



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 12:33 AM UTC

PDB ID : 3SJV / pdb\_00003sjv  
Title : Crystal structure of the RL42 TCR in complex with HLA-B8-FLR  
Authors : Gras, S.; Wilmann, P.G.; Zhenjun, C.; Hanim, H.; Yu Chih, L.; Kjer-Nielsen, L.; Purcell, A.W.; Burrows, S.R.; Mccluskey, J.; Rossjohn, J.  
Deposited on : 2011-06-22  
Resolution : 3.10 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                                                             |

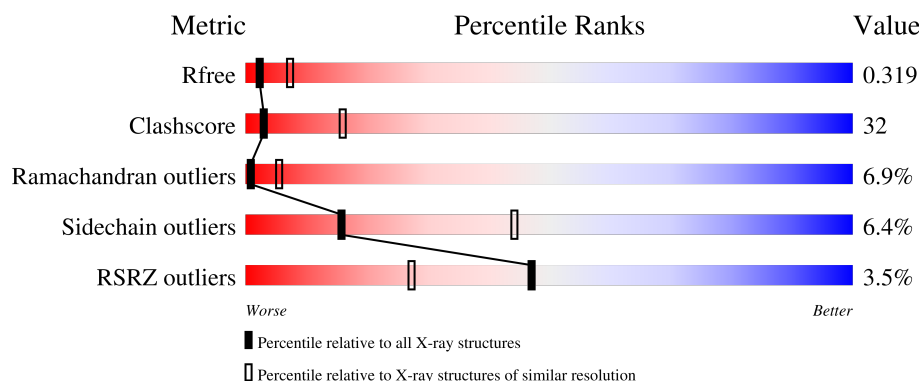
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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                      | 1456 (3.10-3.10)                                      |
| Clashscore            | 190562                      | 1539 (3.10-3.10)                                      |
| Ramachandran outliers | 187476                      | 1467 (3.10-3.10)                                      |
| Sidechain outliers    | 187428                      | 1467 (3.10-3.10)                                      |
| RSRZ outliers         | 180081                      | 1456 (3.10-3.10)                                      |

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     | 277    | <div> <div>7%</div> <div>43%</div> <div>47%</div> <div>10%</div> </div> |
| 1   | F     | 277    | <div> <div>5%</div> <div>44%</div> <div>49%</div> <div>7%</div> </div>  |
| 1   | K     | 277    | <div> <div>7%</div> <div>48%</div> <div>47%</div> <div>5%</div> </div>  |
| 1   | P     | 277    | <div> <div>%</div> <div>47%</div> <div>45%</div> <div>9%</div> </div>   |
| 2   | B     | 100    | <div> <div>%</div> <div>49%</div> <div>40%</div> <div>10%</div> </div>  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 2   | G     | 100    |                  |
| 2   | L     | 100    |                  |
| 2   | Q     | 100    |                  |
| 3   | C     | 9      |                  |
| 3   | H     | 9      |                  |
| 3   | M     | 9      |                  |
| 3   | R     | 9      |                  |
| 4   | D     | 203    |                  |
| 4   | I     | 203    |                  |
| 4   | N     | 203    |                  |
| 4   | S     | 203    |                  |
| 5   | E     | 244    |                  |
| 5   | J     | 244    |                  |
| 5   | O     | 244    |                  |
| 5   | T     | 244    |                  |

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 26455 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 HLA class I histocompatibility antigen, B-8 alpha chain.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | A     | 277      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2258  | 1398 | 412 | 441 | 7 |         |         |       |
| 1   | F     | 277      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2258  | 1398 | 412 | 441 | 7 |         |         |       |
| 1   | K     | 277      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2258  | 1398 | 412 | 441 | 7 |         |         |       |
| 1   | P     | 277      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2258  | 1398 | 412 | 441 | 7 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2   | B     | 99       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 829   | 528 | 140 | 158 | 3 |         |         |       |
| 2   | G     | 99       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 829   | 528 | 140 | 158 | 3 |         |         |       |
| 2   | L     | 100      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 837   | 533 | 141 | 159 | 4 |         |         |       |
| 2   | Q     | 100      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 837   | 533 | 141 | 159 | 4 |         |         |       |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| B     | 0       | MET      | -      | initiating methionine | UNP P61769 |
| G     | 0       | MET      | -      | initiating methionine | UNP P61769 |
| L     | 0       | MET      | -      | initiating methionine | UNP P61769 |
| Q     | 0       | MET      | -      | initiating methionine | UNP P61769 |

- Molecule 3 is a protein called Epstein-Barr nuclear antigen 3.

| Mol | Chain | Residues | Atoms |    |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|---------|-------|
| 3   | C     | 9        | Total | C  | N  | O  | 0       | 0       | 0     |
|     |       |          | 75    | 49 | 15 | 11 |         |         |       |
| 3   | H     | 9        | Total | C  | N  | O  | 0       | 0       | 0     |
|     |       |          | 75    | 49 | 15 | 11 |         |         |       |
| 3   | M     | 9        | Total | C  | N  | O  | 0       | 0       | 0     |
|     |       |          | 75    | 49 | 15 | 11 |         |         |       |
| 3   | R     | 9        | Total | C  | N  | O  | 0       | 0       | 0     |
|     |       |          | 75    | 49 | 15 | 11 |         |         |       |

- Molecule 4 is a protein called RL42 T cell receptor, alpha chain.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 4   | D     | 197      | Total | C   | N   | O   | S | 1       | 0       | 0     |
|     |       |          | 1541  | 962 | 258 | 313 | 8 |         |         |       |
| 4   | I     | 197      | Total | C   | N   | O   | S | 1       | 0       | 0     |
|     |       |          | 1541  | 962 | 258 | 313 | 8 |         |         |       |
| 4   | N     | 197      | Total | C   | N   | O   | S | 1       | 0       | 0     |
|     |       |          | 1541  | 962 | 258 | 313 | 8 |         |         |       |
| 4   | S     | 197      | Total | C   | N   | O   | S | 1       | 0       | 0     |
|     |       |          | 1541  | 962 | 258 | 313 | 8 |         |         |       |

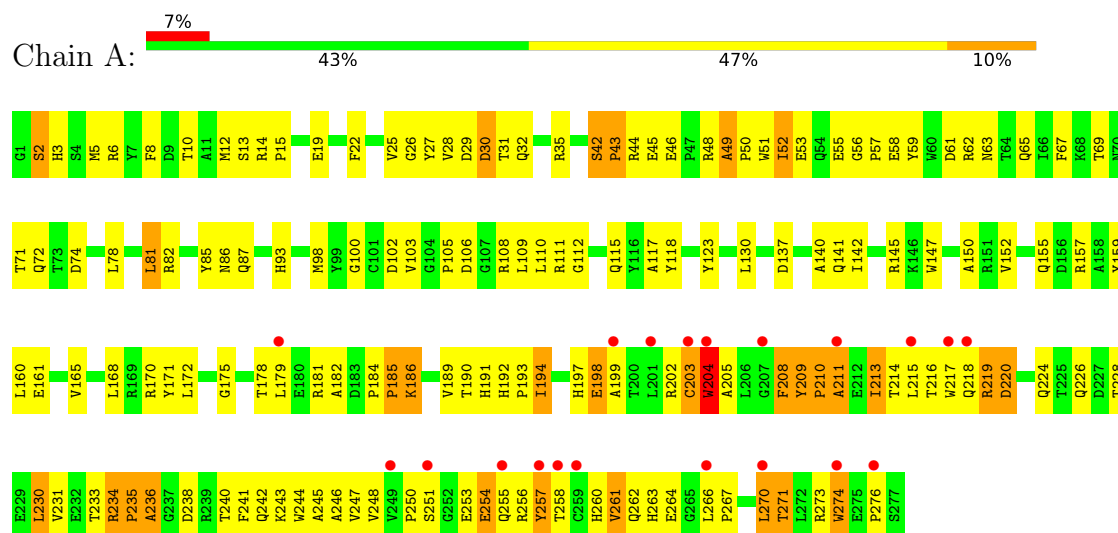
- Molecule 5 is a protein called RL42 T cell receptor, beta chain.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 5   | E     | 241      | Total | C    | N   | O   | S | 2       | 0       | 0     |
|     |       |          | 1908  | 1205 | 331 | 363 | 9 |         |         |       |
| 5   | J     | 240      | Total | C    | N   | O   | S | 2       | 0       | 0     |
|     |       |          | 1903  | 1202 | 330 | 362 | 9 |         |         |       |
| 5   | O     | 241      | Total | C    | N   | O   | S | 2       | 0       | 0     |
|     |       |          | 1908  | 1205 | 331 | 363 | 9 |         |         |       |
| 5   | T     | 241      | Total | C    | N   | O   | S | 2       | 0       | 0     |
|     |       |          | 1908  | 1205 | 331 | 363 | 9 |         |         |       |

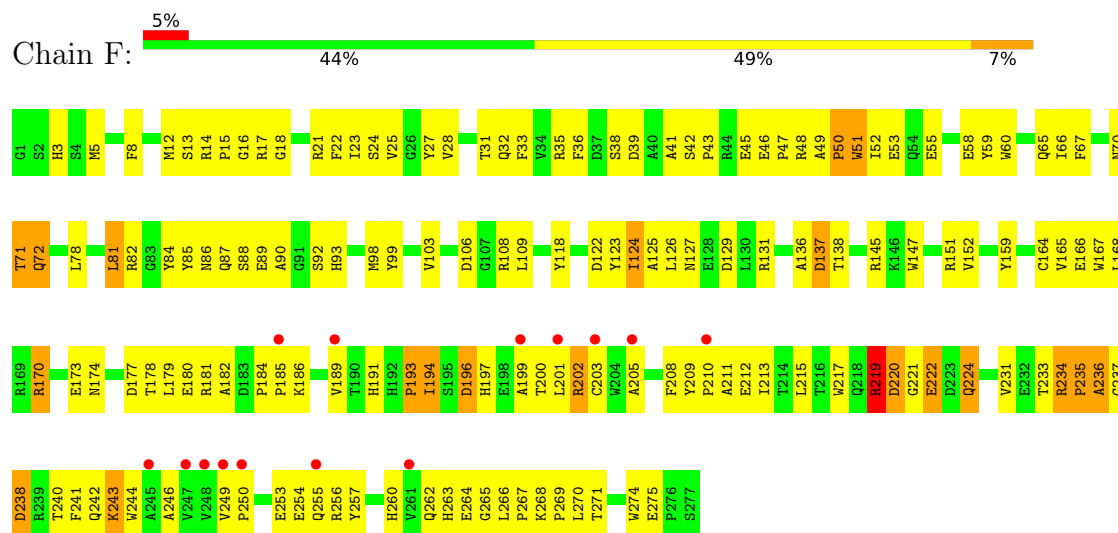
### 3 Residue-property plots

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

- Molecule 1: HLA class I histocompatibility antigen, B-8 alpha chain

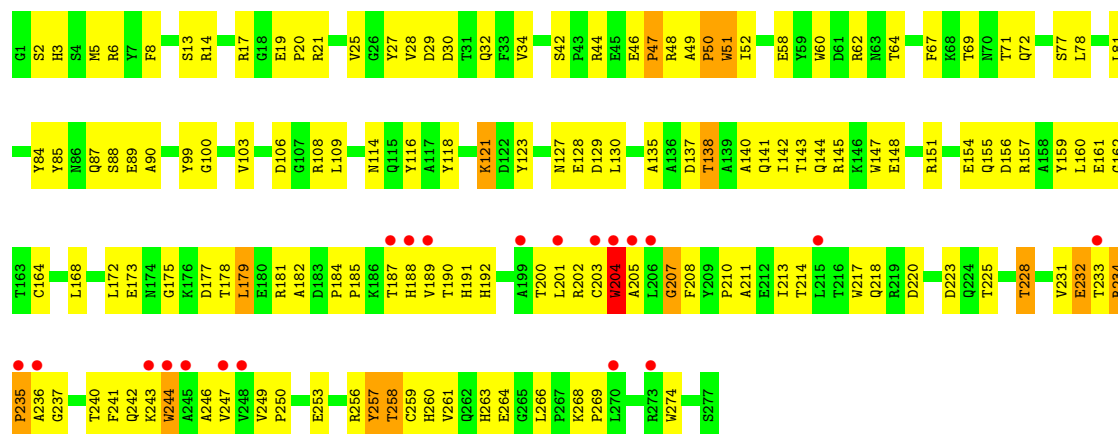


- Molecule 1: HLA class I histocompatibility antigen, B-8 alpha chain

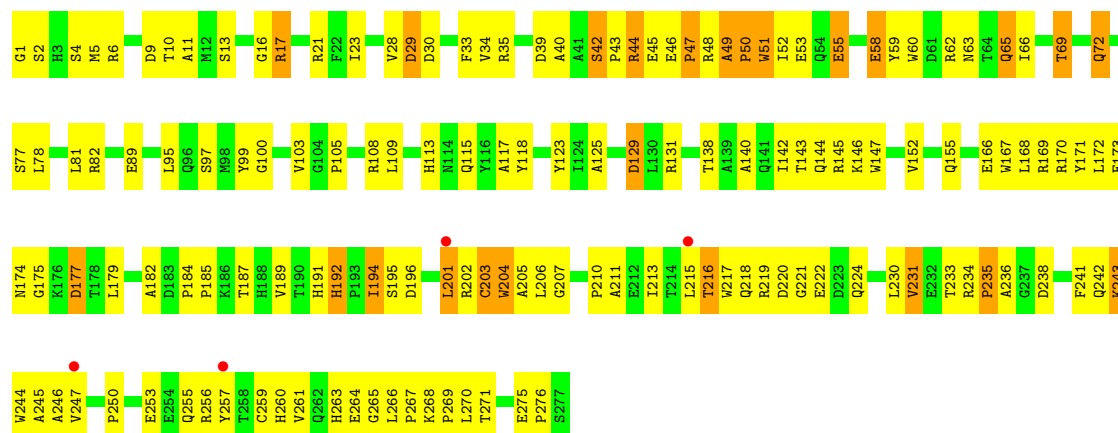


- Molecule 1: HLA class I histocompatibility antigen, B-8 alpha chain





● Molecule 1: HLA class I histocompatibility antigen, B-8 alpha chain



● Molecule 2: Beta-2-microglobulin

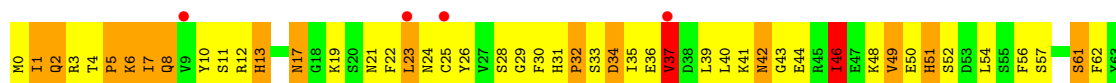


● Molecule 2: Beta-2-microglobulin

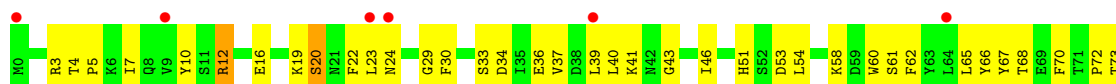




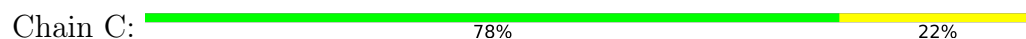
- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin



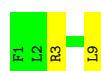
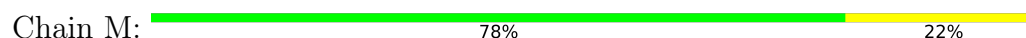
- Molecule 3: Epstein-Barr nuclear antigen 3



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- Molecule 3: Epstein-Barr nuclear antigen 3



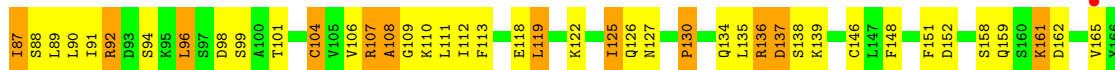
- Molecule 3: Epstein-Barr nuclear antigen 3



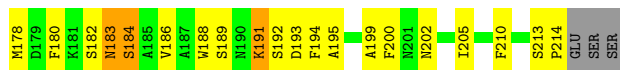
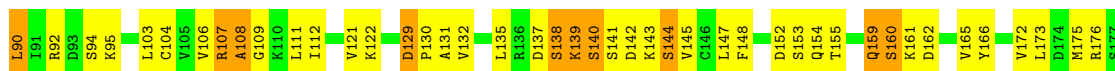




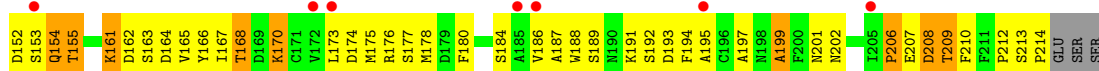
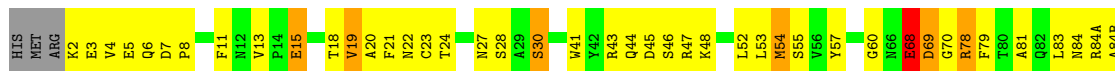
- Molecule 4: RL42 T cell receptor, alpha chain



- Molecule 4: RL42 T cell receptor, alpha chain

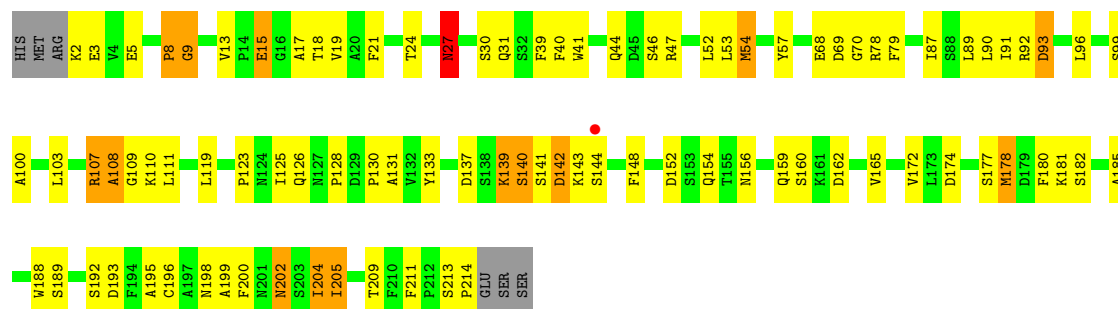


- Molecule 4: RL42 T cell receptor, alpha chain



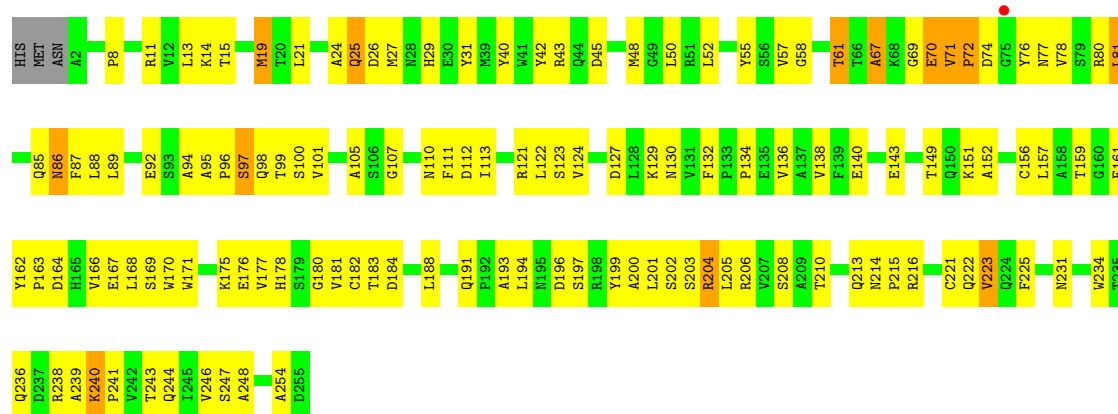
- Molecule 4: RL42 T cell receptor, alpha chain





• Molecule 5: RL42 T cell receptor, beta chain

Chain E: 45% 48% 5% .



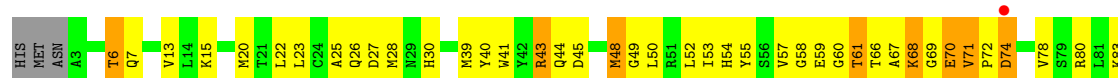
• Molecule 5: RL42 T cell receptor, beta chain

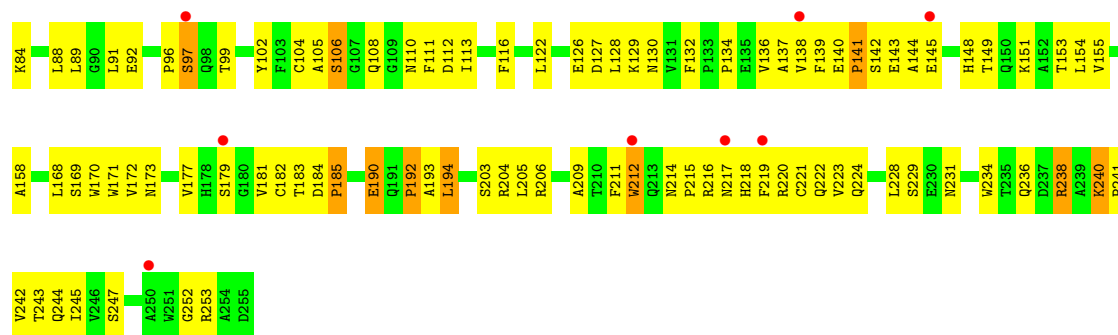
Chain J: 49% 45% . .



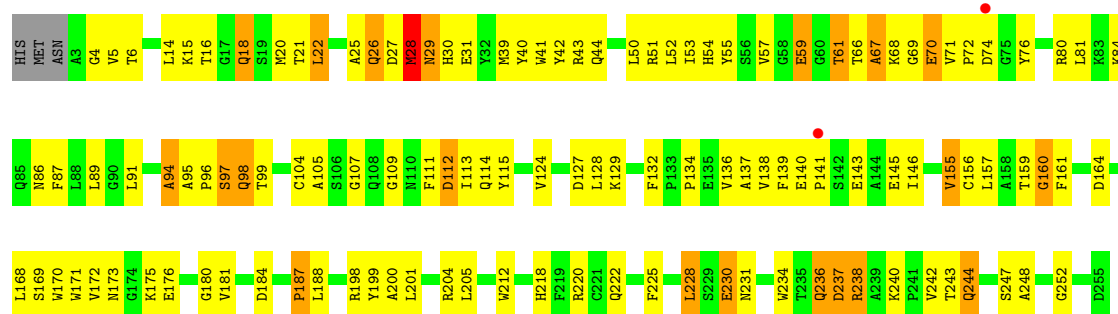
• Molecule 5: RL42 T cell receptor, beta chain

Chain O: 4% 44% 48% 7% .





• Molecule 5: RL42 T cell receptor, beta chain



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 21 21 21                                                  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 100.08Å 185.00Å 217.68Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 19.99 – 3.10<br>19.99 – 3.10                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 90.7 (19.99-3.10)<br>99.5 (19.99-3.10)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.12                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.38 (at 3.09Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX 1.6.1_357                                            | Depositor        |
| R, $R_{free}$                                                           | 0.253 , 0.321<br>0.261 , 0.319                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 3716 reflections (5.04%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 69.3                                                        | Xtriage          |
| Anisotropy                                                              | 0.265                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.22 , 36.7                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.90                                                        | EDS              |
| Total number of atoms                                                   | 26455                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 86.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.73% 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     | 0.30         | 0/2320  | 0.68        | 0/3154          |
| 1   | F     | 0.29         | 0/2320  | 0.70        | 2/3154 (0.1%)   |
| 1   | K     | 0.28         | 0/2320  | 0.69        | 0/3154          |
| 1   | P     | 0.28         | 0/2320  | 0.71        | 2/3154 (0.1%)   |
| 2   | B     | 0.26         | 0/852   | 0.68        | 0/1152          |
| 2   | G     | 0.23         | 0/852   | 0.67        | 0/1152          |
| 2   | L     | 0.23         | 0/860   | 0.67        | 0/1162          |
| 2   | Q     | 0.25         | 0/860   | 0.71        | 0/1162          |
| 3   | C     | 0.25         | 0/76    | 0.65        | 0/98            |
| 3   | H     | 0.27         | 0/76    | 0.59        | 0/98            |
| 3   | M     | 0.27         | 0/76    | 0.60        | 0/98            |
| 3   | R     | 0.28         | 0/76    | 0.53        | 0/98            |
| 4   | D     | 0.29         | 0/1574  | 0.71        | 0/2132          |
| 4   | I     | 0.30         | 0/1574  | 0.76        | 2/2132 (0.1%)   |
| 4   | N     | 0.28         | 0/1574  | 0.73        | 2/2132 (0.1%)   |
| 4   | S     | 0.31         | 0/1574  | 0.77        | 3/2132 (0.1%)   |
| 5   | E     | 0.29         | 0/1959  | 0.72        | 1/2662 (0.0%)   |
| 5   | J     | 0.32         | 0/1954  | 0.77        | 3/2655 (0.1%)   |
| 5   | O     | 0.29         | 0/1959  | 0.74        | 3/2662 (0.1%)   |
| 5   | T     | 0.30         | 0/1959  | 0.72        | 1/2662 (0.0%)   |
| All | All   | 0.29         | 0/27135 | 0.72        | 19/36805 (0.1%) |

There are no bond length outliers.

All (19) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 5   | O     | 68  | LYS  | N-CA-C | 7.14 | 114.64      | 108.78   |
| 5   | E     | 67  | ALA  | N-CA-C | 6.70 | 116.89      | 108.45   |
| 1   | F     | 234 | ARG  | CA-C-N | 6.45 | 127.90      | 119.84   |
| 1   | F     | 234 | ARG  | C-N-CA | 6.45 | 127.90      | 119.84   |
| 4   | I     | 129 | ASP  | CA-C-N | 5.88 | 125.90      | 119.90   |
| 4   | I     | 129 | ASP  | C-N-CA | 5.88 | 125.90      | 119.90   |
| 4   | S     | 9   | GLY  | CA-C-N | 5.82 | 126.01      | 119.90   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4   | S     | 9   | GLY  | C-N-CA  | 5.82  | 126.01      | 119.90   |
| 5   | J     | 140 | GLU  | CA-C-N  | 5.77  | 126.10      | 119.93   |
| 5   | J     | 140 | GLU  | C-N-CA  | 5.77  | 126.10      | 119.93   |
| 1   | P     | 42  | SER  | CA-C-N  | 5.68  | 126.94      | 119.84   |
| 1   | P     | 42  | SER  | C-N-CA  | 5.68  | 126.94      | 119.84   |
| 4   | N     | 129 | ASP  | CA-C-N  | 5.62  | 126.87      | 119.84   |
| 4   | N     | 129 | ASP  | C-N-CA  | 5.62  | 126.87      | 119.84   |
| 5   | O     | 68  | LYS  | CB-CA-C | -5.26 | 109.50      | 117.07   |
| 4   | S     | 78  | ARG  | N-CA-C  | -5.21 | 106.87      | 114.12   |
| 5   | T     | 112 | ASP  | CA-C-O  | 5.11  | 120.91      | 117.94   |
| 5   | O     | 68  | LYS  | CA-C-O  | 5.10  | 120.90      | 117.94   |
| 5   | J     | 86  | ASN  | N-CA-C  | 5.00  | 116.57      | 108.41   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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     | 2258  | 0        | 2098     | 156     | 0            |
| 1   | F     | 2258  | 0        | 2098     | 149     | 0            |
| 1   | K     | 2258  | 0        | 2098     | 137     | 0            |
| 1   | P     | 2258  | 0        | 2098     | 138     | 0            |
| 2   | B     | 829   | 0        | 794      | 54      | 0            |
| 2   | G     | 829   | 0        | 794      | 91      | 0            |
| 2   | L     | 837   | 0        | 803      | 82      | 0            |
| 2   | Q     | 837   | 0        | 803      | 50      | 0            |
| 3   | C     | 75    | 0        | 79       | 3       | 0            |
| 3   | H     | 75    | 0        | 79       | 8       | 0            |
| 3   | M     | 75    | 0        | 79       | 4       | 0            |
| 3   | R     | 75    | 0        | 79       | 5       | 0            |
| 4   | D     | 1541  | 0        | 1466     | 113     | 0            |
| 4   | I     | 1541  | 0        | 1464     | 90      | 0            |
| 4   | N     | 1541  | 0        | 1464     | 154     | 0            |
| 4   | S     | 1541  | 0        | 1464     | 88      | 0            |
| 5   | E     | 1908  | 0        | 1819     | 112     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 5   | J     | 1903  | 0        | 1814     | 101     | 0            |
| 5   | O     | 1908  | 0        | 1819     | 139     | 0            |
| 5   | T     | 1908  | 0        | 1819     | 111     | 0            |
| All | All   | 26455 | 0        | 25031    | 1642    | 0            |

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

All (1642) 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) |
|------------------|------------------|--------------------------|-------------------|
| 4:I:12:ASN:HB3   | 4:I:122:LYS:HE3  | 1.29                     | 1.14              |
| 5:J:96:PRO:HB3   | 5:J:124:VAL:HB   | 1.32                     | 1.07              |
| 5:E:11:ARG:HG2   | 5:E:19:MET:HE3   | 1.39                     | 1.04              |
| 5:O:142:SER:HB3  | 5:O:145:GLU:HB3  | 1.42                     | 0.99              |
| 4:N:207:GLU:N    | 4:N:208:ASP:HB2  | 1.77                     | 0.99              |
| 4:D:30:SER:HA    | 4:D:108:ALA:CB   | 1.92                     | 0.99              |
| 1:A:238:ASP:HB3  | 2:B:12:ARG:HH22  | 1.26                     | 0.98              |
| 4:D:192:SER:N    | 4:D:193:ASP:HA   | 1.79                     | 0.96              |
| 1:F:234:ARG:HH11 | 2:G:10:TYR:HD2   | 1.08                     | 0.96              |
| 4:I:31:GLN:H     | 4:I:108:ALA:HB2  | 1.31                     | 0.96              |
| 4:N:192:SER:N    | 4:N:193:ASP:HA   | 1.81                     | 0.95              |
| 1:F:238:ASP:H    | 2:G:12:ARG:HH21  | 1.07                     | 0.95              |
| 4:S:30:SER:HA    | 4:S:108:ALA:CB   | 1.98                     | 0.94              |
| 2:Q:12:ARG:HG3   | 2:Q:22:PHE:HB3   | 1.50                     | 0.94              |
| 1:P:72:GLN:HG3   | 5:T:57:VAL:HG21  | 1.50                     | 0.93              |
| 2:Q:79:ALA:HB1   | 2:Q:92:ILE:HD11  | 1.51                     | 0.92              |
| 2:G:12:ARG:HB2   | 2:G:22:PHE:HB2   | 1.52                     | 0.91              |
| 1:A:85:TYR:HB2   | 1:A:87:GLN:HE21  | 1.33                     | 0.91              |
| 5:E:96:PRO:HA    | 5:E:97:SER:O     | 1.71                     | 0.91              |
| 4:D:178:MET:HE1  | 5:E:208:SER:HB3  | 1.53                     | 0.90              |
| 4:N:68:GLU:HG2   | 4:N:69:ASP:H     | 1.34                     | 0.90              |
| 1:A:159:TYR:HD2  | 1:A:160:LEU:HD12 | 1.35                     | 0.90              |
| 2:L:81:ARG:HH12  | 2:L:83:ASN:HB3   | 1.35                     | 0.89              |
| 4:D:80:THR:HB    | 4:D:90:LEU:HB2   | 1.55                     | 0.89              |
| 1:P:9:ASP:HB2    | 1:P:97:SER:HB3   | 1.55                     | 0.89              |
| 2:L:29:GLY:HA2   | 2:L:61:SER:HB3   | 1.51                     | 0.89              |
| 2:B:12:ARG:HE    | 2:B:22:PHE:HD2   | 1.17                     | 0.88              |
| 1:F:28:VAL:HG11  | 1:F:179:LEU:HD21 | 1.55                     | 0.88              |
| 4:D:12:ASN:HB3   | 4:D:122:LYS:HE3  | 1.52                     | 0.88              |
| 2:L:12:ARG:HD3   | 2:L:22:PHE:HB2   | 1.55                     | 0.88              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:115:GLN:HG3  | 1:P:125:ALA:HB2  | 1.54                     | 0.87              |
| 5:O:136:VAL:HG21 | 5:O:223:VAL:HG11 | 1.55                     | 0.87              |
| 5:E:193:ALA:HB1  | 5:J:27:MET:HE2   | 1.56                     | 0.87              |
| 4:I:30:SER:HA    | 4:I:108:ALA:CB   | 2.05                     | 0.87              |
| 4:N:122:LYS:HE2  | 4:N:153:SER:HB2  | 1.57                     | 0.86              |
| 4:S:107:ARG:HA   | 4:S:111:LEU:HA   | 1.57                     | 0.86              |
| 5:T:160:GLY:HA2  | 5:T:198:ARG:HB3  | 1.56                     | 0.86              |
| 1:K:202:ARG:HD2  | 1:K:246:ALA:HB2  | 1.57                     | 0.86              |
| 4:D:23:CYS:HB3   | 4:D:87:ILE:HG23  | 1.55                     | 0.86              |
| 4:N:133:TYR:HE2  | 5:O:144:ALA:HB3  | 1.40                     | 0.86              |
| 5:T:96:PRO:HA    | 5:T:97:SER:O     | 1.77                     | 0.85              |
| 1:K:204:TRP:N    | 1:K:204:TRP:HE3  | 1.74                     | 0.85              |
| 4:S:30:SER:HA    | 4:S:108:ALA:HB1  | 1.55                     | 0.85              |
| 1:A:258:THR:HB   | 1:A:273:ARG:HA   | 1.56                     | 0.85              |
| 1:P:13:SER:HB3   | 1:P:78:LEU:HD13  | 1.58                     | 0.85              |
| 1:A:172:LEU:HD23 | 1:A:179:LEU:HD23 | 1.59                     | 0.84              |
| 5:E:213:GLN:HB2  | 5:E:254:ALA:HA   | 1.58                     | 0.84              |
| 5:O:72:PRO:HA    | 5:O:74:ASP:O     | 1.77                     | 0.84              |
| 5:E:13:LEU:HD11  | 5:E:19:MET:HG2   | 1.58                     | 0.84              |
| 4:I:31:GLN:N     | 4:I:108:ALA:HB2  | 1.92                     | 0.84              |
| 4:D:30:SER:HA    | 4:D:108:ALA:HB2  | 1.57                     | 0.84              |
| 5:J:133:PRO:HD3  | 5:J:241:PRO:HB3  | 1.59                     | 0.83              |
| 2:B:1:ILE:HG23   | 2:B:2:GLN:H      | 1.43                     | 0.82              |
| 5:O:68:LYS:HG2   | 5:O:69:GLY:H     | 1.42                     | 0.82              |
| 1:F:70:ASN:HB3   | 3:H:5:ARG:HH21   | 1.45                     | 0.82              |
| 1:K:81:LEU:HD11  | 3:M:9:LEU:HD22   | 1.62                     | 0.81              |
| 1:F:202:ARG:HE   | 1:F:246:ALA:HB2  | 1.44                     | 0.81              |
| 1:P:167:TRP:HA   | 1:P:170:ARG:HB3  | 1.63                     | 0.81              |
| 1:A:217:TRP:HE3  | 1:A:257:TYR:CE1  | 1.99                     | 0.80              |
| 4:N:107:ARG:HA   | 4:N:111:LEU:HA   | 1.61                     | 0.80              |
| 1:K:253:GLU:HG2  | 1:K:256:ARG:HH22 | 1.46                     | 0.80              |
| 4:S:165:VAL:HG23 | 4:S:189:SER:HB2  | 1.64                     | 0.80              |
| 4:N:81:ALA:HA    | 4:N:88:SER:O     | 1.81                     | 0.80              |
| 4:S:213:SER:H    | 4:S:214:PRO:HD2  | 1.45                     | 0.79              |
| 5:J:171:TRP:HB2  | 5:J:220:ARG:HB2  | 1.64                     | 0.79              |
| 1:A:217:TRP:HE3  | 1:A:257:TYR:HH   | 1.30                     | 0.79              |
| 5:O:45:ASP:HB3   | 1:P:145:ARG:HH21 | 1.46                     | 0.79              |
| 1:F:234:ARG:HD2  | 2:G:10:TYR:CD2   | 2.17                     | 0.79              |
| 5:O:44:GLN:HB2   | 5:O:50:LEU:HD23  | 1.65                     | 0.78              |
| 2:Q:36:GLU:HG2   | 2:Q:83:ASN:HB2   | 1.63                     | 0.78              |
| 1:F:35:ARG:CZ    | 2:G:53:ASP:HB3   | 2.13                     | 0.78              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:I:27:ASN:C     | 4:I:27:ASN:HD22  | 1.91                     | 0.78              |
| 1:K:204:TRP:N    | 1:K:204:TRP:CE3  | 2.52                     | 0.78              |
| 4:D:192:SER:H    | 4:D:193:ASP:HA   | 1.49                     | 0.78              |
| 4:S:30:SER:CA    | 4:S:108:ALA:HB2  | 2.14                     | 0.78              |
| 5:E:99:THR:HG23  | 5:E:123:SER:HA   | 1.65                     | 0.78              |
| 1:P:233:THR:HB   | 1:P:243:LYS:HD3  | 1.64                     | 0.77              |
| 4:N:133:TYR:HD1  | 4:N:134:GLN:N    | 1.82                     | 0.77              |
| 2:G:13:HIS:HB3   | 2:G:14:PRO:HD2   | 1.67                     | 0.77              |
| 5:J:71:VAL:H     | 5:J:72:PRO:HD2   | 1.48                     | 0.77              |
| 2:G:24:ASN:HB3   | 2:G:67:TYR:HB3   | 1.65                     | 0.77              |
| 4:I:191:LYS:HE2  | 4:I:191:LYS:HA   | 1.66                     | 0.77              |
| 1:K:202:ARG:HE   | 1:K:244:TRP:HB2  | 1.50                     | 0.77              |
| 4:N:19:VAL:HG12  | 4:N:20:ALA:H     | 1.49                     | 0.77              |
| 4:N:122:LYS:NZ   | 4:N:153:SER:O    | 2.19                     | 0.76              |
| 2:G:46:ILE:HG23  | 2:G:78:TYR:OH    | 1.85                     | 0.76              |
| 5:O:68:LYS:HG2   | 5:O:69:GLY:N     | 1.99                     | 0.76              |
| 4:D:161:LYS:HG2  | 4:D:162:ASP:H    | 1.49                     | 0.75              |
| 4:N:194:PHE:CZ   | 4:N:199:ALA:HA   | 2.22                     | 0.75              |
| 1:A:185:PRO:HB3  | 1:A:263:HIS:CD2  | 2.22                     | 0.75              |
| 5:O:40:TYR:HB2   | 5:O:105:ALA:HB3  | 1.69                     | 0.75              |
| 1:F:233:THR:HG22 | 1:F:243:LYS:HD2  | 1.66                     | 0.74              |
| 1:A:81:LEU:HD23  | 1:A:118:TYR:CD1  | 2.22                     | 0.74              |
| 4:N:176:ARG:HH21 | 5:O:179:SER:HB2  | 1.52                     | 0.74              |
| 5:E:78:VAL:HG23  | 5:E:88:LEU:O     | 1.86                     | 0.74              |
| 4:N:161:LYS:HG3  | 4:N:202:ASN:CG   | 2.12                     | 0.74              |
| 5:O:168:LEU:HA   | 5:O:222:GLN:O    | 1.86                     | 0.74              |
| 1:F:31:THR:HG22  | 1:F:209:TYR:OH   | 1.88                     | 0.74              |
| 1:A:217:TRP:HA   | 1:A:257:TYR:OH   | 1.87                     | 0.74              |
| 4:D:136:ARG:O    | 4:D:137:ASP:HB3  | 1.87                     | 0.74              |
| 1:F:222:GLU:HG2  | 1:F:224:GLN:H    | 1.52                     | 0.74              |
| 4:N:133:TYR:CE2  | 5:O:144:ALA:HB3  | 2.23                     | 0.74              |
| 4:D:12:ASN:CB    | 4:D:122:LYS:HE3  | 2.18                     | 0.73              |
| 2:Q:68:THR:HG21  | 2:Q:78:TYR:HE2   | 1.53                     | 0.73              |
| 1:K:235:PRO:HA   | 1:K:241:PHE:CD1  | 2.23                     | 0.73              |
| 2:L:81:ARG:HH12  | 2:L:83:ASN:CB    | 2.01                     | 0.73              |
| 5:J:25:GLN:HE21  | 5:J:29:HIS:H     | 1.36                     | 0.73              |
| 4:S:192:SER:N    | 4:S:193:ASP:HA   | 2.01                     | 0.73              |
| 2:L:7:ILE:HG12   | 2:L:8:GLN:H      | 1.54                     | 0.73              |
| 1:A:5:MET:HB2    | 1:A:168:LEU:HD13 | 1.70                     | 0.73              |
| 5:O:182:CYS:O    | 5:O:204:ARG:HG2  | 1.88                     | 0.73              |
| 1:A:159:TYR:CD2  | 1:A:160:LEU:HD12 | 2.22                     | 0.73              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:N:122:LYS:CE   | 4:N:153:SER:HB2  | 2.18                     | 0.73              |
| 5:O:96:PRO:HA    | 5:O:97:SER:O     | 1.89                     | 0.73              |
| 5:J:71:VAL:O     | 5:J:74:ASP:N     | 2.22                     | 0.72              |
| 4:S:30:SER:HA    | 4:S:108:ALA:HB2  | 1.70                     | 0.72              |
| 4:S:13:VAL:HG11  | 4:S:19:VAL:HG12  | 1.70                     | 0.72              |
| 5:O:190:GLU:O    | 5:O:192:PRO:HD3  | 1.89                     | 0.72              |
| 1:P:182:ALA:HB1  | 1:P:265:GLY:HA2  | 1.70                     | 0.72              |
| 1:F:220:ASP:OD1  | 1:F:221:GLY:HA3  | 1.88                     | 0.72              |
| 4:I:39:PHE:HD1   | 4:I:106:VAL:HG22 | 1.54                     | 0.72              |
| 4:N:132:VAL:H    | 4:N:209:THR:CG2  | 2.02                     | 0.72              |
| 2:G:39:LEU:HB2   | 2:G:46:ILE:HD11  | 1.72                     | 0.72              |
| 5:J:96:PRO:HB3   | 5:J:124:VAL:CB   | 2.14                     | 0.72              |
| 1:F:202:ARG:HH12 | 2:G:99:MET:HG2   | 1.54                     | 0.72              |
| 5:J:28:ASN:ND2   | 5:J:84:LYS:HE2   | 2.04                     | 0.72              |
| 5:O:228:LEU:HD12 | 5:O:241:PRO:HD2  | 1.72                     | 0.72              |
| 4:D:43:ARG:HH12  | 4:D:98:ASP:HA    | 1.55                     | 0.71              |
| 5:T:222:GLN:HA   | 5:T:247:SER:HB3  | 1.72                     | 0.71              |
| 1:A:13:SER:HB3   | 1:A:78:LEU:HD13  | 1.73                     | 0.71              |
| 5:J:21:LEU:HD13  | 5:J:89:LEU:HD23  | 1.72                     | 0.71              |
| 1:P:222:GLU:HG3  | 1:P:224:GLN:HE22 | 1.55                     | 0.71              |
| 5:T:31:GLU:HG2   | 5:T:84:LYS:HE3   | 1.72                     | 0.71              |
| 5:E:71:VAL:HG13  | 5:E:72:PRO:HD3   | 1.73                     | 0.71              |
| 1:F:234:ARG:HD2  | 2:G:10:TYR:HD2   | 1.55                     | 0.71              |
| 1:A:217:TRP:O    | 1:A:224:GLN:HB3  | 1.90                     | 0.71              |
| 4:I:49:GLU:OE2   | 4:I:51:LYS:HE3   | 1.91                     | 0.71              |
| 4:I:192:SER:HB3  | 4:I:193:ASP:HA   | 1.73                     | 0.71              |
| 4:S:213:SER:N    | 4:S:214:PRO:HD2  | 2.06                     | 0.71              |
| 2:G:26:TYR:HB2   | 2:G:65:LEU:HD13  | 1.73                     | 0.70              |
| 4:I:42:TYR:HB2   | 4:I:103:LEU:HB2  | 1.73                     | 0.70              |
| 4:S:41:TRP:O     | 4:S:53:LEU:HB3   | 1.90                     | 0.70              |
| 4:S:27:ASN:C     | 4:S:27:ASN:HD22  | 1.98                     | 0.70              |
| 4:N:30:SER:HB3   | 4:N:108:ALA:HB2  | 1.74                     | 0.70              |
| 2:L:11:SER:HB2   | 2:L:21:ASN:HD21  | 1.57                     | 0.70              |
| 4:N:13:VAL:HG21  | 4:N:19:VAL:HG13  | 1.72                     | 0.70              |
| 4:D:30:SER:CA    | 4:D:108:ALA:HB2  | 2.21                     | 0.70              |
| 5:O:97:SER:HB3   | 1:P:142:ILE:HD11 | 1.73                     | 0.70              |
| 4:N:68:GLU:CG    | 4:N:69:ASP:H     | 2.03                     | 0.69              |
| 1:P:5:MET:HB2    | 1:P:168:LEU:HD13 | 1.74                     | 0.69              |
| 5:O:234:TRP:HZ2  | 5:O:238:ARG:HG3  | 1.58                     | 0.69              |
| 5:E:101:VAL:HG22 | 5:E:121:ARG:HG3  | 1.74                     | 0.69              |
| 2:L:7:ILE:HG21   | 2:L:93:VAL:HG21  | 1.75                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:219:ARG:NH1  | 1:P:256:ARG:HE   | 1.90                     | 0.69              |
| 2:Q:46:ILE:HB    | 2:Q:78:TYR:OH    | 1.92                     | 0.69              |
| 1:F:201:LEU:HD21 | 1:F:254:GLU:HG3  | 1.73                     | 0.69              |
| 1:K:208:PHE:CE2  | 1:K:241:PHE:HB3  | 2.28                     | 0.69              |
| 4:N:175:MET:HE3  | 4:N:177:SER:HB2  | 1.75                     | 0.69              |
| 2:L:39:LEU:HB3   | 2:L:49:VAL:HG12  | 1.72                     | 0.69              |
| 5:O:172:VAL:HG13 | 5:O:177:VAL:HG21 | 1.73                     | 0.69              |
| 1:A:238:ASP:OD1  | 1:A:240:THR:HG22 | 1.93                     | 0.69              |
| 1:K:14:ARG:HD2   | 1:K:17:ARG:NH2   | 2.08                     | 0.69              |
| 4:N:4:VAL:HG11   | 4:N:113:PHE:O    | 1.93                     | 0.69              |
| 4:N:210:PHE:CZ   | 4:N:212:PRO:HG3  | 2.27                     | 0.69              |
| 1:A:217:TRP:HE3  | 1:A:257:TYR:HE1  | 1.40                     | 0.69              |
| 4:D:79:PHE:CD1   | 4:D:91:ILE:HG22  | 2.28                     | 0.69              |
| 5:E:138:VAL:HG23 | 5:E:248:ALA:HB3  | 1.75                     | 0.68              |
| 1:A:244:TRP:HZ3  | 1:A:246:ALA:HB2  | 1.57                     | 0.68              |
| 4:N:70:GLY:C     | 4:N:79:PHE:H     | 1.99                     | 0.68              |
| 2:G:37:VAL:HG22  | 2:G:82:VAL:HG12  | 1.76                     | 0.68              |
| 2:L:81:ARG:HE    | 2:L:90:PRO:HB3   | 1.59                     | 0.68              |
| 5:O:68:LYS:CG    | 5:O:69:GLY:H     | 2.05                     | 0.68              |
| 2:G:12:ARG:CB    | 2:G:22:PHE:HB2   | 2.23                     | 0.67              |
| 1:K:188:HIS:H    | 1:K:204:TRP:NE1  | 1.90                     | 0.67              |
| 4:N:133:TYR:HD1  | 4:N:134:GLN:H    | 1.42                     | 0.67              |
| 1:A:178:THR:HA   | 1:A:181:ARG:HD3  | 1.75                     | 0.67              |
| 1:F:22:PHE:HB2   | 1:F:38:SER:HB3   | 1.74                     | 0.67              |
| 4:D:96:LEU:HD23  | 4:D:181:LYS:HD3  | 1.75                     | 0.67              |
| 5:E:71:VAL:O     | 5:E:74:ASP:N     | 2.27                     | 0.67              |
| 1:A:184:PRO:HB2  | 1:A:186:LYS:HE3  | 1.76                     | 0.67              |
| 2:G:46:ILE:HD12  | 2:G:46:ILE:H     | 1.58                     | 0.67              |
| 1:P:166:GLU:O    | 1:P:169:ARG:HG2  | 1.94                     | 0.67              |
| 5:E:45:ASP:HB2   | 5:E:48:MET:HG3   | 1.75                     | 0.67              |
| 4:N:70:GLY:O     | 4:N:78:ARG:HG2   | 1.94                     | 0.67              |
| 1:K:142:ILE:HA   | 1:K:145:ARG:NH1  | 2.10                     | 0.67              |
| 4:N:168:THR:HG23 | 4:N:186:VAL:HB   | 1.75                     | 0.67              |
| 4:D:52:LEU:HD22  | 5:E:113:ILE:HG23 | 1.75                     | 0.67              |
| 1:P:202:ARG:HB3  | 1:P:246:ALA:HB2  | 1.77                     | 0.67              |
| 1:A:217:TRP:CE3  | 1:A:257:TYR:HE1  | 2.12                     | 0.67              |
| 4:S:30:SER:CA    | 4:S:108:ALA:CB   | 2.72                     | 0.67              |
| 5:T:22:LEU:HD13  | 5:T:89:LEU:HD23  | 1.77                     | 0.67              |
| 1:F:35:ARG:O     | 1:F:46:GLU:HB3   | 1.95                     | 0.66              |
| 1:F:51:TRP:CD1   | 1:F:51:TRP:H     | 2.13                     | 0.66              |
| 2:Q:24:ASN:HB3   | 2:Q:65:LEU:HD11  | 1.76                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:233:THR:HA   | 1:F:243:LYS:HB2  | 1.77                     | 0.66              |
| 1:K:232:GLU:HG3  | 2:L:6:LYS:HD3    | 1.77                     | 0.66              |
| 1:P:11:ALA:HB3   | 1:P:95:LEU:HB3   | 1.77                     | 0.66              |
| 4:S:31:GLN:H     | 4:S:108:ALA:HB2  | 1.58                     | 0.66              |
| 4:D:27:ASN:C     | 4:D:27:ASN:HD22  | 2.03                     | 0.66              |
| 4:N:207:GLU:HB2  | 4:N:208:ASP:HA   | 1.78                     | 0.66              |
| 1:A:234:ARG:O    | 1:A:234:ARG:HG2  | 1.96                     | 0.66              |
| 2:L:24:ASN:HD21  | 2:L:65:LEU:HB3   | 1.60                     | 0.66              |
| 2:B:1:ILE:HG23   | 2:B:2:GLN:N      | 2.11                     | 0.66              |
| 1:P:50:PRO:HG2   | 1:P:51:TRP:CE3   | 2.30                     | 0.66              |
| 4:I:213:SER:H    | 4:I:214:PRO:HD2  | 1.60                     | 0.66              |
| 2:L:0:MET:HA     | 2:L:1:ILE:HD12   | 1.78                     | 0.66              |
| 1:K:5:MET:HB2    | 1:K:168:LEU:HD13 | 1.78                     | 0.65              |
| 4:N:143:LYS:HG3  | 4:N:144:SER:H    | 1.61                     | 0.65              |
| 1:A:238:ASP:HB3  | 2:B:12:ARG:NH2   | 2.08                     | 0.65              |
| 2:B:73:THR:OG1   | 2:B:76:ASP:HB2   | 1.95                     | 0.65              |
| 4:D:134:GLN:HB2  | 4:D:196:CYS:SG   | 2.35                     | 0.65              |
| 1:K:69:THR:HG23  | 5:O:110:ASN:ND2  | 2.11                     | 0.65              |
| 5:J:174:GLY:HA2  | 5:J:220:ARG:HH12 | 1.61                     | 0.65              |
| 2:B:12:ARG:NE    | 2:B:22:PHE:HD2   | 1.93                     | 0.65              |
| 4:D:192:SER:N    | 4:D:193:ASP:CA   | 2.59                     | 0.65              |
| 4:N:21:PHE:HB2   | 4:N:89:LEU:HB3   | 1.79                     | 0.65              |
| 4:S:39:PHE:CD1   | 4:S:87:ILE:HD11  | 2.32                     | 0.65              |
| 4:N:15:GLU:O     | 4:N:94:SER:HB2   | 1.97                     | 0.65              |
| 4:N:161:LYS:HG3  | 4:N:202:ASN:ND2  | 2.11                     | 0.65              |
| 1:P:28:VAL:HG12  | 1:P:29:ASP:OD1   | 1.97                     | 0.65              |
| 1:P:147:TRP:CD1  | 1:P:152:VAL:HG21 | 2.32                     | 0.65              |
| 5:E:168:LEU:HD12 | 5:E:169:SER:H    | 1.61                     | 0.65              |
| 2:G:45:ARG:HG2   | 2:G:46:ILE:H     | 1.61                     | 0.65              |
| 2:L:4:THR:HG23   | 2:L:86:THR:HB    | 1.77                     | 0.65              |
| 4:N:167:ILE:HG12 | 4:N:187:ALA:HB1  | 1.78                     | 0.65              |
| 4:D:30:SER:HA    | 4:D:108:ALA:HB1  | 1.79                     | 0.64              |
| 4:I:15:GLU:O     | 4:I:94:SER:HB2   | 1.98                     | 0.64              |
| 1:K:244:TRP:N    | 1:K:244:TRP:CD1  | 2.64                     | 0.64              |
| 1:A:49:ALA:HB1   | 1:A:50:PRO:HD2   | 1.79                     | 0.64              |
| 4:I:52:LEU:HD12  | 4:I:53:LEU:H     | 1.62                     | 0.64              |
| 1:K:72:GLN:HG3   | 5:O:57:VAL:HG11  | 1.78                     | 0.64              |
| 1:K:207:GLY:HA2  | 1:K:240:THR:OG1  | 1.97                     | 0.64              |
| 4:S:30:SER:CB    | 4:S:108:ALA:HB2  | 2.28                     | 0.64              |
| 2:B:24:ASN:HB3   | 2:B:67:TYR:HB3   | 1.78                     | 0.64              |
| 5:J:141:PRO:HD2  | 5:J:212:TRP:CZ2  | 2.32                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:113:PHE:CE1  | 5:E:50:LEU:HD12  | 2.31                     | 0.64              |
| 5:O:240:LYS:HG2  | 5:O:242:VAL:HG13 | 1.80                     | 0.64              |
| 4:S:178:MET:HE2  | 4:S:178:MET:HA   | 1.80                     | 0.64              |
| 2:L:40:LEU:HD23  | 2:L:43:GLY:HA2   | 1.79                     | 0.64              |
| 4:N:4:VAL:HG11   | 4:N:114:GLY:HA2  | 1.80                     | 0.64              |
| 3:R:6:ALA:O      | 5:T:109:GLY:HA2  | 1.98                     | 0.64              |
| 2:B:67:TYR:HD2   | 2:B:67:TYR:H     | 1.45                     | 0.64              |
| 1:F:238:ASP:N    | 2:G:12:ARG:HH21  | 1.88                     | 0.64              |
| 5:J:134:PRO:HD3  | 5:J:225:PHE:CD1  | 2.33                     | 0.64              |
| 5:T:97:SER:C     | 5:T:99:THR:H     | 2.04                     | 0.64              |
| 5:T:156:CYS:HB2  | 5:T:170:TRP:CH2  | 2.32                     | 0.64              |
| 4:D:8:PRO:HD2    | 4:D:11:PHE:HZ    | 1.63                     | 0.64              |
| 1:P:65:GLN:HA    | 1:P:65:GLN:HE21  | 1.63                     | 0.64              |
| 1:A:255:GLN:H    | 1:A:255:GLN:CD   | 2.06                     | 0.63              |
| 4:N:210:PHE:O    | 4:N:212:PRO:HD3  | 1.98                     | 0.63              |
| 4:I:30:SER:HA    | 4:I:108:ALA:HB2  | 1.79                     | 0.63              |
| 4:N:28:SER:HA    | 4:N:85:GLN:NE2   | 2.13                     | 0.63              |
| 5:J:78:VAL:HG23  | 5:J:88:LEU:O     | 1.98                     | 0.63              |
| 2:L:2:GLN:OE1    | 2:L:31:HIS:HB2   | 1.98                     | 0.63              |
| 5:J:25:GLN:HG2   | 5:J:27:MET:H     | 1.63                     | 0.63              |
| 1:K:225:THR:O    | 1:K:228:THR:HG22 | 1.98                     | 0.63              |
| 5:T:15:LYS:HE3   | 5:T:128:LEU:HD13 | 1.80                     | 0.63              |
| 1:A:98:MET:HE1   | 2:B:58:LYS:HA    | 1.80                     | 0.63              |
| 5:E:13:LEU:HD11  | 5:E:19:MET:CG    | 2.28                     | 0.63              |
| 4:N:148:PHE:O    | 4:N:184:SER:HA   | 1.99                     | 0.63              |
| 1:F:262:GLN:H    | 1:F:262:GLN:CD   | 2.06                     | 0.63              |
| 1:A:219:ARG:HB2  | 1:A:224:GLN:HB2  | 1.81                     | 0.63              |
| 1:P:260:HIS:HA   | 1:P:271:THR:HG22 | 1.81                     | 0.63              |
| 5:E:210:THR:HA   | 5:E:213:GLN:HE22 | 1.64                     | 0.63              |
| 1:P:103:VAL:HG12 | 1:P:109:LEU:HA   | 1.80                     | 0.63              |
| 5:E:98:GLN:O     | 5:E:122:LEU:HD23 | 1.99                     | 0.63              |
| 4:I:213:SER:N    | 4:I:214:PRO:HD2  | 2.13                     | 0.63              |
| 5:O:170:TRP:CZ3  | 5:O:221:CYS:HB3  | 2.34                     | 0.63              |
| 4:D:79:PHE:HD1   | 4:D:91:ILE:HG22  | 1.62                     | 0.62              |
| 1:F:235:PRO:HB2  | 2:G:65:LEU:HD22  | 1.80                     | 0.62              |
| 1:P:206:LEU:HD23 | 1:P:207:GLY:N    | 2.14                     | 0.62              |
| 1:A:213:ILE:HG13 | 1:A:261:VAL:HG13 | 1.81                     | 0.62              |
| 1:A:242:GLN:O    | 1:A:243:LYS:HB3  | 1.97                     | 0.62              |
| 4:D:91:ILE:O     | 4:D:91:ILE:HG13  | 2.00                     | 0.62              |
| 1:P:58:GLU:O     | 1:P:62:ARG:HG2   | 1.99                     | 0.62              |
| 1:A:218:GLN:HB2  | 1:A:257:TYR:CD2  | 2.34                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:219:ARG:HD2  | 1:F:256:ARG:HB3  | 1.81                     | 0.62              |
| 4:N:7:ASP:HB3    | 4:N:11:PHE:HZ    | 1.65                     | 0.62              |
| 1:P:266:LEU:HD12 | 1:P:267:PRO:HD2  | 1.81                     | 0.62              |
| 2:G:29:GLY:HA2   | 2:G:61:SER:HB3   | 1.81                     | 0.62              |
| 1:K:168:LEU:O    | 1:K:172:LEU:HG   | 2.00                     | 0.62              |
| 5:O:140:GLU:HB3  | 5:O:141:PRO:HD2  | 1.80                     | 0.62              |
| 1:F:5:MET:HB2    | 1:F:168:LEU:HD13 | 1.81                     | 0.62              |
| 4:S:130:PRO:HG2  | 4:S:209:THR:HA   | 1.81                     | 0.62              |
| 5:E:58:GLY:O     | 5:E:80:ARG:HG2   | 1.99                     | 0.62              |
| 1:F:236:ALA:HB1  | 2:G:12:ARG:CZ    | 2.29                     | 0.62              |
| 4:N:44:GLN:HE22  | 5:O:44:GLN:HE22  | 1.47                     | 0.62              |
| 1:F:25:VAL:HG11  | 1:F:35:ARG:CZ    | 2.30                     | 0.62              |
| 5:T:97:SER:O     | 5:T:99:THR:N     | 2.33                     | 0.62              |
| 1:K:188:HIS:C    | 1:K:204:TRP:HE1  | 2.08                     | 0.62              |
| 4:N:30:SER:HA    | 4:N:108:ALA:CB   | 2.30                     | 0.62              |
| 1:K:204:TRP:HE3  | 1:K:204:TRP:H    | 1.47                     | 0.62              |
| 4:N:145:VAL:HG13 | 4:N:187:ALA:H    | 1.63                     | 0.62              |
| 1:A:72:GLN:HG3   | 5:E:57:VAL:HG21  | 1.80                     | 0.62              |
| 5:J:31:TYR:CZ    | 5:J:110:ASN:HB2  | 2.34                     | 0.61              |
| 1:P:182:ALA:HB1  | 1:P:265:GLY:CA   | 2.30                     | 0.61              |
| 5:T:16:THR:HG23  | 5:T:95:ALA:HA    | 1.80                     | 0.61              |
| 5:T:234:TRP:HZ2  | 5:T:238:ARG:HB2  | 1.63                     | 0.61              |
| 4:I:145:VAL:HG12 | 4:I:188:TRP:HB3  | 1.81                     | 0.61              |
| 4:N:137:ASP:OD1  | 5:O:139:PHE:HD1  | 1.83                     | 0.61              |
| 1:A:185:PRO:HB3  | 1:A:263:HIS:HD2  | 1.65                     | 0.61              |
| 2:G:33:SER:HB2   | 2:G:54:LEU:HD11  | 1.83                     | 0.61              |
| 1:K:202:ARG:CD   | 1:K:246:ALA:HB2  | 2.28                     | 0.61              |
| 1:P:21:ARG:NH2   | 1:P:23:ILE:HD11  | 2.14                     | 0.61              |
| 1:A:103:VAL:HG12 | 1:A:109:LEU:HA   | 1.80                     | 0.61              |
| 5:E:45:ASP:HB3   | 1:F:145:ARG:HH21 | 1.66                     | 0.61              |
| 5:T:188:LEU:HB3  | 5:T:200:ALA:HB3  | 1.81                     | 0.61              |
| 4:N:21:PHE:O     | 4:N:88:SER:HA    | 2.00                     | 0.61              |
| 5:T:15:LYS:HB2   | 5:T:128:LEU:HD11 | 1.81                     | 0.61              |
| 5:J:181:VAL:HG12 | 5:J:205:LEU:HD13 | 1.82                     | 0.61              |
| 5:J:212:TRP:HE3  | 5:J:219:PHE:HE1  | 1.48                     | 0.61              |
| 2:L:23:LEU:HD13  | 2:L:70:PHE:CZ    | 2.36                     | 0.61              |
| 4:N:68:GLU:HG2   | 4:N:69:ASP:N     | 2.13                     | 0.61              |
| 1:F:21:ARG:HE    | 1:F:23:ILE:HG13  | 1.66                     | 0.61              |
| 4:N:206:PRO:HB2  | 4:N:208:ASP:HB2  | 1.83                     | 0.61              |
| 1:A:147:TRP:HB3  | 1:A:152:VAL:HB   | 1.83                     | 0.61              |
| 4:D:12:ASN:HB3   | 4:D:122:LYS:CE   | 2.26                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:O:154:LEU:HD11 | 5:O:205:LEU:HB3  | 1.81                     | 0.61              |
| 1:A:35:ARG:CZ    | 2:B:53:ASP:HB3   | 2.30                     | 0.60              |
| 2:L:23:LEU:HD23  | 2:L:78:TYR:HB3   | 1.82                     | 0.60              |
| 1:P:211:ALA:HB2  | 1:P:241:PHE:CD2  | 2.36                     | 0.60              |
| 4:N:30:SER:HA    | 4:N:108:ALA:HB1  | 1.82                     | 0.60              |
| 1:F:159:TYR:CE1  | 3:H:3:ARG:HB2    | 2.37                     | 0.60              |
| 2:G:5:PRO:HA     | 2:G:30:PHE:HB3   | 1.83                     | 0.60              |
| 4:N:112:ILE:HD12 | 4:N:112:ILE:H    | 1.67                     | 0.60              |
| 4:S:18:THR:HG22  | 4:S:93:ASP:H     | 1.66                     | 0.60              |
| 1:A:35:ARG:O     | 1:A:46:GLU:HB3   | 2.01                     | 0.60              |
| 4:N:145:VAL:HG11 | 4:N:186:VAL:HG13 | 1.83                     | 0.60              |
| 5:O:128:LEU:HG   | 5:O:228:LEU:HD21 | 1.84                     | 0.60              |
| 1:A:219:ARG:NH1  | 1:A:219:ARG:HA   | 2.17                     | 0.60              |
| 5:E:97:SER:C     | 5:E:99:THR:H     | 2.09                     | 0.60              |
| 4:D:126:GLN:HG3  | 4:D:127:ASN:N    | 2.16                     | 0.60              |
| 2:L:2:GLN:HE22   | 2:L:31:HIS:H     | 1.50                     | 0.60              |
| 5:T:57:VAL:HG22  | 5:T:61:THR:HG21  | 1.83                     | 0.60              |
| 5:T:164:ASP:CB   | 5:T:187:PRO:HG2  | 2.32                     | 0.60              |
| 5:T:230:GLU:HG3  | 5:T:231:ASN:H    | 1.67                     | 0.60              |
| 4:D:15:GLU:O     | 4:D:94:SER:HB2   | 2.02                     | 0.60              |
| 1:K:187:THR:HB   | 1:K:204:TRP:CZ2  | 2.36                     | 0.60              |
| 4:N:148:PHE:CE2  | 4:N:151:PHE:HB2  | 2.37                     | 0.60              |
| 1:K:51:TRP:CH2   | 1:K:178:THR:HB   | 2.37                     | 0.60              |
| 1:K:69:THR:HA    | 1:K:72:GLN:OE1   | 2.01                     | 0.60              |
| 1:K:257:TYR:HD2  | 1:K:257:TYR:N    | 2.00                     | 0.60              |
| 5:O:136:VAL:HG12 | 5:O:137:ALA:H    | 1.66                     | 0.60              |
| 1:A:217:TRP:CD2  | 1:A:247:VAL:HB   | 2.36                     | 0.60              |
| 1:K:188:HIS:H    | 1:K:204:TRP:HE1  | 1.49                     | 0.60              |
| 4:N:145:VAL:CG1  | 4:N:187:ALA:H    | 2.15                     | 0.60              |
| 2:B:96:ASP:HB3   | 2:B:99:MET:HB3   | 1.83                     | 0.59              |
| 1:A:102:ASP:HB2  | 1:A:110:LEU:HD11 | 1.84                     | 0.59              |
| 5:T:43:ARG:HE    | 5:T:51:ARG:NH2   | 2.00                     | 0.59              |
| 2:Q:68:THR:HG21  | 2:Q:78:TYR:CE2   | 2.36                     | 0.59              |
| 4:N:30:SER:CB    | 4:N:108:ALA:HB2  | 2.31                     | 0.59              |
| 4:I:80:THR:HB    | 4:I:90:LEU:HB2   | 1.84                     | 0.59              |
| 2:Q:36:GLU:CG    | 2:Q:83:ASN:HB2   | 2.32                     | 0.59              |
| 1:A:214:THR:HG22 | 1:A:216:THR:HG23 | 1.83                     | 0.59              |
| 1:F:129:ASP:O    | 1:F:131:ARG:HG3  | 2.03                     | 0.59              |
| 5:J:234:TRP:HZ2  | 5:J:238:ARG:HG3  | 1.68                     | 0.59              |
| 5:T:6:THR:HG23   | 5:T:25:ALA:HB3   | 1.84                     | 0.59              |
| 1:F:177:ASP:O    | 1:F:181:ARG:HB3  | 2.02                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:G:23:LEU:HB2   | 2:G:70:PHE:CE2   | 2.37                     | 0.59              |
| 4:I:52:LEU:HD12  | 4:I:53:LEU:N     | 2.18                     | 0.59              |
| 1:P:2:SER:H      | 1:P:105:PRO:HA   | 1.67                     | 0.59              |
| 1:P:51:TRP:CZ2   | 1:P:179:LEU:HD11 | 2.38                     | 0.59              |
| 1:F:220:ASP:CG   | 1:F:221:GLY:HA3  | 2.28                     | 0.59              |
| 5:J:101:VAL:HG22 | 5:J:121:ARG:HG2  | 1.84                     | 0.59              |
| 1:K:99:TYR:CE1   | 3:M:3:ARG:HB3    | 2.37                     | 0.59              |
| 5:O:170:TRP:HD1  | 5:O:181:VAL:HG23 | 1.67                     | 0.59              |
| 1:P:81:LEU:HD12  | 1:P:118:TYR:CD2  | 2.38                     | 0.59              |
| 1:F:236:ALA:HB1  | 2:G:12:ARG:NH1   | 2.18                     | 0.59              |
| 2:Q:41:LYS:HB2   | 2:Q:46:ILE:HD11  | 1.85                     | 0.59              |
| 4:S:125:ILE:HG21 | 4:S:152:ASP:HA   | 1.85                     | 0.59              |
| 1:A:198:GLU:HG3  | 1:A:248:VAL:HG12 | 1.85                     | 0.58              |
| 4:N:194:PHE:CG   | 4:N:195:ALA:N    | 2.71                     | 0.58              |
| 4:N:194:PHE:HZ   | 4:N:199:ALA:HA   | 1.66                     | 0.58              |
| 1:K:241:PHE:HD1  | 1:K:242:GLN:H    | 1.52                     | 0.58              |
| 4:N:18:THR:HG22  | 4:N:92:ARG:HA    | 1.85                     | 0.58              |
| 5:J:21:LEU:HD12  | 5:J:21:LEU:N     | 2.18                     | 0.58              |
| 1:A:209:TYR:HB3  | 1:A:210:PRO:HD3  | 1.85                     | 0.58              |
| 1:A:219:ARG:HA   | 1:A:219:ARG:HH11 | 1.67                     | 0.58              |
| 4:I:70:GLY:O     | 4:I:78:ARG:HB3   | 2.02                     | 0.58              |
| 4:I:18:THR:HB    | 4:I:92:ARG:HA    | 1.85                     | 0.58              |
| 4:I:195:ALA:O    | 4:I:199:ALA:HB2  | 2.03                     | 0.58              |
| 5:O:26:GLN:HG3   | 5:O:106:SER:HB2  | 1.85                     | 0.58              |
| 1:A:57:PRO:O     | 1:A:61:ASP:HB2   | 2.04                     | 0.58              |
| 1:A:203:CYS:HB2  | 1:A:215:LEU:HD11 | 1.86                     | 0.58              |
| 4:D:58:SER:O     | 4:D:83:LEU:HD23  | 2.03                     | 0.58              |
| 1:K:257:TYR:N    | 1:K:257:TYR:CD2  | 2.69                     | 0.58              |
| 4:N:21:PHE:HZ    | 4:N:119:LEU:HD13 | 1.69                     | 0.58              |
| 1:A:189:VAL:HG22 | 1:A:190:THR:N    | 2.18                     | 0.58              |
| 2:G:7:ILE:HD12   | 2:G:82:VAL:HG21  | 1.84                     | 0.58              |
| 2:L:2:GLN:HE22   | 2:L:31:HIS:N     | 2.01                     | 0.58              |
| 4:N:209:THR:O    | 4:N:210:PHE:HB3  | 2.03                     | 0.58              |
| 2:Q:91:LYS:HG3   | 2:Q:92:ILE:H     | 1.68                     | 0.58              |
| 5:T:5:VAL:HG22   | 5:T:26:GLN:HB2   | 1.85                     | 0.58              |
| 1:K:233:THR:HG23 | 1:K:243:LYS:HG3  | 1.85                     | 0.58              |
| 2:L:3:ARG:HG3    | 2:L:86:THR:HG21  | 1.86                     | 0.58              |
| 1:P:55:GLU:HB2   | 1:P:59:TYR:HB2   | 1.86                     | 0.58              |
| 1:P:269:PRO:O    | 1:P:271:THR:HG23 | 2.04                     | 0.58              |
| 5:O:27:ASP:O     | 5:O:28:MET:HG3   | 2.03                     | 0.58              |
| 2:G:47:GLU:O     | 2:G:48:LYS:HG2   | 2.04                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:191:HIS:NE2  | 1:K:201:LEU:HG   | 2.19                     | 0.58              |
| 4:D:31:GLN:N     | 4:D:108:ALA:HB2  | 2.18                     | 0.57              |
| 2:G:75:LYS:C     | 2:G:77:GLU:H     | 2.12                     | 0.57              |
| 2:L:36:GLU:HG2   | 2:L:37:VAL:H     | 1.68                     | 0.57              |
| 5:O:221:CYS:O    | 5:O:247:SER:HB3  | 2.03                     | 0.57              |
| 2:B:29:GLY:HA2   | 2:B:61:SER:HB2   | 1.86                     | 0.57              |
| 1:F:15:PRO:C     | 1:F:17:ARG:H     | 2.11                     | 0.57              |
| 2:G:17:ASN:HD21  | 2:G:19:LYS:HE3   | 1.69                     | 0.57              |
| 4:D:12:ASN:CG    | 4:D:122:LYS:HE3  | 2.29                     | 0.57              |
| 4:I:165:VAL:HG12 | 4:I:189:SER:OG   | 2.04                     | 0.57              |
| 5:T:4:GLY:HA2    | 5:T:28:MET:HE3   | 1.86                     | 0.57              |
| 2:B:70:PHE:CZ    | 2:B:72:PRO:HG3   | 2.38                     | 0.57              |
| 5:J:42:TYR:HB3   | 5:J:50:LEU:HD22  | 1.86                     | 0.57              |
| 4:N:133:TYR:CD1  | 4:N:134:GLN:N    | 2.68                     | 0.57              |
| 1:A:233:THR:OG1  | 1:A:243:LYS:HE3  | 2.05                     | 0.57              |
| 4:D:52:LEU:HD22  | 5:E:113:ILE:CG2  | 2.34                     | 0.57              |
| 4:N:206:PRO:HB2  | 4:N:208:ASP:CB   | 2.33                     | 0.57              |
| 5:O:216:ARG:HG3  | 5:O:216:ARG:O    | 2.04                     | 0.57              |
| 4:S:137:ASP:HB2  | 5:T:139:PHE:CE2  | 2.39                     | 0.57              |
| 1:A:74:ASP:HB3   | 3:C:5:ARG:NH1    | 2.19                     | 0.57              |
| 5:E:99:THR:CG2   | 5:E:123:SER:HA   | 2.34                     | 0.57              |
| 1:F:35:ARG:HB3   | 1:F:47:PRO:HG2   | 1.86                     | 0.57              |
| 4:N:110:LYS:HG3  | 5:O:111:PHE:CE2  | 2.39                     | 0.57              |
| 4:N:133:TYR:CE2  | 4:N:212:PRO:HG2  | 2.40                     | 0.57              |
| 5:T:171:TRP:CZ3  | 5:T:176:GLU:HB2  | 2.39                     | 0.57              |
| 1:A:142:ILE:HG12 | 1:A:145:ARG:HH12 | 1.69                     | 0.57              |
| 5:E:149:THR:O    | 5:E:151:LYS:HG3  | 2.05                     | 0.57              |
| 4:N:23:CYS:HB3   | 4:N:87:ILE:HG12  | 1.85                     | 0.57              |
| 5:O:138:VAL:HG22 | 5:O:139:PHE:H    | 1.68                     | 0.57              |
| 1:A:85:TYR:CB    | 1:A:87:GLN:HE21  | 2.13                     | 0.57              |
| 4:D:54:MET:HE2   | 4:D:54:MET:HA    | 1.86                     | 0.57              |
| 1:K:203:CYS:O    | 1:K:204:TRP:HB3  | 2.04                     | 0.57              |
| 2:B:54:LEU:HD11  | 2:B:62:PHE:HB3   | 1.87                     | 0.57              |
| 1:F:99:TYR:CE1   | 3:H:3:ARG:HB3    | 2.38                     | 0.57              |
| 1:F:202:ARG:HE   | 1:F:246:ALA:CB   | 2.16                     | 0.57              |
| 2:L:12:ARG:HG3   | 2:L:13:HIS:H     | 1.69                     | 0.57              |
| 4:S:205:ILE:H    | 4:S:205:ILE:HD12 | 1.69                     | 0.57              |
| 1:A:22:PHE:CD1   | 1:A:71:THR:HB    | 2.39                     | 0.57              |
| 2:B:7:ILE:HD12   | 2:B:82:VAL:HG21  | 1.86                     | 0.57              |
| 1:F:215:LEU:HA   | 1:F:262:GLN:HE22 | 1.70                     | 0.57              |
| 4:D:41:TRP:HB2   | 4:D:54:MET:HB2   | 1.87                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:S:52:LEU:HD22  | 5:T:113:ILE:HG23 | 1.86                     | 0.56              |
| 5:T:236:GLN:HG3  | 5:T:237:ASP:H    | 1.70                     | 0.56              |
| 2:B:9:VAL:HG23   | 2:B:93:VAL:HG13  | 1.88                     | 0.56              |
| 2:B:41:LYS:HG2   | 2:B:42:ASN:HD22  | 1.68                     | 0.56              |
| 1:F:220:ASP:CB   | 1:F:221:GLY:HA3  | 2.33                     | 0.56              |
| 1:A:72:GLN:HE21  | 5:E:57:VAL:HG21  | 1.69                     | 0.56              |
| 2:G:7:ILE:O      | 2:G:8:GLN:HG3    | 2.05                     | 0.56              |
| 2:G:11:SER:OG    | 2:G:15:ALA:HB2   | 2.05                     | 0.56              |
| 4:I:132:VAL:HG22 | 4:I:148:PHE:HB2  | 1.86                     | 0.56              |
| 2:L:96:ASP:HB2   | 2:L:99:MET:HB3   | 1.88                     | 0.56              |
| 5:O:6:THR:HG23   | 5:O:25:ALA:HB3   | 1.87                     | 0.56              |
| 5:O:144:ALA:HB1  | 5:O:148:HIS:CE1  | 2.40                     | 0.56              |
| 1:P:21:ARG:HH21  | 1:P:23:ILE:HD11  | 1.70                     | 0.56              |
| 1:P:82:ARG:NH1   | 1:P:89:GLU:HG3   | 2.20                     | 0.56              |
| 1:P:222:GLU:HG3  | 1:P:224:GLN:NE2  | 2.19                     | 0.56              |
| 2:Q:70:PHE:CE1   | 2:Q:72:PRO:HG3   | 2.40                     | 0.56              |
| 5:T:138:VAL:HG23 | 5:T:248:ALA:HB3  | 1.87                     | 0.56              |
| 4:N:52:LEU:HD22  | 5:O:113:ILE:HG23 | 1.87                     | 0.56              |
| 1:P:66:ILE:HD13  | 4:S:109:GLY:HA2  | 1.87                     | 0.56              |
| 4:S:31:GLN:N     | 4:S:108:ALA:HB2  | 2.20                     | 0.56              |
| 4:S:39:PHE:HB3   | 4:S:87:ILE:HD13  | 1.87                     | 0.56              |
| 5:T:71:VAL:HB    | 5:T:72:PRO:HD3   | 1.88                     | 0.56              |
| 1:A:217:TRP:CE3  | 1:A:257:TYR:CE1  | 2.86                     | 0.56              |
| 5:J:54:HIS:CE1   | 5:J:71:VAL:HG21  | 2.40                     | 0.56              |
| 2:L:3:ARG:HE     | 2:L:3:ARG:N      | 2.03                     | 0.56              |
| 1:A:208:PHE:CD1  | 1:A:210:PRO:HD2  | 2.39                     | 0.56              |
| 1:A:217:TRP:HA   | 1:A:257:TYR:CZ   | 2.40                     | 0.56              |
| 5:E:234:TRP:CE2  | 5:E:236:GLN:HB2  | 2.40                     | 0.56              |
| 1:F:191:HIS:CE1  | 1:F:193:PRO:HD3  | 2.41                     | 0.56              |
| 5:J:224:GLN:HE22 | 5:J:245:ILE:HD11 | 1.69                     | 0.56              |
| 2:L:29:GLY:HA2   | 2:L:61:SER:CB    | 2.32                     | 0.56              |
| 5:J:19:MET:SD    | 5:J:122:LEU:HD13 | 2.46                     | 0.56              |
| 1:P:72:GLN:HG3   | 5:T:57:VAL:CG2   | 2.31                     | 0.56              |
| 1:A:218:GLN:HE22 | 1:A:260:HIS:CD2  | 2.24                     | 0.56              |
| 4:D:21:PHE:HZ    | 4:D:119:LEU:HD22 | 1.71                     | 0.56              |
| 5:E:80:ARG:O     | 5:E:81:LEU:C     | 2.49                     | 0.56              |
| 1:F:235:PRO:O    | 1:F:236:ALA:HB2  | 2.05                     | 0.56              |
| 1:K:103:VAL:HG23 | 1:K:108:ARG:C    | 2.29                     | 0.56              |
| 4:N:54:MET:HA    | 4:N:54:MET:HE2   | 1.87                     | 0.56              |
| 4:N:70:GLY:C     | 4:N:79:PHE:N     | 2.63                     | 0.56              |
| 5:O:45:ASP:HB3   | 1:P:145:ARG:NH2  | 2.18                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:217:TRP:CD1  | 1:P:259:CYS:HA   | 2.41                     | 0.56              |
| 1:P:219:ARG:HB3  | 1:P:224:GLN:NE2  | 2.20                     | 0.56              |
| 2:G:45:ARG:HG2   | 2:G:46:ILE:N     | 2.21                     | 0.56              |
| 5:O:26:GLN:HG3   | 5:O:106:SER:CB   | 2.35                     | 0.56              |
| 5:O:44:GLN:HB2   | 5:O:50:LEU:CD2   | 2.35                     | 0.56              |
| 5:O:136:VAL:HG12 | 5:O:137:ALA:N    | 2.21                     | 0.56              |
| 4:S:19:VAL:HG22  | 4:S:91:ILE:HB    | 1.87                     | 0.56              |
| 4:D:78:ARG:HG3   | 4:D:92:ARG:HD3   | 1.88                     | 0.56              |
| 1:K:67:PHE:O     | 1:K:71:THR:HG23  | 2.06                     | 0.56              |
| 5:O:193:ALA:HB1  | 5:T:28:MET:HG2   | 1.86                     | 0.56              |
| 1:P:55:GLU:HB2   | 1:P:59:TYR:CB    | 2.35                     | 0.56              |
| 2:B:21:ASN:HB3   | 2:B:70:PHE:HE1   | 1.70                     | 0.55              |
| 5:J:54:HIS:CE1   | 5:J:71:VAL:HG11  | 2.41                     | 0.55              |
| 1:K:187:THR:HB   | 1:K:204:TRP:CH2  | 2.41                     | 0.55              |
| 1:P:260:HIS:HA   | 1:P:271:THR:CG2  | 2.35                     | 0.55              |
| 4:S:192:SER:H    | 4:S:193:ASP:HA   | 1.70                     | 0.55              |
| 5:T:170:TRP:CD1  | 5:T:181:VAL:HG23 | 2.40                     | 0.55              |
| 4:D:158:SER:HB2  | 4:D:202:ASN:O    | 2.06                     | 0.55              |
| 1:F:70:ASN:HB3   | 3:H:5:ARG:NH2    | 2.18                     | 0.55              |
| 1:K:151:ARG:HD2  | 1:K:154:GLU:OE2  | 2.06                     | 0.55              |
| 5:O:173:ASN:HA   | 5:O:218:HIS:CE1  | 2.41                     | 0.55              |
| 1:P:28:VAL:HG23  | 1:P:33:PHE:CD2   | 2.41                     | 0.55              |
| 2:Q:22:PHE:HZ    | 2:Q:67:TYR:CD2   | 2.24                     | 0.55              |
| 4:N:145:VAL:HG22 | 4:N:187:ALA:C    | 2.31                     | 0.55              |
| 5:O:224:GLN:NE2  | 5:O:245:ILE:HD11 | 2.21                     | 0.55              |
| 5:T:15:LYS:O     | 5:T:18:GLN:HB2   | 2.07                     | 0.55              |
| 2:B:22:PHE:O     | 2:B:23:LEU:HB3   | 2.06                     | 0.55              |
| 5:J:74:ASP:OD1   | 5:J:76:TYR:HD2   | 1.90                     | 0.55              |
| 4:N:128:PRO:HB3  | 4:N:152:ASP:HB3  | 1.87                     | 0.55              |
| 5:E:74:ASP:CG    | 5:E:76:TYR:HD2   | 2.14                     | 0.55              |
| 1:F:211:ALA:HB2  | 1:F:241:PHE:CE2  | 2.41                     | 0.55              |
| 4:I:137:ASP:HA   | 5:J:139:PHE:HA   | 1.88                     | 0.55              |
| 1:K:244:TRP:N    | 1:K:244:TRP:HD1  | 2.03                     | 0.55              |
| 4:S:126:GLN:O    | 4:S:128:PRO:HD3  | 2.06                     | 0.55              |
| 4:I:162:ASP:HB3  | 4:I:165:VAL:HG22 | 1.88                     | 0.55              |
| 1:K:213:ILE:HG22 | 1:K:214:THR:N    | 2.21                     | 0.55              |
| 2:L:12:ARG:HE    | 2:L:13:HIS:CE1   | 2.26                     | 0.55              |
| 5:O:215:PRO:HA   | 5:O:252:GLY:HA3  | 1.89                     | 0.55              |
| 5:O:242:VAL:O    | 5:O:244:GLN:HG2  | 2.07                     | 0.55              |
| 5:J:174:GLY:HA2  | 5:J:220:ARG:NH1  | 2.23                     | 0.54              |
| 1:K:144:GLN:HE21 | 1:K:148:GLU:CD   | 2.15                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:N:132:VAL:H    | 4:N:209:THR:HG21 | 1.73                     | 0.54              |
| 5:O:72:PRO:HA    | 5:O:74:ASP:C     | 2.32                     | 0.54              |
| 2:Q:41:LYS:HA    | 2:Q:78:TYR:HA    | 1.89                     | 0.54              |
| 5:T:128:LEU:HD23 | 5:T:228:LEU:CD1  | 2.36                     | 0.54              |
| 4:D:30:SER:CA    | 4:D:108:ALA:CB   | 2.77                     | 0.54              |
| 1:F:21:ARG:HD3   | 1:F:39:ASP:CG    | 2.32                     | 0.54              |
| 1:F:72:GLN:HG3   | 5:J:57:VAL:HG21  | 1.89                     | 0.54              |
| 1:A:48:ARG:HB3   | 1:A:52:ILE:HD11  | 1.89                     | 0.54              |
| 5:J:156:CYS:C    | 5:J:157:LEU:HD12 | 2.32                     | 0.54              |
| 1:K:211:ALA:O    | 1:K:213:ILE:HG13 | 2.08                     | 0.54              |
| 2:L:3:ARG:N      | 2:L:3:ARG:NE     | 2.56                     | 0.54              |
| 4:N:122:LYS:HZ3  | 4:N:153:SER:HB2  | 1.72                     | 0.54              |
| 1:P:215:LEU:HD12 | 1:P:215:LEU:O    | 2.07                     | 0.54              |
| 5:T:96:PRO:HA    | 5:T:97:SER:C     | 2.32                     | 0.54              |
| 1:A:28:VAL:O     | 1:A:29:ASP:HB2   | 2.06                     | 0.54              |
| 5:E:45:ASP:HB3   | 1:F:145:ARG:NH2  | 2.22                     | 0.54              |
| 1:K:14:ARG:NH2   | 1:K:21:ARG:HB2   | 2.22                     | 0.54              |
| 4:S:211:PHE:HD2  | 4:S:211:PHE:C    | 2.16                     | 0.54              |
| 1:K:81:LEU:HD13  | 1:K:118:TYR:CD1  | 2.41                     | 0.54              |
| 1:K:100:GLY:O    | 1:K:160:LEU:HD22 | 2.08                     | 0.54              |
| 4:N:45:ASP:O     | 4:N:48:LYS:HG2   | 2.07                     | 0.54              |
| 5:O:66:THR:HG22  | 5:O:67:ALA:N     | 2.22                     | 0.54              |
| 1:A:110:LEU:HD12 | 1:A:111:ARG:N    | 2.23                     | 0.54              |
| 5:E:168:LEU:HD21 | 5:E:203:SER:HB2  | 1.89                     | 0.54              |
| 5:J:234:TRP:CD1  | 5:J:240:LYS:HB2  | 2.41                     | 0.54              |
| 4:N:105:VAL:HG13 | 4:N:113:PHE:HA   | 1.90                     | 0.54              |
| 5:O:130:ASN:HA   | 5:O:132:PHE:HE2  | 1.71                     | 0.54              |
| 4:S:21:PHE:HB2   | 4:S:89:LEU:HB3   | 1.90                     | 0.54              |
| 1:A:8:PHE:HB3    | 2:B:56:PHE:CE1   | 2.43                     | 0.54              |
| 5:E:74:ASP:OD1   | 5:E:76:TYR:HD2   | 1.90                     | 0.54              |
| 1:F:182:ALA:HB1  | 1:F:265:GLY:HA2  | 1.88                     | 0.54              |
| 1:K:51:TRP:HH2   | 1:K:178:THR:HB   | 1.72                     | 0.54              |
| 2:L:40:LEU:HB2   | 2:L:78:TYR:CD1   | 2.43                     | 0.54              |
| 5:O:48:MET:HG3   | 5:O:49:GLY:H     | 1.71                     | 0.54              |
| 5:T:228:LEU:HD22 | 5:T:228:LEU:H    | 1.71                     | 0.54              |
| 4:D:159:GLN:H    | 4:D:159:GLN:CD   | 2.16                     | 0.54              |
| 1:F:98:MET:HE2   | 2:G:56:PHE:CE2   | 2.42                     | 0.54              |
| 1:K:156:ASP:O    | 1:K:160:LEU:HG   | 2.07                     | 0.54              |
| 2:L:40:LEU:C     | 2:L:46:ILE:HD11  | 2.32                     | 0.54              |
| 4:N:13:VAL:HG21  | 4:N:19:VAL:HG22  | 1.89                     | 0.54              |
| 4:N:125:ILE:HG23 | 4:N:128:PRO:HG3  | 1.89                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:N:152:ASP:HB2  | 4:N:154:GLN:HE21 | 1.73                     | 0.54              |
| 5:O:194:LEU:HD12 | 5:O:194:LEU:H    | 1.72                     | 0.54              |
| 4:D:25:TYR:CZ    | 4:D:85:GLN:HA    | 2.43                     | 0.54              |
| 5:E:166:VAL:CG1  | 5:E:223:VAL:HG13 | 2.38                     | 0.54              |
| 5:E:238:ARG:HG3  | 5:E:239:ALA:H    | 1.72                     | 0.54              |
| 1:F:220:ASP:CB   | 1:F:221:GLY:CA   | 2.86                     | 0.54              |
| 1:A:178:THR:HG23 | 1:A:179:LEU:HD13 | 1.90                     | 0.53              |
| 5:E:176:GLU:HG3  | 5:E:177:VAL:N    | 2.24                     | 0.53              |
| 1:K:208:PHE:CZ   | 1:K:213:ILE:HD11 | 2.42                     | 0.53              |
| 1:P:2:SER:HB2    | 1:P:105:PRO:HG3  | 1.91                     | 0.53              |
| 1:A:197:HIS:CE1  | 1:A:251:SER:H    | 2.25                     | 0.53              |
| 4:N:44:GLN:NE2   | 5:O:44:GLN:HE22  | 2.05                     | 0.53              |
| 5:O:129:LYS:HE2  | 5:O:236:GLN:OE1  | 2.08                     | 0.53              |
| 5:T:95:ALA:C     | 5:T:124:VAL:HG11 | 2.33                     | 0.53              |
| 1:A:67:PHE:O     | 1:A:71:THR:HG23  | 2.08                     | 0.53              |
| 1:K:233:THR:HG22 | 1:K:241:PHE:CE1  | 2.43                     | 0.53              |
| 2:Q:39:LEU:HB2   | 2:Q:78:TYR:CZ    | 2.43                     | 0.53              |
| 1:A:217:TRP:HE3  | 1:A:257:TYR:CZ   | 2.27                     | 0.53              |
| 1:F:13:SER:O     | 1:F:92:SER:HB2   | 2.08                     | 0.53              |
| 2:G:39:LEU:HB2   | 2:G:46:ILE:CD1   | 2.38                     | 0.53              |
| 1:P:266:LEU:HD21 | 1:P:270:LEU:HD22 | 1.91                     | 0.53              |
| 5:T:55:TYR:CE2   | 5:T:67:ALA:HB3   | 2.43                     | 0.53              |
| 1:A:6:ARG:HA     | 1:A:100:GLY:HA3  | 1.89                     | 0.53              |
| 1:A:26:GLY:O     | 1:A:32:GLN:HA    | 2.09                     | 0.53              |
| 2:B:38:ASP:HB2   | 2:B:81:ARG:HE    | 1.74                     | 0.53              |
| 5:E:55:TYR:CE2   | 5:E:67:ALA:HB3   | 2.44                     | 0.53              |
| 5:E:134:PRO:HB3  | 5:E:161:PHE:HB3  | 1.90                     | 0.53              |
| 1:F:13:SER:HB2   | 1:F:78:LEU:HD13  | 1.89                     | 0.53              |
| 1:F:103:VAL:HG13 | 1:F:168:LEU:HD23 | 1.91                     | 0.53              |
| 1:F:159:TYR:CE2  | 1:F:164:CYS:HB2  | 2.44                     | 0.53              |
| 5:J:40:TYR:N     | 5:J:105:ALA:O    | 2.41                     | 0.53              |
| 4:N:210:PHE:HE1  | 5:O:148:HIS:CE1  | 2.25                     | 0.53              |
| 1:P:263:HIS:CG   | 1:P:264:GLU:H    | 2.26                     | 0.53              |
| 4:S:211:PHE:C    | 4:S:211:PHE:CD2  | 2.87                     | 0.53              |
| 5:T:187:PRO:HB3  | 5:T:199:TYR:HB3  | 1.90                     | 0.53              |
| 4:I:138:SER:O    | 4:I:139:LYS:C    | 2.52                     | 0.53              |
| 5:J:29:HIS:CE1   | 5:J:107:GLY:HA2  | 2.44                     | 0.53              |
| 2:L:87:LEU:HD12  | 2:L:87:LEU:O     | 2.08                     | 0.53              |
| 5:O:58:GLY:O     | 5:O:80:ARG:HG2   | 2.08                     | 0.53              |
| 4:S:68:GLU:HG3   | 4:S:68:GLU:O     | 2.07                     | 0.53              |
| 1:A:218:GLN:N    | 1:A:257:TYR:CE2  | 2.76                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:50:PRO:C     | 1:F:52:ILE:H     | 2.17                     | 0.53              |
| 5:J:58:GLY:O     | 5:J:80:ARG:HD3   | 2.09                     | 0.53              |
| 5:J:71:VAL:N     | 5:J:72:PRO:HD2   | 2.20                     | 0.53              |
| 5:J:110:ASN:O    | 5:J:111:PHE:HB2  | 2.08                     | 0.53              |
| 4:S:18:THR:HB    | 4:S:92:ARG:HA    | 1.89                     | 0.53              |
| 2:B:47:GLU:O     | 2:B:48:LYS:C     | 2.52                     | 0.53              |
| 5:J:71:VAL:O     | 5:J:71:VAL:HG12  | 2.09                     | 0.53              |
| 5:J:182:CYS:O    | 5:J:204:ARG:HD2  | 2.09                     | 0.53              |
| 1:K:244:TRP:CD1  | 1:K:244:TRP:H    | 2.27                     | 0.53              |
| 4:N:30:SER:CA    | 4:N:108:ALA:HB2  | 2.39                     | 0.53              |
| 4:N:152:ASP:HB2  | 4:N:154:GLN:NE2  | 2.24                     | 0.53              |
| 5:T:40:TYR:CD2   | 5:T:114:GLN:NE2  | 2.77                     | 0.53              |
| 1:A:155:GLN:HG2  | 4:D:57:TYR:HB3   | 1.91                     | 0.53              |
| 4:D:161:LYS:NZ   | 4:D:161:LYS:HB3  | 2.24                     | 0.53              |
| 4:I:13:VAL:HG11  | 4:I:19:VAL:HG22  | 1.90                     | 0.53              |
| 4:I:159:GLN:O    | 4:I:160:SER:HB2  | 2.08                     | 0.53              |
| 5:J:194:LEU:HG   | 5:J:196:ASP:H    | 1.74                     | 0.53              |
| 4:N:126:GLN:C    | 4:N:128:PRO:HD3  | 2.33                     | 0.53              |
| 5:O:45:ASP:CB    | 1:P:145:ARG:HH21 | 2.20                     | 0.53              |
| 2:B:24:ASN:HB3   | 2:B:67:TYR:CB    | 2.40                     | 0.52              |
| 5:E:162:TYR:CD1  | 5:E:163:PRO:HA   | 2.43                     | 0.52              |
| 4:I:39:PHE:CD1   | 4:I:106:VAL:HG22 | 2.41                     | 0.52              |
| 1:K:13:SER:HB2   | 1:K:78:LEU:HD13  | 1.91                     | 0.52              |
| 2:L:4:THR:HG21   | 2:L:87:LEU:HB3   | 1.91                     | 0.52              |
| 5:O:154:LEU:O    | 5:O:204:ARG:HA   | 2.09                     | 0.52              |
| 1:P:170:ARG:HH11 | 1:P:174:ASN:ND2  | 2.08                     | 0.52              |
| 4:S:2:LYS:O      | 4:S:3:GLU:HB2    | 2.09                     | 0.52              |
| 1:A:102:ASP:O    | 1:A:110:LEU:HG   | 2.10                     | 0.52              |
| 4:D:136:ARG:NE   | 4:D:136:ARG:HA   | 2.24                     | 0.52              |
| 2:L:23:LEU:HD13  | 2:L:70:PHE:CE1   | 2.44                     | 0.52              |
| 4:N:137:ASP:HB2  | 4:N:142:ASP:OD1  | 2.09                     | 0.52              |
| 5:O:60:GLY:C     | 5:O:61:THR:HG23  | 2.34                     | 0.52              |
| 5:O:170:TRP:CD1  | 5:O:181:VAL:HG23 | 2.44                     | 0.52              |
| 2:Q:29:GLY:HA2   | 2:Q:61:SER:CB    | 2.38                     | 0.52              |
| 5:T:180:GLY:O    | 5:T:205:LEU:HA   | 2.09                     | 0.52              |
| 4:D:136:ARG:O    | 4:D:137:ASP:CB   | 2.57                     | 0.52              |
| 1:F:98:MET:HE2   | 2:G:56:PHE:HE2   | 1.74                     | 0.52              |
| 4:N:145:VAL:HG11 | 4:N:186:VAL:HA   | 1.92                     | 0.52              |
| 1:P:147:TRP:HZ2  | 3:R:9:LEU:HD12   | 1.73                     | 0.52              |
| 5:T:43:ARG:HB2   | 5:T:53:ILE:HD11  | 1.89                     | 0.52              |
| 1:A:189:VAL:HG22 | 1:A:190:THR:H    | 1.74                     | 0.52              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:F:28:VAL:HG23  | 1:F:33:PHE:CD1  | 2.43                     | 0.52              |
| 2:L:81:ARG:NH2   | 2:L:90:PRO:HA   | 2.25                     | 0.52              |
| 1:P:77:SER:O     | 1:P:81:LEU:HD23 | 2.08                     | 0.52              |
| 2:Q:37:VAL:HB    | 2:Q:66:TYR:CZ   | 2.44                     | 0.52              |
| 4:S:141:SER:O    | 4:S:143:LYS:N   | 2.42                     | 0.52              |
| 5:T:59:GLU:O     | 5:T:80:ARG:O    | 2.27                     | 0.52              |
| 5:O:59:GLU:HG2   | 5:O:83:LYS:O    | 2.09                     | 0.52              |
| 4:S:177:SER:O    | 4:S:178:MET:HG2 | 2.09                     | 0.52              |
| 5:T:127:ASP:OD1  | 5:T:129:LYS:HG2 | 2.10                     | 0.52              |
| 5:E:182:CYS:O    | 5:E:204:ARG:HD2 | 2.10                     | 0.52              |
| 4:I:27:ASN:ND2   | 4:I:29:ALA:H    | 2.08                     | 0.52              |
| 4:N:45:ASP:HA    | 4:N:100:ALA:HB1 | 1.90                     | 0.52              |
| 1:F:165:VAL:C    | 1:F:167:TRP:H   | 2.18                     | 0.52              |
| 4:I:70:GLY:O     | 4:I:78:ARG:CB   | 2.58                     | 0.52              |
| 5:J:96:PRO:HA    | 5:J:97:SER:C    | 2.35                     | 0.52              |
| 4:N:4:VAL:O      | 4:N:4:VAL:HG13  | 2.09                     | 0.52              |
| 5:O:155:VAL:HG13 | 5:O:203:SER:O   | 2.09                     | 0.52              |
| 4:S:79:PHE:CD1   | 4:S:91:ILE:HG12 | 2.45                     | 0.52              |
| 5:E:110:ASN:O    | 5:E:111:PHE:HB2 | 2.09                     | 0.52              |
| 4:I:107:ARG:HG2  | 4:I:108:ALA:N   | 2.25                     | 0.52              |
| 5:J:138:VAL:HG22 | 5:J:248:ALA:HB1 | 1.92                     | 0.52              |
| 2:L:95:TRP:CE2   | 2:L:97:ARG:HA   | 2.45                     | 0.52              |
| 5:T:212:TRP:O    | 5:T:252:GLY:HA3 | 2.09                     | 0.52              |
| 2:B:13:HIS:O     | 2:B:14:PRO:C    | 2.53                     | 0.52              |
| 4:D:47:ARG:C     | 4:D:48:LYS:HG2  | 2.35                     | 0.52              |
| 1:K:60:TRP:CZ2   | 1:K:64:THR:HG21 | 2.45                     | 0.52              |
| 4:N:122:LYS:NZ   | 4:N:153:SER:HB2 | 2.23                     | 0.52              |
| 1:P:66:ILE:CD1   | 4:S:109:GLY:HA2 | 2.40                     | 0.52              |
| 4:S:107:ARG:O    | 4:S:108:ALA:C   | 2.52                     | 0.52              |
| 5:T:27:ASP:O     | 5:T:29:ASN:N    | 2.35                     | 0.52              |
| 1:A:211:ALA:C    | 1:A:213:ILE:H   | 2.18                     | 0.52              |
| 5:E:42:TYR:CZ    | 5:E:52:LEU:HD13 | 2.44                     | 0.52              |
| 1:F:220:ASP:OD1  | 1:F:220:ASP:N   | 2.42                     | 0.52              |
| 1:P:50:PRO:O     | 1:P:51:TRP:C    | 2.53                     | 0.52              |
| 4:S:139:LYS:HG3  | 4:S:140:SER:H   | 1.75                     | 0.52              |
| 1:F:122:ASP:OD1  | 2:G:60:TRP:NE1  | 2.42                     | 0.51              |
| 1:F:240:THR:HG22 | 2:G:12:ARG:HH22 | 1.75                     | 0.51              |
| 2:G:10:TYR:CD1   | 2:G:10:TYR:N    | 2.78                     | 0.51              |
| 2:G:27:VAL:HG21  | 2:G:35:ILE:HD13 | 1.92                     | 0.51              |
| 4:I:183:ASN:O    | 4:I:184:SER:HB2 | 2.10                     | 0.51              |
| 1:K:244:TRP:HD1  | 1:K:244:TRP:H   | 1.57                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:215:LEU:HD11 | 1:P:230:LEU:HD13 | 1.92                     | 0.51              |
| 2:Q:29:GLY:HA2   | 2:Q:61:SER:HB2   | 1.91                     | 0.51              |
| 1:F:194:ILE:HG13 | 1:F:199:ALA:HA   | 1.92                     | 0.51              |
| 5:J:31:TYR:CE1   | 5:J:110:ASN:HB2  | 2.45                     | 0.51              |
| 5:J:212:TRP:HE3  | 5:J:219:PHE:CE1  | 2.28                     | 0.51              |
| 4:N:7:ASP:HB2    | 4:N:117:THR:HG21 | 1.92                     | 0.51              |
| 4:N:44:GLN:HE22  | 5:O:44:GLN:NE2   | 2.07                     | 0.51              |
| 4:N:192:SER:H    | 4:N:193:ASP:HA   | 1.73                     | 0.51              |
| 4:N:207:GLU:HB2  | 4:N:208:ASP:CA   | 2.39                     | 0.51              |
| 5:O:182:CYS:HB3  | 5:O:204:ARG:CG   | 2.40                     | 0.51              |
| 1:P:201:LEU:HD13 | 1:P:257:TYR:CZ   | 2.46                     | 0.51              |
| 1:P:213:ILE:HD12 | 1:P:213:ILE:O    | 2.10                     | 0.51              |
| 4:S:200:PHE:C    | 4:S:202:ASN:H    | 2.18                     | 0.51              |
| 4:D:113:PHE:CD1  | 5:E:50:LEU:HD12  | 2.46                     | 0.51              |
| 1:F:236:ALA:HB1  | 2:G:12:ARG:NH2   | 2.25                     | 0.51              |
| 1:P:171:TYR:C    | 1:P:173:GLU:H    | 2.17                     | 0.51              |
| 5:T:143:GLU:O    | 5:T:146:ILE:HG12 | 2.11                     | 0.51              |
| 1:F:266:LEU:HD12 | 1:F:267:PRO:HD2  | 1.91                     | 0.51              |
| 2:G:40:LEU:HD11  | 2:G:81:ARG:HB2   | 1.92                     | 0.51              |
| 4:S:142:ASP:C    | 4:S:144:SER:H    | 2.19                     | 0.51              |
| 1:F:159:TYR:CD1  | 3:H:3:ARG:HB2    | 2.46                     | 0.51              |
| 4:I:12:ASN:CB    | 4:I:122:LYS:HE3  | 2.20                     | 0.51              |
| 4:N:210:PHE:CE1  | 5:O:148:HIS:CE1  | 2.98                     | 0.51              |
| 5:T:95:ALA:O     | 5:T:97:SER:O     | 2.28                     | 0.51              |
| 1:A:209:TYR:H    | 1:A:210:PRO:HD2  | 1.75                     | 0.51              |
| 1:P:217:TRP:CZ3  | 1:P:247:VAL:HG22 | 2.45                     | 0.51              |
| 1:A:244:TRP:CZ3  | 1:A:246:ALA:HB2  | 2.42                     | 0.51              |
| 1:K:127:ASN:O    | 1:K:130:LEU:HD23 | 2.09                     | 0.51              |
| 2:L:6:LYS:O      | 2:L:7:ILE:HG22   | 2.10                     | 0.51              |
| 4:N:143:LYS:O    | 4:N:144:SER:HB3  | 2.11                     | 0.51              |
| 2:Q:54:LEU:HD11  | 2:Q:62:PHE:HB3   | 1.92                     | 0.51              |
| 4:D:111:LEU:HD13 | 5:E:111:PHE:O    | 2.11                     | 0.51              |
| 1:F:234:ARG:O    | 1:F:235:PRO:O    | 2.28                     | 0.51              |
| 1:K:141:GLN:O    | 1:K:144:GLN:HB3  | 2.10                     | 0.51              |
| 1:K:143:THR:O    | 1:K:144:GLN:C    | 2.54                     | 0.51              |
| 1:P:49:ALA:HB1   | 1:P:50:PRO:HD2   | 1.93                     | 0.51              |
| 4:S:111:LEU:HB2  | 5:T:111:PHE:HB3  | 1.91                     | 0.51              |
| 4:D:82:GLN:HB3   | 4:D:88:SER:OG    | 2.11                     | 0.51              |
| 1:F:3:HIS:CE1    | 1:F:180:GLU:HG2  | 2.46                     | 0.51              |
| 2:L:28:SER:HA    | 2:L:62:PHE:O     | 2.11                     | 0.51              |
| 4:N:107:ARG:NH1  | 5:O:110:ASN:O    | 2.44                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:S:139:LYS:CG   | 4:S:140:SER:H    | 2.23                     | 0.51              |
| 5:T:42:TYR:CZ    | 5:T:52:LEU:HD13  | 2.45                     | 0.51              |
| 2:B:4:THR:HG23   | 2:B:5:PRO:HD2    | 1.92                     | 0.51              |
| 4:D:39:PHE:CD1   | 4:D:106:VAL:HG22 | 2.45                     | 0.51              |
| 1:F:85:TYR:HE2   | 1:F:118:TYR:HD2  | 1.59                     | 0.51              |
| 2:L:8:GLN:O      | 2:L:10:TYR:HD1   | 1.94                     | 0.51              |
| 2:L:39:LEU:CB    | 2:L:49:VAL:HG12  | 2.39                     | 0.51              |
| 2:L:42:ASN:HA    | 2:L:77:GLU:O     | 2.11                     | 0.51              |
| 5:T:128:LEU:HD23 | 5:T:228:LEU:HD12 | 1.93                     | 0.51              |
| 4:D:210:PHE:CG   | 4:D:212:PRO:HD3  | 2.46                     | 0.50              |
| 5:E:168:LEU:HD12 | 5:E:169:SER:N    | 2.24                     | 0.50              |
| 1:F:151:ARG:HD2  | 4:I:57:TYR:HD2   | 1.75                     | 0.50              |
| 1:F:234:ARG:HG3  | 1:F:242:GLN:HB2  | 1.92                     | 0.50              |
| 2:G:39:LEU:CB    | 2:G:46:ILE:HD11  | 2.40                     | 0.50              |
| 2:L:17:ASN:OD1   | 2:L:19:LYS:HG3   | 2.11                     | 0.50              |
| 2:L:40:LEU:HB2   | 2:L:78:TYR:HD1   | 1.76                     | 0.50              |
| 4:N:122:LYS:HE3  | 4:N:170:LYS:NZ   | 2.26                     | 0.50              |
| 4:S:188:TRP:CD2  | 5:T:157:LEU:HD11 | 2.45                     | 0.50              |
| 1:A:137:ASP:O    | 1:A:141:GLN:HG3  | 2.10                     | 0.50              |
| 1:A:217:TRP:HD1  | 1:A:228:THR:HG23 | 1.76                     | 0.50              |
| 4:N:132:VAL:H    | 4:N:209:THR:HG23 | 1.76                     | 0.50              |
| 4:N:207:GLU:CA   | 4:N:208:ASP:HB2  | 2.41                     | 0.50              |
| 1:P:65:GLN:OE1   | 4:S:110:LYS:HE3  | 2.11                     | 0.50              |
| 4:S:53:LEU:O     | 4:S:54:MET:HG2   | 2.11                     | 0.50              |
| 4:D:130:PRO:O    | 4:D:209:THR:HA   | 2.11                     | 0.50              |
| 4:D:135:LEU:HB3  | 5:E:140:GLU:O    | 2.11                     | 0.50              |
| 5:E:43:ARG:NH2   | 5:E:97:SER:HB2   | 2.26                     | 0.50              |
| 5:E:43:ARG:HH22  | 5:E:98:GLN:N     | 2.10                     | 0.50              |
| 5:E:223:VAL:O    | 5:E:223:VAL:HG12 | 2.11                     | 0.50              |
| 1:F:65:GLN:HA    | 1:F:65:GLN:OE1   | 2.12                     | 0.50              |
| 1:F:89:GLU:OE1   | 1:F:89:GLU:N     | 2.42                     | 0.50              |
| 1:K:128:GLU:C    | 1:K:130:LEU:H    | 2.18                     | 0.50              |
| 1:P:50:PRO:HG2   | 1:P:51:TRP:CZ3   | 2.46                     | 0.50              |
| 4:S:133:TYR:CD2  | 5:T:145:GLU:HB2  | 2.46                     | 0.50              |
| 1:A:194:ILE:HG12 | 1:A:199:ALA:HA   | 1.93                     | 0.50              |
| 5:J:97:SER:O     | 5:J:99:THR:N     | 2.44                     | 0.50              |
| 1:K:234:ARG:HD2  | 1:K:234:ARG:H    | 1.77                     | 0.50              |
| 4:N:132:VAL:HG13 | 4:N:146:CYS:HB3  | 1.93                     | 0.50              |
| 5:O:102:TYR:HE1  | 5:O:122:LEU:HB3  | 1.77                     | 0.50              |
| 5:O:132:PHE:HA   | 5:O:238:ARG:HH22 | 1.76                     | 0.50              |
| 5:O:183:THR:O    | 5:O:185:PRO:HD3  | 2.11                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:109:LEU:HD23 | 1:A:161:GLU:HG2  | 1.94                     | 0.50              |
| 1:F:48:ARG:O     | 1:F:49:ALA:HB3   | 2.11                     | 0.50              |
| 2:G:23:LEU:HD12  | 2:G:24:ASN:N     | 2.27                     | 0.50              |
| 2:Q:54:LEU:HD11  | 2:Q:62:PHE:CD2   | 2.46                     | 0.50              |
| 5:T:164:ASP:HB3  | 5:T:187:PRO:HG2  | 1.92                     | 0.50              |
| 5:T:172:VAL:O    | 5:T:175:LYS:HG2  | 2.11                     | 0.50              |
| 1:A:123:TYR:CZ   | 1:A:140:ALA:HA   | 2.47                     | 0.50              |
| 1:F:25:VAL:HG11  | 1:F:35:ARG:NH2   | 2.27                     | 0.50              |
| 4:I:40:PHE:HZ    | 5:J:112:ASP:OD1  | 1.94                     | 0.50              |
| 1:K:208:PHE:CE2  | 1:K:213:ILE:HD11 | 2.47                     | 0.50              |
| 4:N:110:LYS:HG2  | 4:N:110:LYS:O    | 2.12                     | 0.50              |
| 5:O:132:PHE:HA   | 5:O:238:ARG:NH2  | 2.26                     | 0.50              |
| 1:P:170:ARG:HH11 | 1:P:174:ASN:HD21 | 1.60                     | 0.50              |
| 2:Q:97:ARG:HG2   | 2:Q:98:ASP:N     | 2.26                     | 0.50              |
| 1:A:234:ARG:O    | 1:A:235:PRO:C    | 2.53                     | 0.50              |
| 4:D:20:ALA:HA    | 4:D:89:LEU:O     | 2.12                     | 0.50              |
| 1:F:13:SER:HB3   | 1:F:93:HIS:H     | 1.77                     | 0.50              |
| 4:I:30:SER:HA    | 4:I:108:ALA:HB1  | 1.88                     | 0.50              |
| 4:I:141:SER:HB3  | 4:I:143:LYS:HE2  | 1.92                     | 0.50              |
| 1:P:143:THR:O    | 1:P:146:LYS:HB3  | 2.12                     | 0.50              |
| 5:T:157:LEU:CD2  | 5:T:159:THR:HG23 | 2.41                     | 0.50              |
| 1:A:250:PRO:O    | 1:A:254:GLU:HG3  | 2.12                     | 0.50              |
| 2:B:73:THR:OG1   | 2:B:74:GLU:N     | 2.45                     | 0.50              |
| 5:E:156:CYS:O    | 5:E:202:SER:HA   | 2.11                     | 0.50              |
| 5:J:127:ASP:C    | 5:J:129:LYS:H    | 2.18                     | 0.50              |
| 1:K:19:GLU:HB3   | 1:K:20:PRO:HD2   | 1.94                     | 0.50              |
| 1:K:228:THR:HA   | 1:K:246:ALA:O    | 2.11                     | 0.50              |
| 2:L:36:GLU:HG2   | 2:L:83:ASN:OD1   | 2.11                     | 0.50              |
| 4:N:23:CYS:HB3   | 4:N:87:ILE:CG1   | 2.41                     | 0.50              |
| 5:J:12:VAL:HG22  | 5:J:123:SER:HB3  | 1.94                     | 0.50              |
| 5:J:70:GLU:O     | 5:J:70:GLU:CD    | 2.54                     | 0.50              |
| 1:K:44:ARG:HD3   | 1:K:48:ARG:HH22  | 1.77                     | 0.50              |
| 1:K:77:SER:HB3   | 3:M:9:LEU:HD13   | 1.92                     | 0.50              |
| 1:A:141:GLN:O    | 1:A:145:ARG:HG3  | 2.12                     | 0.49              |
| 5:E:69:GLY:O     | 5:E:70:GLU:HB2   | 2.12                     | 0.49              |
| 4:I:107:ARG:HG2  | 4:I:108:ALA:H    | 1.76                     | 0.49              |
| 4:I:107:ARG:NH1  | 5:J:110:ASN:O    | 2.44                     | 0.49              |
| 4:N:208:ASP:C    | 4:N:210:PHE:H    | 2.20                     | 0.49              |
| 5:O:39:MET:HA    | 5:O:105:ALA:O    | 2.12                     | 0.49              |
| 5:T:128:LEU:HD12 | 5:T:128:LEU:N    | 2.27                     | 0.49              |
| 4:D:146:CYS:HB2  | 4:D:187:ALA:HB3  | 1.94                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:148:PHE:O    | 4:D:184:SER:HA   | 2.12                     | 0.49              |
| 4:D:172:VAL:HG12 | 4:D:173:LEU:O    | 2.12                     | 0.49              |
| 2:L:23:LEU:O     | 2:L:67:TYR:HB2   | 2.11                     | 0.49              |
| 4:N:213:SER:HB3  | 4:N:214:PRO:HD3  | 1.93                     | 0.49              |
| 1:P:6:ARG:HD3    | 1:P:100:GLY:HA3  | 1.94                     | 0.49              |
| 1:A:215:LEU:HD22 | 1:A:245:ALA:HB3  | 1.93                     | 0.49              |
| 1:F:81:LEU:HD12  | 1:F:84:TYR:HD2   | 1.76                     | 0.49              |
| 1:K:103:VAL:HG23 | 1:K:108:ARG:O    | 2.12                     | 0.49              |
| 2:L:48:LYS:HG2   | 2:L:50:GLU:HG3   | 1.94                     | 0.49              |
| 5:O:136:VAL:HG22 | 5:O:158:ALA:HB2  | 1.94                     | 0.49              |
| 1:P:263:HIS:CG   | 1:P:264:GLU:N    | 2.81                     | 0.49              |
| 5:E:25:GLN:HG2   | 5:E:26:ASP:N     | 2.26                     | 0.49              |
| 5:E:171:TRP:CZ3  | 5:E:222:GLN:HB3  | 2.47                     | 0.49              |
| 5:E:178:HIS:O    | 5:E:181:VAL:HG22 | 2.13                     | 0.49              |
| 5:E:225:PHE:O    | 5:E:243:THR:HG23 | 2.11                     | 0.49              |
| 1:F:12:MET:HE1   | 2:G:34:ASP:OD1   | 2.13                     | 0.49              |
| 2:G:47:GLU:C     | 2:G:48:LYS:HG2   | 2.38                     | 0.49              |
| 3:H:6:ALA:O      | 5:J:109:GLY:HA2  | 2.12                     | 0.49              |
| 5:J:18:SER:HB2   | 5:J:92:GLU:O     | 2.12                     | 0.49              |
| 1:K:44:ARG:HD3   | 1:K:48:ARG:NH2   | 2.27                     | 0.49              |
| 4:N:199:ALA:C    | 4:N:201:ASN:H    | 2.20                     | 0.49              |
| 4:D:208:ASP:HA   | 1:P:108:ARG:HB3  | 1.93                     | 0.49              |
| 5:E:166:VAL:CG1  | 5:E:167:GLU:N    | 2.75                     | 0.49              |
| 5:E:171:TRP:HZ3  | 5:E:222:GLN:HB3  | 1.77                     | 0.49              |
| 5:J:39:MET:HA    | 5:J:106:SER:HA   | 1.93                     | 0.49              |
| 1:K:121:LYS:HZ3  | 2:L:1:ILE:HD11   | 1.77                     | 0.49              |
| 4:N:68:GLU:H     | 4:N:68:GLU:CD    | 2.21                     | 0.49              |
| 4:N:70:GLY:O     | 4:N:78:ARG:CG    | 2.60                     | 0.49              |
| 1:P:35:ARG:CZ    | 2:Q:53:ASP:HB3   | 2.43                     | 0.49              |
| 4:S:148:PHE:HB3  | 4:S:185:ALA:HB3  | 1.93                     | 0.49              |
| 5:T:20:MET:HG2   | 5:T:91:LEU:HD12  | 1.94                     | 0.49              |
| 5:T:95:ALA:O     | 5:T:98:GLN:HB2   | 2.13                     | 0.49              |
| 5:T:136:VAL:HG12 | 5:T:137:ALA:N    | 2.28                     | 0.49              |
| 4:D:25:TYR:OH    | 4:D:85:GLN:HA    | 2.11                     | 0.49              |
| 4:D:107:ARG:HG2  | 4:D:108:ALA:N    | 2.27                     | 0.49              |
| 4:D:167:ILE:C    | 4:D:167:ILE:HD12 | 2.37                     | 0.49              |
| 5:E:94:ALA:O     | 5:E:95:ALA:HB2   | 2.12                     | 0.49              |
| 3:H:9:LEU:HD12   | 3:H:9:LEU:N      | 2.27                     | 0.49              |
| 1:K:159:TYR:CE2  | 1:K:164:CYS:HB2  | 2.47                     | 0.49              |
| 1:K:201:LEU:HD12 | 1:K:201:LEU:N    | 2.28                     | 0.49              |
| 4:N:21:PHE:CZ    | 4:N:119:LEU:HD13 | 2.48                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:J:90:GLY:C     | 5:J:91:LEU:HD23  | 2.37                     | 0.49              |
| 2:L:7:ILE:HA     | 2:L:26:TYR:O     | 2.12                     | 0.49              |
| 2:L:81:ARG:NH1   | 2:L:83:ASN:HB3   | 2.15                     | 0.49              |
| 4:N:2:LYS:O      | 4:N:3:GLU:HB2    | 2.11                     | 0.49              |
| 4:N:206:PRO:C    | 4:N:208:ASP:HB2  | 2.37                     | 0.49              |
| 5:O:182:CYS:HB3  | 5:O:204:ARG:HG3  | 1.93                     | 0.49              |
| 1:A:185:PRO:O    | 1:A:186:LYS:HB2  | 2.12                     | 0.49              |
| 4:D:161:LYS:HB3  | 4:D:161:LYS:HZ2  | 1.78                     | 0.49              |
| 2:G:39:LEU:N     | 2:G:39:LEU:HD12  | 2.28                     | 0.49              |
| 4:I:47:ARG:HD3   | 5:J:186:GLN:HE22 | 1.77                     | 0.49              |
| 5:J:29:HIS:ND1   | 5:J:107:GLY:HA2  | 2.28                     | 0.49              |
| 1:F:123:TYR:HD2  | 1:F:124:ILE:HG22 | 1.78                     | 0.49              |
| 1:F:262:GLN:H    | 1:F:262:GLN:NE2  | 2.10                     | 0.49              |
| 4:I:27:ASN:HD22  | 4:I:29:ALA:H     | 1.60                     | 0.49              |
| 5:O:59:GLU:HG2   | 5:O:84:LYS:HB2   | 1.95                     | 0.49              |
| 5:O:214:ASN:ND2  | 5:O:216:ARG:HB3  | 2.28                     | 0.49              |
| 2:B:29:GLY:HA2   | 2:B:61:SER:CB    | 2.42                     | 0.49              |
| 1:K:109:LEU:HD22 | 1:K:161:GLU:HA   | 1.94                     | 0.49              |
| 1:K:142:ILE:HA   | 1:K:145:ARG:HH11 | 1.76                     | 0.49              |
| 5:O:40:TYR:N     | 5:O:105:ALA:O    | 2.46                     | 0.49              |
| 1:P:45:GLU:O     | 1:P:46:GLU:C     | 2.55                     | 0.49              |
| 4:S:40:PHE:HZ    | 5:T:112:ASP:OD1  | 1.96                     | 0.49              |
| 1:A:6:ARG:HG2    | 1:A:100:GLY:HA3  | 1.94                     | 0.48              |
| 1:F:203:CYS:H    | 1:F:217:TRP:HZ2  | 1.59                     | 0.48              |
| 4:N:167:ILE:HG23 | 4:N:187:ALA:HB2  | 1.96                     | 0.48              |
| 4:N:175:MET:HE2  | 4:N:178:MET:HE2  | 1.95                     | 0.48              |
| 1:A:226:GLN:C    | 1:A:228:THR:H    | 2.21                     | 0.48              |
| 1:K:8:PHE:HB2    | 1:K:25:VAL:HG13  | 1.95                     | 0.48              |
| 4:N:147:LEU:CD2  | 4:N:149:THR:HB   | 2.43                     | 0.48              |
| 5:O:78:VAL:HG23  | 5:O:88:LEU:O     | 2.12                     | 0.48              |
| 5:O:78:VAL:HG23  | 5:O:89:LEU:HA    | 1.95                     | 0.48              |
| 5:O:127:ASP:C    | 5:O:129:LYS:H    | 2.21                     | 0.48              |
| 1:P:115:GLN:HG3  | 1:P:125:ALA:CB   | 2.37                     | 0.48              |
| 1:A:2:SER:H      | 1:A:105:PRO:HG3  | 1.79                     | 0.48              |
| 4:D:68:GLU:O     | 4:D:69:ASP:HB3   | 2.13                     | 0.48              |
| 5:J:172:VAL:HG22 | 5:J:219:PHE:HD2  | 1.78                     | 0.48              |
| 1:K:249:VAL:CG2  | 1:K:250:PRO:HD2  | 2.44                     | 0.48              |
| 2:L:33:SER:O     | 2:L:34:ASP:C     | 2.55                     | 0.48              |
| 5:O:54:HIS:CE1   | 5:O:71:VAL:HG12  | 2.48                     | 0.48              |
| 5:O:54:HIS:HE1   | 5:O:71:VAL:HG12  | 1.78                     | 0.48              |
| 5:O:224:GLN:HE22 | 5:O:245:ILE:HD11 | 1.77                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:S:44:GLN:HE22  | 5:T:44:GLN:HE22  | 1.61                     | 0.48              |
| 5:T:225:PHE:O    | 5:T:243:THR:HG23 | 2.13                     | 0.48              |
| 1:A:217:TRP:HA   | 1:A:257:TYR:HH   | 1.78                     | 0.48              |
| 1:F:88:SER:C     | 1:F:90:ALA:H     | 2.20                     | 0.48              |
| 4:I:161:LYS:HE3  | 4:I:202:ASN:OD1  | 2.13                     | 0.48              |
| 1:K:121:LYS:HG2  | 2:L:1:ILE:CD1    | 2.42                     | 0.48              |
| 1:K:217:TRP:CE3  | 1:K:247:VAL:HB   | 2.48                     | 0.48              |
| 1:P:129:ASP:OD2  | 1:P:131:ARG:HB2  | 2.13                     | 0.48              |
| 4:D:148:PHE:HB2  | 4:D:200:PHE:CE2  | 2.49                     | 0.48              |
| 5:E:8:PRO:HD2    | 5:E:21:LEU:HD22  | 1.96                     | 0.48              |
| 2:G:40:LEU:N     | 2:G:40:LEU:HD12  | 2.29                     | 0.48              |
| 2:G:41:LYS:C     | 2:G:43:GLY:H     | 2.20                     | 0.48              |
| 1:P:189:VAL:HG11 | 1:P:203:CYS:HA   | 1.95                     | 0.48              |
| 1:P:266:LEU:HD21 | 1:P:270:LEU:HB2  | 1.94                     | 0.48              |
| 5:T:54:HIS:CE1   | 5:T:71:VAL:HG22  | 2.49                     | 0.48              |
| 1:A:217:TRP:HZ2  | 1:A:245:ALA:O    | 1.97                     | 0.48              |
| 2:B:27:VAL:HG23  | 2:B:27:VAL:O     | 2.14                     | 0.48              |
| 1:F:67:PHE:O     | 1:F:71:THR:HG23  | 2.14                     | 0.48              |
| 5:J:239:ALA:O    | 5:J:240:LYS:HB3  | 2.14                     | 0.48              |
| 1:K:27:TYR:CE2   | 1:K:32:GLN:HB2   | 2.48                     | 0.48              |
| 2:Q:19:LYS:O     | 2:Q:20:SER:HB2   | 2.13                     | 0.48              |
| 5:T:132:PHE:O    | 5:T:161:PHE:HA   | 2.14                     | 0.48              |
| 4:D:25:TYR:HD2   | 4:D:27:ASN:O     | 1.97                     | 0.48              |
| 1:F:55:GLU:CD    | 1:F:170:ARG:HH22 | 2.21                     | 0.48              |
| 1:F:123:TYR:CE2  | 3:H:9:LEU:HD23   | 2.49                     | 0.48              |
| 1:F:234:ARG:HB2  | 2:G:10:TYR:CE2   | 2.49                     | 0.48              |
| 2:G:46:ILE:HB    | 2:G:47:GLU:H     | 1.41                     | 0.48              |
| 5:O:223:VAL:O    | 5:O:223:VAL:HG13 | 2.14                     | 0.48              |
| 1:P:72:GLN:HG3   | 5:T:57:VAL:HG11  | 1.95                     | 0.48              |
| 1:P:211:ALA:HB2  | 1:P:241:PHE:CG   | 2.48                     | 0.48              |
| 4:S:27:ASN:C     | 4:S:27:ASN:ND2   | 2.67                     | 0.48              |
| 1:A:242:GLN:HE22 | 2:B:12:ARG:HA    | 1.79                     | 0.48              |
| 4:D:168:THR:HB   | 5:E:184:ASP:OD2  | 2.14                     | 0.48              |
| 1:F:55:GLU:CG    | 1:F:170:ARG:HH22 | 2.26                     | 0.48              |
| 1:F:98:MET:HE1   | 2:G:58:LYS:HA    | 1.95                     | 0.48              |
| 1:F:147:TRP:CD1  | 1:F:152:VAL:HG21 | 2.48                     | 0.48              |
| 1:F:201:LEU:HD22 | 1:F:274:TRP:CD1  | 2.49                     | 0.48              |
| 4:I:153:SER:C    | 4:I:155:THR:H    | 2.22                     | 0.48              |
| 4:N:95:LYS:O     | 4:N:121:VAL:HG11 | 2.13                     | 0.48              |
| 5:T:139:PHE:HB2  | 5:T:155:VAL:HG13 | 1.96                     | 0.48              |
| 5:T:157:LEU:HD21 | 5:T:159:THR:HG23 | 1.96                     | 0.48              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 4:D:194:PHE:HD2  | 4:D:194:PHE:H      | 1.62                     | 0.48              |
| 5:J:149:THR:HG23 | 5:J:151:LYS:H      | 1.79                     | 0.48              |
| 5:O:155:VAL:HG13 | 5:O:203:SER:H      | 1.79                     | 0.48              |
| 1:P:143:THR:O    | 1:P:144:GLN:C      | 2.56                     | 0.48              |
| 1:P:206:LEU:HG   | 1:P:242:GLN:HE22   | 1.79                     | 0.48              |
| 2:Q:80:CYS:H     | 2:Q:92:ILE:CD1     | 2.27                     | 0.48              |
| 1:A:67:PHE:CE2   | 1:A:71:THR:HG21    | 2.49                     | 0.48              |
| 5:E:45:ASP:HB2   | 5:E:48:MET:CG      | 2.43                     | 0.48              |
| 5:E:99:THR:HG23  | 5:E:124:VAL:H      | 1.79                     | 0.48              |
| 1:F:211:ALA:HB2  | 1:F:241:PHE:HE2    | 1.79                     | 0.48              |
| 4:N:11:PHE:N     | 4:N:11:PHE:CD2     | 2.82                     | 0.48              |
| 4:N:19:VAL:HG12  | 4:N:20:ALA:N       | 2.24                     | 0.48              |
| 4:N:84:ASN:C     | 4:N:84(B):ALA:H    | 2.21                     | 0.48              |
| 4:N:166:TYR:HD2  | 4:N:188:TRP:NE1    | 2.12                     | 0.48              |
| 4:S:213:SER:N    | 4:S:214:PRO:CD     | 2.77                     | 0.48              |
| 5:E:143:GLU:H    | 5:E:143:GLU:CD     | 2.22                     | 0.47              |
| 4:I:111:LEU:HD13 | 5:J:111:PHE:O      | 2.14                     | 0.47              |
| 4:N:83:LEU:HD21  | 4:N:84(A):ARG:HH11 | 1.79                     | 0.47              |
| 4:N:112:ILE:HD12 | 4:N:112:ILE:N      | 2.29                     | 0.47              |
| 4:N:113:PHE:CE1  | 5:O:50:LEU:HD12    | 2.48                     | 0.47              |
| 2:Q:12:ARG:HG2   | 2:Q:24:ASN:HD21    | 1.79                     | 0.47              |
| 4:S:41:TRP:HA    | 4:S:103:LEU:O      | 2.14                     | 0.47              |
| 5:T:80:ARG:HD2   | 5:T:86:ASN:O       | 2.13                     | 0.47              |
| 5:T:97:SER:C     | 5:T:99:THR:N       | 2.71                     | 0.47              |
| 1:A:82:ARG:HG3   | 1:A:87:GLN:HB2     | 1.95                     | 0.47              |
| 1:A:208:PHE:HD1  | 1:A:209:TYR:N      | 2.12                     | 0.47              |
| 4:D:21:PHE:CZ    | 4:D:119:LEU:HD22   | 2.47                     | 0.47              |
| 5:E:151:LYS:HD3  | 5:E:206:ARG:HD3    | 1.95                     | 0.47              |
| 1:F:72:GLN:HE21  | 5:J:57:VAL:HG21    | 1.79                     | 0.47              |
| 4:N:6:GLN:NE2    | 4:N:102:TYR:O      | 2.47                     | 0.47              |
| 1:P:250:PRO:HG2  | 1:P:253:GLU:HB2    | 1.96                     | 0.47              |
| 4:S:96:LEU:HD21  | 4:S:172:VAL:HG11   | 1.96                     | 0.47              |
| 1:A:253:GLU:HB3  | 1:A:256:ARG:HD3    | 1.96                     | 0.47              |
| 5:E:80:ARG:O     | 5:E:80:ARG:HG3     | 2.15                     | 0.47              |
| 1:F:249:VAL:HB   | 1:F:250:PRO:HD2    | 1.95                     | 0.47              |
| 4:I:162:ASP:HB3  | 4:I:165:VAL:CG2    | 2.44                     | 0.47              |
| 1:K:3:HIS:HB3    | 1:K:29:ASP:OD2     | 2.14                     | 0.47              |
| 2:L:40:LEU:H     | 2:L:78:TYR:HE1     | 1.59                     | 0.47              |
| 4:D:125:ILE:HG13 | 4:D:152:ASP:HA     | 1.97                     | 0.47              |
| 5:E:40:TYR:N     | 5:E:105:ALA:O      | 2.46                     | 0.47              |
| 5:E:127:ASP:OD1  | 5:E:129:LYS:HG3    | 2.15                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:231:VAL:HG13 | 2:G:8:GLN:HE21   | 1.79                     | 0.47              |
| 4:I:200:PHE:O    | 4:I:205:ILE:HD11 | 2.14                     | 0.47              |
| 4:N:115:GLN:HE21 | 5:O:48:MET:HA    | 1.80                     | 0.47              |
| 1:P:231:VAL:HG11 | 1:P:244:TRP:CE2  | 2.49                     | 0.47              |
| 4:S:162:ASP:HB3  | 4:S:165:VAL:HG12 | 1.95                     | 0.47              |
| 5:T:230:GLU:HG3  | 5:T:231:ASN:N    | 2.27                     | 0.47              |
| 1:A:53:GLU:N     | 1:A:53:GLU:OE1   | 2.47                     | 0.47              |
| 1:A:198:GLU:HG3  | 1:A:248:VAL:CG1  | 2.43                     | 0.47              |
| 2:B:12:ARG:O     | 2:B:13:HIS:C     | 2.57                     | 0.47              |
| 5:J:140:GLU:HG2  | 5:J:212:TRP:HH2  | 1.79                     | 0.47              |
| 1:K:172:LEU:HD12 | 1:K:173:GLU:N    | 2.30                     | 0.47              |
| 4:S:44:GLN:O     | 4:S:100:ALA:HB1  | 2.14                     | 0.47              |
| 5:T:41:TRP:CD1   | 5:T:89:LEU:HB2   | 2.49                     | 0.47              |
| 5:T:67:ALA:HB1   | 5:T:68:LYS:HG2   | 1.97                     | 0.47              |
| 5:T:171:TRP:HB2  | 5:T:220:ARG:HB3  | 1.97                     | 0.47              |
| 2:B:9:VAL:CG2    | 2:B:93:VAL:HG13  | 2.45                     | 0.47              |
| 4:D:41:TRP:CZ3   | 4:D:104:CYS:HB2  | 2.50                     | 0.47              |
| 1:F:36:PHE:HA    | 1:F:46:GLU:OE2   | 2.15                     | 0.47              |
| 2:G:38:ASP:C     | 2:G:39:LEU:HD12  | 2.39                     | 0.47              |
| 1:K:218:GLN:HB2  | 1:K:258:THR:OG1  | 2.14                     | 0.47              |
| 5:O:97:SER:C     | 5:O:99:THR:N     | 2.72                     | 0.47              |
| 5:T:164:ASP:HB2  | 5:T:187:PRO:HG2  | 1.94                     | 0.47              |
| 2:B:36:GLU:HB2   | 2:B:83:ASN:HB3   | 1.97                     | 0.47              |
| 5:E:27:MET:HB2   | 5:E:29:HIS:CE1   | 2.49                     | 0.47              |
| 1:F:59:TYR:HE1   | 1:F:167:TRP:CZ3  | 2.32                     | 0.47              |
| 1:F:123:TYR:O    | 1:F:136:ALA:HB3  | 2.14                     | 0.47              |
| 1:F:220:ASP:HB2  | 1:F:221:GLY:CA   | 2.44                     | 0.47              |
| 1:F:240:THR:CG2  | 2:G:12:ARG:HH22  | 2.28                     | 0.47              |
| 1:K:189:VAL:N    | 1:K:204:TRP:CZ2  | 2.82                     | 0.47              |
| 4:N:54:MET:HE2   | 4:N:55:SER:H     | 1.79                     | 0.47              |
| 1:P:123:TYR:OH   | 1:P:140:ALA:HA   | 2.14                     | 0.47              |
| 1:P:147:TRP:CZ2  | 3:R:9:LEU:HD12   | 2.49                     | 0.47              |
| 1:P:191:HIS:ND1  | 1:P:192:HIS:N    | 2.63                     | 0.47              |
| 5:T:66:THR:HG22  | 5:T:67:ALA:N     | 2.30                     | 0.47              |
| 5:T:99:THR:HB    | 5:T:124:VAL:H    | 1.78                     | 0.47              |
| 1:A:258:THR:CB   | 1:A:273:ARG:HA   | 2.37                     | 0.47              |
| 5:J:14:LYS:HB3   | 5:J:17:GLN:HG3   | 1.96                     | 0.47              |
| 1:K:256:ARG:HG3  | 1:K:256:ARG:O    | 2.15                     | 0.47              |
| 4:N:11:PHE:HB2   | 4:N:119:LEU:CD1  | 2.45                     | 0.47              |
| 2:Q:80:CYS:H     | 2:Q:92:ILE:HD11  | 1.80                     | 0.47              |
| 5:T:15:LYS:HB2   | 5:T:128:LEU:CD1  | 2.43                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:27:ASN:ND2   | 4:D:29:ALA:H     | 2.12                     | 0.47              |
| 4:D:39:PHE:HD1   | 4:D:106:VAL:HG22 | 1.80                     | 0.47              |
| 5:E:71:VAL:N     | 5:E:72:PRO:CD    | 2.77                     | 0.47              |
| 2:G:55:SER:HB2   | 2:G:63:TYR:CZ    | 2.49                     | 0.47              |
| 5:O:223:VAL:HG12 | 5:O:247:SER:OG   | 2.15                     | 0.47              |
| 1:P:65:GLN:O     | 1:P:69:THR:HB    | 2.15                     | 0.47              |
| 1:A:14:ARG:NE    | 1:A:19:GLU:O     | 2.48                     | 0.47              |
| 5:J:71:VAL:HA    | 5:J:74:ASP:OD1   | 2.15                     | 0.47              |
| 1:K:173:GLU:C    | 1:K:175:GLY:H    | 2.23                     | 0.47              |
| 5:O:134:PRO:HB2  | 5:O:158:ALA:HB1  | 1.97                     | 0.47              |
| 1:P:184:PRO:HA   | 1:P:185:PRO:HD3  | 1.77                     | 0.47              |
| 2:Q:23:LEU:CD2   | 2:Q:78:TYR:HB3   | 2.45                     | 0.47              |
| 1:A:189:VAL:HG23 | 1:A:203:CYS:HA   | 1.96                     | 0.46              |
| 4:D:46:SER:HA    | 4:D:47:ARG:HA    | 1.63                     | 0.46              |
| 1:F:126:LEU:HD12 | 1:F:127:ASN:H    | 1.79                     | 0.46              |
| 2:G:10:TYR:CE1   | 2:G:24:ASN:CG    | 2.93                     | 0.46              |
| 4:I:44:GLN:HE22  | 5:J:44:GLN:HE22  | 1.62                     | 0.46              |
| 4:N:13:VAL:HG11  | 4:N:19:VAL:HG22  | 1.96                     | 0.46              |
| 4:N:107:ARG:HG2  | 4:N:108:ALA:N    | 2.30                     | 0.46              |
| 5:O:83:LYS:HG3   | 5:O:84:LYS:H     | 1.79                     | 0.46              |
| 1:P:35:ARG:O     | 1:P:46:GLU:HB3   | 2.14                     | 0.46              |
| 1:A:238:ASP:CG   | 2:B:12:ARG:HH12  | 2.24                     | 0.46              |
| 4:D:197:ALA:HA   | 4:D:211:PHE:CE1  | 2.50                     | 0.46              |
| 5:E:238:ARG:HG3  | 5:E:239:ALA:N    | 2.29                     | 0.46              |
| 2:G:17:ASN:ND2   | 2:G:19:LYS:HE3   | 2.30                     | 0.46              |
| 2:L:81:ARG:HH11  | 2:L:81:ARG:HG3   | 1.81                     | 0.46              |
| 4:N:150:ASP:O    | 4:N:151:PHE:C    | 2.58                     | 0.46              |
| 5:O:172:VAL:HG12 | 5:O:219:PHE:HD2  | 1.80                     | 0.46              |
| 2:Q:75:LYS:HB2   | 2:Q:75:LYS:HE2   | 1.70                     | 0.46              |
| 2:Q:89:GLN:O     | 2:Q:89:GLN:HG3   | 2.15                     | 0.46              |
| 1:F:8:PHE:HB3    | 2:G:56:PHE:CE1   | 2.50                     | 0.46              |
| 2:G:1:ILE:HG23   | 2:G:2:GLN:N      | 2.29                     | 0.46              |
| 4:I:24:THR:HG22  | 4:I:85:GLN:O     | 2.15                     | 0.46              |
| 4:I:27:ASN:C     | 4:I:27:ASN:ND2   | 2.63                     | 0.46              |
| 1:K:34:VAL:HA    | 1:K:47:PRO:O     | 2.16                     | 0.46              |
| 1:K:200:THR:C    | 1:K:201:LEU:HD12 | 2.40                     | 0.46              |
| 1:K:253:GLU:CD   | 1:K:253:GLU:H    | 2.23                     | 0.46              |
| 1:P:33:PHE:HB3   | 1:P:51:TRP:HZ2   | 1.81                     | 0.46              |
| 1:P:46:GLU:O     | 1:P:47:PRO:C     | 2.58                     | 0.46              |
| 1:A:266:LEU:HD13 | 1:A:270:LEU:HD23 | 1.97                     | 0.46              |
| 4:D:40:PHE:HZ    | 5:E:112:ASP:OD1  | 1.98                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:101:THR:HA   | 4:D:118:GLU:HA   | 1.97                     | 0.46              |
| 1:F:235:PRO:HG2  | 2:G:26:TYR:CE1   | 2.50                     | 0.46              |
| 1:K:155:GLN:HG2  | 4:N:57:TYR:CD1   | 2.50                     | 0.46              |
| 1:P:203:CYS:O    | 1:P:204:TRP:CD1  | 2.67                     | 0.46              |
| 4:S:30:SER:HB3   | 4:S:108:ALA:HB2  | 1.97                     | 0.46              |
| 4:S:148:PHE:CD1  | 4:S:148:PHE:C    | 2.91                     | 0.46              |
| 2:B:3:ARG:O      | 2:B:30:PHE:HA    | 2.15                     | 0.46              |
| 5:E:157:LEU:HD12 | 5:E:201:LEU:O    | 2.16                     | 0.46              |
| 1:F:255:GLN:HG3  | 1:F:255:GLN:O    | 2.16                     | 0.46              |
| 2:G:40:LEU:C     | 2:G:78:TYR:CD2   | 2.94                     | 0.46              |
| 4:I:83:LEU:HD12  | 4:I:84:ASN:H     | 1.81                     | 0.46              |
| 1:K:88:SER:C     | 1:K:90:ALA:H     | 2.24                     | 0.46              |
| 5:O:138:VAL:HG22 | 5:O:139:PHE:N    | 2.30                     | 0.46              |
| 1:P:266:LEU:CD2  | 1:P:270:LEU:HB2  | 2.45                     | 0.46              |
| 2:Q:10:TYR:HA    | 2:Q:95:TRP:CZ3   | 2.50                     | 0.46              |
| 5:T:14:LEU:HD11  | 5:T:20:MET:HB3   | 1.97                     | 0.46              |
| 5:T:94:ALA:O     | 5:T:95:ALA:HB2   | 2.15                     | 0.46              |
| 4:D:205:ILE:HG23 | 4:D:206:PRO:HD2  | 1.97                     | 0.46              |
| 5:J:191:GLN:C    | 5:J:193:ALA:H    | 2.23                     | 0.46              |
| 1:K:266:LEU:HD12 | 1:K:266:LEU:O    | 2.15                     | 0.46              |
| 2:L:5:PRO:HG3    | 2:L:30:PHE:HB3   | 1.98                     | 0.46              |
| 2:L:40:LEU:HD23  | 2:L:43:GLY:CA    | 2.45                     | 0.46              |
| 5:O:143:GLU:H    | 5:O:143:GLU:CD   | 2.24                     | 0.46              |
| 1:P:217:TRP:HZ3  | 1:P:247:VAL:HG22 | 1.81                     | 0.46              |
| 5:T:105:ALA:HA   | 5:T:115:TYR:O    | 2.14                     | 0.46              |
| 4:D:126:GLN:HG3  | 4:D:127:ASN:H    | 1.81                     | 0.46              |
| 2:G:41:LYS:HB2   | 2:G:78:TYR:CZ    | 2.51                     | 0.46              |
| 4:I:28:SER:HA    | 4:I:85:GLN:NE2   | 2.31                     | 0.46              |
| 5:J:41:TRP:CD1   | 5:J:89:LEU:HB2   | 2.51                     | 0.46              |
| 1:K:218:GLN:HA   | 1:K:223:ASP:HA   | 1.98                     | 0.46              |
| 2:L:7:ILE:HG12   | 2:L:8:GLN:N      | 2.28                     | 0.46              |
| 5:O:220:ARG:CZ   | 5:O:222:GLN:NE2  | 2.79                     | 0.46              |
| 1:A:44:ARG:HB2   | 1:A:48:ARG:HH21  | 1.80                     | 0.46              |
| 5:E:24:ALA:HB2   | 5:E:86:ASN:HB3   | 1.96                     | 0.46              |
| 1:K:130:LEU:HB2  | 1:K:157:ARG:HG3  | 1.98                     | 0.46              |
| 5:O:78:VAL:HG23  | 5:O:88:LEU:C     | 2.41                     | 0.46              |
| 5:T:4:GLY:HA2    | 5:T:28:MET:CE    | 2.45                     | 0.46              |
| 1:A:130:LEU:HB3  | 1:A:157:ARG:HG3  | 1.98                     | 0.46              |
| 5:E:159:THR:HG22 | 5:E:200:ALA:HB1  | 1.97                     | 0.46              |
| 4:N:132:VAL:HG22 | 4:N:146:CYS:HB3  | 1.98                     | 0.46              |
| 1:P:219:ARG:HH11 | 1:P:256:ARG:HE   | 1.60                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:E:134:PRO:O    | 5:E:246:VAL:HG11 | 2.15                     | 0.46              |
| 5:E:168:LEU:HD13 | 5:E:223:VAL:HG23 | 1.98                     | 0.46              |
| 1:K:123:TYR:CZ   | 1:K:140:ALA:HA   | 2.51                     | 0.46              |
| 5:O:234:TRP:CZ2  | 5:O:238:ARG:HG3  | 2.45                     | 0.46              |
| 5:T:40:TYR:O     | 5:T:104:CYS:HA   | 2.16                     | 0.46              |
| 1:A:209:TYR:HB3  | 1:A:210:PRO:CD   | 2.46                     | 0.45              |
| 1:F:151:ARG:HD2  | 4:I:57:TYR:CD2   | 2.50                     | 0.45              |
| 4:I:107:ARG:O    | 4:I:108:ALA:HB3  | 2.16                     | 0.45              |
| 4:I:205:ILE:HD12 | 4:I:205:ILE:N    | 2.31                     | 0.45              |
| 5:J:69:GLY:O     | 5:J:70:GLU:CB    | 2.63                     | 0.45              |
| 5:J:234:TRP:HZ2  | 5:J:238:ARG:CG   | 2.28                     | 0.45              |
| 1:K:14:ARG:HD2   | 1:K:17:ARG:HH21  | 1.78                     | 0.45              |
| 4:N:11:PHE:HB2   | 4:N:119:LEU:HD11 | 1.98                     | 0.45              |
| 4:N:60:GLY:HA2   | 4:N:81:ALA:O     | 2.16                     | 0.45              |
| 1:P:170:ARG:NH1  | 1:P:174:ASN:HD21 | 2.13                     | 0.45              |
| 4:S:196:CYS:HA   | 4:S:199:ALA:HB2  | 1.96                     | 0.45              |
| 1:A:150:ALA:HB3  | 1:A:152:VAL:HG23 | 1.99                     | 0.45              |
| 2:B:41:LYS:O     | 2:B:42:ASN:HB2   | 2.16                     | 0.45              |
| 5:E:130:ASN:HA   | 5:E:132:PHE:CE2  | 2.51                     | 0.45              |
| 1:F:72:GLN:CG    | 5:J:57:VAL:HG11  | 2.47                     | 0.45              |
| 4:I:135:LEU:HD21 | 5:J:153:THR:O    | 2.16                     | 0.45              |
| 1:K:181:ARG:HD2  | 1:K:182:ALA:N    | 2.31                     | 0.45              |
| 1:K:188:HIS:C    | 1:K:204:TRP:NE1  | 2.74                     | 0.45              |
| 5:O:27:ASP:C     | 5:O:28:MET:HG3   | 2.41                     | 0.45              |
| 2:Q:73:THR:O     | 2:Q:74:GLU:HB2   | 2.14                     | 0.45              |
| 4:S:69:ASP:HA    | 4:S:70:GLY:HA2   | 1.57                     | 0.45              |
| 1:A:217:TRP:HE1  | 1:A:246:ALA:N    | 2.15                     | 0.45              |
| 4:D:68:GLU:HG2   | 4:D:69:ASP:N     | 2.30                     | 0.45              |
| 5:E:100:SER:OG   | 5:E:101:VAL:N    | 2.49                     | 0.45              |
| 2:G:24:ASN:HB3   | 2:G:67:TYR:CB    | 2.42                     | 0.45              |
| 4:I:41:TRP:CE2   | 4:I:89:LEU:HB2   | 2.52                     | 0.45              |
| 4:I:44:GLN:OE1   | 4:I:103:LEU:HD11 | 2.16                     | 0.45              |
| 5:O:170:TRP:C    | 5:O:171:TRP:HD1  | 2.24                     | 0.45              |
| 1:P:155:GLN:HG2  | 4:S:57:TYR:CD1   | 2.51                     | 0.45              |
| 5:T:184:ASP:HB2  | 5:T:201:LEU:HD12 | 1.98                     | 0.45              |
| 4:D:27:ASN:C     | 4:D:27:ASN:ND2   | 2.69                     | 0.45              |
| 5:T:127:ASP:OD1  | 5:T:129:LYS:HE3  | 2.17                     | 0.45              |
| 5:T:234:TRP:CZ2  | 5:T:236:GLN:HB3  | 2.52                     | 0.45              |
| 1:A:72:GLN:CG    | 5:E:57:VAL:HG21  | 2.47                     | 0.45              |
| 1:F:124:ILE:HG12 | 1:F:125:ALA:N    | 2.32                     | 0.45              |
| 1:K:106:ASP:OD2  | 1:K:108:ARG:HG2  | 2.16                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:21:ARG:HD3   | 1:P:39:ASP:OD2   | 2.17                     | 0.45              |
| 4:S:110:LYS:HG2  | 4:S:110:LYS:O    | 2.16                     | 0.45              |
| 5:E:222:GLN:HA   | 5:E:247:SER:HB3  | 1.98                     | 0.45              |
| 5:J:74:ASP:O     | 5:J:76:TYR:N     | 2.49                     | 0.45              |
| 5:J:146:ILE:O    | 5:J:150:GLN:HA   | 2.16                     | 0.45              |
| 4:N:132:VAL:HG22 | 4:N:146:CYS:O    | 2.17                     | 0.45              |
| 5:O:59:GLU:O     | 5:O:80:ARG:O     | 2.34                     | 0.45              |
| 1:P:62:ARG:O     | 1:P:65:GLN:HB3   | 2.17                     | 0.45              |
| 1:A:117:ALA:HB2  | 2:B:60:TRP:CE2   | 2.52                     | 0.45              |
| 5:E:166:VAL:HG13 | 5:E:223:VAL:HG13 | 1.98                     | 0.45              |
| 1:F:253:GLU:HA   | 1:F:256:ARG:HH11 | 1.82                     | 0.45              |
| 2:L:96:ASP:O     | 2:L:97:ARG:C     | 2.60                     | 0.45              |
| 5:O:104:CYS:O    | 5:O:116:PHE:HA   | 2.16                     | 0.45              |
| 2:Q:91:LYS:HG3   | 2:Q:92:ILE:N     | 2.32                     | 0.45              |
| 1:A:160:LEU:O    | 1:A:165:VAL:HG23 | 2.16                     | 0.45              |
| 2:B:3:ARG:HH21   | 2:B:61:SER:HB3   | 1.81                     | 0.45              |
| 4:N:5:GLU:HB2    | 4:N:24:THR:OG1   | 2.15                     | 0.45              |
| 1:A:234:ARG:HG3  | 2:B:10:TYR:CD2   | 2.52                     | 0.45              |
| 2:B:1:ILE:HG13   | 2:B:2:GLN:N      | 2.32                     | 0.45              |
| 4:D:49:GLU:OE1   | 4:D:49:GLU:N     | 2.48                     | 0.45              |
| 4:D:79:PHE:HA    | 4:D:90:LEU:O     | 2.16                     | 0.45              |
| 5:E:166:VAL:HG11 | 5:E:223:VAL:HG13 | 1.99                     | 0.45              |
| 1:F:103:VAL:CG1  | 1:F:168:LEU:HD23 | 2.47                     | 0.45              |
| 4:I:27:ASN:HD22  | 4:I:29:ALA:N     | 2.15                     | 0.45              |
| 4:I:192:SER:CB   | 4:I:193:ASP:HA   | 2.36                     | 0.45              |
| 5:J:60:GLY:C     | 5:J:61:THR:OG1   | 2.60                     | 0.45              |
| 5:J:145:GLU:O    | 5:J:149:THR:HG22 | 2.16                     | 0.45              |
| 5:O:184:ASP:HA   | 5:O:185:PRO:HD2  | 1.88                     | 0.45              |
| 1:A:69:THR:HG21  | 4:D:109:GLY:O    | 2.17                     | 0.45              |
| 4:D:41:TRP:O     | 4:D:53:LEU:HB3   | 2.16                     | 0.45              |
| 5:E:168:LEU:CD2  | 5:E:203:SER:HB2  | 2.47                     | 0.45              |
| 1:F:274:TRP:O    | 1:F:275:GLU:HB3  | 2.17                     | 0.45              |
| 1:K:218:GLN:OE1  | 1:K:260:HIS:HB2  | 2.17                     | 0.45              |
| 5:O:128:LEU:O    | 5:O:234:TRP:HZ3  | 1.99                     | 0.45              |
| 4:S:107:ARG:HA   | 4:S:111:LEU:CA   | 2.40                     | 0.45              |
| 2:B:70:PHE:HD2   | 2:B:78:TYR:CZ    | 2.34                     | 0.44              |
| 2:G:31:HIS:CD2   | 2:G:62:PHE:CE1   | 3.05                     | 0.44              |
| 4:N:143:LYS:O    | 4:N:144:SER:CB   | 2.65                     | 0.44              |
| 1:P:44:ARG:HB3   | 1:P:48:ARG:HH21  | 1.82                     | 0.44              |
| 2:Q:39:LEU:C     | 2:Q:40:LEU:HD12  | 2.42                     | 0.44              |
| 4:S:54:MET:HA    | 4:S:54:MET:HE2   | 1.98                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:148:PHE:HB2  | 4:D:200:PHE:CZ   | 2.52                     | 0.44              |
| 1:F:201:LEU:HD21 | 1:F:254:GLU:CG   | 2.44                     | 0.44              |
| 2:G:1:ILE:HG23   | 2:G:2:GLN:H      | 1.82                     | 0.44              |
| 4:I:213:SER:N    | 4:I:214:PRO:CD   | 2.80                     | 0.44              |
| 2:L:35:ILE:HD13  | 2:L:84:HIS:HD2   | 1.83                     | 0.44              |
| 4:N:180:PHE:HD2  | 5:O:206:ARG:NH1  | 2.14                     | 0.44              |
| 4:N:180:PHE:CD2  | 5:O:206:ARG:NH1  | 2.85                     | 0.44              |
| 5:O:20:MET:HE3   | 5:O:20:MET:HB2   | 1.73                     | 0.44              |
| 1:A:219:ARG:CB   | 1:A:224:GLN:HB2  | 2.47                     | 0.44              |
| 1:A:274:TRP:O    | 1:A:274:TRP:CG   | 2.70                     | 0.44              |
| 5:E:238:ARG:CG   | 5:E:239:ALA:H    | 2.30                     | 0.44              |
| 1:F:48:ARG:NH1   | 1:F:60:TRP:CD2   | 2.86                     | 0.44              |
| 1:F:203:CYS:N    | 1:F:217:TRP:HZ2  | 2.15                     | 0.44              |
| 5:J:60:GLY:O     | 5:J:61:THR:OG1   | 2.32                     | 0.44              |
| 5:J:138:VAL:HG13 | 5:J:248:ALA:HB3  | 1.99                     | 0.44              |
| 1:K:188:HIS:N    | 1:K:204:TRP:CZ2  | 2.86                     | 0.44              |
| 1:P:203:CYS:HB2  | 1:P:217:TRP:HZ2  | 1.82                     | 0.44              |
| 4:S:5:GLU:HB3    | 4:S:24:THR:OG1   | 2.17                     | 0.44              |
| 5:T:39:MET:HA    | 5:T:105:ALA:O    | 2.17                     | 0.44              |
| 1:A:235:PRO:HA   | 1:A:241:PHE:HD1  | 1.82                     | 0.44              |
| 4:D:180:PHE:CZ   | 4:D:182:SER:HB3  | 2.53                     | 0.44              |
| 5:E:191:GLN:C    | 5:E:193:ALA:H    | 2.25                     | 0.44              |
| 1:F:66:ILE:HD11  | 4:I:109:GLY:H    | 1.83                     | 0.44              |
| 1:F:88:SER:C     | 1:F:90:ALA:N     | 2.75                     | 0.44              |
| 1:K:220:ASP:OD1  | 1:K:256:ARG:HB2  | 2.18                     | 0.44              |
| 4:N:120:SER:O    | 4:N:121:VAL:C    | 2.60                     | 0.44              |
| 2:Q:77:GLU:H     | 2:Q:77:GLU:CD    | 2.25                     | 0.44              |
| 4:S:89:LEU:C     | 4:S:90:LEU:HD12  | 2.42                     | 0.44              |
| 4:S:152:ASP:CG   | 4:S:154:GLN:HE22 | 2.26                     | 0.44              |
| 1:A:3:HIS:HA     | 1:A:29:ASP:OD1   | 2.18                     | 0.44              |
| 1:A:42:SER:OG    | 1:A:45:GLU:HG3   | 2.17                     | 0.44              |
| 1:A:255:GLN:HB3  | 1:A:274:TRP:NE1  | 2.33                     | 0.44              |
| 1:A:260:HIS:NE2  | 1:A:271:THR:HG23 | 2.33                     | 0.44              |
| 4:D:89:LEU:C     | 4:D:90:LEU:HD12  | 2.42                     | 0.44              |
| 1:F:87:GLN:OE1   | 1:F:93:HIS:NE2   | 2.51                     | 0.44              |
| 5:J:242:VAL:O    | 5:J:243:THR:C    | 2.61                     | 0.44              |
| 1:K:202:ARG:NE   | 1:K:244:TRP:CE3  | 2.85                     | 0.44              |
| 2:L:31:HIS:ND1   | 2:L:32:PRO:HA    | 2.33                     | 0.44              |
| 5:O:155:VAL:HG22 | 5:O:203:SER:O    | 2.18                     | 0.44              |
| 5:T:43:ARG:HH12  | 5:T:98:GLN:HA    | 1.83                     | 0.44              |
| 4:D:151:PHE:CZ   | 4:D:183:ASN:HB3  | 2.53                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:259:CYS:O    | 1:K:261:VAL:HG23 | 2.17                     | 0.44              |
| 2:L:94:LYS:HG3   | 2:L:95:TRP:N     | 2.33                     | 0.44              |
| 5:O:212:TRP:CZ2  | 5:O:253:ARG:HB3  | 2.53                     | 0.44              |
| 5:O:240:LYS:HA   | 5:O:241:PRO:HD3  | 1.81                     | 0.44              |
| 5:T:242:VAL:O    | 5:T:244:GLN:HG2  | 2.17                     | 0.44              |
| 1:A:255:GLN:HA   | 1:A:274:TRP:HE1  | 1.83                     | 0.44              |
| 1:F:50:PRO:HG2   | 1:F:51:TRP:HD1   | 1.83                     | 0.44              |
| 1:F:249:VAL:HG11 | 1:F:257:TYR:CE2  | 2.53                     | 0.44              |
| 5:J:23:CYS:HB3   | 5:J:87:PHE:HB3   | 1.99                     | 0.44              |
| 1:K:84:TYR:CD1   | 1:K:142:ILE:HD12 | 2.53                     | 0.44              |
| 1:K:135:ALA:HB3  | 1:K:141:GLN:HG2  | 2.00                     | 0.44              |
| 1:P:28:VAL:O     | 1:P:30:ASP:N     | 2.51                     | 0.44              |
| 4:S:19:VAL:CG2   | 4:S:91:ILE:HB    | 2.47                     | 0.44              |
| 4:S:131:ALA:HB1  | 4:S:133:TYR:CE1  | 2.53                     | 0.44              |
| 4:S:180:PHE:CE2  | 4:S:182:SER:HB3  | 2.53                     | 0.44              |
| 4:D:210:PHE:CD1  | 4:D:212:PRO:HD3  | 2.53                     | 0.44              |
| 5:E:234:TRP:HZ2  | 5:E:238:ARG:HB3  | 1.82                     | 0.44              |
| 1:F:82:ARG:CZ    | 1:F:89:GLU:HG3   | 2.48                     | 0.44              |
| 1:F:137:ASP:C    | 1:F:137:ASP:OD1  | 2.60                     | 0.44              |
| 1:F:170:ARG:O    | 1:F:173:GLU:HB3  | 2.18                     | 0.44              |
| 4:I:180:PHE:CE2  | 4:I:182:SER:HB3  | 2.53                     | 0.44              |
| 5:J:140:GLU:HA   | 5:J:141:PRO:HD3  | 1.85                     | 0.44              |
| 1:K:268:LYS:HB3  | 1:K:269:PRO:HD2  | 2.00                     | 0.44              |
| 2:L:0:MET:N      | 2:L:1:ILE:HA     | 2.31                     | 0.44              |
| 1:P:117:ALA:HA   | 1:P:123:TYR:H    | 1.83                     | 0.44              |
| 1:P:201:LEU:O    | 1:P:217:TRP:HH2  | 2.01                     | 0.44              |
| 2:Q:23:LEU:HD22  | 2:Q:78:TYR:HB3   | 2.00                     | 0.44              |
| 5:T:168:LEU:HD23 | 5:T:169:SER:N    | 2.32                     | 0.44              |
| 1:A:28:VAL:C     | 1:A:30:ASP:H     | 2.26                     | 0.44              |
| 4:D:2:LYS:O      | 4:D:3:GLU:HB2    | 2.18                     | 0.44              |
| 5:E:43:ARG:HH22  | 5:E:98:GLN:H     | 1.65                     | 0.44              |
| 1:F:196:ASP:CG   | 1:F:197:HIS:H    | 2.26                     | 0.44              |
| 4:I:30:SER:CA    | 4:I:108:ALA:HB2  | 2.46                     | 0.44              |
| 5:O:41:TRP:CD1   | 5:O:89:LEU:HB2   | 2.53                     | 0.44              |
| 5:T:54:HIS:NE2   | 5:T:71:VAL:HG13  | 2.33                     | 0.44              |
| 5:E:31:TYR:HB2   | 5:E:107:GLY:O    | 2.18                     | 0.43              |
| 5:E:71:VAL:H     | 5:E:72:PRO:CD    | 2.31                     | 0.43              |
| 5:E:180:GLY:O    | 5:E:205:LEU:HA   | 2.18                     | 0.43              |
| 1:F:15:PRO:C     | 1:F:17:ARG:N     | 2.76                     | 0.43              |
| 2:G:23:LEU:HB2   | 2:G:70:PHE:CZ    | 2.53                     | 0.43              |
| 4:I:20:ALA:HA    | 4:I:90:LEU:HD12  | 1.99                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:I:145:VAL:HG12 | 4:I:188:TRP:CB   | 2.46                     | 0.43              |
| 5:J:172:VAL:HG22 | 5:J:219:PHE:CD2  | 2.53                     | 0.43              |
| 1:K:58:GLU:O     | 1:K:62:ARG:HG2   | 2.18                     | 0.43              |
| 2:L:56:PHE:HB2   | 2:L:61:SER:O     | 2.18                     | 0.43              |
| 4:N:43:ARG:HB2   | 4:N:53:LEU:HD22  | 2.00                     | 0.43              |
| 1:P:215:LEU:O    | 1:P:216:THR:HG23 | 2.18                     | 0.43              |
| 1:P:219:ARG:O    | 1:P:220:ASP:HB3  | 2.18                     | 0.43              |
| 1:P:234:ARG:HG3  | 2:Q:10:TYR:CG    | 2.53                     | 0.43              |
| 2:Q:4:THR:HA     | 2:Q:5:PRO:HD3    | 1.87                     | 0.43              |
| 5:T:30:HIS:CE1   | 5:T:107:GLY:HA2  | 2.53                     | 0.43              |
| 1:A:217:TRP:CD1  | 1:A:228:THR:HG23 | 2.53                     | 0.43              |
| 2:B:25:CYS:HB2   | 2:B:39:LEU:HD21  | 2.00                     | 0.43              |
| 2:G:64:LEU:HD13  | 2:G:66:TYR:HE1   | 1.83                     | 0.43              |
| 4:N:143:LYS:HG3  | 4:N:144:SER:N    | 2.32                     | 0.43              |
| 4:N:173:LEU:HD23 | 4:N:174:ASP:N    | 2.33                     | 0.43              |
| 1:P:234:ARG:H    | 1:P:234:ARG:HD2  | 1.84                     | 0.43              |
| 1:F:81:LEU:HD12  | 1:F:81:LEU:HA    | 1.81                     | 0.43              |
| 5:J:214:ASN:HA   | 5:J:215:PRO:HD3  | 1.85                     | 0.43              |
| 5:O:53:ILE:O     | 5:O:68:LYS:O     | 2.36                     | 0.43              |
| 1:P:266:LEU:HD21 | 1:P:270:LEU:HD13 | 2.00                     | 0.43              |
| 4:S:140:SER:C    | 4:S:142:ASP:H    | 2.27                     | 0.43              |
| 4:S:156:ASN:H    | 4:S:204:ILE:HD11 | 1.82                     | 0.43              |
| 5:T:74:ASP:C     | 5:T:76:TYR:N     | 2.73                     | 0.43              |
| 1:A:230:LEU:HG   | 1:A:231:VAL:N    | 2.31                     | 0.43              |
| 2:B:22:PHE:HD1   | 2:B:22:PHE:HA    | 1.75                     | 0.43              |
| 4:D:68:GLU:H     | 4:D:68:GLU:CD    | 2.26                     | 0.43              |
| 1:F:221:GLY:O    | 1:F:222:GLU:HB3  | 2.19                     | 0.43              |
| 4:I:152:ASP:OD2  | 4:I:154:GLN:HG2  | 2.18                     | 0.43              |
| 1:K:217:TRP:NE1  | 1:K:259:CYS:SG   | 2.92                     | 0.43              |
| 1:K:263:HIS:ND1  | 1:K:264:GLU:N    | 2.64                     | 0.43              |
| 2:L:94:LYS:HG3   | 2:L:95:TRP:H     | 1.83                     | 0.43              |
| 5:O:110:ASN:O    | 5:O:111:PHE:HB2  | 2.18                     | 0.43              |
| 1:P:51:TRP:NE1   | 1:P:52:ILE:HG12  | 2.33                     | 0.43              |
| 1:P:185:PRO:O    | 1:P:187:THR:HG23 | 2.18                     | 0.43              |
| 2:Q:39:LEU:HA    | 2:Q:80:CYS:HA    | 2.00                     | 0.43              |
| 3:R:6:ALA:HB2    | 4:S:107:ARG:CZ   | 2.48                     | 0.43              |
| 5:T:173:ASN:HA   | 5:T:218:HIS:HB3  | 2.00                     | 0.43              |
| 1:A:62:ARG:O     | 1:A:65:GLN:HB3   | 2.17                     | 0.43              |
| 1:A:130:LEU:CB   | 1:A:157:ARG:HG3  | 2.48                     | 0.43              |
| 1:A:270:LEU:O    | 1:A:271:THR:C    | 2.61                     | 0.43              |
| 4:D:91:ILE:CD1   | 4:D:119:LEU:HD21 | 2.48                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:49:ALA:HB1   | 1:F:50:PRO:CD    | 2.48                     | 0.43              |
| 2:G:10:TYR:N     | 2:G:10:TYR:HD1   | 2.14                     | 0.43              |
| 5:J:14:LYS:O     | 5:J:15:THR:C     | 2.61                     | 0.43              |
| 1:K:159:TYR:CZ   | 3:M:3:ARG:HB2    | 2.53                     | 0.43              |
| 5:O:55:TYR:CE2   | 5:O:67:ALA:HB3   | 2.53                     | 0.43              |
| 1:P:203:CYS:O    | 1:P:204:TRP:HD1  | 2.01                     | 0.43              |
| 1:P:219:ARG:HB3  | 1:P:224:GLN:HE22 | 1.83                     | 0.43              |
| 4:S:192:SER:N    | 4:S:193:ASP:CA   | 2.75                     | 0.43              |
| 4:D:78:ARG:HG3   | 4:D:92:ARG:CD    | 2.48                     | 0.43              |
| 5:E:161:PHE:CE1  | 5:E:199:TYR:HB2  | 2.52                     | 0.43              |
| 4:I:161:LYS:HG3  | 4:I:202:ASN:ND2  | 2.34                     | 0.43              |
| 4:I:192:SER:HA   | 4:I:194:PHE:H    | 1.82                     | 0.43              |
| 5:J:88:LEU:N     | 5:J:88:LEU:HD12  | 2.33                     | 0.43              |
| 5:J:240:LYS:HA   | 5:J:241:PRO:HD3  | 1.77                     | 0.43              |
| 4:N:41:TRP:CE2   | 4:N:89:LEU:HB2   | 2.54                     | 0.43              |
| 1:P:34:VAL:HG22  | 1:P:35:ARG:N     | 2.33                     | 0.43              |
| 5:T:44:GLN:NE2   | 5:T:50:LEU:HD21  | 2.33                     | 0.43              |
| 4:D:138:SER:HA   | 4:D:139:LYS:HA   | 1.48                     | 0.43              |
| 4:D:173:LEU:O    | 4:D:174:ASP:HB2  | 2.18                     | 0.43              |
| 1:F:23:ILE:HG22  | 1:F:24:SER:N     | 2.34                     | 0.43              |
| 2:G:63:TYR:O     | 2:G:63:TYR:CD1   | 2.72                     | 0.43              |
| 5:J:171:TRP:HE1  | 5:J:222:GLN:HB3  | 1.82                     | 0.43              |
| 4:N:164:ASP:O    | 4:N:189:SER:HB2  | 2.19                     | 0.43              |
| 5:O:169:SER:HB3  | 5:O:222:GLN:HB2  | 2.01                     | 0.43              |
| 1:P:72:GLN:CG    | 5:T:57:VAL:HG11  | 2.49                     | 0.43              |
| 2:Q:12:ARG:HG3   | 2:Q:22:PHE:HD2   | 1.84                     | 0.43              |
| 2:Q:91:LYS:CG    | 2:Q:92:ILE:H     | 2.30                     | 0.43              |
| 5:T:74:ASP:O     | 5:T:76:TYR:N     | 2.52                     | 0.43              |
| 1:A:98:MET:HE2   | 2:B:56:PHE:HE2   | 1.83                     | 0.43              |
| 1:A:112:GLY:CA   | 1:A:160:LEU:HD23 | 2.48                     | 0.43              |
| 1:A:204:TRP:O    | 1:A:205:ALA:HB2  | 2.19                     | 0.43              |
| 1:A:236:ALA:O    | 2:B:12:ARG:HD2   | 2.19                     | 0.43              |
| 5:E:168:LEU:HD23 | 5:E:183:THR:CG2  | 2.49                     | 0.43              |
| 1:F:25:VAL:HG12  | 1:F:35:ARG:HG3   | 1.99                     | 0.43              |
| 1:F:205:ALA:HB3  | 1:F:242:GLN:O    | 2.17                     | 0.43              |
| 4:I:131:ALA:CB   | 4:I:210:PHE:HB3  | 2.49                     | 0.43              |
| 1:K:46:GLU:O     | 1:K:48:ARG:HG3   | 2.19                     | 0.43              |
| 1:K:89:GLU:HG2   | 1:K:89:GLU:O     | 2.19                     | 0.43              |
| 4:D:112:ILE:N    | 4:D:112:ILE:HD12 | 2.34                     | 0.43              |
| 5:E:214:ASN:C    | 5:E:216:ARG:H    | 2.25                     | 0.43              |
| 1:F:219:ARG:HB2  | 1:F:257:TYR:HA   | 2.00                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:G:37:VAL:HG22  | 2:G:82:VAL:CG1   | 2.47                     | 0.43              |
| 5:O:141:PRO:HB2  | 5:O:142:SER:H    | 1.69                     | 0.43              |
| 1:P:233:THR:CB   | 1:P:243:LYS:HD3  | 2.44                     | 0.43              |
| 1:A:208:PHE:CD1  | 1:A:209:TYR:N    | 2.86                     | 0.43              |
| 4:D:25:TYR:OH    | 4:D:84(A):ARG:HA | 2.19                     | 0.43              |
| 5:E:97:SER:C     | 5:E:99:THR:N     | 2.68                     | 0.43              |
| 1:F:27:TYR:CE2   | 1:F:32:GLN:HB2   | 2.54                     | 0.43              |
| 2:G:13:HIS:HB3   | 2:G:14:PRO:CD    | 2.45                     | 0.43              |
| 2:G:41:LYS:C     | 2:G:43:GLY:N     | 2.77                     | 0.43              |
| 4:I:13:VAL:HG23  | 4:I:14:PRO:O     | 2.18                     | 0.43              |
| 5:J:28:ASN:CG    | 5:J:84:LYS:HE2   | 2.44                     | 0.43              |
| 2:L:23:LEU:HD12  | 2:L:23:LEU:HA    | 1.82                     | 0.43              |
| 1:P:10:THR:HB    | 1:P:23:ILE:HB    | 2.01                     | 0.43              |
| 1:A:186:LYS:HB2  | 1:A:186:LYS:NZ   | 2.33                     | 0.42              |
| 2:G:41:LYS:HA    | 2:G:78:TYR:CD1   | 2.53                     | 0.42              |
| 2:G:75:LYS:C     | 2:G:77:GLU:N     | 2.77                     | 0.42              |
| 4:I:172:VAL:HG12 | 4:I:173:LEU:O    | 2.19                     | 0.42              |
| 4:N:22:ASN:OD1   | 4:N:86:TYR:HD1   | 2.02                     | 0.42              |
| 4:N:145:VAL:HG22 | 4:N:187:ALA:O    | 2.18                     | 0.42              |
| 1:P:1:GLY:HA3    | 1:P:105:PRO:HA   | 2.01                     | 0.42              |
| 2:Q:7:ILE:HD12   | 2:Q:82:VAL:HG21  | 2.01                     | 0.42              |
| 2:Q:97:ARG:HG2   | 2:Q:98:ASP:H     | 1.84                     | 0.42              |
| 4:S:30:SER:CB    | 4:S:108:ALA:CB   | 2.95                     | 0.42              |
| 4:S:99:SER:HA    | 4:S:119:LEU:O    | 2.19                     | 0.42              |
| 5:T:134:PRO:HA   | 5:T:161:PHE:HB3  | 2.00                     | 0.42              |
| 4:D:138:SER:HA   | 4:D:139:LYS:HD3  | 1.99                     | 0.42              |
| 2:G:39:LEU:HB2   | 2:G:46:ILE:CG1   | 2.49                     | 0.42              |
| 2:G:47:GLU:O     | 2:G:49:VAL:HG13  | 2.19                     | 0.42              |
| 1:K:242:GLN:HE22 | 2:L:12:ARG:HA    | 1.83                     | 0.42              |
| 5:O:23:LEU:HD13  | 5:O:88:LEU:HG    | 2.00                     | 0.42              |
| 1:P:16:GLY:O     | 1:P:17:ARG:C     | 2.62                     | 0.42              |
| 2:Q:29:GLY:CA    | 2:Q:61:SER:HB2   | 2.49                     | 0.42              |
| 1:A:43:PRO:C     | 1:A:44:ARG:HG2   | 2.43                     | 0.42              |
| 1:A:55:GLU:CD    | 1:A:170:ARG:HH12 | 2.24                     | 0.42              |
| 4:D:107:ARG:O    | 4:D:108:ALA:O    | 2.36                     | 0.42              |
| 4:D:167:ILE:HD12 | 4:D:167:ILE:O    | 2.20                     | 0.42              |
| 1:F:209:TYR:O    | 1:F:263:HIS:HE1  | 2.03                     | 0.42              |
| 1:F:268:LYS:HA   | 1:F:269:PRO:HD3  | 1.82                     | 0.42              |
| 2:L:67:TYR:N     | 2:L:67:TYR:CD1   | 2.85                     | 0.42              |
| 5:O:171:TRP:CD2  | 5:O:222:GLN:NE2  | 2.87                     | 0.42              |
| 5:O:228:LEU:N    | 5:O:241:PRO:O    | 2.52                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:123:TYR:CZ   | 1:P:140:ALA:HA   | 2.54                     | 0.42              |
| 5:T:44:GLN:HB2   | 5:T:50:LEU:CD2   | 2.49                     | 0.42              |
| 1:A:257:TYR:CD2  | 1:A:258:THR:N    | 2.88                     | 0.42              |
| 4:D:99:SER:HA    | 4:D:119:LEU:O    | 2.19                     | 0.42              |
| 4:D:208:ASP:N    | 1:P:108:ARG:HH11 | 2.17                     | 0.42              |
| 5:E:43:ARG:HH22  | 5:E:97:SER:HB2   | 1.83                     | 0.42              |
| 5:E:85:GLN:H     | 5:E:85:GLN:CD    | 2.28                     | 0.42              |
| 5:E:171:TRP:HD1  | 5:E:175:LYS:C    | 2.27                     | 0.42              |
| 2:G:23:LEU:HD12  | 2:G:24:ASN:H     | 1.85                     | 0.42              |
| 2:G:24:ASN:N     | 2:G:24:ASN:OD1   | 2.52                     | 0.42              |
| 2:G:77:GLU:HB2   | 2:G:95:TRP:HE3   | 1.84                     | 0.42              |
| 1:K:257:TYR:O    | 1:K:258:THR:HG23 | 2.20                     | 0.42              |
| 2:L:57:SER:OG    | 2:L:61:SER:HB2   | 2.20                     | 0.42              |
| 1:P:266:LEU:HG   | 1:P:268:LYS:O    | 2.20                     | 0.42              |
| 5:T:30:HIS:CG    | 5:T:107:GLY:H    | 2.36                     | 0.42              |
| 1:A:46:GLU:O     | 1:A:48:ARG:HG3   | 2.19                     | 0.42              |
| 1:A:51:TRP:HZ3   | 1:A:171:TYR:CD1  | 2.37                     | 0.42              |
| 1:A:191:HIS:CD2  | 1:A:193:PRO:HG3  | 2.54                     | 0.42              |
| 2:B:21:ASN:HB3   | 2:B:70:PHE:CE1   | 2.53                     | 0.42              |
| 4:D:107:ARG:NH1  | 5:E:110:ASN:O    | 2.46                     | 0.42              |
| 1:F:35:ARG:NH2   | 2:G:53:ASP:HB3   | 2.34                     | 0.42              |
| 4:I:139:LYS:O    | 4:I:140:SER:HB2  | 2.19                     | 0.42              |
| 1:K:3:HIS:HE1    | 1:K:179:LEU:O    | 2.03                     | 0.42              |
| 2:L:12:ARG:HH21  | 2:L:13:HIS:CE1   | 2.37                     | 0.42              |
| 2:L:52:SER:O     | 2:L:64:LEU:HD11  | 2.20                     | 0.42              |
| 4:N:167:ILE:HG12 | 4:N:187:ALA:CB   | 2.47                     | 0.42              |
| 5:O:154:LEU:CD1  | 5:O:205:LEU:HB3  | 2.47                     | 0.42              |
| 1:P:117:ALA:HB2  | 2:Q:60:TRP:CE2   | 2.55                     | 0.42              |
| 4:S:160:SER:HA   | 4:S:202:ASN:HD22 | 1.83                     | 0.42              |
| 5:T:68:LYS:HB2   | 5:T:69:GLY:H     | 1.51                     | 0.42              |
| 1:A:55:GLU:HB3   | 1:A:59:TYR:HB3   | 2.01                     | 0.42              |
| 1:A:181:ARG:HG3  | 1:A:182:ALA:N    | 2.33                     | 0.42              |
| 1:A:184:PRO:CB   | 1:A:186:LYS:HE3  | 2.48                     | 0.42              |
| 5:E:170:TRP:CZ3  | 5:E:221:CYS:HB2  | 2.54                     | 0.42              |
| 2:G:26:TYR:HB2   | 2:G:65:LEU:CD1   | 2.46                     | 0.42              |
| 1:K:234:ARG:HG3  | 2:L:10:TYR:CG    | 2.53                     | 0.42              |
| 4:N:68:GLU:CD    | 4:N:68:GLU:N     | 2.78                     | 0.42              |
| 4:N:168:THR:CG2  | 4:N:186:VAL:HB   | 2.46                     | 0.42              |
| 1:P:175:GLY:C    | 1:P:177:ASP:N    | 2.76                     | 0.42              |
| 4:S:188:TRP:CE2  | 5:T:157:LEU:HD11 | 2.55                     | 0.42              |
| 5:T:128:LEU:HD23 | 5:T:228:LEU:HD11 | 2.01                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:T:140:GLU:HA   | 5:T:141:PRO:HD3  | 1.90                     | 0.42              |
| 1:A:106:ASP:OD1  | 1:A:108:ARG:HG2  | 2.19                     | 0.42              |
| 1:A:190:THR:HG22 | 1:A:191:HIS:N    | 2.35                     | 0.42              |
| 1:A:238:ASP:H    | 2:B:12:ARG:NH1   | 2.18                     | 0.42              |
| 5:E:222:GLN:HA   | 5:E:247:SER:CB   | 2.50                     | 0.42              |
| 1:K:78:LEU:HD23  | 1:K:78:LEU:HA    | 1.84                     | 0.42              |
| 1:K:81:LEU:HD23  | 1:K:84:TYR:HD2   | 1.85                     | 0.42              |
| 1:K:138:THR:HA   | 1:K:141:GLN:HG3  | 2.01                     | 0.42              |
| 1:K:202:ARG:HH22 | 1:K:231:VAL:HG22 | 1.84                     | 0.42              |
| 2:L:48:LYS:HE2   | 2:L:48:LYS:HB3   | 1.87                     | 0.42              |
| 2:L:51:HIS:HB3   | 2:L:66:TYR:CD2   | 2.54                     | 0.42              |
| 5:O:169:SER:O    | 5:O:221:CYS:HA   | 2.20                     | 0.42              |
| 5:O:218:HIS:O    | 5:O:218:HIS:CG   | 2.72                     | 0.42              |
| 5:T:22:LEU:HD12  | 5:T:89:LEU:O     | 2.19                     | 0.42              |
| 5:E:127:ASP:OD1  | 5:E:129:LYS:HE2  | 2.20                     | 0.42              |
| 2:G:5:PRO:HB2    | 2:G:7:ILE:HD11   | 2.02                     | 0.42              |
| 2:G:54:LEU:HD23  | 2:G:54:LEU:C     | 2.44                     | 0.42              |
| 4:I:142:ASP:O    | 4:I:143:LYS:HD3  | 2.20                     | 0.42              |
| 1:K:6:ARG:HA     | 1:K:100:GLY:HA3  | 2.01                     | 0.42              |
| 2:L:31:HIS:CG    | 2:L:32:PRO:HA    | 2.55                     | 0.42              |
| 4:N:137:ASP:OD1  | 5:O:139:PHE:HA   | 2.19                     | 0.42              |
| 5:O:52:LEU:HD21  | 5:O:55:TYR:CD2   | 2.54                     | 0.42              |
| 1:P:202:ARG:HA   | 1:P:245:ALA:O    | 2.19                     | 0.42              |
| 4:D:31:GLN:H     | 4:D:108:ALA:HB2  | 1.84                     | 0.42              |
| 4:D:47:ARG:HG3   | 4:D:47:ARG:O     | 2.20                     | 0.42              |
| 5:E:166:VAL:HG12 | 5:E:167:GLU:N    | 2.35                     | 0.42              |
| 1:K:263:HIS:CG   | 1:K:264:GLU:H    | 2.36                     | 0.42              |
| 2:Q:75:LYS:O     | 2:Q:75:LYS:HD3   | 2.20                     | 0.42              |
| 4:S:200:PHE:C    | 4:S:202:ASN:N    | 2.78                     | 0.42              |
| 5:T:69:GLY:O     | 5:T:70:GLU:HB2   | 2.20                     | 0.42              |
| 1:A:242:GLN:NE2  | 2:B:12:ARG:HA    | 2.34                     | 0.42              |
| 4:N:46:SER:HA    | 4:N:47:ARG:HA    | 1.60                     | 0.42              |
| 4:N:165:VAL:HA   | 4:N:189:SER:HB3  | 2.01                     | 0.42              |
| 5:O:43:ARG:HD3   | 5:O:70:GLU:OE1   | 2.20                     | 0.42              |
| 1:P:51:TRP:CH2   | 1:P:179:LEU:HD11 | 2.55                     | 0.42              |
| 4:D:19:VAL:HB    | 4:D:91:ILE:HD11  | 2.01                     | 0.41              |
| 5:E:240:LYS:HA   | 5:E:241:PRO:HD3  | 1.82                     | 0.41              |
| 4:I:147:LEU:HD13 | 4:I:186:VAL:HG22 | 2.02                     | 0.41              |
| 1:K:137:ASP:C    | 1:K:137:ASP:OD1  | 2.62                     | 0.41              |
| 1:K:184:PRO:HA   | 1:K:185:PRO:HD3  | 1.83                     | 0.41              |
| 1:K:192:HIS:O    | 1:K:200:THR:HB   | 2.19                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:217:TRP:CD1  | 1:K:259:CYS:HA   | 2.55                     | 0.41              |
| 5:O:22:LEU:HD12  | 5:O:22:LEU:N     | 2.35                     | 0.41              |
| 5:O:209:ALA:C    | 5:O:211:PHE:H    | 2.28                     | 0.41              |
| 1:P:238:ASP:HB3  | 2:Q:12:ARG:CZ    | 2.50                     | 0.41              |
| 1:F:21:ARG:HE    | 1:F:23:ILE:CG1   | 2.33                     | 0.41              |
| 4:I:46:SER:HA    | 4:I:47:ARG:HA    | 1.55                     | 0.41              |
| 4:N:143:LYS:HD2  | 4:N:143:LYS:HA   | 1.77                     | 0.41              |
| 4:N:145:VAL:HG21 | 4:N:186:VAL:HG13 | 2.02                     | 0.41              |
| 5:O:130:ASN:HA   | 5:O:132:PHE:CE2  | 2.54                     | 0.41              |
| 5:O:149:THR:O    | 5:O:151:LYS:HG3  | 2.19                     | 0.41              |
| 5:O:220:ARG:NH1  | 5:O:222:GLN:HE21 | 2.19                     | 0.41              |
| 1:A:27:TYR:HA    | 1:A:31:THR:O     | 2.20                     | 0.41              |
| 2:G:39:LEU:H     | 2:G:46:ILE:HD11  | 1.86                     | 0.41              |
| 1:K:50:PRO:HG2   | 1:K:51:TRP:CE3   | 2.55                     | 0.41              |
| 1:K:190:THR:HA   | 1:K:274:TRP:CZ3  | 2.55                     | 0.41              |
| 2:L:41:LYS:N     | 2:L:46:ILE:HD11  | 2.35                     | 0.41              |
| 5:O:153:THR:HA   | 5:O:206:ARG:HB3  | 2.02                     | 0.41              |
| 1:P:78:LEU:O     | 1:P:81:LEU:HB2   | 2.19                     | 0.41              |
| 4:S:46:SER:HA    | 4:S:47:ARG:HA    | 1.50                     | 0.41              |
| 1:A:74:ASP:HB3   | 3:C:5:ARG:HH12   | 1.82                     | 0.41              |
| 1:A:87:GLN:OE1   | 1:A:93:HIS:NE2   | 2.52                     | 0.41              |
| 2:G:39:LEU:O     | 2:G:45:ARG:HA    | 2.20                     | 0.41              |
| 4:I:54:MET:HE2   | 4:I:54:MET:HA    | 2.03                     | 0.41              |
| 4:I:112:ILE:N    | 4:I:112:ILE:HD12 | 2.35                     | 0.41              |
| 5:J:127:ASP:C    | 5:J:129:LYS:N    | 2.78                     | 0.41              |
| 5:J:214:ASN:O    | 5:J:252:GLY:HA3  | 2.20                     | 0.41              |
| 5:J:225:PHE:HE2  | 5:J:227:GLY:HA3  | 1.84                     | 0.41              |
| 4:N:7:ASP:HB3    | 4:N:11:PHE:CZ    | 2.51                     | 0.41              |
| 5:O:15:LYS:HD2   | 5:O:128:LEU:HD13 | 2.02                     | 0.41              |
| 1:P:192:HIS:CE1  | 1:P:202:ARG:HG2  | 2.54                     | 0.41              |
| 1:P:242:GLN:O    | 1:P:243:LYS:HB3  | 2.20                     | 0.41              |
| 1:P:261:VAL:H    | 1:P:271:THR:HG22 | 1.85                     | 0.41              |
| 4:S:15:GLU:O     | 4:S:17:ALA:N     | 2.54                     | 0.41              |
| 4:S:123:PRO:HG3  | 4:S:172:VAL:CG1  | 2.50                     | 0.41              |
| 5:T:43:ARG:NH1   | 5:T:76:TYR:OH    | 2.54                     | 0.41              |
| 1:A:51:TRP:CG    | 1:A:175:GLY:HA3  | 2.54                     | 0.41              |
| 1:A:219:ARG:O    | 1:A:220:ASP:HB2  | 2.20                     | 0.41              |
| 1:A:274:TRP:CD2  | 1:A:274:TRP:C    | 2.96                     | 0.41              |
| 4:D:15:GLU:OE1   | 4:D:181:LYS:HE3  | 2.20                     | 0.41              |
| 5:E:136:VAL:HG21 | 5:E:223:VAL:HB   | 2.03                     | 0.41              |
| 5:E:234:TRP:CZ2  | 5:E:236:GLN:HB2  | 2.55                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:184:PRO:HA   | 1:F:185:PRO:HD3  | 1.84                     | 0.41              |
| 2:G:37:VAL:HB    | 2:G:66:TYR:CE1   | 2.55                     | 0.41              |
| 4:I:84(C):SER:O  | 4:I:85:GLN:HB2   | 2.21                     | 0.41              |
| 5:J:184:ASP:HA   | 5:J:185:PRO:HD3  | 1.91                     | 0.41              |
| 5:J:212:TRP:C    | 5:J:214:ASN:H    | 2.28                     | 0.41              |
| 1:K:49:ALA:HB1   | 1:K:50:PRO:HD2   | 2.02                     | 0.41              |
| 1:K:188:HIS:N    | 1:K:204:TRP:HE1  | 2.16                     | 0.41              |
| 1:K:201:LEU:HD13 | 1:K:247:VAL:O    | 2.20                     | 0.41              |
| 2:L:39:LEU:HD22  | 2:L:49:VAL:HA    | 2.02                     | 0.41              |
| 1:P:194:ILE:HG22 | 1:P:195:SER:N    | 2.36                     | 0.41              |
| 1:P:213:ILE:HG22 | 1:P:263:HIS:ND1  | 2.35                     | 0.41              |
| 2:B:70:PHE:CD1   | 2:B:70:PHE:C     | 2.97                     | 0.41              |
| 2:B:73:THR:HG1   | 2:B:76:ASP:HB2   | 1.86                     | 0.41              |
| 1:F:215:LEU:C    | 1:F:215:LEU:HD12 | 2.46                     | 0.41              |
| 2:G:41:LYS:HB2   | 2:G:78:TYR:CE1   | 2.55                     | 0.41              |
| 4:I:95:LYS:C     | 4:I:121:VAL:HG11 | 2.45                     | 0.41              |
| 1:K:28:VAL:O     | 1:K:29:ASP:HB2   | 2.20                     | 0.41              |
| 1:K:48:ARG:O     | 1:K:52:ILE:HB    | 2.20                     | 0.41              |
| 2:L:54:LEU:HD11  | 2:L:62:PHE:HD1   | 1.86                     | 0.41              |
| 5:T:72:PRO:HA    | 5:T:74:ASP:HA    | 1.35                     | 0.41              |
| 1:A:189:VAL:CG2  | 1:A:190:THR:N    | 2.83                     | 0.41              |
| 4:D:30:SER:C     | 4:D:108:ALA:HB2  | 2.45                     | 0.41              |
| 1:F:174:ASN:HD22 | 1:F:174:ASN:H    | 1.69                     | 0.41              |
| 1:F:185:PRO:C    | 1:F:186:LYS:HD2  | 2.46                     | 0.41              |
| 4:I:166:TYR:HD2  | 4:I:188:TRP:NE1  | 2.17                     | 0.41              |
| 1:K:50:PRO:C     | 1:K:52:ILE:H     | 2.29                     | 0.41              |
| 2:L:2:GLN:NE2    | 2:L:31:HIS:N     | 2.68                     | 0.41              |
| 4:N:27:ASN:HB3   | 4:N:30:SER:OG    | 2.21                     | 0.41              |
| 5:O:99:THR:HG23  | 5:O:99:THR:O     | 2.21                     | 0.41              |
| 1:P:51:TRP:CD1   | 1:P:52:ILE:HG12  | 2.55                     | 0.41              |
| 1:P:95:LEU:HD12  | 1:P:117:ALA:O    | 2.20                     | 0.41              |
| 4:S:8:PRO:HB2    | 4:S:9:GLY:H      | 1.50                     | 0.41              |
| 1:A:254:GLU:H    | 1:A:254:GLU:CD   | 2.28                     | 0.41              |
| 1:A:257:TYR:CG   | 1:A:258:THR:N    | 2.86                     | 0.41              |
| 2:B:9:VAL:HG22   | 2:B:80:CYS:HB2   | 2.02                     | 0.41              |
| 4:D:165:VAL:HA   | 4:D:189:SER:HB2  | 2.02                     | 0.41              |
| 4:D:208:ASP:HA   | 1:P:108:ARG:CB   | 2.50                     | 0.41              |
| 1:F:45:GLU:OE2   | 1:F:45:GLU:HA    | 2.20                     | 0.41              |
| 4:I:53:LEU:C     | 4:I:54:MET:HG2   | 2.45                     | 0.41              |
| 4:I:70:GLY:C     | 4:I:79:PHE:H     | 2.27                     | 0.41              |
| 5:J:172:VAL:HA   | 5:J:218:HIS:O    | 2.21                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:L:7:ILE:HD11   | 2:L:25:CYS:HB3   | 2.03                     | 0.41              |
| 2:L:39:LEU:HG    | 2:L:46:ILE:HD12  | 2.03                     | 0.41              |
| 1:P:147:TRP:CG   | 1:P:152:VAL:HG21 | 2.56                     | 0.41              |
| 1:A:5:MET:O      | 1:A:100:GLY:HA3  | 2.21                     | 0.41              |
| 4:D:135:LEU:H    | 4:D:135:LEU:HD12 | 1.85                     | 0.41              |
| 5:E:77:ASN:O     | 5:E:89:LEU:HD12  | 2.21                     | 0.41              |
| 1:F:72:GLN:HG3   | 5:J:57:VAL:HG11  | 2.03                     | 0.41              |
| 1:F:194:ILE:HD11 | 1:F:200:THR:HG23 | 2.01                     | 0.41              |
| 1:F:244:TRP:HH2  | 2:G:99:MET:HE2   | 1.86                     | 0.41              |
| 2:G:57:SER:HB2   | 2:G:59:ASP:OD1   | 2.21                     | 0.41              |
| 5:J:31:TYR:CE1   | 5:J:57:VAL:HG12  | 2.56                     | 0.41              |
| 1:K:116:TYR:CE2  | 1:K:147:TRP:CH2  | 3.09                     | 0.41              |
| 1:K:189:VAL:HB   | 1:K:204:TRP:CZ2  | 2.55                     | 0.41              |
| 2:L:36:GLU:H     | 2:L:36:GLU:CD    | 2.29                     | 0.41              |
| 2:L:95:TRP:CD1   | 2:L:96:ASP:N     | 2.89                     | 0.41              |
| 5:O:234:TRP:CZ2  | 5:O:236:GLN:HB2  | 2.56                     | 0.41              |
| 1:P:6:ARG:NH1    | 1:P:113:HIS:HB2  | 2.35                     | 0.41              |
| 2:Q:3:ARG:HG2    | 2:Q:29:GLY:O     | 2.21                     | 0.41              |
| 2:Q:5:PRO:HA     | 2:Q:30:PHE:HB3   | 2.01                     | 0.41              |
| 2:Q:12:ARG:HG3   | 2:Q:22:PHE:CD2   | 2.55                     | 0.41              |
| 2:Q:33:SER:O     | 2:Q:34:ASP:C     | 2.64                     | 0.41              |
| 4:S:125:ILE:HD13 | 4:S:181:LYS:O    | 2.21                     | 0.41              |
| 4:S:160:SER:HA   | 4:S:202:ASN:ND2  | 2.35                     | 0.41              |
| 1:A:8:PHE:HB2    | 1:A:25:VAL:CG1   | 2.51                     | 0.41              |
| 1:A:49:ALA:HB1   | 1:A:50:PRO:CD    | 2.50                     | 0.41              |
| 4:D:18:THR:HG22  | 4:D:92:ARG:HA    | 2.02                     | 0.41              |
| 5:E:152:ALA:O    | 5:E:206:ARG:HA   | 2.21                     | 0.41              |
| 1:F:14:ARG:HA    | 1:F:15:PRO:HD3   | 1.83                     | 0.41              |
| 1:F:16:GLY:C     | 1:F:18:GLY:H     | 2.29                     | 0.41              |
| 1:F:85:TYR:HB3   | 1:F:87:GLN:HE21  | 1.85                     | 0.41              |
| 1:F:219:ARG:HG3  | 1:F:256:ARG:C    | 2.46                     | 0.41              |
| 2:G:46:ILE:HD13  | 2:G:49:VAL:HG21  | 2.02                     | 0.41              |
| 4:I:137:ASP:HB3  | 5:J:139:PHE:CE2  | 2.55                     | 0.41              |
| 4:I:143:LYS:HB2  | 4:I:144:SER:H    | 1.70                     | 0.41              |
| 5:J:71:VAL:H     | 5:J:72:PRO:CD    | 2.23                     | 0.41              |
| 5:J:163:PRO:HB2  | 5:J:165:HIS:CE1  | 2.56                     | 0.41              |
| 4:S:178:MET:HA   | 4:S:178:MET:CE   | 2.50                     | 0.41              |
| 5:T:15:LYS:HE3   | 5:T:128:LEU:CD1  | 2.49                     | 0.41              |
| 1:A:263:HIS:HB3  | 1:A:264:GLU:H    | 1.67                     | 0.40              |
| 2:B:39:LEU:C     | 2:B:40:LEU:HD12  | 2.46                     | 0.40              |
| 4:D:213:SER:HB3  | 4:D:214:PRO:HD3  | 2.02                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:E:19:MET:HE2   | 5:E:19:MET:HB2   | 1.85                     | 0.40              |
| 5:E:97:SER:OG    | 5:E:98:GLN:N     | 2.50                     | 0.40              |
| 4:I:84:ASN:ND2   | 4:I:84(C):SER:OG | 2.54                     | 0.40              |
| 5:J:153:THR:OG1  | 5:J:206:ARG:HB2  | 2.21                     | 0.40              |
| 2:L:7:ILE:HD12   | 2:L:82:VAL:CG2   | 2.50                     | 0.40              |
| 4:N:145:VAL:HG13 | 4:N:187:ALA:N    | 2.34                     | 0.40              |
| 5:O:30:HIS:CD2   | 5:O:108:GLN:N    | 2.89                     | 0.40              |
| 5:O:129:LYS:HE2  | 5:O:236:GLN:CD   | 2.46                     | 0.40              |
| 1:P:46:GLU:OE1   | 1:P:60:TRP:HZ2   | 2.03                     | 0.40              |
| 1:P:99:TYR:CZ    | 3:R:3:ARG:HB3    | 2.56                     | 0.40              |
| 1:P:175:GLY:C    | 1:P:177:ASP:H    | 2.29                     | 0.40              |
| 4:D:27:ASN:HD22  | 4:D:29:ALA:N     | 2.19                     | 0.40              |
| 1:F:178:THR:HA   | 1:F:181:ARG:HH11 | 1.87                     | 0.40              |
| 1:F:208:PHE:CE2  | 1:F:242:GLN:O    | 2.74                     | 0.40              |
| 4:I:6:GLN:CD     | 4:I:104:CYS:HB3  | 2.46                     | 0.40              |
| 5:J:53:ILE:HG22  | 5:J:54:HIS:CD2   | 2.56                     | 0.40              |
| 1:K:51:TRP:CH2   | 1:K:179:LEU:HD13 | 2.56                     | 0.40              |
| 2:L:96:ASP:CB    | 2:L:99:MET:HB3   | 2.51                     | 0.40              |
| 4:N:151:PHE:HZ   | 4:N:155:THR:C    | 2.29                     | 0.40              |
| 1:P:205:ALA:O    | 1:P:206:LEU:HB2  | 2.20                     | 0.40              |
| 5:T:115:TYR:CD2  | 5:T:115:TYR:N    | 2.88                     | 0.40              |
| 1:A:202:ARG:HA   | 1:A:245:ALA:O    | 2.21                     | 0.40              |
| 2:B:67:TYR:CD2   | 2:B:67:TYR:N     | 2.84                     | 0.40              |
| 5:E:171:TRP:CD1  | 5:E:175:LYS:C    | 3.00                     | 0.40              |
| 1:F:50:PRO:HA    | 1:F:53:GLU:OE1   | 2.21                     | 0.40              |
| 1:F:58:GLU:O     | 1:F:59:TYR:C     | 2.65                     | 0.40              |
| 1:F:260:HIS:CD2  | 1:F:271:THR:HB   | 2.56                     | 0.40              |
| 1:F:268:LYS:O    | 1:F:270:LEU:HD12 | 2.20                     | 0.40              |
| 2:G:33:SER:HB3   | 2:G:62:PHE:CE2   | 2.55                     | 0.40              |
| 4:I:175:MET:O    | 4:I:176:ARG:C    | 2.65                     | 0.40              |
| 1:K:69:THR:HG23  | 5:O:110:ASN:HD21 | 1.83                     | 0.40              |
| 1:K:121:LYS:HD3  | 1:K:121:LYS:HA   | 1.89                     | 0.40              |
| 1:K:203:CYS:O    | 1:K:204:TRP:CB   | 2.69                     | 0.40              |
| 4:N:87:ILE:HD11  | 4:N:104:CYS:SG   | 2.61                     | 0.40              |
| 5:O:7:GLN:HB3    | 5:O:104:CYS:SG   | 2.61                     | 0.40              |
| 5:T:20:MET:HB2   | 5:T:20:MET:HE3   | 1.76                     | 0.40              |
| 3:C:9:LEU:HD12   | 3:C:9:LEU:N      | 2.37                     | 0.40              |
| 4:D:197:ALA:HA   | 4:D:211:PHE:CD1  | 2.57                     | 0.40              |
| 4:I:129:ASP:HA   | 4:I:130:PRO:HD2  | 1.84                     | 0.40              |
| 4:I:210:PHE:C    | 4:I:210:PHE:CD2  | 2.99                     | 0.40              |
| 5:J:71:VAL:C     | 5:J:74:ASP:N     | 2.79                     | 0.40              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:K:85:TYR:HB2  | 1:K:87:GLN:NE2   | 2.35                     | 0.40              |
| 4:N:30:SER:CA   | 4:N:108:ALA:CB   | 2.97                     | 0.40              |
| 4:N:165:VAL:O   | 4:N:167:ILE:HG13 | 2.22                     | 0.40              |
| 5:O:139:PHE:HB2 | 5:O:155:VAL:O    | 2.22                     | 0.40              |
| 1:P:235:PRO:HG2 | 2:Q:10:TYR:OH    | 2.21                     | 0.40              |
| 5:T:42:TYR:CE2  | 5:T:52:LEU:HB2   | 2.56                     | 0.40              |
| 2:B:4:THR:HG23  | 2:B:5:PRO:CD     | 2.52                     | 0.40              |
| 5:E:14:LYS:O    | 5:E:15:THR:C     | 2.64                     | 0.40              |
| 5:E:176:GLU:HG2 | 5:E:178:HIS:HE1  | 1.87                     | 0.40              |
| 2:G:44:GLU:OE1  | 2:G:44:GLU:HA    | 2.22                     | 0.40              |
| 1:K:129:ASP:O   | 1:K:130:LEU:C    | 2.64                     | 0.40              |
| 2:L:81:ARG:NH1  | 2:L:81:ARG:HG3   | 2.37                     | 0.40              |
| 4:N:152:ASP:C   | 4:N:154:GLN:H    | 2.29                     | 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     | 275/277 (99%) | 193 (70%) | 54 (20%) | 28 (10%) | 0           | 3   |
| 1   | F     | 275/277 (99%) | 196 (71%) | 57 (21%) | 22 (8%)  | 1           | 4   |
| 1   | K     | 275/277 (99%) | 196 (71%) | 62 (22%) | 17 (6%)  | 1           | 7   |
| 1   | P     | 275/277 (99%) | 210 (76%) | 43 (16%) | 22 (8%)  | 1           | 4   |
| 2   | B     | 97/100 (97%)  | 77 (79%)  | 15 (16%) | 5 (5%)   | 1           | 10  |
| 2   | G     | 97/100 (97%)  | 75 (77%)  | 16 (16%) | 6 (6%)   | 1           | 7   |
| 2   | L     | 98/100 (98%)  | 70 (71%)  | 17 (17%) | 11 (11%) | 0           | 2   |
| 2   | Q     | 98/100 (98%)  | 72 (74%)  | 20 (20%) | 6 (6%)   | 1           | 7   |
| 3   | C     | 7/9 (78%)     | 6 (86%)   | 1 (14%)  | 0        | 100         | 100 |
| 3   | H     | 7/9 (78%)     | 6 (86%)   | 1 (14%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|-----------|----------|-------------|-----|
| 3   | M     | 7/9 (78%)       | 5 (71%)    | 2 (29%)   | 0        | 100         | 100 |
| 3   | R     | 7/9 (78%)       | 7 (100%)   | 0         | 0        | 100         | 100 |
| 4   | D     | 195/203 (96%)   | 139 (71%)  | 39 (20%)  | 17 (9%)  | 0           | 4   |
| 4   | I     | 195/203 (96%)   | 140 (72%)  | 42 (22%)  | 13 (7%)  | 1           | 6   |
| 4   | N     | 195/203 (96%)   | 120 (62%)  | 54 (28%)  | 21 (11%) | 0           | 2   |
| 4   | S     | 195/203 (96%)   | 146 (75%)  | 37 (19%)  | 12 (6%)  | 1           | 7   |
| 5   | E     | 239/244 (98%)   | 192 (80%)  | 40 (17%)  | 7 (3%)   | 3           | 19  |
| 5   | J     | 238/244 (98%)   | 191 (80%)  | 35 (15%)  | 12 (5%)  | 1           | 11  |
| 5   | O     | 239/244 (98%)   | 172 (72%)  | 54 (23%)  | 13 (5%)  | 1           | 9   |
| 5   | T     | 239/244 (98%)   | 196 (82%)  | 31 (13%)  | 12 (5%)  | 1           | 11  |
| All | All   | 3253/3332 (98%) | 2409 (74%) | 620 (19%) | 224 (7%) | 1           | 5   |

All (224) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 30  | ASP  |
| 1   | A     | 211 | ALA  |
| 1   | A     | 235 | PRO  |
| 1   | A     | 267 | PRO  |
| 2   | B     | 14  | PRO  |
| 4   | D     | 8   | PRO  |
| 4   | D     | 108 | ALA  |
| 4   | D     | 136 | ARG  |
| 4   | D     | 137 | ASP  |
| 5   | E     | 70  | GLU  |
| 5   | E     | 97  | SER  |
| 1   | F     | 106 | ASP  |
| 1   | F     | 235 | PRO  |
| 1   | F     | 236 | ALA  |
| 2   | G     | 12  | ARG  |
| 4   | I     | 8   | PRO  |
| 4   | I     | 139 | LYS  |
| 4   | I     | 159 | GLN  |
| 5   | J     | 70  | GLU  |
| 5   | J     | 96  | PRO  |
| 1   | K     | 210 | PRO  |
| 1   | K     | 235 | PRO  |
| 1   | K     | 236 | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | L     | 5   | PRO  |
| 2   | L     | 6   | LYS  |
| 2   | L     | 7   | ILE  |
| 2   | L     | 34  | ASP  |
| 2   | L     | 37  | VAL  |
| 4   | N     | 15  | GLU  |
| 4   | N     | 30  | SER  |
| 4   | N     | 68  | GLU  |
| 4   | N     | 107 | ARG  |
| 4   | N     | 162 | ASP  |
| 1   | P     | 29  | ASP  |
| 1   | P     | 43  | PRO  |
| 1   | P     | 47  | PRO  |
| 1   | P     | 50  | PRO  |
| 1   | P     | 177 | ASP  |
| 1   | P     | 196 | ASP  |
| 2   | Q     | 12  | ARG  |
| 2   | Q     | 20  | SER  |
| 4   | S     | 142 | ASP  |
| 5   | T     | 70  | GLU  |
| 5   | T     | 97  | SER  |
| 5   | T     | 98  | GLN  |
| 1   | A     | 185 | PRO  |
| 1   | A     | 194 | ILE  |
| 1   | A     | 203 | CYS  |
| 1   | A     | 208 | PHE  |
| 1   | A     | 210 | PRO  |
| 1   | A     | 236 | ALA  |
| 1   | A     | 254 | GLU  |
| 2   | B     | 48  | LYS  |
| 4   | D     | 125 | ILE  |
| 4   | D     | 170 | LYS  |
| 4   | D     | 174 | ASP  |
| 4   | D     | 208 | ASP  |
| 5   | E     | 61  | THR  |
| 5   | E     | 72  | PRO  |
| 1   | F     | 213 | ILE  |
| 2   | G     | 16  | GLU  |
| 4   | I     | 107 | ARG  |
| 4   | I     | 138 | SER  |
| 4   | I     | 140 | SER  |
| 4   | I     | 144 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | I     | 160 | SER  |
| 4   | I     | 178 | MET  |
| 4   | I     | 184 | SER  |
| 5   | J     | 98  | GLN  |
| 1   | K     | 30  | ASP  |
| 1   | K     | 207 | GLY  |
| 2   | L     | 8   | GLN  |
| 2   | L     | 42  | ASN  |
| 4   | N     | 8   | PRO  |
| 4   | N     | 78  | ARG  |
| 4   | N     | 108 | ALA  |
| 4   | N     | 121 | VAL  |
| 4   | N     | 142 | ASP  |
| 4   | N     | 151 | PHE  |
| 4   | N     | 199 | ALA  |
| 5   | O     | 74  | ASP  |
| 5   | O     | 97  | SER  |
| 5   | O     | 141 | PRO  |
| 5   | O     | 229 | SER  |
| 1   | P     | 17  | ARG  |
| 1   | P     | 40  | ALA  |
| 1   | P     | 51  | TRP  |
| 1   | P     | 235 | PRO  |
| 1   | P     | 255 | GLN  |
| 4   | S     | 8   | PRO  |
| 4   | S     | 108 | ALA  |
| 4   | S     | 139 | LYS  |
| 5   | T     | 28  | MET  |
| 1   | A     | 204 | TRP  |
| 1   | A     | 209 | TYR  |
| 1   | A     | 276 | PRO  |
| 2   | B     | 19  | LYS  |
| 4   | D     | 15  | GLU  |
| 4   | D     | 191 | LYS  |
| 1   | F     | 51  | TRP  |
| 1   | F     | 86  | ASN  |
| 1   | F     | 219 | ARG  |
| 1   | F     | 222 | GLU  |
| 1   | F     | 243 | LYS  |
| 2   | G     | 52  | SER  |
| 2   | G     | 74  | GLU  |
| 2   | G     | 77  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | I     | 108 | ALA  |
| 4   | I     | 183 | ASN  |
| 5   | J     | 67  | ALA  |
| 5   | J     | 72  | PRO  |
| 5   | J     | 233 | GLU  |
| 1   | K     | 177 | ASP  |
| 1   | K     | 204 | TRP  |
| 1   | K     | 205 | ALA  |
| 1   | K     | 232 | GLU  |
| 2   | L     | 61  | SER  |
| 4   | N     | 143 | LYS  |
| 4   | N     | 144 | SER  |
| 4   | N     | 170 | LYS  |
| 4   | N     | 191 | LYS  |
| 4   | N     | 197 | ALA  |
| 4   | N     | 206 | PRO  |
| 4   | N     | 208 | ASP  |
| 5   | O     | 106 | SER  |
| 5   | O     | 240 | LYS  |
| 1   | P     | 42  | SER  |
| 1   | P     | 194 | ILE  |
| 1   | P     | 221 | GLY  |
| 1   | P     | 236 | ALA  |
| 4   | S     | 159 | GLN  |
| 4   | S     | 195 | ALA  |
| 5   | T     | 18  | GLN  |
| 5   | T     | 94  | ALA  |
| 1   | A     | 2   | SER  |
| 1   | A     | 86  | ASN  |
| 1   | A     | 220 | ASP  |
| 1   | A     | 262 | GLN  |
| 1   | A     | 271 | THR  |
| 4   | D     | 3   | GLU  |
| 4   | D     | 107 | ARG  |
| 4   | D     | 119 | LEU  |
| 5   | E     | 92  | GLU  |
| 5   | E     | 240 | LYS  |
| 1   | F     | 41  | ALA  |
| 1   | F     | 166 | GLU  |
| 1   | F     | 196 | ASP  |
| 1   | F     | 202 | ARG  |
| 1   | F     | 212 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 224 | GLN  |
| 5   | J     | 66  | THR  |
| 5   | J     | 75  | GLY  |
| 5   | J     | 240 | LYS  |
| 1   | K     | 2   | SER  |
| 1   | K     | 51  | TRP  |
| 1   | K     | 114 | ASN  |
| 1   | K     | 162 | GLY  |
| 1   | K     | 237 | GLY  |
| 2   | L     | 32  | PRO  |
| 4   | N     | 130 | PRO  |
| 5   | O     | 112 | ASP  |
| 5   | O     | 217 | ASN  |
| 1   | P     | 210 | PRO  |
| 2   | Q     | 43  | GLY  |
| 2   | Q     | 79  | ALA  |
| 4   | S     | 15  | GLU  |
| 4   | S     | 27  | ASN  |
| 4   | S     | 93  | ASP  |
| 4   | S     | 140 | SER  |
| 4   | S     | 174 | ASP  |
| 5   | T     | 67  | ALA  |
| 5   | T     | 238 | ARG  |
| 5   | T     | 240 | LYS  |
| 1   | A     | 42  | SER  |
| 2   | B     | 23  | LEU  |
| 2   | B     | 47  | GLU  |
| 4   | D     | 30  | SER  |
| 4   | D     | 110 | LYS  |
| 1   | F     | 43  | PRO  |
| 1   | F     | 264 | GLU  |
| 2   | G     | 46  | ILE  |
| 1   | K     | 47  | PRO  |
| 2   | L     | 46  | ILE  |
| 4   | N     | 163 | SER  |
| 5   | O     | 92  | GLU  |
| 5   | O     | 190 | GLU  |
| 5   | O     | 243 | THR  |
| 1   | P     | 4   | SER  |
| 1   | P     | 58  | GLU  |
| 1   | P     | 172 | LEU  |
| 1   | P     | 243 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 58  | GLU  |
| 1   | A     | 192 | HIS  |
| 4   | D     | 175 | MET  |
| 1   | F     | 237 | GLY  |
| 5   | J     | 71  | VAL  |
| 5   | J     | 192 | PRO  |
| 2   | Q     | 16  | GLU  |
| 4   | S     | 107 | ARG  |
| 5   | T     | 236 | GLN  |
| 1   | A     | 56  | GLY  |
| 4   | D     | 130 | PRO  |
| 1   | F     | 193 | PRO  |
| 1   | K     | 42  | SER  |
| 1   | K     | 50  | PRO  |
| 2   | L     | 49  | VAL  |
| 5   | T     | 187 | PRO  |
| 1   | A     | 213 | ILE  |
| 1   | P     | 49  | ALA  |
| 1   | P     | 276 | PRO  |
| 2   | Q     | 90  | PRO  |
| 5   | T     | 160 | GLY  |
| 1   | F     | 50  | PRO  |
| 4   | I     | 9   | GLY  |
| 5   | O     | 185 | PRO  |
| 1   | A     | 15  | PRO  |
| 1   | A     | 261 | VAL  |
| 1   | F     | 194 | ILE  |
| 5   | J     | 49  | GLY  |
| 1   | A     | 43  | PRO  |
| 1   | A     | 49  | ALA  |
| 5   | E     | 215 | PRO  |
| 5   | O     | 192 | PRO  |
| 1   | F     | 210 | 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     | 236/236 (100%)  | 221 (94%)  | 15 (6%)  | 16          | 44  |
| 1   | F     | 236/236 (100%)  | 222 (94%)  | 14 (6%)  | 18          | 48  |
| 1   | K     | 236/236 (100%)  | 227 (96%)  | 9 (4%)   | 29          | 60  |
| 1   | P     | 236/236 (100%)  | 219 (93%)  | 17 (7%)  | 13          | 40  |
| 2   | B     | 94/95 (99%)     | 87 (93%)   | 7 (7%)   | 13          | 40  |
| 2   | G     | 94/95 (99%)     | 85 (90%)   | 9 (10%)  | 8           | 30  |
| 2   | L     | 95/95 (100%)    | 83 (87%)   | 12 (13%) | 4           | 19  |
| 2   | Q     | 95/95 (100%)    | 90 (95%)   | 5 (5%)   | 20          | 51  |
| 3   | C     | 6/6 (100%)      | 6 (100%)   | 0        | 100         | 100 |
| 3   | H     | 6/6 (100%)      | 5 (83%)    | 1 (17%)  | 2           | 10  |
| 3   | M     | 6/6 (100%)      | 6 (100%)   | 0        | 100         | 100 |
| 3   | R     | 6/6 (100%)      | 6 (100%)   | 0        | 100         | 100 |
| 4   | D     | 177/183 (97%)   | 164 (93%)  | 13 (7%)  | 13          | 40  |
| 4   | I     | 177/183 (97%)   | 169 (96%)  | 8 (4%)   | 24          | 56  |
| 4   | N     | 177/183 (97%)   | 163 (92%)  | 14 (8%)  | 11          | 37  |
| 4   | S     | 177/183 (97%)   | 170 (96%)  | 7 (4%)   | 28          | 60  |
| 5   | E     | 205/208 (99%)   | 189 (92%)  | 16 (8%)  | 11          | 38  |
| 5   | J     | 205/208 (99%)   | 196 (96%)  | 9 (4%)   | 25          | 56  |
| 5   | O     | 205/208 (99%)   | 192 (94%)  | 13 (6%)  | 16          | 45  |
| 5   | T     | 205/208 (99%)   | 190 (93%)  | 15 (7%)  | 13          | 40  |
| All | All   | 2874/2912 (99%) | 2690 (94%) | 184 (6%) | 16          | 44  |

All (184) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 10  | THR  |
| 1   | A     | 12  | MET  |
| 1   | A     | 52  | ILE  |
| 1   | A     | 63  | ASN  |
| 1   | A     | 81  | LEU  |
| 1   | A     | 115 | GLN  |
| 1   | A     | 186 | LYS  |
| 1   | A     | 198 | GLU  |
| 1   | A     | 204 | TRP  |
| 1   | A     | 219 | ARG  |
| 1   | A     | 230 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 234 | ARG  |
| 1   | A     | 257 | TYR  |
| 1   | A     | 270 | LEU  |
| 1   | A     | 274 | TRP  |
| 2   | B     | 12  | ARG  |
| 2   | B     | 22  | PHE  |
| 2   | B     | 24  | ASN  |
| 2   | B     | 31  | HIS  |
| 2   | B     | 58  | LYS  |
| 2   | B     | 67  | TYR  |
| 2   | B     | 70  | PHE  |
| 4   | D     | 19  | VAL  |
| 4   | D     | 27  | ASN  |
| 4   | D     | 48  | LYS  |
| 4   | D     | 54  | MET  |
| 4   | D     | 68  | GLU  |
| 4   | D     | 87  | ILE  |
| 4   | D     | 92  | ARG  |
| 4   | D     | 96  | LEU  |
| 4   | D     | 104 | CYS  |
| 4   | D     | 161 | LYS  |
| 4   | D     | 171 | CYS  |
| 4   | D     | 194 | PHE  |
| 4   | D     | 207 | GLU  |
| 5   | E     | 19  | MET  |
| 5   | E     | 25  | GLN  |
| 5   | E     | 61  | THR  |
| 5   | E     | 71  | VAL  |
| 5   | E     | 81  | LEU  |
| 5   | E     | 86  | ASN  |
| 5   | E     | 87  | PHE  |
| 5   | E     | 164 | ASP  |
| 5   | E     | 188 | LEU  |
| 5   | E     | 194 | LEU  |
| 5   | E     | 196 | ASP  |
| 5   | E     | 197 | SER  |
| 5   | E     | 204 | ARG  |
| 5   | E     | 223 | VAL  |
| 5   | E     | 231 | ASN  |
| 5   | E     | 244 | GLN  |
| 1   | F     | 42  | SER  |
| 1   | F     | 71  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 72  | GLN  |
| 1   | F     | 81  | LEU  |
| 1   | F     | 108 | ARG  |
| 1   | F     | 109 | LEU  |
| 1   | F     | 124 | ILE  |
| 1   | F     | 137 | ASP  |
| 1   | F     | 138 | THR  |
| 1   | F     | 170 | ARG  |
| 1   | F     | 189 | VAL  |
| 1   | F     | 219 | ARG  |
| 1   | F     | 220 | ASP  |
| 1   | F     | 238 | ASP  |
| 2   | G     | 7   | ILE  |
| 2   | G     | 10  | TYR  |
| 2   | G     | 23  | LEU  |
| 2   | G     | 39  | LEU  |
| 2   | G     | 40  | LEU  |
| 2   | G     | 46  | ILE  |
| 2   | G     | 51  | HIS  |
| 2   | G     | 78  | TYR  |
| 2   | G     | 85  | VAL  |
| 3   | H     | 5   | ARG  |
| 4   | I     | 18  | THR  |
| 4   | I     | 24  | THR  |
| 4   | I     | 27  | ASN  |
| 4   | I     | 48  | LYS  |
| 4   | I     | 54  | MET  |
| 4   | I     | 87  | ILE  |
| 4   | I     | 90  | LEU  |
| 4   | I     | 191 | LYS  |
| 5   | J     | 20  | THR  |
| 5   | J     | 21  | LEU  |
| 5   | J     | 48  | MET  |
| 5   | J     | 87  | PHE  |
| 5   | J     | 99  | THR  |
| 5   | J     | 126 | GLU  |
| 5   | J     | 128 | LEU  |
| 5   | J     | 165 | HIS  |
| 5   | J     | 236 | GLN  |
| 1   | K     | 121 | LYS  |
| 1   | K     | 138 | THR  |
| 1   | K     | 179 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | K     | 204 | TRP  |
| 1   | K     | 228 | THR  |
| 1   | K     | 234 | ARG  |
| 1   | K     | 244 | TRP  |
| 1   | K     | 257 | TYR  |
| 1   | K     | 258 | THR  |
| 2   | L     | 1   | ILE  |
| 2   | L     | 2   | GLN  |
| 2   | L     | 13  | HIS  |
| 2   | L     | 17  | ASN  |
| 2   | L     | 23  | LEU  |
| 2   | L     | 37  | VAL  |
| 2   | L     | 44  | GLU  |
| 2   | L     | 46  | ILE  |
| 2   | L     | 51  | HIS  |
| 2   | L     | 67  | TYR  |
| 2   | L     | 85  | VAL  |
| 2   | L     | 93  | VAL  |
| 4   | N     | 19  | VAL  |
| 4   | N     | 54  | MET  |
| 4   | N     | 68  | GLU  |
| 4   | N     | 69  | ASP  |
| 4   | N     | 106 | VAL  |
| 4   | N     | 113 | PHE  |
| 4   | N     | 125 | ILE  |
| 4   | N     | 127 | ASN  |
| 4   | N     | 132 | VAL  |
| 4   | N     | 154 | GLN  |
| 4   | N     | 155 | THR  |
| 4   | N     | 161 | LYS  |
| 4   | N     | 168 | THR  |
| 4   | N     | 209 | THR  |
| 5   | O     | 6   | THR  |
| 5   | O     | 13  | VAL  |
| 5   | O     | 43  | ARG  |
| 5   | O     | 48  | MET  |
| 5   | O     | 61  | THR  |
| 5   | O     | 70  | GLU  |
| 5   | O     | 71  | VAL  |
| 5   | O     | 91  | LEU  |
| 5   | O     | 126 | GLU  |
| 5   | O     | 194 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | O     | 212 | TRP  |
| 5   | O     | 231 | ASN  |
| 5   | O     | 238 | ARG  |
| 1   | P     | 44  | ARG  |
| 1   | P     | 53  | GLU  |
| 1   | P     | 55  | GLU  |
| 1   | P     | 63  | ASN  |
| 1   | P     | 65  | GLN  |
| 1   | P     | 69  | THR  |
| 1   | P     | 72  | GLN  |
| 1   | P     | 129 | ASP  |
| 1   | P     | 138 | THR  |
| 1   | P     | 192 | HIS  |
| 1   | P     | 201 | LEU  |
| 1   | P     | 203 | CYS  |
| 1   | P     | 204 | TRP  |
| 1   | P     | 216 | THR  |
| 1   | P     | 218 | GLN  |
| 1   | P     | 231 | VAL  |
| 1   | P     | 275 | GLU  |
| 2   | Q     | 51  | HIS  |
| 2   | Q     | 58  | LYS  |
| 2   | Q     | 75  | LYS  |
| 2   | Q     | 83  | ASN  |
| 2   | Q     | 97  | ARG  |
| 4   | S     | 27  | ASN  |
| 4   | S     | 54  | MET  |
| 4   | S     | 178 | MET  |
| 4   | S     | 198 | ASN  |
| 4   | S     | 202 | ASN  |
| 4   | S     | 204 | ILE  |
| 4   | S     | 205 | ILE  |
| 5   | T     | 21  | THR  |
| 5   | T     | 22  | LEU  |
| 5   | T     | 26  | GLN  |
| 5   | T     | 28  | MET  |
| 5   | T     | 29  | ASN  |
| 5   | T     | 59  | GLU  |
| 5   | T     | 61  | THR  |
| 5   | T     | 81  | LEU  |
| 5   | T     | 87  | PHE  |
| 5   | T     | 155 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | T     | 204 | ARG  |
| 5   | T     | 228 | LEU  |
| 5   | T     | 230 | GLU  |
| 5   | T     | 237 | ASP  |
| 5   | T     | 244 | GLN  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (82) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 63  | ASN  |
| 1   | A     | 72  | GLN  |
| 1   | A     | 113 | HIS  |
| 1   | A     | 115 | GLN  |
| 1   | A     | 191 | HIS  |
| 1   | A     | 197 | HIS  |
| 1   | A     | 218 | GLN  |
| 1   | A     | 263 | HIS  |
| 2   | B     | 42  | ASN  |
| 4   | D     | 27  | ASN  |
| 5   | E     | 25  | GLN  |
| 5   | E     | 86  | ASN  |
| 5   | E     | 98  | GLN  |
| 5   | E     | 114 | GLN  |
| 5   | E     | 178 | HIS  |
| 5   | E     | 213 | GLN  |
| 5   | E     | 231 | ASN  |
| 5   | E     | 244 | GLN  |
| 1   | F     | 72  | GLN  |
| 1   | F     | 96  | GLN  |
| 1   | F     | 115 | GLN  |
| 1   | F     | 174 | ASN  |
| 1   | F     | 191 | HIS  |
| 1   | F     | 255 | GLN  |
| 1   | F     | 260 | HIS  |
| 1   | F     | 262 | GLN  |
| 2   | G     | 8   | GLN  |
| 2   | G     | 83  | ASN  |
| 4   | I     | 27  | ASN  |
| 5   | J     | 25  | GLN  |
| 5   | J     | 28  | ASN  |
| 5   | J     | 44  | GLN  |
| 5   | J     | 54  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | J     | 86  | ASN  |
| 5   | J     | 98  | GLN  |
| 5   | J     | 114 | GLN  |
| 5   | J     | 165 | HIS  |
| 5   | J     | 178 | HIS  |
| 5   | J     | 186 | GLN  |
| 5   | J     | 224 | GLN  |
| 5   | J     | 236 | GLN  |
| 1   | K     | 3   | HIS  |
| 1   | K     | 63  | ASN  |
| 1   | K     | 144 | GLN  |
| 1   | K     | 224 | GLN  |
| 1   | K     | 226 | GLN  |
| 1   | K     | 242 | GLN  |
| 1   | K     | 262 | GLN  |
| 2   | L     | 2   | GLN  |
| 2   | L     | 13  | HIS  |
| 4   | N     | 44  | GLN  |
| 4   | N     | 115 | GLN  |
| 4   | N     | 154 | GLN  |
| 4   | N     | 202 | ASN  |
| 5   | O     | 44  | GLN  |
| 5   | O     | 54  | HIS  |
| 5   | O     | 98  | GLN  |
| 5   | O     | 110 | ASN  |
| 5   | O     | 148 | HIS  |
| 5   | O     | 218 | HIS  |
| 5   | O     | 222 | GLN  |
| 5   | O     | 224 | GLN  |
| 5   | O     | 244 | GLN  |
| 1   | P     | 65  | GLN  |
| 1   | P     | 141 | GLN  |
| 1   | P     | 174 | ASN  |
| 1   | P     | 242 | GLN  |
| 1   | P     | 262 | GLN  |
| 2   | Q     | 2   | GLN  |
| 2   | Q     | 24  | ASN  |
| 2   | Q     | 31  | HIS  |
| 4   | S     | 27  | ASN  |
| 4   | S     | 44  | GLN  |
| 4   | S     | 85  | GLN  |
| 4   | S     | 202 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | T     | 44  | GLN  |
| 5   | T     | 54  | HIS  |
| 5   | T     | 86  | ASN  |
| 5   | T     | 98  | GLN  |
| 5   | T     | 114 | GLN  |
| 5   | T     | 191 | GLN  |
| 5   | T     | 244 | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

### 5.7 Other polymers ⓘ

There are no such residues in this entry.

### 5.8 Polymer linkage issues ⓘ

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     | 277/277 (100%)  | 0.24   | 20 (7%) 21 11  | 21, 78, 193, 223      | 0      |
| 1   | F     | 277/277 (100%)  | 0.29   | 14 (5%) 33 18  | 30, 82, 214, 249      | 0      |
| 1   | K     | 277/277 (100%)  | 0.35   | 20 (7%) 21 11  | 31, 93, 215, 245      | 0      |
| 1   | P     | 277/277 (100%)  | 0.21   | 4 (1%) 73 53   | 25, 87, 200, 220      | 0      |
| 2   | B     | 99/100 (99%)    | 0.00   | 1 (1%) 79 61   | 34, 67, 116, 130      | 0      |
| 2   | G     | 99/100 (99%)    | 0.49   | 6 (6%) 27 15   | 49, 100, 159, 188     | 0      |
| 2   | L     | 100/100 (100%)  | 1.07   | 9 (9%) 15 8    | 66, 193, 228, 236     | 0      |
| 2   | Q     | 100/100 (100%)  | 0.64   | 8 (8%) 18 10   | 45, 136, 184, 191     | 0      |
| 3   | C     | 9/9 (100%)      | -0.32  | 0 100 100      | 27, 31, 41, 48        | 0      |
| 3   | H     | 9/9 (100%)      | -0.45  | 0 100 100      | 22, 34, 43, 45        | 0      |
| 3   | M     | 9/9 (100%)      | -0.14  | 0 100 100      | 29, 34, 52, 62        | 0      |
| 3   | R     | 9/9 (100%)      | -0.63  | 0 100 100      | 22, 27, 46, 54        | 0      |
| 4   | D     | 197/203 (97%)   | 0.21   | 2 (1%) 79 61   | 31, 78, 133, 162      | 0      |
| 4   | I     | 197/203 (97%)   | -0.23  | 0 100 100      | 20, 46, 116, 143      | 0      |
| 4   | N     | 197/203 (97%)   | 0.74   | 17 (8%) 16 9   | 35, 97, 178, 201      | 0      |
| 4   | S     | 197/203 (97%)   | -0.04  | 1 (0%) 87 73   | 21, 51, 132, 166      | 0      |
| 5   | E     | 241/244 (98%)   | -0.06  | 1 (0%) 88 76   | 28, 64, 113, 133      | 2 (0%) |
| 5   | J     | 240/244 (98%)   | -0.33  | 1 (0%) 88 76   | 20, 41, 90, 137       | 2 (0%) |
| 5   | O     | 241/244 (98%)   | 0.19   | 9 (3%) 45 25   | 27, 61, 176, 189      | 2 (0%) |
| 5   | T     | 241/244 (98%)   | -0.13  | 2 (0%) 82 65   | 20, 52, 114, 145      | 2 (0%) |
| All | All   | 3293/3332 (98%) | 0.17   | 115 (3%) 47 27 | 20, 72, 193, 249      | 8 (0%) |

All (115) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | Q     | 78  | TYR  | 6.1  |
| 2   | L     | 78  | TYR  | 5.5  |
| 2   | L     | 23  | LEU  | 5.4  |
| 2   | Q     | 79  | ALA  | 4.8  |
| 4   | N     | 172 | VAL  | 4.1  |
| 1   | F     | 201 | LEU  | 4.1  |
| 4   | N     | 131 | ALA  | 3.8  |
| 1   | F     | 261 | VAL  | 3.8  |
| 1   | A     | 266 | LEU  | 3.8  |
| 1   | A     | 217 | TRP  | 3.6  |
| 1   | P     | 257 | TYR  | 3.6  |
| 1   | K     | 215 | LEU  | 3.5  |
| 2   | L     | 9   | VAL  | 3.4  |
| 2   | G     | 23  | LEU  | 3.4  |
| 1   | A     | 215 | LEU  | 3.4  |
| 1   | A     | 179 | LEU  | 3.2  |
| 2   | L     | 25  | CYS  | 3.2  |
| 1   | A     | 259 | CYS  | 3.2  |
| 5   | E     | 75  | GLY  | 3.2  |
| 1   | F     | 255 | GLN  | 3.1  |
| 2   | G     | 78  | TYR  | 3.1  |
| 5   | T     | 74  | ASP  | 3.0  |
| 1   | K     | 235 | PRO  | 3.0  |
| 1   | P     | 201 | LEU  | 2.8  |
| 1   | A     | 201 | LEU  | 2.8  |
| 1   | A     | 274 | TRP  | 2.8  |
| 1   | A     | 218 | GLN  | 2.8  |
| 2   | G     | 40  | LEU  | 2.8  |
| 2   | L     | 82  | VAL  | 2.7  |
| 2   | Q     | 23  | LEU  | 2.7  |
| 4   | N     | 153 | SER  | 2.7  |
| 1   | A     | 199 | ALA  | 2.7  |
| 4   | D     | 165 | VAL  | 2.6  |
| 4   | N     | 195 | ALA  | 2.6  |
| 5   | O     | 138 | VAL  | 2.6  |
| 4   | N     | 205 | ILE  | 2.6  |
| 1   | F     | 249 | VAL  | 2.6  |
| 1   | K     | 205 | ALA  | 2.6  |
| 4   | N     | 185 | ALA  | 2.6  |
| 1   | A     | 255 | GLN  | 2.6  |
| 1   | K     | 203 | CYS  | 2.6  |
| 1   | K     | 245 | ALA  | 2.6  |
| 2   | L     | 85  | VAL  | 2.6  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 5   | O     | 219 | PHE  | 2.6  |
| 2   | G     | 14  | PRO  | 2.6  |
| 1   | A     | 211 | ALA  | 2.6  |
| 4   | N     | 133 | TYR  | 2.5  |
| 1   | A     | 276 | PRO  | 2.5  |
| 4   | D     | 207 | GLU  | 2.5  |
| 2   | Q     | 0   | MET  | 2.5  |
| 5   | T     | 141 | PRO  | 2.5  |
| 1   | A     | 249 | VAL  | 2.5  |
| 1   | K     | 206 | LEU  | 2.5  |
| 1   | F     | 247 | VAL  | 2.5  |
| 1   | A     | 270 | LEU  | 2.4  |
| 4   | N     | 173 | LEU  | 2.4  |
| 1   | F     | 248 | VAL  | 2.4  |
| 4   | N     | 123 | PRO  | 2.4  |
| 5   | O     | 250 | ALA  | 2.4  |
| 1   | F     | 185 | PRO  | 2.4  |
| 4   | N     | 130 | PRO  | 2.4  |
| 5   | O     | 74  | ASP  | 2.4  |
| 1   | K     | 199 | ALA  | 2.3  |
| 1   | P     | 215 | LEU  | 2.3  |
| 1   | P     | 247 | VAL  | 2.3  |
| 1   | A     | 204 | TRP  | 2.3  |
| 5   | O     | 212 | TRP  | 2.3  |
| 4   | S     | 144 | SER  | 2.3  |
| 5   | J     | 72  | PRO  | 2.3  |
| 2   | L     | 79  | ALA  | 2.3  |
| 1   | A     | 257 | TYR  | 2.3  |
| 1   | A     | 207 | GLY  | 2.2  |
| 4   | N     | 108 | ALA  | 2.2  |
| 2   | G     | 95  | TRP  | 2.2  |
| 1   | K     | 233 | THR  | 2.2  |
| 5   | O     | 97  | SER  | 2.2  |
| 1   | K     | 273 | ARG  | 2.2  |
| 2   | L     | 37  | VAL  | 2.2  |
| 2   | Q     | 24  | ASN  | 2.2  |
| 1   | K     | 187 | THR  | 2.2  |
| 1   | A     | 251 | SER  | 2.2  |
| 4   | N     | 150 | ASP  | 2.2  |
| 1   | F     | 210 | PRO  | 2.2  |
| 1   | K     | 236 | ALA  | 2.2  |
| 1   | K     | 270 | LEU  | 2.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | F     | 199 | ALA  | 2.2  |
| 1   | K     | 243 | LYS  | 2.2  |
| 4   | N     | 132 | VAL  | 2.1  |
| 2   | Q     | 64  | LEU  | 2.1  |
| 5   | O     | 217 | ASN  | 2.1  |
| 1   | F     | 203 | CYS  | 2.1  |
| 1   | K     | 248 | VAL  | 2.1  |
| 1   | A     | 258 | THR  | 2.1  |
| 1   | K     | 201 | LEU  | 2.1  |
| 2   | Q     | 39  | LEU  | 2.1  |
| 1   | F     | 205 | ALA  | 2.1  |
| 2   | L     | 88  | SER  | 2.1  |
| 1   | F     | 189 | VAL  | 2.1  |
| 1   | K     | 189 | VAL  | 2.1  |
| 1   | K     | 244 | TRP  | 2.1  |
| 1   | F     | 245 | ALA  | 2.1  |
| 5   | O     | 179 | SER  | 2.1  |
| 2   | B     | 23  | LEU  | 2.1  |
| 2   | G     | 11  | SER  | 2.1  |
| 4   | N     | 120 | SER  | 2.1  |
| 4   | N     | 145 | VAL  | 2.1  |
| 1   | K     | 188 | HIS  | 2.1  |
| 1   | K     | 204 | TRP  | 2.1  |
| 4   | N     | 186 | VAL  | 2.0  |
| 1   | A     | 203 | CYS  | 2.0  |
| 1   | F     | 250 | PRO  | 2.0  |
| 1   | K     | 247 | VAL  | 2.0  |
| 2   | Q     | 9   | VAL  | 2.0  |
| 4   | N     | 149 | THR  | 2.0  |
| 5   | O     | 145 | GLU  | 2.0  |

## 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.