
| 1:M:27:GLU:CG    | 1:M:60:LYS:HD2   | 2.29                     | 0.63              |
| 1:O:4:LEU:HD21   | 1:O:87:VAL:HG21  | 1.81                     | 0.63              |
| 1:A:102:THR:CA   | 2:B:171:THR:HG22 | 2.28                     | 0.63              |
| 2:F:67:VAL:HG23  | 2:F:126:ILE:HG12 | 1.81                     | 0.63              |
| 1:G:94:ASP:HB3   | 1:G:96:SER:OG    | 1.98                     | 0.63              |
| 2:J:32:GLN:O     | 2:J:110:THR:HG23 | 1.99                     | 0.63              |
| 1:O:162:LEU:HD21 | 1:O:178:PRO:CD   | 2.29                     | 0.63              |
| 1:C:138:ASN:C    | 1:C:177:LEU:HB3  | 2.24                     | 0.62              |
| 2:H:90:THR:HG23  | 2:H:91:PRO:O     | 1.98                     | 0.62              |
| 1:I:4:LEU:HD21   | 1:I:87:VAL:HG21  | 1.80                     | 0.62              |
| 1:I:27:GLU:HA    | 1:I:60:LYS:HG3   | 1.80                     | 0.62              |
| 1:M:135:ARG:NH1  | 1:M:177:LEU:HD11 | 2.13                     | 0.62              |
| 1:O:27:GLU:HA    | 1:O:60:LYS:HG3   | 1.80                     | 0.62              |
| 1:A:140:LEU:HD23 | 1:A:141:THR:N    | 2.14                     | 0.62              |
| 2:P:32:GLN:O     | 2:P:110:THR:HG23 | 1.99                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:185:ILE:HB   | 1:A:202:GLY:HA3  | 1.82                     | 0.62              |
| 1:C:140:LEU:HD23 | 1:C:141:THR:N    | 2.15                     | 0.62              |
| 1:C:185:ILE:HB   | 1:C:202:GLY:HA3  | 1.81                     | 0.62              |
| 2:D:192:ASN:ND2  | 2:D:279:GLN:HE22 | 1.94                     | 0.62              |
| 1:E:12:PRO:HB2   | 1:E:15:GLN:HG3   | 1.82                     | 0.62              |
| 1:E:138:ASN:C    | 1:E:177:LEU:HB3  | 2.24                     | 0.62              |
| 1:G:185:ILE:HB   | 1:G:202:GLY:HA3  | 1.81                     | 0.62              |
| 1:I:135:ARG:NH1  | 1:I:177:LEU:HD11 | 2.13                     | 0.62              |
| 2:D:172:LEU:O    | 2:D:172:LEU:HD23 | 1.99                     | 0.62              |
| 2:J:20:VAL:HG21  | 2:J:42:ILE:HD11  | 1.81                     | 0.62              |
| 2:N:59:GLN:CG    | 2:N:132:ARG:HB2  | 2.28                     | 0.62              |
| 2:N:184:THR:HA   | 2:N:249:SER:HA   | 1.81                     | 0.62              |
| 2:B:59:GLN:CG    | 2:B:132:ARG:HD2  | 2.30                     | 0.62              |
| 1:E:156:ASN:HB2  | 1:E:186:THR:OG1  | 2.00                     | 0.62              |
| 1:G:156:ASN:HB2  | 1:G:186:THR:OG1  | 2.00                     | 0.62              |
| 1:G:191:ASN:HD21 | 1:G:195:ALA:HB3  | 1.64                     | 0.62              |
| 1:K:24:ASN:HB2   | 1:K:57:MET:HE3   | 1.80                     | 0.62              |
| 1:K:156:ASN:C    | 1:K:158:GLY:H    | 2.07                     | 0.62              |
| 2:N:32:GLN:O     | 2:N:110:THR:HG23 | 2.00                     | 0.62              |
| 2:P:43:PHE:HA    | 2:P:102:PRO:HA   | 1.79                     | 0.62              |
| 2:P:59:GLN:CG    | 2:P:132:ARG:HB2  | 2.29                     | 0.62              |
| 1:A:94:ASP:HB3   | 1:A:96:SER:OG    | 2.00                     | 0.62              |
| 1:C:94:ASP:HB3   | 1:C:96:SER:OG    | 1.99                     | 0.62              |
| 2:F:90:THR:HG23  | 2:F:91:PRO:O     | 1.98                     | 0.62              |
| 2:J:59:GLN:CG    | 2:J:132:ARG:HB2  | 2.29                     | 0.62              |
| 1:K:162:LEU:HD21 | 1:K:178:PRO:CD   | 2.29                     | 0.62              |
| 2:P:67:VAL:HG13  | 2:P:109:LEU:HD13 | 1.80                     | 0.62              |
| 2:B:170:VAL:CG1  | 2:B:172:LEU:HB2  | 2.27                     | 0.62              |
| 1:C:156:ASN:HB2  | 1:C:186:THR:OG1  | 2.00                     | 0.62              |
| 2:J:67:VAL:HG13  | 2:J:109:LEU:HD13 | 1.80                     | 0.62              |
| 2:L:59:GLN:CG    | 2:L:132:ARG:HB2  | 2.29                     | 0.62              |
| 2:L:184:THR:HA   | 2:L:249:SER:HA   | 1.81                     | 0.62              |
| 1:A:135:ARG:HH22 | 1:A:181:ALA:CB   | 2.13                     | 0.62              |
| 2:B:172:LEU:O    | 2:B:172:LEU:HD23 | 2.00                     | 0.62              |
| 2:J:21:TYR:HB3   | 2:J:151:ASN:ND2  | 2.15                     | 0.61              |
| 1:K:4:LEU:HD21   | 1:K:87:VAL:HG21  | 1.81                     | 0.61              |
| 1:M:156:ASN:C    | 1:M:158:GLY:H    | 2.06                     | 0.61              |
| 1:C:135:ARG:HH22 | 1:C:181:ALA:CB   | 2.13                     | 0.61              |
| 1:E:104:GLN:HG3  | 2:F:168:VAL:HG23 | 1.82                     | 0.61              |
| 2:F:59:GLN:CG    | 2:F:132:ARG:HD2  | 2.30                     | 0.61              |
| 1:G:138:ASN:C    | 1:G:177:LEU:HB3  | 2.25                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:135:ARG:HH22 | 1:E:181:ALA:CB   | 2.14                     | 0.61              |
| 2:H:172:LEU:O    | 2:H:172:LEU:HD23 | 2.00                     | 0.61              |
| 2:J:201:THR:CG2  | 2:J:206:ASN:HA   | 2.24                     | 0.61              |
| 2:F:172:LEU:O    | 2:F:172:LEU:HD23 | 2.01                     | 0.61              |
| 1:G:135:ARG:HH22 | 1:G:181:ALA:CB   | 2.13                     | 0.61              |
| 1:I:162:LEU:HD21 | 1:I:178:PRO:CD   | 2.29                     | 0.61              |
| 2:J:19:ASN:HD21  | 2:L:219:GLN:HE22 | 1.48                     | 0.61              |
| 2:L:32:GLN:O     | 2:L:110:THR:HG23 | 1.99                     | 0.61              |
| 2:D:136:ASN:C    | 2:D:136:ASN:HD22 | 2.08                     | 0.61              |
| 1:E:185:ILE:HB   | 1:E:202:GLY:HA3  | 1.82                     | 0.61              |
| 1:E:191:ASN:HD21 | 1:E:195:ALA:HB3  | 1.63                     | 0.61              |
| 2:L:74:THR:HG22  | 2:L:83:PRO:HA    | 1.83                     | 0.61              |
| 2:H:67:VAL:HG23  | 2:H:126:ILE:HG12 | 1.83                     | 0.61              |
| 2:B:67:VAL:HG23  | 2:B:126:ILE:HG12 | 1.82                     | 0.61              |
| 1:E:140:LEU:HD23 | 1:E:141:THR:N    | 2.15                     | 0.61              |
| 1:G:11:TYR:HB2   | 1:G:113:LEU:HD11 | 1.81                     | 0.61              |
| 2:H:59:GLN:CG    | 2:H:132:ARG:HD2  | 2.30                     | 0.61              |
| 1:I:7:THR:O      | 1:I:111:ILE:HB   | 2.01                     | 0.61              |
| 2:J:184:THR:HA   | 2:J:249:SER:HA   | 1.81                     | 0.61              |
| 2:N:19:ASN:HD21  | 2:P:219:GLN:HE22 | 1.46                     | 0.61              |
| 1:A:104:GLN:HG3  | 2:B:168:VAL:HG23 | 1.82                     | 0.61              |
| 2:F:170:VAL:CG1  | 2:F:172:LEU:HB2  | 2.26                     | 0.61              |
| 1:I:4:LEU:O      | 2:J:160:GLY:N    | 2.33                     | 0.61              |
| 2:L:20:VAL:HG21  | 2:L:42:ILE:HD11  | 1.82                     | 0.61              |
| 2:P:175:TYR:OH   | 2:P:263:VAL:HB   | 2.00                     | 0.61              |
| 1:C:177:LEU:HD12 | 1:C:178:PRO:HD2  | 1.83                     | 0.61              |
| 2:N:21:TYR:HB3   | 2:N:151:ASN:ND2  | 2.15                     | 0.61              |
| 1:A:188:ARG:NH1  | 1:A:199:LYS:HB2  | 2.16                     | 0.61              |
| 2:N:175:TYR:N    | 2:N:176:PRO:HD2  | 2.16                     | 0.61              |
| 2:P:184:THR:HA   | 2:P:249:SER:HA   | 1.81                     | 0.61              |
| 1:C:102:THR:HA   | 2:D:171:THR:HG22 | 1.82                     | 0.60              |
| 2:H:92:ARG:HG3   | 2:H:92:ARG:NH1   | 2.11                     | 0.60              |
| 2:H:174:ASP:O    | 2:H:176:PRO:N    | 2.34                     | 0.60              |
| 2:N:193:LEU:HB3  | 2:N:240:LEU:HD12 | 1.83                     | 0.60              |
| 2:P:20:VAL:HG21  | 2:P:42:ILE:HD11  | 1.81                     | 0.60              |
| 2:D:175:TYR:O    | 2:D:256:TYR:CD1  | 2.54                     | 0.60              |
| 2:L:193:LEU:HB3  | 2:L:240:LEU:HD12 | 1.82                     | 0.60              |
| 1:M:7:THR:O      | 1:M:111:ILE:HB   | 2.01                     | 0.60              |
| 1:O:27:GLU:CG    | 1:O:60:LYS:HD2   | 2.29                     | 0.60              |
| 1:C:118:ALA:O    | 1:C:119:LYS:HB2  | 2.02                     | 0.60              |
| 2:D:207:SER:O    | 2:D:224:GLN:HG3  | 2.02                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:188:ARG:NH1  | 1:E:199:LYS:HB2  | 2.17                     | 0.60              |
| 2:D:170:VAL:CG1  | 2:D:172:LEU:HB2  | 2.26                     | 0.60              |
| 1:E:102:THR:HA   | 2:F:171:THR:HG22 | 1.83                     | 0.60              |
| 2:J:74:THR:HG22  | 2:J:83:PRO:HA    | 1.82                     | 0.60              |
| 1:K:7:THR:O      | 1:K:111:ILE:HB   | 2.00                     | 0.60              |
| 2:N:20:VAL:HG21  | 2:N:42:ILE:HD11  | 1.82                     | 0.60              |
| 1:A:11:TYR:HB2   | 1:A:113:LEU:HD11 | 1.83                     | 0.60              |
| 2:H:192:ASN:ND2  | 2:H:279:GLN:HE22 | 1.96                     | 0.60              |
| 2:J:175:TYR:OH   | 2:J:263:VAL:HB   | 2.01                     | 0.60              |
| 2:L:14:GLY:HA2   | 2:L:142:PHE:CE1  | 2.37                     | 0.60              |
| 2:P:21:TYR:HB3   | 2:P:151:ASN:ND2  | 2.15                     | 0.60              |
| 2:P:74:THR:HG22  | 2:P:83:PRO:HA    | 1.82                     | 0.60              |
| 2:J:175:TYR:N    | 2:J:176:PRO:HD2  | 2.16                     | 0.60              |
| 2:L:125:LEU:HD12 | 2:L:148:ILE:O    | 2.02                     | 0.60              |
| 1:A:177:LEU:HD12 | 1:A:178:PRO:HD2  | 1.83                     | 0.60              |
| 1:A:191:ASN:HD21 | 1:A:195:ALA:HB3  | 1.66                     | 0.60              |
| 1:C:104:GLN:HG3  | 2:D:168:VAL:HG23 | 1.84                     | 0.60              |
| 2:F:131:LEU:HD23 | 2:F:131:LEU:C    | 2.27                     | 0.60              |
| 2:L:201:THR:CG2  | 2:L:206:ASN:HA   | 2.24                     | 0.60              |
| 1:O:117:PRO:O    | 1:O:120:LEU:HG   | 2.02                     | 0.60              |
| 2:F:227:ARG:HB3  | 2:F:232:ILE:HD11 | 1.84                     | 0.60              |
| 2:L:175:TYR:N    | 2:L:176:PRO:HD2  | 2.16                     | 0.60              |
| 2:B:167:ASP:OD2  | 2:B:168:VAL:N    | 2.35                     | 0.60              |
| 2:B:175:TYR:O    | 2:B:256:TYR:CD1  | 2.55                     | 0.60              |
| 2:B:184:THR:HG22 | 2:B:249:SER:HA   | 1.82                     | 0.60              |
| 1:G:141:THR:HG23 | 1:G:174:THR:HG22 | 1.83                     | 0.60              |
| 2:J:193:LEU:HB3  | 2:J:240:LEU:HD12 | 1.83                     | 0.60              |
| 1:A:1:GLY:H1     | 1:A:26:ASP:CG    | 2.10                     | 0.60              |
| 2:B:174:ASP:O    | 2:B:176:PRO:N    | 2.35                     | 0.60              |
| 1:E:94:ASP:HB3   | 1:E:96:SER:OG    | 2.01                     | 0.60              |
| 1:E:177:LEU:HD12 | 1:E:178:PRO:HD2  | 1.83                     | 0.60              |
| 2:F:174:ASP:O    | 2:F:176:PRO:N    | 2.35                     | 0.60              |
| 2:H:131:LEU:HD23 | 2:H:131:LEU:C    | 2.27                     | 0.60              |
| 2:L:175:TYR:OH   | 2:L:263:VAL:HB   | 2.01                     | 0.60              |
| 2:P:175:TYR:N    | 2:P:176:PRO:HD2  | 2.16                     | 0.60              |
| 1:K:4:LEU:O      | 2:L:160:GLY:N    | 2.33                     | 0.59              |
| 2:L:21:TYR:HB3   | 2:L:151:ASN:ND2  | 2.16                     | 0.59              |
| 2:N:74:THR:HG22  | 2:N:83:PRO:HA    | 1.82                     | 0.59              |
| 2:N:175:TYR:OH   | 2:N:263:VAL:HB   | 2.00                     | 0.59              |
| 2:P:193:LEU:HB3  | 2:P:240:LEU:HD12 | 1.82                     | 0.59              |
| 2:B:136:ASN:C    | 2:B:136:ASN:HD22 | 2.09                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:184:THR:HG22 | 2:F:249:SER:HA   | 1.83                     | 0.59              |
| 1:G:82:LEU:HD12  | 1:G:83:PHE:N     | 2.16                     | 0.59              |
| 1:G:179:SER:C    | 1:G:181:ALA:N    | 2.50                     | 0.59              |
| 1:I:101:ASN:ND2  | 2:J:268:VAL:HG23 | 2.17                     | 0.59              |
| 1:M:117:PRO:O    | 1:M:120:LEU:HG   | 2.02                     | 0.59              |
| 2:P:125:LEU:HD12 | 2:P:148:ILE:O    | 2.02                     | 0.59              |
| 1:A:102:THR:HA   | 2:B:171:THR:HG22 | 1.82                     | 0.59              |
| 1:A:179:SER:C    | 1:A:181:ALA:N    | 2.50                     | 0.59              |
| 1:C:82:LEU:HD12  | 1:C:83:PHE:N     | 2.17                     | 0.59              |
| 2:H:163:VAL:HG22 | 2:H:185:VAL:HG12 | 1.84                     | 0.59              |
| 2:H:175:TYR:O    | 2:H:256:TYR:CD1  | 2.55                     | 0.59              |
| 1:I:27:GLU:CG    | 1:I:60:LYS:HD2   | 2.29                     | 0.59              |
| 1:E:118:ALA:O    | 1:E:119:LYS:HB2  | 2.02                     | 0.59              |
| 2:F:211:ASN:HD22 | 2:F:211:ASN:C    | 2.11                     | 0.59              |
| 2:H:167:ASP:OD2  | 2:H:168:VAL:N    | 2.36                     | 0.59              |
| 1:I:117:PRO:O    | 1:I:120:LEU:HG   | 2.02                     | 0.59              |
| 2:J:14:GLY:HA2   | 2:J:142:PHE:CE1  | 2.38                     | 0.59              |
| 1:K:101:ASN:ND2  | 2:L:268:VAL:HG23 | 2.17                     | 0.59              |
| 2:L:177:GLY:HA3  | 2:L:256:TYR:CE1  | 2.38                     | 0.59              |
| 1:M:188:ARG:HH11 | 1:M:199:LYS:HB2  | 1.67                     | 0.59              |
| 2:D:67:VAL:HG23  | 2:D:126:ILE:HG12 | 1.85                     | 0.59              |
| 2:D:174:ASP:O    | 2:D:176:PRO:N    | 2.35                     | 0.59              |
| 1:E:11:TYR:HB2   | 1:E:113:LEU:HD11 | 1.83                     | 0.59              |
| 1:G:102:THR:HA   | 2:H:171:THR:HG22 | 1.82                     | 0.59              |
| 1:G:188:ARG:NH1  | 1:G:199:LYS:HB2  | 2.17                     | 0.59              |
| 1:K:117:PRO:O    | 1:K:120:LEU:HG   | 2.02                     | 0.59              |
| 1:A:135:ARG:HH22 | 1:A:181:ALA:HB1  | 1.68                     | 0.59              |
| 1:G:177:LEU:HD12 | 1:G:178:PRO:HD2  | 1.84                     | 0.59              |
| 1:K:11:TYR:HB2   | 1:K:113:LEU:HD11 | 1.85                     | 0.59              |
| 1:M:11:TYR:HB2   | 1:M:113:LEU:HD11 | 1.85                     | 0.59              |
| 1:O:7:THR:O      | 1:O:111:ILE:HB   | 2.01                     | 0.59              |
| 2:D:131:LEU:HD23 | 2:D:131:LEU:C    | 2.28                     | 0.59              |
| 2:D:184:THR:HG22 | 2:D:249:SER:HA   | 1.85                     | 0.59              |
| 1:G:141:THR:CG2  | 1:G:174:THR:HG22 | 2.33                     | 0.59              |
| 2:N:14:GLY:HA2   | 2:N:142:PHE:CE1  | 2.37                     | 0.59              |
| 2:P:177:GLY:HA3  | 2:P:256:TYR:CE1  | 2.38                     | 0.59              |
| 2:H:227:ARG:HB3  | 2:H:232:ILE:HD11 | 1.85                     | 0.59              |
| 1:A:82:LEU:HD12  | 1:A:83:PHE:N     | 2.18                     | 0.59              |
| 2:F:13:ILE:HG13  | 4:F:1539:HOH:O   | 2.03                     | 0.59              |
| 2:F:136:ASN:HD22 | 2:F:136:ASN:C    | 2.09                     | 0.59              |
| 2:F:170:VAL:C    | 2:F:172:LEU:H    | 2.10                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:175:TYR:O    | 2:F:256:TYR:CD1  | 2.55                     | 0.59              |
| 1:G:118:ALA:O    | 1:G:119:LYS:HB2  | 2.02                     | 0.59              |
| 2:H:184:THR:HG22 | 2:H:249:SER:HA   | 1.84                     | 0.59              |
| 1:M:4:LEU:O      | 2:N:160:GLY:N    | 2.33                     | 0.59              |
| 1:C:191:ASN:HD21 | 1:C:195:ALA:HB3  | 1.67                     | 0.59              |
| 1:E:82:LEU:HD12  | 1:E:83:PHE:N     | 2.17                     | 0.59              |
| 2:F:167:ASP:OD2  | 2:F:168:VAL:N    | 2.36                     | 0.59              |
| 2:F:172:LEU:O    | 2:F:173:PRO:C    | 2.46                     | 0.59              |
| 2:N:24:LEU:HD11  | 2:N:126:ILE:HD11 | 1.84                     | 0.59              |
| 1:I:188:ARG:HH11 | 1:I:199:LYS:HB2  | 1.68                     | 0.58              |
| 1:K:27:GLU:HG2   | 1:K:60:LYS:CD    | 2.32                     | 0.58              |
| 2:N:177:GLY:HA3  | 2:N:256:TYR:CE1  | 2.37                     | 0.58              |
| 2:P:14:GLY:HA2   | 2:P:142:PHE:CE1  | 2.37                     | 0.58              |
| 1:C:188:ARG:NH1  | 1:C:199:LYS:HB2  | 2.17                     | 0.58              |
| 1:G:27:GLU:HA    | 1:G:60:LYS:HG3   | 1.85                     | 0.58              |
| 1:O:79:ARG:HA    | 1:O:147:PRO:HB2  | 1.85                     | 0.58              |
| 1:A:118:ALA:O    | 1:A:119:LYS:HB2  | 2.01                     | 0.58              |
| 1:C:27:GLU:HA    | 1:C:60:LYS:HG3   | 1.85                     | 0.58              |
| 1:E:183:SER:C    | 1:E:185:ILE:H    | 2.12                     | 0.58              |
| 2:F:5:THR:HG22   | 2:F:8:GLY:H      | 1.67                     | 0.58              |
| 1:G:47:ARG:HH22  | 1:G:74:GLN:HB2   | 1.69                     | 0.58              |
| 1:I:103:LEU:O    | 2:J:168:VAL:HG23 | 2.03                     | 0.58              |
| 1:K:27:GLU:CG    | 1:K:60:LYS:HD2   | 2.30                     | 0.58              |
| 2:B:227:ARG:HB3  | 2:B:232:ILE:HD11 | 1.86                     | 0.58              |
| 2:D:59:GLN:CG    | 2:D:132:ARG:HD2  | 2.31                     | 0.58              |
| 2:H:114:SER:HB3  | 2:L:80:SER:HB3   | 1.85                     | 0.58              |
| 2:J:24:LEU:HD11  | 2:J:126:ILE:HD11 | 1.85                     | 0.58              |
| 1:K:188:ARG:HH11 | 1:K:199:LYS:HB2  | 1.68                     | 0.58              |
| 1:A:183:SER:C    | 1:A:185:ILE:H    | 2.12                     | 0.58              |
| 1:I:11:TYR:HB2   | 1:I:113:LEU:HD11 | 1.85                     | 0.58              |
| 1:I:135:ARG:NH1  | 1:I:181:ALA:CB   | 2.53                     | 0.58              |
| 1:M:103:LEU:O    | 2:N:168:VAL:HG23 | 2.04                     | 0.58              |
| 2:N:125:LEU:HD12 | 2:N:148:ILE:O    | 2.02                     | 0.58              |
| 2:P:24:LEU:HD11  | 2:P:126:ILE:HD11 | 1.85                     | 0.58              |
| 2:B:58:LEU:H     | 2:B:90:THR:CG2   | 2.16                     | 0.58              |
| 2:B:179:VAL:O    | 2:B:253:THR:HG23 | 2.03                     | 0.58              |
| 1:G:183:SER:C    | 1:G:185:ILE:H    | 2.12                     | 0.58              |
| 1:M:101:ASN:ND2  | 2:N:268:VAL:HG23 | 2.17                     | 0.58              |
| 1:C:188:ARG:HH12 | 1:C:199:LYS:H    | 1.50                     | 0.58              |
| 2:F:92:ARG:HG3   | 2:F:92:ARG:NH1   | 2.12                     | 0.58              |
| 1:G:135:ARG:NH2  | 1:G:181:ALA:HB1  | 2.19                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:188:ARG:HH12 | 1:G:199:LYS:H    | 1.51                     | 0.58              |
| 2:H:136:ASN:HD22 | 2:H:136:ASN:C    | 2.09                     | 0.58              |
| 1:I:197:THR:HB   | 1:I:198:PRO:HD2  | 1.86                     | 0.58              |
| 2:N:84:PHE:CD1   | 2:N:85:PRO:HA    | 2.39                     | 0.58              |
| 2:N:131:LEU:HB3  | 2:N:144:PHE:HB2  | 1.86                     | 0.58              |
| 1:O:11:TYR:HB2   | 1:O:113:LEU:HD11 | 1.85                     | 0.58              |
| 1:O:103:LEU:O    | 2:P:168:VAL:HG23 | 2.04                     | 0.58              |
| 2:F:192:ASN:ND2  | 2:F:279:GLN:HE22 | 1.99                     | 0.58              |
| 1:G:135:ARG:HH22 | 1:G:181:ALA:HB1  | 1.68                     | 0.58              |
| 2:H:58:LEU:H     | 2:H:90:THR:CG2   | 2.16                     | 0.58              |
| 2:H:170:VAL:CG1  | 2:H:172:LEU:HB2  | 2.27                     | 0.58              |
| 2:N:201:THR:CG2  | 2:N:206:ASN:HA   | 2.24                     | 0.58              |
| 2:B:131:LEU:C    | 2:B:131:LEU:HD23 | 2.29                     | 0.58              |
| 1:C:135:ARG:HH22 | 1:C:181:ALA:HB1  | 1.68                     | 0.58              |
| 1:E:135:ARG:NH2  | 1:E:181:ALA:HB1  | 2.19                     | 0.58              |
| 1:K:122:LEU:HD11 | 1:K:126:GLN:O    | 2.04                     | 0.58              |
| 1:O:122:LEU:HD11 | 1:O:126:GLN:O    | 2.04                     | 0.58              |
| 2:H:172:LEU:O    | 2:H:173:PRO:C    | 2.46                     | 0.58              |
| 2:L:223:VAL:HG12 | 2:L:224:GLN:N    | 2.19                     | 0.58              |
| 1:M:27:GLU:HG2   | 1:M:60:LYS:CD    | 2.32                     | 0.58              |
| 1:M:79:ARG:HA    | 1:M:147:PRO:HB2  | 1.85                     | 0.58              |
| 1:A:27:GLU:HA    | 1:A:60:LYS:HG3   | 1.86                     | 0.57              |
| 2:B:68:LEU:O     | 2:P:87:THR:HG21  | 2.03                     | 0.57              |
| 2:B:170:VAL:C    | 2:B:172:LEU:H    | 2.11                     | 0.57              |
| 2:D:167:ASP:OD2  | 2:D:168:VAL:N    | 2.35                     | 0.57              |
| 2:F:58:LEU:H     | 2:F:90:THR:CG2   | 2.16                     | 0.57              |
| 2:H:68:LEU:O     | 2:L:87:THR:HG21  | 2.04                     | 0.57              |
| 2:J:177:GLY:HA3  | 2:J:256:TYR:CE1  | 2.38                     | 0.57              |
| 1:K:6:ALA:HB3    | 1:K:20:LEU:HD11  | 1.86                     | 0.57              |
| 1:O:4:LEU:O      | 2:P:160:GLY:N    | 2.33                     | 0.57              |
| 1:O:197:THR:HB   | 1:O:198:PRO:HD2  | 1.86                     | 0.57              |
| 2:P:201:THR:CG2  | 2:P:206:ASN:HA   | 2.24                     | 0.57              |
| 1:A:24:ASN:O     | 1:A:60:LYS:HA    | 2.05                     | 0.57              |
| 2:B:172:LEU:O    | 2:B:173:PRO:C    | 2.47                     | 0.57              |
| 2:D:170:VAL:C    | 2:D:172:LEU:H    | 2.12                     | 0.57              |
| 1:E:27:GLU:HA    | 1:E:60:LYS:HG3   | 1.87                     | 0.57              |
| 1:G:135:ARG:CZ   | 1:G:181:ALA:HB1  | 2.34                     | 0.57              |
| 1:G:158:GLY:HA2  | 1:G:184:ASN:HD22 | 1.69                     | 0.57              |
| 2:H:211:ASN:HD22 | 2:H:211:ASN:C    | 2.10                     | 0.57              |
| 1:I:27:GLU:HG2   | 1:I:60:LYS:CD    | 2.32                     | 0.57              |
| 1:I:122:LEU:HD11 | 1:I:126:GLN:O    | 2.04                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:79:ARG:HA    | 1:K:147:PRO:HB2  | 1.85                     | 0.57              |
| 1:O:6:ALA:HB3    | 1:O:20:LEU:HD11  | 1.86                     | 0.57              |
| 1:G:1:GLY:H1     | 1:G:26:ASP:CG    | 2.12                     | 0.57              |
| 2:L:131:LEU:HB3  | 2:L:144:PHE:HB2  | 1.87                     | 0.57              |
| 1:O:101:ASN:ND2  | 2:P:268:VAL:HG23 | 2.17                     | 0.57              |
| 1:O:188:ARG:HH11 | 1:O:199:LYS:HB2  | 1.68                     | 0.57              |
| 2:B:120:ILE:CG2  | 2:B:126:ILE:HD11 | 2.31                     | 0.57              |
| 1:C:135:ARG:NH2  | 1:C:181:ALA:HB1  | 2.19                     | 0.57              |
| 2:L:84:PHE:CD1   | 2:L:85:PRO:HA    | 2.40                     | 0.57              |
| 2:P:84:PHE:CD1   | 2:P:85:PRO:HA    | 2.39                     | 0.57              |
| 2:B:211:ASN:HD22 | 2:B:211:ASN:C    | 2.12                     | 0.57              |
| 1:C:134:ARG:CD   | 1:C:141:THR:CG2  | 2.83                     | 0.57              |
| 2:D:5:THR:HG22   | 2:D:8:GLY:H      | 1.69                     | 0.57              |
| 1:E:179:SER:C    | 1:E:181:ALA:N    | 2.50                     | 0.57              |
| 2:J:125:LEU:HD12 | 2:J:148:ILE:O    | 2.03                     | 0.57              |
| 1:A:135:ARG:NH2  | 1:A:181:ALA:HB1  | 2.19                     | 0.57              |
| 1:A:183:SER:OG   | 1:A:204:MET:HE3  | 2.05                     | 0.57              |
| 2:B:114:SER:HB3  | 2:P:80:SER:HB3   | 1.85                     | 0.57              |
| 1:C:135:ARG:CZ   | 1:C:181:ALA:HB1  | 2.34                     | 0.57              |
| 1:C:158:GLY:HA2  | 1:C:184:ASN:HD22 | 1.69                     | 0.57              |
| 1:E:197:THR:HB   | 1:E:198:PRO:HD2  | 1.87                     | 0.57              |
| 2:F:179:VAL:O    | 2:F:253:THR:HG23 | 2.03                     | 0.57              |
| 1:K:103:LEU:O    | 2:L:168:VAL:HG23 | 2.04                     | 0.57              |
| 2:L:24:LEU:HD11  | 2:L:126:ILE:HD11 | 1.84                     | 0.57              |
| 2:L:71:PHE:CE2   | 2:L:111:PRO:HG3  | 2.39                     | 0.57              |
| 2:N:71:PHE:CE2   | 2:N:111:PRO:HG3  | 2.39                     | 0.57              |
| 2:D:163:VAL:HG22 | 2:D:185:VAL:HG12 | 1.87                     | 0.57              |
| 2:D:211:ASN:HD22 | 2:D:211:ASN:C    | 2.12                     | 0.57              |
| 2:F:163:VAL:HG22 | 2:F:185:VAL:HG12 | 1.86                     | 0.57              |
| 1:I:79:ARG:HA    | 1:I:147:PRO:HB2  | 1.85                     | 0.57              |
| 2:J:71:PHE:CE2   | 2:J:111:PRO:HG3  | 2.40                     | 0.57              |
| 2:J:131:LEU:HB3  | 2:J:144:PHE:HB2  | 1.87                     | 0.57              |
| 2:L:96:ASN:HD22  | 2:L:96:ASN:H     | 1.53                     | 0.57              |
| 1:M:6:ALA:HB3    | 1:M:20:LEU:HD11  | 1.87                     | 0.57              |
| 1:M:197:THR:HB   | 1:M:198:PRO:HD2  | 1.86                     | 0.57              |
| 2:N:66:GLY:O     | 2:N:70:ASN:HB2   | 2.05                     | 0.57              |
| 1:C:134:ARG:NH1  | 1:C:141:THR:HG21 | 2.19                     | 0.57              |
| 2:D:58:LEU:H     | 2:D:90:THR:CG2   | 2.18                     | 0.57              |
| 2:P:71:PHE:CE2   | 2:P:111:PRO:HG3  | 2.40                     | 0.57              |
| 2:P:131:LEU:HB3  | 2:P:144:PHE:HB2  | 1.87                     | 0.57              |
| 2:P:227:ARG:HH22 | 2:P:230:THR:HG21 | 1.70                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:5:THR:HG22   | 2:B:8:GLY:H      | 1.69                     | 0.57              |
| 2:J:223:VAL:HG12 | 2:J:224:GLN:N    | 2.19                     | 0.57              |
| 2:L:227:ARG:HH22 | 2:L:230:THR:HG21 | 1.70                     | 0.57              |
| 2:L:267:ASN:HB3  | 2:L:269:GLN:HG3  | 1.87                     | 0.57              |
| 1:M:28:ASN:N     | 1:M:28:ASN:HD22  | 2.03                     | 0.57              |
| 2:N:224:GLN:HG2  | 2:N:231:ILE:CG2  | 2.35                     | 0.57              |
| 1:A:135:ARG:CZ   | 1:A:181:ALA:HB1  | 2.34                     | 0.57              |
| 1:C:183:SER:C    | 1:C:185:ILE:H    | 2.12                     | 0.57              |
| 1:C:188:ARG:NH1  | 1:C:199:LYS:N    | 2.53                     | 0.57              |
| 1:E:135:ARG:HH22 | 1:E:181:ALA:HB1  | 1.68                     | 0.57              |
| 2:H:5:THR:HG22   | 2:H:8:GLY:H      | 1.70                     | 0.57              |
| 2:J:84:PHE:CD1   | 2:J:85:PRO:HA    | 2.40                     | 0.57              |
| 1:M:122:LEU:HD11 | 1:M:126:GLN:O    | 2.04                     | 0.57              |
| 1:E:135:ARG:CZ   | 1:E:181:ALA:HB1  | 2.34                     | 0.56              |
| 1:E:158:GLY:HA2  | 1:E:184:ASN:HD22 | 1.69                     | 0.56              |
| 2:J:96:ASN:HD22  | 2:J:96:ASN:H     | 1.53                     | 0.56              |
| 1:K:197:THR:HB   | 1:K:198:PRO:HD2  | 1.86                     | 0.56              |
| 1:O:11:TYR:CE2   | 1:O:69:ASP:HB2   | 2.40                     | 0.56              |
| 2:P:224:GLN:HG2  | 2:P:231:ILE:CG2  | 2.35                     | 0.56              |
| 1:K:28:ASN:HD22  | 1:K:28:ASN:N     | 2.03                     | 0.56              |
| 1:O:78:ASP:O     | 1:O:170:MET:HE1  | 2.05                     | 0.56              |
| 1:A:158:GLY:HA2  | 1:A:184:ASN:HD22 | 1.69                     | 0.56              |
| 2:B:219:GLN:HG2  | 2:B:220:GLY:N    | 2.20                     | 0.56              |
| 2:D:179:VAL:O    | 2:D:253:THR:HG23 | 2.05                     | 0.56              |
| 2:D:219:GLN:HG2  | 2:D:220:GLY:N    | 2.19                     | 0.56              |
| 1:E:24:ASN:O     | 1:E:60:LYS:HA    | 2.05                     | 0.56              |
| 1:E:193:TYR:O    | 2:F:158:THR:HG22 | 2.06                     | 0.56              |
| 1:G:193:TYR:O    | 2:H:158:THR:HG22 | 2.06                     | 0.56              |
| 2:H:28:VAL:O     | 2:H:156:VAL:HA   | 2.06                     | 0.56              |
| 2:J:66:GLY:O     | 2:J:70:ASN:HB2   | 2.05                     | 0.56              |
| 2:J:250:LEU:HB2  | 2:J:252:LEU:HG   | 1.87                     | 0.56              |
| 2:L:11:ILE:HD12  | 2:L:146:TRP:CZ2  | 2.40                     | 0.56              |
| 1:M:11:TYR:CE2   | 1:M:69:ASP:HB2   | 2.40                     | 0.56              |
| 2:P:267:ASN:HB3  | 2:P:269:GLN:HG3  | 1.87                     | 0.56              |
| 1:A:188:ARG:NH1  | 1:A:199:LYS:N    | 2.53                     | 0.56              |
| 2:F:226:THR:HG22 | 2:F:253:THR:HB   | 1.88                     | 0.56              |
| 2:H:170:VAL:C    | 2:H:172:LEU:H    | 2.12                     | 0.56              |
| 2:H:179:VAL:O    | 2:H:253:THR:HG23 | 2.05                     | 0.56              |
| 1:I:11:TYR:CE2   | 1:I:69:ASP:HB2   | 2.40                     | 0.56              |
| 2:N:11:ILE:HD12  | 2:N:146:TRP:CZ2  | 2.40                     | 0.56              |
| 2:N:227:ARG:HH22 | 2:N:230:THR:HG21 | 1.70                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:154:GLU:OE2  | 1:O:188:ARG:HD3  | 2.06                     | 0.56              |
| 1:C:183:SER:OG   | 1:C:204:MET:HE3  | 2.05                     | 0.56              |
| 2:D:172:LEU:O    | 2:D:173:PRO:C    | 2.47                     | 0.56              |
| 2:D:227:ARG:HB3  | 2:D:232:ILE:HD11 | 1.88                     | 0.56              |
| 1:G:188:ARG:NH1  | 1:G:199:LYS:N    | 2.54                     | 0.56              |
| 2:H:120:ILE:HD13 | 2:H:126:ILE:HD11 | 1.87                     | 0.56              |
| 2:J:30:VAL:HA    | 2:J:111:PRO:HB2  | 1.87                     | 0.56              |
| 2:N:224:GLN:HG2  | 2:N:231:ILE:HG21 | 1.87                     | 0.56              |
| 2:P:264:THR:CG2  | 2:P:265:ALA:H    | 2.15                     | 0.56              |
| 1:C:47:ARG:HH22  | 1:C:74:GLN:HB2   | 1.70                     | 0.56              |
| 1:E:188:ARG:HH12 | 1:E:199:LYS:H    | 1.52                     | 0.56              |
| 1:I:6:ALA:HB3    | 1:I:20:LEU:HD11  | 1.86                     | 0.56              |
| 2:J:227:ARG:HH22 | 2:J:230:THR:HG21 | 1.70                     | 0.56              |
| 1:K:189:THR:O    | 1:K:196:LEU:HA   | 2.06                     | 0.56              |
| 1:O:189:THR:O    | 1:O:196:LEU:HA   | 2.06                     | 0.56              |
| 2:P:223:VAL:HG12 | 2:P:224:GLN:N    | 2.19                     | 0.56              |
| 2:B:163:VAL:HG22 | 2:B:185:VAL:HG12 | 1.88                     | 0.56              |
| 1:C:193:TYR:O    | 2:D:158:THR:HG22 | 2.06                     | 0.56              |
| 2:D:167:ASP:CG   | 2:D:168:VAL:N    | 2.50                     | 0.56              |
| 1:G:197:THR:HB   | 1:G:198:PRO:HD2  | 1.88                     | 0.56              |
| 2:H:50:GLU:H     | 2:H:50:GLU:CD    | 2.14                     | 0.56              |
| 1:I:135:ARG:HH12 | 1:I:181:ALA:HB2  | 1.69                     | 0.56              |
| 1:I:162:LEU:CD2  | 1:I:178:PRO:HD3  | 2.36                     | 0.56              |
| 2:J:224:GLN:HG2  | 2:J:231:ILE:CG2  | 2.35                     | 0.56              |
| 1:K:78:ASP:O     | 1:K:170:MET:HE1  | 2.06                     | 0.56              |
| 1:K:80:GLU:HG3   | 1:K:147:PRO:O    | 2.05                     | 0.56              |
| 2:L:215:PHE:C    | 2:L:215:PHE:CD2  | 2.84                     | 0.56              |
| 2:L:224:GLN:HG2  | 2:L:231:ILE:CG2  | 2.35                     | 0.56              |
| 2:N:267:ASN:HB3  | 2:N:269:GLN:HG3  | 1.87                     | 0.56              |
| 2:B:28:VAL:O     | 2:B:156:VAL:HA   | 2.05                     | 0.56              |
| 1:E:142:LEU:H    | 1:E:142:LEU:CD2  | 2.19                     | 0.56              |
| 2:J:11:ILE:HD12  | 2:J:146:TRP:CZ2  | 2.41                     | 0.56              |
| 1:M:22:VAL:CG2   | 1:M:65:LEU:HG    | 2.36                     | 0.56              |
| 1:O:27:GLU:HG2   | 1:O:60:LYS:CD    | 2.32                     | 0.56              |
| 1:O:80:GLU:HG3   | 1:O:147:PRO:O    | 2.06                     | 0.56              |
| 2:P:60:ARG:HG3   | 2:P:61:GLY:N     | 2.21                     | 0.56              |
| 2:P:66:GLY:O     | 2:P:70:ASN:HB2   | 2.06                     | 0.56              |
| 1:E:188:ARG:NH1  | 1:E:199:LYS:N    | 2.54                     | 0.56              |
| 1:K:11:TYR:CE2   | 1:K:69:ASP:HB2   | 2.40                     | 0.56              |
| 2:N:223:VAL:HG12 | 2:N:224:GLN:N    | 2.20                     | 0.56              |
| 2:P:224:GLN:HG2  | 2:P:231:ILE:HG21 | 1.88                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:188:ARG:HH12 | 1:A:199:LYS:H    | 1.51                     | 0.56              |
| 2:B:226:THR:HG22 | 2:B:253:THR:HB   | 1.88                     | 0.56              |
| 2:F:28:VAL:O     | 2:F:156:VAL:HA   | 2.05                     | 0.56              |
| 2:F:219:GLN:HG2  | 2:F:220:GLY:N    | 2.20                     | 0.56              |
| 1:I:78:ASP:O     | 1:I:170:MET:HE1  | 2.06                     | 0.56              |
| 2:L:60:ARG:HG3   | 2:L:61:GLY:N     | 2.21                     | 0.56              |
| 1:A:197:THR:HB   | 1:A:198:PRO:HD2  | 1.88                     | 0.55              |
| 2:D:28:VAL:O     | 2:D:156:VAL:HA   | 2.07                     | 0.55              |
| 1:E:47:ARG:HH22  | 1:E:74:GLN:HB2   | 1.69                     | 0.55              |
| 1:G:141:THR:CB   | 1:G:174:THR:HG22 | 2.35                     | 0.55              |
| 2:H:207:SER:O    | 2:H:224:GLN:HG3  | 2.06                     | 0.55              |
| 2:H:219:GLN:HG2  | 2:H:220:GLY:N    | 2.20                     | 0.55              |
| 2:J:267:ASN:HB3  | 2:J:269:GLN:HG3  | 1.87                     | 0.55              |
| 1:K:22:VAL:CG2   | 1:K:65:LEU:HG    | 2.36                     | 0.55              |
| 1:K:162:LEU:CD2  | 1:K:178:PRO:HD3  | 2.36                     | 0.55              |
| 2:L:20:VAL:HG12  | 2:L:22:VAL:HG13  | 1.88                     | 0.55              |
| 1:M:80:GLU:HG3   | 1:M:147:PRO:O    | 2.06                     | 0.55              |
| 2:P:30:VAL:HA    | 2:P:111:PRO:HB2  | 1.89                     | 0.55              |
| 2:P:250:LEU:HB2  | 2:P:252:LEU:HG   | 1.87                     | 0.55              |
| 1:A:47:ARG:HH22  | 1:A:74:GLN:HB2   | 1.71                     | 0.55              |
| 1:E:183:SER:OG   | 1:E:204:MET:HE3  | 2.05                     | 0.55              |
| 2:F:71:PHE:CE2   | 2:F:111:PRO:HG3  | 2.41                     | 0.55              |
| 1:I:154:GLU:OE2  | 1:I:188:ARG:HD3  | 2.06                     | 0.55              |
| 2:N:264:THR:CG2  | 2:N:265:ALA:H    | 2.16                     | 0.55              |
| 2:B:207:SER:O    | 2:B:224:GLN:HG3  | 2.06                     | 0.55              |
| 2:D:120:ILE:HD13 | 2:D:126:ILE:HD11 | 1.87                     | 0.55              |
| 2:H:226:THR:HG22 | 2:H:253:THR:HB   | 1.88                     | 0.55              |
| 1:I:22:VAL:CG2   | 1:I:65:LEU:HG    | 2.37                     | 0.55              |
| 2:N:220:GLY:HA2  | 2:N:259:THR:OG1  | 2.07                     | 0.55              |
| 1:O:22:VAL:CG2   | 1:O:65:LEU:HG    | 2.36                     | 0.55              |
| 1:O:28:ASN:HD22  | 1:O:28:ASN:N     | 2.03                     | 0.55              |
| 2:P:96:ASN:HD22  | 2:P:96:ASN:H     | 1.54                     | 0.55              |
| 2:P:220:GLY:HA2  | 2:P:259:THR:OG1  | 2.07                     | 0.55              |
| 1:A:142:LEU:CD2  | 1:A:142:LEU:H    | 2.20                     | 0.55              |
| 2:B:201:THR:CG2  | 2:B:206:ASN:HA   | 2.29                     | 0.55              |
| 2:F:83:PRO:O     | 2:F:86:THR:HA    | 2.07                     | 0.55              |
| 2:F:201:THR:CG2  | 2:F:206:ASN:HD22 | 2.18                     | 0.55              |
| 1:G:142:LEU:H    | 1:G:142:LEU:CD2  | 2.19                     | 0.55              |
| 1:I:104:GLN:O    | 2:J:271:ILE:HA   | 2.07                     | 0.55              |
| 2:L:66:GLY:O     | 2:L:70:ASN:HB2   | 2.05                     | 0.55              |
| 2:N:20:VAL:HG12  | 2:N:22:VAL:HG13  | 1.89                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:P:11:ILE:HD12  | 2:P:146:TRP:CZ2  | 2.40                     | 0.55              |
| 1:G:183:SER:OG   | 1:G:204:MET:HE3  | 2.07                     | 0.55              |
| 1:I:28:ASN:HD22  | 1:I:28:ASN:N     | 2.03                     | 0.55              |
| 2:L:30:VAL:HA    | 2:L:111:PRO:HB2  | 1.87                     | 0.55              |
| 1:M:104:GLN:O    | 2:N:271:ILE:HA   | 2.07                     | 0.55              |
| 1:M:162:LEU:CD2  | 1:M:178:PRO:HD3  | 2.36                     | 0.55              |
| 2:N:19:ASN:ND2   | 2:P:219:GLN:NE2  | 2.53                     | 0.55              |
| 2:P:117:GLY:O    | 2:P:155:VAL:HA   | 2.06                     | 0.55              |
| 1:C:94:ASP:CG    | 2:D:168:VAL:HG11 | 2.32                     | 0.55              |
| 2:J:28:VAL:O     | 2:J:156:VAL:HA   | 2.07                     | 0.55              |
| 2:J:215:PHE:C    | 2:J:215:PHE:CD2  | 2.84                     | 0.55              |
| 2:F:120:ILE:CG2  | 2:F:126:ILE:HD11 | 2.29                     | 0.55              |
| 1:I:28:ASN:N     | 1:I:28:ASN:ND2   | 2.54                     | 0.55              |
| 1:I:80:GLU:HG3   | 1:I:147:PRO:O    | 2.06                     | 0.55              |
| 1:I:189:THR:O    | 1:I:196:LEU:HA   | 2.07                     | 0.55              |
| 2:J:73:GLY:HA2   | 4:J:1611:HOH:O   | 2.06                     | 0.55              |
| 1:M:154:GLU:OE2  | 1:M:188:ARG:HD3  | 2.06                     | 0.55              |
| 1:M:184:ASN:O    | 1:M:186:THR:HG23 | 2.07                     | 0.55              |
| 2:N:250:LEU:HB2  | 2:N:252:LEU:HG   | 1.88                     | 0.55              |
| 1:O:135:ARG:HH12 | 1:O:181:ALA:HB2  | 1.68                     | 0.55              |
| 2:P:215:PHE:C    | 2:P:215:PHE:CD2  | 2.84                     | 0.55              |
| 1:C:142:LEU:H    | 1:C:142:LEU:CD2  | 2.20                     | 0.55              |
| 2:F:117:GLY:O    | 2:F:155:VAL:HA   | 2.07                     | 0.55              |
| 2:J:19:ASN:ND2   | 2:L:219:GLN:NE2  | 2.54                     | 0.55              |
| 2:J:117:GLY:O    | 2:J:155:VAL:HA   | 2.07                     | 0.55              |
| 2:L:4:LYS:HA     | 2:L:10:ALA:HA    | 1.89                     | 0.55              |
| 1:M:28:ASN:HD22  | 1:M:28:ASN:H     | 1.54                     | 0.55              |
| 1:M:78:ASP:O     | 1:M:170:MET:HE1  | 2.06                     | 0.55              |
| 2:H:201:THR:CG2  | 2:H:206:ASN:HD22 | 2.18                     | 0.55              |
| 2:L:71:PHE:HE2   | 2:L:111:PRO:HG3  | 1.72                     | 0.55              |
| 2:D:201:THR:CG2  | 2:D:206:ASN:HD22 | 2.18                     | 0.55              |
| 1:E:140:LEU:HB2  | 1:E:177:LEU:HD22 | 1.89                     | 0.55              |
| 2:F:50:GLU:CD    | 2:F:50:GLU:H     | 2.14                     | 0.55              |
| 2:L:250:LEU:HB2  | 2:L:252:LEU:HG   | 1.87                     | 0.55              |
| 1:M:28:ASN:N     | 1:M:28:ASN:ND2   | 2.54                     | 0.55              |
| 2:H:71:PHE:CE2   | 2:H:111:PRO:HG3  | 2.42                     | 0.54              |
| 2:J:224:GLN:HG2  | 2:J:231:ILE:HG21 | 1.88                     | 0.54              |
| 1:K:28:ASN:HD22  | 1:K:28:ASN:H     | 1.54                     | 0.54              |
| 2:N:215:PHE:C    | 2:N:215:PHE:CD2  | 2.84                     | 0.54              |
| 1:O:184:ASN:O    | 1:O:186:THR:HG23 | 2.08                     | 0.54              |
| 1:A:174:THR:HG23 | 1:A:174:THR:O    | 2.06                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:50:GLU:CD    | 2:D:50:GLU:H     | 2.15                     | 0.54              |
| 2:J:4:LYS:HA     | 2:J:10:ALA:HA    | 1.89                     | 0.54              |
| 1:M:115:TYR:O    | 1:M:117:PRO:HD3  | 2.08                     | 0.54              |
| 1:K:28:ASN:N     | 1:K:28:ASN:ND2   | 2.54                     | 0.54              |
| 1:K:115:TYR:O    | 1:K:117:PRO:HD3  | 2.07                     | 0.54              |
| 1:K:184:ASN:O    | 1:K:186:THR:HG23 | 2.07                     | 0.54              |
| 2:L:200:THR:O    | 2:L:209:PHE:HA   | 2.07                     | 0.54              |
| 1:M:189:THR:O    | 1:M:196:LEU:HA   | 2.06                     | 0.54              |
| 2:P:28:VAL:O     | 2:P:156:VAL:HA   | 2.07                     | 0.54              |
| 2:P:200:THR:O    | 2:P:209:PHE:HA   | 2.07                     | 0.54              |
| 2:B:50:GLU:H     | 2:B:50:GLU:CD    | 2.14                     | 0.54              |
| 1:C:24:ASN:O     | 1:C:60:LYS:HA    | 2.06                     | 0.54              |
| 2:F:120:ILE:HD13 | 2:F:126:ILE:HD11 | 1.89                     | 0.54              |
| 2:J:200:THR:O    | 2:J:209:PHE:HA   | 2.07                     | 0.54              |
| 1:K:104:GLN:O    | 2:L:271:ILE:HA   | 2.07                     | 0.54              |
| 2:L:162:ASP:O    | 2:L:185:VAL:HG13 | 2.07                     | 0.54              |
| 1:A:94:ASP:CG    | 2:B:168:VAL:HG11 | 2.32                     | 0.54              |
| 1:G:94:ASP:CG    | 2:H:168:VAL:HG11 | 2.33                     | 0.54              |
| 2:H:117:GLY:O    | 2:H:155:VAL:HA   | 2.07                     | 0.54              |
| 2:J:162:ASP:O    | 2:J:185:VAL:HG13 | 2.07                     | 0.54              |
| 2:L:224:GLN:HG2  | 2:L:231:ILE:HG21 | 1.88                     | 0.54              |
| 2:D:71:PHE:CE2   | 2:D:111:PRO:HG3  | 2.42                     | 0.54              |
| 1:I:185:ILE:HD12 | 1:I:204:MET:SD   | 2.48                     | 0.54              |
| 2:N:60:ARG:HG3   | 2:N:61:GLY:N     | 2.22                     | 0.54              |
| 2:N:200:THR:O    | 2:N:209:PHE:HA   | 2.08                     | 0.54              |
| 1:O:162:LEU:CD2  | 1:O:178:PRO:HD3  | 2.36                     | 0.54              |
| 1:A:156:ASN:C    | 1:A:158:GLY:H    | 2.16                     | 0.54              |
| 2:F:5:THR:HG23   | 2:F:7:ASN:H      | 1.72                     | 0.54              |
| 1:G:24:ASN:O     | 1:G:60:LYS:HA    | 2.07                     | 0.54              |
| 1:I:115:TYR:O    | 1:I:117:PRO:HD3  | 2.07                     | 0.54              |
| 2:J:20:VAL:HG12  | 2:J:22:VAL:HG13  | 1.88                     | 0.54              |
| 2:J:201:THR:HA   | 2:J:209:PHE:HA   | 1.90                     | 0.54              |
| 2:J:264:THR:CG2  | 2:J:265:ALA:H    | 2.16                     | 0.54              |
| 1:K:135:ARG:HH12 | 1:K:181:ALA:HB2  | 1.69                     | 0.54              |
| 2:L:74:THR:HB    | 2:L:82:TYR:O     | 2.07                     | 0.54              |
| 2:L:264:THR:CG2  | 2:L:265:ALA:H    | 2.15                     | 0.54              |
| 2:N:96:ASN:H     | 2:N:96:ASN:HD22  | 1.55                     | 0.54              |
| 1:O:28:ASN:HD22  | 1:O:28:ASN:H     | 1.55                     | 0.54              |
| 1:E:94:ASP:CG    | 2:F:168:VAL:HG11 | 2.32                     | 0.54              |
| 1:I:28:ASN:HD22  | 1:I:28:ASN:H     | 1.54                     | 0.54              |
| 1:K:154:GLU:OE2  | 1:K:188:ARG:HD3  | 2.06                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:98:LEU:HD13  | 1:M:98:LEU:C     | 2.33                     | 0.54              |
| 2:N:117:GLY:O    | 2:N:155:VAL:HA   | 2.07                     | 0.54              |
| 2:P:162:ASP:O    | 2:P:185:VAL:HG13 | 2.07                     | 0.54              |
| 2:D:83:PRO:O     | 2:D:86:THR:HA    | 2.07                     | 0.54              |
| 1:I:131:LEU:HD12 | 1:I:143:ILE:O    | 2.08                     | 0.54              |
| 2:J:220:GLY:HA2  | 2:J:259:THR:OG1  | 2.07                     | 0.54              |
| 1:K:185:ILE:HD12 | 1:K:204:MET:SD   | 2.48                     | 0.54              |
| 2:L:40:THR:O     | 2:L:40:THR:HG22  | 2.08                     | 0.54              |
| 2:L:201:THR:HA   | 2:L:209:PHE:HA   | 1.90                     | 0.54              |
| 2:N:28:VAL:O     | 2:N:156:VAL:HA   | 2.07                     | 0.54              |
| 2:N:74:THR:HB    | 2:N:82:TYR:O     | 2.07                     | 0.54              |
| 1:O:28:ASN:N     | 1:O:28:ASN:ND2   | 2.54                     | 0.54              |
| 2:B:201:THR:CG2  | 2:B:206:ASN:HD22 | 2.20                     | 0.54              |
| 2:F:207:SER:O    | 2:F:224:GLN:HG3  | 2.08                     | 0.54              |
| 2:H:201:THR:CG2  | 2:H:206:ASN:HA   | 2.29                     | 0.54              |
| 1:O:39:ASN:CG    | 1:O:43:VAL:HG13  | 2.33                     | 0.54              |
| 1:O:104:GLN:O    | 2:P:271:ILE:HA   | 2.07                     | 0.54              |
| 1:O:115:TYR:O    | 1:O:117:PRO:HD3  | 2.08                     | 0.54              |
| 1:O:133:PHE:CE1  | 1:O:202:GLY:HA2  | 2.43                     | 0.54              |
| 1:A:193:TYR:O    | 2:B:158:THR:HG22 | 2.06                     | 0.53              |
| 1:C:134:ARG:HD2  | 1:C:141:THR:HG22 | 1.91                     | 0.53              |
| 1:G:133:PHE:CD2  | 1:G:140:LEU:HD21 | 2.31                     | 0.53              |
| 1:G:140:LEU:HB2  | 1:G:177:LEU:HD22 | 1.90                     | 0.53              |
| 1:K:131:LEU:HD12 | 1:K:143:ILE:O    | 2.08                     | 0.53              |
| 1:M:185:ILE:HD12 | 1:M:204:MET:SD   | 2.48                     | 0.53              |
| 2:P:71:PHE:HE2   | 2:P:111:PRO:HG3  | 1.74                     | 0.53              |
| 2:P:192:ASN:HB2  | 2:P:279:GLN:NE2  | 2.23                     | 0.53              |
| 2:B:71:PHE:CE2   | 2:B:111:PRO:HG3  | 2.43                     | 0.53              |
| 1:G:156:ASN:C    | 1:G:158:GLY:H    | 2.16                     | 0.53              |
| 2:J:192:ASN:HB2  | 2:J:279:GLN:NE2  | 2.24                     | 0.53              |
| 1:K:98:LEU:HD13  | 1:K:98:LEU:C     | 2.33                     | 0.53              |
| 2:N:162:ASP:O    | 2:N:185:VAL:HG13 | 2.07                     | 0.53              |
| 2:N:192:ASN:HB2  | 2:N:279:GLN:NE2  | 2.23                     | 0.53              |
| 1:O:185:ILE:HD12 | 1:O:204:MET:SD   | 2.48                     | 0.53              |
| 1:E:174:THR:HG23 | 1:E:174:THR:O    | 2.07                     | 0.53              |
| 1:I:39:ASN:CG    | 1:I:43:VAL:HG13  | 2.32                     | 0.53              |
| 2:J:74:THR:HB    | 2:J:82:TYR:O     | 2.08                     | 0.53              |
| 2:J:224:GLN:NE2  | 2:J:231:ILE:HD13 | 2.23                     | 0.53              |
| 2:J:270:SER:C    | 2:J:271:ILE:HD12 | 2.33                     | 0.53              |
| 2:L:117:GLY:O    | 2:L:155:VAL:HA   | 2.08                     | 0.53              |
| 2:L:131:LEU:HD23 | 2:L:131:LEU:C    | 2.33                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:L:270:SER:C    | 2:L:271:ILE:HD12 | 2.33                     | 0.53              |
| 2:N:30:VAL:HA    | 2:N:111:PRO:HB2  | 1.88                     | 0.53              |
| 2:N:40:THR:HG22  | 2:N:40:THR:O     | 2.09                     | 0.53              |
| 2:N:224:GLN:NE2  | 2:N:231:ILE:HD13 | 2.24                     | 0.53              |
| 2:P:74:THR:HB    | 2:P:82:TYR:O     | 2.08                     | 0.53              |
| 1:C:140:LEU:HB2  | 1:C:177:LEU:HD22 | 1.90                     | 0.53              |
| 1:C:184:ASN:O    | 1:C:186:THR:HG23 | 2.09                     | 0.53              |
| 2:D:120:ILE:CG2  | 2:D:126:ILE:HD11 | 2.30                     | 0.53              |
| 2:H:5:THR:HG23   | 2:H:7:ASN:H      | 1.73                     | 0.53              |
| 2:J:174:ASP:HB3  | 2:J:176:PRO:HD2  | 1.91                     | 0.53              |
| 1:K:101:ASN:ND2  | 2:L:268:VAL:H    | 2.07                     | 0.53              |
| 1:M:101:ASN:ND2  | 2:N:268:VAL:H    | 2.07                     | 0.53              |
| 2:P:40:THR:O     | 2:P:40:THR:HG22  | 2.08                     | 0.53              |
| 2:P:224:GLN:NE2  | 2:P:231:ILE:HD13 | 2.24                     | 0.53              |
| 2:L:28:VAL:O     | 2:L:156:VAL:HA   | 2.08                     | 0.53              |
| 2:N:270:SER:C    | 2:N:271:ILE:HD12 | 2.33                     | 0.53              |
| 1:A:140:LEU:HB2  | 1:A:177:LEU:HD22 | 1.91                     | 0.53              |
| 1:C:205:GLU:OXT  | 1:C:205:GLU:HG3  | 2.09                     | 0.53              |
| 1:G:205:GLU:HG3  | 1:G:205:GLU:OXT  | 2.09                     | 0.53              |
| 2:P:270:SER:C    | 2:P:271:ILE:HD12 | 2.33                     | 0.53              |
| 2:H:83:PRO:O     | 2:H:86:THR:HA    | 2.08                     | 0.53              |
| 2:H:173:PRO:HG3  | 2:H:179:VAL:CG1  | 2.39                     | 0.53              |
| 1:I:133:PHE:CE1  | 1:I:202:GLY:HA2  | 2.43                     | 0.53              |
| 1:K:133:PHE:CE1  | 1:K:202:GLY:HA2  | 2.44                     | 0.53              |
| 1:M:39:ASN:CG    | 1:M:43:VAL:HG13  | 2.33                     | 0.53              |
| 2:N:71:PHE:HE2   | 2:N:111:PRO:HG3  | 1.73                     | 0.53              |
| 2:N:131:LEU:HD23 | 2:N:131:LEU:C    | 2.34                     | 0.53              |
| 2:P:4:LYS:HA     | 2:P:10:ALA:HA    | 1.90                     | 0.53              |
| 2:P:20:VAL:HG12  | 2:P:22:VAL:HG13  | 1.89                     | 0.53              |
| 1:C:186:THR:HG21 | 1:C:199:LYS:NZ   | 2.23                     | 0.53              |
| 2:D:63:ALA:HB1   | 2:D:67:VAL:HG12  | 1.89                     | 0.53              |
| 2:L:174:ASP:HB3  | 2:L:176:PRO:HD2  | 1.91                     | 0.53              |
| 1:C:197:THR:HB   | 1:C:198:PRO:HD2  | 1.90                     | 0.53              |
| 1:G:184:ASN:O    | 1:G:186:THR:HG23 | 2.08                     | 0.53              |
| 2:H:7:ASN:HB2    | 4:H:1661:HOH:O   | 2.09                     | 0.53              |
| 1:I:101:ASN:ND2  | 2:J:268:VAL:H    | 2.07                     | 0.53              |
| 2:J:60:ARG:HG3   | 2:J:61:GLY:N     | 2.23                     | 0.53              |
| 2:L:192:ASN:HB2  | 2:L:279:GLN:NE2  | 2.24                     | 0.53              |
| 2:L:220:GLY:HA2  | 2:L:259:THR:OG1  | 2.06                     | 0.53              |
| 1:M:191:ASN:HD21 | 1:M:195:ALA:HB3  | 1.74                     | 0.53              |
| 1:O:98:LEU:C     | 1:O:98:LEU:HD13  | 2.33                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:186:THR:HG21 | 1:E:199:LYS:NZ   | 2.24                     | 0.53              |
| 1:M:133:PHE:CE1  | 1:M:202:GLY:HA2  | 2.44                     | 0.53              |
| 2:N:4:LYS:HA     | 2:N:10:ALA:HA    | 1.90                     | 0.53              |
| 2:N:201:THR:HA   | 2:N:209:PHE:HA   | 1.90                     | 0.53              |
| 1:O:46:GLY:O     | 1:O:70:ALA:HB3   | 2.09                     | 0.53              |
| 2:P:34:LEU:HD12  | 2:P:35:VAL:N     | 2.20                     | 0.53              |
| 2:P:174:ASP:HB3  | 2:P:176:PRO:HD2  | 1.91                     | 0.53              |
| 2:L:224:GLN:NE2  | 2:L:231:ILE:HD13 | 2.24                     | 0.52              |
| 1:M:28:ASN:O     | 1:M:29:SER:HB3   | 2.09                     | 0.52              |
| 2:N:174:ASP:HB3  | 2:N:176:PRO:HD2  | 1.91                     | 0.52              |
| 2:L:78:SER:H     | 2:L:104:PRO:HB2  | 1.74                     | 0.52              |
| 1:M:46:GLY:O     | 1:M:70:ALA:HB3   | 2.10                     | 0.52              |
| 1:E:156:ASN:C    | 1:E:158:GLY:H    | 2.17                     | 0.52              |
| 1:I:98:LEU:C     | 1:I:98:LEU:HD13  | 2.33                     | 0.52              |
| 2:J:71:PHE:HE2   | 2:J:111:PRO:HG3  | 1.73                     | 0.52              |
| 2:B:185:VAL:HG23 | 2:B:243:VAL:HG11 | 1.90                     | 0.52              |
| 2:D:136:ASN:ND2  | 2:D:136:ASN:C    | 2.67                     | 0.52              |
| 1:E:22:VAL:CG2   | 1:E:65:LEU:HG    | 2.39                     | 0.52              |
| 2:J:78:SER:H     | 2:J:104:PRO:HB2  | 1.75                     | 0.52              |
| 1:K:39:ASN:CG    | 1:K:43:VAL:HG13  | 2.33                     | 0.52              |
| 1:O:131:LEU:HD12 | 1:O:143:ILE:O    | 2.09                     | 0.52              |
| 2:P:78:SER:H     | 2:P:104:PRO:HB2  | 1.75                     | 0.52              |
| 2:P:201:THR:HA   | 2:P:209:PHE:HA   | 1.90                     | 0.52              |
| 2:P:207:SER:O    | 2:P:224:GLN:HG3  | 2.10                     | 0.52              |
| 2:B:120:ILE:HD13 | 2:B:126:ILE:HD11 | 1.90                     | 0.52              |
| 2:D:117:GLY:O    | 2:D:155:VAL:HA   | 2.08                     | 0.52              |
| 2:J:131:LEU:C    | 2:J:131:LEU:HD23 | 2.34                     | 0.52              |
| 2:L:208:ILE:HG21 | 2:L:259:THR:HG22 | 1.91                     | 0.52              |
| 1:A:184:ASN:O    | 1:A:186:THR:HG23 | 2.08                     | 0.52              |
| 2:D:22:VAL:HG23  | 2:D:22:VAL:O     | 2.09                     | 0.52              |
| 1:E:1:GLY:N      | 1:E:26:ASP:CG    | 2.66                     | 0.52              |
| 1:G:1:GLY:N      | 1:G:26:ASP:CG    | 2.68                     | 0.52              |
| 1:I:46:GLY:O     | 1:I:70:ALA:HB3   | 2.09                     | 0.52              |
| 1:I:184:ASN:O    | 1:I:186:THR:HG23 | 2.08                     | 0.52              |
| 1:M:135:ARG:HH12 | 1:M:181:ALA:HB2  | 1.68                     | 0.52              |
| 1:O:101:ASN:ND2  | 2:P:268:VAL:H    | 2.07                     | 0.52              |
| 2:B:174:ASP:O    | 2:B:176:PRO:CD   | 2.58                     | 0.52              |
| 1:C:122:LEU:CD1  | 1:C:126:GLN:HB3  | 2.40                     | 0.52              |
| 2:D:174:ASP:O    | 2:D:176:PRO:CD   | 2.58                     | 0.52              |
| 1:E:184:ASN:O    | 1:E:186:THR:HG23 | 2.08                     | 0.52              |
| 1:G:186:THR:HG21 | 1:G:199:LYS:HZ1  | 1.75                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:186:THR:HG21 | 1:G:199:LYS:NZ   | 2.23                     | 0.52              |
| 2:H:185:VAL:HG23 | 2:H:243:VAL:HG11 | 1.92                     | 0.52              |
| 1:I:140:LEU:HD23 | 1:I:141:THR:N    | 2.25                     | 0.52              |
| 1:K:28:ASN:O     | 1:K:29:SER:HB3   | 2.09                     | 0.52              |
| 2:N:13:ILE:HG23  | 3:N:1506:MAN:C2  | 2.40                     | 0.52              |
| 2:N:208:ILE:HG21 | 2:N:259:THR:HG22 | 1.92                     | 0.52              |
| 1:O:191:ASN:HD21 | 1:O:195:ALA:HB3  | 1.74                     | 0.52              |
| 2:P:131:LEU:HD23 | 2:P:131:LEU:C    | 2.33                     | 0.52              |
| 2:B:83:PRO:O     | 2:B:86:THR:HA    | 2.08                     | 0.52              |
| 1:M:131:LEU:HD12 | 1:M:143:ILE:O    | 2.08                     | 0.52              |
| 2:N:14:GLY:HA2   | 2:N:142:PHE:CD1  | 2.45                     | 0.52              |
| 1:O:140:LEU:HD23 | 1:O:141:THR:N    | 2.25                     | 0.52              |
| 2:H:174:ASP:O    | 2:H:176:PRO:CD   | 2.58                     | 0.52              |
| 1:K:46:GLY:O     | 1:K:70:ALA:HB3   | 2.09                     | 0.52              |
| 1:K:191:ASN:HD21 | 1:K:195:ALA:HB3  | 1.74                     | 0.52              |
| 2:L:43:PHE:CD1   | 2:L:43:PHE:N     | 2.78                     | 0.52              |
| 1:O:28:ASN:O     | 1:O:29:SER:HB3   | 2.09                     | 0.52              |
| 2:B:5:THR:HG23   | 2:B:7:ASN:H      | 1.73                     | 0.52              |
| 2:F:136:ASN:ND2  | 2:F:136:ASN:C    | 2.68                     | 0.52              |
| 1:G:140:LEU:HD23 | 1:G:140:LEU:C    | 2.35                     | 0.52              |
| 2:J:40:THR:O     | 2:J:40:THR:HG22  | 2.09                     | 0.52              |
| 1:K:140:LEU:HD23 | 1:K:141:THR:N    | 2.25                     | 0.52              |
| 2:P:14:GLY:HA2   | 2:P:142:PHE:CD1  | 2.45                     | 0.52              |
| 2:B:173:PRO:HG3  | 2:B:179:VAL:CG1  | 2.39                     | 0.51              |
| 1:C:186:THR:HG21 | 1:C:199:LYS:HZ1  | 1.75                     | 0.51              |
| 1:E:205:GLU:HG3  | 1:E:205:GLU:OXT  | 2.09                     | 0.51              |
| 1:I:191:ASN:HD21 | 1:I:195:ALA:HB3  | 1.74                     | 0.51              |
| 2:N:164:SER:HB2  | 2:N:184:THR:O    | 2.10                     | 0.51              |
| 1:A:85:MET:O     | 1:A:110:ARG:HA   | 2.10                     | 0.51              |
| 1:A:140:LEU:HD23 | 1:A:140:LEU:C    | 2.35                     | 0.51              |
| 1:A:186:THR:HG21 | 1:A:199:LYS:NZ   | 2.25                     | 0.51              |
| 1:C:144:ASN:OD1  | 1:C:146:THR:HG23 | 2.10                     | 0.51              |
| 2:F:33:ASN:ND2   | 2:F:110:THR:OG1  | 2.44                     | 0.51              |
| 2:F:185:VAL:HG23 | 2:F:243:VAL:HG11 | 1.91                     | 0.51              |
| 2:H:63:ALA:HB1   | 2:H:67:VAL:HG12  | 1.91                     | 0.51              |
| 2:L:14:GLY:HA2   | 2:L:142:PHE:CD1  | 2.45                     | 0.51              |
| 2:N:34:LEU:HD12  | 2:N:35:VAL:N     | 2.20                     | 0.51              |
| 2:N:78:SER:H     | 2:N:104:PRO:HB2  | 1.75                     | 0.51              |
| 1:O:160:ARG:CG   | 1:O:178:PRO:HG3  | 2.41                     | 0.51              |
| 1:A:133:PHE:CD2  | 1:A:140:LEU:HD21 | 2.30                     | 0.51              |
| 1:C:156:ASN:C    | 1:C:158:GLY:H    | 2.17                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:85:MET:O     | 1:E:110:ARG:HA   | 2.10                     | 0.51              |
| 1:M:160:ARG:CG   | 1:M:178:PRO:HG3  | 2.41                     | 0.51              |
| 1:A:144:ASN:OD1  | 1:A:146:THR:HG23 | 2.10                     | 0.51              |
| 1:E:122:LEU:CD1  | 1:E:126:GLN:HB3  | 2.40                     | 0.51              |
| 1:G:144:ASN:OD1  | 1:G:146:THR:HG23 | 2.11                     | 0.51              |
| 2:H:211:ASN:ND2  | 2:H:269:GLN:H    | 2.09                     | 0.51              |
| 1:I:28:ASN:O     | 1:I:29:SER:HB3   | 2.09                     | 0.51              |
| 2:N:207:SER:O    | 2:N:224:GLN:HG3  | 2.10                     | 0.51              |
| 2:P:208:ILE:HG21 | 2:P:259:THR:HG22 | 1.92                     | 0.51              |
| 1:C:140:LEU:HD23 | 1:C:140:LEU:C    | 2.35                     | 0.51              |
| 2:D:211:ASN:HD21 | 2:D:269:GLN:H    | 1.58                     | 0.51              |
| 2:H:215:PHE:O    | 2:H:216:SER:C    | 2.54                     | 0.51              |
| 1:A:122:LEU:CD1  | 1:A:126:GLN:HB3  | 2.40                     | 0.51              |
| 2:B:117:GLY:O    | 2:B:155:VAL:HA   | 2.09                     | 0.51              |
| 2:B:211:ASN:C    | 2:B:211:ASN:ND2  | 2.68                     | 0.51              |
| 1:C:13:ALA:HB3   | 1:C:118:ALA:H    | 1.76                     | 0.51              |
| 2:F:211:ASN:HD21 | 2:F:269:GLN:H    | 1.57                     | 0.51              |
| 1:K:160:ARG:CG   | 1:K:178:PRO:HG3  | 2.41                     | 0.51              |
| 2:N:43:PHE:N     | 2:N:43:PHE:CD1   | 2.78                     | 0.51              |
| 2:H:120:ILE:CG2  | 2:H:126:ILE:HD11 | 2.31                     | 0.51              |
| 2:J:67:VAL:HG21  | 2:J:126:ILE:CG2  | 2.35                     | 0.51              |
| 2:J:208:ILE:HG21 | 2:J:259:THR:HG22 | 1.91                     | 0.51              |
| 2:N:38:LEU:C     | 2:N:40:THR:N     | 2.67                     | 0.51              |
| 1:A:22:VAL:CG2   | 1:A:65:LEU:HG    | 2.41                     | 0.51              |
| 1:A:94:ASP:C     | 1:A:96:SER:H     | 2.18                     | 0.51              |
| 1:C:102:THR:C    | 2:D:171:THR:HG22 | 2.36                     | 0.51              |
| 2:F:67:VAL:CG2   | 2:F:126:ILE:HG12 | 2.41                     | 0.51              |
| 1:I:66:ARG:HG2   | 1:I:66:ARG:HH11  | 1.75                     | 0.51              |
| 2:J:43:PHE:N     | 2:J:43:PHE:CD1   | 2.79                     | 0.51              |
| 1:M:66:ARG:HG2   | 1:M:66:ARG:HH11  | 1.76                     | 0.51              |
| 1:M:140:LEU:HD23 | 1:M:141:THR:N    | 2.25                     | 0.51              |
| 2:P:190:SER:HA   | 2:P:244:GLY:HA2  | 1.93                     | 0.51              |
| 1:C:22:VAL:CG2   | 1:C:65:LEU:HG    | 2.41                     | 0.51              |
| 2:D:5:THR:HG23   | 2:D:7:ASN:H      | 1.76                     | 0.51              |
| 2:F:174:ASP:O    | 2:F:176:PRO:CD   | 2.59                     | 0.51              |
| 2:H:211:ASN:HD21 | 2:H:269:GLN:H    | 1.57                     | 0.51              |
| 1:K:66:ARG:HG2   | 1:K:66:ARG:HH11  | 1.76                     | 0.51              |
| 2:N:19:ASN:HD21  | 2:P:219:GLN:CD   | 2.19                     | 0.51              |
| 2:P:43:PHE:N     | 2:P:43:PHE:CD1   | 2.78                     | 0.51              |
| 1:A:205:GLU:HG3  | 1:A:205:GLU:OXT  | 2.10                     | 0.51              |
| 2:B:215:PHE:O    | 2:B:216:SER:C    | 2.54                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:174:ASP:O    | 2:D:176:PRO:HD2  | 2.11                     | 0.51              |
| 2:H:174:ASP:O    | 2:H:176:PRO:HD2  | 2.11                     | 0.51              |
| 1:I:160:ARG:CG   | 1:I:178:PRO:HG3  | 2.41                     | 0.51              |
| 1:O:67:ILE:N     | 1:O:67:ILE:HD12  | 2.26                     | 0.51              |
| 2:P:164:SER:HB2  | 2:P:184:THR:O    | 2.11                     | 0.51              |
| 2:B:163:VAL:CG1  | 2:B:183:LEU:HD21 | 2.41                     | 0.50              |
| 2:F:215:PHE:O    | 2:F:216:SER:C    | 2.54                     | 0.50              |
| 1:G:122:LEU:CD1  | 1:G:126:GLN:HB3  | 2.40                     | 0.50              |
| 2:L:96:ASN:N     | 2:L:96:ASN:ND2   | 2.58                     | 0.50              |
| 1:M:47:ARG:HH22  | 1:M:74:GLN:HB2   | 1.76                     | 0.50              |
| 2:N:190:SER:HA   | 2:N:244:GLY:HA2  | 1.93                     | 0.50              |
| 2:B:131:LEU:HB3  | 2:B:144:PHE:HB2  | 1.93                     | 0.50              |
| 2:B:227:ARG:HA   | 2:B:251:GLY:O    | 2.11                     | 0.50              |
| 2:D:226:THR:HG22 | 2:D:253:THR:HB   | 1.94                     | 0.50              |
| 1:E:140:LEU:HD23 | 1:E:140:LEU:C    | 2.36                     | 0.50              |
| 1:I:9:VAL:O      | 1:I:113:LEU:HA   | 2.11                     | 0.50              |
| 2:L:163:VAL:HA   | 2:L:185:VAL:CG2  | 2.35                     | 0.50              |
| 1:A:13:ALA:HB3   | 1:A:118:ALA:H    | 1.76                     | 0.50              |
| 2:B:174:ASP:O    | 2:B:176:PRO:HD2  | 2.11                     | 0.50              |
| 1:E:133:PHE:CD2  | 1:E:140:LEU:HD21 | 2.31                     | 0.50              |
| 2:H:33:ASN:ND2   | 2:H:110:THR:OG1  | 2.44                     | 0.50              |
| 2:H:184:THR:HG22 | 2:H:249:SER:CA   | 2.41                     | 0.50              |
| 2:J:96:ASN:N     | 2:J:96:ASN:ND2   | 2.59                     | 0.50              |
| 2:L:202:ALA:HB2  | 2:L:210:THR:CG2  | 2.34                     | 0.50              |
| 2:P:96:ASN:N     | 2:P:96:ASN:ND2   | 2.59                     | 0.50              |
| 2:B:136:ASN:ND2  | 2:B:136:ASN:C    | 2.68                     | 0.50              |
| 1:E:94:ASP:C     | 1:E:96:SER:H     | 2.19                     | 0.50              |
| 1:E:102:THR:C    | 2:F:171:THR:HG22 | 2.36                     | 0.50              |
| 1:E:144:ASN:OD1  | 1:E:146:THR:HG23 | 2.12                     | 0.50              |
| 2:J:14:GLY:HA2   | 2:J:142:PHE:CD1  | 2.47                     | 0.50              |
| 2:J:207:SER:O    | 2:J:224:GLN:HG3  | 2.10                     | 0.50              |
| 1:K:47:ARG:HH22  | 1:K:74:GLN:HB2   | 1.76                     | 0.50              |
| 1:K:67:ILE:HD12  | 1:K:67:ILE:N     | 2.26                     | 0.50              |
| 2:L:66:GLY:HA3   | 2:L:119:ALA:O    | 2.11                     | 0.50              |
| 2:B:184:THR:HG22 | 2:B:249:SER:CA   | 2.40                     | 0.50              |
| 2:D:211:ASN:ND2  | 2:D:269:GLN:H    | 2.10                     | 0.50              |
| 1:E:132:ARG:HB3  | 1:E:205:GLU:HB3  | 1.92                     | 0.50              |
| 1:G:85:MET:O     | 1:G:110:ARG:HA   | 2.11                     | 0.50              |
| 1:I:101:ASN:HD22 | 2:J:268:VAL:CG2  | 2.24                     | 0.50              |
| 2:N:66:GLY:HA3   | 2:N:119:ALA:O    | 2.11                     | 0.50              |
| 1:A:194:GLY:O    | 2:B:158:THR:HG21 | 2.11                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:94:ASP:C     | 1:C:96:SER:H     | 2.19                     | 0.50              |
| 1:C:133:PHE:CD2  | 1:C:140:LEU:HD21 | 2.31                     | 0.50              |
| 1:C:194:GLY:O    | 2:D:158:THR:HG21 | 2.12                     | 0.50              |
| 2:D:215:PHE:O    | 2:D:216:SER:C    | 2.54                     | 0.50              |
| 2:F:184:THR:HG22 | 2:F:249:SER:CA   | 2.42                     | 0.50              |
| 1:G:114:TYR:CE2  | 1:G:149:TYR:HB2  | 2.47                     | 0.50              |
| 2:H:163:VAL:CG1  | 2:H:183:LEU:HD21 | 2.41                     | 0.50              |
| 1:O:66:ARG:HG2   | 1:O:66:ARG:HH11  | 1.77                     | 0.50              |
| 2:H:166:ARG:O    | 2:H:167:ASP:HB2  | 2.12                     | 0.50              |
| 2:H:211:ASN:C    | 2:H:211:ASN:ND2  | 2.66                     | 0.50              |
| 1:I:67:ILE:HD12  | 1:I:67:ILE:N     | 2.26                     | 0.50              |
| 2:B:126:ILE:CD1  | 2:B:150:ALA:HB2  | 2.24                     | 0.50              |
| 1:C:85:MET:O     | 1:C:110:ARG:HA   | 2.11                     | 0.50              |
| 1:E:12:PRO:HD2   | 1:E:15:GLN:HG3   | 1.92                     | 0.50              |
| 1:E:194:GLY:O    | 2:F:158:THR:HG21 | 2.12                     | 0.50              |
| 2:F:167:ASP:CG   | 2:F:168:VAL:HG12 | 2.37                     | 0.50              |
| 2:F:211:ASN:ND2  | 2:F:269:GLN:H    | 2.10                     | 0.50              |
| 1:G:186:THR:CG2  | 1:G:199:LYS:NZ   | 2.75                     | 0.50              |
| 2:H:22:VAL:O     | 2:H:22:VAL:HG23  | 2.12                     | 0.50              |
| 2:H:136:ASN:ND2  | 2:H:136:ASN:C    | 2.68                     | 0.50              |
| 2:J:66:GLY:HA3   | 2:J:119:ALA:O    | 2.11                     | 0.50              |
| 2:L:207:SER:O    | 2:L:224:GLN:HG3  | 2.10                     | 0.50              |
| 1:M:149:TYR:CD2  | 1:M:168:PRO:HA   | 2.47                     | 0.50              |
| 2:D:185:VAL:HG23 | 2:D:243:VAL:HG11 | 1.93                     | 0.50              |
| 2:F:174:ASP:O    | 2:F:176:PRO:HD2  | 2.12                     | 0.50              |
| 2:H:67:VAL:CG2   | 2:H:126:ILE:HG12 | 2.42                     | 0.50              |
| 2:J:190:SER:HA   | 2:J:244:GLY:HA2  | 1.93                     | 0.50              |
| 1:K:9:VAL:O      | 1:K:113:LEU:HA   | 2.11                     | 0.50              |
| 1:O:9:VAL:O      | 1:O:113:LEU:HA   | 2.11                     | 0.50              |
| 1:O:47:ARG:HH22  | 1:O:74:GLN:HB2   | 1.76                     | 0.50              |
| 2:P:126:ILE:HD12 | 2:P:148:ILE:HG22 | 1.94                     | 0.50              |
| 1:A:102:THR:C    | 2:B:171:THR:HG22 | 2.37                     | 0.49              |
| 2:B:211:ASN:ND2  | 2:B:269:GLN:H    | 2.10                     | 0.49              |
| 2:B:211:ASN:HD21 | 2:B:269:GLN:H    | 1.57                     | 0.49              |
| 1:C:11:TYR:CE2   | 1:C:69:ASP:HB2   | 2.47                     | 0.49              |
| 1:C:132:ARG:HB3  | 1:C:205:GLU:HB3  | 1.92                     | 0.49              |
| 1:E:186:THR:HG21 | 1:E:199:LYS:HZ1  | 1.77                     | 0.49              |
| 2:F:173:PRO:HG3  | 2:F:179:VAL:CG1  | 2.39                     | 0.49              |
| 1:G:22:VAL:CG2   | 1:G:65:LEU:HG    | 2.42                     | 0.49              |
| 1:G:102:THR:C    | 2:H:171:THR:HG22 | 2.37                     | 0.49              |
| 1:G:122:LEU:C    | 1:G:122:LEU:HD12 | 2.37                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:149:TYR:CD2  | 1:O:168:PRO:HA   | 2.47                     | 0.49              |
| 2:B:22:VAL:HG23  | 2:B:22:VAL:O     | 2.11                     | 0.49              |
| 1:E:142:LEU:H    | 1:E:142:LEU:HD22 | 1.77                     | 0.49              |
| 2:L:190:SER:HA   | 2:L:244:GLY:HA2  | 1.93                     | 0.49              |
| 1:M:67:ILE:N     | 1:M:67:ILE:HD12  | 2.26                     | 0.49              |
| 1:O:179:SER:C    | 1:O:181:ALA:H    | 2.21                     | 0.49              |
| 1:A:1:GLY:N      | 1:A:26:ASP:CG    | 2.69                     | 0.49              |
| 1:A:12:PRO:HD2   | 1:A:15:GLN:HG3   | 1.93                     | 0.49              |
| 2:B:163:VAL:HG13 | 2:B:183:LEU:HD21 | 1.95                     | 0.49              |
| 1:C:1:GLY:N      | 1:C:26:ASP:CG    | 2.70                     | 0.49              |
| 2:F:227:ARG:HA   | 2:F:251:GLY:O    | 2.12                     | 0.49              |
| 1:G:94:ASP:C     | 1:G:96:SER:H     | 2.18                     | 0.49              |
| 2:H:167:ASP:CG   | 2:H:168:VAL:HG12 | 2.38                     | 0.49              |
| 1:I:47:ARG:HH22  | 1:I:74:GLN:HB2   | 1.76                     | 0.49              |
| 1:I:149:TYR:CD2  | 1:I:168:PRO:HA   | 2.47                     | 0.49              |
| 1:I:179:SER:C    | 1:I:181:ALA:H    | 2.20                     | 0.49              |
| 2:J:225:LEU:O    | 2:J:231:ILE:HG23 | 2.12                     | 0.49              |
| 2:L:271:ILE:HD12 | 2:L:271:ILE:N    | 2.28                     | 0.49              |
| 1:C:186:THR:CG2  | 1:C:199:LYS:NZ   | 2.75                     | 0.49              |
| 2:J:75:VAL:O     | 2:J:75:VAL:HG13  | 2.11                     | 0.49              |
| 2:J:145:VAL:HG12 | 2:J:146:TRP:N    | 2.27                     | 0.49              |
| 2:J:253:THR:HG22 | 2:J:255:ASN:ND2  | 2.21                     | 0.49              |
| 1:K:11:TYR:CZ    | 1:K:69:ASP:HB2   | 2.47                     | 0.49              |
| 1:K:149:TYR:CD2  | 1:K:168:PRO:HA   | 2.47                     | 0.49              |
| 2:N:208:ILE:HG23 | 2:N:257:ALA:CB   | 2.40                     | 0.49              |
| 2:N:227:ARG:HA   | 2:N:251:GLY:O    | 2.13                     | 0.49              |
| 2:P:145:VAL:HG12 | 2:P:146:TRP:N    | 2.27                     | 0.49              |
| 2:P:271:ILE:HD12 | 2:P:271:ILE:N    | 2.28                     | 0.49              |
| 1:G:194:GLY:O    | 2:H:158:THR:HG21 | 2.11                     | 0.49              |
| 2:H:163:VAL:HG13 | 2:H:183:LEU:HD21 | 1.94                     | 0.49              |
| 2:J:164:SER:HB2  | 2:J:184:THR:O    | 2.11                     | 0.49              |
| 1:K:41:ASP:HB2   | 1:K:43:VAL:HG12  | 1.94                     | 0.49              |
| 2:L:21:TYR:CB    | 2:L:151:ASN:HD21 | 2.24                     | 0.49              |
| 1:M:9:VAL:O      | 1:M:113:LEU:HA   | 2.11                     | 0.49              |
| 2:N:225:LEU:O    | 2:N:231:ILE:HG23 | 2.12                     | 0.49              |
| 1:O:41:ASP:HB2   | 1:O:43:VAL:HG12  | 1.94                     | 0.49              |
| 1:A:132:ARG:HB3  | 1:A:205:GLU:HB3  | 1.93                     | 0.49              |
| 2:D:163:VAL:CG1  | 2:D:183:LEU:HD21 | 2.43                     | 0.49              |
| 2:F:211:ASN:C    | 2:F:211:ASN:ND2  | 2.66                     | 0.49              |
| 1:I:11:TYR:CZ    | 1:I:69:ASP:HB2   | 2.47                     | 0.49              |
| 2:L:164:SER:HB2  | 2:L:184:THR:O    | 2.11                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:140:LEU:HD22 | 1:M:142:LEU:HD22 | 1.95                     | 0.49              |
| 2:N:145:VAL:HG12 | 2:N:146:TRP:N    | 2.27                     | 0.49              |
| 1:O:11:TYR:CZ    | 1:O:69:ASP:HB2   | 2.47                     | 0.49              |
| 2:P:38:LEU:C     | 2:P:40:THR:N     | 2.67                     | 0.49              |
| 2:P:66:GLY:HA3   | 2:P:119:ALA:O    | 2.12                     | 0.49              |
| 2:P:227:ARG:HA   | 2:P:251:GLY:O    | 2.13                     | 0.49              |
| 2:D:38:LEU:C     | 2:D:40:THR:N     | 2.69                     | 0.49              |
| 1:E:13:ALA:HB3   | 1:E:118:ALA:H    | 1.76                     | 0.49              |
| 1:G:132:ARG:HB3  | 1:G:205:GLU:HB3  | 1.93                     | 0.49              |
| 1:M:101:ASN:HD22 | 2:N:268:VAL:CG2  | 2.23                     | 0.49              |
| 1:A:12:PRO:HB2   | 1:A:15:GLN:HG2   | 1.93                     | 0.49              |
| 2:D:185:VAL:HG11 | 2:D:276:PHE:CE2  | 2.48                     | 0.49              |
| 2:J:45:HIS:HB3   | 2:J:100:ASP:HA   | 1.95                     | 0.49              |
| 2:J:126:ILE:HD12 | 2:J:148:ILE:HG22 | 1.94                     | 0.49              |
| 1:K:140:LEU:HD22 | 1:K:142:LEU:HD22 | 1.95                     | 0.49              |
| 2:N:271:ILE:HD12 | 2:N:271:ILE:N    | 2.27                     | 0.49              |
| 1:O:140:LEU:HD22 | 1:O:142:LEU:HD22 | 1.95                     | 0.49              |
| 2:B:67:VAL:CG2   | 2:B:126:ILE:HG12 | 2.42                     | 0.49              |
| 2:D:211:ASN:C    | 2:D:211:ASN:ND2  | 2.67                     | 0.49              |
| 2:F:185:VAL:HG11 | 2:F:276:PHE:CE2  | 2.48                     | 0.49              |
| 2:H:185:VAL:HG11 | 2:H:276:PHE:CE2  | 2.48                     | 0.49              |
| 2:D:163:VAL:HG13 | 2:D:183:LEU:HD21 | 1.95                     | 0.49              |
| 1:E:122:LEU:C    | 1:E:122:LEU:HD12 | 2.38                     | 0.49              |
| 2:F:163:VAL:CG1  | 2:F:183:LEU:HD21 | 2.42                     | 0.49              |
| 2:F:173:PRO:O    | 2:F:256:TYR:HE1  | 1.96                     | 0.49              |
| 1:I:47:ARG:HH22  | 1:I:74:GLN:NE2   | 1.92                     | 0.49              |
| 2:J:271:ILE:HD12 | 2:J:271:ILE:N    | 2.27                     | 0.49              |
| 1:M:11:TYR:CZ    | 1:M:69:ASP:HB2   | 2.47                     | 0.49              |
| 2:P:163:VAL:HA   | 2:P:185:VAL:CG2  | 2.35                     | 0.49              |
| 2:P:225:LEU:O    | 2:P:231:ILE:HG23 | 2.13                     | 0.49              |
| 1:C:1:GLY:H1     | 1:C:26:ASP:CG    | 2.20                     | 0.48              |
| 1:C:12:PRO:HD2   | 1:C:15:GLN:HG3   | 1.94                     | 0.48              |
| 2:F:66:GLY:HA3   | 2:F:119:ALA:O    | 2.13                     | 0.48              |
| 2:H:227:ARG:HA   | 2:H:251:GLY:O    | 2.13                     | 0.48              |
| 1:I:27:GLU:HA    | 1:I:60:LYS:CG    | 2.43                     | 0.48              |
| 1:I:140:LEU:HD22 | 1:I:142:LEU:HD22 | 1.95                     | 0.48              |
| 2:J:34:LEU:HD12  | 2:J:35:VAL:N     | 2.21                     | 0.48              |
| 1:M:39:ASN:HB3   | 1:M:45:ASP:OD2   | 2.13                     | 0.48              |
| 2:N:267:ASN:HB3  | 2:N:269:GLN:HE21 | 1.78                     | 0.48              |
| 1:A:122:LEU:C    | 1:A:122:LEU:HD12 | 2.38                     | 0.48              |
| 1:G:13:ALA:HB3   | 1:G:118:ALA:H    | 1.76                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:66:GLY:HA3   | 2:H:119:ALA:O    | 2.14                     | 0.48              |
| 2:J:38:LEU:C     | 2:J:40:THR:N     | 2.66                     | 0.48              |
| 2:J:202:ALA:HB2  | 2:J:210:THR:CG2  | 2.34                     | 0.48              |
| 1:K:39:ASN:HB3   | 1:K:45:ASP:OD2   | 2.13                     | 0.48              |
| 1:K:101:ASN:HD22 | 2:L:268:VAL:CG2  | 2.24                     | 0.48              |
| 2:L:126:ILE:HD12 | 2:L:148:ILE:HG22 | 1.95                     | 0.48              |
| 2:N:164:SER:O    | 2:N:183:LEU:HD23 | 2.13                     | 0.48              |
| 2:P:75:VAL:O     | 2:P:75:VAL:HG13  | 2.13                     | 0.48              |
| 2:P:267:ASN:HB3  | 2:P:269:GLN:HE21 | 1.78                     | 0.48              |
| 1:A:142:LEU:H    | 1:A:142:LEU:HD22 | 1.78                     | 0.48              |
| 1:A:187:TYR:C    | 1:A:187:TYR:CD1  | 2.91                     | 0.48              |
| 2:B:63:ALA:HB1   | 2:B:67:VAL:HG12  | 1.94                     | 0.48              |
| 1:I:41:ASP:HB2   | 1:I:43:VAL:HG12  | 1.94                     | 0.48              |
| 2:L:267:ASN:HB3  | 2:L:269:GLN:HE21 | 1.79                     | 0.48              |
| 1:M:6:ALA:HB3    | 1:M:20:LEU:CD1   | 2.44                     | 0.48              |
| 1:O:101:ASN:HD22 | 2:P:268:VAL:CG2  | 2.23                     | 0.48              |
| 2:B:166:ARG:O    | 2:B:167:ASP:HB2  | 2.13                     | 0.48              |
| 1:E:11:TYR:CE2   | 1:E:69:ASP:HB2   | 2.49                     | 0.48              |
| 2:H:131:LEU:HB3  | 2:H:144:PHE:HB2  | 1.96                     | 0.48              |
| 2:H:181:ILE:HB   | 2:H:252:LEU:HB2  | 1.96                     | 0.48              |
| 1:I:39:ASN:HB3   | 1:I:45:ASP:OD2   | 2.13                     | 0.48              |
| 2:J:19:ASN:HD21  | 2:L:219:GLN:CD   | 2.21                     | 0.48              |
| 2:J:96:ASN:HD22  | 2:J:96:ASN:N     | 2.10                     | 0.48              |
| 1:K:179:SER:C    | 1:K:181:ALA:H    | 2.20                     | 0.48              |
| 2:L:8:GLY:O      | 2:L:9:THR:C      | 2.57                     | 0.48              |
| 2:L:145:VAL:HG12 | 2:L:146:TRP:N    | 2.28                     | 0.48              |
| 2:D:33:ASN:ND2   | 2:D:110:THR:OG1  | 2.46                     | 0.48              |
| 2:D:66:GLY:HA3   | 2:D:119:ALA:O    | 2.13                     | 0.48              |
| 2:H:172:LEU:N    | 2:H:173:PRO:CD   | 2.75                     | 0.48              |
| 2:P:45:HIS:HB3   | 2:P:100:ASP:HA   | 1.96                     | 0.48              |
| 1:A:71:THR:HG23  | 1:A:71:THR:O     | 2.14                     | 0.48              |
| 2:B:33:ASN:ND2   | 2:B:110:THR:OG1  | 2.46                     | 0.48              |
| 2:B:66:GLY:HA3   | 2:B:119:ALA:O    | 2.13                     | 0.48              |
| 2:B:181:ILE:HB   | 2:B:252:LEU:HB2  | 1.95                     | 0.48              |
| 2:D:167:ASP:CG   | 2:D:168:VAL:HG12 | 2.37                     | 0.48              |
| 1:G:11:TYR:CE2   | 1:G:69:ASP:HB2   | 2.48                     | 0.48              |
| 2:J:17:SER:HB2   | 2:L:262:GLN:OE1  | 2.13                     | 0.48              |
| 1:K:6:ALA:HB3    | 1:K:20:LEU:CD1   | 2.43                     | 0.48              |
| 1:O:39:ASN:HB3   | 1:O:45:ASP:OD2   | 2.13                     | 0.48              |
| 2:P:253:THR:HG22 | 2:P:255:ASN:ND2  | 2.22                     | 0.48              |
| 2:B:172:LEU:N    | 2:B:173:PRO:CD   | 2.76                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:140:LEU:H    | 1:C:177:LEU:HB2  | 1.79                     | 0.48              |
| 2:F:166:ARG:O    | 2:F:167:ASP:HB2  | 2.14                     | 0.48              |
| 2:L:45:HIS:HB3   | 2:L:100:ASP:HA   | 1.96                     | 0.48              |
| 2:L:225:LEU:O    | 2:L:231:ILE:HG23 | 2.12                     | 0.48              |
| 2:L:227:ARG:CD   | 2:L:232:ILE:HD11 | 2.44                     | 0.48              |
| 1:M:27:GLU:HA    | 1:M:60:LYS:CG    | 2.43                     | 0.48              |
| 1:M:37:VAL:HG11  | 1:M:48:PHE:HB2   | 1.96                     | 0.48              |
| 1:M:179:SER:C    | 1:M:181:ALA:H    | 2.20                     | 0.48              |
| 2:N:17:SER:HB2   | 2:P:262:GLN:OE1  | 2.13                     | 0.48              |
| 2:N:227:ARG:CD   | 2:N:232:ILE:HD11 | 2.44                     | 0.48              |
| 1:C:179:SER:C    | 1:C:181:ALA:N    | 2.51                     | 0.48              |
| 2:D:77:TYR:CE2   | 2:D:90:THR:HG21  | 2.49                     | 0.48              |
| 2:D:166:ARG:O    | 2:D:167:ASP:HB2  | 2.14                     | 0.48              |
| 2:D:173:PRO:O    | 2:D:256:TYR:HE1  | 1.97                     | 0.48              |
| 1:E:140:LEU:H    | 1:E:177:LEU:HB2  | 1.78                     | 0.48              |
| 1:G:140:LEU:H    | 1:G:177:LEU:HB2  | 1.78                     | 0.48              |
| 2:L:227:ARG:HA   | 2:L:251:GLY:O    | 2.13                     | 0.48              |
| 1:A:186:THR:CG2  | 1:A:199:LYS:NZ   | 2.76                     | 0.48              |
| 2:D:173:PRO:HG3  | 2:D:179:VAL:CG1  | 2.40                     | 0.48              |
| 1:E:1:GLY:N      | 1:E:26:ASP:OD1   | 2.46                     | 0.48              |
| 1:G:132:ARG:C    | 1:G:133:PHE:CD1  | 2.92                     | 0.48              |
| 2:J:267:ASN:HB3  | 2:J:269:GLN:HE21 | 1.78                     | 0.48              |
| 1:K:37:VAL:HG11  | 1:K:48:PHE:HB2   | 1.96                     | 0.48              |
| 2:N:96:ASN:HD22  | 2:N:96:ASN:N     | 2.12                     | 0.48              |
| 2:N:218:ALA:HA   | 2:N:264:THR:HB   | 1.96                     | 0.48              |
| 2:P:164:SER:O    | 2:P:183:LEU:HD23 | 2.13                     | 0.48              |
| 2:D:227:ARG:HA   | 2:D:251:GLY:O    | 2.13                     | 0.48              |
| 1:E:187:TYR:CD1  | 1:E:187:TYR:C    | 2.92                     | 0.48              |
| 1:I:133:PHE:HD2  | 1:I:140:LEU:HD21 | 1.79                     | 0.48              |
| 2:L:75:VAL:HG13  | 2:L:75:VAL:O     | 2.14                     | 0.48              |
| 2:L:96:ASN:H     | 2:L:96:ASN:ND2   | 2.11                     | 0.48              |
| 2:N:45:HIS:HB3   | 2:N:100:ASP:HA   | 1.95                     | 0.48              |
| 1:A:132:ARG:C    | 1:A:133:PHE:CD1  | 2.92                     | 0.47              |
| 1:E:186:THR:CG2  | 1:E:199:LYS:NZ   | 2.76                     | 0.47              |
| 1:G:71:THR:O     | 1:G:71:THR:HG23  | 2.13                     | 0.47              |
| 2:H:173:PRO:O    | 2:H:256:TYR:HE1  | 1.97                     | 0.47              |
| 2:L:164:SER:O    | 2:L:183:LEU:HD23 | 2.13                     | 0.47              |
| 1:M:41:ASP:HB2   | 1:M:43:VAL:HG12  | 1.94                     | 0.47              |
| 1:M:135:ARG:HH22 | 1:M:181:ALA:CB   | 2.27                     | 0.47              |
| 2:B:173:PRO:O    | 2:B:256:TYR:HE1  | 1.98                     | 0.47              |
| 1:C:71:THR:HG23  | 1:C:71:THR:O     | 2.14                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:134:ARG:NE   | 1:C:141:THR:HG21 | 2.28                     | 0.47              |
| 1:C:187:TYR:CD1  | 1:C:187:TYR:C    | 2.92                     | 0.47              |
| 2:D:181:ILE:HB   | 2:D:252:LEU:HB2  | 1.96                     | 0.47              |
| 1:I:135:ARG:HH22 | 1:I:181:ALA:CB   | 2.27                     | 0.47              |
| 2:J:164:SER:O    | 2:J:183:LEU:HD23 | 2.14                     | 0.47              |
| 1:K:135:ARG:HH22 | 1:K:181:ALA:CB   | 2.27                     | 0.47              |
| 1:M:41:ASP:C     | 1:M:43:VAL:H     | 2.22                     | 0.47              |
| 1:A:1:GLY:N      | 1:A:26:ASP:OD1   | 2.47                     | 0.47              |
| 2:B:167:ASP:CG   | 2:B:168:VAL:HG12 | 2.38                     | 0.47              |
| 1:C:1:GLY:N      | 1:C:26:ASP:OD1   | 2.47                     | 0.47              |
| 2:F:163:VAL:HG13 | 2:F:183:LEU:HD21 | 1.96                     | 0.47              |
| 2:H:77:TYR:CE2   | 2:H:90:THR:HG21  | 2.49                     | 0.47              |
| 1:K:41:ASP:C     | 1:K:43:VAL:H     | 2.22                     | 0.47              |
| 2:N:126:ILE:HD12 | 2:N:148:ILE:HG22 | 1.94                     | 0.47              |
| 1:O:41:ASP:C     | 1:O:43:VAL:H     | 2.22                     | 0.47              |
| 1:O:135:ARG:HH22 | 1:O:181:ALA:CB   | 2.27                     | 0.47              |
| 2:P:48:TYR:H     | 3:P:1607:MAN:H62 | 1.80                     | 0.47              |
| 2:P:155:VAL:HG12 | 2:P:157:PRO:CD   | 2.43                     | 0.47              |
| 1:A:186:THR:HG21 | 1:A:199:LYS:HZ1  | 1.79                     | 0.47              |
| 2:D:38:LEU:C     | 2:D:40:THR:H     | 2.21                     | 0.47              |
| 2:D:184:THR:HG22 | 2:D:249:SER:CA   | 2.43                     | 0.47              |
| 1:G:187:TYR:CD1  | 1:G:187:TYR:C    | 2.92                     | 0.47              |
| 1:I:6:ALA:HB3    | 1:I:20:LEU:CD1   | 2.44                     | 0.47              |
| 1:I:41:ASP:C     | 1:I:43:VAL:H     | 2.22                     | 0.47              |
| 1:M:47:ARG:NH2   | 1:M:74:GLN:NE2   | 2.59                     | 0.47              |
| 1:M:93:MET:HE1   | 1:M:98:LEU:HD23  | 1.96                     | 0.47              |
| 2:P:227:ARG:CD   | 2:P:232:ILE:HD11 | 2.44                     | 0.47              |
| 2:P:267:ASN:CB   | 2:P:269:GLN:HE21 | 2.28                     | 0.47              |
| 1:C:114:TYR:CE2  | 1:C:149:TYR:HB2  | 2.50                     | 0.47              |
| 1:E:12:PRO:HB2   | 1:E:15:GLN:HG2   | 1.96                     | 0.47              |
| 1:E:71:THR:HG23  | 1:E:71:THR:O     | 2.15                     | 0.47              |
| 1:E:114:TYR:CE2  | 1:E:149:TYR:HB2  | 2.49                     | 0.47              |
| 2:F:181:ILE:HB   | 2:F:252:LEU:HB2  | 1.97                     | 0.47              |
| 1:K:136:SER:C    | 1:K:177:LEU:HD23 | 2.39                     | 0.47              |
| 2:L:218:ALA:HA   | 2:L:264:THR:HB   | 1.96                     | 0.47              |
| 2:N:163:VAL:HA   | 2:N:185:VAL:CG2  | 2.36                     | 0.47              |
| 1:O:6:ALA:HB3    | 1:O:20:LEU:CD1   | 2.44                     | 0.47              |
| 1:O:27:GLU:HA    | 1:O:60:LYS:CG    | 2.43                     | 0.47              |
| 1:O:133:PHE:HD2  | 1:O:140:LEU:HD21 | 1.79                     | 0.47              |
| 2:P:218:ALA:HA   | 2:P:264:THR:HB   | 1.96                     | 0.47              |
| 1:A:11:TYR:CE2   | 1:A:69:ASP:HB2   | 2.50                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:60:ARG:HB2   | 2:B:60:ARG:CZ    | 2.45                     | 0.47              |
| 2:B:77:TYR:CE2   | 2:B:90:THR:HG21  | 2.50                     | 0.47              |
| 1:I:185:ILE:O    | 1:I:202:GLY:N    | 2.35                     | 0.47              |
| 2:J:41:GLN:C     | 2:J:42:ILE:HG13  | 2.40                     | 0.47              |
| 2:J:227:ARG:CD   | 2:J:232:ILE:HD11 | 2.44                     | 0.47              |
| 1:K:178:PRO:O    | 1:K:179:SER:HB3  | 2.15                     | 0.47              |
| 2:L:66:GLY:HA2   | 2:L:70:ASN:HD22  | 1.79                     | 0.47              |
| 2:P:53:THR:H     | 2:P:136:ASN:ND2  | 2.13                     | 0.47              |
| 1:A:30:THR:HG22  | 1:A:31:TYR:N     | 2.30                     | 0.47              |
| 1:A:95:LYS:HD3   | 1:A:95:LYS:N     | 2.30                     | 0.47              |
| 1:C:33:ILE:O     | 1:C:54:LEU:HA    | 2.15                     | 0.47              |
| 1:C:132:ARG:C    | 1:C:133:PHE:CD1  | 2.93                     | 0.47              |
| 1:C:141:THR:HB   | 1:C:174:THR:CG2  | 2.41                     | 0.47              |
| 1:C:142:LEU:H    | 1:C:142:LEU:HD22 | 1.78                     | 0.47              |
| 2:D:240:LEU:HD21 | 2:D:250:LEU:HD22 | 1.96                     | 0.47              |
| 1:E:30:THR:HG22  | 1:E:31:TYR:N     | 2.30                     | 0.47              |
| 1:E:95:LYS:HD3   | 1:E:95:LYS:N     | 2.30                     | 0.47              |
| 1:I:47:ARG:NH2   | 1:I:74:GLN:NE2   | 2.58                     | 0.47              |
| 2:J:8:GLY:O      | 2:J:9:THR:C      | 2.57                     | 0.47              |
| 2:J:218:ALA:HA   | 2:J:264:THR:HB   | 1.96                     | 0.47              |
| 2:J:227:ARG:HA   | 2:J:251:GLY:O    | 2.13                     | 0.47              |
| 1:K:27:GLU:HA    | 1:K:60:LYS:CG    | 2.44                     | 0.47              |
| 1:K:47:ARG:HH22  | 1:K:74:GLN:NE2   | 1.92                     | 0.47              |
| 1:K:102:THR:H    | 2:L:269:GLN:HG2  | 1.80                     | 0.47              |
| 2:L:179:VAL:O    | 2:L:179:VAL:HG23 | 2.15                     | 0.47              |
| 1:M:11:TYR:OH    | 1:M:69:ASP:HB2   | 2.14                     | 0.47              |
| 2:N:75:VAL:HG13  | 2:N:75:VAL:O     | 2.14                     | 0.47              |
| 2:N:226:THR:CG2  | 2:N:253:THR:HB   | 2.42                     | 0.47              |
| 1:O:178:PRO:O    | 1:O:179:SER:HB3  | 2.15                     | 0.47              |
| 2:P:41:GLN:C     | 2:P:42:ILE:HG13  | 2.40                     | 0.47              |
| 2:P:66:GLY:HA2   | 2:P:70:ASN:HD22  | 1.79                     | 0.47              |
| 2:P:226:THR:CG2  | 2:P:253:THR:HB   | 2.43                     | 0.47              |
| 2:D:195:TYR:CE1  | 2:D:238:VAL:HB   | 2.50                     | 0.47              |
| 2:D:201:THR:HG23 | 2:D:203:ASP:H    | 1.79                     | 0.47              |
| 2:F:41:GLN:NE2   | 4:F:1523:HOH:O   | 2.48                     | 0.47              |
| 1:G:1:GLY:N      | 1:G:26:ASP:OD1   | 2.48                     | 0.47              |
| 1:G:142:LEU:H    | 1:G:142:LEU:HD22 | 1.78                     | 0.47              |
| 2:H:41:GLN:NE2   | 4:H:1627:HOH:O   | 2.47                     | 0.47              |
| 1:I:11:TYR:OH    | 1:I:69:ASP:HB2   | 2.14                     | 0.47              |
| 2:J:267:ASN:CB   | 2:J:269:GLN:HE21 | 2.28                     | 0.47              |
| 1:K:11:TYR:OH    | 1:K:69:ASP:HB2   | 2.14                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:133:PHE:HD2  | 1:K:140:LEU:HD21 | 1.79                     | 0.47              |
| 2:L:13:ILE:HG23  | 3:L:1504:MAN:C2  | 2.45                     | 0.47              |
| 1:M:178:PRO:O    | 1:M:179:SER:HB3  | 2.15                     | 0.47              |
| 2:N:1:PHE:HD1    | 2:N:144:PHE:CZ   | 2.33                     | 0.47              |
| 2:N:8:GLY:O      | 2:N:9:THR:C      | 2.57                     | 0.47              |
| 2:N:179:VAL:HG23 | 2:N:179:VAL:O    | 2.15                     | 0.47              |
| 2:F:170:VAL:C    | 2:F:172:LEU:N    | 2.73                     | 0.47              |
| 1:K:156:ASN:C    | 1:K:158:GLY:N    | 2.73                     | 0.47              |
| 2:L:224:GLN:HE21 | 2:L:231:ILE:HD13 | 1.80                     | 0.47              |
| 1:M:95:LYS:HD3   | 1:M:95:LYS:N     | 2.30                     | 0.47              |
| 1:M:160:ARG:HG3  | 1:M:178:PRO:HG3  | 1.97                     | 0.47              |
| 1:A:140:LEU:H    | 1:A:177:LEU:HB2  | 1.79                     | 0.47              |
| 2:B:185:VAL:HG11 | 2:B:276:PHE:CE2  | 2.50                     | 0.47              |
| 2:B:195:TYR:CE1  | 2:B:238:VAL:HB   | 2.50                     | 0.47              |
| 2:D:192:ASN:HA   | 2:D:241:GLY:O    | 2.15                     | 0.47              |
| 2:H:201:THR:HG23 | 2:H:203:ASP:H    | 1.80                     | 0.47              |
| 1:I:37:VAL:HG11  | 1:I:48:PHE:HB2   | 1.96                     | 0.47              |
| 1:I:136:SER:C    | 1:I:177:LEU:HD23 | 2.39                     | 0.47              |
| 2:J:103:TRP:CE2  | 2:J:105:VAL:HG21 | 2.50                     | 0.47              |
| 1:M:61:LYS:O     | 1:M:62:GLU:HB2   | 2.15                     | 0.47              |
| 2:N:96:ASN:N     | 2:N:96:ASN:ND2   | 2.60                     | 0.47              |
| 1:O:37:VAL:HG11  | 1:O:48:PHE:HB2   | 1.96                     | 0.47              |
| 2:P:222:GLY:C    | 2:P:257:ALA:HB3  | 2.40                     | 0.47              |
| 2:D:201:THR:CG2  | 2:D:206:ASN:HA   | 2.29                     | 0.46              |
| 2:F:22:VAL:HG23  | 2:F:22:VAL:O     | 2.13                     | 0.46              |
| 1:G:12:PRO:HD2   | 1:G:15:GLN:HG3   | 1.95                     | 0.46              |
| 2:H:29:ASN:HA    | 4:H:1629:HOH:O   | 2.13                     | 0.46              |
| 2:J:96:ASN:H     | 2:J:96:ASN:ND2   | 2.12                     | 0.46              |
| 2:L:1:PHE:HD1    | 2:L:144:PHE:CZ   | 2.33                     | 0.46              |
| 2:L:250:LEU:HD13 | 2:L:252:LEU:HD11 | 1.97                     | 0.46              |
| 2:L:253:THR:HG22 | 2:L:255:ASN:ND2  | 2.22                     | 0.46              |
| 1:M:133:PHE:HD2  | 1:M:140:LEU:HD21 | 1.79                     | 0.46              |
| 2:N:41:GLN:C     | 2:N:42:ILE:HG13  | 2.40                     | 0.46              |
| 2:N:96:ASN:H     | 2:N:96:ASN:ND2   | 2.13                     | 0.46              |
| 1:C:122:LEU:C    | 1:C:122:LEU:HD12 | 2.38                     | 0.46              |
| 1:G:141:THR:HG23 | 1:G:174:THR:CG2  | 2.45                     | 0.46              |
| 1:G:160:ARG:HG2  | 1:G:178:PRO:HG3  | 1.97                     | 0.46              |
| 2:H:60:ARG:CZ    | 2:H:60:ARG:HB2   | 2.45                     | 0.46              |
| 1:I:95:LYS:HD3   | 1:I:95:LYS:N     | 2.30                     | 0.46              |
| 1:I:178:PRO:O    | 1:I:179:SER:HB3  | 2.15                     | 0.46              |
| 2:J:1:PHE:HD1    | 2:J:144:PHE:CZ   | 2.33                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:93:MET:HE1   | 1:K:98:LEU:HD23  | 1.96                     | 0.46              |
| 2:N:53:THR:H     | 2:N:136:ASN:ND2  | 2.13                     | 0.46              |
| 2:N:66:GLY:HA2   | 2:N:70:ASN:HD22  | 1.80                     | 0.46              |
| 1:O:11:TYR:OH    | 1:O:69:ASP:HB2   | 2.14                     | 0.46              |
| 2:P:8:GLY:O      | 2:P:9:THR:C      | 2.57                     | 0.46              |
| 1:A:72:ASN:O     | 1:A:74:GLN:HG3   | 2.16                     | 0.46              |
| 1:E:132:ARG:C    | 1:E:133:PHE:CD1  | 2.93                     | 0.46              |
| 2:F:63:ALA:HB1   | 2:F:67:VAL:HG12  | 1.96                     | 0.46              |
| 1:G:12:PRO:HB2   | 1:G:15:GLN:HG2   | 1.96                     | 0.46              |
| 2:J:21:TYR:CB    | 2:J:151:ASN:HD21 | 2.24                     | 0.46              |
| 1:M:156:ASN:C    | 1:M:158:GLY:N    | 2.73                     | 0.46              |
| 1:O:156:ASN:C    | 1:O:158:GLY:N    | 2.73                     | 0.46              |
| 1:O:160:ARG:HG3  | 1:O:178:PRO:HG3  | 1.98                     | 0.46              |
| 1:A:12:PRO:CB    | 1:A:15:GLN:HG3   | 2.45                     | 0.46              |
| 2:B:113:SER:OG   | 2:P:81:SER:N     | 2.47                     | 0.46              |
| 1:E:86:ASN:ND2   | 1:E:110:ARG:HB2  | 2.30                     | 0.46              |
| 2:F:77:TYR:CE2   | 2:F:90:THR:HG21  | 2.51                     | 0.46              |
| 1:G:33:ILE:O     | 1:G:54:LEU:HA    | 2.15                     | 0.46              |
| 2:H:195:TYR:CE1  | 2:H:238:VAL:HB   | 2.49                     | 0.46              |
| 1:I:142:LEU:HB2  | 1:I:173:SER:O    | 2.16                     | 0.46              |
| 2:J:165:ALA:O    | 2:J:166:ARG:C    | 2.59                     | 0.46              |
| 2:L:195:TYR:O    | 2:L:237:THR:HA   | 2.15                     | 0.46              |
| 2:P:195:TYR:O    | 2:P:237:THR:HA   | 2.15                     | 0.46              |
| 1:A:28:ASN:O     | 1:A:29:SER:HB3   | 2.16                     | 0.46              |
| 1:A:33:ILE:O     | 1:A:54:LEU:HA    | 2.15                     | 0.46              |
| 1:C:12:PRO:HB2   | 1:C:15:GLN:HG2   | 1.95                     | 0.46              |
| 1:C:30:THR:HG22  | 1:C:31:TYR:N     | 2.30                     | 0.46              |
| 1:E:33:ILE:O     | 1:E:54:LEU:HA    | 2.14                     | 0.46              |
| 2:F:38:LEU:C     | 2:F:40:THR:H     | 2.22                     | 0.46              |
| 2:F:60:ARG:CZ    | 2:F:60:ARG:HB2   | 2.45                     | 0.46              |
| 2:F:88:SER:HA    | 4:F:1572:HOH:O   | 2.16                     | 0.46              |
| 1:I:156:ASN:C    | 1:I:158:GLY:N    | 2.73                     | 0.46              |
| 1:K:47:ARG:NH2   | 1:K:74:GLN:NE2   | 2.58                     | 0.46              |
| 1:M:136:SER:C    | 1:M:177:LEU:HD23 | 2.40                     | 0.46              |
| 2:N:165:ALA:O    | 2:N:166:ARG:C    | 2.59                     | 0.46              |
| 1:O:47:ARG:HH22  | 1:O:74:GLN:NE2   | 1.92                     | 0.46              |
| 2:P:1:PHE:HD1    | 2:P:144:PHE:CZ   | 2.33                     | 0.46              |
| 2:P:197:LEU:CD1  | 2:P:225:LEU:HD12 | 2.42                     | 0.46              |
| 1:C:95:LYS:N     | 1:C:95:LYS:HD3   | 2.30                     | 0.46              |
| 2:F:201:THR:HG23 | 2:F:203:ASP:H    | 1.80                     | 0.46              |
| 1:I:102:THR:H    | 2:J:269:GLN:HG2  | 1.80                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:J:24:LEU:O     | 2:J:26:PRO:N     | 2.49                     | 0.46              |
| 2:L:83:PRO:O     | 2:L:86:THR:HA    | 2.15                     | 0.46              |
| 1:M:102:THR:H    | 2:N:269:GLN:HG2  | 1.80                     | 0.46              |
| 1:O:140:LEU:HD23 | 1:O:140:LEU:C    | 2.41                     | 0.46              |
| 1:O:177:LEU:HD12 | 1:O:178:PRO:CD   | 2.40                     | 0.46              |
| 2:P:250:LEU:HD13 | 2:P:252:LEU:HD11 | 1.97                     | 0.46              |
| 1:A:138:ASN:CA   | 1:A:177:LEU:HB3  | 2.46                     | 0.46              |
| 2:B:38:LEU:C     | 2:B:40:THR:N     | 2.72                     | 0.46              |
| 2:B:135:ASN:HD21 | 2:B:138:ASN:HD21 | 1.63                     | 0.46              |
| 2:B:170:VAL:C    | 2:B:172:LEU:N    | 2.74                     | 0.46              |
| 1:C:72:ASN:O     | 1:C:74:GLN:HG3   | 2.16                     | 0.46              |
| 2:D:172:LEU:N    | 2:D:173:PRO:CD   | 2.77                     | 0.46              |
| 1:E:181:ALA:HB1  | 1:E:182:GLY:H    | 1.53                     | 0.46              |
| 1:G:95:LYS:HD3   | 1:G:95:LYS:N     | 2.31                     | 0.46              |
| 2:H:38:LEU:C     | 2:H:40:THR:N     | 2.71                     | 0.46              |
| 2:J:53:THR:H     | 2:J:136:ASN:ND2  | 2.13                     | 0.46              |
| 2:J:66:GLY:HA2   | 2:J:70:ASN:HD22  | 1.80                     | 0.46              |
| 2:J:179:VAL:HG23 | 2:J:179:VAL:O    | 2.15                     | 0.46              |
| 2:J:208:ILE:HG23 | 2:J:257:ALA:CB   | 2.40                     | 0.46              |
| 2:J:250:LEU:HD13 | 2:J:252:LEU:HD11 | 1.96                     | 0.46              |
| 1:K:39:ASN:HD21  | 1:K:43:VAL:CG1   | 2.18                     | 0.46              |
| 1:K:136:SER:HB2  | 1:K:139:SER:H    | 1.81                     | 0.46              |
| 2:N:203:ASP:OD1  | 2:N:208:ILE:HD12 | 2.16                     | 0.46              |
| 2:P:203:ASP:OD1  | 2:P:208:ILE:HD12 | 2.16                     | 0.46              |
| 2:P:224:GLN:HE21 | 2:P:231:ILE:HD13 | 1.81                     | 0.46              |
| 2:B:13:ILE:HG13  | 4:B:1545:HOH:O   | 2.15                     | 0.46              |
| 1:C:160:ARG:HG2  | 1:C:178:PRO:HG3  | 1.98                     | 0.46              |
| 1:C:183:SER:C    | 1:C:185:ILE:N    | 2.74                     | 0.46              |
| 2:D:131:LEU:HB3  | 2:D:144:PHE:HB2  | 1.97                     | 0.46              |
| 1:G:86:ASN:ND2   | 1:G:110:ARG:HB2  | 2.31                     | 0.46              |
| 2:J:203:ASP:OD1  | 2:J:208:ILE:HD12 | 2.16                     | 0.46              |
| 1:K:12:PRO:HB2   | 1:K:15:GLN:HG3   | 1.97                     | 0.46              |
| 1:K:95:LYS:N     | 1:K:95:LYS:HD3   | 2.30                     | 0.46              |
| 1:K:99:THR:C     | 1:K:100:GLU:HG3  | 2.41                     | 0.46              |
| 1:K:140:LEU:HD23 | 1:K:140:LEU:C    | 2.41                     | 0.46              |
| 2:L:184:THR:OG1  | 2:L:247:ALA:HB1  | 2.16                     | 0.46              |
| 2:L:222:GLY:C    | 2:L:257:ALA:HB3  | 2.41                     | 0.46              |
| 1:M:136:SER:HB2  | 1:M:139:SER:H    | 1.81                     | 0.46              |
| 2:N:103:TRP:CE2  | 2:N:105:VAL:HG21 | 2.51                     | 0.46              |
| 2:P:96:ASN:H     | 2:P:96:ASN:ND2   | 2.12                     | 0.46              |
| 1:A:46:GLY:O     | 1:A:70:ALA:HB3   | 2.16                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:67:VAL:CG2   | 2:D:126:ILE:HG12 | 2.46                     | 0.46              |
| 2:F:138:ASN:C    | 2:F:138:ASN:HD22 | 2.23                     | 0.46              |
| 1:G:183:SER:C    | 1:G:185:ILE:N    | 2.74                     | 0.46              |
| 2:J:175:TYR:N    | 2:J:176:PRO:CD   | 2.79                     | 0.46              |
| 2:L:60:ARG:HG2   | 4:L:1505:HOH:O   | 2.14                     | 0.46              |
| 2:L:203:ASP:OD1  | 2:L:208:ILE:HD12 | 2.15                     | 0.46              |
| 2:N:24:LEU:O     | 2:N:26:PRO:N     | 2.49                     | 0.46              |
| 2:N:195:TYR:O    | 2:N:237:THR:HA   | 2.16                     | 0.46              |
| 1:O:102:THR:H    | 2:P:269:GLN:HG2  | 1.80                     | 0.46              |
| 2:P:24:LEU:O     | 2:P:26:PRO:N     | 2.49                     | 0.46              |
| 2:P:83:PRO:O     | 2:P:86:THR:HA    | 2.16                     | 0.46              |
| 1:A:160:ARG:HG2  | 1:A:178:PRO:HG3  | 1.98                     | 0.46              |
| 1:G:72:ASN:O     | 1:G:74:GLN:HG3   | 2.16                     | 0.46              |
| 1:G:93:MET:CE    | 1:G:98:LEU:HD23  | 2.43                     | 0.46              |
| 1:G:129:GLU:H    | 1:G:129:GLU:HG3  | 1.52                     | 0.46              |
| 1:K:142:LEU:HB2  | 1:K:173:SER:O    | 2.16                     | 0.46              |
| 1:M:99:THR:C     | 1:M:100:GLU:HG3  | 2.41                     | 0.46              |
| 2:N:267:ASN:CB   | 2:N:269:GLN:HE21 | 2.28                     | 0.46              |
| 1:O:57:MET:HA    | 1:O:61:LYS:CE    | 2.46                     | 0.46              |
| 1:O:95:LYS:HD3   | 1:O:95:LYS:N     | 2.30                     | 0.46              |
| 2:P:103:TRP:CE2  | 2:P:105:VAL:HG21 | 2.51                     | 0.46              |
| 2:P:165:ALA:O    | 2:P:166:ARG:C    | 2.59                     | 0.46              |
| 1:A:86:ASN:ND2   | 1:A:110:ARG:HB2  | 2.31                     | 0.45              |
| 1:E:72:ASN:O     | 1:E:74:GLN:HG3   | 2.16                     | 0.45              |
| 1:E:160:ARG:HG2  | 1:E:178:PRO:HG3  | 1.98                     | 0.45              |
| 1:E:191:ASN:ND2  | 1:E:195:ALA:HB3  | 2.31                     | 0.45              |
| 1:I:57:MET:HA    | 1:I:61:LYS:CE    | 2.46                     | 0.45              |
| 2:L:250:LEU:CD1  | 2:L:252:LEU:HD11 | 2.47                     | 0.45              |
| 2:L:267:ASN:CB   | 2:L:269:GLN:HE21 | 2.28                     | 0.45              |
| 1:M:57:MET:HA    | 1:M:61:LYS:CE    | 2.46                     | 0.45              |
| 2:N:83:PRO:O     | 2:N:86:THR:HA    | 2.17                     | 0.45              |
| 2:N:250:LEU:HD13 | 2:N:252:LEU:HD11 | 1.97                     | 0.45              |
| 1:O:136:SER:C    | 1:O:177:LEU:HD23 | 2.39                     | 0.45              |
| 2:P:184:THR:OG1  | 2:P:247:ALA:HB1  | 2.16                     | 0.45              |
| 2:P:208:ILE:HG23 | 2:P:257:ALA:CB   | 2.40                     | 0.45              |
| 1:E:28:ASN:O     | 1:E:29:SER:HB3   | 2.17                     | 0.45              |
| 1:G:140:LEU:C    | 1:G:140:LEU:CD2  | 2.89                     | 0.45              |
| 2:J:250:LEU:CD1  | 2:J:252:LEU:HD11 | 2.47                     | 0.45              |
| 1:K:57:MET:HA    | 1:K:61:LYS:CE    | 2.46                     | 0.45              |
| 2:L:34:LEU:HD12  | 2:L:35:VAL:N     | 2.21                     | 0.45              |
| 2:L:38:LEU:C     | 2:L:40:THR:N     | 2.67                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:93:MET:HE1   | 1:O:98:LEU:HD23  | 1.97                     | 0.45              |
| 2:P:179:VAL:HG23 | 2:P:179:VAL:O    | 2.15                     | 0.45              |
| 1:A:51:THR:HA    | 1:A:52:PRO:C     | 2.41                     | 0.45              |
| 1:A:186:THR:HB   | 1:A:199:LYS:NZ   | 2.32                     | 0.45              |
| 1:C:141:THR:HA   | 1:C:174:THR:HA   | 1.98                     | 0.45              |
| 2:D:184:THR:HB   | 2:D:247:ALA:HB1  | 1.98                     | 0.45              |
| 2:F:131:LEU:HB3  | 2:F:144:PHE:HB2  | 1.98                     | 0.45              |
| 1:G:28:ASN:ND2   | 1:G:28:ASN:O     | 2.49                     | 0.45              |
| 2:H:170:VAL:C    | 2:H:172:LEU:N    | 2.74                     | 0.45              |
| 2:H:240:LEU:HD21 | 2:H:250:LEU:HD22 | 1.98                     | 0.45              |
| 1:I:99:THR:C     | 1:I:100:GLU:HG3  | 2.41                     | 0.45              |
| 1:I:136:SER:HB2  | 1:I:139:SER:H    | 1.81                     | 0.45              |
| 1:I:140:LEU:HD23 | 1:I:140:LEU:C    | 2.41                     | 0.45              |
| 2:J:83:PRO:O     | 2:J:86:THR:HA    | 2.16                     | 0.45              |
| 2:J:222:GLY:C    | 2:J:257:ALA:HB3  | 2.41                     | 0.45              |
| 2:J:224:GLN:HE21 | 2:J:231:ILE:HD13 | 1.80                     | 0.45              |
| 2:L:41:GLN:C     | 2:L:42:ILE:HG13  | 2.40                     | 0.45              |
| 2:L:53:THR:H     | 2:L:136:ASN:ND2  | 2.13                     | 0.45              |
| 2:L:165:ALA:O    | 2:L:166:ARG:C    | 2.59                     | 0.45              |
| 1:M:140:LEU:HD23 | 1:M:140:LEU:C    | 2.41                     | 0.45              |
| 2:N:96:ASN:O     | 2:N:97:SER:HB2   | 2.17                     | 0.45              |
| 2:N:222:GLY:C    | 2:N:257:ALA:HB3  | 2.41                     | 0.45              |
| 2:P:175:TYR:N    | 2:P:176:PRO:CD   | 2.80                     | 0.45              |
| 1:C:86:ASN:ND2   | 1:C:110:ARG:HB2  | 2.32                     | 0.45              |
| 1:C:162:LEU:HD21 | 1:C:178:PRO:CD   | 2.47                     | 0.45              |
| 2:F:195:TYR:CE1  | 2:F:238:VAL:HB   | 2.51                     | 0.45              |
| 2:F:201:THR:CG2  | 2:F:206:ASN:HA   | 2.31                     | 0.45              |
| 1:G:186:THR:HB   | 1:G:199:LYS:NZ   | 2.31                     | 0.45              |
| 1:I:12:PRO:HB2   | 1:I:15:GLN:HG3   | 1.97                     | 0.45              |
| 1:I:177:LEU:HD12 | 1:I:178:PRO:CD   | 2.40                     | 0.45              |
| 2:J:155:VAL:HG12 | 2:J:157:PRO:CD   | 2.43                     | 0.45              |
| 1:M:142:LEU:HB2  | 1:M:173:SER:O    | 2.16                     | 0.45              |
| 2:P:154:VAL:HG12 | 2:P:155:VAL:N    | 2.32                     | 0.45              |
| 1:A:114:TYR:CE2  | 1:A:149:TYR:HB2  | 2.51                     | 0.45              |
| 1:A:154:GLU:OE2  | 1:A:188:ARG:HD3  | 2.16                     | 0.45              |
| 1:A:156:ASN:O    | 1:A:185:ILE:HA   | 2.16                     | 0.45              |
| 2:B:138:ASN:C    | 2:B:138:ASN:HD22 | 2.24                     | 0.45              |
| 1:C:28:ASN:O     | 1:C:29:SER:HB3   | 2.15                     | 0.45              |
| 2:D:5:THR:CG2    | 2:D:8:GLY:H      | 2.29                     | 0.45              |
| 2:D:60:ARG:HB2   | 2:D:60:ARG:CZ    | 2.47                     | 0.45              |
| 2:D:158:THR:HG23 | 4:D:1617:HOH:O   | 2.15                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:38:LEU:C     | 2:F:40:THR:N     | 2.70                     | 0.45              |
| 1:G:46:GLY:O     | 1:G:70:ALA:HB3   | 2.16                     | 0.45              |
| 1:G:51:THR:HA    | 1:G:52:PRO:C     | 2.41                     | 0.45              |
| 2:H:38:LEU:C     | 2:H:40:THR:H     | 2.24                     | 0.45              |
| 1:I:93:MET:HE1   | 1:I:98:LEU:HD23  | 1.97                     | 0.45              |
| 1:K:79:ARG:HB3   | 1:K:170:MET:HE1  | 1.96                     | 0.45              |
| 2:L:103:TRP:CE2  | 2:L:105:VAL:HG21 | 2.51                     | 0.45              |
| 1:M:12:PRO:HB2   | 1:M:15:GLN:HG3   | 1.97                     | 0.45              |
| 2:N:184:THR:OG1  | 2:N:247:ALA:HB1  | 2.16                     | 0.45              |
| 2:N:195:TYR:HB2  | 2:N:275:THR:O    | 2.17                     | 0.45              |
| 1:O:99:THR:C     | 1:O:100:GLU:HG3  | 2.42                     | 0.45              |
| 1:O:142:LEU:HB2  | 1:O:173:SER:O    | 2.16                     | 0.45              |
| 2:P:250:LEU:CD1  | 2:P:252:LEU:HD11 | 2.47                     | 0.45              |
| 1:E:183:SER:C    | 1:E:185:ILE:N    | 2.74                     | 0.45              |
| 1:I:160:ARG:HG3  | 1:I:178:PRO:HG3  | 1.98                     | 0.45              |
| 2:J:226:THR:CG2  | 2:J:253:THR:HB   | 2.42                     | 0.45              |
| 1:O:61:LYS:O     | 1:O:62:GLU:HB2   | 2.15                     | 0.45              |
| 2:B:184:THR:HB   | 2:B:247:ALA:HB1  | 1.98                     | 0.45              |
| 1:C:138:ASN:CA   | 1:C:177:LEU:HB3  | 2.47                     | 0.45              |
| 1:C:167:VAL:HA   | 1:C:168:PRO:HD2  | 1.77                     | 0.45              |
| 1:E:138:ASN:CA   | 1:E:177:LEU:HB3  | 2.47                     | 0.45              |
| 2:F:167:ASP:OD1  | 2:F:168:VAL:HG12 | 2.17                     | 0.45              |
| 1:I:61:LYS:O     | 1:I:62:GLU:HB2   | 2.16                     | 0.45              |
| 1:K:160:ARG:HG3  | 1:K:178:PRO:HG3  | 1.98                     | 0.45              |
| 1:O:144:ASN:HB3  | 1:O:167:VAL:HG12 | 1.99                     | 0.45              |
| 1:A:122:LEU:HD11 | 1:A:126:GLN:C    | 2.42                     | 0.45              |
| 1:A:140:LEU:C    | 1:A:140:LEU:CD2  | 2.90                     | 0.45              |
| 1:C:46:GLY:O     | 1:C:70:ALA:HB3   | 2.16                     | 0.45              |
| 2:D:4:LYS:HB2    | 2:D:4:LYS:NZ     | 2.31                     | 0.45              |
| 1:G:125:ASP:OD1  | 1:G:126:GLN:N    | 2.50                     | 0.45              |
| 1:I:144:ASN:HB3  | 1:I:167:VAL:HG12 | 1.99                     | 0.45              |
| 2:J:195:TYR:HB2  | 2:J:275:THR:O    | 2.16                     | 0.45              |
| 2:J:195:TYR:O    | 2:J:237:THR:HA   | 2.16                     | 0.45              |
| 1:M:79:ARG:HB3   | 1:M:170:MET:HE1  | 1.96                     | 0.45              |
| 1:O:144:ASN:HB3  | 1:O:167:VAL:CG1  | 2.47                     | 0.45              |
| 2:B:240:LEU:HD21 | 2:B:250:LEU:HD22 | 1.97                     | 0.45              |
| 1:C:201:THR:O    | 1:C:203:VAL:HG23 | 2.17                     | 0.45              |
| 1:E:186:THR:HB   | 1:E:199:LYS:NZ   | 2.32                     | 0.45              |
| 2:F:118:VAL:O    | 2:F:118:VAL:HG12 | 2.17                     | 0.45              |
| 2:J:96:ASN:O     | 2:J:97:SER:HB2   | 2.17                     | 0.45              |
| 1:K:61:LYS:O     | 1:K:62:GLU:HB2   | 2.16                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:47:ARG:HH22  | 1:M:74:GLN:NE2   | 1.92                     | 0.45              |
| 1:M:149:TYR:CD1  | 1:M:169:PRO:HD3  | 2.52                     | 0.45              |
| 2:N:227:ARG:NE   | 2:N:232:ILE:HD11 | 2.32                     | 0.45              |
| 1:O:79:ARG:HB3   | 1:O:170:MET:HE1  | 1.96                     | 0.45              |
| 1:C:144:ASN:HB3  | 1:C:167:VAL:HG12 | 1.98                     | 0.45              |
| 1:G:141:THR:HA   | 1:G:174:THR:HA   | 1.99                     | 0.45              |
| 2:H:201:THR:CB   | 2:H:206:ASN:ND2  | 2.81                     | 0.45              |
| 2:L:24:LEU:O     | 2:L:26:PRO:N     | 2.49                     | 0.45              |
| 2:L:96:ASN:O     | 2:L:97:SER:HB2   | 2.17                     | 0.45              |
| 1:O:47:ARG:NH2   | 1:O:74:GLN:NE2   | 2.58                     | 0.45              |
| 1:O:136:SER:HB2  | 1:O:139:SER:H    | 1.81                     | 0.45              |
| 1:A:186:THR:CG2  | 1:A:199:LYS:HZ2  | 2.30                     | 0.44              |
| 1:C:82:LEU:HD12  | 1:C:83:PHE:H     | 1.82                     | 0.44              |
| 1:E:46:GLY:O     | 1:E:70:ALA:HB3   | 2.17                     | 0.44              |
| 1:E:156:ASN:O    | 1:E:185:ILE:HA   | 2.17                     | 0.44              |
| 1:G:30:THR:HG22  | 1:G:31:TYR:N     | 2.31                     | 0.44              |
| 2:N:42:ILE:HG23  | 2:N:146:TRP:CH2  | 2.52                     | 0.44              |
| 2:N:197:LEU:CD1  | 2:N:225:LEU:HD12 | 2.43                     | 0.44              |
| 2:P:195:TYR:HB2  | 2:P:275:THR:O    | 2.16                     | 0.44              |
| 2:P:227:ARG:NE   | 2:P:232:ILE:HD11 | 2.32                     | 0.44              |
| 1:A:144:ASN:HB3  | 1:A:167:VAL:HG12 | 1.98                     | 0.44              |
| 1:C:154:GLU:OE2  | 1:C:188:ARG:HD3  | 2.17                     | 0.44              |
| 1:C:156:ASN:O    | 1:C:185:ILE:HA   | 2.16                     | 0.44              |
| 1:E:71:THR:O     | 1:E:73:ASN:N     | 2.51                     | 0.44              |
| 1:E:201:THR:O    | 1:E:203:VAL:HG23 | 2.18                     | 0.44              |
| 2:F:136:ASN:HD22 | 2:F:136:ASN:N    | 2.15                     | 0.44              |
| 1:G:28:ASN:O     | 1:G:29:SER:HB3   | 2.16                     | 0.44              |
| 1:G:144:ASN:HB3  | 1:G:167:VAL:HG12 | 1.98                     | 0.44              |
| 2:H:138:ASN:C    | 2:H:138:ASN:HD22 | 2.24                     | 0.44              |
| 2:J:154:VAL:HG12 | 2:J:155:VAL:N    | 2.32                     | 0.44              |
| 2:J:184:THR:OG1  | 2:J:247:ALA:HB1  | 2.17                     | 0.44              |
| 2:N:253:THR:HG22 | 2:N:255:ASN:ND2  | 2.22                     | 0.44              |
| 1:O:82:LEU:HB2   | 1:O:149:TYR:CE1  | 2.53                     | 0.44              |
| 1:I:39:ASN:OD1   | 1:I:43:VAL:HG13  | 2.18                     | 0.44              |
| 1:I:57:MET:HA    | 1:I:61:LYS:HE3   | 2.00                     | 0.44              |
| 1:I:144:ASN:HB3  | 1:I:167:VAL:CG1  | 2.48                     | 0.44              |
| 2:J:42:ILE:HG23  | 2:J:146:TRP:CH2  | 2.53                     | 0.44              |
| 1:K:71:THR:HG23  | 1:K:71:THR:O     | 2.17                     | 0.44              |
| 1:K:85:MET:O     | 1:K:110:ARG:HA   | 2.17                     | 0.44              |
| 1:K:177:LEU:HD12 | 1:K:178:PRO:CD   | 2.40                     | 0.44              |
| 2:N:154:VAL:HG12 | 2:N:155:VAL:N    | 2.32                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:N:175:TYR:N    | 2:N:176:PRO:CD   | 2.80                     | 0.44              |
| 2:N:224:GLN:HE21 | 2:N:231:ILE:HD13 | 1.80                     | 0.44              |
| 1:O:85:MET:O     | 1:O:110:ARG:HA   | 2.17                     | 0.44              |
| 2:B:201:THR:HG23 | 2:B:203:ASP:H    | 1.82                     | 0.44              |
| 1:C:140:LEU:C    | 1:C:140:LEU:CD2  | 2.89                     | 0.44              |
| 2:F:172:LEU:N    | 2:F:173:PRO:CD   | 2.76                     | 0.44              |
| 1:G:201:THR:O    | 1:G:203:VAL:HG23 | 2.18                     | 0.44              |
| 2:H:135:ASN:HD21 | 2:H:138:ASN:HD21 | 1.64                     | 0.44              |
| 1:I:85:MET:O     | 1:I:110:ARG:HA   | 2.17                     | 0.44              |
| 1:I:190:ILE:HD12 | 2:J:279:GLN:HG2  | 1.99                     | 0.44              |
| 2:L:155:VAL:HG12 | 2:L:157:PRO:CD   | 2.43                     | 0.44              |
| 2:N:59:GLN:HG3   | 2:N:132:ARG:HD3  | 2.00                     | 0.44              |
| 2:N:250:LEU:CD1  | 2:N:252:LEU:HD11 | 2.47                     | 0.44              |
| 1:O:50:VAL:HG21  | 1:O:85:MET:HE1   | 1.99                     | 0.44              |
| 1:O:186:THR:HB   | 1:O:199:LYS:NZ   | 2.32                     | 0.44              |
| 1:A:47:ARG:NH2   | 1:A:74:GLN:HB2   | 2.33                     | 0.44              |
| 1:C:28:ASN:O     | 1:C:28:ASN:ND2   | 2.51                     | 0.44              |
| 1:E:141:THR:HA   | 1:E:174:THR:HA   | 2.00                     | 0.44              |
| 1:I:82:LEU:HB2   | 1:I:149:TYR:CE1  | 2.52                     | 0.44              |
| 2:L:267:ASN:OD1  | 2:L:269:GLN:NE2  | 2.51                     | 0.44              |
| 1:M:144:ASN:HB3  | 1:M:167:VAL:CG1  | 2.47                     | 0.44              |
| 1:M:190:ILE:HD12 | 2:N:279:GLN:HG2  | 2.00                     | 0.44              |
| 1:O:12:PRO:HD2   | 1:O:15:GLN:HG3   | 1.99                     | 0.44              |
| 2:P:61:GLY:HA3   | 2:P:86:THR:HG23  | 2.00                     | 0.44              |
| 2:P:96:ASN:O     | 2:P:97:SER:HB2   | 2.17                     | 0.44              |
| 1:A:177:LEU:HA   | 1:A:178:PRO:HD2  | 1.88                     | 0.44              |
| 1:G:138:ASN:CA   | 1:G:177:LEU:HB3  | 2.48                     | 0.44              |
| 1:G:154:GLU:OE2  | 1:G:188:ARG:HD3  | 2.17                     | 0.44              |
| 1:I:186:THR:HB   | 1:I:199:LYS:NZ   | 2.32                     | 0.44              |
| 2:L:195:TYR:HB2  | 2:L:275:THR:O    | 2.17                     | 0.44              |
| 1:M:50:VAL:HG21  | 1:M:85:MET:HE1   | 1.99                     | 0.44              |
| 1:M:82:LEU:HB2   | 1:M:149:TYR:CE1  | 2.53                     | 0.44              |
| 2:N:168:VAL:HG13 | 2:N:168:VAL:O    | 2.18                     | 0.44              |
| 1:O:71:THR:O     | 1:O:71:THR:HG23  | 2.18                     | 0.44              |
| 2:P:58:LEU:H     | 2:P:90:THR:HG21  | 1.79                     | 0.44              |
| 2:B:184:THR:HA   | 2:B:248:VAL:O    | 2.18                     | 0.44              |
| 1:C:71:THR:O     | 1:C:73:ASN:N     | 2.51                     | 0.44              |
| 2:D:5:THR:HG22   | 2:D:9:THR:N      | 2.32                     | 0.44              |
| 1:E:47:ARG:NH2   | 1:E:74:GLN:HB2   | 2.32                     | 0.44              |
| 1:E:123:PRO:HA   | 1:E:124:PRO:HD2  | 1.84                     | 0.44              |
| 1:E:140:LEU:C    | 1:E:140:LEU:CD2  | 2.90                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:4:LYS:HB2    | 2:H:4:LYS:NZ     | 2.33                     | 0.44              |
| 2:H:192:ASN:HA   | 2:H:241:GLY:O    | 2.18                     | 0.44              |
| 1:I:71:THR:HG23  | 1:I:71:THR:O     | 2.18                     | 0.44              |
| 2:J:44:CYS:O     | 2:J:101:LYS:N    | 2.50                     | 0.44              |
| 2:J:61:GLY:HA3   | 2:J:86:THR:HG23  | 1.99                     | 0.44              |
| 2:J:168:VAL:O    | 2:J:168:VAL:HG13 | 2.18                     | 0.44              |
| 2:J:211:ASN:HD22 | 2:J:212:THR:N    | 2.16                     | 0.44              |
| 2:J:215:PHE:O    | 2:J:216:SER:C    | 2.61                     | 0.44              |
| 1:K:39:ASN:OD1   | 1:K:43:VAL:HG13  | 2.18                     | 0.44              |
| 1:M:45:ASP:OD1   | 1:M:47:ARG:HB2   | 2.18                     | 0.44              |
| 1:M:186:THR:HB   | 1:M:199:LYS:NZ   | 2.33                     | 0.44              |
| 2:N:267:ASN:OD1  | 2:N:269:GLN:NE2  | 2.51                     | 0.44              |
| 1:O:12:PRO:HB2   | 1:O:15:GLN:HG3   | 1.98                     | 0.44              |
| 1:O:149:TYR:CD1  | 1:O:169:PRO:HD3  | 2.52                     | 0.44              |
| 2:P:42:ILE:HG23  | 2:P:146:TRP:CH2  | 2.53                     | 0.44              |
| 2:P:202:ALA:HB2  | 2:P:210:THR:CG2  | 2.34                     | 0.44              |
| 2:P:211:ASN:HD22 | 2:P:212:THR:N    | 2.16                     | 0.44              |
| 2:P:267:ASN:OD1  | 2:P:269:GLN:NE2  | 2.50                     | 0.44              |
| 1:A:191:ASN:ND2  | 1:A:195:ALA:HB3  | 2.33                     | 0.44              |
| 2:B:167:ASP:OD1  | 2:B:168:VAL:HG12 | 2.18                     | 0.44              |
| 1:C:12:PRO:CB    | 1:C:15:GLN:HG3   | 2.45                     | 0.44              |
| 1:C:186:THR:HB   | 1:C:199:LYS:NZ   | 2.32                     | 0.44              |
| 2:D:138:ASN:C    | 2:D:138:ASN:HD22 | 2.24                     | 0.44              |
| 2:D:167:ASP:OD1  | 2:D:168:VAL:HG12 | 2.18                     | 0.44              |
| 1:G:162:LEU:HD21 | 1:G:178:PRO:CD   | 2.48                     | 0.44              |
| 1:K:190:ILE:HD12 | 2:L:279:GLN:HG2  | 2.00                     | 0.44              |
| 2:L:211:ASN:HD22 | 2:L:212:THR:N    | 2.16                     | 0.44              |
| 1:M:144:ASN:HB3  | 1:M:167:VAL:HG12 | 1.99                     | 0.44              |
| 1:O:190:ILE:HD12 | 2:P:279:GLN:HG2  | 2.00                     | 0.44              |
| 2:P:21:TYR:CB    | 2:P:151:ASN:HD21 | 2.24                     | 0.44              |
| 2:P:59:GLN:HG3   | 2:P:132:ARG:HD3  | 2.00                     | 0.44              |
| 2:P:267:ASN:CG   | 2:P:269:GLN:HE21 | 2.26                     | 0.44              |
| 1:E:154:GLU:OE2  | 1:E:188:ARG:HD3  | 2.18                     | 0.44              |
| 2:F:184:THR:HB   | 2:F:247:ALA:HB1  | 1.98                     | 0.44              |
| 1:G:122:LEU:HD11 | 1:G:126:GLN:C    | 2.42                     | 0.44              |
| 1:G:156:ASN:O    | 1:G:185:ILE:HA   | 2.17                     | 0.44              |
| 1:I:50:VAL:HG21  | 1:I:85:MET:HE1   | 1.99                     | 0.44              |
| 1:I:160:ARG:HG2  | 1:I:178:PRO:HG3  | 2.00                     | 0.44              |
| 1:K:45:ASP:OD1   | 1:K:47:ARG:HB2   | 2.18                     | 0.44              |
| 1:K:144:ASN:HB3  | 1:K:167:VAL:HG12 | 1.99                     | 0.44              |
| 1:K:149:TYR:CD1  | 1:K:169:PRO:HD3  | 2.52                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:L:42:ILE:HG23  | 2:L:146:TRP:CH2  | 2.53                     | 0.44              |
| 2:L:59:GLN:HG3   | 2:L:132:ARG:HD3  | 2.00                     | 0.44              |
| 2:L:227:ARG:NE   | 2:L:232:ILE:HD11 | 2.32                     | 0.44              |
| 1:M:71:THR:HG23  | 1:M:71:THR:O     | 2.18                     | 0.44              |
| 1:A:147:PRO:HB3  | 1:A:170:MET:HE2  | 2.00                     | 0.43              |
| 1:A:162:LEU:HD21 | 1:A:178:PRO:CD   | 2.47                     | 0.43              |
| 2:B:38:LEU:C     | 2:B:40:THR:H     | 2.25                     | 0.43              |
| 1:C:47:ARG:NH2   | 1:C:74:GLN:HB2   | 2.33                     | 0.43              |
| 1:E:93:MET:CE    | 1:E:98:LEU:HD23  | 2.45                     | 0.43              |
| 1:E:162:LEU:HD21 | 1:E:178:PRO:CD   | 2.48                     | 0.43              |
| 1:I:79:ARG:HB3   | 1:I:170:MET:HE1  | 1.96                     | 0.43              |
| 1:K:183:SER:C    | 1:K:185:ILE:H    | 2.26                     | 0.43              |
| 1:K:186:THR:HB   | 1:K:199:LYS:NZ   | 2.32                     | 0.43              |
| 2:L:154:VAL:HG12 | 2:L:155:VAL:N    | 2.32                     | 0.43              |
| 2:L:175:TYR:N    | 2:L:176:PRO:CD   | 2.80                     | 0.43              |
| 2:L:215:PHE:O    | 2:L:216:SER:C    | 2.61                     | 0.43              |
| 2:N:61:GLY:HA3   | 2:N:86:THR:HG23  | 2.00                     | 0.43              |
| 2:P:215:PHE:O    | 2:P:216:SER:C    | 2.61                     | 0.43              |
| 1:A:169:PRO:O    | 1:A:170:MET:C    | 2.61                     | 0.43              |
| 1:C:122:LEU:HD11 | 1:C:126:GLN:C    | 2.42                     | 0.43              |
| 2:D:184:THR:HA   | 2:D:248:VAL:O    | 2.18                     | 0.43              |
| 1:E:31:TYR:O     | 1:E:56:ALA:HA    | 2.18                     | 0.43              |
| 1:E:155:LEU:HD12 | 1:E:187:TYR:HB3  | 2.01                     | 0.43              |
| 2:H:118:VAL:O    | 2:H:118:VAL:HG12 | 2.18                     | 0.43              |
| 2:H:184:THR:HB   | 2:H:247:ALA:HB1  | 1.99                     | 0.43              |
| 2:J:41:GLN:O     | 2:J:42:ILE:HG13  | 2.18                     | 0.43              |
| 1:K:50:VAL:HG21  | 1:K:85:MET:HE1   | 1.99                     | 0.43              |
| 1:K:82:LEU:HB2   | 1:K:149:TYR:CE1  | 2.53                     | 0.43              |
| 2:L:135:ASN:ND2  | 3:L:1504:MAN:O4  | 2.52                     | 0.43              |
| 2:N:211:ASN:HD22 | 2:N:212:THR:N    | 2.16                     | 0.43              |
| 1:O:160:ARG:HG2  | 1:O:178:PRO:HG3  | 2.00                     | 0.43              |
| 2:F:201:THR:CB   | 2:F:206:ASN:ND2  | 2.81                     | 0.43              |
| 2:H:173:PRO:O    | 2:H:174:ASP:C    | 2.62                     | 0.43              |
| 2:H:184:THR:HA   | 2:H:248:VAL:O    | 2.18                     | 0.43              |
| 2:J:1:PHE:CD1    | 2:J:133:GLN:HG3  | 2.53                     | 0.43              |
| 2:J:267:ASN:OD1  | 2:J:269:GLN:NE2  | 2.51                     | 0.43              |
| 2:L:67:VAL:HG21  | 2:L:126:ILE:CG2  | 2.35                     | 0.43              |
| 2:N:58:LEU:H     | 2:N:90:THR:HG21  | 1.80                     | 0.43              |
| 2:N:267:ASN:CG   | 2:N:269:GLN:HE21 | 2.26                     | 0.43              |
| 2:P:1:PHE:CD1    | 2:P:133:GLN:HG3  | 2.53                     | 0.43              |
| 2:P:192:ASN:HA   | 2:P:241:GLY:O    | 2.18                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:125:ASP:OD1  | 1:A:126:GLN:N    | 2.51                     | 0.43              |
| 2:D:262:GLN:HE21 | 2:D:262:GLN:CA   | 2.25                     | 0.43              |
| 1:G:186:THR:CG2  | 1:G:199:LYS:HZ2  | 2.31                     | 0.43              |
| 2:H:5:THR:CG2    | 2:H:8:GLY:H      | 2.31                     | 0.43              |
| 2:J:267:ASN:CG   | 2:J:269:GLN:HE21 | 2.26                     | 0.43              |
| 1:K:185:ILE:O    | 1:K:202:GLY:N    | 2.35                     | 0.43              |
| 2:L:30:VAL:HG23  | 2:L:156:VAL:CG1  | 2.49                     | 0.43              |
| 2:L:41:GLN:O     | 2:L:42:ILE:HG13  | 2.18                     | 0.43              |
| 1:M:50:VAL:HG12  | 1:M:51:THR:N     | 2.34                     | 0.43              |
| 2:N:30:VAL:HG23  | 2:N:156:VAL:CG1  | 2.49                     | 0.43              |
| 1:O:57:MET:HA    | 1:O:61:LYS:HE3   | 2.00                     | 0.43              |
| 1:C:147:PRO:HB3  | 1:C:170:MET:HE2  | 2.00                     | 0.43              |
| 2:D:45:HIS:CD2   | 2:D:45:HIS:C     | 2.96                     | 0.43              |
| 1:E:144:ASN:HB3  | 1:E:167:VAL:HG12 | 1.98                     | 0.43              |
| 1:I:183:SER:C    | 1:I:185:ILE:H    | 2.27                     | 0.43              |
| 2:J:30:VAL:HG23  | 2:J:156:VAL:CG1  | 2.48                     | 0.43              |
| 1:K:52:PRO:HG2   | 1:K:55:PHE:CE2   | 2.53                     | 0.43              |
| 1:K:144:ASN:HB3  | 1:K:167:VAL:CG1  | 2.47                     | 0.43              |
| 1:M:85:MET:O     | 1:M:110:ARG:HA   | 2.18                     | 0.43              |
| 1:O:39:ASN:OD1   | 1:O:43:VAL:HG13  | 2.18                     | 0.43              |
| 1:A:28:ASN:O     | 1:A:28:ASN:ND2   | 2.51                     | 0.43              |
| 1:A:201:THR:O    | 1:A:203:VAL:HG23 | 2.18                     | 0.43              |
| 2:B:221:VAL:HG12 | 2:B:222:GLY:N    | 2.33                     | 0.43              |
| 1:E:186:THR:CG2  | 1:E:199:LYS:HZ2  | 2.32                     | 0.43              |
| 1:G:155:LEU:HD12 | 1:G:187:TYR:HB3  | 2.01                     | 0.43              |
| 1:G:168:PRO:HA   | 1:G:169:PRO:HD3  | 1.87                     | 0.43              |
| 2:H:5:THR:HG22   | 2:H:9:THR:N      | 2.33                     | 0.43              |
| 2:H:167:ASP:OD1  | 2:H:168:VAL:HG12 | 2.18                     | 0.43              |
| 1:I:135:ARG:NH2  | 1:I:181:ALA:CB   | 2.82                     | 0.43              |
| 1:I:149:TYR:CG   | 1:I:169:PRO:HD3  | 2.54                     | 0.43              |
| 1:I:149:TYR:CD1  | 1:I:169:PRO:HD3  | 2.52                     | 0.43              |
| 2:J:227:ARG:NE   | 2:J:232:ILE:HD11 | 2.33                     | 0.43              |
| 1:M:39:ASN:OD1   | 1:M:43:VAL:HG13  | 2.18                     | 0.43              |
| 1:M:182:GLY:O    | 1:M:183:SER:CB   | 2.65                     | 0.43              |
| 2:N:21:TYR:CB    | 2:N:151:ASN:HD21 | 2.24                     | 0.43              |
| 2:N:41:GLN:O     | 2:N:42:ILE:HG13  | 2.19                     | 0.43              |
| 2:P:41:GLN:O     | 2:P:42:ILE:HG13  | 2.18                     | 0.43              |
| 1:A:94:ASP:C     | 1:A:96:SER:N     | 2.76                     | 0.43              |
| 1:A:141:THR:HA   | 1:A:174:THR:HA   | 1.99                     | 0.43              |
| 1:C:186:THR:CG2  | 1:C:199:LYS:HZ2  | 2.32                     | 0.43              |
| 1:E:125:ASP:OD1  | 1:E:126:GLN:N    | 2.51                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:184:THR:HA   | 2:F:248:VAL:O    | 2.18                     | 0.43              |
| 2:J:122:ALA:N    | 2:J:153:ASP:OD1  | 2.52                     | 0.43              |
| 2:J:192:ASN:HA   | 2:J:241:GLY:O    | 2.19                     | 0.43              |
| 2:J:241:GLY:O    | 2:J:243:VAL:HG23 | 2.19                     | 0.43              |
| 1:K:25:ASN:O     | 1:K:26:ASP:C     | 2.61                     | 0.43              |
| 1:K:135:ARG:NH2  | 1:K:181:ALA:CB   | 2.82                     | 0.43              |
| 1:K:135:ARG:NH2  | 1:K:181:ALA:HB1  | 2.34                     | 0.43              |
| 2:L:192:ASN:HA   | 2:L:241:GLY:O    | 2.19                     | 0.43              |
| 2:L:208:ILE:HG23 | 2:L:257:ALA:CB   | 2.40                     | 0.43              |
| 2:L:267:ASN:CG   | 2:L:269:GLN:HE21 | 2.26                     | 0.43              |
| 2:N:30:VAL:HG12  | 2:N:31:GLY:N     | 2.33                     | 0.43              |
| 2:N:155:VAL:HG12 | 2:N:157:PRO:CD   | 2.43                     | 0.43              |
| 1:O:13:ALA:HB3   | 1:O:118:ALA:H    | 1.84                     | 0.43              |
| 1:O:135:ARG:NH2  | 1:O:181:ALA:CB   | 2.81                     | 0.43              |
| 1:O:183:SER:C    | 1:O:185:ILE:H    | 2.27                     | 0.43              |
| 1:O:188:ARG:NH1  | 1:O:199:LYS:N    | 2.67                     | 0.43              |
| 2:P:168:VAL:O    | 2:P:168:VAL:HG13 | 2.18                     | 0.43              |
| 1:A:31:TYR:O     | 1:A:56:ALA:HA    | 2.19                     | 0.43              |
| 1:A:47:ARG:NH2   | 1:A:74:GLN:NE2   | 2.54                     | 0.43              |
| 2:D:170:VAL:C    | 2:D:172:LEU:N    | 2.74                     | 0.43              |
| 1:G:31:TYR:O     | 1:G:56:ALA:HA    | 2.19                     | 0.43              |
| 1:G:47:ARG:NH2   | 1:G:74:GLN:HB2   | 2.31                     | 0.43              |
| 1:I:52:PRO:HG2   | 1:I:55:PHE:CE2   | 2.53                     | 0.43              |
| 2:L:241:GLY:O    | 2:L:243:VAL:HG23 | 2.19                     | 0.43              |
| 2:N:95:TYR:OH    | 2:N:103:TRP:CA   | 2.66                     | 0.43              |
| 2:N:241:GLY:O    | 2:N:243:VAL:HG23 | 2.19                     | 0.43              |
| 2:B:1:PHE:CG     | 2:B:133:GLN:HG3  | 2.54                     | 0.43              |
| 2:B:5:THR:CG2    | 2:B:8:GLY:H      | 2.32                     | 0.43              |
| 1:C:31:TYR:O     | 1:C:56:ALA:HA    | 2.18                     | 0.43              |
| 1:E:51:THR:HA    | 1:E:52:PRO:C     | 2.43                     | 0.43              |
| 1:E:122:LEU:HD12 | 1:E:123:PRO:N    | 2.34                     | 0.43              |
| 1:G:94:ASP:C     | 1:G:96:SER:N     | 2.76                     | 0.43              |
| 2:J:63:ALA:C     | 2:J:64:TYR:CD1   | 2.97                     | 0.43              |
| 2:J:197:LEU:CD1  | 2:J:225:LEU:HD12 | 2.42                     | 0.43              |
| 1:K:177:LEU:HA   | 1:K:178:PRO:HD2  | 1.79                     | 0.43              |
| 1:M:57:MET:HA    | 1:M:61:LYS:HE3   | 2.00                     | 0.43              |
| 1:M:129:GLU:C    | 1:M:131:LEU:H    | 2.27                     | 0.43              |
| 1:M:135:ARG:NH2  | 1:M:181:ALA:CB   | 2.81                     | 0.43              |
| 1:O:45:ASP:OD1   | 1:O:47:ARG:HB2   | 2.19                     | 0.43              |
| 1:O:52:PRO:HG2   | 1:O:55:PHE:CE2   | 2.54                     | 0.43              |
| 2:B:4:LYS:HB2    | 2:B:4:LYS:NZ     | 2.34                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:173:PRO:O    | 2:B:174:ASP:C    | 2.62                     | 0.43              |
| 2:B:212:THR:O    | 2:B:269:GLN:HB2  | 2.19                     | 0.43              |
| 1:C:94:ASP:C     | 1:C:96:SER:N     | 2.77                     | 0.43              |
| 1:C:125:ASP:OD1  | 1:C:126:GLN:N    | 2.52                     | 0.43              |
| 2:D:173:PRO:O    | 2:D:174:ASP:C    | 2.62                     | 0.43              |
| 1:E:28:ASN:O     | 1:E:28:ASN:ND2   | 2.52                     | 0.43              |
| 1:G:122:LEU:HD12 | 1:G:123:PRO:N    | 2.34                     | 0.43              |
| 2:H:116:GLY:HA2  | 2:H:189:LYS:CE   | 2.48                     | 0.43              |
| 2:J:13:ILE:HG23  | 3:J:1605:MAN:C2  | 2.48                     | 0.43              |
| 1:K:160:ARG:HG2  | 1:K:178:PRO:HG3  | 2.00                     | 0.43              |
| 2:L:53:THR:H     | 2:L:136:ASN:HD21 | 1.67                     | 0.43              |
| 1:M:135:ARG:NH2  | 1:M:181:ALA:HB1  | 2.34                     | 0.43              |
| 2:B:111:PRO:HB3  | 2:B:156:VAL:HG21 | 2.01                     | 0.42              |
| 2:F:173:PRO:O    | 2:F:174:ASP:C    | 2.63                     | 0.42              |
| 1:G:38:GLU:OE1   | 1:G:110:ARG:NH2  | 2.46                     | 0.42              |
| 1:G:67:ILE:N     | 1:G:67:ILE:HD12  | 2.34                     | 0.42              |
| 2:H:221:VAL:HG12 | 2:H:222:GLY:N    | 2.34                     | 0.42              |
| 1:I:12:PRO:HD2   | 1:I:15:GLN:HG3   | 2.00                     | 0.42              |
| 2:J:135:ASN:ND2  | 3:J:1605:MAN:O4  | 2.52                     | 0.42              |
| 1:K:129:GLU:C    | 1:K:131:LEU:H    | 2.28                     | 0.42              |
| 2:L:126:ILE:HD11 | 2:L:150:ALA:HB2  | 2.01                     | 0.42              |
| 1:M:77:GLN:HA    | 1:M:77:GLN:NE2   | 2.34                     | 0.42              |
| 1:M:160:ARG:HG2  | 1:M:178:PRO:HG3  | 2.01                     | 0.42              |
| 1:O:135:ARG:NH2  | 1:O:181:ALA:HB1  | 2.34                     | 0.42              |
| 2:P:126:ILE:HD11 | 2:P:150:ALA:HB2  | 2.01                     | 0.42              |
| 2:P:196:TYR:CD1  | 2:P:196:TYR:C    | 2.97                     | 0.42              |
| 2:P:207:SER:HB3  | 2:P:233:PRO:HB3  | 2.01                     | 0.42              |
| 1:C:93:MET:CE    | 1:C:98:LEU:HD23  | 2.45                     | 0.42              |
| 2:F:196:TYR:CD1  | 2:F:196:TYR:C    | 2.97                     | 0.42              |
| 2:H:126:ILE:CD1  | 2:H:150:ALA:HB2  | 2.26                     | 0.42              |
| 2:J:59:GLN:HG3   | 2:J:132:ARG:HD3  | 2.00                     | 0.42              |
| 1:K:149:TYR:CG   | 1:K:169:PRO:HD3  | 2.54                     | 0.42              |
| 2:L:29:ASN:OD1   | 2:L:157:PRO:HD2  | 2.19                     | 0.42              |
| 1:M:39:ASN:HD21  | 1:M:43:VAL:CG1   | 2.18                     | 0.42              |
| 1:M:52:PRO:HG2   | 1:M:55:PHE:CE2   | 2.54                     | 0.42              |
| 2:N:29:ASN:OD1   | 2:N:157:PRO:HD2  | 2.19                     | 0.42              |
| 1:O:31:TYR:O     | 1:O:56:ALA:HA    | 2.19                     | 0.42              |
| 2:P:122:ALA:N    | 2:P:153:ASP:OD1  | 2.52                     | 0.42              |
| 1:A:93:MET:CE    | 1:A:98:LEU:HD23  | 2.44                     | 0.42              |
| 1:A:155:LEU:HD12 | 1:A:187:TYR:HB3  | 2.01                     | 0.42              |
| 1:C:117:PRO:O    | 1:C:120:LEU:HG   | 2.19                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:226:THR:HG22 | 2:D:255:ASN:HD21 | 1.84                     | 0.42              |
| 2:F:4:LYS:HB2    | 2:F:4:LYS:NZ     | 2.34                     | 0.42              |
| 2:F:45:HIS:C     | 2:F:45:HIS:CD2   | 2.97                     | 0.42              |
| 1:G:117:PRO:O    | 1:G:120:LEU:HG   | 2.19                     | 0.42              |
| 2:H:201:THR:HB   | 2:H:206:ASN:ND2  | 2.34                     | 0.42              |
| 1:I:13:ALA:HB3   | 1:I:118:ALA:H    | 1.84                     | 0.42              |
| 2:L:168:VAL:HG13 | 2:L:168:VAL:O    | 2.18                     | 0.42              |
| 1:O:50:VAL:HG12  | 1:O:51:THR:N     | 2.34                     | 0.42              |
| 1:C:51:THR:HA    | 1:C:52:PRO:C     | 2.43                     | 0.42              |
| 2:D:226:THR:CG2  | 2:D:255:ASN:HD21 | 2.32                     | 0.42              |
| 1:E:169:PRO:O    | 1:E:170:MET:C    | 2.62                     | 0.42              |
| 2:F:240:LEU:HD21 | 2:F:250:LEU:HD22 | 2.00                     | 0.42              |
| 1:G:10:ILE:O     | 1:G:12:PRO:HD3   | 2.19                     | 0.42              |
| 1:G:191:ASN:ND2  | 1:G:195:ALA:HB3  | 2.32                     | 0.42              |
| 2:H:33:ASN:HD22  | 2:H:33:ASN:HA    | 1.59                     | 0.42              |
| 2:J:181:ILE:HA   | 2:J:182:PRO:HD3  | 1.93                     | 0.42              |
| 2:J:223:VAL:CG1  | 2:J:224:GLN:N    | 2.82                     | 0.42              |
| 1:K:13:ALA:HB3   | 1:K:118:ALA:H    | 1.84                     | 0.42              |
| 1:K:50:VAL:HG12  | 1:K:51:THR:N     | 2.34                     | 0.42              |
| 2:L:61:GLY:HA3   | 2:L:86:THR:HG23  | 2.00                     | 0.42              |
| 1:O:25:ASN:O     | 1:O:26:ASP:C     | 2.61                     | 0.42              |
| 1:O:134:ARG:HD2  | 1:O:141:THR:OG1  | 2.20                     | 0.42              |
| 1:O:188:ARG:NH1  | 1:O:199:LYS:H    | 2.17                     | 0.42              |
| 2:P:29:ASN:OD1   | 2:P:157:PRO:HD2  | 2.20                     | 0.42              |
| 2:P:30:VAL:HG23  | 2:P:156:VAL:CG1  | 2.49                     | 0.42              |
| 2:P:136:ASN:N    | 2:P:136:ASN:HD22 | 2.17                     | 0.42              |
| 2:P:223:VAL:CG1  | 2:P:224:GLN:N    | 2.82                     | 0.42              |
| 1:A:117:PRO:O    | 1:A:120:LEU:HG   | 2.19                     | 0.42              |
| 1:C:155:LEU:HD12 | 1:C:187:TYR:HB3  | 2.01                     | 0.42              |
| 2:D:7:ASN:HB2    | 4:D:1654:HOH:O   | 2.19                     | 0.42              |
| 1:E:98:LEU:HD13  | 1:E:98:LEU:C     | 2.45                     | 0.42              |
| 2:F:192:ASN:HA   | 2:F:241:GLY:O    | 2.19                     | 0.42              |
| 1:G:98:LEU:C     | 1:G:98:LEU:HD13  | 2.44                     | 0.42              |
| 2:H:113:SER:OG   | 2:L:81:SER:N     | 2.47                     | 0.42              |
| 2:H:136:ASN:HD22 | 2:H:136:ASN:N    | 2.18                     | 0.42              |
| 1:I:45:ASP:OD1   | 1:I:47:ARG:HB2   | 2.18                     | 0.42              |
| 1:K:13:ALA:CB    | 1:K:117:PRO:HA   | 2.50                     | 0.42              |
| 1:K:188:ARG:NH1  | 1:K:199:LYS:N    | 2.67                     | 0.42              |
| 2:L:250:LEU:CB   | 2:L:252:LEU:HG   | 2.50                     | 0.42              |
| 1:M:12:PRO:HD2   | 1:M:15:GLN:HG3   | 2.00                     | 0.42              |
| 1:M:188:ARG:NH1  | 1:M:199:LYS:N    | 2.67                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:N:122:ALA:N    | 2:N:153:ASP:OD1  | 2.53                     | 0.42              |
| 2:N:192:ASN:HA   | 2:N:241:GLY:O    | 2.19                     | 0.42              |
| 2:N:215:PHE:O    | 2:N:216:SER:C    | 2.61                     | 0.42              |
| 2:P:241:GLY:O    | 2:P:243:VAL:HG23 | 2.19                     | 0.42              |
| 1:A:79:ARG:HB3   | 1:A:170:MET:HE3  | 2.01                     | 0.42              |
| 2:B:116:GLY:HA2  | 2:B:189:LYS:CE   | 2.47                     | 0.42              |
| 2:D:118:VAL:O    | 2:D:118:VAL:HG12 | 2.19                     | 0.42              |
| 2:D:126:ILE:CD1  | 2:D:150:ALA:HB2  | 2.24                     | 0.42              |
| 1:I:28:ASN:O     | 1:I:29:SER:CB    | 2.68                     | 0.42              |
| 1:I:39:ASN:HD21  | 1:I:43:VAL:CG1   | 2.18                     | 0.42              |
| 2:J:20:VAL:CG1   | 2:J:22:VAL:HG13  | 2.50                     | 0.42              |
| 2:J:30:VAL:HG12  | 2:J:31:GLY:N     | 2.34                     | 0.42              |
| 2:J:184:THR:HA   | 2:J:248:VAL:O    | 2.19                     | 0.42              |
| 2:L:1:PHE:CD1    | 2:L:133:GLN:HG3  | 2.55                     | 0.42              |
| 1:M:25:ASN:O     | 1:M:26:ASP:C     | 2.61                     | 0.42              |
| 1:M:31:TYR:O     | 1:M:56:ALA:HA    | 2.20                     | 0.42              |
| 1:M:134:ARG:HD2  | 1:M:141:THR:OG1  | 2.20                     | 0.42              |
| 1:M:149:TYR:CG   | 1:M:169:PRO:HD3  | 2.54                     | 0.42              |
| 1:M:183:SER:C    | 1:M:185:ILE:H    | 2.27                     | 0.42              |
| 2:N:11:ILE:HA    | 2:N:12:PRO:HD2   | 1.89                     | 0.42              |
| 2:N:63:ALA:C     | 2:N:64:TYR:CD1   | 2.98                     | 0.42              |
| 2:N:126:ILE:HD11 | 2:N:150:ALA:HB2  | 2.02                     | 0.42              |
| 2:P:169:THR:OG1  | 2:P:181:ILE:HG23 | 2.19                     | 0.42              |
| 1:A:67:ILE:HD12  | 1:A:67:ILE:N     | 2.34                     | 0.42              |
| 1:A:122:LEU:HD12 | 1:A:123:PRO:N    | 2.35                     | 0.42              |
| 1:A:142:LEU:HD22 | 1:A:142:LEU:N    | 2.35                     | 0.42              |
| 2:D:135:ASN:HD21 | 2:D:138:ASN:HD21 | 1.66                     | 0.42              |
| 2:D:212:THR:O    | 2:D:269:GLN:HB2  | 2.20                     | 0.42              |
| 1:E:142:LEU:HD22 | 1:E:142:LEU:N    | 2.34                     | 0.42              |
| 1:I:50:VAL:HG12  | 1:I:51:THR:N     | 2.34                     | 0.42              |
| 1:I:135:ARG:CZ   | 1:I:177:LEU:HD21 | 2.50                     | 0.42              |
| 2:J:24:LEU:O     | 2:J:25:ALA:C     | 2.63                     | 0.42              |
| 2:L:95:TYR:OH    | 2:L:103:TRP:CA   | 2.66                     | 0.42              |
| 1:M:177:LEU:HD12 | 1:M:178:PRO:CD   | 2.40                     | 0.42              |
| 1:A:107:ILE:HG12 | 4:A:213:HOH:O    | 2.19                     | 0.42              |
| 1:C:177:LEU:HA   | 1:C:178:PRO:HD2  | 1.87                     | 0.42              |
| 2:D:201:THR:CB   | 2:D:206:ASN:ND2  | 2.83                     | 0.42              |
| 2:F:136:ASN:ND2  | 2:F:136:ASN:H    | 2.17                     | 0.42              |
| 2:F:212:THR:O    | 2:F:269:GLN:HB2  | 2.20                     | 0.42              |
| 1:I:117:PRO:O    | 1:I:119:LYS:N    | 2.53                     | 0.42              |
| 1:I:122:LEU:CD1  | 1:I:126:GLN:HB3  | 2.50                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:135:ARG:NH2  | 1:I:181:ALA:HB1  | 2.34                     | 0.42              |
| 1:I:188:ARG:NH1  | 1:I:199:LYS:H    | 2.18                     | 0.42              |
| 2:J:13:ILE:HG23  | 3:J:1605:MAN:O2  | 2.20                     | 0.42              |
| 2:J:58:LEU:H     | 2:J:90:THR:HG21  | 1.79                     | 0.42              |
| 1:K:57:MET:HA    | 1:K:61:LYS:HE3   | 2.00                     | 0.42              |
| 2:L:30:VAL:HG12  | 2:L:31:GLY:N     | 2.34                     | 0.42              |
| 2:L:48:TYR:HB2   | 2:L:52:ILE:CD1   | 2.48                     | 0.42              |
| 1:M:135:ARG:CZ   | 1:M:177:LEU:HD21 | 2.50                     | 0.42              |
| 1:O:117:PRO:O    | 1:O:119:LYS:N    | 2.53                     | 0.42              |
| 2:P:24:LEU:O     | 2:P:25:ALA:C     | 2.63                     | 0.42              |
| 2:P:184:THR:HA   | 2:P:248:VAL:O    | 2.19                     | 0.42              |
| 2:P:184:THR:HG1  | 2:P:247:ALA:HB1  | 1.85                     | 0.42              |
| 2:D:215:PHE:HD1  | 2:D:267:ASN:OD1  | 2.03                     | 0.42              |
| 2:D:221:VAL:HG12 | 2:D:222:GLY:N    | 2.35                     | 0.42              |
| 1:E:122:LEU:HD11 | 1:E:126:GLN:C    | 2.44                     | 0.42              |
| 1:I:31:TYR:O     | 1:I:56:ALA:HA    | 2.20                     | 0.42              |
| 1:I:188:ARG:NH1  | 1:I:199:LYS:N    | 2.67                     | 0.42              |
| 2:L:40:THR:C     | 2:L:41:GLN:HG2   | 2.45                     | 0.42              |
| 2:L:58:LEU:H     | 2:L:90:THR:HG21  | 1.78                     | 0.42              |
| 2:L:96:ASN:HD22  | 2:L:96:ASN:N     | 2.10                     | 0.42              |
| 1:M:108:ILE:HB   | 2:N:275:THR:HG23 | 2.02                     | 0.42              |
| 2:N:169:THR:OG1  | 2:N:181:ILE:HG23 | 2.20                     | 0.42              |
| 1:O:77:GLN:NE2   | 1:O:77:GLN:HA    | 2.35                     | 0.42              |
| 2:P:14:GLY:HA2   | 2:P:142:PHE:CZ   | 2.55                     | 0.42              |
| 2:P:95:TYR:OH    | 2:P:103:TRP:CA   | 2.66                     | 0.42              |
| 1:A:94:ASP:OD1   | 2:B:168:VAL:HG11 | 2.20                     | 0.42              |
| 1:C:94:ASP:OD1   | 2:D:168:VAL:HG11 | 2.20                     | 0.42              |
| 1:C:122:LEU:HD12 | 1:C:123:PRO:N    | 2.35                     | 0.42              |
| 2:F:111:PRO:HB3  | 2:F:156:VAL:HG21 | 2.02                     | 0.42              |
| 2:F:221:VAL:HG12 | 2:F:222:GLY:N    | 2.35                     | 0.42              |
| 1:I:25:ASN:O     | 1:I:26:ASP:C     | 2.61                     | 0.42              |
| 2:J:207:SER:HB3  | 2:J:233:PRO:HB3  | 2.01                     | 0.42              |
| 1:K:134:ARG:HD2  | 1:K:141:THR:OG1  | 2.20                     | 0.42              |
| 2:L:63:ALA:C     | 2:L:64:TYR:CD1   | 2.98                     | 0.42              |
| 2:L:207:SER:HB3  | 2:L:233:PRO:HB3  | 2.01                     | 0.42              |
| 2:L:223:VAL:CG1  | 2:L:224:GLN:N    | 2.82                     | 0.42              |
| 2:N:184:THR:HG1  | 2:N:247:ALA:HB1  | 1.85                     | 0.42              |
| 1:O:13:ALA:CB    | 1:O:117:PRO:HA   | 2.50                     | 0.42              |
| 1:O:142:LEU:HD22 | 1:O:142:LEU:N    | 2.35                     | 0.42              |
| 1:O:149:TYR:CG   | 1:O:169:PRO:HD3  | 2.54                     | 0.42              |
| 2:P:63:ALA:C     | 2:P:64:TYR:CD1   | 2.97                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:71:THR:O     | 1:A:73:ASN:N     | 2.51                     | 0.41              |
| 2:B:196:TYR:CD1  | 2:B:196:TYR:C    | 2.98                     | 0.41              |
| 2:B:226:THR:HG22 | 2:B:255:ASN:HD21 | 1.84                     | 0.41              |
| 1:C:67:ILE:HD12  | 1:C:67:ILE:N     | 2.34                     | 0.41              |
| 1:C:142:LEU:HD22 | 1:C:142:LEU:N    | 2.34                     | 0.41              |
| 2:D:90:THR:HG23  | 2:D:91:PRO:N     | 2.34                     | 0.41              |
| 2:D:196:TYR:CD1  | 2:D:196:TYR:C    | 2.98                     | 0.41              |
| 1:E:67:ILE:N     | 1:E:67:ILE:HD12  | 2.34                     | 0.41              |
| 1:I:77:GLN:NE2   | 1:I:77:GLN:HA    | 2.35                     | 0.41              |
| 2:J:136:ASN:N    | 2:J:136:ASN:HD22 | 2.18                     | 0.41              |
| 2:J:163:VAL:HA   | 2:J:185:VAL:CG2  | 2.36                     | 0.41              |
| 2:J:196:TYR:CD1  | 2:J:196:TYR:C    | 2.98                     | 0.41              |
| 1:K:28:ASN:O     | 1:K:29:SER:CB    | 2.68                     | 0.41              |
| 2:L:14:GLY:HA2   | 2:L:142:PHE:CZ   | 2.54                     | 0.41              |
| 2:L:64:TYR:CE1   | 2:L:128:VAL:HG23 | 2.55                     | 0.41              |
| 2:L:122:ALA:N    | 2:L:153:ASP:OD1  | 2.53                     | 0.41              |
| 2:N:184:THR:HA   | 2:N:248:VAL:O    | 2.20                     | 0.41              |
| 2:N:196:TYR:C    | 2:N:196:TYR:CD1  | 2.98                     | 0.41              |
| 1:A:98:LEU:C     | 1:A:98:LEU:HD13  | 2.45                     | 0.41              |
| 2:B:201:THR:CB   | 2:B:206:ASN:ND2  | 2.83                     | 0.41              |
| 1:C:79:ARG:HB3   | 1:C:170:MET:HE3  | 2.02                     | 0.41              |
| 1:C:169:PRO:O    | 1:C:170:MET:C    | 2.62                     | 0.41              |
| 2:D:136:ASN:HD22 | 2:D:136:ASN:N    | 2.16                     | 0.41              |
| 1:E:117:PRO:O    | 1:E:120:LEU:HG   | 2.20                     | 0.41              |
| 1:I:134:ARG:HD2  | 1:I:141:THR:OG1  | 2.20                     | 0.41              |
| 2:J:53:THR:H     | 2:J:136:ASN:HD21 | 1.68                     | 0.41              |
| 2:J:116:GLY:O    | 2:J:156:VAL:O    | 2.38                     | 0.41              |
| 2:J:126:ILE:HD11 | 2:J:150:ALA:HB2  | 2.02                     | 0.41              |
| 1:K:12:PRO:HD2   | 1:K:15:GLN:HG3   | 2.00                     | 0.41              |
| 1:K:122:LEU:CD1  | 1:K:126:GLN:HB3  | 2.50                     | 0.41              |
| 1:M:122:LEU:CD1  | 1:M:126:GLN:HB3  | 2.50                     | 0.41              |
| 2:N:14:GLY:HA2   | 2:N:142:PHE:CZ   | 2.55                     | 0.41              |
| 1:O:129:GLU:C    | 1:O:131:LEU:H    | 2.27                     | 0.41              |
| 2:P:19:ASN:OD1   | 2:P:147:ASN:HB2  | 2.20                     | 0.41              |
| 2:P:30:VAL:HG12  | 2:P:31:GLY:N     | 2.34                     | 0.41              |
| 2:P:116:GLY:O    | 2:P:156:VAL:O    | 2.38                     | 0.41              |
| 2:B:192:ASN:HA   | 2:B:241:GLY:O    | 2.20                     | 0.41              |
| 1:C:181:ALA:HB1  | 1:C:182:GLY:H    | 1.53                     | 0.41              |
| 2:D:201:THR:HB   | 2:D:206:ASN:ND2  | 2.36                     | 0.41              |
| 1:E:12:PRO:CB    | 1:E:15:GLN:HG3   | 2.48                     | 0.41              |
| 1:G:142:LEU:HD22 | 1:G:142:LEU:N    | 2.34                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:135:ARG:HH12 | 1:I:177:LEU:HD11 | 1.82                     | 0.41              |
| 2:J:227:ARG:HG2  | 2:J:232:ILE:HD11 | 2.02                     | 0.41              |
| 1:K:77:GLN:HA    | 1:K:77:GLN:NE2   | 2.35                     | 0.41              |
| 2:L:44:CYS:O     | 2:L:101:LYS:N    | 2.50                     | 0.41              |
| 2:L:116:GLY:O    | 2:L:156:VAL:O    | 2.38                     | 0.41              |
| 1:M:185:ILE:O    | 1:M:202:GLY:N    | 2.35                     | 0.41              |
| 1:M:188:ARG:NH1  | 1:M:199:LYS:H    | 2.17                     | 0.41              |
| 2:N:1:PHE:CD1    | 2:N:133:GLN:HG3  | 2.54                     | 0.41              |
| 2:N:207:SER:HB3  | 2:N:233:PRO:HB3  | 2.01                     | 0.41              |
| 1:O:28:ASN:O     | 1:O:29:SER:CB    | 2.68                     | 0.41              |
| 1:O:122:LEU:CD1  | 1:O:126:GLN:HB3  | 2.50                     | 0.41              |
| 1:C:38:GLU:OE1   | 1:C:110:ARG:NH2  | 2.46                     | 0.41              |
| 2:D:136:ASN:ND2  | 2:D:136:ASN:H    | 2.17                     | 0.41              |
| 1:E:79:ARG:HB3   | 1:E:170:MET:HE3  | 2.03                     | 0.41              |
| 2:F:126:ILE:CD1  | 2:F:150:ALA:HB2  | 2.25                     | 0.41              |
| 2:F:162:ASP:HB3  | 2:F:186:TYR:CZ   | 2.55                     | 0.41              |
| 1:G:147:PRO:HB3  | 1:G:170:MET:HE2  | 2.02                     | 0.41              |
| 2:H:45:HIS:CD2   | 2:H:45:HIS:C     | 2.98                     | 0.41              |
| 1:I:13:ALA:CB    | 1:I:117:PRO:HA   | 2.50                     | 0.41              |
| 2:J:19:ASN:OD1   | 2:J:147:ASN:HB2  | 2.20                     | 0.41              |
| 2:J:250:LEU:CB   | 2:J:252:LEU:HG   | 2.50                     | 0.41              |
| 1:K:31:TYR:O     | 1:K:56:ALA:HA    | 2.19                     | 0.41              |
| 1:K:135:ARG:CZ   | 1:K:177:LEU:HD21 | 2.50                     | 0.41              |
| 2:L:196:TYR:CD1  | 2:L:196:TYR:C    | 2.97                     | 0.41              |
| 1:M:132:ARG:C    | 1:M:133:PHE:CD1  | 2.99                     | 0.41              |
| 1:O:135:ARG:CZ   | 1:O:177:LEU:HD21 | 2.50                     | 0.41              |
| 2:P:53:THR:H     | 2:P:136:ASN:HD21 | 1.66                     | 0.41              |
| 2:P:227:ARG:HG2  | 2:P:232:ILE:HD11 | 2.03                     | 0.41              |
| 2:F:201:THR:HB   | 2:F:206:ASN:ND2  | 2.35                     | 0.41              |
| 1:G:169:PRO:O    | 1:G:170:MET:C    | 2.63                     | 0.41              |
| 1:K:117:PRO:O    | 1:K:119:LYS:N    | 2.53                     | 0.41              |
| 1:K:188:ARG:NH1  | 1:K:199:LYS:H    | 2.18                     | 0.41              |
| 2:L:169:THR:OG1  | 2:L:181:ILE:HG23 | 2.20                     | 0.41              |
| 2:L:184:THR:HA   | 2:L:248:VAL:O    | 2.20                     | 0.41              |
| 2:L:197:LEU:CD1  | 2:L:225:LEU:HD12 | 2.43                     | 0.41              |
| 2:L:227:ARG:HG2  | 2:L:232:ILE:HD11 | 2.03                     | 0.41              |
| 2:N:24:LEU:O     | 2:N:25:ALA:C     | 2.63                     | 0.41              |
| 1:O:39:ASN:HD21  | 1:O:43:VAL:CG1   | 2.18                     | 0.41              |
| 1:O:108:ILE:HB   | 2:P:275:THR:HG23 | 2.03                     | 0.41              |
| 2:P:40:THR:C     | 2:P:41:GLN:HG2   | 2.45                     | 0.41              |
| 2:B:5:THR:HG22   | 2:B:9:THR:N      | 2.35                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:178:PRO:O    | 1:C:179:SER:HB3  | 2.20                     | 0.41              |
| 1:E:94:ASP:C     | 1:E:96:SER:N     | 2.77                     | 0.41              |
| 2:H:136:ASN:ND2  | 2:H:136:ASN:H    | 2.18                     | 0.41              |
| 2:J:29:ASN:OD1   | 2:J:157:PRO:HD2  | 2.20                     | 0.41              |
| 2:J:169:THR:OG1  | 2:J:181:ILE:HG23 | 2.20                     | 0.41              |
| 1:M:80:GLU:HG3   | 1:M:148:TYR:HA   | 2.02                     | 0.41              |
| 2:N:40:THR:C     | 2:N:41:GLN:HG2   | 2.46                     | 0.41              |
| 2:N:116:GLY:O    | 2:N:156:VAL:O    | 2.37                     | 0.41              |
| 2:P:44:CYS:O     | 2:P:101:LYS:N    | 2.51                     | 0.41              |
| 1:A:178:PRO:O    | 1:A:179:SER:HB3  | 2.21                     | 0.41              |
| 2:B:45:HIS:CD2   | 2:B:45:HIS:C     | 2.97                     | 0.41              |
| 1:E:147:PRO:HB3  | 1:E:170:MET:HE2  | 2.02                     | 0.41              |
| 2:L:20:VAL:CG1   | 2:L:22:VAL:HG13  | 2.50                     | 0.41              |
| 2:L:24:LEU:O     | 2:L:25:ALA:C     | 2.63                     | 0.41              |
| 1:M:135:ARG:HH12 | 1:M:177:LEU:HD11 | 1.82                     | 0.41              |
| 2:N:19:ASN:OD1   | 2:N:147:ASN:HB2  | 2.21                     | 0.41              |
| 2:N:20:VAL:CG1   | 2:N:22:VAL:HG13  | 2.50                     | 0.41              |
| 2:N:22:VAL:HG12  | 2:N:41:GLN:HG3   | 2.02                     | 0.41              |
| 2:N:90:THR:HG23  | 2:N:91:PRO:O     | 2.21                     | 0.41              |
| 1:O:132:ARG:C    | 1:O:133:PHE:CD1  | 2.99                     | 0.41              |
| 2:B:207:SER:HB3  | 2:B:233:PRO:HB3  | 2.02                     | 0.41              |
| 2:B:215:PHE:HD1  | 2:B:267:ASN:OD1  | 2.04                     | 0.41              |
| 2:D:1:PHE:CG     | 2:D:133:GLN:HG3  | 2.56                     | 0.41              |
| 1:E:94:ASP:OD1   | 2:F:168:VAL:HG11 | 2.20                     | 0.41              |
| 1:G:107:ILE:HG12 | 4:G:216:HOH:O    | 2.21                     | 0.41              |
| 2:H:196:TYR:CD1  | 2:H:196:TYR:C    | 2.98                     | 0.41              |
| 2:H:215:PHE:HD1  | 2:H:267:ASN:OD1  | 2.03                     | 0.41              |
| 1:I:133:PHE:HB3  | 1:I:134:ARG:H    | 1.70                     | 0.41              |
| 2:L:136:ASN:HD22 | 2:L:136:ASN:N    | 2.17                     | 0.41              |
| 1:M:13:ALA:CB    | 1:M:117:PRO:HA   | 2.50                     | 0.41              |
| 2:N:53:THR:H     | 2:N:136:ASN:HD21 | 1.67                     | 0.41              |
| 2:N:227:ARG:HG2  | 2:N:232:ILE:HD11 | 2.03                     | 0.41              |
| 2:P:46:ASN:HD22  | 2:P:96:ASN:HA    | 1.85                     | 0.41              |
| 2:P:67:VAL:CG2   | 2:P:126:ILE:HG23 | 2.36                     | 0.41              |
| 2:P:250:LEU:CB   | 2:P:252:LEU:HG   | 2.50                     | 0.41              |
| 1:A:129:GLU:H    | 1:A:129:GLU:HG3  | 1.51                     | 0.41              |
| 1:A:174:THR:O    | 1:A:174:THR:CG2  | 2.68                     | 0.41              |
| 1:A:181:ALA:HB1  | 1:A:182:GLY:H    | 1.53                     | 0.41              |
| 1:A:183:SER:C    | 1:A:185:ILE:N    | 2.74                     | 0.41              |
| 1:A:198:PRO:O    | 1:A:200:MET:HG2  | 2.21                     | 0.41              |
| 2:B:33:ASN:HD22  | 2:B:33:ASN:HA    | 1.60                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:81:SER:C     | 2:B:82:TYR:CD1   | 2.99                     | 0.41              |
| 2:B:226:THR:CG2  | 2:B:255:ASN:HD21 | 2.33                     | 0.41              |
| 1:C:132:ARG:C    | 1:C:143:ILE:HG23 | 2.46                     | 0.41              |
| 2:D:116:GLY:HA2  | 2:D:189:LYS:CE   | 2.47                     | 0.41              |
| 1:E:198:PRO:O    | 1:E:200:MET:HG2  | 2.21                     | 0.41              |
| 2:F:84:PHE:CA    | 2:F:85:PRO:C     | 2.92                     | 0.41              |
| 2:F:92:ARG:NH1   | 2:F:92:ARG:CG    | 2.83                     | 0.41              |
| 2:F:168:VAL:O    | 2:F:168:VAL:HG22 | 2.21                     | 0.41              |
| 1:G:71:THR:O     | 1:G:73:ASN:N     | 2.51                     | 0.41              |
| 2:H:201:THR:CB   | 2:H:206:ASN:HD22 | 2.34                     | 0.41              |
| 2:H:212:THR:O    | 2:H:269:GLN:HB2  | 2.20                     | 0.41              |
| 1:I:129:GLU:C    | 1:I:131:LEU:H    | 2.28                     | 0.41              |
| 2:J:20:VAL:CG2   | 2:J:42:ILE:HD11  | 2.50                     | 0.41              |
| 2:J:40:THR:C     | 2:J:41:GLN:HG2   | 2.45                     | 0.41              |
| 1:K:126:GLN:O    | 1:K:126:GLN:HG2  | 2.21                     | 0.41              |
| 1:K:132:ARG:C    | 1:K:133:PHE:CD1  | 2.99                     | 0.41              |
| 2:L:262:GLN:HE21 | 2:L:262:GLN:HA   | 1.85                     | 0.41              |
| 1:M:13:ALA:HB3   | 1:M:118:ALA:H    | 1.84                     | 0.41              |
| 1:M:117:PRO:O    | 1:M:119:LYS:N    | 2.53                     | 0.41              |
| 1:M:133:PHE:HB3  | 1:M:134:ARG:H    | 1.71                     | 0.41              |
| 2:N:64:TYR:CE1   | 2:N:128:VAL:HG23 | 2.56                     | 0.41              |
| 2:N:67:VAL:HG21  | 2:N:126:ILE:CG2  | 2.36                     | 0.41              |
| 2:N:136:ASN:N    | 2:N:136:ASN:HD22 | 2.18                     | 0.41              |
| 2:N:262:GLN:HA   | 2:N:262:GLN:HE21 | 1.85                     | 0.41              |
| 1:O:135:ARG:HH12 | 1:O:177:LEU:HD11 | 1.83                     | 0.41              |
| 2:P:20:VAL:CG1   | 2:P:22:VAL:HG13  | 2.51                     | 0.41              |
| 2:P:262:GLN:HA   | 2:P:262:GLN:HE21 | 1.86                     | 0.41              |
| 1:A:27:GLU:CG    | 1:A:60:LYS:HD2   | 2.49                     | 0.41              |
| 1:C:198:PRO:O    | 1:C:200:MET:HG2  | 2.21                     | 0.41              |
| 2:D:5:THR:N      | 2:D:9:THR:O      | 2.51                     | 0.41              |
| 1:E:167:VAL:HA   | 1:E:168:PRO:HD2  | 1.75                     | 0.41              |
| 2:F:135:ASN:HD21 | 2:F:138:ASN:HD21 | 1.67                     | 0.41              |
| 1:G:80:GLU:HA    | 1:G:115:TYR:O    | 2.21                     | 0.41              |
| 1:I:184:ASN:O    | 1:I:184:ASN:CG   | 2.64                     | 0.41              |
| 2:J:84:PHE:CA    | 2:J:85:PRO:C     | 2.92                     | 0.41              |
| 1:K:80:GLU:HG3   | 1:K:148:TYR:HA   | 2.03                     | 0.41              |
| 1:M:142:LEU:HD22 | 1:M:142:LEU:N    | 2.35                     | 0.41              |
| 2:N:84:PHE:CA    | 2:N:85:PRO:C     | 2.92                     | 0.41              |
| 2:P:120:ILE:O    | 2:P:153:ASP:HA   | 2.21                     | 0.41              |
| 2:P:175:TYR:CZ   | 2:P:263:VAL:HB   | 2.56                     | 0.41              |
| 1:C:168:PRO:HA   | 1:C:169:PRO:HD3  | 1.87                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:132:ARG:C    | 1:E:143:ILE:HG23 | 2.46                     | 0.40              |
| 2:F:81:SER:C     | 2:F:82:TYR:CD1   | 2.99                     | 0.40              |
| 2:F:90:THR:HG23  | 2:F:91:PRO:N     | 2.35                     | 0.40              |
| 1:G:188:ARG:HG2  | 1:G:199:LYS:HA   | 2.04                     | 0.40              |
| 2:H:162:ASP:HB3  | 2:H:186:TYR:CZ   | 2.56                     | 0.40              |
| 1:I:142:LEU:HD22 | 1:I:142:LEU:N    | 2.36                     | 0.40              |
| 2:L:19:ASN:OD1   | 2:L:147:ASN:HB2  | 2.21                     | 0.40              |
| 2:L:175:TYR:CZ   | 2:L:263:VAL:HB   | 2.57                     | 0.40              |
| 1:M:126:GLN:O    | 1:M:126:GLN:HG2  | 2.21                     | 0.40              |
| 2:N:46:ASN:HD22  | 2:N:96:ASN:HA    | 1.86                     | 0.40              |
| 2:N:128:VAL:O    | 2:N:128:VAL:HG12 | 2.21                     | 0.40              |
| 2:N:202:ALA:HB2  | 2:N:210:THR:CG2  | 2.34                     | 0.40              |
| 1:O:182:GLY:O    | 1:O:183:SER:CB   | 2.65                     | 0.40              |
| 1:O:185:ILE:O    | 1:O:202:GLY:N    | 2.35                     | 0.40              |
| 2:P:52:ILE:HD12  | 3:P:1607:MAN:H61 | 2.04                     | 0.40              |
| 2:B:90:THR:HG23  | 2:B:91:PRO:N     | 2.36                     | 0.40              |
| 1:C:191:ASN:ND2  | 1:C:195:ALA:HB3  | 2.34                     | 0.40              |
| 2:D:59:GLN:HG2   | 2:D:132:ARG:CD   | 2.43                     | 0.40              |
| 2:D:111:PRO:HB3  | 2:D:156:VAL:HG21 | 2.02                     | 0.40              |
| 2:D:168:VAL:O    | 2:D:168:VAL:HG22 | 2.20                     | 0.40              |
| 1:G:39:ASN:OD1   | 1:G:39:ASN:C     | 2.63                     | 0.40              |
| 1:G:198:PRO:O    | 1:G:200:MET:HG2  | 2.21                     | 0.40              |
| 2:H:168:VAL:O    | 2:H:168:VAL:HG22 | 2.22                     | 0.40              |
| 2:H:228:ASN:N    | 2:H:228:ASN:HD22 | 2.19                     | 0.40              |
| 1:I:80:GLU:HG3   | 1:I:148:TYR:HA   | 2.03                     | 0.40              |
| 1:I:108:ILE:HB   | 2:J:275:THR:HG23 | 2.02                     | 0.40              |
| 1:M:101:ASN:ND2  | 2:N:268:VAL:N    | 2.69                     | 0.40              |
| 2:N:175:TYR:CZ   | 2:N:263:VAL:HB   | 2.56                     | 0.40              |
| 1:A:82:LEU:HD12  | 1:A:83:PHE:H     | 1.84                     | 0.40              |
| 1:A:167:VAL:HA   | 1:A:168:PRO:HD2  | 1.76                     | 0.40              |
| 1:C:188:ARG:HG2  | 1:C:199:LYS:HA   | 2.03                     | 0.40              |
| 2:D:218:ALA:HB2  | 2:D:266:GLY:CA   | 2.51                     | 0.40              |
| 1:G:167:VAL:HA   | 1:G:168:PRO:HD2  | 1.76                     | 0.40              |
| 1:K:184:ASN:O    | 1:K:184:ASN:CG   | 2.64                     | 0.40              |
| 2:L:254:ALA:C    | 2:L:255:ASN:HD22 | 2.30                     | 0.40              |
| 1:O:193:TYR:HB3  | 2:P:157:PRO:HG3  | 2.03                     | 0.40              |
| 1:A:155:LEU:HA   | 1:A:186:THR:O    | 2.22                     | 0.40              |
| 2:B:136:ASN:HD22 | 2:B:136:ASN:N    | 2.18                     | 0.40              |
| 1:E:129:GLU:H    | 1:E:129:GLU:HG3  | 1.52                     | 0.40              |
| 1:E:155:LEU:HA   | 1:E:186:THR:O    | 2.22                     | 0.40              |
| 1:G:178:PRO:O    | 1:G:179:SER:HB3  | 2.21                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:191:ASN:O    | 1:G:194:GLY:N    | 2.46                     | 0.40              |
| 2:H:1:PHE:CG     | 2:H:133:GLN:HG3  | 2.57                     | 0.40              |
| 2:J:22:VAL:HG12  | 2:J:41:GLN:HG3   | 2.03                     | 0.40              |
| 2:J:33:ASN:C     | 2:J:33:ASN:HD22  | 2.29                     | 0.40              |
| 2:J:46:ASN:HD22  | 2:J:96:ASN:HA    | 1.86                     | 0.40              |
| 1:K:8:ARG:NH1    | 1:K:190:ILE:CG2  | 2.85                     | 0.40              |
| 1:K:142:LEU:HD22 | 1:K:142:LEU:N    | 2.36                     | 0.40              |
| 2:L:64:TYR:CD1   | 2:L:64:TYR:N     | 2.89                     | 0.40              |
| 2:L:128:VAL:O    | 2:L:128:VAL:HG12 | 2.21                     | 0.40              |
| 2:N:24:LEU:O     | 2:N:152:ASN:ND2  | 2.51                     | 0.40              |
| 2:N:223:VAL:CG1  | 2:N:224:GLN:N    | 2.83                     | 0.40              |
| 1:O:103:LEU:HD23 | 2:P:181:ILE:HD11 | 2.03                     | 0.40              |
| 2:P:11:ILE:HA    | 2:P:12:PRO:HD2   | 1.89                     | 0.40              |
| 2:P:106:ALA:CB   | 2:P:108:TYR:HE1  | 2.35                     | 0.40              |
| 1:A:132:ARG:C    | 1:A:143:ILE:HG23 | 2.47                     | 0.40              |
| 2:B:118:VAL:O    | 2:B:118:VAL:HG12 | 2.20                     | 0.40              |
| 2:B:262:GLN:HE21 | 2:B:262:GLN:CA   | 2.25                     | 0.40              |
| 1:C:98:LEU:HD13  | 1:C:98:LEU:C     | 2.45                     | 0.40              |
| 1:E:47:ARG:NH2   | 1:E:74:GLN:NE2   | 2.55                     | 0.40              |
| 2:F:116:GLY:HA2  | 2:F:189:LYS:CE   | 2.47                     | 0.40              |
| 1:I:132:ARG:C    | 1:I:133:PHE:CD1  | 2.99                     | 0.40              |
| 2:J:120:ILE:O    | 2:J:153:ASP:HA   | 2.21                     | 0.40              |
| 2:L:22:VAL:HG12  | 2:L:41:GLN:HG3   | 2.02                     | 0.40              |
| 2:L:90:THR:HG23  | 2:L:91:PRO:O     | 2.22                     | 0.40              |
| 2:L:231:ILE:CG2  | 2:L:232:ILE:N    | 2.84                     | 0.40              |
| 1:M:193:TYR:HB3  | 2:N:157:PRO:HG3  | 2.04                     | 0.40              |
| 2:N:209:PHE:CE2  | 2:N:272:ILE:HG23 | 2.57                     | 0.40              |
| 2:N:231:ILE:CG2  | 2:N:232:ILE:N    | 2.85                     | 0.40              |
| 1:O:101:ASN:ND2  | 2:P:268:VAL:N    | 2.69                     | 0.40              |
| 1:O:126:GLN:O    | 1:O:126:GLN:HG2  | 2.21                     | 0.40              |
| 2:P:22:VAL:HG12  | 2:P:41:GLN:HG3   | 2.03                     | 0.40              |
| 2:P:162:ASP:O    | 2:P:185:VAL:HA   | 2.22                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

of similar resolution.

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

| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|-----------|----------|-------------|----|
| 1   | A     | 203/205 (99%)   | 163 (80%)  | 29 (14%)  | 11 (5%)  | 1           | 4  |
| 1   | C     | 203/205 (99%)   | 164 (81%)  | 28 (14%)  | 11 (5%)  | 1           | 4  |
| 1   | E     | 203/205 (99%)   | 163 (80%)  | 29 (14%)  | 11 (5%)  | 1           | 4  |
| 1   | G     | 203/205 (99%)   | 164 (81%)  | 28 (14%)  | 11 (5%)  | 1           | 4  |
| 1   | I     | 203/205 (99%)   | 162 (80%)  | 29 (14%)  | 12 (6%)  | 1           | 3  |
| 1   | K     | 203/205 (99%)   | 162 (80%)  | 29 (14%)  | 12 (6%)  | 1           | 3  |
| 1   | M     | 203/205 (99%)   | 162 (80%)  | 29 (14%)  | 12 (6%)  | 1           | 3  |
| 1   | O     | 203/205 (99%)   | 163 (80%)  | 28 (14%)  | 12 (6%)  | 1           | 3  |
| 2   | B     | 277/279 (99%)   | 244 (88%)  | 24 (9%)   | 9 (3%)   | 3           | 11 |
| 2   | D     | 277/279 (99%)   | 243 (88%)  | 24 (9%)   | 10 (4%)  | 2           | 10 |
| 2   | F     | 277/279 (99%)   | 244 (88%)  | 23 (8%)   | 10 (4%)  | 2           | 10 |
| 2   | H     | 277/279 (99%)   | 243 (88%)  | 24 (9%)   | 10 (4%)  | 2           | 10 |
| 2   | J     | 277/279 (99%)   | 195 (70%)  | 60 (22%)  | 22 (8%)  | 1           | 1  |
| 2   | L     | 277/279 (99%)   | 195 (70%)  | 60 (22%)  | 22 (8%)  | 1           | 1  |
| 2   | N     | 277/279 (99%)   | 195 (70%)  | 60 (22%)  | 22 (8%)  | 1           | 1  |
| 2   | P     | 277/279 (99%)   | 196 (71%)  | 59 (21%)  | 22 (8%)  | 1           | 1  |
| All | All   | 3840/3872 (99%) | 3058 (80%) | 563 (15%) | 219 (6%) | 1           | 4  |

All (219) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 29  | SER  |
| 1   | A     | 119 | LYS  |
| 1   | A     | 181 | ALA  |
| 1   | A     | 183 | SER  |
| 2   | B     | 175 | TYR  |
| 2   | B     | 218 | ALA  |
| 1   | C     | 29  | SER  |
| 1   | C     | 119 | LYS  |
| 1   | C     | 181 | ALA  |
| 1   | C     | 183 | SER  |
| 2   | D     | 175 | TYR  |
| 2   | D     | 218 | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 29  | SER  |
| 1   | E     | 119 | LYS  |
| 1   | E     | 181 | ALA  |
| 1   | E     | 183 | SER  |
| 2   | F     | 175 | TYR  |
| 2   | F     | 218 | ALA  |
| 1   | G     | 29  | SER  |
| 1   | G     | 119 | LYS  |
| 1   | G     | 181 | ALA  |
| 1   | G     | 183 | SER  |
| 2   | H     | 175 | TYR  |
| 2   | H     | 218 | ALA  |
| 1   | I     | 29  | SER  |
| 1   | I     | 119 | LYS  |
| 1   | I     | 181 | ALA  |
| 1   | I     | 183 | SER  |
| 1   | K     | 29  | SER  |
| 1   | K     | 119 | LYS  |
| 1   | K     | 181 | ALA  |
| 1   | K     | 183 | SER  |
| 2   | L     | 264 | THR  |
| 1   | M     | 29  | SER  |
| 1   | M     | 119 | LYS  |
| 1   | M     | 181 | ALA  |
| 1   | M     | 183 | SER  |
| 2   | N     | 264 | THR  |
| 1   | O     | 29  | SER  |
| 1   | O     | 119 | LYS  |
| 1   | O     | 181 | ALA  |
| 1   | O     | 183 | SER  |
| 2   | P     | 264 | THR  |
| 1   | A     | 26  | ASP  |
| 1   | A     | 192 | ASP  |
| 2   | B     | 116 | GLY  |
| 2   | B     | 167 | ASP  |
| 2   | B     | 173 | PRO  |
| 2   | B     | 174 | ASP  |
| 2   | B     | 215 | PHE  |
| 2   | B     | 221 | VAL  |
| 1   | C     | 26  | ASP  |
| 1   | C     | 192 | ASP  |
| 2   | D     | 116 | GLY  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | D     | 167 | ASP  |
| 2   | D     | 173 | PRO  |
| 2   | D     | 174 | ASP  |
| 2   | D     | 215 | PHE  |
| 2   | D     | 221 | VAL  |
| 1   | E     | 26  | ASP  |
| 1   | E     | 192 | ASP  |
| 2   | F     | 116 | GLY  |
| 2   | F     | 167 | ASP  |
| 2   | F     | 173 | PRO  |
| 2   | F     | 174 | ASP  |
| 2   | F     | 215 | PHE  |
| 2   | F     | 221 | VAL  |
| 1   | G     | 26  | ASP  |
| 1   | G     | 192 | ASP  |
| 2   | H     | 116 | GLY  |
| 2   | H     | 167 | ASP  |
| 2   | H     | 173 | PRO  |
| 2   | H     | 174 | ASP  |
| 2   | H     | 215 | PHE  |
| 2   | H     | 221 | VAL  |
| 1   | I     | 62  | GLU  |
| 2   | J     | 9   | THR  |
| 2   | J     | 22  | VAL  |
| 2   | J     | 32  | GLN  |
| 2   | J     | 116 | GLY  |
| 2   | J     | 157 | PRO  |
| 2   | J     | 168 | VAL  |
| 2   | J     | 190 | SER  |
| 2   | J     | 247 | ALA  |
| 2   | J     | 264 | THR  |
| 1   | K     | 62  | GLU  |
| 2   | L     | 9   | THR  |
| 2   | L     | 22  | VAL  |
| 2   | L     | 32  | GLN  |
| 2   | L     | 116 | GLY  |
| 2   | L     | 157 | PRO  |
| 2   | L     | 168 | VAL  |
| 2   | L     | 190 | SER  |
| 2   | L     | 247 | ALA  |
| 1   | M     | 62  | GLU  |
| 2   | N     | 9   | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | N     | 22  | VAL  |
| 2   | N     | 116 | GLY  |
| 2   | N     | 157 | PRO  |
| 2   | N     | 168 | VAL  |
| 2   | N     | 190 | SER  |
| 2   | N     | 247 | ALA  |
| 1   | O     | 62  | GLU  |
| 2   | P     | 9   | THR  |
| 2   | P     | 22  | VAL  |
| 2   | P     | 32  | GLN  |
| 2   | P     | 116 | GLY  |
| 2   | P     | 157 | PRO  |
| 2   | P     | 168 | VAL  |
| 2   | P     | 190 | SER  |
| 2   | P     | 247 | ALA  |
| 1   | A     | 134 | ARG  |
| 1   | A     | 138 | ASN  |
| 1   | C     | 134 | ARG  |
| 1   | C     | 138 | ASN  |
| 1   | E     | 134 | ARG  |
| 1   | E     | 138 | ASN  |
| 1   | G     | 134 | ARG  |
| 1   | G     | 138 | ASN  |
| 1   | I     | 26  | ASP  |
| 2   | J     | 97  | SER  |
| 2   | J     | 173 | PRO  |
| 2   | J     | 206 | ASN  |
| 2   | J     | 235 | ASN  |
| 2   | J     | 242 | ALA  |
| 1   | K     | 26  | ASP  |
| 2   | L     | 97  | SER  |
| 2   | L     | 173 | PRO  |
| 2   | L     | 206 | ASN  |
| 2   | L     | 235 | ASN  |
| 2   | L     | 242 | ALA  |
| 1   | M     | 26  | ASP  |
| 2   | N     | 32  | GLN  |
| 2   | N     | 97  | SER  |
| 2   | N     | 173 | PRO  |
| 2   | N     | 206 | ASN  |
| 2   | N     | 235 | ASN  |
| 2   | N     | 242 | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | O     | 26  | ASP  |
| 2   | P     | 97  | SER  |
| 2   | P     | 173 | PRO  |
| 2   | P     | 206 | ASN  |
| 2   | P     | 235 | ASN  |
| 2   | P     | 242 | ALA  |
| 1   | A     | 72  | ASN  |
| 1   | A     | 91  | PRO  |
| 1   | C     | 72  | ASN  |
| 1   | C     | 91  | PRO  |
| 1   | E     | 72  | ASN  |
| 1   | G     | 72  | ASN  |
| 1   | G     | 91  | PRO  |
| 1   | I     | 91  | PRO  |
| 1   | I     | 121 | ALA  |
| 1   | I     | 134 | ARG  |
| 1   | I     | 138 | ASN  |
| 2   | J     | 166 | ARG  |
| 2   | J     | 261 | GLY  |
| 1   | K     | 91  | PRO  |
| 1   | K     | 121 | ALA  |
| 1   | K     | 134 | ARG  |
| 1   | K     | 138 | ASN  |
| 2   | L     | 166 | ARG  |
| 2   | L     | 261 | GLY  |
| 1   | M     | 91  | PRO  |
| 1   | M     | 121 | ALA  |
| 1   | M     | 134 | ARG  |
| 1   | M     | 138 | ASN  |
| 2   | N     | 166 | ARG  |
| 2   | N     | 261 | GLY  |
| 1   | O     | 91  | PRO  |
| 1   | O     | 121 | ALA  |
| 1   | O     | 134 | ARG  |
| 1   | O     | 138 | ASN  |
| 2   | P     | 166 | ARG  |
| 2   | P     | 261 | GLY  |
| 1   | E     | 91  | PRO  |
| 1   | I     | 164 | ASN  |
| 2   | J     | 40  | THR  |
| 2   | J     | 100 | ASP  |
| 1   | K     | 164 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | L     | 40  | THR  |
| 2   | L     | 100 | ASP  |
| 1   | M     | 164 | ASN  |
| 2   | N     | 40  | THR  |
| 2   | N     | 100 | ASP  |
| 2   | N     | 217 | PRO  |
| 1   | O     | 164 | ASN  |
| 2   | P     | 40  | THR  |
| 2   | P     | 100 | ASP  |
| 1   | A     | 147 | PRO  |
| 1   | C     | 147 | PRO  |
| 2   | D     | 260 | GLY  |
| 1   | E     | 147 | PRO  |
| 2   | F     | 260 | GLY  |
| 1   | G     | 147 | PRO  |
| 2   | H     | 260 | GLY  |
| 2   | J     | 217 | PRO  |
| 2   | L     | 217 | PRO  |
| 2   | P     | 217 | PRO  |
| 2   | B     | 260 | GLY  |
| 2   | J     | 26  | PRO  |
| 1   | I     | 42  | GLY  |
| 2   | J     | 273 | GLY  |
| 2   | J     | 274 | VAL  |
| 1   | K     | 42  | GLY  |
| 2   | L     | 26  | PRO  |
| 2   | L     | 273 | GLY  |
| 2   | L     | 274 | VAL  |
| 1   | M     | 42  | GLY  |
| 2   | N     | 26  | PRO  |
| 2   | N     | 273 | GLY  |
| 1   | O     | 42  | GLY  |
| 2   | P     | 26  | PRO  |
| 2   | P     | 273 | GLY  |
| 2   | P     | 274 | VAL  |
| 2   | N     | 274 | VAL  |
| 2   | D     | 104 | PRO  |
| 2   | F     | 104 | PRO  |
| 2   | H     | 104 | PRO  |



### 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     | 176/176 (100%)   | 157 (89%)  | 19 (11%) | 6           | 21 |
| 1   | C     | 176/176 (100%)   | 157 (89%)  | 19 (11%) | 6           | 21 |
| 1   | E     | 176/176 (100%)   | 157 (89%)  | 19 (11%) | 6           | 21 |
| 1   | G     | 176/176 (100%)   | 157 (89%)  | 19 (11%) | 6           | 21 |
| 1   | I     | 176/176 (100%)   | 163 (93%)  | 13 (7%)  | 13          | 37 |
| 1   | K     | 176/176 (100%)   | 163 (93%)  | 13 (7%)  | 13          | 37 |
| 1   | M     | 176/176 (100%)   | 163 (93%)  | 13 (7%)  | 13          | 37 |
| 1   | O     | 176/176 (100%)   | 163 (93%)  | 13 (7%)  | 13          | 37 |
| 2   | B     | 226/226 (100%)   | 205 (91%)  | 21 (9%)  | 8           | 27 |
| 2   | D     | 226/226 (100%)   | 204 (90%)  | 22 (10%) | 8           | 25 |
| 2   | F     | 226/226 (100%)   | 203 (90%)  | 23 (10%) | 7           | 23 |
| 2   | H     | 226/226 (100%)   | 205 (91%)  | 21 (9%)  | 8           | 27 |
| 2   | J     | 226/226 (100%)   | 218 (96%)  | 8 (4%)   | 32          | 67 |
| 2   | L     | 226/226 (100%)   | 218 (96%)  | 8 (4%)   | 32          | 67 |
| 2   | N     | 226/226 (100%)   | 219 (97%)  | 7 (3%)   | 35          | 70 |
| 2   | P     | 226/226 (100%)   | 218 (96%)  | 8 (4%)   | 32          | 67 |
| All | All   | 3216/3216 (100%) | 2970 (92%) | 246 (8%) | 12          | 36 |

All (246) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 8   | ARG  |
| 1   | A     | 22  | VAL  |
| 1   | A     | 23  | THR  |
| 1   | A     | 28  | ASN  |
| 1   | A     | 43  | VAL  |
| 1   | A     | 44  | LYS  |
| 1   | A     | 61  | LYS  |
| 1   | A     | 62  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 92  | SER  |
| 1   | A     | 104 | GLN  |
| 1   | A     | 113 | LEU  |
| 1   | A     | 129 | GLU  |
| 1   | A     | 135 | ARG  |
| 1   | A     | 142 | LEU  |
| 1   | A     | 143 | ILE  |
| 1   | A     | 146 | THR  |
| 1   | A     | 173 | SER  |
| 1   | A     | 200 | MET  |
| 1   | A     | 205 | GLU  |
| 2   | B     | 4   | LYS  |
| 2   | B     | 5   | THR  |
| 2   | B     | 33  | ASN  |
| 2   | B     | 36  | VAL  |
| 2   | B     | 40  | THR  |
| 2   | B     | 57  | THR  |
| 2   | B     | 59  | GLN  |
| 2   | B     | 81  | SER  |
| 2   | B     | 90  | THR  |
| 2   | B     | 94  | VAL  |
| 2   | B     | 96  | ASN  |
| 2   | B     | 107 | LEU  |
| 2   | B     | 126 | ILE  |
| 2   | B     | 136 | ASN  |
| 2   | B     | 138 | ASN  |
| 2   | B     | 190 | SER  |
| 2   | B     | 201 | THR  |
| 2   | B     | 226 | THR  |
| 2   | B     | 253 | THR  |
| 2   | B     | 262 | GLN  |
| 2   | B     | 271 | ILE  |
| 1   | C     | 8   | ARG  |
| 1   | C     | 22  | VAL  |
| 1   | C     | 23  | THR  |
| 1   | C     | 28  | ASN  |
| 1   | C     | 43  | VAL  |
| 1   | C     | 44  | LYS  |
| 1   | C     | 61  | LYS  |
| 1   | C     | 62  | GLU  |
| 1   | C     | 104 | GLN  |
| 1   | C     | 113 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 129 | GLU  |
| 1   | C     | 135 | ARG  |
| 1   | C     | 142 | LEU  |
| 1   | C     | 143 | ILE  |
| 1   | C     | 146 | THR  |
| 1   | C     | 173 | SER  |
| 1   | C     | 174 | THR  |
| 1   | C     | 200 | MET  |
| 1   | C     | 205 | GLU  |
| 2   | D     | 4   | LYS  |
| 2   | D     | 5   | THR  |
| 2   | D     | 33  | ASN  |
| 2   | D     | 36  | VAL  |
| 2   | D     | 40  | THR  |
| 2   | D     | 53  | THR  |
| 2   | D     | 57  | THR  |
| 2   | D     | 59  | GLN  |
| 2   | D     | 81  | SER  |
| 2   | D     | 90  | THR  |
| 2   | D     | 94  | VAL  |
| 2   | D     | 96  | ASN  |
| 2   | D     | 107 | LEU  |
| 2   | D     | 126 | ILE  |
| 2   | D     | 136 | ASN  |
| 2   | D     | 138 | ASN  |
| 2   | D     | 190 | SER  |
| 2   | D     | 201 | THR  |
| 2   | D     | 226 | THR  |
| 2   | D     | 253 | THR  |
| 2   | D     | 262 | GLN  |
| 2   | D     | 271 | ILE  |
| 1   | E     | 8   | ARG  |
| 1   | E     | 22  | VAL  |
| 1   | E     | 23  | THR  |
| 1   | E     | 28  | ASN  |
| 1   | E     | 43  | VAL  |
| 1   | E     | 44  | LYS  |
| 1   | E     | 61  | LYS  |
| 1   | E     | 62  | GLU  |
| 1   | E     | 92  | SER  |
| 1   | E     | 104 | GLN  |
| 1   | E     | 113 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 129 | GLU  |
| 1   | E     | 135 | ARG  |
| 1   | E     | 142 | LEU  |
| 1   | E     | 143 | ILE  |
| 1   | E     | 146 | THR  |
| 1   | E     | 173 | SER  |
| 1   | E     | 200 | MET  |
| 1   | E     | 205 | GLU  |
| 2   | F     | 4   | LYS  |
| 2   | F     | 5   | THR  |
| 2   | F     | 33  | ASN  |
| 2   | F     | 36  | VAL  |
| 2   | F     | 40  | THR  |
| 2   | F     | 53  | THR  |
| 2   | F     | 57  | THR  |
| 2   | F     | 59  | GLN  |
| 2   | F     | 81  | SER  |
| 2   | F     | 90  | THR  |
| 2   | F     | 94  | VAL  |
| 2   | F     | 96  | ASN  |
| 2   | F     | 107 | LEU  |
| 2   | F     | 126 | ILE  |
| 2   | F     | 136 | ASN  |
| 2   | F     | 138 | ASN  |
| 2   | F     | 179 | VAL  |
| 2   | F     | 190 | SER  |
| 2   | F     | 201 | THR  |
| 2   | F     | 226 | THR  |
| 2   | F     | 253 | THR  |
| 2   | F     | 262 | GLN  |
| 2   | F     | 271 | ILE  |
| 1   | G     | 8   | ARG  |
| 1   | G     | 22  | VAL  |
| 1   | G     | 23  | THR  |
| 1   | G     | 28  | ASN  |
| 1   | G     | 43  | VAL  |
| 1   | G     | 44  | LYS  |
| 1   | G     | 61  | LYS  |
| 1   | G     | 62  | GLU  |
| 1   | G     | 92  | SER  |
| 1   | G     | 104 | GLN  |
| 1   | G     | 113 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 129 | GLU  |
| 1   | G     | 135 | ARG  |
| 1   | G     | 142 | LEU  |
| 1   | G     | 143 | ILE  |
| 1   | G     | 146 | THR  |
| 1   | G     | 173 | SER  |
| 1   | G     | 200 | MET  |
| 1   | G     | 205 | GLU  |
| 2   | H     | 4   | LYS  |
| 2   | H     | 5   | THR  |
| 2   | H     | 33  | ASN  |
| 2   | H     | 36  | VAL  |
| 2   | H     | 40  | THR  |
| 2   | H     | 57  | THR  |
| 2   | H     | 59  | GLN  |
| 2   | H     | 81  | SER  |
| 2   | H     | 90  | THR  |
| 2   | H     | 94  | VAL  |
| 2   | H     | 96  | ASN  |
| 2   | H     | 107 | LEU  |
| 2   | H     | 126 | ILE  |
| 2   | H     | 136 | ASN  |
| 2   | H     | 138 | ASN  |
| 2   | H     | 190 | SER  |
| 2   | H     | 201 | THR  |
| 2   | H     | 226 | THR  |
| 2   | H     | 253 | THR  |
| 2   | H     | 262 | GLN  |
| 2   | H     | 271 | ILE  |
| 1   | I     | 8   | ARG  |
| 1   | I     | 22  | VAL  |
| 1   | I     | 28  | ASN  |
| 1   | I     | 43  | VAL  |
| 1   | I     | 44  | LYS  |
| 1   | I     | 61  | LYS  |
| 1   | I     | 62  | GLU  |
| 1   | I     | 92  | SER  |
| 1   | I     | 129 | GLU  |
| 1   | I     | 135 | ARG  |
| 1   | I     | 176 | LYS  |
| 1   | I     | 183 | SER  |
| 1   | I     | 205 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | J     | 37  | ASP  |
| 2   | J     | 43  | PHE  |
| 2   | J     | 57  | THR  |
| 2   | J     | 96  | ASN  |
| 2   | J     | 136 | ASN  |
| 2   | J     | 157 | PRO  |
| 2   | J     | 183 | LEU  |
| 2   | J     | 184 | THR  |
| 1   | K     | 8   | ARG  |
| 1   | K     | 22  | VAL  |
| 1   | K     | 28  | ASN  |
| 1   | K     | 43  | VAL  |
| 1   | K     | 44  | LYS  |
| 1   | K     | 61  | LYS  |
| 1   | K     | 62  | GLU  |
| 1   | K     | 92  | SER  |
| 1   | K     | 129 | GLU  |
| 1   | K     | 135 | ARG  |
| 1   | K     | 176 | LYS  |
| 1   | K     | 183 | SER  |
| 1   | K     | 205 | GLU  |
| 2   | L     | 37  | ASP  |
| 2   | L     | 43  | PHE  |
| 2   | L     | 57  | THR  |
| 2   | L     | 96  | ASN  |
| 2   | L     | 136 | ASN  |
| 2   | L     | 157 | PRO  |
| 2   | L     | 183 | LEU  |
| 2   | L     | 184 | THR  |
| 1   | M     | 8   | ARG  |
| 1   | M     | 22  | VAL  |
| 1   | M     | 28  | ASN  |
| 1   | M     | 43  | VAL  |
| 1   | M     | 44  | LYS  |
| 1   | M     | 61  | LYS  |
| 1   | M     | 62  | GLU  |
| 1   | M     | 92  | SER  |
| 1   | M     | 129 | GLU  |
| 1   | M     | 135 | ARG  |
| 1   | M     | 176 | LYS  |
| 1   | M     | 183 | SER  |
| 1   | M     | 205 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | N     | 43  | PHE  |
| 2   | N     | 57  | THR  |
| 2   | N     | 96  | ASN  |
| 2   | N     | 136 | ASN  |
| 2   | N     | 157 | PRO  |
| 2   | N     | 183 | LEU  |
| 2   | N     | 184 | THR  |
| 1   | O     | 8   | ARG  |
| 1   | O     | 22  | VAL  |
| 1   | O     | 28  | ASN  |
| 1   | O     | 43  | VAL  |
| 1   | O     | 44  | LYS  |
| 1   | O     | 61  | LYS  |
| 1   | O     | 62  | GLU  |
| 1   | O     | 92  | SER  |
| 1   | O     | 129 | GLU  |
| 1   | O     | 135 | ARG  |
| 1   | O     | 176 | LYS  |
| 1   | O     | 183 | SER  |
| 1   | O     | 205 | GLU  |
| 2   | P     | 37  | ASP  |
| 2   | P     | 43  | PHE  |
| 2   | P     | 57  | THR  |
| 2   | P     | 96  | ASN  |
| 2   | P     | 136 | ASN  |
| 2   | P     | 157 | PRO  |
| 2   | P     | 183 | LEU  |
| 2   | P     | 184 | THR  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (207) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 15  | GLN  |
| 1   | A     | 19  | GLN  |
| 1   | A     | 28  | ASN  |
| 1   | A     | 72  | ASN  |
| 1   | A     | 74  | GLN  |
| 1   | A     | 77  | GLN  |
| 1   | A     | 86  | ASN  |
| 1   | A     | 126 | GLN  |
| 1   | A     | 184 | ASN  |
| 2   | B     | 23  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 29  | ASN  |
| 2   | B     | 32  | GLN  |
| 2   | B     | 33  | ASN  |
| 2   | B     | 70  | ASN  |
| 2   | B     | 136 | ASN  |
| 2   | B     | 138 | ASN  |
| 2   | B     | 206 | ASN  |
| 2   | B     | 211 | ASN  |
| 2   | B     | 219 | GLN  |
| 2   | B     | 224 | GLN  |
| 2   | B     | 228 | ASN  |
| 2   | B     | 255 | ASN  |
| 2   | B     | 262 | GLN  |
| 2   | B     | 267 | ASN  |
| 2   | B     | 279 | GLN  |
| 1   | C     | 15  | GLN  |
| 1   | C     | 19  | GLN  |
| 1   | C     | 28  | ASN  |
| 1   | C     | 72  | ASN  |
| 1   | C     | 74  | GLN  |
| 1   | C     | 77  | GLN  |
| 1   | C     | 86  | ASN  |
| 1   | C     | 126 | GLN  |
| 1   | C     | 184 | ASN  |
| 2   | D     | 23  | ASN  |
| 2   | D     | 29  | ASN  |
| 2   | D     | 32  | GLN  |
| 2   | D     | 33  | ASN  |
| 2   | D     | 70  | ASN  |
| 2   | D     | 136 | ASN  |
| 2   | D     | 138 | ASN  |
| 2   | D     | 206 | ASN  |
| 2   | D     | 211 | ASN  |
| 2   | D     | 219 | GLN  |
| 2   | D     | 224 | GLN  |
| 2   | D     | 228 | ASN  |
| 2   | D     | 255 | ASN  |
| 2   | D     | 262 | GLN  |
| 2   | D     | 267 | ASN  |
| 2   | D     | 279 | GLN  |
| 1   | E     | 15  | GLN  |
| 1   | E     | 28  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 72  | ASN  |
| 1   | E     | 74  | GLN  |
| 1   | E     | 77  | GLN  |
| 1   | E     | 86  | ASN  |
| 1   | E     | 126 | GLN  |
| 1   | E     | 184 | ASN  |
| 2   | F     | 23  | ASN  |
| 2   | F     | 29  | ASN  |
| 2   | F     | 32  | GLN  |
| 2   | F     | 33  | ASN  |
| 2   | F     | 41  | GLN  |
| 2   | F     | 70  | ASN  |
| 2   | F     | 136 | ASN  |
| 2   | F     | 138 | ASN  |
| 2   | F     | 192 | ASN  |
| 2   | F     | 206 | ASN  |
| 2   | F     | 211 | ASN  |
| 2   | F     | 219 | GLN  |
| 2   | F     | 224 | GLN  |
| 2   | F     | 228 | ASN  |
| 2   | F     | 255 | ASN  |
| 2   | F     | 262 | GLN  |
| 2   | F     | 267 | ASN  |
| 2   | F     | 279 | GLN  |
| 1   | G     | 15  | GLN  |
| 1   | G     | 28  | ASN  |
| 1   | G     | 72  | ASN  |
| 1   | G     | 74  | GLN  |
| 1   | G     | 77  | GLN  |
| 1   | G     | 86  | ASN  |
| 1   | G     | 126 | GLN  |
| 1   | G     | 184 | ASN  |
| 2   | H     | 23  | ASN  |
| 2   | H     | 29  | ASN  |
| 2   | H     | 32  | GLN  |
| 2   | H     | 33  | ASN  |
| 2   | H     | 41  | GLN  |
| 2   | H     | 70  | ASN  |
| 2   | H     | 136 | ASN  |
| 2   | H     | 138 | ASN  |
| 2   | H     | 206 | ASN  |
| 2   | H     | 211 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | H     | 219 | GLN  |
| 2   | H     | 224 | GLN  |
| 2   | H     | 228 | ASN  |
| 2   | H     | 255 | ASN  |
| 2   | H     | 262 | GLN  |
| 2   | H     | 267 | ASN  |
| 2   | H     | 279 | GLN  |
| 1   | I     | 28  | ASN  |
| 1   | I     | 34  | GLN  |
| 1   | I     | 72  | ASN  |
| 1   | I     | 74  | GLN  |
| 1   | I     | 77  | GLN  |
| 1   | I     | 86  | ASN  |
| 1   | I     | 101 | ASN  |
| 1   | I     | 104 | GLN  |
| 1   | I     | 126 | GLN  |
| 1   | I     | 184 | ASN  |
| 2   | J     | 19  | ASN  |
| 2   | J     | 33  | ASN  |
| 2   | J     | 41  | GLN  |
| 2   | J     | 70  | ASN  |
| 2   | J     | 96  | ASN  |
| 2   | J     | 136 | ASN  |
| 2   | J     | 138 | ASN  |
| 2   | J     | 143 | GLN  |
| 2   | J     | 151 | ASN  |
| 2   | J     | 191 | GLN  |
| 2   | J     | 211 | ASN  |
| 2   | J     | 224 | GLN  |
| 2   | J     | 228 | ASN  |
| 2   | J     | 255 | ASN  |
| 2   | J     | 262 | GLN  |
| 2   | J     | 269 | GLN  |
| 2   | J     | 279 | GLN  |
| 1   | K     | 28  | ASN  |
| 1   | K     | 34  | GLN  |
| 1   | K     | 72  | ASN  |
| 1   | K     | 74  | GLN  |
| 1   | K     | 77  | GLN  |
| 1   | K     | 86  | ASN  |
| 1   | K     | 101 | ASN  |
| 1   | K     | 104 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | K     | 126 | GLN  |
| 1   | K     | 184 | ASN  |
| 2   | L     | 33  | ASN  |
| 2   | L     | 41  | GLN  |
| 2   | L     | 70  | ASN  |
| 2   | L     | 96  | ASN  |
| 2   | L     | 136 | ASN  |
| 2   | L     | 138 | ASN  |
| 2   | L     | 143 | GLN  |
| 2   | L     | 151 | ASN  |
| 2   | L     | 191 | GLN  |
| 2   | L     | 211 | ASN  |
| 2   | L     | 219 | GLN  |
| 2   | L     | 224 | GLN  |
| 2   | L     | 228 | ASN  |
| 2   | L     | 255 | ASN  |
| 2   | L     | 269 | GLN  |
| 2   | L     | 279 | GLN  |
| 1   | M     | 28  | ASN  |
| 1   | M     | 34  | GLN  |
| 1   | M     | 72  | ASN  |
| 1   | M     | 74  | GLN  |
| 1   | M     | 77  | GLN  |
| 1   | M     | 86  | ASN  |
| 1   | M     | 101 | ASN  |
| 1   | M     | 104 | GLN  |
| 1   | M     | 126 | GLN  |
| 1   | M     | 184 | ASN  |
| 2   | N     | 19  | ASN  |
| 2   | N     | 33  | ASN  |
| 2   | N     | 41  | GLN  |
| 2   | N     | 70  | ASN  |
| 2   | N     | 96  | ASN  |
| 2   | N     | 136 | ASN  |
| 2   | N     | 138 | ASN  |
| 2   | N     | 143 | GLN  |
| 2   | N     | 151 | ASN  |
| 2   | N     | 191 | GLN  |
| 2   | N     | 192 | ASN  |
| 2   | N     | 211 | ASN  |
| 2   | N     | 224 | GLN  |
| 2   | N     | 228 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | N     | 255 | ASN  |
| 2   | N     | 262 | GLN  |
| 2   | N     | 269 | GLN  |
| 2   | N     | 279 | GLN  |
| 1   | O     | 28  | ASN  |
| 1   | O     | 34  | GLN  |
| 1   | O     | 72  | ASN  |
| 1   | O     | 74  | GLN  |
| 1   | O     | 77  | GLN  |
| 1   | O     | 86  | ASN  |
| 1   | O     | 101 | ASN  |
| 1   | O     | 104 | GLN  |
| 1   | O     | 126 | GLN  |
| 2   | P     | 33  | ASN  |
| 2   | P     | 41  | GLN  |
| 2   | P     | 70  | ASN  |
| 2   | P     | 96  | ASN  |
| 2   | P     | 136 | ASN  |
| 2   | P     | 138 | ASN  |
| 2   | P     | 143 | GLN  |
| 2   | P     | 151 | ASN  |
| 2   | P     | 191 | GLN  |
| 2   | P     | 211 | ASN  |
| 2   | P     | 219 | GLN  |
| 2   | P     | 224 | GLN  |
| 2   | P     | 228 | ASN  |
| 2   | P     | 255 | ASN  |
| 2   | P     | 269 | GLN  |
| 2   | P     | 279 | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

8 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 3   | MAN  | H     | 1603 | -    | 12,12,12     | 0.40 | 0           | 17,17,17    | 0.47 | 0           |
| 3   | MAN  | D     | 1601 | -    | 12,12,12     | 0.35 | 0           | 17,17,17    | 0.49 | 0           |
| 3   | MAN  | B     | 1500 | -    | 12,12,12     | 0.38 | 0           | 17,17,17    | 0.37 | 0           |
| 3   | MAN  | N     | 1506 | -    | 12,12,12     | 0.26 | 0           | 17,17,17    | 0.43 | 0           |
| 3   | MAN  | P     | 1607 | -    | 12,12,12     | 0.29 | 0           | 17,17,17    | 0.39 | 0           |
| 3   | MAN  | J     | 1605 | -    | 12,12,12     | 0.29 | 0           | 17,17,17    | 0.35 | 0           |
| 3   | MAN  | L     | 1504 | -    | 12,12,12     | 0.30 | 0           | 17,17,17    | 0.44 | 0           |
| 3   | MAN  | F     | 1502 | -    | 12,12,12     | 0.37 | 0           | 17,17,17    | 0.53 | 0           |

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

| Mol | Type | Chain | Res  | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|------|------|---------|-----------|---------|
| 3   | MAN  | H     | 1603 | -    | -       | 2/2/22/22 | 0/1/1/1 |
| 3   | MAN  | D     | 1601 | -    | -       | 1/2/22/22 | 0/1/1/1 |
| 3   | MAN  | B     | 1500 | -    | -       | 2/2/22/22 | 0/1/1/1 |
| 3   | MAN  | N     | 1506 | -    | -       | 0/2/22/22 | 0/1/1/1 |
| 3   | MAN  | P     | 1607 | -    | -       | 0/2/22/22 | 0/1/1/1 |
| 3   | MAN  | J     | 1605 | -    | -       | 0/2/22/22 | 0/1/1/1 |
| 3   | MAN  | L     | 1504 | -    | -       | 0/2/22/22 | 0/1/1/1 |
| 3   | MAN  | F     | 1502 | -    | -       | 1/2/22/22 | 0/1/1/1 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       |
|-----|-------|------|------|-------------|
| 3   | H     | 1603 | MAN  | C4-C5-C6-O6 |
| 3   | B     | 1500 | MAN  | C4-C5-C6-O6 |
| 3   | B     | 1500 | MAN  | O5-C5-C6-O6 |
| 3   | H     | 1603 | MAN  | O5-C5-C6-O6 |
| 3   | D     | 1601 | MAN  | C4-C5-C6-O6 |
| 3   | F     | 1502 | MAN  | C4-C5-C6-O6 |

There are no ring outliers.

4 monomers are involved in 8 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 3   | N     | 1506 | MAN  | 1       | 0            |
| 3   | P     | 1607 | MAN  | 2       | 0            |
| 3   | J     | 1605 | MAN  | 3       | 0            |
| 3   | L     | 1504 | MAN  | 2       | 0            |

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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     | 205/205 (100%)   | -1.24  | 0 100 100    | 20, 55, 108, 132      | 0     |
| 1   | C     | 205/205 (100%)   | -1.29  | 0 100 100    | 20, 57, 108, 130      | 0     |
| 1   | E     | 205/205 (100%)   | -1.25  | 0 100 100    | 20, 59, 108, 129      | 0     |
| 1   | G     | 205/205 (100%)   | -1.28  | 0 100 100    | 19, 58, 110, 132      | 0     |
| 1   | I     | 205/205 (100%)   | -0.61  | 0 100 100    | 20, 168, 190, 196     | 0     |
| 1   | K     | 205/205 (100%)   | -0.59  | 0 100 100    | 20, 171, 195, 198     | 0     |
| 1   | M     | 205/205 (100%)   | -0.53  | 0 100 100    | 20, 170, 193, 198     | 0     |
| 1   | O     | 205/205 (100%)   | -0.61  | 2 (0%) 79 72 | 20, 168, 193, 198     | 0     |
| 2   | B     | 279/279 (100%)   | -1.36  | 0 100 100    | 17, 40, 79, 114       | 0     |
| 2   | D     | 279/279 (100%)   | -1.36  | 0 100 100    | 18, 41, 80, 116       | 0     |
| 2   | F     | 279/279 (100%)   | -1.34  | 0 100 100    | 18, 41, 83, 112       | 0     |
| 2   | H     | 279/279 (100%)   | -1.34  | 0 100 100    | 17, 42, 83, 114       | 0     |
| 2   | J     | 279/279 (100%)   | -0.74  | 0 100 100    | 51, 112, 192, 200     | 0     |
| 2   | L     | 279/279 (100%)   | -0.70  | 0 100 100    | 56, 113, 190, 200     | 0     |
| 2   | N     | 279/279 (100%)   | -0.75  | 0 100 100    | 53, 115, 193, 200     | 0     |
| 2   | P     | 279/279 (100%)   | -0.78  | 0 100 100    | 50, 112, 191, 200     | 0     |
| All | All   | 3872/3872 (100%) | -1.00  | 2 (0%) 92 90 | 17, 85, 186, 200      | 0     |

All (2) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | O     | 105 | LEU  | 2.9  |
| 1   | O     | 103 | LEU  | 2.4  |

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 3   | MAN  | H     | 1603 | 12/12 | 0.98 | 0.04 | 28,34,39,39                 | 0     |
| 3   | MAN  | L     | 1504 | 12/12 | 0.98 | 0.04 | 96,99,103,106               | 0     |
| 3   | MAN  | N     | 1506 | 12/12 | 0.98 | 0.05 | 90,94,100,101               | 0     |
| 3   | MAN  | B     | 1500 | 12/12 | 0.99 | 0.04 | 30,35,39,39                 | 0     |
| 3   | MAN  | J     | 1605 | 12/12 | 0.99 | 0.05 | 96,100,105,106              | 0     |
| 3   | MAN  | D     | 1601 | 12/12 | 0.99 | 0.03 | 28,36,41,41                 | 0     |
| 3   | MAN  | F     | 1502 | 12/12 | 0.99 | 0.05 | 29,35,41,41                 | 0     |
| 3   | MAN  | P     | 1607 | 12/12 | 0.99 | 0.04 | 110,112,116,117             | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.