



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:08 PM UTC

PDB ID : 5E6I / pdb\_00005e6i  
Title : Crystal structure of TCR PF8 in complex with flu MP(58-66) epitope presented by HLA-A2  
Authors : Gao, M.; Mariuzza, R.  
Deposited on : 2015-10-09  
Resolution : 4.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

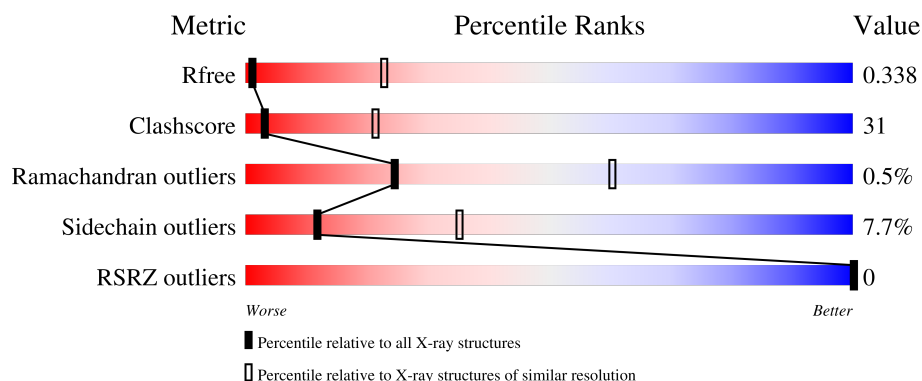
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 4.00 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.



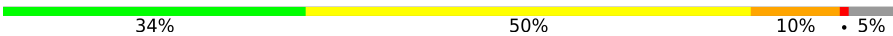
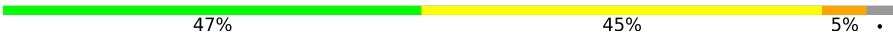
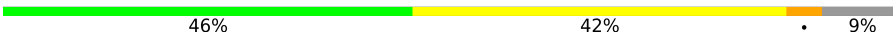
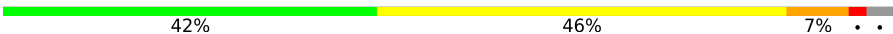
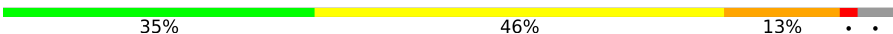
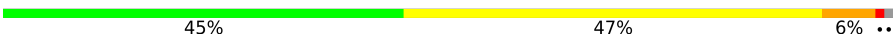
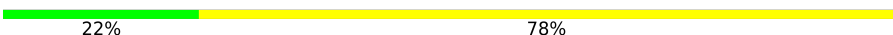
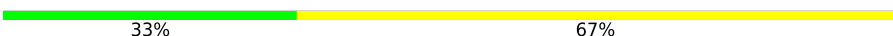
| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 1082 (4.20-3.80)                                      |
| Clashscore            | 190562                      | 1129 (4.20-3.80)                                      |
| Ramachandran outliers | 187476                      | 1064 (4.20-3.80)                                      |
| Sidechain outliers    | 187428                      | 1055 (4.20-3.80)                                      |
| RSRZ outliers         | 180081                      | 1082 (4.20-3.80)                                      |

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     | 208    |                  |
| 1   | F     | 208    |                  |
| 1   | G     | 208    |                  |
| 1   | P     | 208    |                  |
| 2   | B     | 243    |                  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 2   | H     | 243    |    |
| 2   | L     | 243    |    |
| 2   | Q     | 243    |    |
| 3   | C     | 276    |    |
| 3   | I     | 276    |    |
| 3   | M     | 276    |    |
| 3   | R     | 276    |    |
| 4   | D     | 100    |    |
| 4   | J     | 100    |    |
| 4   | N     | 100    |    |
| 4   | U     | 100    |    |
| 5   | E     | 9      |   |
| 5   | K     | 9      |  |
| 5   | O     | 9      |  |
| 5   | T     | 9      |  |

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 24882 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 TCR alpha chain, Human nkt tcr alpha chain.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | G     | 201      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1535  | 961 | 252 | 313 | 9 |         |         |       |
| 1   | A     | 196      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1459  | 910 | 241 | 300 | 8 |         |         |       |
| 1   | F     | 198      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1486  | 930 | 243 | 304 | 9 |         |         |       |
| 1   | P     | 191      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1426  | 895 | 232 | 292 | 7 |         |         |       |

- Molecule 2 is a protein called T-cell receptor beta-2 chain C region.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2   | H     | 239      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1878  | 1189 | 320 | 361 | 8 |         |         |       |
| 2   | B     | 241      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1870  | 1179 | 316 | 367 | 8 |         |         |       |
| 2   | L     | 242      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1891  | 1199 | 314 | 370 | 8 |         |         |       |
| 2   | Q     | 238      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1840  | 1164 | 312 | 356 | 8 |         |         |       |

There are 64 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference      |
|-------|---------|----------|--------|----------|----------------|
| H     | 0       | MET      | LEU    | conflict | UNP A0A087WZ08 |
| H     | 18      | GLU      | LYS    | conflict | UNP A0A087WZ08 |
| H     | ?       | -        | SER    | deletion | UNP A0A087WZ08 |
| H     | 96      | ILE      | THR    | conflict | UNP A0A087WZ08 |
| H     | 97      | TYR      | VAL    | conflict | UNP A0A087WZ08 |
| H     | 98      | PRO      | LEU    | conflict | UNP A0A087WZ08 |
| H     | 99      | GLY      | HIS    | conflict | UNP A0A087WZ08 |
| H     | 100     | GLU      | SER    | conflict | UNP A0A087WZ08 |

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| Chain | Residue | Modelled | Actual | Comment  | Reference      |
|-------|---------|----------|--------|----------|----------------|
| H     | 101     | LEU      | GLN    | conflict | UNP A0A087WZ08 |
| H     | 102     | PHE      | TYR    | conflict | UNP A0A087WZ08 |
| H     | 105     | GLU      | PRO    | conflict | UNP A0A087WZ08 |
| H     | 107     | SER      | THR    | conflict | UNP A0A087WZ08 |
| H     | 110     | THR      | LEU    | conflict | UNP A0A087WZ08 |
| H     | 122     | GLU      | LYS    | conflict | UNP A0A087WZ08 |
| H     | 169     | CYS      | SER    | conflict | UNP A0A087WZ08 |
| H     | 187     | ALA      | CYS    | conflict | UNP A0A087WZ08 |
| B     | 0       | MET      | LEU    | conflict | UNP A0A087WZ08 |
| B     | 18      | GLU      | LYS    | conflict | UNP A0A087WZ08 |
| B     | ?       | -        | SER    | deletion | UNP A0A087WZ08 |
| B     | 96      | ILE      | THR    | conflict | UNP A0A087WZ08 |
| B     | 97      | TYR      | VAL    | conflict | UNP A0A087WZ08 |
| B     | 98      | PRO      | LEU    | conflict | UNP A0A087WZ08 |
| B     | 99      | GLY      | HIS    | conflict | UNP A0A087WZ08 |
| B     | 100     | GLU      | SER    | conflict | UNP A0A087WZ08 |
| B     | 101     | LEU      | GLN    | conflict | UNP A0A087WZ08 |
| B     | 102     | PHE      | TYR    | conflict | UNP A0A087WZ08 |
| B     | 105     | GLU      | PRO    | conflict | UNP A0A087WZ08 |
| B     | 107     | SER      | THR    | conflict | UNP A0A087WZ08 |
| B     | 110     | THR      | LEU    | conflict | UNP A0A087WZ08 |
| B     | 122     | GLU      | LYS    | conflict | UNP A0A087WZ08 |
| B     | 169     | CYS      | SER    | conflict | UNP A0A087WZ08 |
| B     | 187     | ALA      | CYS    | conflict | UNP A0A087WZ08 |
| L     | 0       | MET      | LEU    | conflict | UNP A0A087WZ08 |
| L     | 18      | GLU      | LYS    | conflict | UNP A0A087WZ08 |
| L     | ?       | -        | SER    | deletion | UNP A0A087WZ08 |
| L     | 96      | ILE      | THR    | conflict | UNP A0A087WZ08 |
| L     | 97      | TYR      | VAL    | conflict | UNP A0A087WZ08 |
| L     | 98      | PRO      | LEU    | conflict | UNP A0A087WZ08 |
| L     | 99      | GLY      | HIS    | conflict | UNP A0A087WZ08 |
| L     | 100     | GLU      | SER    | conflict | UNP A0A087WZ08 |
| L     | 101     | LEU      | GLN    | conflict | UNP A0A087WZ08 |
| L     | 102     | PHE      | TYR    | conflict | UNP A0A087WZ08 |
| L     | 105     | GLU      | PRO    | conflict | UNP A0A087WZ08 |
| L     | 107     | SER      | THR    | conflict | UNP A0A087WZ08 |
| L     | 110     | THR      | LEU    | conflict | UNP A0A087WZ08 |
| L     | 122     | GLU      | LYS    | conflict | UNP A0A087WZ08 |
| L     | 169     | CYS      | SER    | conflict | UNP A0A087WZ08 |
| L     | 187     | ALA      | CYS    | conflict | UNP A0A087WZ08 |
| Q     | 0       | MET      | LEU    | conflict | UNP A0A087WZ08 |
| Q     | 18      | GLU      | LYS    | conflict | UNP A0A087WZ08 |

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| Chain | Residue | Modelled | Actual | Comment  | Reference      |
|-------|---------|----------|--------|----------|----------------|
| Q     | ?       | -        | SER    | deletion | UNP A0A087WZ08 |
| Q     | 96      | ILE      | THR    | conflict | UNP A0A087WZ08 |
| Q     | 97      | TYR      | VAL    | conflict | UNP A0A087WZ08 |
| Q     | 98      | PRO      | LEU    | conflict | UNP A0A087WZ08 |
| Q     | 99      | GLY      | HIS    | conflict | UNP A0A087WZ08 |
| Q     | 100     | GLU      | SER    | conflict | UNP A0A087WZ08 |
| Q     | 101     | LEU      | GLN    | conflict | UNP A0A087WZ08 |
| Q     | 102     | PHE      | TYR    | conflict | UNP A0A087WZ08 |
| Q     | 105     | GLU      | PRO    | conflict | UNP A0A087WZ08 |
| Q     | 107     | SER      | THR    | conflict | UNP A0A087WZ08 |
| Q     | 110     | THR      | LEU    | conflict | UNP A0A087WZ08 |
| Q     | 122     | GLU      | LYS    | conflict | UNP A0A087WZ08 |
| Q     | 169     | CYS      | SER    | conflict | UNP A0A087WZ08 |
| Q     | 187     | ALA      | CYS    | conflict | UNP A0A087WZ08 |

- Molecule 3 is a protein called HLA class I histocompatibility antigen, A-2 alpha chain.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3   | I     | 261      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2072  | 1297 | 378 | 388 | 9 |         |         |       |
| 3   | C     | 258      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2034  | 1273 | 363 | 389 | 9 |         |         |       |
| 3   | M     | 268      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2076  | 1294 | 375 | 399 | 8 |         |         |       |
| 3   | R     | 251      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1994  | 1249 | 360 | 376 | 9 |         |         |       |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| I     | 0       | MET      | -      | initiating methionine | UNP P01892 |
| C     | 0       | MET      | -      | initiating methionine | UNP P01892 |
| M     | 0       | MET      | -      | initiating methionine | UNP P01892 |
| R     | 0       | MET      | -      | initiating methionine | UNP P01892 |

- Molecule 4 is a protein called Beta-2-microglobulin.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 4   | J     | 96       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 772   | 489 | 131 | 149 | 3 |         |         |       |
| 4   | D     | 97       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 787   | 503 | 131 | 150 | 3 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 4   | N     | 92       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 697   | 440 | 123 | 132 | 2 |         |         |       |
| 4   | U     | 99       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 793   | 504 | 133 | 153 | 3 |         |         |       |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| J     | 0       | MET      | -      | initiating methionine | UNP P61769 |
| D     | 0       | MET      | -      | initiating methionine | UNP P61769 |
| N     | 0       | MET      | -      | initiating methionine | UNP P61769 |
| U     | 0       | MET      | -      | initiating methionine | UNP P61769 |

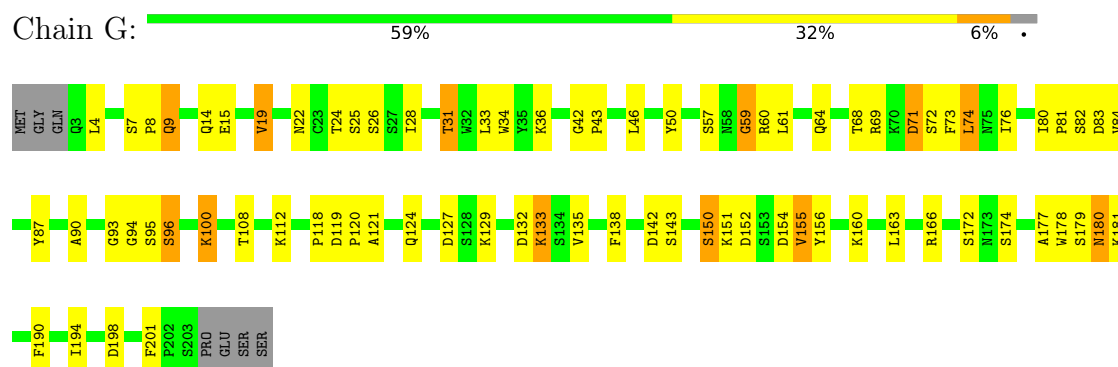
- Molecule 5 is a protein called Matrix protein 1.

| Mol | Chain | Residues | Atoms |    |   |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|---------|-------|
| 5   | K     | 9        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 68    | 49 | 9 | 10 |         |         |       |
| 5   | E     | 9        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 68    | 49 | 9 | 10 |         |         |       |
| 5   | O     | 9        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 68    | 49 | 9 | 10 |         |         |       |
| 5   | T     | 9        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 68    | 49 | 9 | 10 |         |         |       |

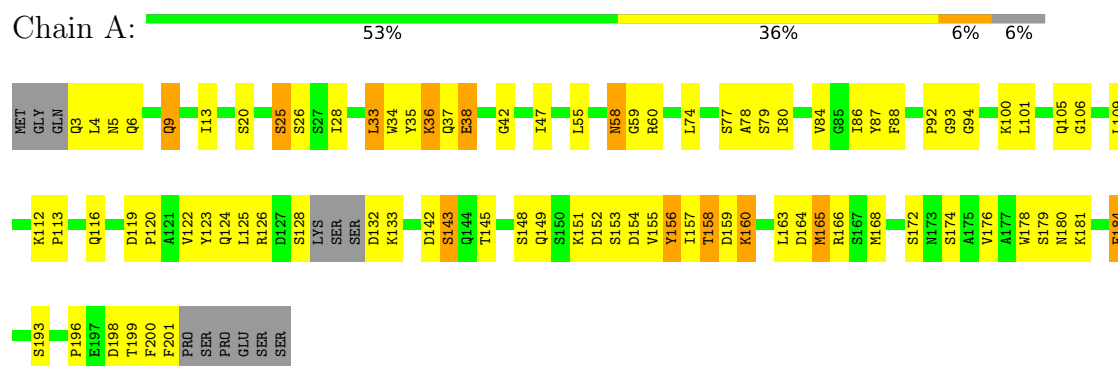
### 3 Residue-property plots [i](#)

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

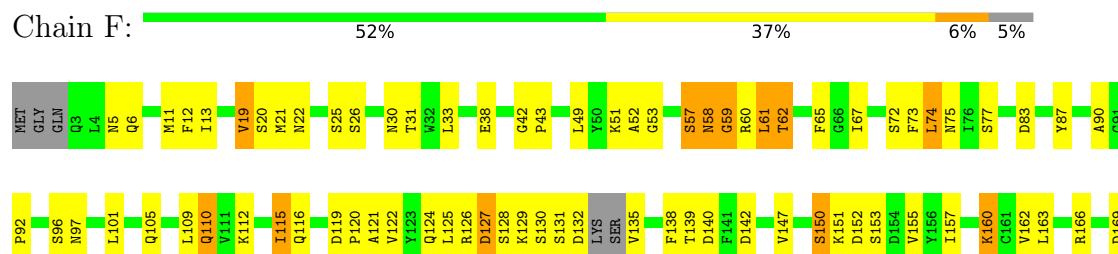
- Molecule 1: TCR alpha chain, Human nkt tcr alpha chain



- Molecule 1: TCR alpha chain, Human nkt tcr alpha chain



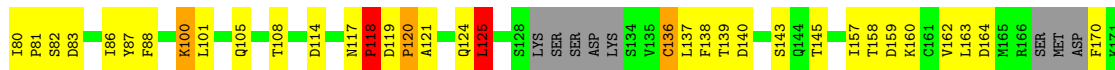
- Molecule 1: TCR alpha chain, Human nkt tcr alpha chain





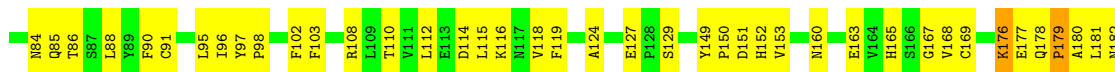
- Molecule 1: TCR alpha chain, Human nkt tcr alpha chain

Chain P: 55% 34% 8%



- Molecule 2: T-cell receptor beta-2 chain C region

Chain H: 56% 37% 5%



- Molecule 2: T-cell receptor beta-2 chain C region

Chain B: 57% 38% 2%



- Molecule 2: T-cell receptor beta-2 chain C region

Chain L: 59% 37% 2%

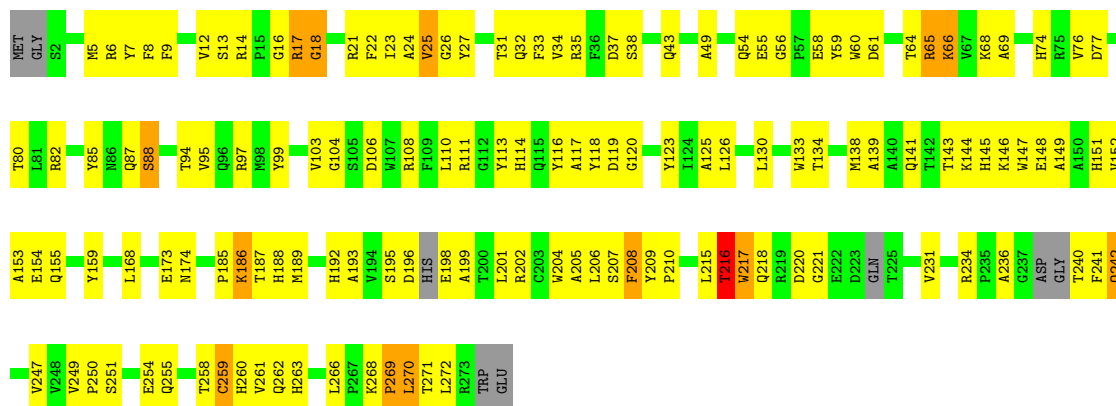






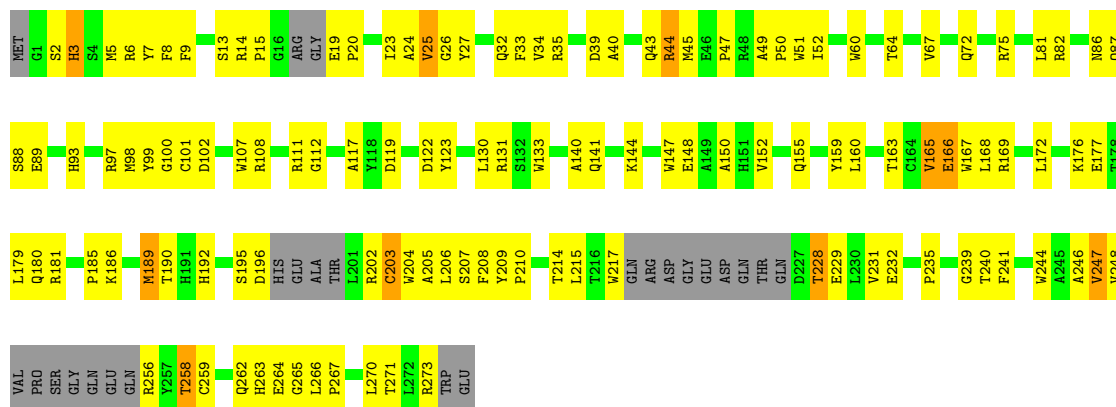
- Molecule 3: HLA class I histocompatibility antigen, A-2 alpha chain

Chain M: 47% 45% 5% .



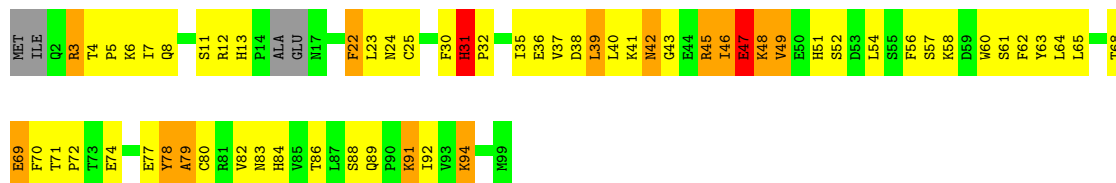
- Molecule 3: HLA class I histocompatibility antigen, A-2 alpha chain

Chain R: 46% 42% 9% .



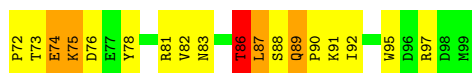
- Molecule 4: Beta-2-microglobulin

Chain J: 35% 46% 13% . .

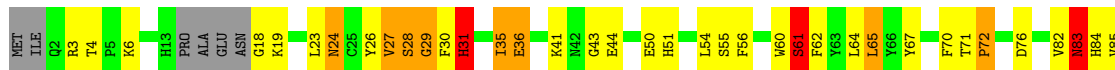


- Molecule 4: Beta-2-microglobulin

Chain D: 42% 46% 7% . .



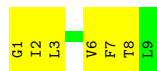
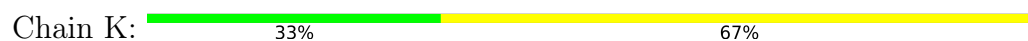
• Molecule 4: Beta-2-microglobulin



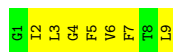
• Molecule 4: Beta-2-microglobulin



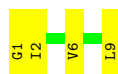
• Molecule 5: Matrix protein 1



• Molecule 5: Matrix protein 1



• Molecule 5: Matrix protein 1



• Molecule 5: Matrix protein 1



|    |    |    |  |
|----|----|----|--|
| G1 |    |    |  |
|    | V6 |    |  |
|    | F7 |    |  |
|    |    | T8 |  |
|    |    | L9 |  |

## 4 Data and refinement statistics

| Property                                                                | Value                                                               | Source           |
|-------------------------------------------------------------------------|---------------------------------------------------------------------|------------------|
| Space group                                                             | P 1                                                                 | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 71.85Å 123.61Å 139.04Å<br>83.66° 74.87° 73.17°                      | Depositor        |
| Resolution (Å)                                                          | 36.56 – 4.00<br>36.56 – 4.00                                        | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 91.0 (36.56-4.00)<br>80.3 (36.56-4.00)                              | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.16                                                                | Depositor        |
| $R_{sym}$                                                               | (Not available)                                                     | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.16 (at 4.00Å)                                                     | Xtriage          |
| Refinement program                                                      | PHENIX                                                              | Depositor        |
| R, $R_{free}$                                                           | 0.259 , 0.338<br>0.268 , 0.338                                      | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 1661 reflections (4.46%)                                            | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 94.3                                                                | Xtriage          |
| Anisotropy                                                              | 0.549                                                               | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.24 , 455.5                                                        | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.53$ , $\langle L^2 \rangle = 0.36$         | Xtriage          |
| Estimated twinning fraction                                             | 0.277 for h,h-k,h-l<br>0.000 for -h,-h+k,-l<br>0.000 for -h,-k,-h+l | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.92                                                                | EDS              |
| Total number of atoms                                                   | 24882                                                               | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 108.0                                                               | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.77% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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

| Mol | Chain | Bond lengths |                | Bond angles |                  |
|-----|-------|--------------|----------------|-------------|------------------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5          |
| 1   | A     | 0.51         | 0/1486         | 1.04        | 8/2013 (0.4%)    |
| 1   | F     | 0.52         | 0/1517         | 1.05        | 10/2060 (0.5%)   |
| 1   | G     | 0.49         | 1/1567 (0.1%)  | 0.96        | 11/2125 (0.5%)   |
| 1   | P     | 0.52         | 0/1454         | 1.01        | 8/1977 (0.4%)    |
| 2   | B     | 0.51         | 1/1917 (0.1%)  | 0.98        | 8/2616 (0.3%)    |
| 2   | H     | 0.48         | 0/1930         | 0.97        | 9/2635 (0.3%)    |
| 2   | L     | 0.47         | 0/1944         | 0.97        | 6/2659 (0.2%)    |
| 2   | Q     | 0.50         | 0/1891         | 1.08        | 12/2583 (0.5%)   |
| 3   | C     | 0.53         | 1/2091 (0.0%)  | 1.09        | 21/2841 (0.7%)   |
| 3   | I     | 0.62         | 2/2129 (0.1%)  | 1.16        | 18/2887 (0.6%)   |
| 3   | M     | 0.64         | 0/2130         | 1.14        | 17/2890 (0.6%)   |
| 3   | R     | 0.47         | 0/2048         | 0.95        | 8/2777 (0.3%)    |
| 4   | D     | 0.57         | 1/809 (0.1%)   | 1.14        | 6/1098 (0.5%)    |
| 4   | J     | 0.56         | 0/793          | 1.22        | 9/1075 (0.8%)    |
| 4   | N     | 0.69         | 0/715          | 1.40        | 12/962 (1.2%)    |
| 4   | U     | 0.60         | 2/815 (0.2%)   | 1.21        | 9/1104 (0.8%)    |
| 5   | E     | 0.39         | 0/69           | 0.88        | 1/92 (1.1%)      |
| 5   | K     | 0.66         | 0/69           | 1.01        | 0/92             |
| 5   | O     | 0.30         | 0/69           | 0.83        | 0/92             |
| 5   | T     | 0.38         | 0/69           | 0.70        | 0/92             |
| All | All   | 0.54         | 8/25512 (0.0%) | 1.06        | 173/34670 (0.5%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 1                   |
| 1   | F     | 0                   | 1                   |
| 1   | P     | 0                   | 1                   |
| 2   | Q     | 0                   | 1                   |
| 3   | C     | 0                   | 2                   |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 3   | I     | 0                   | 1                   |
| 3   | M     | 0                   | 2                   |
| 3   | R     | 0                   | 2                   |
| 4   | D     | 0                   | 1                   |
| 4   | J     | 0                   | 2                   |
| 4   | N     | 0                   | 1                   |
| All | All   | 0                   | 15                  |

All (8) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 1   | G     | 201 | PHE  | C-N   | 5.77 | 1.41        | 1.33     |
| 3   | I     | 151 | HIS  | CA-C  | 5.67 | 1.59        | 1.52     |
| 4   | D     | 89  | GLN  | C-N   | 5.53 | 1.41        | 1.33     |
| 3   | I     | 155 | GLN  | CA-C  | 5.39 | 1.59        | 1.52     |
| 4   | U     | 89  | GLN  | C-N   | 5.33 | 1.40        | 1.33     |
| 2   | B     | 150 | PRO  | N-CD  | 5.22 | 1.55        | 1.47     |
| 3   | C     | 250 | PRO  | N-CD  | 5.17 | 1.54        | 1.47     |
| 4   | U     | 90  | PRO  | N-CD  | 5.11 | 1.54        | 1.47     |

All (173) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 4   | N     | 19  | LYS  | N-CA-C  | -15.15 | 88.24       | 108.24   |
| 4   | J     | 47  | GLU  | N-CA-C  | 13.19  | 125.73      | 111.36   |
| 3   | I     | 155 | GLN  | N-CA-C  | 12.40  | 124.34      | 111.07   |
| 3   | M     | 192 | HIS  | N-CA-C  | 11.48  | 127.08      | 111.24   |
| 3   | M     | 207 | SER  | N-CA-C  | 11.46  | 126.91      | 112.24   |
| 2   | B     | 147 | GLY  | N-CA-C  | 10.80  | 133.20      | 113.76   |
| 4   | J     | 48  | LYS  | N-CA-C  | 10.75  | 126.14      | 112.92   |
| 2   | Q     | 127 | GLU  | CA-C-N  | 10.34  | 132.77      | 119.84   |
| 2   | Q     | 127 | GLU  | C-N-CA  | 10.34  | 132.77      | 119.84   |
| 2   | H     | 231 | GLN  | N-CA-CB | 9.78   | 126.79      | 111.24   |
| 1   | F     | 112 | LYS  | CA-C-N  | 9.08   | 128.92      | 120.21   |
| 1   | F     | 112 | LYS  | C-N-CA  | 9.08   | 128.92      | 120.21   |
| 2   | Q     | 149 | TYR  | C-N-CD  | 8.91   | 140.19      | 120.60   |
| 3   | C     | 178 | THR  | N-CA-C  | 8.89   | 121.05      | 111.36   |
| 3   | M     | 269 | PRO  | N-CA-C  | -8.84  | 97.41       | 111.03   |
| 3   | M     | 208 | PHE  | N-CA-C  | 8.55   | 123.62      | 110.36   |
| 1   | F     | 196 | PRO  | CA-N-CD | -8.50  | 100.10      | 112.00   |
| 2   | B     | 149 | TYR  | C-N-CD  | 8.43   | 139.14      | 120.60   |
| 3   | I     | 218 | GLN  | N-CA-C  | 8.39   | 119.71      | 107.88   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | M     | 64  | THR  | N-CA-C  | -8.24 | 102.30      | 111.28   |
| 4   | N     | 86  | THR  | N-CA-C  | 8.24  | 120.04      | 111.14   |
| 1   | P     | 57  | SER  | N-CA-C  | 8.23  | 123.63      | 112.68   |
| 4   | N     | 35  | ILE  | N-CA-C  | 8.20  | 120.59      | 108.45   |
| 4   | N     | 28  | SER  | N-CA-C  | 8.16  | 120.85      | 107.23   |
| 2   | L     | 119 | PHE  | CA-C-N  | 7.83  | 128.44      | 120.38   |
| 2   | L     | 119 | PHE  | C-N-CA  | 7.83  | 128.44      | 120.38   |
| 3   | C     | 206 | LEU  | N-CA-C  | 7.62  | 117.94      | 107.73   |
| 1   | G     | 112 | LYS  | CA-C-N  | -7.38 | 112.61      | 120.66   |
| 1   | G     | 112 | LYS  | C-N-CA  | -7.38 | 112.61      | 120.66   |
| 4   | J     | 42  | ASN  | N-CA-C  | -7.37 | 97.11       | 108.31   |
| 1   | A     | 42  | GLY  | CA-C-N  | 7.34  | 127.79      | 119.93   |
| 1   | A     | 42  | GLY  | C-N-CA  | 7.34  | 127.79      | 119.93   |
| 4   | D     | 89  | GLN  | CA-C-N  | -7.25 | 112.51      | 119.76   |
| 4   | D     | 89  | GLN  | C-N-CA  | -7.25 | 112.51      | 119.76   |
| 4   | U     | 28  | SER  | N-CA-C  | 7.16  | 119.25      | 107.73   |
| 3   | I     | 255 | GLN  | N-CA-C  | -7.15 | 104.54      | 113.55   |
| 1   | F     | 151 | LYS  | CB-CA-C | -7.09 | 108.39      | 116.54   |
| 2   | B     | 146 | THR  | N-CA-C  | -6.94 | 101.58      | 110.53   |
| 4   | D     | 4   | THR  | CA-C-N  | 6.94  | 127.11      | 120.31   |
| 4   | D     | 4   | THR  | C-N-CA  | 6.94  | 127.11      | 120.31   |
| 1   | P     | 55  | LEU  | CB-CA-C | 6.93  | 121.13      | 109.48   |
| 3   | C     | 70  | HIS  | N-CA-C  | -6.89 | 103.78      | 111.71   |
| 1   | F     | 58  | ASN  | N-CA-C  | -6.85 | 104.79      | 113.01   |
| 3   | M     | 199 | ALA  | N-CA-C  | -6.84 | 97.95       | 108.76   |
| 3   | C     | 248 | VAL  | N-CA-C  | 6.83  | 117.36      | 108.35   |
| 4   | N     | 31  | HIS  | N-CA-C  | 6.77  | 116.10      | 108.25   |
| 4   | U     | 89  | GLN  | CA-C-N  | -6.76 | 112.80      | 119.76   |
| 4   | U     | 89  | GLN  | C-N-CA  | -6.76 | 112.80      | 119.76   |
| 2   | H     | 127 | GLU  | CA-C-N  | 6.72  | 126.76      | 119.90   |
| 2   | H     | 127 | GLU  | C-N-CA  | 6.72  | 126.76      | 119.90   |
| 2   | Q     | 119 | PHE  | N-CA-C  | 6.69  | 114.24      | 108.22   |
| 3   | R     | 239 | GLY  | N-CA-C  | -6.68 | 105.85      | 115.27   |
| 1   | G     | 201 | PHE  | CA-C-N  | -6.59 | 112.97      | 119.76   |
| 1   | G     | 201 | PHE  | C-N-CA  | -6.59 | 112.97      | 119.76   |
| 2   | H     | 203 | ARG  | CA-C-N  | -6.54 | 112.41      | 122.62   |
| 2   | H     | 203 | ARG  | C-N-CA  | -6.54 | 112.41      | 122.62   |
| 2   | H     | 228 | PRO  | N-CA-C  | 6.53  | 122.81      | 113.47   |
| 3   | M     | 242 | GLN  | N-CA-C  | 6.53  | 118.47      | 108.42   |
| 4   | J     | 79  | ALA  | CA-C-N  | -6.50 | 113.64      | 122.86   |
| 4   | J     | 79  | ALA  | C-N-CA  | -6.50 | 113.64      | 122.86   |
| 3   | I     | 62  | GLY  | N-CA-C  | -6.43 | 107.26      | 114.40   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 3   | M     | 193 | ALA  | N-CA-C   | 6.43  | 117.95      | 111.07   |
| 1   | F     | 189 | ALA  | N-CA-C   | 6.41  | 117.93      | 111.07   |
| 3   | C     | 207 | SER  | N-CA-C   | -6.33 | 105.13      | 112.86   |
| 3   | M     | 270 | LEU  | N-CA-C   | -6.32 | 99.73       | 109.52   |
| 3   | I     | 170 | ARG  | N-CA-C   | -6.30 | 104.41      | 111.28   |
| 3   | I     | 203 | CYS  | CA-CB-SG | 6.26  | 128.80      | 114.40   |
| 4   | D     | 47  | GLU  | N-CA-C   | -6.20 | 102.78      | 110.41   |
| 3   | M     | 259 | CYS  | N-CA-C   | 6.16  | 119.57      | 107.98   |
| 4   | J     | 49  | VAL  | N-CA-C   | 6.13  | 119.47      | 109.78   |
| 1   | G     | 59  | GLY  | N-CA-C   | -6.02 | 103.31      | 112.51   |
| 2   | H     | 119 | PHE  | CA-C-N   | 6.00  | 126.56      | 120.38   |
| 2   | H     | 119 | PHE  | C-N-CA   | 6.00  | 126.56      | 120.38   |
| 1   | A     | 160 | LYS  | N-CA-C   | 6.00  | 118.26      | 110.53   |
| 4   | J     | 51  | HIS  | N-CA-C   | 5.95  | 118.34      | 108.99   |
| 2   | L     | 51  | ASN  | CB-CA-C  | -5.93 | 108.73      | 115.79   |
| 2   | Q     | 150 | PRO  | CA-N-CD  | -5.92 | 103.22      | 111.50   |
| 4   | N     | 29  | GLY  | N-CA-C   | 5.91  | 127.19      | 113.18   |
| 3   | C     | 200 | THR  | N-CA-C   | 5.90  | 118.73      | 108.76   |
| 2   | L     | 178 | GLN  | N-CA-C   | 5.89  | 118.05      | 110.39   |
| 3   | C     | 177 | GLU  | CA-C-N   | 5.87  | 128.62      | 120.29   |
| 3   | C     | 177 | GLU  | C-N-CA   | 5.87  | 128.62      | 120.29   |
| 4   | N     | 61  | SER  | N-CA-C   | 5.86  | 117.95      | 108.34   |
| 1   | P     | 53  | GLY  | N-CA-C   | -5.86 | 99.30       | 113.18   |
| 1   | P     | 118 | PRO  | CA-N-CD  | -5.84 | 103.83      | 112.00   |
| 2   | Q     | 113 | GLU  | N-CA-C   | 5.81  | 117.69      | 111.36   |
| 3   | I     | 192 | HIS  | N-CA-C   | 5.80  | 116.21      | 108.38   |
| 4   | N     | 27  | VAL  | N-CA-C   | 5.79  | 121.37      | 109.34   |
| 1   | F     | 96  | SER  | N-CA-C   | -5.78 | 106.21      | 113.72   |
| 3   | C     | 179 | LEU  | CA-CB-CG | 5.78  | 136.52      | 116.30   |
| 4   | U     | 29  | GLY  | N-CA-C   | -5.75 | 107.05      | 115.72   |
| 3   | R     | 166 | GLU  | N-CA-C   | -5.71 | 105.06      | 111.28   |
| 3   | I     | 254 | GLU  | N-CA-C   | 5.71  | 118.98      | 111.28   |
| 4   | D     | 4   | THR  | N-CA-C   | 5.70  | 116.99      | 109.93   |
| 3   | C     | 249 | VAL  | CA-C-N   | -5.69 | 112.73      | 119.84   |
| 3   | C     | 249 | VAL  | C-N-CA   | -5.69 | 112.73      | 119.84   |
| 3   | R     | 52  | ILE  | N-CA-C   | -5.63 | 108.36      | 113.71   |
| 4   | U     | 79  | ALA  | N-CA-C   | 5.62  | 115.66      | 108.24   |
| 1   | G     | 119 | ASP  | CA-C-N   | 5.61  | 125.52      | 119.85   |
| 1   | G     | 119 | ASP  | C-N-CA   | 5.61  | 125.52      | 119.85   |
| 3   | M     | 216 | THR  | N-CA-C   | -5.60 | 100.27      | 109.40   |
| 3   | C     | 37  | ASP  | CA-C-N   | 5.60  | 128.24      | 120.29   |
| 3   | C     | 37  | ASP  | C-N-CA   | 5.60  | 128.24      | 120.29   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4   | N     | 88  | SER  | CB-CA-C | -5.57 | 110.17      | 116.63   |
| 3   | I     | 147 | TRP  | N-CA-C  | -5.55 | 106.51      | 113.28   |
| 3   | M     | 66  | LYS  | N-CA-C  | 5.55  | 117.01      | 111.07   |
| 3   | C     | 38  | SER  | N-CA-C  | 5.55  | 117.41      | 111.36   |
| 3   | C     | 171 | TYR  | N-CA-C  | -5.51 | 106.69      | 113.41   |
| 3   | I     | 256 | ARG  | N-CA-C  | 5.51  | 117.39      | 108.08   |
| 4   | U     | 89  | GLN  | N-CA-C  | -5.49 | 102.29      | 110.20   |
| 2   | L     | 173 | GLN  | CA-C-N  | 5.49  | 125.49      | 119.89   |
| 2   | L     | 173 | GLN  | C-N-CA  | 5.49  | 125.49      | 119.89   |
| 4   | N     | 89  | GLN  | CA-C-N  | 5.49  | 125.41      | 119.76   |
| 4   | N     | 89  | GLN  | C-N-CA  | 5.49  | 125.41      | 119.76   |
| 2   | B     | 148 | PHE  | N-CA-C  | 5.48  | 117.89      | 109.07   |
| 4   | J     | 46  | ILE  | CB-CA-C | -5.46 | 105.58      | 111.59   |
| 4   | U     | 80  | CYS  | N-CA-C  | 5.46  | 118.36      | 109.24   |
| 2   | B     | 178 | GLN  | CA-C-N  | 5.46  | 125.15      | 119.64   |
| 2   | B     | 178 | GLN  | C-N-CA  | 5.46  | 125.15      | 119.64   |
| 2   | Q     | 135 | HIS  | CA-C-N  | 5.46  | 131.97      | 121.54   |
| 2   | Q     | 135 | HIS  | C-N-CA  | 5.46  | 131.97      | 121.54   |
| 4   | J     | 31  | HIS  | N-CA-C  | 5.45  | 113.03      | 108.13   |
| 3   | M     | 139 | ALA  | N-CA-C  | -5.45 | 106.67      | 113.15   |
| 1   | P     | 125 | LEU  | N-CA-C  | 5.45  | 116.80      | 108.52   |
| 1   | A     | 38  | GLU  | CA-C-N  | 5.44  | 126.64      | 119.84   |
| 1   | A     | 38  | GLU  | C-N-CA  | 5.44  | 126.64      | 119.84   |
| 3   | C     | 121 | LYS  | N-CA-C  | 5.44  | 115.46      | 108.34   |
| 4   | U     | 4   | THR  | CA-C-N  | 5.43  | 125.33      | 119.85   |
| 4   | U     | 4   | THR  | C-N-CA  | 5.43  | 125.33      | 119.85   |
| 3   | M     | 208 | PHE  | N-CA-CB | -5.39 | 102.25      | 110.49   |
| 3   | R     | 205 | ALA  | N-CA-C  | 5.38  | 116.86      | 107.49   |
| 3   | R     | 122 | ASP  | N-CA-C  | 5.38  | 117.24      | 110.24   |
| 3   | I     | 191 | HIS  | N-CA-C  | 5.38  | 117.27      | 108.55   |
| 2   | Q     | 220 | GLU  | N-CA-C  | 5.35  | 118.27      | 109.76   |
| 1   | G     | 150 | SER  | CA-C-N  | 5.34  | 131.31      | 121.70   |
| 1   | G     | 150 | SER  | C-N-CA  | 5.34  | 131.31      | 121.70   |
| 1   | G     | 155 | VAL  | N-CA-C  | 5.33  | 116.89      | 109.80   |
| 3   | C     | 46  | GLU  | CA-C-N  | 5.33  | 125.30      | 120.03   |
| 3   | C     | 46  | GLU  | C-N-CA  | 5.33  | 125.30      | 120.03   |
| 3   | I     | 207 | SER  | N-CA-C  | 5.32  | 118.58      | 111.24   |
| 1   | F     | 150 | SER  | N-CA-C  | 5.31  | 117.93      | 110.23   |
| 3   | R     | 202 | ARG  | N-CA-C  | 5.31  | 117.33      | 108.99   |
| 2   | H     | 230 | THR  | N-CA-C  | -5.30 | 100.39      | 109.24   |
| 3   | I     | 143 | THR  | N-CA-C  | -5.30 | 104.97      | 111.75   |
| 3   | C     | 43  | GLN  | N-CA-C  | -5.28 | 106.42      | 112.86   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | A     | 36  | LYS  | N-CA-C   | 5.25  | 117.05      | 108.55   |
| 2   | Q     | 167 | GLY  | N-CA-C   | -5.20 | 108.44      | 115.36   |
| 5   | E     | 6   | VAL  | N-CA-C   | 5.19  | 116.13      | 108.45   |
| 1   | G     | 127 | ASP  | N-CA-C   | 5.18  | 117.55      | 110.55   |
| 3   | I     | 241 | PHE  | N-CA-C   | 5.18  | 115.89      | 108.74   |
| 3   | R     | 44  | ARG  | N-CA-C   | -5.18 | 102.09      | 110.32   |
| 1   | A     | 165 | MET  | N-CA-C   | 5.17  | 116.26      | 108.46   |
| 3   | M     | 59  | TYR  | N-CA-C   | -5.17 | 99.80       | 110.80   |
| 2   | B     | 171 | ASP  | CA-C-N   | 5.16  | 124.83      | 119.56   |
| 2   | B     | 171 | ASP  | C-N-CA   | 5.16  | 124.83      | 119.56   |
| 1   | P     | 56  | THR  | N-CA-C   | -5.15 | 100.77      | 108.96   |
| 1   | P     | 117 | ASN  | CA-C-N   | -5.15 | 113.41      | 119.84   |
| 1   | P     | 117 | ASN  | C-N-CA   | -5.15 | 113.41      | 119.84   |
| 3   | I     | 14  | ARG  | CA-C-N   | 5.13  | 126.25      | 119.84   |
| 3   | I     | 14  | ARG  | C-N-CA   | 5.13  | 126.25      | 119.84   |
| 3   | C     | 56  | GLY  | CA-C-N   | 5.12  | 125.41      | 119.47   |
| 3   | C     | 56  | GLY  | C-N-CA   | 5.12  | 125.41      | 119.47   |
| 1   | F     | 127 | ASP  | N-CA-C   | 5.10  | 117.98      | 110.59   |
| 3   | I     | 54  | GLN  | N-CA-C   | 5.09  | 116.83      | 111.28   |
| 3   | I     | 180 | GLN  | CA-CB-CG | 5.08  | 124.26      | 114.10   |
| 1   | F     | 62  | THR  | N-CA-C   | 5.05  | 116.61      | 108.32   |
| 4   | N     | 83  | ASN  | N-CA-C   | 5.05  | 114.90      | 108.24   |
| 2   | Q     | 115 | LEU  | N-CA-C   | 5.04  | 116.77      | 111.28   |
| 3   | R     | 190 | THR  | N-CA-C   | 5.04  | 116.38      | 107.61   |
| 1   | A     | 25  | SER  | N-CA-C   | 5.03  | 115.69      | 108.74   |
| 2   | Q     | 51  | ASN  | CB-CA-C  | -5.02 | 110.77      | 116.54   |
| 3   | M     | 49  | ALA  | CA-C-N   | 5.01  | 124.67      | 119.56   |
| 3   | M     | 49  | ALA  | C-N-CA   | 5.01  | 124.67      | 119.56   |

There are no chirality outliers.

All (15) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | A     | 158 | THR  | Peptide |
| 3   | C     | 178 | THR  | Peptide |
| 3   | C     | 233 | THR  | Peptide |
| 4   | D     | 86  | THR  | Peptide |
| 1   | F     | 57  | SER  | Peptide |
| 3   | I     | 131 | ARG  | Peptide |
| 4   | J     | 47  | GLU  | Peptide |
| 4   | J     | 68  | THR  | Peptide |
| 3   | M     | 217 | TRP  | Peptide |

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| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 3   | M     | 88  | SER  | Peptide |
| 4   | N     | 83  | ASN  | Peptide |
| 1   | P     | 197 | GLU  | Peptide |
| 2   | Q     | 135 | HIS  | Peptide |
| 3   | R     | 258 | THR  | Peptide |
| 3   | R     | 43  | GLN  | Peptide |

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 1459  | 0        | 1369     | 71      | 0            |
| 1   | F     | 1486  | 0        | 1377     | 76      | 0            |
| 1   | G     | 1535  | 0        | 1459     | 89      | 0            |
| 1   | P     | 1426  | 0        | 1324     | 78      | 0            |
| 2   | B     | 1870  | 0        | 1737     | 111     | 0            |
| 2   | H     | 1878  | 0        | 1760     | 104     | 0            |
| 2   | L     | 1891  | 0        | 1754     | 111     | 0            |
| 2   | Q     | 1840  | 0        | 1701     | 90      | 0            |
| 3   | C     | 2034  | 0        | 1862     | 113     | 0            |
| 3   | I     | 2072  | 0        | 1914     | 215     | 0            |
| 3   | M     | 2076  | 0        | 1865     | 145     | 0            |
| 3   | R     | 1994  | 0        | 1836     | 123     | 0            |
| 4   | D     | 787   | 0        | 736      | 79      | 0            |
| 4   | J     | 772   | 0        | 706      | 80      | 0            |
| 4   | N     | 697   | 0        | 612      | 52      | 0            |
| 4   | U     | 793   | 0        | 732      | 72      | 0            |
| 5   | E     | 68    | 0        | 75       | 8       | 0            |
| 5   | K     | 68    | 0        | 75       | 18      | 0            |
| 5   | O     | 68    | 0        | 75       | 7       | 0            |
| 5   | T     | 68    | 0        | 75       | 4       | 0            |
| All | All   | 24882 | 0        | 23044    | 1488    | 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 31.

All (1488) 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:G:133:LYS:CB  | 1:G:180:ASN:HD21 | 1.15                     | 1.51              |
| 1:P:47:ILE:CD1  | 1:P:57:SER:HB2   | 1.37                     | 1.50              |
| 1:G:59:GLY:CA   | 1:G:61:LEU:H     | 1.24                     | 1.50              |
| 1:G:59:GLY:HA3  | 1:G:61:LEU:N     | 1.32                     | 1.44              |
| 1:G:133:LYS:CB  | 1:G:180:ASN:ND2  | 1.89                     | 1.33              |
| 1:G:133:LYS:HB3 | 1:G:180:ASN:ND2  | 1.43                     | 1.28              |
| 2:H:97:TYR:O    | 3:I:152:VAL:HG12 | 1.23                     | 1.25              |
| 4:D:73:THR:HB   | 4:D:76:ASP:OD2   | 1.27                     | 1.24              |
| 2:Q:136:THR:OG1 | 2:Q:137:GLN:HA   | 1.37                     | 1.21              |
| 2:B:145:ALA:HB1 | 2:B:148:PHE:CZ   | 1.76                     | 1.20              |
| 2:B:121:PRO:CB  | 2:B:148:PHE:HE1  | 1.54                     | 1.19              |
| 2:L:96:ILE:CD1  | 3:M:146:LYS:HE2  | 1.73                     | 1.18              |
| 4:N:18:GLY:HA2  | 4:N:72:PRO:O     | 1.38                     | 1.18              |
| 2:L:96:ILE:HD12 | 3:M:146:LYS:CE   | 1.74                     | 1.17              |
| 4:J:4:THR:HB    | 4:J:86:THR:CG2   | 1.75                     | 1.16              |
| 2:B:222:THR:HB  | 2:B:223:GLN:CG   | 1.74                     | 1.16              |
| 1:P:47:ILE:HD12 | 1:P:57:SER:CB    | 1.75                     | 1.15              |
| 2:H:97:TYR:C    | 3:I:152:VAL:HG12 | 1.72                     | 1.15              |
| 2:H:97:TYR:O    | 3:I:152:VAL:CG1  | 1.95                     | 1.13              |
| 1:G:133:LYS:CA  | 1:G:180:ASN:HD21 | 1.62                     | 1.12              |
| 1:P:47:ILE:CD1  | 1:P:57:SER:CB    | 2.27                     | 1.11              |
| 4:N:84:HIS:CD2  | 4:N:86:THR:H     | 1.69                     | 1.11              |
| 4:U:58:LYS:HA   | 4:U:60:TRP:H     | 1.13                     | 1.10              |
| 3:I:63:GLU:HA   | 3:I:66:LYS:HZ2   | 1.14                     | 1.09              |
| 1:P:47:ILE:CG1  | 1:P:57:SER:HB2   | 1.83                     | 1.08              |
| 2:B:145:ALA:HB1 | 2:B:148:PHE:HZ   | 1.05                     | 1.07              |
| 1:G:133:LYS:CG  | 1:G:180:ASN:HD21 | 1.68                     | 1.06              |
| 2:B:222:THR:HB  | 2:B:223:GLN:HG3  | 1.12                     | 1.06              |
| 2:B:96:ILE:HD12 | 3:C:146:LYS:HE2  | 1.32                     | 1.06              |
| 3:C:49:ALA:HB1  | 3:C:51:TRP:CZ3   | 1.90                     | 1.06              |
| 4:J:45:ARG:H    | 4:J:45:ARG:HD2   | 1.22                     | 1.05              |
| 4:U:83:ASN:HB2  | 4:U:90:PRO:HB3   | 1.11                     | 1.05              |
| 2:L:96:ILE:HD11 | 3:M:146:LYS:NZ   | 1.73                     | 1.04              |
| 2:H:96:ILE:HG22 | 3:I:152:VAL:HG11 | 1.39                     | 1.04              |
| 2:B:149:TYR:CE2 | 2:B:150:PRO:HB3  | 1.94                     | 1.03              |
| 1:G:57:SER:O    | 1:G:59:GLY:N     | 1.89                     | 1.03              |
| 4:D:76:ASP:HB3  | 4:D:78:TYR:HE2   | 1.23                     | 1.03              |
| 2:Q:119:PHE:HB2 | 2:Q:120:PRO:HD2  | 1.38                     | 1.03              |
| 2:L:96:ILE:CD1  | 3:M:146:LYS:CE   | 2.34                     | 1.02              |
| 3:I:218:GLN:HG3 | 3:I:219:ARG:H    | 1.25                     | 1.01              |
| 1:G:132:ASP:O   | 1:G:180:ASN:OD1  | 1.78                     | 1.01              |
| 4:N:84:HIS:HD2  | 4:N:86:THR:HG22  | 1.22                     | 1.00              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:Q:132:GLU:O    | 2:Q:136:THR:HA   | 1.59                     | 1.00              |
| 4:N:84:HIS:CD2   | 4:N:86:THR:HB    | 1.98                     | 0.99              |
| 4:J:4:THR:HB     | 4:J:86:THR:HG21  | 1.02                     | 0.99              |
| 4:N:84:HIS:HD2   | 4:N:86:THR:CG2   | 1.74                     | 0.99              |
| 4:D:76:ASP:HB3   | 4:D:78:TYR:CE2   | 1.99                     | 0.98              |
| 2:B:121:PRO:CB   | 2:B:148:PHE:CE1  | 2.47                     | 0.98              |
| 1:G:133:LYS:HA   | 1:G:180:ASN:ND2  | 1.77                     | 0.98              |
| 3:I:155:GLN:O    | 3:I:157:ARG:N    | 1.97                     | 0.98              |
| 3:M:55:GLU:HB3   | 3:M:58:GLU:HG3   | 1.44                     | 0.97              |
| 3:C:173:GLU:HG3  | 3:C:174:ASN:N    | 1.76                     | 0.97              |
| 1:G:60:ARG:NH2   | 1:G:83:ASP:OD2   | 1.97                     | 0.96              |
| 2:L:227:LYS:O    | 2:L:229:VAL:HG23 | 1.65                     | 0.96              |
| 4:N:84:HIS:NE2   | 4:N:86:THR:HB    | 1.80                     | 0.96              |
| 2:B:222:THR:CB   | 2:B:223:GLN:HG3  | 1.95                     | 0.95              |
| 2:Q:134:SER:O    | 2:Q:136:THR:HB   | 1.67                     | 0.95              |
| 1:G:133:LYS:CA   | 1:G:180:ASN:ND2  | 2.24                     | 0.95              |
| 4:D:74:GLU:OE2   | 4:D:74:GLU:N     | 2.00                     | 0.94              |
| 3:M:65:ARG:O     | 3:M:68:LYS:CD    | 2.16                     | 0.94              |
| 4:J:46:ILE:CD1   | 4:J:70:PHE:HZ    | 1.80                     | 0.94              |
| 2:B:121:PRO:HA   | 2:B:148:PHE:CE1  | 2.02                     | 0.94              |
| 3:M:126:LEU:HD21 | 3:M:130:LEU:HA   | 1.49                     | 0.94              |
| 4:J:4:THR:CB     | 4:J:86:THR:HG21  | 1.97                     | 0.93              |
| 4:U:58:LYS:HA    | 4:U:60:TRP:N     | 1.83                     | 0.93              |
| 3:M:32:GLN:OE1   | 3:M:34:VAL:N     | 2.02                     | 0.93              |
| 3:M:17:ARG:HG2   | 3:M:17:ARG:HH11  | 1.34                     | 0.92              |
| 4:N:84:HIS:CD2   | 4:N:86:THR:CB    | 2.52                     | 0.92              |
| 3:I:218:GLN:HG3  | 3:I:219:ARG:N    | 1.84                     | 0.91              |
| 2:Q:134:SER:C    | 2:Q:136:THR:HB   | 1.94                     | 0.91              |
| 4:D:73:THR:CB    | 4:D:76:ASP:OD2   | 2.19                     | 0.91              |
| 4:N:18:GLY:CA    | 4:N:72:PRO:O     | 2.19                     | 0.90              |
| 2:L:96:ILE:HD11  | 3:M:146:LYS:HZ3  | 1.36                     | 0.90              |
| 3:M:6:ARG:HH12   | 3:M:113:TYR:HD2  | 1.17                     | 0.90              |
| 2:Q:149:TYR:CE1  | 2:Q:150:PRO:HB3  | 2.07                     | 0.90              |
| 2:B:96:ILE:HD12  | 3:C:146:LYS:CE   | 2.02                     | 0.90              |
| 1:G:133:LYS:HB3  | 1:G:180:ASN:HD22 | 1.36                     | 0.89              |
| 4:J:46:ILE:HD13  | 4:J:70:PHE:CZ    | 2.07                     | 0.89              |
| 1:G:59:GLY:CA    | 1:G:61:LEU:N     | 2.07                     | 0.89              |
| 3:M:65:ARG:HG3   | 3:M:65:ARG:HH11  | 1.35                     | 0.89              |
| 1:P:47:ILE:CG1   | 1:P:57:SER:CB    | 2.50                     | 0.89              |
| 4:U:28:SER:HB3   | 4:U:63:TYR:HA    | 1.54                     | 0.89              |
| 3:C:66:LYS:HD2   | 5:E:4:GLY:HA2    | 1.51                     | 0.89              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:228:PRO:O    | 2:H:229:VAL:HG22 | 1.72                     | 0.89              |
| 1:P:52:ALA:HA    | 1:P:65:PHE:HB3   | 1.52                     | 0.89              |
| 2:Q:136:THR:OG1  | 2:Q:137:GLN:CA   | 2.21                     | 0.89              |
| 4:D:75:LYS:O     | 4:D:76:ASP:OD1   | 1.91                     | 0.89              |
| 1:F:115:ILE:HD13 | 1:F:142:ASP:HA   | 1.53                     | 0.89              |
| 3:C:146:LYS:NZ   | 5:E:9:LEU:O      | 2.04                     | 0.88              |
| 2:L:50:MET:HE1   | 5:O:6:VAL:H      | 1.38                     | 0.88              |
| 3:R:263:HIS:ND1  | 3:R:265:GLY:N    | 2.22                     | 0.88              |
| 3:M:65:ARG:O     | 3:M:68:LYS:HD3   | 1.73                     | 0.88              |
| 2:L:96:ILE:HD12  | 3:M:146:LYS:HE2  | 0.89                     | 0.87              |
| 1:G:60:ARG:HH12  | 1:G:83:ASP:CG    | 1.81                     | 0.87              |
| 4:D:76:ASP:CB    | 4:D:78:TYR:HE2   | 1.87                     | 0.87              |
| 2:B:121:PRO:CA   | 2:B:148:PHE:CE1  | 2.58                     | 0.87              |
| 4:D:5:PRO:HB3    | 4:D:30:PHE:HB3   | 1.56                     | 0.87              |
| 3:R:207:SER:HA   | 3:R:240:THR:HB   | 1.55                     | 0.87              |
| 2:L:95:LEU:HD12  | 2:L:96:ILE:N     | 1.90                     | 0.86              |
| 1:P:47:ILE:HG13  | 1:P:57:SER:CB    | 2.05                     | 0.86              |
| 4:J:46:ILE:CD1   | 4:J:70:PHE:CZ    | 2.58                     | 0.86              |
| 3:I:218:GLN:CG   | 3:I:219:ARG:H    | 1.88                     | 0.86              |
| 3:M:215:LEU:HB3  | 3:M:261:VAL:HG12 | 1.57                     | 0.86              |
| 4:J:89:GLN:HB2   | 4:J:91:LYS:HG2   | 1.58                     | 0.86              |
| 3:R:185:PRO:HD3  | 3:R:263:HIS:CD2  | 2.10                     | 0.86              |
| 2:H:47:TYR:HE1   | 2:H:61:PRO:HA    | 1.39                     | 0.86              |
| 3:I:145:HIS:O    | 3:I:148:GLU:N    | 2.08                     | 0.85              |
| 4:J:3:ARG:O      | 4:J:30:PHE:HA    | 1.76                     | 0.85              |
| 2:Q:149:TYR:CD1  | 2:Q:150:PRO:HB3  | 2.10                     | 0.85              |
| 3:I:183:ASP:OD2  | 3:I:207:SER:O    | 1.95                     | 0.85              |
| 4:J:46:ILE:HD13  | 4:J:70:PHE:HZ    | 1.38                     | 0.85              |
| 3:C:173:GLU:HG3  | 3:C:174:ASN:H    | 1.37                     | 0.85              |
| 4:N:18:GLY:HA2   | 4:N:72:PRO:C     | 2.01                     | 0.85              |
| 2:B:7:ASN:ND2    | 2:B:22:THR:OG1   | 2.08                     | 0.85              |
| 1:P:47:ILE:HD12  | 1:P:57:SER:HB2   | 0.87                     | 0.85              |
| 4:N:88:SER:OG    | 4:N:89:GLN:N     | 2.10                     | 0.85              |
| 2:B:53:GLU:O     | 3:C:68:LYS:HE2   | 1.76                     | 0.84              |
| 1:F:129:LYS:HG3  | 1:F:131:SER:H    | 1.43                     | 0.84              |
| 3:I:263:HIS:CE1  | 3:I:265:GLY:H    | 1.94                     | 0.84              |
| 4:D:83:ASN:HB2   | 4:D:90:PRO:HB3   | 1.60                     | 0.84              |
| 1:A:158:THR:HG22 | 1:A:159:ASP:H    | 1.42                     | 0.84              |
| 4:N:84:HIS:CD2   | 4:N:86:THR:N     | 2.46                     | 0.83              |
| 1:P:37:GLN:HB3   | 1:P:86:ILE:HD11  | 1.59                     | 0.83              |
| 2:Q:214:GLY:H    | 2:Q:230:THR:HB   | 1.42                     | 0.83              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:J:41:LYS:HG3   | 4:J:78:TYR:HD1   | 1.43                     | 0.83              |
| 2:L:96:ILE:CD1   | 3:M:146:LYS:NZ   | 2.41                     | 0.83              |
| 3:I:202:ARG:HG2  | 3:I:246:ALA:HA   | 1.59                     | 0.83              |
| 2:L:20:THR:HA    | 2:L:77:ILE:HG22  | 1.59                     | 0.83              |
| 3:M:65:ARG:O     | 3:M:68:LYS:CE    | 2.27                     | 0.83              |
| 4:D:46:ILE:HG12  | 4:D:47:GLU:H     | 1.43                     | 0.82              |
| 4:N:24:ASN:HB3   | 4:N:67:TYR:HB3   | 1.61                     | 0.82              |
| 3:I:6:ARG:NH1    | 3:I:99:TYR:O     | 2.11                     | 0.82              |
| 3:I:93:HIS:ND1   | 3:I:118:TYR:OH   | 2.12                     | 0.82              |
| 2:H:25:GLN:HE22  | 2:H:29:HIS:CD2   | 1.96                     | 0.82              |
| 2:L:36:ARG:HB2   | 2:L:46:ILE:HD11  | 1.61                     | 0.82              |
| 3:R:35:ARG:NH1   | 4:U:53:ASP:HB3   | 1.93                     | 0.82              |
| 3:C:234:ARG:HD2  | 4:D:8:GLN:HE22   | 1.43                     | 0.82              |
| 1:G:150:SER:HA   | 1:G:151:LYS:HB2  | 1.60                     | 0.82              |
| 3:M:220:ASP:CB   | 3:M:221:GLY:HA3  | 2.09                     | 0.82              |
| 4:J:45:ARG:HD2   | 4:J:45:ARG:N     | 1.94                     | 0.82              |
| 3:M:26:GLY:O     | 3:M:32:GLN:NE2   | 2.11                     | 0.82              |
| 3:M:259:CYS:HB3  | 3:M:272:LEU:HB2  | 1.61                     | 0.82              |
| 3:I:155:GLN:O    | 3:I:158:ALA:N    | 2.12                     | 0.81              |
| 3:M:65:ARG:O     | 3:M:68:LYS:HE2   | 1.79                     | 0.81              |
| 3:I:150:ALA:O    | 3:I:151:HIS:HB2  | 1.80                     | 0.81              |
| 1:F:127:ASP:OD1  | 1:F:128:SER:N    | 2.12                     | 0.81              |
| 3:C:49:ALA:CB    | 3:C:51:TRP:CZ3   | 2.63                     | 0.81              |
| 3:M:215:LEU:HD12 | 3:M:215:LEU:O    | 1.81                     | 0.80              |
| 1:P:198:ASP:OD1  | 1:P:199:THR:N    | 2.13                     | 0.80              |
| 2:B:121:PRO:CA   | 2:B:148:PHE:HE1  | 1.92                     | 0.80              |
| 2:L:148:PHE:HB2  | 2:L:186:TYR:HB2  | 1.62                     | 0.80              |
| 3:I:133:TRP:CZ2  | 3:I:153:ALA:HB1  | 2.17                     | 0.80              |
| 2:L:27:MET:HB3   | 2:L:29:HIS:CD2   | 2.16                     | 0.80              |
| 3:C:64:THR:HA    | 3:C:67:VAL:HG12  | 1.62                     | 0.80              |
| 4:N:84:HIS:CD2   | 4:N:86:THR:CG2   | 2.63                     | 0.80              |
| 1:F:57:SER:O     | 1:F:61:LEU:O     | 2.00                     | 0.80              |
| 3:I:213:ILE:HD12 | 3:I:263:HIS:CD2  | 2.17                     | 0.79              |
| 3:I:144:LYS:HD3  | 3:I:148:GLU:OE2  | 1.81                     | 0.79              |
| 2:H:96:ILE:CG2   | 3:I:152:VAL:HG11 | 2.12                     | 0.79              |
| 2:H:178:GLN:CD   | 2:H:178:GLN:H    | 1.90                     | 0.79              |
| 3:I:133:TRP:HZ2  | 3:I:153:ALA:CB   | 1.95                     | 0.79              |
| 4:N:84:HIS:CD2   | 4:N:86:THR:HG22  | 2.14                     | 0.79              |
| 2:B:108:ARG:NH2  | 2:B:150:PRO:HG2  | 1.98                     | 0.79              |
| 1:G:133:LYS:CG   | 1:G:180:ASN:ND2  | 2.36                     | 0.79              |
| 1:A:158:THR:CG2  | 1:A:159:ASP:H    | 1.95                     | 0.79              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:9:ARG:NH1    | 2:B:213:TYR:OH   | 2.16                     | 0.79              |
| 2:B:149:TYR:CD2  | 2:B:150:PRO:HB3  | 2.18                     | 0.78              |
| 3:C:37:ASP:OD1   | 3:C:38:SER:N     | 2.16                     | 0.78              |
| 1:A:156:TYR:HB3  | 1:A:178:TRP:O    | 1.84                     | 0.78              |
| 1:F:129:LYS:HE2  | 1:F:132:ASP:HA   | 1.64                     | 0.78              |
| 3:I:147:TRP:CZ2  | 5:K:7:PHE:CE1    | 2.71                     | 0.78              |
| 4:J:41:LYS:HD2   | 4:J:46:ILE:HD11  | 1.66                     | 0.78              |
| 3:R:263:HIS:CE1  | 3:R:265:GLY:H    | 2.01                     | 0.78              |
| 1:G:133:LYS:HG2  | 1:G:180:ASN:ND2  | 1.99                     | 0.78              |
| 2:B:22:THR:HA    | 2:B:75:PRO:HA    | 1.67                     | 0.77              |
| 1:G:135:VAL:HG12 | 1:G:178:TRP:HB3  | 1.67                     | 0.77              |
| 3:I:85:TYR:HB3   | 3:I:87:GLN:HG2   | 1.66                     | 0.77              |
| 2:B:108:ARG:HH22 | 2:B:150:PRO:HG2  | 1.47                     | 0.77              |
| 2:L:38:ASP:OD2   | 2:L:44:ARG:NH2   | 2.17                     | 0.77              |
| 3:R:35:ARG:HH12  | 4:U:53:ASP:HB3   | 1.50                     | 0.77              |
| 3:I:99:TYR:HB3   | 3:I:114:HIS:HD2  | 1.49                     | 0.77              |
| 1:F:57:SER:O     | 1:F:61:LEU:HB2   | 1.85                     | 0.77              |
| 2:Q:119:PHE:HB2  | 2:Q:120:PRO:CD   | 2.14                     | 0.77              |
| 3:M:7:TYR:HA     | 3:M:26:GLY:HA2   | 1.66                     | 0.77              |
| 2:Q:215:LEU:HD13 | 2:Q:219:ASP:HB2  | 1.67                     | 0.77              |
| 3:C:203:CYS:N    | 3:C:245:ALA:O    | 2.18                     | 0.76              |
| 4:D:18:GLY:H     | 4:D:72:PRO:HG2   | 1.50                     | 0.76              |
| 3:M:186:LYS:O    | 3:M:206:LEU:N    | 2.19                     | 0.76              |
| 2:H:88:LEU:HD12  | 2:H:108:ARG:HB3  | 1.68                     | 0.76              |
| 3:C:55:GLU:OE2   | 3:C:170:ARG:NH2  | 2.19                     | 0.76              |
| 3:C:85:TYR:HD2   | 3:C:87:GLN:HB2   | 1.51                     | 0.76              |
| 3:I:72:GLN:OE1   | 3:I:75:ARG:NH1   | 2.16                     | 0.76              |
| 3:M:138:MET:HA   | 3:M:141:GLN:HG2  | 1.66                     | 0.75              |
| 3:C:5:MET:HB2    | 3:C:168:LEU:HD13 | 1.66                     | 0.75              |
| 3:C:66:LYS:CD    | 5:E:4:GLY:HA2    | 2.16                     | 0.75              |
| 4:U:24:ASN:OD1   | 4:U:65:LEU:HD11  | 1.85                     | 0.75              |
| 3:M:217:TRP:NE1  | 3:M:258:THR:O    | 2.19                     | 0.75              |
| 2:L:112:LEU:HD11 | 2:L:149:TYR:HE2  | 1.52                     | 0.75              |
| 3:M:85:TYR:HD2   | 3:M:87:GLN:HE22  | 1.35                     | 0.75              |
| 2:Q:132:GLU:O    | 2:Q:136:THR:CA   | 2.35                     | 0.75              |
| 3:R:163:THR:O    | 3:R:167:TRP:HD1  | 1.70                     | 0.75              |
| 2:Q:125:VAL:HG23 | 2:Q:235:ALA:HB3  | 1.69                     | 0.75              |
| 1:G:121:ALA:HA   | 1:G:198:ASP:HB3  | 1.68                     | 0.75              |
| 3:I:133:TRP:CZ2  | 3:I:153:ALA:CB   | 2.70                     | 0.75              |
| 1:A:142:ASP:OD1  | 1:A:143:SER:N    | 2.20                     | 0.75              |
| 2:H:228:PRO:C    | 2:H:229:VAL:HG22 | 2.11                     | 0.74              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:I:5:MET:HB2    | 3:I:168:LEU:HD13 | 1.69                     | 0.74              |
| 3:R:25:VAL:HG11  | 4:U:54:LEU:O     | 1.88                     | 0.74              |
| 1:F:127:ASP:HB3  | 1:F:129:LYS:HG2  | 1.68                     | 0.74              |
| 3:M:215:LEU:HD12 | 3:M:215:LEU:C    | 2.12                     | 0.74              |
| 2:H:37:GLN:HB2   | 2:H:43:LEU:HD12  | 1.70                     | 0.74              |
| 3:M:38:SER:O     | 3:M:43:GLN:NE2   | 2.21                     | 0.74              |
| 4:N:27:VAL:O     | 4:N:28:SER:OG    | 2.03                     | 0.74              |
| 1:G:60:ARG:NH2   | 1:G:80:ILE:HB    | 2.02                     | 0.73              |
| 4:D:89:GLN:HB2   | 4:D:90:PRO:HD2   | 1.70                     | 0.73              |
| 3:R:185:PRO:HD3  | 3:R:263:HIS:HD2  | 1.51                     | 0.73              |
| 3:M:82:ARG:NH1   | 3:M:118:TYR:OH   | 2.21                     | 0.73              |
| 2:H:61:PRO:O     | 2:H:64:TYR:HD2   | 1.71                     | 0.73              |
| 3:I:99:TYR:HB3   | 3:I:114:HIS:CD2  | 2.23                     | 0.73              |
| 3:M:17:ARG:HG2   | 3:M:17:ARG:NH1   | 2.02                     | 0.73              |
| 3:C:35:ARG:HH11  | 3:C:35:ARG:HG2   | 1.54                     | 0.73              |
| 4:J:40:LEU:HD11  | 4:J:45:ARG:HE    | 1.53                     | 0.73              |
| 1:F:126:ARG:NH1  | 1:F:127:ASP:H    | 1.86                     | 0.73              |
| 2:H:25:GLN:HE22  | 2:H:29:HIS:HD2   | 1.33                     | 0.73              |
| 2:H:229:VAL:HG23 | 2:H:230:THR:N    | 2.03                     | 0.73              |
| 4:D:73:THR:CG2   | 4:D:74:GLU:OE2   | 2.37                     | 0.73              |
| 1:P:118:PRO:O    | 1:P:119:ASP:OD1  | 2.06                     | 0.73              |
| 2:Q:221:TRP:CH2  | 2:Q:223:GLN:C    | 2.67                     | 0.73              |
| 1:G:50:TYR:CZ    | 3:I:151:HIS:NE2  | 2.57                     | 0.72              |
| 3:I:137:ASP:O    | 3:I:141:GLN:HB2  | 1.89                     | 0.72              |
| 3:I:169:ARG:NH2  | 3:I:173:GLU:OE1  | 2.23                     | 0.72              |
| 3:C:36:PHE:HB2   | 3:C:45:MET:HB3   | 1.71                     | 0.72              |
| 2:L:27:MET:CB    | 2:L:29:HIS:CD2   | 2.72                     | 0.72              |
| 1:G:133:LYS:HA   | 1:G:180:ASN:CG   | 2.15                     | 0.72              |
| 1:F:160:LYS:HD3  | 1:F:160:LYS:N    | 2.05                     | 0.72              |
| 3:I:145:HIS:O    | 3:I:149:ALA:N    | 2.21                     | 0.72              |
| 1:A:163:LEU:HD23 | 1:A:172:SER:HB2  | 1.70                     | 0.72              |
| 1:A:13:ILE:HG12  | 1:A:109:LEU:HD11 | 1.70                     | 0.72              |
| 2:B:28:ASN:OD1   | 2:B:71:LYS:NZ    | 2.22                     | 0.72              |
| 2:L:25:GLN:NE2   | 2:L:27:MET:SD    | 2.63                     | 0.72              |
| 1:A:5:ASN:OD1    | 1:A:6:GLN:N      | 2.21                     | 0.72              |
| 3:I:104:GLY:H    | 3:I:110:LEU:HD13 | 1.54                     | 0.72              |
| 4:J:57:SER:HB3   | 4:J:61:SER:H     | 1.53                     | 0.72              |
| 2:L:25:GLN:CD    | 2:L:27:MET:HG2   | 2.14                     | 0.72              |
| 3:M:6:ARG:O      | 3:M:27:TYR:N     | 2.22                     | 0.71              |
| 2:B:164:VAL:HG22 | 2:B:166:SER:H    | 1.55                     | 0.71              |
| 1:G:42:GLY:HA2   | 2:H:90:PHE:HE2   | 1.54                     | 0.71              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:158:THR:HG22 | 1:A:159:ASP:N    | 2.03                     | 0.71              |
| 3:R:34:VAL:HG12  | 3:R:47:PRO:HA    | 1.72                     | 0.71              |
| 4:D:52:SER:HB3   | 4:D:65:LEU:HB3   | 1.72                     | 0.71              |
| 1:A:165:MET:HE3  | 1:A:166:ARG:H    | 1.56                     | 0.71              |
| 3:I:145:HIS:C    | 3:I:148:GLU:H    | 1.98                     | 0.71              |
| 1:F:20:SER:HA    | 1:F:75:ASN:HA    | 1.72                     | 0.71              |
| 2:L:144:LEU:HD22 | 2:L:189:SER:OG   | 1.91                     | 0.71              |
| 3:I:175:GLY:O    | 3:I:179:LEU:HB2  | 1.91                     | 0.71              |
| 4:D:73:THR:HG23  | 4:D:74:GLU:OE2   | 1.91                     | 0.70              |
| 4:D:88:SER:CB    | 4:D:89:GLN:HA    | 2.20                     | 0.70              |
| 3:R:263:HIS:CE1  | 3:R:265:GLY:N    | 2.60                     | 0.70              |
| 1:G:60:ARG:NH1   | 1:G:83:ASP:OD2   | 2.24                     | 0.70              |
| 2:Q:163:GLU:OE1  | 2:Q:163:GLU:N    | 2.24                     | 0.70              |
| 3:M:201:LEU:HD13 | 3:M:217:TRP:HZ3  | 1.56                     | 0.70              |
| 3:M:263:HIS:H    | 3:M:266:LEU:HB2  | 1.56                     | 0.70              |
| 3:I:62:GLY:O     | 3:I:66:LYS:HD3   | 1.91                     | 0.70              |
| 3:R:180:GLN:N    | 3:R:180:GLN:OE1  | 2.25                     | 0.70              |
| 3:C:6:ARG:HD2    | 3:C:98:MET:HE1   | 1.74                     | 0.70              |
| 1:A:33:LEU:HD13  | 1:A:35:TYR:HE1   | 1.56                     | 0.70              |
| 1:G:59:GLY:HA2   | 1:G:60:ARG:HB3   | 1.74                     | 0.69              |
| 1:G:59:GLY:HA3   | 1:G:61:LEU:CA    | 2.22                     | 0.69              |
| 2:Q:115:LEU:H    | 2:Q:115:LEU:HD12 | 1.57                     | 0.69              |
| 1:A:36:LYS:HE3   | 1:A:87:TYR:CE2   | 2.28                     | 0.69              |
| 1:P:86:ILE:HG22  | 1:P:108:THR:HG22 | 1.73                     | 0.69              |
| 2:L:144:LEU:CD2  | 2:L:189:SER:OG   | 2.40                     | 0.69              |
| 3:M:120:GLY:HA2  | 4:N:60:TRP:HD1   | 1.57                     | 0.69              |
| 3:R:6:ARG:HD3    | 3:R:100:GLY:HA3  | 1.73                     | 0.69              |
| 4:J:41:LYS:HG2   | 4:J:42:ASN:N     | 2.07                     | 0.69              |
| 1:G:9:GLN:HB3    | 2:L:198:PHE:HZ   | 1.58                     | 0.69              |
| 1:F:30:ASN:ND2   | 3:M:154:GLU:HB3  | 2.08                     | 0.69              |
| 2:L:87:SER:HB3   | 2:L:89:TYR:HE1   | 1.57                     | 0.69              |
| 4:N:29:GLY:HA2   | 4:N:61:SER:OG    | 1.93                     | 0.69              |
| 2:H:221:TRP:NE1  | 2:H:223:GLN:O    | 2.26                     | 0.68              |
| 3:I:155:GLN:C    | 3:I:157:ARG:N    | 2.46                     | 0.68              |
| 3:C:81:LEU:HA    | 3:C:84:TYR:HD2   | 1.59                     | 0.68              |
| 4:D:41:LYS:O     | 4:D:41:LYS:HG2   | 1.91                     | 0.68              |
| 3:C:37:ASP:OD2   | 3:C:40:ALA:HB2   | 1.94                     | 0.68              |
| 2:H:215:LEU:O    | 2:H:229:VAL:HA   | 1.94                     | 0.68              |
| 3:I:51:TRP:CE2   | 3:I:179:LEU:HD11 | 2.28                     | 0.68              |
| 4:J:35:ILE:HB    | 4:J:84:HIS:HD2   | 1.59                     | 0.68              |
| 1:F:126:ARG:HH11 | 1:F:127:ASP:H    | 1.39                     | 0.68              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 4:D:88:SER:HB3   | 4:D:89:GLN:HA   | 1.74                     | 0.68              |
| 4:N:27:VAL:N     | 4:N:64:LEU:O    | 2.27                     | 0.68              |
| 4:N:84:HIS:HD2   | 4:N:86:THR:CB   | 1.97                     | 0.68              |
| 2:B:36:ARG:HB2   | 2:B:46:ILE:HD11 | 1.74                     | 0.68              |
| 4:D:87:LEU:HD12  | 4:D:87:LEU:O    | 1.94                     | 0.68              |
| 2:H:98:PRO:HD2   | 3:I:152:VAL:HA  | 1.75                     | 0.67              |
| 3:I:155:GLN:C    | 3:I:157:ARG:H   | 2.03                     | 0.67              |
| 3:M:187:THR:HG22 | 3:M:205:ALA:HA  | 1.76                     | 0.67              |
| 1:P:47:ILE:HG13  | 1:P:57:SER:OG   | 1.94                     | 0.67              |
| 2:H:221:TRP:CG   | 2:H:227:LYS:HG2 | 2.30                     | 0.67              |
| 2:Q:137:GLN:O    | 2:Q:196:ALA:HB2 | 1.95                     | 0.67              |
| 3:R:228:THR:OG1  | 3:R:247:VAL:HB  | 1.94                     | 0.67              |
| 4:U:58:LYS:CA    | 4:U:60:TRP:H    | 2.01                     | 0.67              |
| 4:J:41:LYS:HG3   | 4:J:78:TYR:CD1  | 2.27                     | 0.67              |
| 2:B:88:LEU:HD22  | 2:B:108:ARG:HA  | 1.77                     | 0.67              |
| 2:B:100:GLU:HB3  | 2:B:102:PHE:CE1 | 2.29                     | 0.67              |
| 4:D:74:GLU:H     | 4:D:74:GLU:CD   | 1.92                     | 0.67              |
| 3:R:177:GLU:HA   | 3:R:180:GLN:HB2 | 1.77                     | 0.67              |
| 2:B:86:THR:HG23  | 2:B:110:THR:HA  | 1.76                     | 0.67              |
| 2:H:214:GLY:CA   | 2:H:229:VAL:O   | 2.43                     | 0.67              |
| 4:U:38:ASP:OD2   | 4:U:45:ARG:NH2  | 2.28                     | 0.67              |
| 4:J:41:LYS:O     | 4:J:42:ASN:C    | 2.35                     | 0.66              |
| 2:B:145:ALA:CB   | 2:B:148:PHE:CZ  | 2.67                     | 0.66              |
| 2:H:195:SER:HB2  | 2:H:198:PHE:HB2 | 1.78                     | 0.66              |
| 3:M:120:GLY:HA3  | 4:N:31:HIS:NE2  | 2.10                     | 0.66              |
| 1:F:177:ALA:HB3  | 1:F:190:PHE:CE1 | 2.31                     | 0.66              |
| 2:Q:164:VAL:HG12 | 2:Q:166:SER:H   | 1.61                     | 0.66              |
| 3:R:8:PHE:HB2    | 3:R:25:VAL:HG22 | 1.77                     | 0.66              |
| 4:J:39:LEU:HD23  | 4:J:49:VAL:HG11 | 1.77                     | 0.66              |
| 3:C:234:ARG:HD2  | 4:D:8:GLN:NE2   | 2.11                     | 0.66              |
| 4:D:46:ILE:HG12  | 4:D:47:GLU:N    | 2.10                     | 0.66              |
| 2:L:38:ASP:OD1   | 2:L:87:SER:OG   | 2.12                     | 0.66              |
| 3:I:127:LYS:HD2  | 3:I:128:GLU:H   | 1.61                     | 0.66              |
| 1:A:60:ARG:HB2   | 1:A:77:SER:OG   | 1.96                     | 0.66              |
| 4:D:7:ILE:HD13   | 4:D:27:VAL:HG22 | 1.77                     | 0.66              |
| 4:D:83:ASN:ND2   | 4:D:90:PRO:HD3  | 2.10                     | 0.66              |
| 2:L:229:VAL:O    | 2:L:230:THR:C   | 2.38                     | 0.66              |
| 2:L:229:VAL:O    | 2:L:231:GLN:HB2 | 1.95                     | 0.66              |
| 1:P:47:ILE:HG21  | 1:P:57:SER:HB3  | 1.77                     | 0.66              |
| 1:G:60:ARG:CZ    | 1:G:83:ASP:OD2  | 2.44                     | 0.66              |
| 4:D:83:ASN:CB    | 4:D:90:PRO:HB3  | 2.24                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:177:ALA:HB3  | 1:F:190:PHE:HE1  | 1.60                     | 0.66              |
| 3:R:98:MET:HE2   | 4:U:58:LYS:HZ1   | 1.60                     | 0.66              |
| 4:J:4:THR:OG1    | 4:J:5:PRO:HD2    | 1.96                     | 0.66              |
| 3:R:107:TRP:O    | 3:R:169:ARG:NH1  | 2.29                     | 0.66              |
| 4:D:81:ARG:HA    | 4:D:92:ILE:HG22  | 1.77                     | 0.65              |
| 2:H:214:GLY:HA3  | 2:H:229:VAL:O    | 1.96                     | 0.65              |
| 3:M:148:GLU:HA   | 3:M:151:HIS:H    | 1.59                     | 0.65              |
| 3:M:215:LEU:CB   | 3:M:261:VAL:HG12 | 2.25                     | 0.65              |
| 3:R:263:HIS:ND1  | 3:R:264:GLU:N    | 2.44                     | 0.65              |
| 3:I:151:HIS:O    | 3:I:154:GLU:N    | 2.30                     | 0.65              |
| 3:R:98:MET:HE2   | 4:U:58:LYS:NZ    | 2.11                     | 0.65              |
| 3:I:7:TYR:CD2    | 5:K:2:ILE:HD12   | 2.31                     | 0.65              |
| 3:R:189:MET:SD   | 3:R:273:ARG:HD2  | 2.37                     | 0.65              |
| 3:M:188:HIS:CG   | 3:M:189:MET:H    | 2.15                     | 0.65              |
| 2:L:94:SER:HB2   | 2:L:100:GLU:O    | 1.96                     | 0.65              |
| 2:L:157:TRP:O    | 2:L:163:GLU:HB2  | 1.97                     | 0.65              |
| 3:M:254:GLU:HG3  | 3:M:255:GLN:HG3  | 1.79                     | 0.65              |
| 2:B:145:ALA:HB1  | 2:B:148:PHE:CE2  | 2.29                     | 0.65              |
| 2:L:25:GLN:NE2   | 2:L:27:MET:CG    | 2.60                     | 0.65              |
| 3:R:217:TRP:HD1  | 3:R:258:THR:HA   | 1.62                     | 0.65              |
| 1:G:50:TYR:CE1   | 3:I:151:HIS:CD2  | 2.85                     | 0.65              |
| 3:I:6:ARG:NH1    | 3:I:7:TYR:H      | 1.95                     | 0.65              |
| 3:C:258:THR:HG22 | 3:C:273:ARG:HD2  | 1.78                     | 0.64              |
| 3:C:236:ALA:HB1  | 4:D:12:ARG:HG2   | 1.78                     | 0.64              |
| 3:M:262:GLN:HB2  | 3:M:269:PRO:HB3  | 1.78                     | 0.64              |
| 2:H:227:LYS:O    | 2:H:229:VAL:HG13 | 1.97                     | 0.64              |
| 3:I:63:GLU:CA    | 3:I:66:LYS:HZ2   | 2.02                     | 0.64              |
| 3:I:169:ARG:CZ   | 3:I:173:GLU:HA   | 2.28                     | 0.64              |
| 1:P:158:THR:HG21 | 1:P:176:VAL:H    | 1.62                     | 0.64              |
| 1:F:163:LEU:HB3  | 2:L:169:CYS:HB2  | 1.79                     | 0.64              |
| 2:Q:120:PRO:HD3  | 2:Q:228:PRO:HB3  | 1.78                     | 0.64              |
| 3:I:213:ILE:CD1  | 3:I:263:HIS:CD2  | 2.80                     | 0.64              |
| 2:L:96:ILE:HD11  | 3:M:146:LYS:CE   | 2.17                     | 0.64              |
| 3:M:185:PRO:HB3  | 3:M:208:PHE:HB3  | 1.79                     | 0.64              |
| 4:N:88:SER:HG    | 4:N:89:GLN:H     | 1.43                     | 0.64              |
| 3:C:33:PHE:CD2   | 3:C:51:TRP:HZ2   | 2.16                     | 0.64              |
| 2:Q:158:TRP:HB2  | 2:Q:207:ARG:HB3  | 1.80                     | 0.64              |
| 1:G:163:LEU:HB3  | 2:H:169:CYS:HB3  | 1.79                     | 0.64              |
| 2:H:204:ASN:OD1  | 2:H:204:ASN:N    | 2.31                     | 0.64              |
| 3:I:186:LYS:HB2  | 3:I:206:LEU:HD22 | 1.78                     | 0.64              |
| 2:B:222:THR:HB   | 2:B:223:GLN:CB   | 2.28                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:R:163:THR:HG22 | 3:R:167:TRP:NE1  | 2.13                     | 0.64              |
| 1:A:158:THR:CG2  | 1:A:159:ASP:N    | 2.59                     | 0.63              |
| 2:L:1:GLU:OE1    | 2:L:1:GLU:N      | 2.28                     | 0.63              |
| 1:P:51:LYS:HE2   | 3:R:131:ARG:HE   | 1.63                     | 0.63              |
| 3:I:142:THR:O    | 3:I:143:THR:C    | 2.40                     | 0.63              |
| 1:A:9:GLN:HE21   | 1:A:105:GLN:HE22 | 1.45                     | 0.63              |
| 3:R:72:GLN:N     | 3:R:72:GLN:OE1   | 2.30                     | 0.63              |
| 3:R:159:TYR:OH   | 5:T:1:GLY:O      | 2.17                     | 0.63              |
| 3:M:14:ARG:HD3   | 3:M:21:ARG:HH12  | 1.63                     | 0.63              |
| 3:M:198:GLU:O    | 3:M:251:SER:HB3  | 1.99                     | 0.63              |
| 1:G:59:GLY:HA3   | 1:G:61:LEU:H     | 0.49                     | 0.63              |
| 1:G:80:ILE:HG22  | 1:G:82:SER:H     | 1.63                     | 0.63              |
| 4:J:88:SER:OG    | 4:J:89:GLN:NE2   | 2.31                     | 0.63              |
| 4:D:87:LEU:HD12  | 4:D:87:LEU:C     | 2.23                     | 0.63              |
| 3:M:155:GLN:HE21 | 3:M:155:GLN:HA   | 1.64                     | 0.63              |
| 4:N:30:PHE:CE2   | 4:N:84:HIS:CE1   | 2.86                     | 0.63              |
| 4:D:86:THR:HG22  | 4:D:87:LEU:H     | 1.64                     | 0.63              |
| 3:M:32:GLN:HG2   | 3:M:35:ARG:HH11  | 1.63                     | 0.63              |
| 2:L:36:ARG:NH1   | 2:L:38:ASP:OD2   | 2.31                     | 0.63              |
| 3:C:236:ALA:O    | 4:D:12:ARG:NE    | 2.32                     | 0.63              |
| 1:F:60:ARG:HB2   | 1:F:77:SER:O     | 1.98                     | 0.63              |
| 2:L:221:TRP:CG   | 2:L:227:LYS:HG2  | 2.34                     | 0.63              |
| 1:G:57:SER:C     | 1:G:59:GLY:N     | 2.52                     | 0.62              |
| 3:M:77:ASP:HB3   | 5:O:9:LEU:HD12   | 1.81                     | 0.62              |
| 2:H:86:THR:HG23  | 2:H:110:THR:HA   | 1.80                     | 0.62              |
| 4:J:46:ILE:HD12  | 4:J:70:PHE:HZ    | 1.61                     | 0.62              |
| 1:F:162:VAL:HG12 | 1:F:173:ASN:HA   | 1.80                     | 0.62              |
| 1:P:158:THR:OG1  | 1:P:159:ASP:N    | 2.30                     | 0.62              |
| 2:Q:13:THR:HB    | 2:Q:111:VAL:HG12 | 1.81                     | 0.62              |
| 1:P:158:THR:CG2  | 1:P:176:VAL:H    | 2.11                     | 0.62              |
| 2:Q:207:ARG:NH2  | 2:Q:209:GLN:OE1  | 2.31                     | 0.62              |
| 4:U:83:ASN:CB    | 4:U:90:PRO:HB3   | 2.07                     | 0.62              |
| 1:F:52:ALA:HB1   | 1:F:67:ILE:HG22  | 1.81                     | 0.62              |
| 3:R:93:HIS:ND1   | 3:R:119:ASP:OD1  | 2.23                     | 0.62              |
| 2:H:20:THR:HG22  | 2:H:77:ILE:HG12  | 1.80                     | 0.62              |
| 2:H:228:PRO:O    | 2:H:229:VAL:CG2  | 2.47                     | 0.62              |
| 1:A:60:ARG:NE    | 1:A:78:ALA:O     | 2.31                     | 0.62              |
| 3:M:54:GLN:NE2   | 3:M:174:ASN:OD1  | 2.33                     | 0.62              |
| 1:A:36:LYS:HD2   | 1:A:87:TYR:CE1   | 2.33                     | 0.62              |
| 2:Q:51:ASN:O     | 2:Q:68:ARG:NH1   | 2.28                     | 0.62              |
| 2:H:96:ILE:HG22  | 3:I:152:VAL:CG1  | 2.24                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:47:ILE:HG23  | 1:A:55:LEU:HD11  | 1.81                     | 0.62              |
| 4:D:54:LEU:HD11  | 4:D:62:PHE:HD1   | 1.65                     | 0.62              |
| 2:L:27:MET:HB3   | 2:L:29:HIS:NE2   | 2.14                     | 0.62              |
| 4:N:70:PHE:CE2   | 4:N:71:THR:O     | 2.53                     | 0.62              |
| 4:N:86:THR:HG23  | 4:N:87:LEU:N     | 2.14                     | 0.62              |
| 4:J:6:LYS:HD2    | 4:J:7:ILE:H      | 1.64                     | 0.62              |
| 2:B:100:GLU:HB3  | 2:B:102:PHE:HE1  | 1.64                     | 0.62              |
| 3:C:34:VAL:HG11  | 3:C:45:MET:HE3   | 1.82                     | 0.62              |
| 1:F:147:VAL:O    | 1:F:160:LYS:NZ   | 2.32                     | 0.62              |
| 1:P:47:ILE:CG2   | 1:P:57:SER:HB3   | 2.30                     | 0.62              |
| 1:A:100:LYS:NZ   | 2:B:59:ASP:OD1   | 2.27                     | 0.61              |
| 1:A:198:ASP:OD1  | 1:A:199:THR:N    | 2.33                     | 0.61              |
| 1:F:6:GLN:O      | 1:F:105:GLN:NE2  | 2.33                     | 0.61              |
| 1:F:33:LEU:N     | 1:F:90:ALA:O     | 2.32                     | 0.61              |
| 3:M:65:ARG:HG3   | 3:M:65:ARG:NH1   | 2.09                     | 0.61              |
| 4:U:28:SER:HA    | 4:U:30:PHE:HD1   | 1.63                     | 0.61              |
| 4:D:35:ILE:HD13  | 4:D:64:LEU:HD12  | 1.81                     | 0.61              |
| 2:Q:46:ILE:HG22  | 2:Q:47:TYR:HD1   | 1.65                     | 0.61              |
| 3:R:163:THR:HG22 | 3:R:167:TRP:CD1  | 2.35                     | 0.61              |
| 3:C:242:GLN:OE1  | 4:D:10:TYR:HE1   | 1.82                     | 0.61              |
| 2:Q:3:GLN:HG2    | 2:Q:4:VAL:H      | 1.64                     | 0.61              |
| 2:Q:137:GLN:O    | 2:Q:196:ALA:CB   | 2.48                     | 0.61              |
| 3:C:35:ARG:HG2   | 3:C:35:ARG:NH1   | 2.15                     | 0.61              |
| 3:I:68:LYS:HG3   | 3:I:69:ALA:N     | 2.15                     | 0.61              |
| 1:F:43:PRO:HD2   | 2:L:103:PHE:CG   | 2.36                     | 0.61              |
| 3:R:47:PRO:HB3   | 3:R:60:TRP:CH2   | 2.36                     | 0.61              |
| 4:U:23:LEU:HD21  | 4:U:39:LEU:HD22  | 1.82                     | 0.61              |
| 3:I:98:MET:HE3   | 3:I:115:GLN:HB3  | 1.82                     | 0.61              |
| 3:I:129:ASP:OD1  | 3:I:131:ARG:HG2  | 2.00                     | 0.61              |
| 2:L:168:VAL:HG12 | 2:L:192:LEU:HD13 | 1.81                     | 0.61              |
| 2:Q:52:VAL:HG12  | 2:Q:53:GLU:HG2   | 1.83                     | 0.61              |
| 2:B:22:THR:HG22  | 2:B:75:PRO:HB3   | 1.83                     | 0.61              |
| 2:Q:170:THR:HG22 | 2:Q:190:SER:HB2  | 1.83                     | 0.61              |
| 3:I:49:ALA:O     | 3:I:52:ILE:HG22  | 2.01                     | 0.61              |
| 3:I:229:GLU:HB2  | 3:I:246:ALA:HB3  | 1.83                     | 0.61              |
| 2:B:158:TRP:HB2  | 2:B:207:ARG:HB3  | 1.83                     | 0.61              |
| 1:P:33:LEU:HD23  | 1:P:45:LEU:HD13  | 1.82                     | 0.61              |
| 4:U:23:LEU:HD22  | 4:U:41:LYS:NZ    | 2.15                     | 0.61              |
| 1:G:71:ASP:OD1   | 1:G:71:ASP:N     | 2.33                     | 0.61              |
| 3:I:45:MET:HB3   | 3:I:60:TRP:HE3   | 1.66                     | 0.61              |
| 4:J:46:ILE:HG22  | 4:J:47:GLU:N     | 2.16                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:101:LEU:HD22 | 2:L:101:LEU:HD11 | 1.81                     | 0.61              |
| 4:J:45:ARG:H     | 4:J:45:ARG:CD    | 2.06                     | 0.60              |
| 3:I:182:THR:HB   | 3:I:265:GLY:HA2  | 1.82                     | 0.60              |
| 4:D:76:ASP:CB    | 4:D:78:TYR:CE2   | 2.72                     | 0.60              |
| 3:I:66:LYS:HE2   | 5:K:2:ILE:HG22   | 1.83                     | 0.60              |
| 2:B:47:TYR:HE1   | 2:B:61:PRO:HA    | 1.66                     | 0.60              |
| 3:C:170:ARG:HG2  | 3:C:173:GLU:CD   | 2.26                     | 0.60              |
| 2:L:20:THR:HA    | 2:L:77:ILE:CG2   | 2.29                     | 0.60              |
| 1:P:124:GLN:HA   | 1:P:136:CYS:HB3  | 1.84                     | 0.60              |
| 3:I:176:LYS:HG3  | 3:I:177:GLU:HG2  | 1.84                     | 0.60              |
| 4:U:46:ILE:HD11  | 4:U:49:VAL:HG13  | 1.83                     | 0.60              |
| 3:I:244:TRP:HZ3  | 3:I:246:ALA:HB2  | 1.65                     | 0.60              |
| 3:R:263:HIS:CG   | 3:R:265:GLY:H    | 2.16                     | 0.60              |
| 2:H:221:TRP:HB2  | 2:H:227:LYS:HD3  | 1.83                     | 0.60              |
| 4:U:41:LYS:HD2   | 4:U:78:TYR:HD1   | 1.67                     | 0.60              |
| 3:I:218:GLN:CG   | 3:I:219:ARG:N    | 2.51                     | 0.60              |
| 3:I:263:HIS:ND1  | 3:I:264:GLU:N    | 2.49                     | 0.60              |
| 2:L:152:HIS:HB3  | 2:L:213:TYR:HB2  | 1.82                     | 0.60              |
| 3:M:217:TRP:HE1  | 3:M:259:CYS:HA   | 1.65                     | 0.60              |
| 3:M:236:ALA:O    | 3:M:240:THR:OG1  | 2.12                     | 0.60              |
| 3:R:163:THR:O    | 3:R:167:TRP:CD1  | 2.53                     | 0.60              |
| 3:C:28:VAL:HB    | 3:C:33:PHE:HE1   | 1.66                     | 0.59              |
| 3:C:69:ALA:O     | 3:C:73:THR:N     | 2.28                     | 0.59              |
| 1:G:60:ARG:HH22  | 1:G:80:ILE:HB    | 1.68                     | 0.59              |
| 1:G:68:THR:HG22  | 1:A:20:SER:HB2   | 1.85                     | 0.59              |
| 2:B:96:ILE:CD1   | 3:C:146:LYS:HE2  | 2.20                     | 0.59              |
| 2:B:149:TYR:CD2  | 2:B:150:PRO:CA   | 2.85                     | 0.59              |
| 3:C:206:LEU:HB2  | 3:C:242:GLN:HG2  | 1.83                     | 0.59              |
| 3:I:82:ARG:HA    | 3:I:85:TYR:HB2   | 1.84                     | 0.59              |
| 4:J:54:LEU:HD12  | 4:J:64:LEU:HD21  | 1.83                     | 0.59              |
| 1:F:196:PRO:O    | 1:F:198:ASP:OD1  | 2.20                     | 0.59              |
| 3:R:159:TYR:HD2  | 3:R:160:LEU:HD12 | 1.68                     | 0.59              |
| 4:U:75:LYS:HB2   | 4:U:75:LYS:NZ    | 2.17                     | 0.59              |
| 3:I:172:LEU:HD23 | 3:I:179:LEU:HD23 | 1.85                     | 0.59              |
| 1:F:122:VAL:HG22 | 1:F:138:PHE:HB2  | 1.84                     | 0.59              |
| 1:G:42:GLY:HA2   | 2:H:90:PHE:CE2   | 2.37                     | 0.59              |
| 2:L:112:LEU:HD11 | 2:L:149:TYR:CE2  | 2.37                     | 0.59              |
| 3:I:141:GLN:NE2  | 3:I:144:LYS:HE3  | 2.17                     | 0.59              |
| 3:I:155:GLN:O    | 3:I:156:LEU:C    | 2.46                     | 0.59              |
| 3:M:206:LEU:CA   | 3:M:242:GLN:HE22 | 2.16                     | 0.59              |
| 2:H:29:HIS:CB    | 2:H:32:MET:HE1   | 2.33                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:J:52:SER:HB3   | 4:J:65:LEU:H     | 1.68                     | 0.59              |
| 3:C:69:ALA:O     | 3:C:72:GLN:N     | 2.36                     | 0.58              |
| 1:F:125:LEU:HD22 | 2:L:128:PRO:HA   | 1.84                     | 0.58              |
| 1:P:125:LEU:HD21 | 2:Q:128:PRO:HA   | 1.84                     | 0.58              |
| 4:U:52:SER:HB3   | 4:U:65:LEU:H     | 1.68                     | 0.58              |
| 1:G:50:TYR:CZ    | 3:I:151:HIS:CE1  | 2.91                     | 0.58              |
| 2:B:7:ASN:HD22   | 2:B:22:THR:HG1   | 1.44                     | 0.58              |
| 2:B:149:TYR:CD2  | 2:B:150:PRO:CB   | 2.85                     | 0.58              |
| 3:M:23:ILE:HD12  | 4:N:54:LEU:HD22  | 1.84                     | 0.58              |
| 3:I:61:ASP:O     | 3:I:65:ARG:HG3   | 2.03                     | 0.58              |
| 4:J:54:LEU:HA    | 4:J:64:LEU:HD21  | 1.84                     | 0.58              |
| 1:F:121:ALA:HA   | 1:F:198:ASP:HB3  | 1.84                     | 0.58              |
| 3:M:5:MET:HB2    | 3:M:168:LEU:HD13 | 1.84                     | 0.58              |
| 3:C:173:GLU:CG   | 3:C:174:ASN:N    | 2.61                     | 0.58              |
| 3:M:74:HIS:HA    | 3:M:77:ASP:HB2   | 1.85                     | 0.58              |
| 1:P:60:ARG:NH1   | 1:P:78:ALA:O     | 2.31                     | 0.58              |
| 4:U:23:LEU:N     | 4:U:68:THR:O     | 2.30                     | 0.58              |
| 2:L:25:GLN:HG2   | 2:L:27:MET:HG2   | 1.85                     | 0.58              |
| 1:P:31:THR:HG22  | 1:P:50:TYR:HD1   | 1.69                     | 0.58              |
| 4:J:39:LEU:CD2   | 4:J:49:VAL:HG11  | 2.34                     | 0.58              |
| 2:L:71:LYS:HD3   | 2:L:71:LYS:N     | 2.19                     | 0.58              |
| 3:M:259:CYS:CB   | 3:M:272:LEU:HB2  | 2.33                     | 0.58              |
| 4:U:7:ILE:HD12   | 4:U:27:VAL:HG12  | 1.85                     | 0.58              |
| 1:G:28:ILE:HD11  | 1:G:69:ARG:CZ    | 2.35                     | 0.57              |
| 3:C:173:GLU:CG   | 3:C:174:ASN:H    | 2.14                     | 0.57              |
| 1:G:33:LEU:O     | 1:G:90:ALA:N     | 2.35                     | 0.57              |
| 2:H:98:PRO:N     | 3:I:152:VAL:HG12 | 2.17                     | 0.57              |
| 3:I:85:TYR:HB3   | 3:I:87:GLN:CG    | 2.35                     | 0.57              |
| 4:J:78:TYR:CD2   | 4:J:78:TYR:N     | 2.73                     | 0.57              |
| 4:U:7:ILE:HG13   | 4:U:82:VAL:HG21  | 1.86                     | 0.57              |
| 3:I:133:TRP:HZ2  | 3:I:153:ALA:HB1  | 1.59                     | 0.57              |
| 2:B:149:TYR:HD2  | 2:B:150:PRO:N    | 2.00                     | 0.57              |
| 2:L:27:MET:O     | 2:L:28:ASN:HB2   | 2.03                     | 0.57              |
| 2:L:145:ALA:HB1  | 2:L:148:PHE:CE2  | 2.39                     | 0.57              |
| 3:R:102:ASP:N    | 3:R:111:ARG:O    | 2.29                     | 0.57              |
| 3:R:266:LEU:HD12 | 3:R:267:PRO:HD2  | 1.86                     | 0.57              |
| 3:C:59:TYR:O     | 3:C:63:GLU:N     | 2.35                     | 0.57              |
| 4:D:46:ILE:HG23  | 4:D:47:GLU:O     | 2.04                     | 0.57              |
| 1:F:30:ASN:HD22  | 3:M:154:GLU:HB3  | 1.67                     | 0.57              |
| 2:L:178:GLN:OE1  | 2:L:178:GLN:HA   | 2.05                     | 0.57              |
| 4:N:85:VAL:HG12  | 4:N:85:VAL:O     | 2.04                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:I:171:TYR:OH   | 5:K:1:GLY:N      | 2.32                     | 0.57              |
| 1:A:9:GLN:NE2    | 1:A:105:GLN:HE22 | 2.03                     | 0.57              |
| 1:A:180:ASN:HD22 | 1:A:180:ASN:C    | 2.11                     | 0.57              |
| 2:L:150:PRO:HD2  | 2:L:152:HIS:HD2  | 1.69                     | 0.57              |
| 3:R:27:TYR:CE1   | 3:R:32:GLN:HG2   | 2.39                     | 0.57              |
| 3:R:98:MET:HG3   | 4:U:58:LYS:HZ1   | 1.69                     | 0.57              |
| 4:J:37:VAL:HG13  | 4:J:82:VAL:HG22  | 1.87                     | 0.57              |
| 4:U:21:ASN:OD1   | 4:U:22:PHE:N     | 2.37                     | 0.57              |
| 2:H:47:TYR:HE1   | 2:H:61:PRO:CA    | 2.14                     | 0.56              |
| 2:Q:38:ASP:OD1   | 2:Q:87:SER:OG    | 2.23                     | 0.56              |
| 3:R:32:GLN:OE1   | 3:R:35:ARG:NH2   | 2.38                     | 0.56              |
| 2:H:97:TYR:C     | 3:I:152:VAL:CG1  | 2.61                     | 0.56              |
| 3:I:17:ARG:HB3   | 3:I:18:GLY:HA2   | 1.87                     | 0.56              |
| 3:I:28:VAL:O     | 3:I:31:THR:OG1   | 2.21                     | 0.56              |
| 3:I:137:ASP:OD1  | 3:I:137:ASP:N    | 2.38                     | 0.56              |
| 2:B:10:TYR:CD1   | 2:B:108:ARG:HB2  | 2.41                     | 0.56              |
| 2:B:149:TYR:CD2  | 2:B:150:PRO:N    | 2.73                     | 0.56              |
| 1:F:135:VAL:HG11 | 2:L:126:PHE:CD1  | 2.40                     | 0.56              |
| 2:L:86:THR:HG23  | 2:L:110:THR:HA   | 1.87                     | 0.56              |
| 3:M:144:LYS:O    | 3:M:147:TRP:N    | 2.38                     | 0.56              |
| 2:H:151:ASP:O    | 2:H:152:HIS:ND1  | 2.38                     | 0.56              |
| 3:I:58:GLU:OE1   | 3:I:58:GLU:N     | 2.32                     | 0.56              |
| 4:J:24:ASN:HB3   | 4:J:65:LEU:HD11  | 1.86                     | 0.56              |
| 4:D:24:ASN:OD1   | 4:D:24:ASN:N     | 2.39                     | 0.56              |
| 3:I:25:VAL:HG11  | 3:I:32:GLN:HE21  | 1.71                     | 0.56              |
| 1:A:184:PHE:CD1  | 1:A:184:PHE:N    | 2.72                     | 0.56              |
| 3:C:60:TRP:O     | 3:C:64:THR:HG23  | 2.05                     | 0.56              |
| 1:G:59:GLY:HA2   | 1:G:60:ARG:CB    | 2.33                     | 0.56              |
| 3:I:169:ARG:NH2  | 3:I:173:GLU:HA   | 2.21                     | 0.56              |
| 2:B:57:LYS:HE2   | 2:B:61:PRO:HB2   | 1.87                     | 0.56              |
| 4:D:38:ASP:OD2   | 4:D:45:ARG:NH1   | 2.39                     | 0.56              |
| 1:F:74:LEU:HD13  | 1:F:74:LEU:O     | 2.04                     | 0.56              |
| 3:M:56:GLY:N     | 3:M:58:GLU:HG2   | 2.20                     | 0.56              |
| 1:G:25:SER:OG    | 1:G:26:SER:N     | 2.38                     | 0.56              |
| 1:P:47:ILE:CG2   | 1:P:57:SER:CB    | 2.83                     | 0.56              |
| 4:U:13:HIS:HB3   | 4:U:14:PRO:HD2   | 1.86                     | 0.56              |
| 2:H:176:LYS:HE2  | 2:H:182:ASN:H    | 1.71                     | 0.56              |
| 4:J:57:SER:OG    | 4:J:58:LYS:N     | 2.36                     | 0.56              |
| 4:U:65:LEU:HD12  | 4:U:66:TYR:N     | 2.21                     | 0.56              |
| 1:G:19:VAL:HG13  | 1:G:76:ILE:HB    | 1.88                     | 0.56              |
| 3:I:81:LEU:HB3   | 3:I:85:TYR:HE2   | 1.71                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:148:SER:H    | 1:A:193:SER:HB3  | 1.69                     | 0.56              |
| 2:B:89:TYR:O     | 2:B:107:SER:OG   | 2.24                     | 0.56              |
| 2:L:140:THR:HG23 | 2:L:193:ARG:HB2  | 1.88                     | 0.56              |
| 4:N:70:PHE:CZ    | 4:N:71:THR:O     | 2.57                     | 0.56              |
| 4:U:23:LEU:HD22  | 4:U:41:LYS:HZ3   | 1.71                     | 0.56              |
| 3:I:106:ASP:O    | 3:I:107:TRP:HB2  | 2.05                     | 0.55              |
| 1:A:88:PHE:HA    | 1:A:106:GLY:HA2  | 1.87                     | 0.55              |
| 2:B:88:LEU:HD22  | 2:B:108:ARG:HG3  | 1.89                     | 0.55              |
| 2:B:125:VAL:HG23 | 2:B:235:ALA:HB3  | 1.88                     | 0.55              |
| 2:B:145:ALA:CB   | 2:B:148:PHE:CE2  | 2.89                     | 0.55              |
| 1:G:31:THR:OG1   | 3:I:155:GLN:NE2  | 2.38                     | 0.55              |
| 2:H:221:TRP:NE1  | 2:H:225:ARG:O    | 2.38                     | 0.55              |
| 3:M:31:THR:OG1   | 3:M:209:TYR:OH   | 2.24                     | 0.55              |
| 2:Q:136:THR:OG1  | 2:Q:137:GLN:OE1  | 2.24                     | 0.55              |
| 3:M:234:ARG:N    | 3:M:242:GLN:O    | 2.38                     | 0.55              |
| 3:R:163:THR:HG22 | 3:R:167:TRP:HE1  | 1.70                     | 0.55              |
| 3:I:217:TRP:NE1  | 3:I:259:CYS:HB3  | 2.22                     | 0.55              |
| 3:M:117:ALA:HA   | 3:M:123:TYR:HB3  | 1.86                     | 0.55              |
| 1:G:163:LEU:HD11 | 2:H:193:ARG:HD3  | 1.89                     | 0.55              |
| 3:I:15:PRO:HG2   | 3:I:91:GLY:N     | 2.22                     | 0.55              |
| 3:I:160:LEU:O    | 3:I:164:CYS:HB3  | 2.07                     | 0.55              |
| 4:D:73:THR:HG22  | 4:D:74:GLU:OE2   | 2.07                     | 0.55              |
| 2:L:27:MET:O     | 2:L:29:HIS:HD2   | 1.90                     | 0.55              |
| 2:Q:221:TRP:CZ2  | 2:Q:223:GLN:C    | 2.84                     | 0.55              |
| 3:I:263:HIS:ND1  | 3:I:263:HIS:C    | 2.64                     | 0.55              |
| 1:A:58:ASN:C     | 1:A:58:ASN:HD22  | 2.14                     | 0.55              |
| 2:L:44:ARG:HD2   | 2:L:60:VAL:HG21  | 1.88                     | 0.55              |
| 3:C:213:ILE:HD11 | 3:C:261:VAL:HG13 | 1.88                     | 0.55              |
| 3:M:104:GLY:C    | 3:M:106:ASP:H    | 2.13                     | 0.55              |
| 1:G:154:ASP:CG   | 1:G:181:LYS:O    | 2.50                     | 0.55              |
| 3:I:213:ILE:HD12 | 3:I:263:HIS:HD2  | 1.66                     | 0.55              |
| 2:H:160:ASN:HA   | 2:H:205:HIS:HB2  | 1.88                     | 0.55              |
| 3:I:73:THR:HG23  | 5:K:8:THR:HG22   | 1.89                     | 0.55              |
| 1:A:166:ARG:HG3  | 1:A:168:MET:O    | 2.07                     | 0.55              |
| 2:L:64:TYR:HB3   | 2:L:76:LEU:HD11  | 1.89                     | 0.55              |
| 3:M:188:HIS:CG   | 3:M:189:MET:N    | 2.75                     | 0.54              |
| 1:G:83:ASP:O     | 1:G:87:TYR:OH    | 2.21                     | 0.54              |
| 3:I:104:GLY:C    | 3:I:106:ASP:H    | 2.14                     | 0.54              |
| 3:I:125:ALA:HB3  | 3:I:134:THR:HB   | 1.89                     | 0.54              |
| 2:B:46:ILE:HG22  | 2:B:47:TYR:N     | 2.22                     | 0.54              |
| 3:R:270:LEU:HD22 | 3:R:271:THR:H    | 1.73                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:J:22:PHE:CD1   | 4:J:69:GLU:HA    | 2.42                     | 0.54              |
| 1:F:92:PRO:HG2   | 3:M:155:GLN:OE1  | 2.07                     | 0.54              |
| 1:A:38:GLU:N     | 1:A:38:GLU:OE1   | 2.40                     | 0.54              |
| 4:N:24:ASN:OD1   | 4:N:24:ASN:N     | 2.40                     | 0.54              |
| 1:P:88:PHE:CZ    | 2:Q:43:LEU:HD12  | 2.42                     | 0.54              |
| 2:Q:170:THR:HA   | 2:Q:190:SER:HA   | 1.88                     | 0.54              |
| 3:I:14:ARG:CB    | 3:I:19:GLU:H     | 2.19                     | 0.54              |
| 3:C:12:VAL:HG12  | 3:C:94:THR:HG23  | 1.89                     | 0.54              |
| 3:R:186:LYS:N    | 3:R:206:LEU:O    | 2.36                     | 0.54              |
| 3:R:206:LEU:HD12 | 3:R:207:SER:H    | 1.73                     | 0.54              |
| 4:U:28:SER:HA    | 4:U:30:PHE:CD1   | 2.41                     | 0.54              |
| 1:P:105:GLN:HA   | 2:Q:42:GLY:HA3   | 1.89                     | 0.54              |
| 4:J:5:PRO:HB3    | 4:J:30:PHE:CD2   | 2.43                     | 0.54              |
| 3:C:74:HIS:HA    | 3:C:77:ASP:HB2   | 1.88                     | 0.54              |
| 1:F:11:MET:HG3   | 1:F:109:LEU:HD12 | 1.88                     | 0.54              |
| 3:R:82:ARG:HH21  | 3:R:88:SER:HA    | 1.73                     | 0.54              |
| 1:F:126:ARG:NH1  | 1:F:127:ASP:N    | 2.56                     | 0.54              |
| 1:P:51:LYS:HE2   | 3:R:131:ARG:NE   | 2.23                     | 0.54              |
| 3:I:73:THR:OG1   | 5:K:6:VAL:HG11   | 2.08                     | 0.54              |
| 1:F:129:LYS:HG3  | 1:F:131:SER:N    | 2.18                     | 0.54              |
| 2:L:25:GLN:CG    | 2:L:27:MET:HG2   | 2.37                     | 0.54              |
| 4:U:45:ARG:HG3   | 4:U:46:ILE:N     | 2.21                     | 0.54              |
| 3:C:116:TYR:HB2  | 3:C:124:ILE:HG22 | 1.89                     | 0.53              |
| 2:Q:118:VAL:HG23 | 2:Q:118:VAL:O    | 2.07                     | 0.53              |
| 3:I:151:HIS:O    | 3:I:154:GLU:HB2  | 2.07                     | 0.53              |
| 5:K:2:ILE:HG13   | 5:K:3:LEU:H      | 1.72                     | 0.53              |
| 2:L:18:GLU:HG3   | 2:L:79:GLU:HA    | 1.90                     | 0.53              |
| 2:L:126:PHE:CE2  | 2:L:144:LEU:HD12 | 2.42                     | 0.53              |
| 1:G:34:TRP:CE2   | 1:G:74:LEU:HB2   | 2.44                     | 0.53              |
| 4:D:10:TYR:HB2   | 4:D:24:ASN:O     | 2.08                     | 0.53              |
| 3:R:144:LYS:NZ   | 3:R:148:GLU:OE2  | 2.41                     | 0.53              |
| 3:I:141:GLN:HE22 | 3:I:144:LYS:HE3  | 1.73                     | 0.53              |
| 2:B:21:VAL:O     | 2:B:76:LEU:N     | 2.40                     | 0.53              |
| 3:C:33:PHE:HZ    | 3:C:171:TYR:HB3  | 1.74                     | 0.53              |
| 3:C:49:ALA:CB    | 3:C:51:TRP:CH2   | 2.91                     | 0.53              |
| 1:P:49:LEU:HD21  | 1:P:63:ALA:HB3   | 1.91                     | 0.53              |
| 4:D:56:PHE:CZ    | 4:D:60:TRP:HA    | 2.42                     | 0.53              |
| 2:L:45:GLN:OE1   | 2:L:48:TYR:HB3   | 2.08                     | 0.53              |
| 3:M:65:ARG:HH11  | 3:M:65:ARG:CG    | 2.13                     | 0.53              |
| 3:I:81:LEU:O     | 3:I:84:TYR:N     | 2.42                     | 0.53              |
| 3:I:231:VAL:HG22 | 3:I:232:GLU:O    | 2.09                     | 0.53              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 4:J:11:SER:OG   | 4:J:13:HIS:O     | 2.27                     | 0.53              |
| 2:B:10:TYR:CD1  | 2:B:108:ARG:CB   | 2.92                     | 0.53              |
| 3:C:234:ARG:O   | 4:D:10:TYR:OH    | 2.27                     | 0.53              |
| 3:M:120:GLY:HA2 | 4:N:60:TRP:CD1   | 2.41                     | 0.53              |
| 2:Q:36:ARG:NH2  | 2:Q:84:ASN:O     | 2.23                     | 0.53              |
| 1:G:9:GLN:HB3   | 2:L:198:PHE:CZ   | 2.42                     | 0.53              |
| 1:G:36:LYS:HG2  | 1:G:46:LEU:HG    | 1.90                     | 0.53              |
| 3:I:202:ARG:HB2 | 3:I:204:TRP:CZ3  | 2.43                     | 0.53              |
| 4:J:56:PHE:HA   | 4:J:62:PHE:CD1   | 2.44                     | 0.53              |
| 3:C:42:SER:O    | 3:C:43:GLN:HB3   | 2.08                     | 0.53              |
| 1:P:51:LYS:HE2  | 3:R:131:ARG:HH21 | 1.74                     | 0.53              |
| 3:R:23:ILE:HD11 | 4:U:54:LEU:HD22  | 1.91                     | 0.53              |
| 3:R:117:ALA:HB2 | 4:U:60:TRP:CH2   | 2.44                     | 0.53              |
| 4:U:54:LEU:HD21 | 4:U:62:PHE:CE1   | 2.44                     | 0.53              |
| 3:I:54:GLN:O    | 3:I:55:GLU:C     | 2.50                     | 0.53              |
| 1:A:148:SER:HB2 | 1:A:193:SER:HB3  | 1.91                     | 0.53              |
| 1:F:83:ASP:O    | 1:F:87:TYR:OH    | 2.22                     | 0.53              |
| 3:R:5:MET:HB2   | 3:R:168:LEU:HD13 | 1.90                     | 0.53              |
| 4:U:65:LEU:HD12 | 4:U:66:TYR:H     | 1.74                     | 0.53              |
| 2:H:190:SER:OG  | 2:H:191:ARG:N    | 2.42                     | 0.52              |
| 1:F:49:LEU:HD13 | 1:F:65:PHE:HB2   | 1.92                     | 0.52              |
| 2:Q:131:ALA:O   | 2:Q:134:SER:OG   | 2.19                     | 0.52              |
| 4:U:46:ILE:CD1  | 4:U:49:VAL:HG13  | 2.39                     | 0.52              |
| 4:D:26:TYR:HA   | 4:D:64:LEU:O     | 2.09                     | 0.52              |
| 1:F:177:ALA:HA  | 1:F:178:TRP:CE3  | 2.44                     | 0.52              |
| 3:M:262:GLN:CB  | 3:M:269:PRO:HB3  | 2.38                     | 0.52              |
| 3:I:31:THR:HG23 | 3:I:209:TYR:OH   | 2.09                     | 0.52              |
| 2:Q:95:LEU:HD12 | 2:Q:95:LEU:H     | 1.73                     | 0.52              |
| 3:I:32:GLN:O    | 3:I:49:ALA:HB2   | 2.09                     | 0.52              |
| 3:I:81:LEU:HB3  | 3:I:85:TYR:CE2   | 2.44                     | 0.52              |
| 4:J:41:LYS:HA   | 4:J:78:TYR:HB3   | 1.91                     | 0.52              |
| 3:C:99:TYR:HH   | 5:E:3:LEU:H      | 1.55                     | 0.52              |
| 1:A:133:LYS:HB2 | 2:B:126:PHE:HE1  | 1.74                     | 0.52              |
| 2:L:25:GLN:CD   | 2:L:27:MET:CG    | 2.82                     | 0.52              |
| 2:L:29:HIS:HA   | 2:L:95:LEU:HA    | 1.91                     | 0.52              |
| 2:L:145:ALA:HB1 | 2:L:148:PHE:CZ   | 2.45                     | 0.52              |
| 4:U:48:LYS:HZ3  | 4:U:69:GLU:HB2   | 1.74                     | 0.52              |
| 2:B:10:TYR:HD1  | 2:B:108:ARG:CB   | 2.23                     | 0.52              |
| 1:P:60:ARG:NH1  | 1:P:83:ASP:OD2   | 2.43                     | 0.52              |
| 3:R:214:THR:H   | 3:R:262:GLN:HB2  | 1.75                     | 0.52              |
| 3:I:139:ALA:O   | 3:I:142:THR:CG2  | 2.57                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:K:7:PHE:CD1    | 5:K:7:PHE:C      | 2.88                     | 0.52              |
| 1:F:22:ASN:HB3   | 1:F:73:PHE:CD2   | 2.45                     | 0.52              |
| 4:N:30:PHE:CG    | 4:N:31:HIS:N     | 2.77                     | 0.52              |
| 2:Q:47:TYR:HA    | 2:Q:57:LYS:CB    | 2.39                     | 0.52              |
| 3:R:98:MET:HG3   | 4:U:58:LYS:NZ    | 2.24                     | 0.52              |
| 3:R:217:TRP:CD1  | 3:R:258:THR:HA   | 2.44                     | 0.52              |
| 4:U:37:VAL:HG22  | 4:U:82:VAL:HA    | 1.91                     | 0.52              |
| 1:G:14:GLN:HG2   | 1:G:15:GLU:N     | 2.25                     | 0.52              |
| 2:H:203:ARG:C    | 2:H:204:ASN:OD1  | 2.53                     | 0.52              |
| 2:L:95:LEU:HD12  | 2:L:95:LEU:C     | 2.35                     | 0.52              |
| 2:H:34:TRP:CH2   | 2:H:91:CYS:HB2   | 2.45                     | 0.52              |
| 3:I:123:TYR:CZ   | 3:I:140:ALA:HA   | 2.44                     | 0.52              |
| 4:J:12:ARG:HG3   | 4:J:13:HIS:CE1   | 2.45                     | 0.52              |
| 2:B:20:THR:HA    | 2:B:77:ILE:HG22  | 1.90                     | 0.52              |
| 1:F:57:SER:C     | 1:F:61:LEU:HB2   | 2.33                     | 0.52              |
| 3:I:213:ILE:HG23 | 3:I:263:HIS:HB3  | 1.91                     | 0.52              |
| 1:A:156:TYR:CD1  | 1:A:156:TYR:C    | 2.86                     | 0.52              |
| 2:B:96:ILE:CD1   | 3:C:146:LYS:CE   | 2.81                     | 0.52              |
| 3:C:87:GLN:HG2   | 3:C:93:HIS:CE1   | 2.45                     | 0.52              |
| 2:L:34:TRP:CD1   | 2:L:76:LEU:HB2   | 2.45                     | 0.51              |
| 5:O:2:ILE:HD12   | 5:O:2:ILE:H      | 1.76                     | 0.51              |
| 3:R:256:ARG:HD3  | 3:R:256:ARG:N    | 2.24                     | 0.51              |
| 4:U:9:VAL:HG13   | 4:U:24:ASN:O     | 2.09                     | 0.51              |
| 3:C:33:PHE:CG    | 3:C:51:TRP:HZ2   | 2.29                     | 0.51              |
| 2:L:148:PHE:HE1  | 2:L:153:VAL:HG11 | 1.74                     | 0.51              |
| 3:M:56:GLY:C     | 3:M:58:GLU:HG2   | 2.35                     | 0.51              |
| 4:U:75:LYS:HB2   | 4:U:75:LYS:HZ3   | 1.75                     | 0.51              |
| 2:H:169:CYS:SG   | 2:H:191:ARG:NE   | 2.75                     | 0.51              |
| 1:F:21:MET:HE1   | 1:F:87:TYR:CD2   | 2.45                     | 0.51              |
| 1:F:152:ASP:OD1  | 1:F:153:SER:N    | 2.44                     | 0.51              |
| 3:M:133:TRP:HE1  | 3:M:153:ALA:HB2  | 1.76                     | 0.51              |
| 1:G:24:THR:HA    | 1:G:71:ASP:HB3   | 1.93                     | 0.51              |
| 1:G:50:TYR:OH    | 3:I:151:HIS:CE1  | 2.63                     | 0.51              |
| 2:H:229:VAL:HG23 | 2:H:230:THR:O    | 2.10                     | 0.51              |
| 3:I:12:VAL:O     | 3:I:20:PRO:HA    | 2.10                     | 0.51              |
| 1:A:36:LYS:HG3   | 1:A:87:TYR:HA    | 1.93                     | 0.51              |
| 2:L:27:MET:HB2   | 2:L:29:HIS:CD2   | 2.46                     | 0.51              |
| 3:M:7:TYR:CD1    | 3:M:26:GLY:HA3   | 2.45                     | 0.51              |
| 3:M:76:VAL:O     | 3:M:80:THR:N     | 2.44                     | 0.51              |
| 2:Q:137:GLN:O    | 2:Q:137:GLN:HG3  | 2.10                     | 0.51              |
| 2:Q:173:GLN:OE1  | 2:Q:174:PRO:HD2  | 2.10                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:R:9:PHE:HB2    | 3:R:97:ARG:HB3   | 1.91                     | 0.51              |
| 3:I:263:HIS:CE1  | 3:I:265:GLY:N    | 2.72                     | 0.51              |
| 1:P:80:ILE:HG22  | 1:P:82:SER:H     | 1.75                     | 0.51              |
| 2:Q:20:THR:HG23  | 2:Q:77:ILE:HG22  | 1.91                     | 0.51              |
| 3:I:145:HIS:O    | 3:I:148:GLU:CA   | 2.59                     | 0.51              |
| 1:F:196:PRO:O    | 1:F:196:PRO:HD2  | 2.09                     | 0.51              |
| 1:P:13:ILE:HD13  | 1:P:19:VAL:HG21  | 1.93                     | 0.51              |
| 4:U:24:ASN:OD1   | 4:U:25:CYS:N     | 2.44                     | 0.51              |
| 3:I:81:LEU:O     | 3:I:82:ARG:C     | 2.54                     | 0.51              |
| 3:I:230:LEU:HD12 | 3:I:231:VAL:N    | 2.25                     | 0.51              |
| 3:C:183:ASP:OD1  | 3:C:184:ALA:N    | 2.44                     | 0.51              |
| 3:M:263:HIS:HB3  | 3:M:266:LEU:HG   | 1.93                     | 0.51              |
| 2:Q:14:VAL:HA    | 2:Q:112:LEU:O    | 2.11                     | 0.51              |
| 2:Q:25:GLN:NE2   | 2:Q:29:HIS:O     | 2.38                     | 0.51              |
| 4:J:4:THR:HB     | 4:J:86:THR:CB    | 2.40                     | 0.51              |
| 4:J:5:PRO:HB3    | 4:J:30:PHE:HB3   | 1.93                     | 0.51              |
| 4:J:40:LEU:CD1   | 4:J:45:ARG:HE    | 2.22                     | 0.51              |
| 2:L:7:ASN:H      | 2:L:22:THR:HB    | 1.74                     | 0.51              |
| 3:M:202:ARG:HG3  | 3:M:204:TRP:HE1  | 1.76                     | 0.51              |
| 2:Q:119:PHE:O    | 2:Q:148:PHE:HA   | 2.11                     | 0.51              |
| 3:I:116:TYR:HB2  | 3:I:124:ILE:HG22 | 1.93                     | 0.51              |
| 3:M:68:LYS:HG2   | 3:M:69:ALA:N     | 2.26                     | 0.51              |
| 4:U:28:SER:HB3   | 4:U:63:TYR:CA    | 2.36                     | 0.51              |
| 3:I:6:ARG:NH2    | 3:I:98:MET:HG2   | 2.26                     | 0.51              |
| 1:A:154:ASP:CG   | 1:A:181:LYS:HD3  | 2.35                     | 0.51              |
| 2:B:108:ARG:HH22 | 2:B:150:PRO:CG   | 2.22                     | 0.51              |
| 3:C:122:ASP:OD1  | 4:D:60:TRP:NE1   | 2.43                     | 0.51              |
| 1:F:5:ASN:OD1    | 1:F:6:GLN:N      | 2.44                     | 0.51              |
| 2:L:224:ASP:OD1  | 2:L:224:ASP:N    | 2.35                     | 0.51              |
| 3:R:235:PRO:HG2  | 4:U:65:LEU:HD22  | 1.92                     | 0.51              |
| 4:U:47:GLU:HG2   | 4:U:48:LYS:H     | 1.76                     | 0.51              |
| 2:H:38:ASP:N     | 2:H:38:ASP:OD1   | 2.44                     | 0.50              |
| 2:B:178:GLN:N    | 2:B:178:GLN:OE1  | 2.43                     | 0.50              |
| 3:C:45:MET:HG2   | 3:C:64:THR:HG22  | 1.93                     | 0.50              |
| 2:L:144:LEU:HD23 | 2:L:189:SER:OG   | 2.11                     | 0.50              |
| 2:Q:63:GLY:O     | 2:Q:85:GLN:NE2   | 2.44                     | 0.50              |
| 2:Q:196:ALA:O    | 2:Q:200:GLN:HG2  | 2.11                     | 0.50              |
| 3:I:66:LYS:O     | 3:I:69:ALA:N     | 2.43                     | 0.50              |
| 3:I:66:LYS:CE    | 5:K:2:ILE:HG22   | 2.41                     | 0.50              |
| 4:J:37:VAL:HG22  | 4:J:82:VAL:HG13  | 1.93                     | 0.50              |
| 4:J:39:LEU:HD12  | 4:J:80:CYS:HB3   | 1.94                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:149:TYR:CD2  | 2:B:149:TYR:C    | 2.88                     | 0.50              |
| 1:P:29:PHE:HB2   | 1:P:32:TRP:NE1   | 2.26                     | 0.50              |
| 4:J:56:PHE:HA    | 4:J:62:PHE:CE1   | 2.47                     | 0.50              |
| 2:B:10:TYR:HD1   | 2:B:108:ARG:HB3  | 1.77                     | 0.50              |
| 2:B:151:ASP:OD1  | 2:B:151:ASP:O    | 2.29                     | 0.50              |
| 2:H:181:LEU:HD22 | 1:F:169:ASP:HB2  | 1.93                     | 0.50              |
| 4:D:55:SER:OG    | 4:D:56:PHE:N     | 2.45                     | 0.50              |
| 4:N:30:PHE:C     | 4:N:30:PHE:CD2   | 2.89                     | 0.50              |
| 1:P:47:ILE:HD12  | 1:P:57:SER:CA    | 2.38                     | 0.50              |
| 2:Q:51:ASN:O     | 2:Q:68:ARG:HD3   | 2.12                     | 0.50              |
| 3:R:51:TRP:CH2   | 3:R:179:LEU:HD11 | 2.47                     | 0.50              |
| 4:U:75:LYS:NZ    | 4:U:75:LYS:CB    | 2.73                     | 0.50              |
| 1:P:158:THR:HG1  | 1:P:159:ASP:H    | 1.58                     | 0.50              |
| 2:H:29:HIS:HB2   | 2:H:32:MET:HE1   | 1.94                     | 0.50              |
| 3:I:126:LEU:HB2  | 3:I:133:TRP:CZ3  | 2.46                     | 0.50              |
| 3:I:133:TRP:CE2  | 3:I:153:ALA:HB1  | 2.46                     | 0.50              |
| 3:M:99:TYR:HB3   | 3:M:114:HIS:HA   | 1.94                     | 0.50              |
| 1:P:125:LEU:HD11 | 2:Q:128:PRO:C    | 2.36                     | 0.50              |
| 4:U:23:LEU:CD2   | 4:U:39:LEU:HD22  | 2.42                     | 0.50              |
| 4:J:40:LEU:HA    | 4:J:45:ARG:HA    | 1.93                     | 0.50              |
| 2:L:25:GLN:NE2   | 2:L:27:MET:HG2   | 2.26                     | 0.50              |
| 3:M:148:GLU:HA   | 3:M:151:HIS:N    | 2.26                     | 0.50              |
| 1:G:9:GLN:HE21   | 2:L:198:PHE:HE2  | 1.57                     | 0.50              |
| 3:R:72:GLN:HA    | 3:R:75:ARG:HB2   | 1.94                     | 0.50              |
| 1:G:43:PRO:HD2   | 2:H:103:PHE:CD1  | 2.47                     | 0.50              |
| 3:I:217:TRP:HA   | 3:I:258:THR:O    | 2.12                     | 0.50              |
| 2:H:229:VAL:HG23 | 2:H:230:THR:H    | 1.76                     | 0.49              |
| 3:M:99:TYR:HB3   | 3:M:114:HIS:ND1  | 2.26                     | 0.49              |
| 4:N:24:ASN:HD22  | 4:N:65:LEU:HD13  | 1.77                     | 0.49              |
| 4:U:60:TRP:HA    | 4:U:60:TRP:CE3   | 2.46                     | 0.49              |
| 2:H:61:PRO:O     | 2:H:64:TYR:CD2   | 2.58                     | 0.49              |
| 4:J:35:ILE:HG13  | 4:J:83:ASN:O     | 2.12                     | 0.49              |
| 3:M:262:GLN:NE2  | 3:M:266:LEU:O    | 2.44                     | 0.49              |
| 2:Q:98:PRO:HG3   | 3:R:155:GLN:HG2  | 1.94                     | 0.49              |
| 3:I:17:ARG:CB    | 3:I:18:GLY:HA2   | 2.42                     | 0.49              |
| 3:I:60:TRP:O     | 3:I:64:THR:HG23  | 2.12                     | 0.49              |
| 3:M:117:ALA:HB3  | 4:N:60:TRP:CE2   | 2.47                     | 0.49              |
| 1:P:15:GLU:OE2   | 1:P:81:PRO:HG3   | 2.13                     | 0.49              |
| 3:I:133:TRP:HE1  | 3:I:153:ALA:CB   | 2.25                     | 0.49              |
| 3:I:142:THR:O    | 3:I:144:LYS:N    | 2.45                     | 0.49              |
| 1:A:165:MET:HE3  | 1:A:166:ARG:N    | 2.24                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:81:LEU:HD23  | 3:C:84:TYR:HB2   | 1.95                     | 0.49              |
| 3:C:234:ARG:NH1  | 3:C:244:TRP:CD1  | 2.80                     | 0.49              |
| 4:D:95:TRP:CZ2   | 4:D:97:ARG:HB2   | 2.47                     | 0.49              |
| 2:L:95:LEU:HD12  | 2:L:96:ILE:CB    | 2.43                     | 0.49              |
| 3:M:103:VAL:HG23 | 3:M:108:ARG:O    | 2.12                     | 0.49              |
| 3:I:144:LYS:CD   | 3:I:148:GLU:OE2  | 2.55                     | 0.49              |
| 1:A:3:GLN:O      | 1:A:4:LEU:HD23   | 2.13                     | 0.49              |
| 1:A:87:TYR:HE2   | 1:A:109:LEU:HB3  | 1.78                     | 0.49              |
| 2:L:110:THR:OG1  | 2:L:152:HIS:NE2  | 2.41                     | 0.49              |
| 4:N:54:LEU:HD21  | 4:N:62:PHE:CE2   | 2.47                     | 0.49              |
| 1:G:9:GLN:NE2    | 2:L:198:PHE:HE2  | 2.10                     | 0.49              |
| 2:B:123:VAL:HG13 | 2:B:144:LEU:O    | 2.12                     | 0.49              |
| 3:C:197:HIS:NE2  | 3:C:250:PRO:CB   | 2.76                     | 0.49              |
| 4:D:91:LYS:O     | 4:D:92:ILE:HG23  | 2.11                     | 0.49              |
| 3:I:169:ARG:HD2  | 3:I:172:LEU:HB2  | 1.95                     | 0.49              |
| 3:C:155:GLN:OE1  | 3:C:155:GLN:HA   | 2.12                     | 0.49              |
| 4:D:37:VAL:HB    | 4:D:66:TYR:CE1   | 2.47                     | 0.49              |
| 2:L:48:TYR:O     | 2:L:49:SER:OG    | 2.27                     | 0.49              |
| 3:M:22:PHE:CE2   | 3:M:24:ALA:HB2   | 2.48                     | 0.49              |
| 3:M:201:LEU:HD11 | 3:M:247:VAL:HB   | 1.94                     | 0.49              |
| 3:R:133:TRP:HB2  | 3:R:144:LYS:NZ   | 2.27                     | 0.49              |
| 4:U:16:GLU:O     | 4:U:18:GLY:HA2   | 2.13                     | 0.49              |
| 2:H:221:TRP:CB   | 2:H:227:LYS:HD3  | 2.43                     | 0.49              |
| 3:I:15:PRO:HB3   | 3:I:89:GLU:O     | 2.11                     | 0.49              |
| 2:B:25:GLN:NE2   | 2:B:72:ARG:HA    | 2.28                     | 0.49              |
| 3:C:229:GLU:HG2  | 3:C:244:TRP:CZ3  | 2.48                     | 0.49              |
| 4:D:83:ASN:ND2   | 4:D:90:PRO:HB3   | 2.28                     | 0.49              |
| 3:M:133:TRP:NE1  | 3:M:153:ALA:HB2  | 2.27                     | 0.49              |
| 3:I:147:TRP:CZ2  | 5:K:7:PHE:CD1    | 3.01                     | 0.49              |
| 3:R:7:TYR:HD2    | 3:R:99:TYR:CE1   | 2.31                     | 0.49              |
| 1:G:34:TRP:CZ2   | 1:G:74:LEU:HB2   | 2.48                     | 0.49              |
| 4:J:32:PRO:O     | 4:J:84:HIS:NE2   | 2.44                     | 0.49              |
| 4:J:40:LEU:HD11  | 4:J:45:ARG:NE    | 2.26                     | 0.49              |
| 3:C:64:THR:CA    | 3:C:67:VAL:HG12  | 2.37                     | 0.49              |
| 3:M:6:ARG:HG2    | 3:M:8:PHE:CE1    | 2.48                     | 0.49              |
| 2:H:5:THR:O      | 2:H:23:CYS:HA    | 2.13                     | 0.48              |
| 2:H:112:LEU:HD23 | 2:H:115:LEU:HD23 | 1.94                     | 0.48              |
| 1:F:190:PHE:C    | 1:F:192:ASN:H    | 2.19                     | 0.48              |
| 1:G:150:SER:HB3  | 1:G:152:ASP:N    | 2.28                     | 0.48              |
| 1:G:155:VAL:HG12 | 1:G:156:TYR:N    | 2.28                     | 0.48              |
| 2:H:216:SER:O    | 2:H:218:ASN:N    | 2.43                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:I:139:ALA:O    | 3:I:142:THR:HG22 | 2.13                     | 0.48              |
| 3:I:145:HIS:HA   | 3:I:148:GLU:HB2  | 1.95                     | 0.48              |
| 4:J:4:THR:CB     | 4:J:86:THR:CG2   | 2.69                     | 0.48              |
| 3:M:117:ALA:HB3  | 4:N:60:TRP:CZ2   | 2.48                     | 0.48              |
| 2:H:36:ARG:NH1   | 2:H:84:ASN:O     | 2.46                     | 0.48              |
| 1:F:51:LYS:HE2   | 1:F:53:GLY:HA3   | 1.96                     | 0.48              |
| 1:P:16:GLY:N     | 1:P:79:SER:OG    | 2.39                     | 0.48              |
| 1:P:137:LEU:HD23 | 1:P:138:PHE:N    | 2.27                     | 0.48              |
| 3:I:96:GLN:HG2   | 4:J:62:PHE:CZ    | 2.48                     | 0.48              |
| 3:I:229:GLU:O    | 3:I:246:ALA:N    | 2.46                     | 0.48              |
| 4:J:40:LEU:CD1   | 4:J:45:ARG:HG3   | 2.43                     | 0.48              |
| 4:J:83:ASN:OD1   | 4:J:84:HIS:N     | 2.47                     | 0.48              |
| 1:A:126:ARG:O    | 2:B:127:GLU:N    | 2.36                     | 0.48              |
| 4:D:87:LEU:C     | 4:D:87:LEU:CD1   | 2.85                     | 0.48              |
| 3:M:65:ARG:O     | 3:M:68:LYS:CG    | 2.61                     | 0.48              |
| 3:R:82:ARG:O     | 3:R:86:ASN:N     | 2.44                     | 0.48              |
| 3:I:9:PHE:HZ     | 5:K:2:ILE:HD11   | 1.78                     | 0.48              |
| 3:I:61:ASP:C     | 3:I:63:GLU:N     | 2.71                     | 0.48              |
| 3:I:115:GLN:HG2  | 4:J:60:TRP:HZ2   | 1.78                     | 0.48              |
| 2:B:146:THR:HG22 | 2:B:147:GLY:N    | 2.28                     | 0.48              |
| 2:L:77:ILE:HA    | 2:L:78:LEU:HD12  | 1.94                     | 0.48              |
| 1:A:160:LYS:HA   | 1:A:174:SER:O    | 2.13                     | 0.48              |
| 2:L:95:LEU:HD13  | 3:M:146:LYS:CE   | 2.44                     | 0.48              |
| 4:N:30:PHE:CZ    | 4:N:84:HIS:CE1   | 3.01                     | 0.48              |
| 2:H:165:HIS:O    | 2:H:168:VAL:HG12 | 2.12                     | 0.48              |
| 2:H:221:TRP:HB2  | 2:H:227:LYS:CD   | 2.43                     | 0.48              |
| 1:A:36:LYS:HE3   | 1:A:87:TYR:CD2   | 2.48                     | 0.48              |
| 2:B:48:TYR:CZ    | 2:B:56:ASP:HB2   | 2.48                     | 0.48              |
| 2:B:130:GLU:CD   | 2:B:130:GLU:H    | 2.21                     | 0.48              |
| 4:D:50:GLU:O     | 4:D:67:TYR:N     | 2.33                     | 0.48              |
| 3:M:65:ARG:NH1   | 3:M:65:ARG:CG    | 2.73                     | 0.48              |
| 4:J:63:TYR:O     | 4:J:64:LEU:HD23  | 2.14                     | 0.48              |
| 3:C:229:GLU:HB3  | 3:C:246:ALA:O    | 2.14                     | 0.48              |
| 3:C:234:ARG:HG2  | 4:D:10:TYR:CE2   | 2.48                     | 0.48              |
| 2:L:91:CYS:O     | 2:L:104:GLY:N    | 2.45                     | 0.48              |
| 1:G:43:PRO:HB2   | 2:H:103:PHE:CE2  | 2.49                     | 0.48              |
| 1:G:118:PRO:O    | 1:G:120:PRO:HD3  | 2.14                     | 0.48              |
| 1:F:119:ASP:O    | 1:F:140:ASP:HB2  | 2.14                     | 0.48              |
| 1:F:139:THR:HG23 | 1:F:140:ASP:OD2  | 2.14                     | 0.48              |
| 4:U:46:ILE:HD11  | 4:U:49:VAL:HG22  | 1.95                     | 0.48              |
| 3:I:176:LYS:HG3  | 3:I:177:GLU:N    | 2.29                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:K:7:PHE:CD1    | 5:K:7:PHE:O      | 2.67                     | 0.48              |
| 1:P:114:ASP:OD1  | 1:P:114:ASP:N    | 2.42                     | 0.48              |
| 3:I:52:ILE:HG12  | 3:I:60:TRP:CZ2   | 2.49                     | 0.47              |
| 3:I:150:ALA:O    | 3:I:151:HIS:CB   | 2.51                     | 0.47              |
| 3:I:186:LYS:O    | 3:I:206:LEU:HD13 | 2.13                     | 0.47              |
| 3:I:202:ARG:HD2  | 3:I:204:TRP:CH2  | 2.49                     | 0.47              |
| 3:C:7:TYR:CE1    | 5:E:2:ILE:HB     | 2.49                     | 0.47              |
| 3:C:34:VAL:HG12  | 3:C:35:ARG:H     | 1.79                     | 0.47              |
| 3:C:125:ALA:HB3  | 3:C:134:THR:HB   | 1.95                     | 0.47              |
| 1:F:19:VAL:O     | 1:F:75:ASN:HB2   | 2.14                     | 0.47              |
| 3:M:270:LEU:HD12 | 3:M:270:LEU:HA   | 1.70                     | 0.47              |
| 4:J:40:LEU:HD12  | 4:J:45:ARG:HG3   | 1.95                     | 0.47              |
| 1:A:123:TYR:HB3  | 2:B:129:SER:HB2  | 1.96                     | 0.47              |
| 4:D:89:GLN:HG3   | 4:D:90:PRO:O     | 2.15                     | 0.47              |
| 2:L:3:GLN:HA     | 2:L:25:GLN:NE2   | 2.28                     | 0.47              |
| 2:Q:216:SER:O    | 2:Q:218:ASN:N    | 2.47                     | 0.47              |
| 3:I:81:LEU:O     | 3:I:83:GLY:N     | 2.47                     | 0.47              |
| 3:I:93:HIS:HB3   | 3:I:118:TYR:CE1  | 2.49                     | 0.47              |
| 4:N:86:THR:CG2   | 4:N:87:LEU:N     | 2.77                     | 0.47              |
| 3:I:218:GLN:HG3  | 3:I:219:ARG:HG2  | 1.96                     | 0.47              |
| 4:J:38:ASP:O     | 4:J:80:CYS:HB2   | 2.15                     | 0.47              |
| 4:J:46:ILE:CG2   | 4:J:47:GLU:N     | 2.77                     | 0.47              |
| 3:C:185:PRO:HG3  | 3:C:263:HIS:ND1  | 2.29                     | 0.47              |
| 4:D:41:LYS:O     | 4:D:42:ASN:HB2   | 2.15                     | 0.47              |
| 1:F:58:ASN:H     | 1:F:61:LEU:HD22  | 1.80                     | 0.47              |
| 3:R:23:ILE:HD13  | 4:U:54:LEU:HB3   | 1.96                     | 0.47              |
| 1:G:142:ASP:OD1  | 1:G:143:SER:N    | 2.48                     | 0.47              |
| 2:H:6:GLN:HE22   | 2:H:90:PHE:HA    | 1.79                     | 0.47              |
| 4:J:3:ARG:O      | 4:J:31:HIS:N     | 2.47                     | 0.47              |
| 2:L:95:LEU:HD12  | 2:L:96:ILE:HG13  | 1.96                     | 0.47              |
| 3:M:271:THR:OG1  | 3:M:272:LEU:N    | 2.46                     | 0.47              |
| 4:D:78:TYR:O     | 4:D:95:TRP:HB3   | 2.15                     | 0.47              |
| 3:M:138:MET:SD   | 3:M:141:GLN:NE2  | 2.87                     | 0.47              |
| 3:R:172:LEU:O    | 3:R:180:GLN:NE2  | 2.48                     | 0.47              |
| 3:R:235:PRO:HG2  | 4:U:65:LEU:CD2   | 2.44                     | 0.47              |
| 2:H:55:THR:OG1   | 3:I:65:ARG:NH2   | 2.47                     | 0.47              |
| 4:J:79:ALA:HB2   | 4:J:94:LYS:HA    | 1.97                     | 0.47              |
| 2:B:32:MET:SD    | 2:B:68:ARG:NH1   | 2.86                     | 0.47              |
| 3:C:170:ARG:O    | 3:C:173:GLU:HG2  | 2.14                     | 0.47              |
| 2:L:150:PRO:HD2  | 2:L:152:HIS:CD2  | 2.49                     | 0.47              |
| 2:L:152:HIS:O    | 2:L:213:TYR:HD2  | 1.97                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:51:LYS:HE2   | 3:R:131:ARG:NH2  | 2.29                     | 0.47              |
| 3:R:9:PHE:CD1    | 3:R:97:ARG:HG2   | 2.50                     | 0.47              |
| 3:R:163:THR:CG2  | 3:R:167:TRP:HE1  | 2.27                     | 0.47              |
| 3:I:59:TYR:O     | 3:I:63:GLU:HG2   | 2.14                     | 0.47              |
| 3:I:129:ASP:OD1  | 3:I:130:LEU:N    | 2.48                     | 0.47              |
| 3:C:33:PHE:CZ    | 3:C:171:TYR:HB3  | 2.50                     | 0.47              |
| 4:D:8:GLN:O      | 4:D:8:GLN:HG3    | 2.14                     | 0.47              |
| 3:M:189:MET:HE3  | 3:M:217:TRP:HH2  | 1.80                     | 0.47              |
| 1:P:170:PHE:CE1  | 1:P:172:SER:HB2  | 2.50                     | 0.47              |
| 4:U:23:LEU:HB2   | 4:U:70:PHE:CD2   | 2.50                     | 0.47              |
| 2:H:80:SER:OG    | 3:R:270:LEU:HG   | 2.15                     | 0.47              |
| 3:I:245:ALA:O    | 3:I:247:VAL:HG23 | 2.15                     | 0.47              |
| 1:F:160:LYS:N    | 1:F:160:LYS:CD   | 2.77                     | 0.47              |
| 4:N:84:HIS:CG    | 4:N:85:VAL:N     | 2.83                     | 0.47              |
| 2:B:6:GLN:HE21   | 2:B:91:CYS:H     | 1.62                     | 0.47              |
| 3:C:13:SER:HB3   | 3:C:78:LEU:HD22  | 1.96                     | 0.47              |
| 3:C:81:LEU:HA    | 3:C:84:TYR:CD2   | 2.44                     | 0.47              |
| 2:L:49:SER:HB3   | 2:L:54:VAL:O     | 2.14                     | 0.47              |
| 3:M:147:TRP:CZ2  | 5:O:9:LEU:HD23   | 2.49                     | 0.47              |
| 2:Q:98:PRO:O     | 3:R:150:ALA:HB1  | 2.15                     | 0.47              |
| 1:G:124:GLN:O    | 2:H:129:SER:HB2  | 2.14                     | 0.46              |
| 2:H:110:THR:HG21 | 2:H:150:PRO:HG2  | 1.96                     | 0.46              |
| 2:H:114:ASP:OD1  | 2:H:116:LYS:HG3  | 2.15                     | 0.46              |
| 2:H:150:PRO:HD2  | 2:H:152:HIS:CD2  | 2.50                     | 0.46              |
| 3:I:84:TYR:HD2   | 3:I:85:TYR:CE2   | 2.33                     | 0.46              |
| 4:J:3:ARG:O      | 4:J:30:PHE:CA    | 2.58                     | 0.46              |
| 4:J:80:CYS:C     | 4:J:92:ILE:HG23  | 2.39                     | 0.46              |
| 4:D:37:VAL:HB    | 4:D:66:TYR:CZ    | 2.50                     | 0.46              |
| 3:M:262:GLN:CG   | 3:M:269:PRO:HB3  | 2.45                     | 0.46              |
| 2:Q:208:CYS:O    | 2:Q:234:SER:HB3  | 2.15                     | 0.46              |
| 2:H:31:TYR:HD1   | 2:H:50:MET:HA    | 1.79                     | 0.46              |
| 2:H:61:PRO:HG2   | 2:H:62:GLU:N     | 2.30                     | 0.46              |
| 1:P:159:ASP:OD1  | 1:P:160:LYS:N    | 2.48                     | 0.46              |
| 3:I:228:THR:HG23 | 3:I:247:VAL:HG22 | 1.98                     | 0.46              |
| 2:B:149:TYR:HD2  | 2:B:149:TYR:C    | 2.24                     | 0.46              |
| 4:D:5:PRO:CB     | 4:D:30:PHE:HB3   | 2.39                     | 0.46              |
| 2:L:228:PRO:C    | 2:L:229:VAL:HG23 | 2.39                     | 0.46              |
| 3:M:16:GLY:HA2   | 3:M:18:GLY:HA2   | 1.98                     | 0.46              |
| 1:P:157:ILE:HG22 | 1:P:158:THR:H    | 1.79                     | 0.46              |
| 3:R:19:GLU:OE1   | 3:R:19:GLU:N     | 2.49                     | 0.46              |
| 2:H:13:THR:OG1   | 2:H:14:VAL:N     | 2.48                     | 0.46              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 3:I:125:ALA:O    | 3:I:134:THR:N   | 2.47                     | 0.46              |
| 3:I:129:ASP:CG   | 3:I:131:ARG:HG2 | 2.41                     | 0.46              |
| 1:A:157:ILE:HA   | 1:A:176:VAL:O   | 2.16                     | 0.46              |
| 4:D:54:LEU:HA    | 4:D:64:LEU:HD21 | 1.96                     | 0.46              |
| 3:M:110:LEU:HG   | 3:M:111:ARG:HG3 | 1.98                     | 0.46              |
| 1:P:26:SER:C     | 1:P:70:LYS:HD2  | 2.40                     | 0.46              |
| 3:I:63:GLU:HA    | 3:I:66:LYS:NZ   | 2.03                     | 0.46              |
| 3:I:82:ARG:NH1   | 3:I:89:GLU:HB3  | 2.30                     | 0.46              |
| 3:I:96:GLN:HG2   | 4:J:62:PHE:HZ   | 1.81                     | 0.46              |
| 4:J:31:HIS:HE1   | 4:J:62:PHE:CD2  | 2.33                     | 0.46              |
| 1:A:199:THR:O    | 1:A:199:THR:OG1 | 2.29                     | 0.46              |
| 2:B:146:THR:O    | 2:B:148:PHE:CE2 | 2.68                     | 0.46              |
| 3:C:65:ARG:O     | 3:C:65:ARG:HG2  | 2.15                     | 0.46              |
| 3:C:140:ALA:O    | 3:C:144:LYS:N   | 2.44                     | 0.46              |
| 3:M:249:VAL:HG22 | 3:M:250:PRO:N   | 2.30                     | 0.46              |
| 1:P:121:ALA:HA   | 1:P:198:ASP:OD1 | 2.16                     | 0.46              |
| 3:R:98:MET:CE    | 4:U:58:LYS:HZ1  | 2.27                     | 0.46              |
| 4:U:46:ILE:HD12  | 4:U:48:LYS:N    | 2.29                     | 0.46              |
| 3:I:3:HIS:NE2    | 3:I:180:GLN:HB2 | 2.29                     | 0.46              |
| 3:I:64:THR:O     | 3:I:68:LYS:HB3  | 2.16                     | 0.46              |
| 3:I:135:ALA:CB   | 3:I:141:GLN:OE1 | 2.64                     | 0.46              |
| 3:I:144:LYS:O    | 3:I:148:GLU:N   | 2.49                     | 0.46              |
| 1:A:25:SER:OG    | 1:A:26:SER:N    | 2.49                     | 0.46              |
| 2:B:70:GLU:N     | 2:B:70:GLU:OE1  | 2.48                     | 0.46              |
| 3:C:7:TYR:HE1    | 5:E:2:ILE:HB    | 1.80                     | 0.46              |
| 4:D:83:ASN:CG    | 4:D:90:PRO:HB3  | 2.40                     | 0.46              |
| 3:I:7:TYR:OH     | 5:K:1:GLY:N     | 2.39                     | 0.46              |
| 1:A:116:GLN:N    | 1:A:116:GLN:OE1 | 2.49                     | 0.46              |
| 4:D:12:ARG:NH1   | 4:D:22:PHE:HD2  | 2.14                     | 0.46              |
| 3:M:61:ASP:O     | 3:M:65:ARG:N    | 2.41                     | 0.46              |
| 2:Q:136:THR:HG23 | 2:Q:137:GLN:N   | 2.30                     | 0.46              |
| 2:Q:149:TYR:HA   | 2:Q:150:PRO:HA  | 1.58                     | 0.46              |
| 3:R:98:MET:CG    | 4:U:58:LYS:HZ1  | 2.29                     | 0.46              |
| 3:I:32:GLN:CD    | 3:I:48:ARG:HD2  | 2.41                     | 0.46              |
| 1:A:128:SER:HB3  | 1:A:133:LYS:HE2 | 1.98                     | 0.46              |
| 2:B:38:ASP:OD1   | 2:B:38:ASP:N    | 2.48                     | 0.46              |
| 3:C:5:MET:C      | 3:C:6:ARG:HG2   | 2.41                     | 0.46              |
| 3:C:67:VAL:O     | 3:C:67:VAL:HG22 | 2.15                     | 0.46              |
| 1:F:126:ARG:HD2  | 1:F:126:ARG:HA  | 1.84                     | 0.46              |
| 1:F:129:LYS:HZ3  | 1:F:132:ASP:N   | 2.13                     | 0.46              |
| 3:M:254:GLU:CG   | 3:M:255:GLN:HG3 | 2.45                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:N:43:GLY:HA2   | 4:N:44:GLU:HA    | 1.48                     | 0.46              |
| 4:N:55:SER:OG    | 4:N:56:PHE:N     | 2.49                     | 0.46              |
| 2:Q:82:SER:O     | 2:Q:111:VAL:HG21 | 2.16                     | 0.46              |
| 3:I:124:ILE:HD13 | 3:I:147:TRP:CZ3  | 2.50                     | 0.46              |
| 3:C:35:ARG:HD3   | 4:D:53:ASP:CG    | 2.41                     | 0.46              |
| 1:F:124:GLN:HG2  | 1:F:186:CYS:SG   | 2.56                     | 0.46              |
| 1:G:150:SER:HA   | 1:G:151:LYS:CB   | 2.41                     | 0.46              |
| 3:I:103:VAL:HG22 | 3:I:109:PHE:HA   | 1.97                     | 0.46              |
| 3:C:234:ARG:NH1  | 3:C:244:TRP:HD1  | 2.14                     | 0.46              |
| 2:L:4:VAL:HG13   | 2:L:104:GLY:HA2  | 1.98                     | 0.46              |
| 2:Q:82:SER:OG    | 2:Q:84:ASN:HB3   | 2.16                     | 0.46              |
| 3:R:51:TRP:H     | 3:R:51:TRP:CD1   | 2.33                     | 0.46              |
| 1:G:138:PHE:CB   | 1:G:190:PHE:HE2  | 2.29                     | 0.45              |
| 2:H:167:GLY:O    | 2:H:192:LEU:HD12 | 2.16                     | 0.45              |
| 3:I:10:THR:HB    | 3:I:23:ILE:HD11  | 1.97                     | 0.45              |
| 1:G:64:GLN:O     | 1:G:72:SER:HB2   | 2.16                     | 0.45              |
| 2:B:222:THR:HB   | 2:B:223:GLN:CA   | 2.46                     | 0.45              |
| 4:D:88:SER:CB    | 4:D:89:GLN:CA    | 2.93                     | 0.45              |
| 2:Q:31:TYR:HB3   | 2:Q:94:SER:HB3   | 1.97                     | 0.45              |
| 3:R:192:HIS:NE2  | 4:U:98:ASP:HB2   | 2.31                     | 0.45              |
| 2:H:18:GLU:HG2   | 2:H:79:GLU:HA    | 1.97                     | 0.45              |
| 3:I:141:GLN:HE22 | 3:I:144:LYS:CE   | 2.29                     | 0.45              |
| 3:I:236:ALA:O    | 4:J:12:ARG:NE    | 2.50                     | 0.45              |
| 4:J:22:PHE:CD1   | 4:J:22:PHE:N     | 2.82                     | 0.45              |
| 1:A:36:LYS:HZ3   | 1:A:84:VAL:C     | 2.24                     | 0.45              |
| 1:A:132:ASP:O    | 1:A:133:LYS:HD3  | 2.16                     | 0.45              |
| 1:A:145:THR:HG21 | 1:A:196:PRO:HD3  | 1.98                     | 0.45              |
| 3:C:197:HIS:NE2  | 3:C:250:PRO:HB3  | 2.31                     | 0.45              |
| 4:D:89:GLN:HB2   | 4:D:90:PRO:CD    | 2.43                     | 0.45              |
| 1:F:197:GLU:C    | 1:F:198:ASP:OD1  | 2.59                     | 0.45              |
| 3:R:101:CYS:HA   | 3:R:112:GLY:HA2  | 1.99                     | 0.45              |
| 1:G:60:ARG:NH1   | 1:G:83:ASP:CG    | 2.60                     | 0.45              |
| 1:G:174:SER:OG   | 2:H:191:ARG:HD2  | 2.17                     | 0.45              |
| 2:H:118:VAL:O    | 2:H:228:PRO:HG3  | 2.16                     | 0.45              |
| 1:A:93:GLY:HA2   | 1:A:94:GLY:HA3   | 1.74                     | 0.45              |
| 3:C:231:VAL:HG21 | 3:C:244:TRP:CE2  | 2.52                     | 0.45              |
| 4:D:88:SER:HB3   | 4:D:89:GLN:CA    | 2.44                     | 0.45              |
| 1:F:38:GLU:N     | 1:F:38:GLU:OE1   | 2.50                     | 0.45              |
| 2:L:47:TYR:OH    | 2:L:55:THR:HB    | 2.17                     | 0.45              |
| 1:G:7:SER:OG     | 1:G:8:PRO:HA     | 2.17                     | 0.45              |
| 1:G:19:VAL:CG1   | 1:G:76:ILE:HB    | 2.46                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:I:207:SER:O    | 3:I:207:SER:OG   | 2.27                     | 0.45              |
| 2:B:4:VAL:HG23   | 2:B:4:VAL:O      | 2.16                     | 0.45              |
| 2:B:46:ILE:C     | 2:B:47:TYR:HD1   | 2.25                     | 0.45              |
| 2:B:173:GLN:CD   | 2:B:173:GLN:H    | 2.23                     | 0.45              |
| 2:L:56:ASP:OD1   | 3:M:68:LYS:NZ    | 2.50                     | 0.45              |
| 1:P:86:ILE:HD13  | 1:P:88:PHE:CE2   | 2.52                     | 0.45              |
| 1:P:139:THR:OG1  | 1:P:140:ASP:OD1  | 2.23                     | 0.45              |
| 1:A:152:ASP:C    | 1:A:154:ASP:H    | 2.25                     | 0.45              |
| 2:L:158:TRP:HA   | 2:L:163:GLU:HA   | 1.99                     | 0.45              |
| 1:P:101:LEU:HD23 | 2:Q:101:LEU:HD11 | 1.98                     | 0.45              |
| 1:P:118:PRO:O    | 1:P:118:PRO:HD2  | 2.17                     | 0.45              |
| 2:Q:119:PHE:CB   | 2:Q:120:PRO:CD   | 2.82                     | 0.45              |
| 3:R:3:HIS:ND1    | 3:R:3:HIS:N      | 2.65                     | 0.45              |
| 3:R:45:MET:HE3   | 3:R:67:VAL:HB    | 1.98                     | 0.45              |
| 3:R:97:ARG:NH2   | 5:T:7:PHE:HZ     | 2.15                     | 0.45              |
| 3:R:231:VAL:HG21 | 3:R:244:TRP:CE3  | 2.51                     | 0.45              |
| 3:I:45:MET:HB3   | 3:I:60:TRP:CE3   | 2.48                     | 0.45              |
| 4:D:91:LYS:O     | 4:D:92:ILE:CG2   | 2.65                     | 0.45              |
| 3:M:220:ASP:CB   | 3:M:221:GLY:CA   | 2.91                     | 0.45              |
| 2:Q:2:ALA:HA     | 2:Q:26:ASN:HD21  | 1.80                     | 0.45              |
| 3:R:25:VAL:HG12  | 3:R:35:ARG:NH1   | 2.32                     | 0.45              |
| 3:R:195:SER:HA   | 3:R:196:ASP:HA   | 1.65                     | 0.45              |
| 2:H:114:ASP:OD1  | 2:H:115:LEU:N    | 2.50                     | 0.45              |
| 3:C:114:HIS:CE1  | 5:E:7:PHE:HZ     | 2.35                     | 0.45              |
| 3:C:182:THR:HG22 | 3:C:210:PRO:HD3  | 1.98                     | 0.45              |
| 2:L:148:PHE:CB   | 2:L:186:TYR:HB2  | 2.42                     | 0.45              |
| 4:N:31:HIS:HB2   | 4:N:62:PHE:CE1   | 2.52                     | 0.45              |
| 1:P:25:SER:OG    | 1:P:26:SER:N     | 2.49                     | 0.45              |
| 1:P:31:THR:HG22  | 1:P:50:TYR:CD1   | 2.50                     | 0.45              |
| 4:U:26:TYR:HA    | 4:U:65:LEU:HD13  | 1.97                     | 0.45              |
| 4:U:64:LEU:HD12  | 4:U:64:LEU:HA    | 1.59                     | 0.45              |
| 3:I:81:LEU:C     | 3:I:85:TYR:HD2   | 2.25                     | 0.45              |
| 3:I:107:TRP:CH2  | 3:I:169:ARG:CZ   | 3.00                     | 0.45              |
| 3:I:115:GLN:HG3  | 3:I:124:ILE:O    | 2.17                     | 0.45              |
| 1:A:163:LEU:HB3  | 1:A:172:SER:O    | 2.17                     | 0.45              |
| 3:C:200:THR:OG1  | 3:C:248:VAL:HG21 | 2.17                     | 0.45              |
| 2:L:34:TRP:CH2   | 2:L:91:CYS:HB2   | 2.52                     | 0.45              |
| 3:M:32:GLN:OE1   | 3:M:33:PHE:N     | 2.49                     | 0.45              |
| 3:R:14:ARG:HE    | 3:R:14:ARG:HB3   | 1.53                     | 0.45              |
| 4:U:54:LEU:HA    | 4:U:64:LEU:HD13  | 1.99                     | 0.45              |
| 2:H:13:THR:HG21  | 2:H:19:LEU:HD11  | 1.99                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:I:216:THR:C    | 3:I:217:TRP:HD1  | 2.24                     | 0.45              |
| 1:A:37:GLN:HE22  | 2:B:37:GLN:CD    | 2.25                     | 0.45              |
| 3:C:141:GLN:N    | 3:C:141:GLN:OE1  | 2.50                     | 0.45              |
| 2:L:6:GLN:NE2    | 2:L:34:TRP:CH2   | 2.84                     | 0.45              |
| 2:L:87:SER:HB3   | 2:L:89:TYR:CE1   | 2.46                     | 0.45              |
| 2:L:115:LEU:O    | 2:L:118:VAL:HG22 | 2.16                     | 0.45              |
| 3:M:85:TYR:HB3   | 3:M:87:GLN:NE2   | 2.32                     | 0.45              |
| 3:M:117:ALA:HA   | 3:M:123:TYR:CB   | 2.47                     | 0.45              |
| 3:R:189:MET:HE3  | 3:R:189:MET:HB2  | 1.73                     | 0.45              |
| 3:R:270:LEU:CD2  | 3:R:271:THR:H    | 2.30                     | 0.45              |
| 4:J:54:LEU:HA    | 4:J:64:LEU:CD2   | 2.46                     | 0.44              |
| 1:A:155:VAL:HA   | 1:A:179:SER:HB2  | 1.98                     | 0.44              |
| 2:B:53:GLU:OE1   | 3:C:72:GLN:NE2   | 2.50                     | 0.44              |
| 3:M:104:GLY:C    | 3:M:106:ASP:N    | 2.75                     | 0.44              |
| 3:M:123:TYR:HE2  | 3:M:143:THR:HG21 | 1.81                     | 0.44              |
| 3:M:215:LEU:HB2  | 3:M:260:HIS:O    | 2.17                     | 0.44              |
| 3:M:216:THR:O    | 3:M:217:TRP:CD1  | 2.70                     | 0.44              |
| 3:R:15:PRO:HB3   | 3:R:89:GLU:O     | 2.17                     | 0.44              |
| 3:R:263:HIS:CE1  | 3:R:265:GLY:CA   | 3.00                     | 0.44              |
| 3:I:85:TYR:CZ    | 3:I:118:TYR:CE2  | 3.05                     | 0.44              |
| 1:A:78:ALA:O     | 1:A:80:ILE:N     | 2.47                     | 0.44              |
| 1:A:163:LEU:HD21 | 2:B:193:ARG:HD2  | 1.99                     | 0.44              |
| 1:F:155:VAL:HG12 | 1:F:179:SER:HB2  | 1.99                     | 0.44              |
| 2:L:10:TYR:CD1   | 2:L:108:ARG:HB2  | 2.52                     | 0.44              |
| 2:L:159:VAL:N    | 2:L:162:LYS:O    | 2.48                     | 0.44              |
| 3:M:9:PHE:HB2    | 3:M:97:ARG:CB    | 2.47                     | 0.44              |
| 3:M:216:THR:O    | 3:M:217:TRP:HD1  | 2.01                     | 0.44              |
| 2:Q:216:SER:HA   | 2:Q:229:VAL:CG1  | 2.47                     | 0.44              |
| 1:G:46:LEU:HD23  | 1:G:46:LEU:HA    | 1.73                     | 0.44              |
| 1:G:178:TRP:O    | 1:G:179:SER:OG   | 2.34                     | 0.44              |
| 3:I:218:GLN:CD   | 3:I:219:ARG:H    | 2.25                     | 0.44              |
| 4:J:46:ILE:HD12  | 4:J:70:PHE:CZ    | 2.43                     | 0.44              |
| 2:B:209:GLN:HG3  | 2:B:234:SER:OG   | 2.17                     | 0.44              |
| 2:L:128:PRO:HG3  | 2:L:141:LEU:HG   | 2.00                     | 0.44              |
| 3:R:7:TYR:HD2    | 3:R:99:TYR:HE1   | 1.65                     | 0.44              |
| 4:U:13:HIS:HB2   | 4:U:21:ASN:ND2   | 2.32                     | 0.44              |
| 2:H:3:GLN:OE1    | 2:H:4:VAL:N      | 2.50                     | 0.44              |
| 2:H:26:ASN:HA    | 2:H:27:MET:HA    | 1.49                     | 0.44              |
| 2:H:61:PRO:CG    | 2:H:62:GLU:N     | 2.80                     | 0.44              |
| 4:J:25:CYS:O     | 4:J:65:LEU:HD12  | 2.17                     | 0.44              |
| 1:A:58:ASN:HA    | 1:A:59:GLY:HA2   | 1.44                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:109:PHE:CD1  | 3:C:165:VAL:HG21 | 2.52                     | 0.44              |
| 3:C:234:ARG:HB3  | 3:C:242:GLN:O    | 2.17                     | 0.44              |
| 4:D:56:PHE:CZ    | 4:D:60:TRP:HE3   | 2.35                     | 0.44              |
| 1:F:25:SER:OG    | 1:F:26:SER:N     | 2.49                     | 0.44              |
| 1:F:59:GLY:C     | 1:F:61:LEU:H     | 2.25                     | 0.44              |
| 1:F:157:ILE:HA   | 1:F:177:ALA:HB2  | 1.99                     | 0.44              |
| 2:Q:29:HIS:NE2   | 2:Q:95:LEU:HG    | 2.32                     | 0.44              |
| 2:H:25:GLN:HB3   | 2:H:72:ARG:O     | 2.18                     | 0.44              |
| 2:H:47:TYR:OH    | 2:H:61:PRO:HB2   | 2.18                     | 0.44              |
| 3:I:146:LYS:HA   | 3:I:146:LYS:HD2  | 1.67                     | 0.44              |
| 2:L:27:MET:C     | 2:L:29:HIS:HD2   | 2.26                     | 0.44              |
| 3:I:28:VAL:HG23  | 3:I:33:PHE:CE1   | 2.52                     | 0.44              |
| 3:I:82:ARG:O     | 3:I:86:ASN:N     | 2.46                     | 0.44              |
| 1:A:124:GLN:O    | 1:A:125:LEU:HD23 | 2.17                     | 0.44              |
| 3:C:170:ARG:HG2  | 3:C:173:GLU:OE2  | 2.17                     | 0.44              |
| 3:M:56:GLY:O     | 3:M:60:TRP:HD1   | 2.01                     | 0.44              |
| 3:M:159:TYR:OH   | 5:O:1:GLY:O      | 2.30                     | 0.44              |
| 4:N:3:ARG:H      | 4:N:30:PHE:HE1   | 1.64                     | 0.44              |
| 3:R:263:HIS:CE1  | 3:R:265:GLY:HA3  | 2.52                     | 0.44              |
| 3:I:89:GLU:OE1   | 3:I:89:GLU:N     | 2.51                     | 0.44              |
| 4:J:41:LYS:O     | 4:J:43:GLY:N     | 2.51                     | 0.44              |
| 3:I:52:ILE:CD1   | 3:I:60:TRP:CH2   | 3.01                     | 0.44              |
| 3:I:81:LEU:C     | 3:I:83:GLY:N     | 2.75                     | 0.44              |
| 1:A:34:TRP:CE3   | 1:A:74:LEU:HD22  | 2.53                     | 0.44              |
| 3:C:172:LEU:O    | 3:C:176:LYS:HG3  | 2.18                     | 0.44              |
| 3:M:217:TRP:NE1  | 3:M:259:CYS:HA   | 2.32                     | 0.44              |
| 1:P:47:ILE:CG2   | 1:P:57:SER:HB2   | 2.48                     | 0.44              |
| 1:P:125:LEU:HG   | 2:Q:127:GLU:O    | 2.17                     | 0.44              |
| 1:A:148:SER:CB   | 1:A:193:SER:HB3  | 2.47                     | 0.44              |
| 2:B:101:LEU:C    | 2:B:102:PHE:HD1  | 2.26                     | 0.44              |
| 3:C:47:PRO:HD3   | 3:C:60:TRP:CH2   | 2.53                     | 0.44              |
| 4:U:47:GLU:H     | 4:U:47:GLU:CD    | 2.26                     | 0.44              |
| 4:D:56:PHE:CE2   | 4:D:60:TRP:CE3   | 3.06                     | 0.43              |
| 2:Q:201:ASN:HA   | 2:Q:202:PRO:HD3  | 1.85                     | 0.43              |
| 4:U:27:VAL:HG11  | 4:U:37:VAL:HG21  | 2.00                     | 0.43              |
| 3:I:217:TRP:HE1  | 3:I:259:CYS:HB3  | 1.82                     | 0.43              |
| 1:A:165:MET:HG3  | 2:B:166:SER:OG   | 2.18                     | 0.43              |
| 3:C:234:ARG:HH12 | 3:C:244:TRP:CD1  | 2.35                     | 0.43              |
| 1:P:24:THR:OG1   | 1:P:25:SER:N     | 2.50                     | 0.43              |
| 1:P:13:ILE:HD13  | 1:P:19:VAL:CG2   | 2.47                     | 0.43              |
| 1:P:74:LEU:HD22  | 1:P:74:LEU:HA    | 1.88                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:Q:22:THR:OG1   | 2:Q:23:CYS:N     | 2.50                     | 0.43              |
| 3:R:3:HIS:HD2    | 3:R:172:LEU:HD21 | 1.84                     | 0.43              |
| 3:I:66:LYS:HE2   | 5:K:2:ILE:CG2    | 2.46                     | 0.43              |
| 3:I:133:TRP:CZ2  | 3:I:153:ALA:HB2  | 2.51                     | 0.43              |
| 4:J:31:HIS:CE1   | 4:J:62:PHE:CD2   | 3.06                     | 0.43              |
| 2:B:121:PRO:O    | 2:B:233:VAL:HG21 | 2.19                     | 0.43              |
| 2:B:173:GLN:HA   | 2:B:174:PRO:HD3  | 1.74                     | 0.43              |
| 2:L:13:THR:HG21  | 2:L:19:LEU:HD23  | 2.00                     | 0.43              |
| 2:L:102:PHE:N    | 2:L:102:PHE:CD1  | 2.85                     | 0.43              |
| 3:M:13:SER:OG    | 3:M:82:ARG:NH2   | 2.51                     | 0.43              |
| 3:M:201:LEU:HD13 | 3:M:217:TRP:CZ3  | 2.45                     | 0.43              |
| 2:Q:8:PRO:HD2    | 2:Q:21:VAL:HG22  | 2.00                     | 0.43              |
| 4:U:41:LYS:HB3   | 4:U:78:TYR:CE1   | 2.54                     | 0.43              |
| 3:I:138:MET:HA   | 3:I:141:GLN:HB3  | 2.01                     | 0.43              |
| 3:C:33:PHE:CE2   | 3:C:51:TRP:CZ2   | 3.07                     | 0.43              |
| 3:C:85:TYR:HE2   | 3:C:87:GLN:NE2   | 2.16                     | 0.43              |
| 3:C:200:THR:HA   | 3:C:248:VAL:HG23 | 2.00                     | 0.43              |
| 2:L:136:THR:HG21 | 2:L:193:ARG:NH2  | 2.34                     | 0.43              |
| 3:M:215:LEU:C    | 3:M:215:LEU:CD1  | 2.86                     | 0.43              |
| 2:Q:66:VAL:HG12  | 2:Q:76:LEU:HA    | 2.00                     | 0.43              |
| 3:R:51:TRP:CD1   | 3:R:51:TRP:N     | 2.87                     | 0.43              |
| 4:J:42:ASN:HB3   | 4:J:43:GLY:H     | 1.64                     | 0.43              |
| 3:C:84:TYR:HB3   | 3:C:139:ALA:HB1  | 2.00                     | 0.43              |
| 3:C:102:ASP:O    | 3:C:110:LEU:HB3  | 2.17                     | 0.43              |
| 4:D:81:ARG:CA    | 4:D:92:ILE:HG22  | 2.45                     | 0.43              |
| 1:F:139:THR:OG1  | 1:F:140:ASP:N    | 2.51                     | 0.43              |
| 1:P:60:ARG:HH12  | 1:P:80:ILE:H     | 1.66                     | 0.43              |
| 1:P:100:LYS:HG2  | 2:Q:45:GLN:OE1   | 2.18                     | 0.43              |
| 3:R:228:THR:HB   | 3:R:229:GLU:H    | 1.52                     | 0.43              |
| 1:G:81:PRO:O     | 1:G:84:VAL:HG23  | 2.17                     | 0.43              |
| 3:I:127:LYS:CD   | 3:I:128:GLU:H    | 2.29                     | 0.43              |
| 1:A:101:LEU:HD22 | 2:B:101:LEU:HD11 | 2.00                     | 0.43              |
| 2:B:143:CYS:SG   | 2:B:155:LEU:HD11 | 2.59                     | 0.43              |
| 3:C:195:SER:HA   | 3:C:196:ASP:HA   | 1.70                     | 0.43              |
| 3:C:234:ARG:HG2  | 4:D:10:TYR:CZ    | 2.54                     | 0.43              |
| 4:D:64:LEU:HD23  | 4:D:64:LEU:HA    | 1.75                     | 0.43              |
| 2:L:137:GLN:C    | 2:L:196:ALA:HB2  | 2.44                     | 0.43              |
| 3:M:209:TYR:CD1  | 3:M:210:PRO:HA   | 2.53                     | 0.43              |
| 1:P:124:GLN:O    | 1:P:125:LEU:HD13 | 2.19                     | 0.43              |
| 2:Q:221:TRP:CH2  | 2:Q:223:GLN:O    | 2.72                     | 0.43              |
| 1:G:129:LYS:HE2  | 2:H:124:ALA:HB2  | 2.01                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:177:ALA:HB3  | 1:G:190:PHE:HE1  | 1.83                     | 0.43              |
| 3:I:126:LEU:HD11 | 3:I:130:LEU:HA   | 1.99                     | 0.43              |
| 1:A:156:TYR:O    | 1:A:156:TYR:CG   | 2.70                     | 0.43              |
| 2:L:126:PHE:HD2  | 2:L:142:VAL:O    | 2.02                     | 0.43              |
| 1:P:50:TYR:C     | 1:P:51:LYS:HG2   | 2.43                     | 0.43              |
| 2:Q:136:THR:CB   | 2:Q:137:GLN:HA   | 2.38                     | 0.43              |
| 2:Q:150:PRO:HD2  | 2:Q:150:PRO:O    | 2.19                     | 0.43              |
| 3:R:81:LEU:HD23  | 3:R:81:LEU:HA    | 1.77                     | 0.43              |
| 4:U:5:PRO:HB2    | 4:U:7:ILE:HD11   | 2.00                     | 0.43              |
| 3:I:3:HIS:O      | 3:I:4:SER:OG     | 2.32                     | 0.43              |
| 3:I:95:VAL:HG22  | 3:I:118:TYR:HD1  | 1.83                     | 0.43              |
| 3:I:141:GLN:HE22 | 3:I:144:LYS:NZ   | 2.17                     | 0.43              |
| 1:A:36:LYS:NZ    | 1:A:84:VAL:C     | 2.77                     | 0.43              |
| 2:B:10:TYR:CD1   | 2:B:108:ARG:HB3  | 2.54                     | 0.43              |
| 2:B:167:GLY:O    | 2:B:192:LEU:HA   | 2.18                     | 0.43              |
| 2:B:225:ARG:O    | 2:B:226:ALA:C    | 2.61                     | 0.43              |
| 4:N:36:GLU:O     | 4:N:82:VAL:HG13  | 2.19                     | 0.43              |
| 1:P:61:LEU:HD23  | 1:P:76:ILE:HG12  | 2.01                     | 0.43              |
| 3:I:7:TYR:HE2    | 5:K:1:GLY:O      | 2.01                     | 0.43              |
| 3:I:180:GLN:HG3  | 3:I:180:GLN:O    | 2.19                     | 0.43              |
| 2:B:12:ILE:HD11  | 2:B:108:ARG:HH21 | 1.83                     | 0.43              |
| 2:B:13:THR:OG1   | 2:B:14:VAL:N     | 2.52                     | 0.43              |
| 2:B:149:TYR:HA   | 2:B:150:PRO:HA   | 1.75                     | 0.43              |
| 3:C:197:HIS:NE2  | 3:C:250:PRO:HB2  | 2.34                     | 0.43              |
| 4:N:91:LYS:HE2   | 4:N:91:LYS:HB3   | 1.76                     | 0.43              |
| 1:P:163:LEU:HD11 | 1:P:172:SER:HB3  | 2.01                     | 0.43              |
| 3:R:168:LEU:O    | 3:R:172:LEU:N    | 2.52                     | 0.43              |
| 1:G:22:ASN:HB3   | 1:G:73:PHE:CD2   | 2.53                     | 0.42              |
| 1:G:172:SER:OG   | 2:H:193:ARG:NH1  | 2.52                     | 0.42              |
| 2:H:64:TYR:O     | 2:H:65:LYS:HG3   | 2.18                     | 0.42              |
| 3:I:34:VAL:HG12  | 3:I:35:ARG:H     | 1.84                     | 0.42              |
| 4:D:39:LEU:HB2   | 4:D:46:ILE:HG21  | 2.01                     | 0.42              |
| 1:F:60:ARG:HH12  | 1:F:83:ASP:CG    | 2.26                     | 0.42              |
| 2:L:139:ALA:O    | 2:L:193:ARG:HA   | 2.18                     | 0.42              |
| 3:M:99:TYR:CB    | 3:M:114:HIS:HA   | 2.49                     | 0.42              |
| 3:M:126:LEU:HD21 | 3:M:130:LEU:HD23 | 2.00                     | 0.42              |
| 1:P:100:LYS:HE3  | 1:P:100:LYS:HB3  | 1.87                     | 0.42              |
| 1:G:93:GLY:HA2   | 1:G:94:GLY:HA3   | 1.62                     | 0.42              |
| 3:I:55:GLU:OE1   | 3:I:170:ARG:NH2  | 2.52                     | 0.42              |
| 1:A:116:GLN:H    | 1:A:116:GLN:CD   | 2.26                     | 0.42              |
| 2:Q:8:PRO:HD2    | 2:Q:21:VAL:HG13  | 2.01                     | 0.42              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 3:R:33:PHE:CD1  | 3:R:34:VAL:HG22  | 2.54                     | 0.42              |
| 3:R:204:TRP:HH2 | 4:U:99:MET:HA    | 1.84                     | 0.42              |
| 4:J:4:THR:OG1   | 4:J:5:PRO:CD     | 2.65                     | 0.42              |
| 3:M:146:LYS:HA  | 3:M:149:ALA:HB3  | 2.01                     | 0.42              |
| 4:N:30:PHE:O    | 4:N:62:PHE:HB2   | 2.20                     | 0.42              |
| 1:G:59:GLY:C    | 1:G:61:LEU:N     | 2.69                     | 0.42              |
| 2:H:8:PRO:HG3   | 2:H:11:LEU:HD12  | 2.02                     | 0.42              |
| 2:B:8:PRO:HG3   | 2:B:11:LEU:HD12  | 2.00                     | 0.42              |
| 2:B:64:TYR:CD1  | 2:B:78:LEU:HG    | 2.54                     | 0.42              |
| 1:F:135:VAL:HA  | 1:F:178:TRP:HB3  | 2.00                     | 0.42              |
| 3:M:262:GLN:NE2 | 3:M:263:HIS:O    | 2.52                     | 0.42              |
| 1:P:164:ASP:O   | 2:Q:167:GLY:N    | 2.44                     | 0.42              |
| 2:Q:128:PRO:HD2 | 2:Q:199:TRP:CZ2  | 2.54                     | 0.42              |
| 2:Q:215:LEU:O   | 2:Q:229:VAL:HG13 | 2.19                     | 0.42              |
| 1:F:120:PRO:HG3 | 1:F:196:PRO:HG2  | 2.01                     | 0.42              |
| 3:M:95:VAL:HG22 | 3:M:118:TYR:HD1  | 1.84                     | 0.42              |
| 4:N:30:PHE:CD2  | 4:N:31:HIS:N     | 2.88                     | 0.42              |
| 3:R:165:VAL:O   | 3:R:166:GLU:C    | 2.60                     | 0.42              |
| 2:H:46:ILE:C    | 2:H:47:TYR:HD1   | 2.28                     | 0.42              |
| 3:I:12:VAL:HG22 | 3:I:94:THR:HG23  | 2.01                     | 0.42              |
| 2:B:88:LEU:HD22 | 2:B:108:ARG:CA   | 2.48                     | 0.42              |
| 2:Q:86:THR:HG23 | 2:Q:110:THR:HA   | 2.01                     | 0.42              |
| 3:R:214:THR:C   | 3:R:215:LEU:HD23 | 2.44                     | 0.42              |
| 5:T:6:VAL:HB    | 5:T:7:PHE:H      | 1.68                     | 0.42              |
| 3:I:33:PHE:O    | 3:I:52:ILE:CD1   | 2.68                     | 0.42              |
| 1:A:119:ASP:HA  | 1:A:120:PRO:HD2  | 1.87                     | 0.42              |
| 2:B:34:TRP:CG   | 2:B:76:LEU:HD22  | 2.55                     | 0.42              |
| 3:C:37:ASP:HB3  | 3:C:40:ALA:HB3   | 2.02                     | 0.42              |
| 3:R:39:ASP:OD1  | 3:R:40:ALA:N     | 2.52                     | 0.42              |
| 3:R:144:LYS:O   | 3:R:148:GLU:N    | 2.51                     | 0.42              |
| 4:U:23:LEU:HB3  | 4:U:68:THR:HG23  | 2.01                     | 0.42              |
| 2:H:30:GLU:H    | 2:H:95:LEU:HA    | 1.84                     | 0.42              |
| 2:H:160:ASN:CA  | 2:H:205:HIS:HB2  | 2.50                     | 0.42              |
| 3:I:139:ALA:O   | 3:I:142:THR:HG23 | 2.20                     | 0.42              |
| 3:I:180:GLN:O   | 3:I:180:GLN:CG   | 2.68                     | 0.42              |
| 3:I:215:LEU:HA  | 3:I:260:HIS:O    | 2.20                     | 0.42              |
| 1:A:92:PRO:HG2  | 3:C:155:GLN:NE2  | 2.34                     | 0.42              |
| 2:B:7:ASN:HA    | 2:B:8:PRO:HA     | 1.73                     | 0.42              |
| 4:D:51:HIS:HB3  | 4:D:66:TYR:CD1   | 2.54                     | 0.42              |
| 2:L:50:MET:H    | 2:L:50:MET:HG3   | 1.50                     | 0.42              |
| 2:L:228:PRO:C   | 2:L:229:VAL:CG2  | 2.93                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:143:SER:C    | 1:P:145:THR:H    | 2.27                     | 0.42              |
| 1:P:157:ILE:HG22 | 1:P:158:THR:N    | 2.35                     | 0.42              |
| 2:Q:29:HIS:HB3   | 2:Q:94:SER:O     | 2.19                     | 0.42              |
| 3:R:49:ALA:HA    | 3:R:50:PRO:HD3   | 1.88                     | 0.42              |
| 1:A:153:SER:O    | 1:A:153:SER:OG   | 2.34                     | 0.42              |
| 3:M:148:GLU:CA   | 3:M:151:HIS:H    | 2.30                     | 0.42              |
| 3:M:241:PHE:N    | 3:M:241:PHE:CD1  | 2.86                     | 0.42              |
| 3:R:35:ARG:HA    | 3:R:35:ARG:HD3   | 1.76                     | 0.42              |
| 2:H:149:TYR:HA   | 2:H:150:PRO:HA   | 1.90                     | 0.42              |
| 2:B:8:PRO:HG2    | 2:B:11:LEU:HB2   | 2.02                     | 0.42              |
| 3:R:64:THR:O     | 3:R:67:VAL:HG12  | 2.20                     | 0.42              |
| 3:R:177:GLU:O    | 3:R:181:ARG:N    | 2.53                     | 0.42              |
| 2:H:79:GLU:O     | 3:R:270:LEU:HD21 | 2.20                     | 0.41              |
| 2:H:84:ASN:OD1   | 2:H:85:GLN:HG3   | 2.19                     | 0.41              |
| 3:I:104:GLY:C    | 3:I:106:ASP:N    | 2.78                     | 0.41              |
| 2:B:171:ASP:OD1  | 2:B:189:SER:HB3  | 2.20                     | 0.41              |
| 3:C:21:ARG:NH1   | 3:C:21:ARG:HG2   | 2.35                     | 0.41              |
| 3:M:116:TYR:CD2  | 5:O:9:LEU:HD21   | 2.54                     | 0.41              |
| 3:M:125:ALA:HB3  | 3:M:134:THR:OG1  | 2.19                     | 0.41              |
| 3:M:143:THR:OG1  | 3:M:144:LYS:N    | 2.54                     | 0.41              |
| 2:Q:135:HIS:ND1  | 2:Q:135:HIS:O    | 2.53                     | 0.41              |
| 3:R:27:TYR:HE1   | 3:R:32:GLN:HG2   | 1.84                     | 0.41              |
| 3:R:123:TYR:CZ   | 3:R:140:ALA:HA   | 2.55                     | 0.41              |
| 2:H:7:ASN:HB2    | 2:H:22:THR:HG23  | 2.01                     | 0.41              |
| 2:H:12:ILE:HD13  | 2:H:214:GLY:HA2  | 2.01                     | 0.41              |
| 3:I:126:LEU:HD21 | 3:I:130:LEU:HD22 | 2.01                     | 0.41              |
| 3:I:231:VAL:HG21 | 4:J:8:GLN:HE22   | 1.85                     | 0.41              |
| 3:C:59:TYR:CZ    | 3:C:63:GLU:HG3   | 2.55                     | 0.41              |
| 3:C:87:GLN:OE1   | 3:C:88:SER:N     | 2.37                     | 0.41              |
| 3:C:250:PRO:O    | 3:C:250:PRO:HG2  | 2.20                     | 0.41              |
| 1:P:139:THR:OG1  | 1:P:140:ASP:N    | 2.53                     | 0.41              |
| 2:Q:9:ARG:HA     | 2:Q:107:SER:HB2  | 2.00                     | 0.41              |
| 3:I:7:TYR:CG     | 5:K:2:ILE:HD12   | 2.55                     | 0.41              |
| 3:I:51:TRP:NE1   | 3:I:179:LEU:HD11 | 2.35                     | 0.41              |
| 3:I:208:PHE:CE1  | 3:I:213:ILE:HG13 | 2.56                     | 0.41              |
| 4:D:76:ASP:HB3   | 4:D:78:TYR:CD2   | 2.53                     | 0.41              |
| 4:J:3:ARG:HD2    | 4:J:3:ARG:HA     | 1.81                     | 0.41              |
| 3:C:33:PHE:CD2   | 3:C:51:TRP:CZ2   | 3.02                     | 0.41              |
| 3:C:109:PHE:HD1  | 3:C:165:VAL:HG21 | 1.86                     | 0.41              |
| 1:F:97:ASN:O     | 3:M:66:LYS:NZ    | 2.49                     | 0.41              |
| 2:L:95:LEU:HD12  | 2:L:96:ILE:CG1   | 2.50                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:Q:137:GLN:O    | 2:Q:196:ALA:HB3  | 2.21                     | 0.41              |
| 3:R:185:PRO:CD   | 3:R:263:HIS:HD2  | 2.25                     | 0.41              |
| 3:R:209:TYR:CD1  | 3:R:210:PRO:HA   | 2.55                     | 0.41              |
| 3:R:244:TRP:HB3  | 4:U:99:MET:HE1   | 2.01                     | 0.41              |
| 1:G:59:GLY:CA    | 1:G:60:ARG:CB    | 2.98                     | 0.41              |
| 2:H:25:GLN:NE2   | 2:H:29:HIS:CD2   | 2.77                     | 0.41              |
| 2:H:27:MET:O     | 2:H:27:MET:SD    | 2.79                     | 0.41              |
| 2:H:178:GLN:H    | 2:H:178:GLN:NE2  | 2.18                     | 0.41              |
| 3:I:84:TYR:CD2   | 3:I:139:ALA:HB2  | 2.55                     | 0.41              |
| 3:I:178:THR:C    | 3:I:179:LEU:HD12 | 2.45                     | 0.41              |
| 3:I:186:LYS:O    | 3:I:206:LEU:HB2  | 2.19                     | 0.41              |
| 2:B:10:TYR:HA    | 2:B:108:ARG:HB3  | 2.03                     | 0.41              |
| 3:C:33:PHE:CE2   | 3:C:51:TRP:HZ2   | 2.38                     | 0.41              |
| 1:F:11:MET:HE3   | 1:F:11:MET:HB2   | 1.81                     | 0.41              |
| 1:F:42:GLY:HA2   | 2:L:90:PHE:CE1   | 2.56                     | 0.41              |
| 1:F:126:ARG:NH1  | 1:F:129:LYS:NZ   | 2.69                     | 0.41              |
| 3:M:103:VAL:HG23 | 3:M:108:ARG:C    | 2.45                     | 0.41              |
| 4:N:64:LEU:HD23  | 4:N:64:LEU:HA    | 1.75                     | 0.41              |
| 2:Q:215:LEU:O    | 2:Q:215:LEU:HD12 | 2.21                     | 0.41              |
| 3:R:7:TYR:HD1    | 3:R:26:GLY:HA2   | 1.85                     | 0.41              |
| 1:G:59:GLY:HA3   | 1:G:61:LEU:CB    | 2.50                     | 0.41              |
| 3:I:74:HIS:HA    | 3:I:77:ASP:HB2   | 2.01                     | 0.41              |
| 1:A:163:LEU:HD12 | 1:A:164:ASP:H    | 1.84                     | 0.41              |
| 3:C:101:CYS:HA   | 3:C:112:GLY:HA2  | 2.01                     | 0.41              |
| 3:C:176:LYS:O    | 3:C:177:GLU:C    | 2.63                     | 0.41              |
| 1:F:147:VAL:HB   | 1:F:160:LYS:NZ   | 2.35                     | 0.41              |
| 3:M:23:ILE:HA    | 3:M:37:ASP:HB3   | 2.02                     | 0.41              |
| 3:M:147:TRP:O    | 3:M:152:VAL:HB   | 2.20                     | 0.41              |
| 2:Q:27:MET:HB3   | 2:Q:29:HIS:CD2   | 2.56                     | 0.41              |
| 3:R:3:HIS:CD2    | 3:R:172:LEU:HD11 | 2.56                     | 0.41              |
| 3:R:203:CYS:HB2  | 3:R:217:TRP:CZ2  | 2.56                     | 0.41              |
| 2:H:190:SER:O    | 2:H:191:ARG:HG3  | 2.21                     | 0.41              |
| 3:I:52:ILE:HD13  | 3:I:60:TRP:CH2   | 2.56                     | 0.41              |
| 3:I:175:GLY:HA3  | 3:I:179:LEU:HD22 | 2.03                     | 0.41              |
| 5:K:7:PHE:C      | 5:K:7:PHE:HD1    | 2.28                     | 0.41              |
| 1:A:125:LEU:HD22 | 2:B:128:PRO:HA   | 2.03                     | 0.41              |
| 4:D:47:GLU:H     | 4:D:47:GLU:HG2   | 1.57                     | 0.41              |
| 1:F:129:LYS:HZ3  | 1:F:131:SER:C    | 2.29                     | 0.41              |
| 2:L:97:TYR:HA    | 2:L:98:PRO:HA    | 1.84                     | 0.41              |
| 3:M:12:VAL:HG12  | 3:M:94:THR:HG23  | 2.01                     | 0.41              |
| 2:Q:178:GLN:HB2  | 2:Q:181:LEU:HD13 | 2.02                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:R:208:PHE:O    | 3:R:241:PHE:N    | 2.50                     | 0.41              |
| 2:H:179:PRO:O    | 2:H:180:ALA:C    | 2.63                     | 0.41              |
| 4:J:5:PRO:HB3    | 4:J:30:PHE:HD2   | 1.83                     | 0.41              |
| 4:D:22:PHE:CD1   | 4:D:69:GLU:HA    | 2.56                     | 0.41              |
| 3:M:17:ARG:NH1   | 3:M:17:ARG:CG    | 2.73                     | 0.41              |
| 3:M:201:LEU:HD23 | 3:M:249:VAL:HG11 | 2.01                     | 0.41              |
| 3:R:141:GLN:HA   | 3:R:144:LYS:HB3  | 2.03                     | 0.41              |
| 1:G:50:TYR:CE1   | 3:I:151:HIS:NE2  | 2.89                     | 0.41              |
| 1:G:166:ARG:H    | 1:G:166:ARG:HG2  | 1.69                     | 0.41              |
| 2:H:29:HIS:HE1   | 2:H:102:PHE:CE2  | 2.39                     | 0.41              |
| 4:D:37:VAL:HG22  | 4:D:82:VAL:HG22  | 2.02                     | 0.41              |
| 1:F:13:ILE:HD13  | 1:F:19:VAL:HG22  | 2.02                     | 0.41              |
| 4:N:18:GLY:N     | 4:N:72:PRO:O     | 2.52                     | 0.41              |
| 1:P:21:MET:HE1   | 1:P:87:TYR:CG    | 2.56                     | 0.41              |
| 2:Q:216:SER:C    | 2:Q:218:ASN:H    | 2.29                     | 0.41              |
| 3:R:44:ARG:HA    | 3:R:64:THR:HG21  | 2.03                     | 0.41              |
| 3:R:97:ARG:CZ    | 5:T:7:PHE:HZ     | 2.34                     | 0.41              |
| 3:R:117:ALA:CB   | 4:U:60:TRP:CZ3   | 3.04                     | 0.41              |
| 3:R:147:TRP:CD1  | 3:R:152:VAL:HG21 | 2.56                     | 0.41              |
| 4:U:23:LEU:HD12  | 4:U:24:ASN:H     | 1.86                     | 0.41              |
| 4:U:35:ILE:HG22  | 4:U:84:HIS:CG    | 2.54                     | 0.41              |
| 4:U:73:THR:HG22  | 4:U:75:LYS:H     | 1.85                     | 0.41              |
| 4:U:75:LYS:HZ3   | 4:U:75:LYS:CB    | 2.33                     | 0.41              |
| 2:H:34:TRP:CZ3   | 2:H:91:CYS:HB2   | 2.55                     | 0.41              |
| 2:H:205:HIS:HD2  | 2:H:236:GLU:OE2  | 2.03                     | 0.41              |
| 3:I:133:TRP:NE1  | 3:I:153:ALA:CB   | 2.84                     | 0.41              |
| 3:I:185:PRO:HB3  | 3:I:208:PHE:HB3  | 2.02                     | 0.41              |
| 3:I:229:GLU:CB   | 3:I:246:ALA:HB3  | 2.50                     | 0.41              |
| 4:J:71:THR:HA    | 4:J:72:PRO:HD3   | 1.92                     | 0.41              |
| 2:B:6:GLN:HE22   | 2:B:90:PHE:HA    | 1.86                     | 0.41              |
| 3:C:42:SER:C     | 3:C:44:ARG:N     | 2.78                     | 0.41              |
| 4:D:10:TYR:HB3   | 4:D:24:ASN:OD1   | 2.21                     | 0.41              |
| 1:P:159:ASP:CG   | 1:P:160:LYS:N    | 2.79                     | 0.41              |
| 3:R:82:ARG:NE    | 3:R:87:GLN:O     | 2.53                     | 0.41              |
| 1:G:24:THR:HG22  | 1:G:71:ASP:HB3   | 2.03                     | 0.40              |
| 1:G:36:LYS:HE3   | 1:G:36:LYS:HB2   | 1.92                     | 0.40              |
| 2:H:27:MET:SD    | 2:H:27:MET:C     | 3.04                     | 0.40              |
| 2:H:150:PRO:HG2  | 2:H:152:HIS:NE2  | 2.36                     | 0.40              |
| 2:B:6:GLN:NE2    | 2:B:90:PHE:HA    | 2.36                     | 0.40              |
| 2:B:121:PRO:HA   | 2:B:148:PHE:CD1  | 2.52                     | 0.40              |
| 2:B:129:SER:O    | 2:B:133:ILE:HG13 | 2.21                     | 0.40              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 4:D:37:VAL:HG13 | 4:D:82:VAL:HG22 | 2.02                     | 0.40              |
| 1:F:12:PHE:HD1  | 1:F:110:GLN:H   | 1.69                     | 0.40              |
| 1:F:147:VAL:HB  | 1:F:160:LYS:HZ2 | 1.85                     | 0.40              |
| 2:L:6:GLN:HE21  | 2:L:34:TRP:HH2  | 1.69                     | 0.40              |
| 4:N:41:LYS:NZ   | 4:N:76:ASP:OD2  | 2.32                     | 0.40              |
| 2:Q:115:LEU:H   | 2:Q:115:LEU:CD1 | 2.19                     | 0.40              |
| 3:R:24:ALA:O    | 3:R:35:ARG:HD3  | 2.21                     | 0.40              |
| 3:R:217:TRP:HD1 | 3:R:258:THR:CA  | 2.33                     | 0.40              |
| 4:J:41:LYS:CG   | 4:J:78:TYR:HD1  | 2.23                     | 0.40              |
| 2:B:50:MET:O    | 2:B:54:VAL:HB   | 2.21                     | 0.40              |
| 1:F:129:LYS:HG3 | 1:F:130:SER:N   | 2.35                     | 0.40              |
| 1:G:100:LYS:HE2 | 1:G:100:LYS:HB2 | 1.78                     | 0.40              |
| 1:A:112:LYS:HA  | 1:A:113:PRO:HD3 | 1.97                     | 0.40              |
| 2:B:7:ASN:O     | 2:B:21:VAL:HG13 | 2.22                     | 0.40              |
| 2:B:50:MET:HE1  | 5:E:5:PHE:HA    | 2.01                     | 0.40              |
| 2:B:68:ARG:HD2  | 2:B:74:PHE:CD1  | 2.56                     | 0.40              |
| 2:B:88:LEU:CD2  | 2:B:108:ARG:HG3 | 2.49                     | 0.40              |
| 2:B:222:THR:HA  | 2:B:223:GLN:HA  | 1.69                     | 0.40              |
| 3:C:49:ALA:HB3  | 3:C:51:TRP:CH2  | 2.56                     | 0.40              |
| 3:M:16:GLY:HA2  | 3:M:17:ARG:HA   | 1.50                     | 0.40              |
| 3:M:85:TYR:HB3  | 3:M:87:GLN:HE22 | 1.86                     | 0.40              |
| 3:M:116:TYR:HD2 | 5:O:9:LEU:HD21  | 1.85                     | 0.40              |
| 4:N:96:ASP:OD1  | 4:N:97:ARG:N    | 2.53                     | 0.40              |
| 1:P:43:PRO:HD2  | 2:Q:103:PHE:CG  | 2.56                     | 0.40              |
| 1:P:180:ASN:O   | 1:P:181:LYS:HB3 | 2.21                     | 0.40              |
| 3:R:244:TRP:HE1 | 3:R:246:ALA:HB2 | 1.86                     | 0.40              |
| 1:G:94:GLY:C    | 1:G:96:SER:N    | 2.77                     | 0.40              |
| 2:H:221:TRP:CD2 | 2:H:227:LYS:HG2 | 2.57                     | 0.40              |
| 3:I:116:TYR:OH  | 5:K:7:PHE:CE1   | 2.73                     | 0.40              |
| 1:A:200:PHE:CG  | 1:A:201:PHE:N   | 2.89                     | 0.40              |
| 2:B:120:PRO:HD3 | 2:B:228:PRO:HB3 | 2.03                     | 0.40              |
| 3:C:216:THR:O   | 3:C:260:HIS:CE1 | 2.74                     | 0.40              |
| 1:F:20:SER:HB2  | 1:P:68:THR:HG22 | 2.04                     | 0.40              |
| 1:F:124:GLN:O   | 2:L:129:SER:HB2 | 2.21                     | 0.40              |
| 3:M:8:PHE:N     | 3:M:25:VAL:O    | 2.55                     | 0.40              |
| 1:P:47:ILE:HG23 | 1:P:57:SER:CB   | 2.51                     | 0.40              |
| 1:P:119:ASP:O   | 1:P:120:PRO:C   | 2.63                     | 0.40              |
| 3:R:13:SER:HA   | 3:R:20:PRO:HB3  | 2.03                     | 0.40              |
| 1:G:4:LEU:HD13  | 1:G:25:SER:HB2  | 2.02                     | 0.40              |
| 3:I:87:GLN:NE2  | 3:I:87:GLN:HA   | 2.36                     | 0.40              |
| 3:I:262:GLN:HB3 | 3:I:269:PRO:HB3 | 2.03                     | 0.40              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 4:J:23:LEU:HG    | 4:J:70:PHE:HD2  | 1.85                     | 0.40              |
| 2:L:229:VAL:HG12 | 2:L:230:THR:N   | 2.36                     | 0.40              |
| 3:M:14:ARG:HD3   | 3:M:21:ARG:NH1  | 2.32                     | 0.40              |
| 3:M:119:ASP:C    | 4:N:31:HIS:CE1  | 2.99                     | 0.40              |
| 3:M:195:SER:O    | 3:M:196:ASP:HB2 | 2.22                     | 0.40              |
| 4:N:54:LEU:HD21  | 4:N:62:PHE:HE2  | 1.86                     | 0.40              |
| 1:P:30:ASN:HA    | 1:P:65:PHE:HZ   | 1.87                     | 0.40              |
| 1:P:37:GLN:O     | 1:P:86:ILE:HG13 | 2.22                     | 0.40              |
| 2:Q:65:LYS:HB2   | 2:Q:65:LYS:HE3  | 1.85                     | 0.40              |
| 2:Q:82:SER:HG    | 2:Q:84:ASN:HB3  | 1.85                     | 0.40              |
| 3:R:130:LEU:O    | 3:R:131:ARG:HG3 | 2.22                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 1   | A     | 192/208 (92%) | 161 (84%) | 31 (16%) | 0        | 100         | 100 |
| 1   | F     | 194/208 (93%) | 173 (89%) | 20 (10%) | 1 (0%)   | 24          | 60  |
| 1   | G     | 199/208 (96%) | 176 (88%) | 23 (12%) | 0        | 100         | 100 |
| 1   | P     | 185/208 (89%) | 151 (82%) | 32 (17%) | 2 (1%)   | 11          | 44  |
| 2   | B     | 239/243 (98%) | 212 (89%) | 26 (11%) | 1 (0%)   | 30          | 65  |
| 2   | H     | 237/243 (98%) | 201 (85%) | 32 (14%) | 4 (2%)   | 7           | 36  |
| 2   | L     | 240/243 (99%) | 213 (89%) | 27 (11%) | 0        | 100         | 100 |
| 2   | Q     | 234/243 (96%) | 211 (90%) | 21 (9%)  | 2 (1%)   | 14          | 48  |
| 3   | C     | 252/276 (91%) | 223 (88%) | 29 (12%) | 0        | 100         | 100 |
| 3   | I     | 253/276 (92%) | 218 (86%) | 34 (13%) | 1 (0%)   | 30          | 65  |
| 3   | M     | 260/276 (94%) | 225 (86%) | 33 (13%) | 2 (1%)   | 16          | 52  |

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| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|-----------|----------|-------------|-----|
| 3   | R     | 241/276 (87%)   | 210 (87%)  | 31 (13%)  | 0        | 100         | 100 |
| 4   | D     | 95/100 (95%)    | 82 (86%)   | 13 (14%)  | 0        | 100         | 100 |
| 4   | J     | 92/100 (92%)    | 86 (94%)   | 6 (6%)    | 0        | 100         | 100 |
| 4   | N     | 88/100 (88%)    | 76 (86%)   | 10 (11%)  | 2 (2%)   | 5           | 31  |
| 4   | U     | 97/100 (97%)    | 82 (84%)   | 14 (14%)  | 1 (1%)   | 12          | 45  |
| 5   | E     | 7/9 (78%)       | 7 (100%)   | 0         | 0        | 100         | 100 |
| 5   | K     | 7/9 (78%)       | 7 (100%)   | 0         | 0        | 100         | 100 |
| 5   | O     | 7/9 (78%)       | 5 (71%)    | 2 (29%)   | 0        | 100         | 100 |
| 5   | T     | 7/9 (78%)       | 5 (71%)    | 2 (29%)   | 0        | 100         | 100 |
| All | All   | 3126/3344 (94%) | 2724 (87%) | 386 (12%) | 16 (0%)  | 24          | 60  |

All (16) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | I     | 156 | LEU  |
| 4   | N     | 26  | TYR  |
| 4   | N     | 72  | PRO  |
| 2   | Q     | 136 | THR  |
| 2   | H     | 61  | PRO  |
| 3   | M     | 218 | GLN  |
| 1   | P     | 118 | PRO  |
| 4   | U     | 87  | LEU  |
| 2   | H     | 229 | VAL  |
| 2   | B     | 145 | ALA  |
| 3   | M     | 18  | GLY  |
| 2   | Q     | 150 | PRO  |
| 1   | F     | 59  | GLY  |
| 2   | H     | 75  | PRO  |
| 1   | P     | 120 | PRO  |
| 2   | H     | 179 | 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     | 162/183 (88%)   | 150 (93%)  | 12 (7%)  | 13          | 36  |
| 1   | F     | 165/183 (90%)   | 152 (92%)  | 13 (8%)  | 11          | 35  |
| 1   | G     | 175/183 (96%)   | 162 (93%)  | 13 (7%)  | 13          | 36  |
| 1   | P     | 157/183 (86%)   | 151 (96%)  | 6 (4%)   | 29          | 51  |
| 2   | B     | 201/217 (93%)   | 188 (94%)  | 13 (6%)  | 15          | 40  |
| 2   | H     | 204/217 (94%)   | 193 (95%)  | 11 (5%)  | 20          | 44  |
| 2   | L     | 205/217 (94%)   | 193 (94%)  | 12 (6%)  | 18          | 42  |
| 2   | Q     | 198/217 (91%)   | 183 (92%)  | 15 (8%)  | 12          | 36  |
| 3   | C     | 205/232 (88%)   | 185 (90%)  | 20 (10%) | 7           | 27  |
| 3   | I     | 206/232 (89%)   | 181 (88%)  | 25 (12%) | 5           | 21  |
| 3   | M     | 203/232 (88%)   | 193 (95%)  | 10 (5%)  | 22          | 46  |
| 3   | R     | 201/232 (87%)   | 188 (94%)  | 13 (6%)  | 15          | 40  |
| 4   | D     | 87/95 (92%)     | 77 (88%)   | 10 (12%) | 5           | 22  |
| 4   | J     | 85/95 (90%)     | 72 (85%)   | 13 (15%) | 3           | 15  |
| 4   | N     | 70/95 (74%)     | 58 (83%)   | 12 (17%) | 2           | 13  |
| 4   | U     | 87/95 (92%)     | 81 (93%)   | 6 (7%)   | 14          | 39  |
| 5   | E     | 7/7 (100%)      | 7 (100%)   | 0        | 100         | 100 |
| 5   | K     | 7/7 (100%)      | 7 (100%)   | 0        | 100         | 100 |
| 5   | O     | 7/7 (100%)      | 7 (100%)   | 0        | 100         | 100 |
| 5   | T     | 7/7 (100%)      | 7 (100%)   | 0        | 100         | 100 |
| All | All   | 2639/2936 (90%) | 2435 (92%) | 204 (8%) | 12          | 35  |

All (204) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 9   | GLN  |
| 1   | G     | 19  | VAL  |
| 1   | G     | 31  | THR  |
| 1   | G     | 71  | ASP  |
| 1   | G     | 74  | LEU  |
| 1   | G     | 95  | SER  |
| 1   | G     | 96  | SER  |
| 1   | G     | 100 | LYS  |
| 1   | G     | 108 | THR  |
| 1   | G     | 133 | LYS  |
| 1   | G     | 160 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 180 | ASN  |
| 1   | G     | 194 | ILE  |
| 2   | H     | 6   | GLN  |
| 2   | H     | 32  | MET  |
| 2   | H     | 43  | LEU  |
| 2   | H     | 62  | GLU  |
| 2   | H     | 153 | VAL  |
| 2   | H     | 163 | GLU  |
| 2   | H     | 176 | LYS  |
| 2   | H     | 177 | GLU  |
| 2   | H     | 204 | ASN  |
| 2   | H     | 216 | SER  |
| 2   | H     | 217 | GLU  |
| 3   | I     | 13  | SER  |
| 3   | I     | 23  | ILE  |
| 3   | I     | 34  | VAL  |
| 3   | I     | 66  | LYS  |
| 3   | I     | 68  | LYS  |
| 3   | I     | 75  | ARG  |
| 3   | I     | 87  | GLN  |
| 3   | I     | 89  | GLU  |
| 3   | I     | 103 | VAL  |
| 3   | I     | 119 | ASP  |
| 3   | I     | 142 | THR  |
| 3   | I     | 146 | LYS  |
| 3   | I     | 165 | VAL  |
| 3   | I     | 177 | GLU  |
| 3   | I     | 180 | GLN  |
| 3   | I     | 191 | HIS  |
| 3   | I     | 207 | SER  |
| 3   | I     | 213 | ILE  |
| 3   | I     | 231 | VAL  |
| 3   | I     | 238 | ASP  |
| 3   | I     | 248 | VAL  |
| 3   | I     | 258 | THR  |
| 3   | I     | 263 | HIS  |
| 3   | I     | 268 | LYS  |
| 3   | I     | 273 | ARG  |
| 4   | J     | 3   | ARG  |
| 4   | J     | 22  | PHE  |
| 4   | J     | 31  | HIS  |
| 4   | J     | 36  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | J     | 39  | LEU  |
| 4   | J     | 45  | ARG  |
| 4   | J     | 48  | LYS  |
| 4   | J     | 69  | GLU  |
| 4   | J     | 74  | GLU  |
| 4   | J     | 77  | GLU  |
| 4   | J     | 78  | TYR  |
| 4   | J     | 91  | LYS  |
| 4   | J     | 94  | LYS  |
| 1   | A     | 9   | GLN  |
| 1   | A     | 28  | ILE  |
| 1   | A     | 33  | LEU  |
| 1   | A     | 58  | ASN  |
| 1   | A     | 79  | SER  |
| 1   | A     | 86  | ILE  |
| 1   | A     | 122 | VAL  |
| 1   | A     | 143 | SER  |
| 1   | A     | 149 | GLN  |
| 1   | A     | 151 | LYS  |
| 1   | A     | 156 | TYR  |
| 1   | A     | 184 | PHE  |
| 2   | B     | 25  | GLN  |
| 2   | B     | 27  | MET  |
| 2   | B     | 79  | GLU  |
| 2   | B     | 127 | GLU  |
| 2   | B     | 130 | GLU  |
| 2   | B     | 136 | THR  |
| 2   | B     | 141 | LEU  |
| 2   | B     | 150 | PRO  |
| 2   | B     | 156 | SER  |
| 2   | B     | 181 | LEU  |
| 2   | B     | 197 | THR  |
| 2   | B     | 215 | LEU  |
| 2   | B     | 224 | ASP  |
| 3   | C     | 25  | VAL  |
| 3   | C     | 34  | VAL  |
| 3   | C     | 35  | ARG  |
| 3   | C     | 42  | SER  |
| 3   | C     | 44  | ARG  |
| 3   | C     | 102 | ASP  |
| 3   | C     | 124 | ILE  |
| 3   | C     | 138 | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 155 | GLN  |
| 3   | C     | 160 | LEU  |
| 3   | C     | 170 | ARG  |
| 3   | C     | 201 | LEU  |
| 3   | C     | 203 | CYS  |
| 3   | C     | 213 | ILE  |
| 3   | C     | 214 | THR  |
| 3   | C     | 215 | LEU  |
| 3   | C     | 248 | VAL  |
| 3   | C     | 262 | GLN  |
| 3   | C     | 268 | LYS  |
| 3   | C     | 270 | LEU  |
| 4   | D     | 10  | TYR  |
| 4   | D     | 24  | ASN  |
| 4   | D     | 41  | LYS  |
| 4   | D     | 47  | GLU  |
| 4   | D     | 48  | LYS  |
| 4   | D     | 58  | LYS  |
| 4   | D     | 74  | GLU  |
| 4   | D     | 75  | LYS  |
| 4   | D     | 86  | THR  |
| 4   | D     | 87  | LEU  |
| 1   | F     | 19  | VAL  |
| 1   | F     | 31  | THR  |
| 1   | F     | 61  | LEU  |
| 1   | F     | 62  | THR  |
| 1   | F     | 72  | SER  |
| 1   | F     | 74  | LEU  |
| 1   | F     | 110 | GLN  |
| 1   | F     | 115 | ILE  |
| 1   | F     | 116 | GLN  |
| 1   | F     | 150 | SER  |
| 1   | F     | 160 | LYS  |
| 1   | F     | 166 | ARG  |
| 1   | F     | 176 | VAL  |
| 2   | L     | 3   | GLN  |
| 2   | L     | 4   | VAL  |
| 2   | L     | 6   | GLN  |
| 2   | L     | 45  | GLN  |
| 2   | L     | 50  | MET  |
| 2   | L     | 69  | LYS  |
| 2   | L     | 118 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | L     | 141 | LEU  |
| 2   | L     | 178 | GLN  |
| 2   | L     | 224 | ASP  |
| 2   | L     | 233 | VAL  |
| 2   | L     | 240 | ARG  |
| 3   | M     | 17  | ARG  |
| 3   | M     | 25  | VAL  |
| 3   | M     | 65  | ARG  |
| 3   | M     | 88  | SER  |
| 3   | M     | 145 | HIS  |
| 3   | M     | 173 | GLU  |
| 3   | M     | 186 | LYS  |
| 3   | M     | 216 | THR  |
| 3   | M     | 231 | VAL  |
| 3   | M     | 268 | LYS  |
| 4   | N     | 4   | THR  |
| 4   | N     | 6   | LYS  |
| 4   | N     | 23  | LEU  |
| 4   | N     | 24  | ASN  |
| 4   | N     | 31  | HIS  |
| 4   | N     | 35  | ILE  |
| 4   | N     | 36  | GLU  |
| 4   | N     | 50  | GLU  |
| 4   | N     | 51  | HIS  |
| 4   | N     | 61  | SER  |
| 4   | N     | 65  | LEU  |
| 4   | N     | 83  | ASN  |
| 1   | P     | 18  | ASP  |
| 1   | P     | 74  | LEU  |
| 1   | P     | 100 | LYS  |
| 1   | P     | 125 | LEU  |
| 1   | P     | 136 | CYS  |
| 1   | P     | 162 | VAL  |
| 2   | Q     | 14  | VAL  |
| 2   | Q     | 43  | LEU  |
| 2   | Q     | 53  | GLU  |
| 2   | Q     | 60  | VAL  |
| 2   | Q     | 65  | LYS  |
| 2   | Q     | 82  | SER  |
| 2   | Q     | 95  | LEU  |
| 2   | Q     | 115 | LEU  |
| 2   | Q     | 132 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | Q     | 154 | GLU  |
| 2   | Q     | 173 | GLN  |
| 2   | Q     | 193 | ARG  |
| 2   | Q     | 200 | GLN  |
| 2   | Q     | 215 | LEU  |
| 2   | Q     | 223 | GLN  |
| 3   | R     | 2   | SER  |
| 3   | R     | 3   | HIS  |
| 3   | R     | 25  | VAL  |
| 3   | R     | 108 | ARG  |
| 3   | R     | 165 | VAL  |
| 3   | R     | 176 | LYS  |
| 3   | R     | 189 | MET  |
| 3   | R     | 203 | CYS  |
| 3   | R     | 228 | THR  |
| 3   | R     | 232 | GLU  |
| 3   | R     | 247 | VAL  |
| 3   | R     | 248 | VAL  |
| 3   | R     | 259 | CYS  |
| 4   | U     | 16  | GLU  |
| 4   | U     | 28  | SER  |
| 4   | U     | 45  | ARG  |
| 4   | U     | 49  | VAL  |
| 4   | U     | 75  | LYS  |
| 4   | U     | 89  | GLN  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 3   | GLN  |
| 1   | G     | 6   | GLN  |
| 1   | G     | 37  | GLN  |
| 1   | G     | 180 | ASN  |
| 2   | H     | 25  | GLN  |
| 2   | H     | 29  | HIS  |
| 2   | H     | 37  | GLN  |
| 2   | H     | 85  | GLN  |
| 2   | H     | 182 | ASN  |
| 2   | H     | 200 | GLN  |
| 3   | I     | 114 | HIS  |
| 3   | I     | 141 | GLN  |
| 3   | I     | 151 | HIS  |

*Continued on next page...*

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | I     | 155 | GLN  |
| 4   | J     | 24  | ASN  |
| 4   | J     | 89  | GLN  |
| 1   | A     | 9   | GLN  |
| 1   | A     | 149 | GLN  |
| 2   | B     | 7   | ASN  |
| 2   | B     | 51  | ASN  |
| 2   | B     | 204 | ASN  |
| 3   | C     | 96  | GLN  |
| 3   | C     | 151 | HIS  |
| 3   | C     | 192 | HIS  |
| 3   | C     | 260 | HIS  |
| 4   | D     | 13  | HIS  |
| 1   | F     | 192 | ASN  |
| 2   | L     | 6   | GLN  |
| 2   | L     | 25  | GLN  |
| 2   | L     | 51  | ASN  |
| 2   | L     | 205 | HIS  |
| 3   | M     | 145 | HIS  |
| 3   | M     | 155 | GLN  |
| 3   | M     | 253 | GLN  |
| 4   | N     | 42  | ASN  |
| 4   | N     | 84  | HIS  |
| 1   | P     | 5   | ASN  |
| 1   | P     | 6   | GLN  |
| 1   | P     | 37  | GLN  |
| 1   | P     | 110 | GLN  |
| 2   | Q     | 37  | GLN  |
| 2   | Q     | 152 | HIS  |
| 2   | Q     | 160 | ASN  |
| 2   | Q     | 218 | ASN  |
| 3   | R     | 115 | GLN  |
| 4   | U     | 83  | ASN  |

### 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 [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2   | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|-----------|-----------------------|-------|
| 1   | A     | 196/208 (94%)   | -0.94  | 0 100 100 | 57, 111, 150, 165     | 0     |
| 1   | F     | 198/208 (95%)   | -0.94  | 0 100 100 | 57, 94, 135, 145      | 0     |
| 1   | G     | 201/208 (96%)   | -0.94  | 0 100 100 | 50, 92, 133, 156      | 0     |
| 1   | P     | 191/208 (91%)   | -0.87  | 0 100 100 | 60, 101, 146, 158     | 0     |
| 2   | B     | 241/243 (99%)   | -0.95  | 0 100 100 | 61, 99, 139, 160      | 0     |
| 2   | H     | 239/243 (98%)   | -0.89  | 0 100 100 | 65, 92, 132, 144      | 0     |
| 2   | L     | 242/243 (99%)   | -0.94  | 0 100 100 | 70, 91, 131, 165      | 0     |
| 2   | Q     | 238/243 (97%)   | -0.89  | 0 100 100 | 77, 102, 130, 151     | 0     |
| 3   | C     | 258/276 (93%)   | -0.90  | 0 100 100 | 74, 110, 154, 176     | 0     |
| 3   | I     | 261/276 (94%)   | -0.88  | 0 100 100 | 91, 119, 150, 182     | 0     |
| 3   | M     | 268/276 (97%)   | -0.83  | 0 100 100 | 83, 122, 159, 176     | 0     |
| 3   | R     | 251/276 (90%)   | -0.92  | 0 100 100 | 72, 106, 145, 152     | 0     |
| 4   | D     | 97/100 (97%)    | -0.86  | 0 100 100 | 84, 127, 157, 167     | 0     |
| 4   | J     | 96/100 (96%)    | -0.83  | 0 100 100 | 106, 135, 164, 170    | 0     |
| 4   | N     | 92/100 (92%)    | -0.91  | 0 100 100 | 100, 136, 168, 174    | 0     |
| 4   | U     | 99/100 (99%)    | -0.89  | 0 100 100 | 79, 130, 151, 174     | 0     |
| 5   | E     | 9/9 (100%)      | -1.01  | 0 100 100 | 80, 83, 89, 92        | 0     |
| 5   | K     | 9/9 (100%)      | -0.81  | 0 100 100 | 91, 97, 103, 106      | 0     |
| 5   | O     | 9/9 (100%)      | -0.70  | 0 100 100 | 87, 104, 113, 114     | 0     |
| 5   | T     | 9/9 (100%)      | -0.87  | 0 100 100 | 78, 83, 90, 91        | 0     |
| All | All   | 3204/3344 (95%) | -0.90  | 0 100 100 | 50, 107, 149, 182     | 0     |

There are no RSRZ outliers to report.

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.