



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 05:07 PM UTC

PDB ID : 8GS5 / pdb\_00008gs5  
Title : Crystal structure of a constitutively active mutant of human IDH3 holoenzyme in apo form  
Authors : Sun, P.; Chen, X.; Ding, J.  
Deposited on : 2022-09-04  
Resolution : 4.49 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

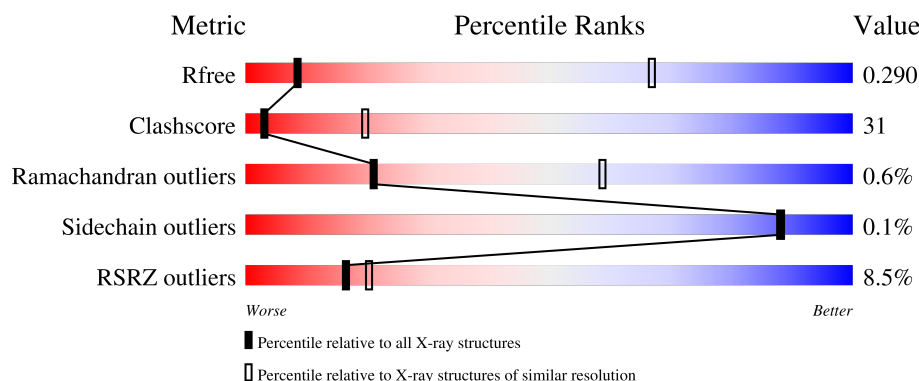
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.49 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                      | 1124 (5.06-3.90)                                      |
| Clashscore            | 190562                      | 1028 (5.04-3.92)                                      |
| Ramachandran outliers | 187476                      | 1058 (5.06-3.90)                                      |
| Sidechain outliers    | 187428                      | 1041 (5.06-3.90)                                      |
| RSRZ outliers         | 180081                      | 1119 (5.06-3.90)                                      |

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     | 339    | <div> <div>8%</div> <div>60%</div> <div>40%</div> <div>.</div> </div>   |
| 1   | C     | 339    | <div> <div>17%</div> <div>67%</div> <div>30%</div> <div>.</div> </div>  |
| 1   | E     | 339    | <div> <div>17%</div> <div>63%</div> <div>35%</div> <div>..</div> </div> |
| 1   | G     | 339    | <div> <div>10%</div> <div>71%</div> <div>24%</div> <div>..</div> </div> |
| 1   | I     | 339    | <div> <div>8%</div> <div>67%</div> <div>29%</div> <div>..</div> </div>  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | K     | 339    |                  |
| 1   | M     | 339    |                  |
| 1   | O     | 339    |                  |
| 2   | D     | 354    |                  |
| 2   | H     | 354    |                  |
| 2   | L     | 354    |                  |
| 2   | P     | 354    |                  |
| 3   | B     | 352    |                  |
| 3   | F     | 352    |                  |
| 3   | J     | 352    |                  |
| 3   | N     | 352    |                  |

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 39351 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 Isocitrate dehydrogenase [NAD] subunit alpha, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | C     | 328      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2389  | 1503 | 406 | 459 | 21 |         |         |       |
| 1   | A     | 336      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2412  | 1510 | 412 | 470 | 20 |         |         |       |
| 1   | G     | 324      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2444  | 1537 | 417 | 470 | 20 |         |         |       |
| 1   | E     | 336      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2400  | 1502 | 411 | 465 | 22 |         |         |       |
| 1   | K     | 327      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2480  | 1561 | 424 | 473 | 22 |         |         |       |
| 1   | I     | 336      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2439  | 1530 | 414 | 473 | 22 |         |         |       |
| 1   | O     | 329      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2454  | 1546 | 419 | 467 | 22 |         |         |       |
| 1   | M     | 336      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2436  | 1524 | 416 | 474 | 22 |         |         |       |

There are 8 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| C     | 139     | ALA      | GLN    | engineered mutation | UNP P50213 |
| A     | 139     | ALA      | GLN    | engineered mutation | UNP P50213 |
| G     | 139     | ALA      | GLN    | engineered mutation | UNP P50213 |
| E     | 139     | ALA      | GLN    | engineered mutation | UNP P50213 |
| K     | 139     | ALA      | GLN    | engineered mutation | UNP P50213 |
| I     | 139     | ALA      | GLN    | engineered mutation | UNP P50213 |
| O     | 139     | ALA      | GLN    | engineered mutation | UNP P50213 |
| M     | 139     | ALA      | GLN    | engineered mutation | UNP P50213 |

- Molecule 2 is a protein called Isocitrate dehydrogenase [NAD] subunit gamma, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 2   | D     | 339      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2496  | 1556 | 456 | 466 | 18 |         |         |       |
| 2   | H     | 347      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2555  | 1594 | 467 | 476 | 18 |         |         |       |
| 2   | L     | 347      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2569  | 1606 | 469 | 477 | 17 |         |         |       |
| 2   | P     | 346      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2539  | 1590 | 462 | 469 | 18 |         |         |       |

- Molecule 3 is a protein called Isoform A of Isocitrate dehydrogenase [NAD] subunit beta, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 3   | B     | 335      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2466  | 1557 | 425 | 465 | 19 |         |         |       |
| 3   | F     | 335      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2400  | 1516 | 420 | 446 | 18 |         |         |       |
| 3   | J     | 335      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2465  | 1557 | 429 | 459 | 20 |         |         |       |
| 3   | N     | 334      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2407  | 1515 | 417 | 456 | 19 |         |         |       |

There are 48 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference    |
|-------|---------|----------|--------|----------------|--------------|
| B     | 341     | GLU      | -      | expression tag | UNP O43837-2 |
| B     | 342     | ILE      | -      | expression tag | UNP O43837-2 |
| B     | 343     | CYS      | -      | expression tag | UNP O43837-2 |
| B     | 344     | ARG      | -      | expression tag | UNP O43837-2 |
| B     | 345     | ARG      | -      | expression tag | UNP O43837-2 |
| B     | 346     | VAL      | -      | expression tag | UNP O43837-2 |
| B     | 347     | LYS      | -      | expression tag | UNP O43837-2 |
| B     | 348     | ASP      | -      | expression tag | UNP O43837-2 |
| B     | 349     | LEU      | -      | expression tag | UNP O43837-2 |
| B     | 350     | ASP      | -      | expression tag | UNP O43837-2 |
| B     | 351     | GLU      | -      | expression tag | UNP O43837-2 |
| B     | 352     | ASN      | -      | expression tag | UNP O43837-2 |
| F     | 341     | GLU      | -      | expression tag | UNP O43837-2 |
| F     | 342     | ILE      | -      | expression tag | UNP O43837-2 |
| F     | 343     | CYS      | -      | expression tag | UNP O43837-2 |
| F     | 344     | ARG      | -      | expression tag | UNP O43837-2 |
| F     | 345     | ARG      | -      | expression tag | UNP O43837-2 |
| F     | 346     | VAL      | -      | expression tag | UNP O43837-2 |

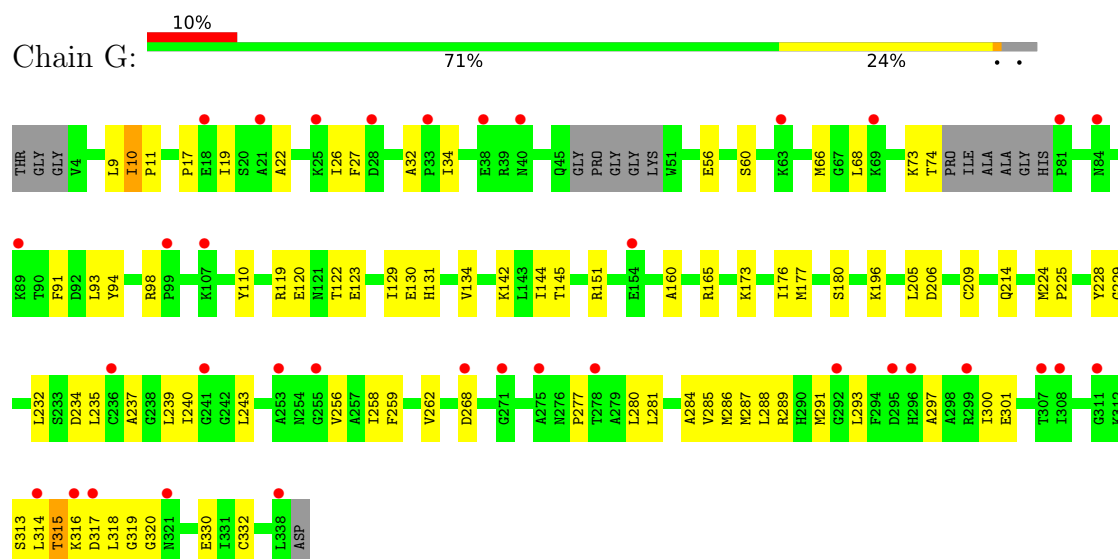
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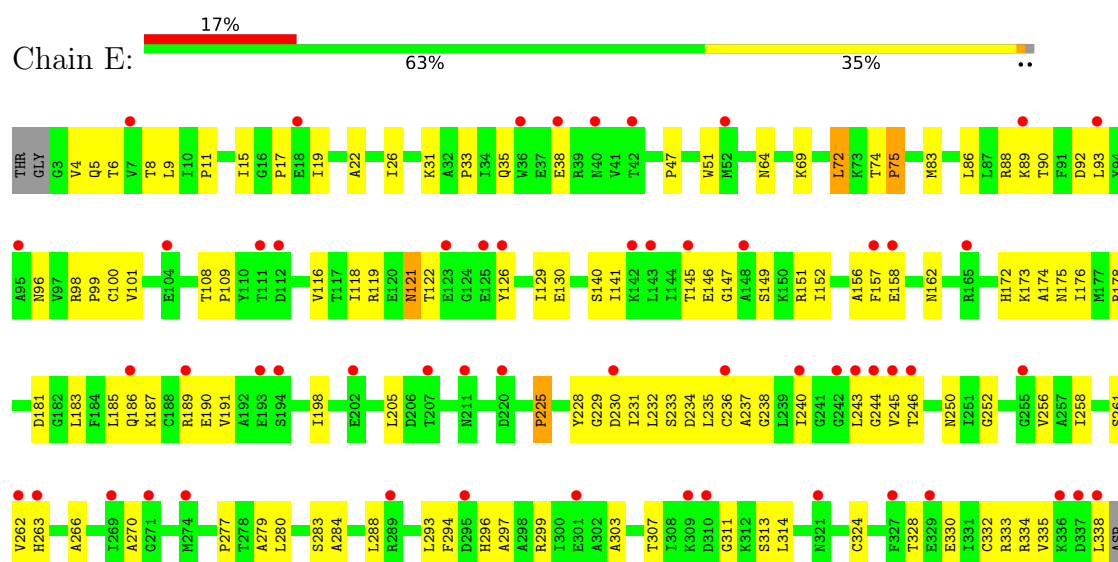
| Chain | Residue | Modelled | Actual | Comment        | Reference    |
|-------|---------|----------|--------|----------------|--------------|
| F     | 347     | LYS      | -      | expression tag | UNP O43837-2 |
| F     | 348     | ASP      | -      | expression tag | UNP O43837-2 |
| F     | 349     | LEU      | -      | expression tag | UNP O43837-2 |
| F     | 350     | ASP      | -      | expression tag | UNP O43837-2 |
| F     | 351     | GLU      | -      | expression tag | UNP O43837-2 |
| F     | 352     | ASN      | -      | expression tag | UNP O43837-2 |
| J     | 341     | GLU      | -      | expression tag | UNP O43837-2 |
| J     | 342     | ILE      | -      | expression tag | UNP O43837-2 |
| J     | 343     | CYS      | -      | expression tag | UNP O43837-2 |
| J     | 344     | ARG      | -      | expression tag | UNP O43837-2 |
| J     | 345     | ARG      | -      | expression tag | UNP O43837-2 |
| J     | 346     | VAL      | -      | expression tag | UNP O43837-2 |
| J     | 347     | LYS      | -      | expression tag | UNP O43837-2 |
| J     | 348     | ASP      | -      | expression tag | UNP O43837-2 |
| J     | 349     | LEU      | -      | expression tag | UNP O43837-2 |
| J     | 350     | ASP      | -      | expression tag | UNP O43837-2 |
| J     | 351     | GLU      | -      | expression tag | UNP O43837-2 |
| J     | 352     | ASN      | -      | expression tag | UNP O43837-2 |
| N     | 341     | GLU      | -      | expression tag | UNP O43837-2 |
| N     | 342     | ILE      | -      | expression tag | UNP O43837-2 |
| N     | 343     | CYS      | -      | expression tag | UNP O43837-2 |
| N     | 344     | ARG      | -      | expression tag | UNP O43837-2 |
| N     | 345     | ARG      | -      | expression tag | UNP O43837-2 |
| N     | 346     | VAL      | -      | expression tag | UNP O43837-2 |
| N     | 347     | LYS      | -      | expression tag | UNP O43837-2 |
| N     | 348     | ASP      | -      | expression tag | UNP O43837-2 |
| N     | 349     | LEU      | -      | expression tag | UNP O43837-2 |
| N     | 350     | ASP      | -      | expression tag | UNP O43837-2 |
| N     | 351     | GLU      | -      | expression tag | UNP O43837-2 |
| N     | 352     | ASN      | -      | expression tag | UNP O43837-2 |



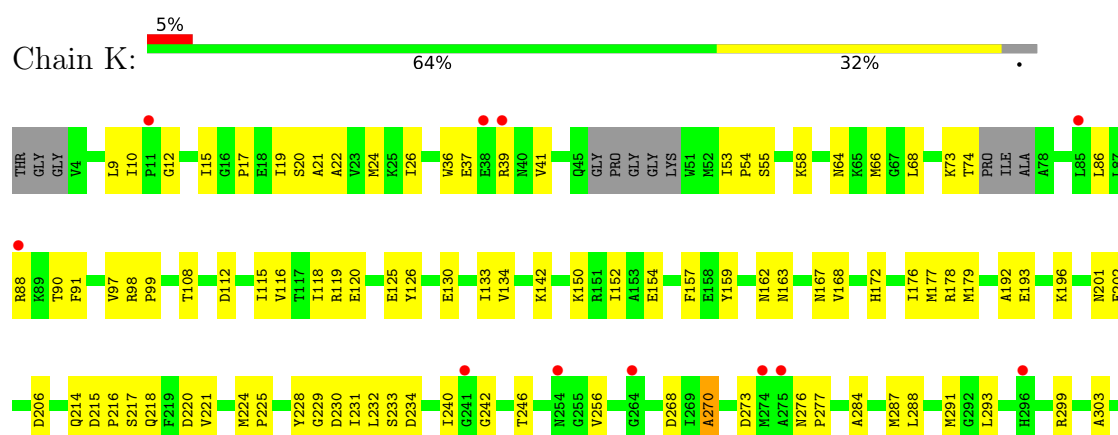
• Molecule 1: Isocitrate dehydrogenase [NAD] subunit alpha, mitochondrial

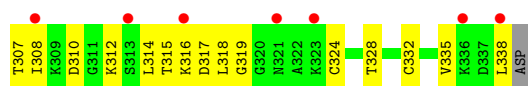


• Molecule 1: Isocitrate dehydrogenase [NAD] subunit alpha, mitochondrial

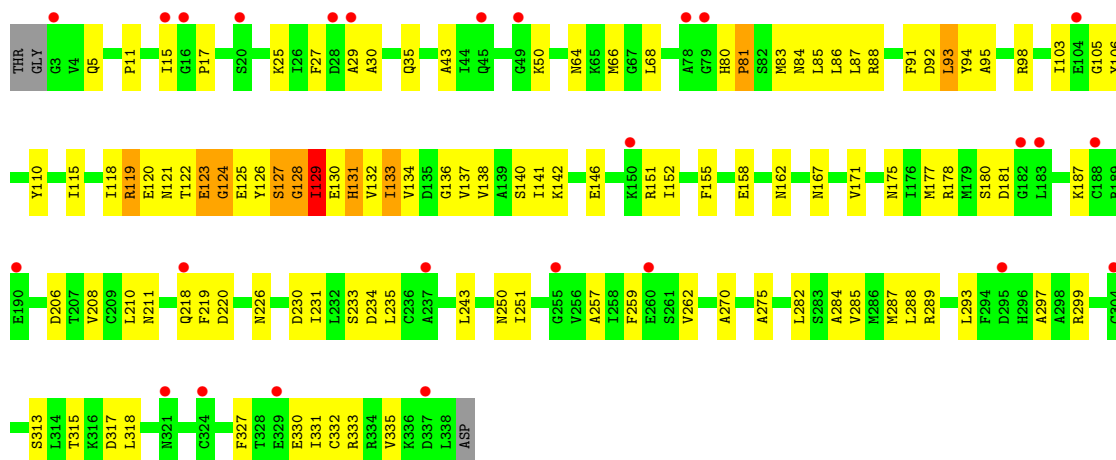


• Molecule 1: Isocitrate dehydrogenase [NAD] subunit alpha, mitochondrial

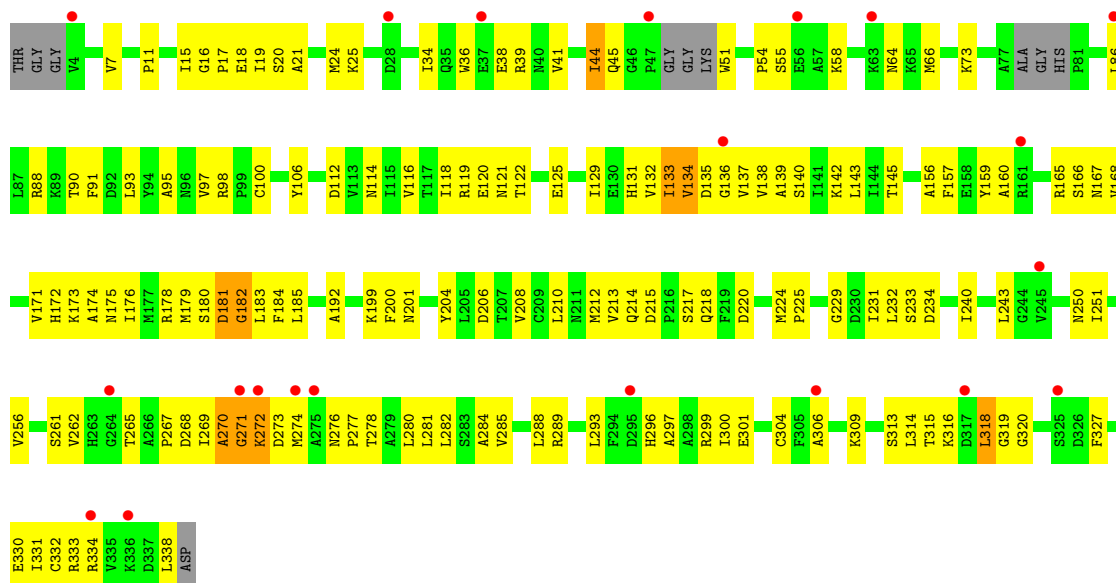




- Molecule 1: Isocitrate dehydrogenase [NAD] subunit alpha, mitochondrial

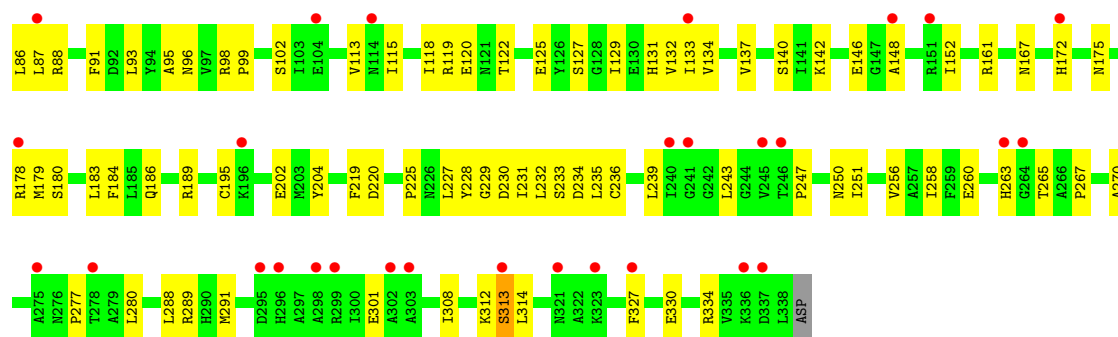


- Molecule 1: Isocitrate dehydrogenase [NAD] subunit alpha, mitochondrial

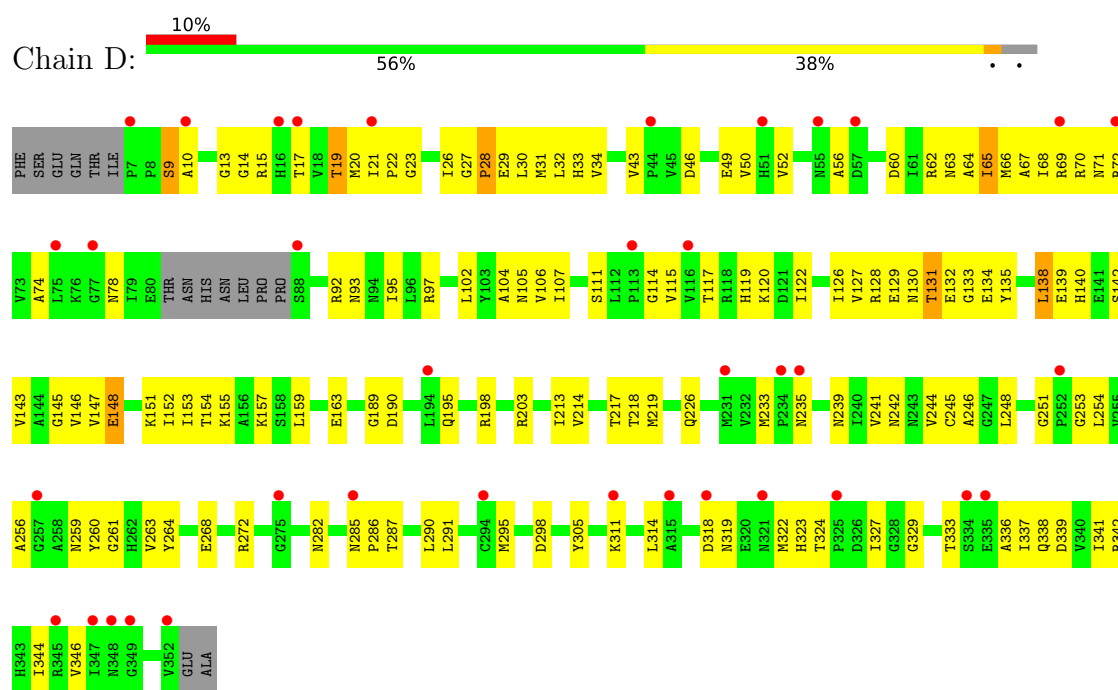


- Molecule 1: Isocitrate dehydrogenase [NAD] subunit alpha, mitochondrial

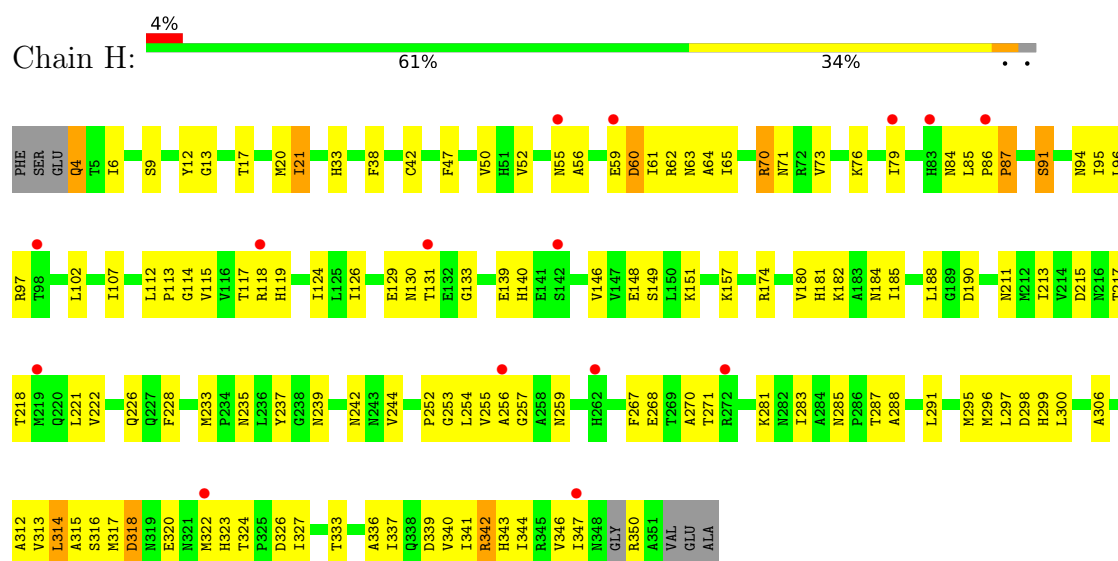




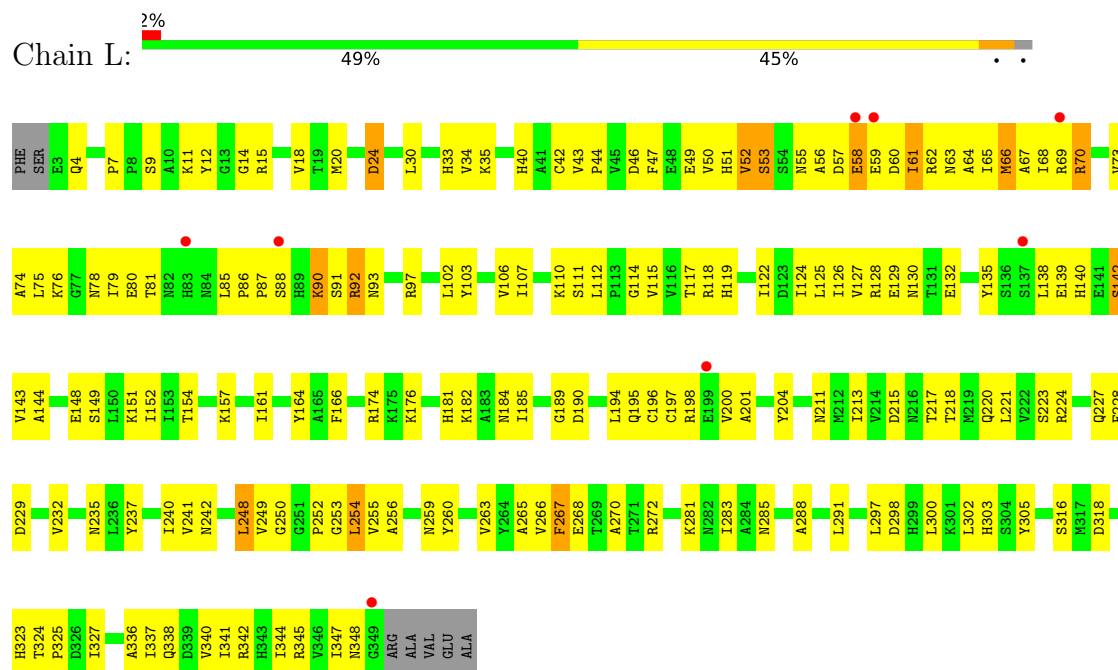
• Molecule 2: Isocitrate dehydrogenase [NAD] subunit gamma, mitochondrial



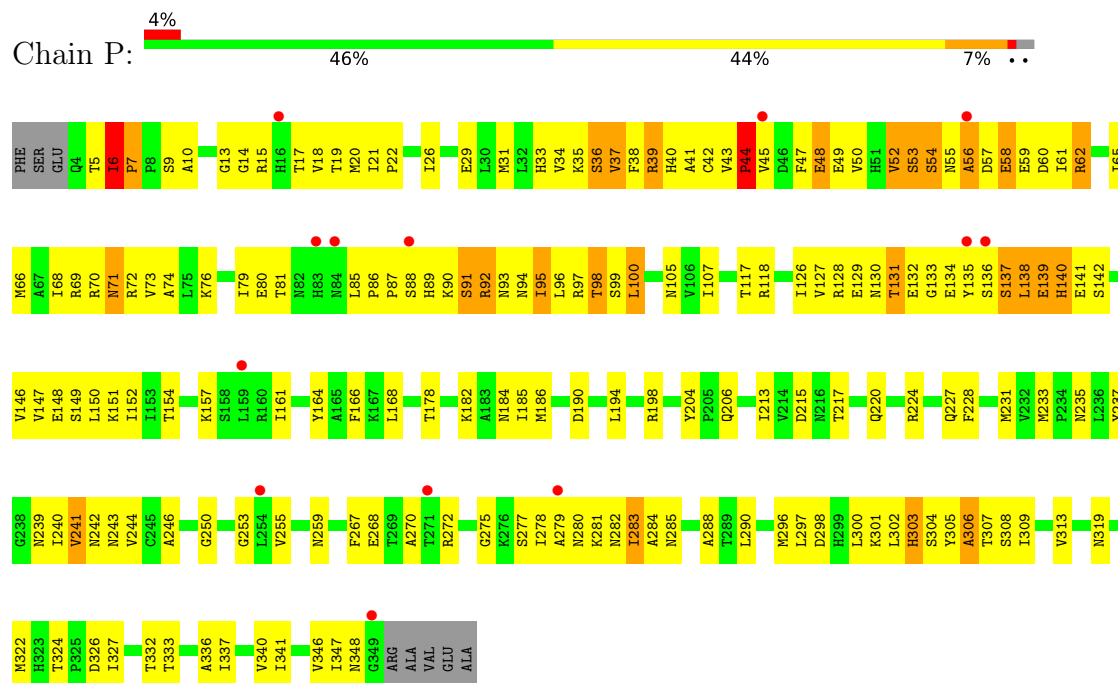
• Molecule 2: Isocitrate dehydrogenase [NAD] subunit gamma, mitochondrial



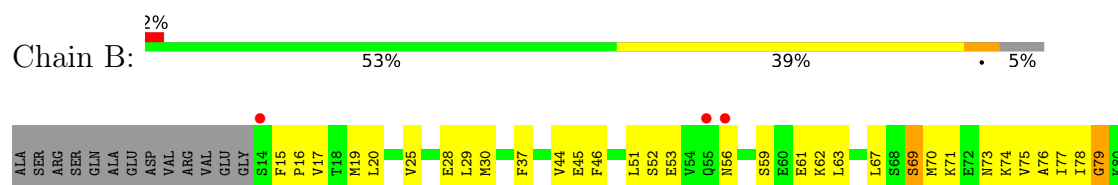
• Molecule 2: Isocitrate dehydrogenase [NAD] subunit gamma, mitochondrial

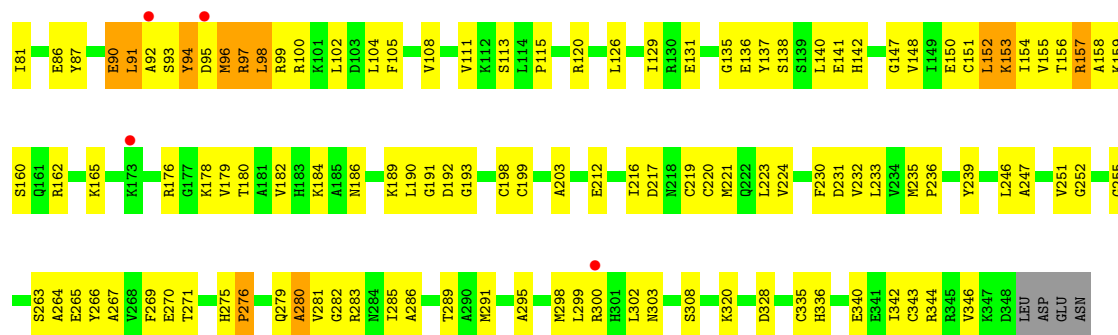


• Molecule 2: Isocitrate dehydrogenase [NAD] subunit gamma, mitochondrial



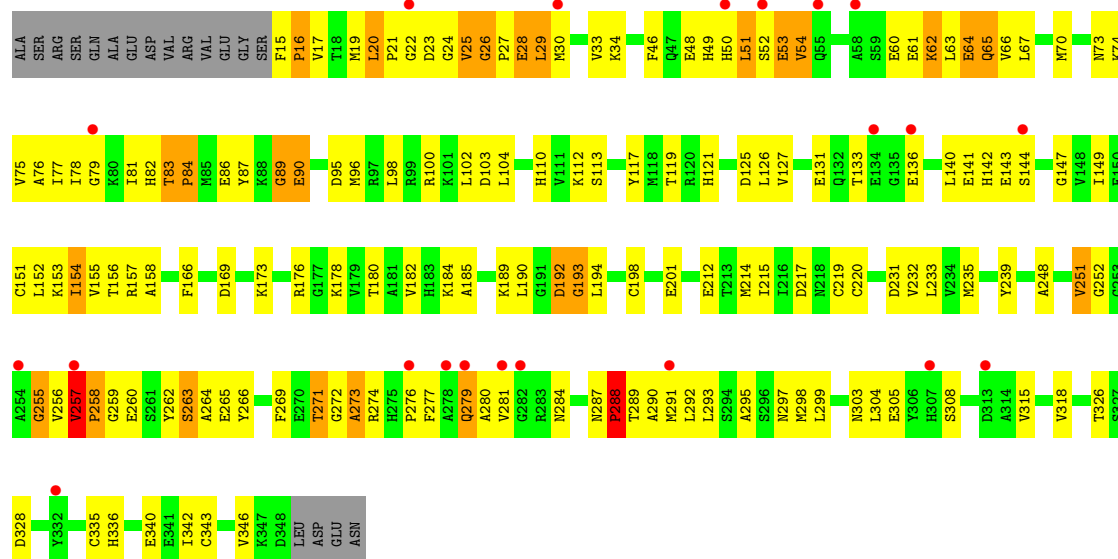
• Molecule 3: Isoform A of Isocitrate dehydrogenase [NAD] subunit beta, mitochondrial







- Molecule 3: Isoform A of Isocitrate dehydrogenase [NAD] subunit beta, mitochondrial



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | C 2 2 21                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 159.26Å 490.33Å 330.46Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 30.54 – 4.49<br>30.54 – 4.49                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 84.4 (30.54-4.49)<br>84.1 (30.54-4.49)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.20                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.26 (at 4.42Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX 1.14_3260                                            | Depositor        |
| R, $R_{free}$                                                           | 0.268 , 0.286<br>0.270 , 0.290                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 3251 reflections (4.18%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 76.0                                                        | Xtriage          |
| Anisotropy                                                              | 0.651                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.23 , 49.8                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.82                                                        | EDS              |
| Total number of atoms                                                   | 39351                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 107.0                                                       | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% 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     | 0.39         | 0/2452          | 0.73        | 5/3339 (0.1%)    |
| 1   | C     | 0.19         | 0/2427          | 0.40        | 1/3295 (0.0%)    |
| 1   | E     | 0.48         | 2/2439 (0.1%)   | 0.71        | 6/3321 (0.2%)    |
| 1   | G     | 0.14         | 0/2482          | 0.46        | 2/3355 (0.1%)    |
| 1   | I     | 0.51         | 3/2482 (0.1%)   | 0.81        | 16/3379 (0.5%)   |
| 1   | K     | 0.18         | 0/2518          | 0.56        | 6/3400 (0.2%)    |
| 1   | M     | 0.44         | 2/2476 (0.1%)   | 0.55        | 1/3366 (0.0%)    |
| 1   | O     | 0.38         | 0/2493          | 0.72        | 10/3372 (0.3%)   |
| 2   | D     | 0.41         | 0/2534          | 0.80        | 15/3438 (0.4%)   |
| 2   | H     | 0.44         | 0/2592          | 0.84        | 12/3516 (0.3%)   |
| 2   | L     | 0.58         | 1/2609 (0.0%)   | 1.09        | 24/3541 (0.7%)   |
| 2   | P     | 0.66         | 1/2578 (0.0%)   | 1.05        | 35/3501 (1.0%)   |
| 3   | B     | 0.60         | 1/2508 (0.0%)   | 1.11        | 26/3402 (0.8%)   |
| 3   | F     | 0.48         | 0/2442          | 1.03        | 18/3322 (0.5%)   |
| 3   | J     | 0.58         | 2/2507 (0.1%)   | 0.99        | 19/3400 (0.6%)   |
| 3   | N     | 0.54         | 1/2447 (0.0%)   | 1.02        | 30/3324 (0.9%)   |
| All | All   | 0.46         | 13/39986 (0.0%) | 0.84        | 226/54271 (0.4%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | E     | 0                   | 1                   |
| 2   | H     | 0                   | 1                   |
| 3   | B     | 0                   | 1                   |
| 3   | F     | 0                   | 1                   |
| All | All   | 0                   | 4                   |

All (13) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 1   | I     | 81  | PRO  | N-CD  | -14.16 | 1.27        | 1.47     |
| 1   | E     | 75  | PRO  | N-CD  | -13.03 | 1.29        | 1.47     |
| 3   | B     | 91  | LEU  | CA-C  | 9.86   | 1.66        | 1.53     |
| 1   | M     | 313 | SER  | N-CA  | -7.47  | 1.36        | 1.46     |
| 1   | M     | 312 | LYS  | CA-C  | 7.18   | 1.62        | 1.52     |
| 2   | P     | 44  | PRO  | N-CD  | 6.17   | 1.56        | 1.47     |
| 1   | E     | 109 | PRO  | N-CD  | 6.13   | 1.56        | 1.47     |
| 3   | J     | 261 | SER  | CA-CB | -5.89  | 1.44        | 1.53     |
| 2   | L     | 252 | PRO  | C-O   | -5.80  | 1.16        | 1.24     |
| 3   | J     | 84  | PRO  | N-CD  | -5.17  | 1.40        | 1.47     |
| 1   | I     | 123 | GLU  | CA-C  | -5.16  | 1.46        | 1.52     |
| 1   | I     | 127 | SER  | CA-C  | -5.09  | 1.46        | 1.52     |
| 3   | N     | 288 | PRO  | N-CD  | -5.07  | 1.40        | 1.47     |

All (226) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 3   | F     | 230 | PHE  | CB-CA-C | -23.82 | 66.59       | 109.70   |
| 2   | L     | 70  | ARG  | N-CA-C  | 23.10  | 136.67      | 111.03   |
| 3   | B     | 252 | GLY  | N-CA-C  | -21.11 | 79.63       | 110.88   |
| 3   | B     | 92  | ALA  | N-CA-C  | -17.86 | 81.97       | 110.20   |
| 1   | A     | 312 | LYS  | N-CA-C  | 16.41  | 135.10      | 111.96   |
| 2   | L     | 58  | GLU  | N-CA-C  | 15.94  | 128.12      | 111.07   |
| 2   | P     | 302 | LEU  | CB-CA-C | -13.77 | 90.10       | 111.17   |
| 1   | I     | 124 | GLY  | N-CA-C  | -12.98 | 93.06       | 110.58   |
| 3   | F     | 230 | PHE  | CA-C-N  | 12.61  | 141.97      | 122.42   |
| 3   | F     | 230 | PHE  | C-N-CA  | 12.61  | 141.97      | 122.42   |
| 3   | J     | 190 | LEU  | N-CA-C  | 11.49  | 123.88      | 111.36   |
| 2   | L     | 70  | ARG  | CB-CA-C | -11.25 | 93.51       | 110.95   |
| 3   | N     | 25  | VAL  | N-CA-C  | 11.25  | 122.09      | 110.62   |
| 3   | J     | 187 | ILE  | N-CA-C  | 11.17  | 122.28      | 111.67   |
| 1   | E     | 176 | ILE  | CB-CA-C | -10.70 | 99.18       | 111.80   |
| 3   | J     | 276 | PRO  | N-CA-C  | -10.50 | 92.99       | 110.21   |
| 2   | P     | 44  | PRO  | CA-N-CD | -10.17 | 97.76       | 112.00   |
| 2   | L     | 81  | THR  | N-CA-C  | -10.16 | 96.18       | 110.50   |
| 1   | K     | 134 | VAL  | CB-CA-C | 10.15  | 126.46      | 110.52   |
| 1   | I     | 127 | SER  | N-CA-C  | -9.88  | 96.56       | 110.50   |
| 1   | A     | 312 | LYS  | CB-CA-C | -9.70  | 93.71       | 110.88   |
| 3   | N     | 53  | GLU  | N-CA-CB | -9.61  | 94.25       | 110.49   |
| 2   | L     | 7   | PRO  | N-CA-C  | -9.54  | 99.06       | 110.70   |
| 1   | K     | 176 | ILE  | CB-CA-C | -9.47  | 102.44      | 111.44   |
| 3   | B     | 90  | GLU  | N-CA-C  | -9.46  | 102.31      | 114.04   |
| 3   | F     | 230 | PHE  | N-CA-C  | 9.13   | 124.19      | 108.76   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | E     | 176 | ILE  | N-CA-C   | 8.63  | 119.86      | 111.67   |
| 1   | O     | 318 | LEU  | N-CA-C   | 8.62  | 120.68      | 111.28   |
| 3   | J     | 188 | MET  | N-CA-C   | -8.45 | 92.10       | 107.98   |
| 3   | N     | 271 | THR  | N-CA-C   | -8.37 | 94.94       | 108.41   |
| 3   | F     | 97  | ARG  | CA-C-N   | -8.36 | 108.93      | 120.38   |
| 3   | F     | 97  | ARG  | C-N-CA   | -8.36 | 108.93      | 120.38   |
| 3   | N     | 251 | VAL  | N-CA-C   | 8.19  | 118.23      | 110.53   |
| 3   | F     | 286 | ALA  | CA-C-N   | 8.17  | 134.40      | 121.17   |
| 3   | F     | 286 | ALA  | C-N-CA   | 8.17  | 134.40      | 121.17   |
| 3   | B     | 53  | GLU  | CB-CA-C  | -7.92 | 97.54       | 109.90   |
| 1   | G     | 315 | THR  | CB-CA-C  | -7.87 | 95.85       | 111.60   |
| 3   | N     | 26  | GLY  | O-C-N    | 7.84  | 123.89      | 121.07   |
| 3   | N     | 255 | GLY  | N-CA-C   | 7.82  | 122.11      | 112.73   |
| 3   | N     | 65  | GLN  | N-CA-C   | -7.81 | 102.77      | 111.28   |
| 2   | P     | 277 | SER  | N-CA-C   | -7.74 | 102.84      | 111.28   |
| 3   | N     | 28  | GLU  | N-CA-C   | -7.70 | 102.97      | 111.36   |
| 3   | F     | 276 | PRO  | N-CA-C   | -7.65 | 96.72       | 112.47   |
| 3   | N     | 288 | PRO  | CB-CA-C  | -7.64 | 98.95       | 111.56   |
| 1   | O     | 270 | ALA  | N-CA-C   | -7.55 | 103.05      | 111.28   |
| 1   | I     | 131 | HIS  | CA-CB-CG | -7.51 | 106.29      | 113.80   |
| 2   | P     | 44  | PRO  | N-CD-CG  | -7.43 | 92.06       | 103.20   |
| 2   | D     | 19  | THR  | CB-CA-C  | -7.40 | 98.35       | 109.90   |
| 3   | B     | 276 | PRO  | N-CA-C   | -7.39 | 99.63       | 110.80   |
| 3   | N     | 89  | GLY  | N-CA-C   | -7.39 | 103.86      | 112.73   |
| 3   | B     | 62  | LYS  | N-CA-C   | -7.38 | 103.36      | 112.88   |
| 3   | F     | 84  | PRO  | N-CA-C   | 7.37  | 125.26      | 114.80   |
| 1   | O     | 178 | ARG  | N-CA-C   | 7.34  | 119.28      | 111.28   |
| 2   | P     | 131 | THR  | N-CA-C   | -7.31 | 103.32      | 112.90   |
| 3   | N     | 154 | ILE  | CB-CA-C  | -7.31 | 99.44       | 110.55   |
| 1   | A     | 176 | ILE  | N-CA-C   | 7.19  | 124.29      | 109.34   |
| 2   | P     | 91  | SER  | N-CA-C   | -7.18 | 99.19       | 109.96   |
| 3   | N     | 279 | GLN  | N-CA-C   | -7.17 | 103.40      | 111.14   |
| 3   | F     | 84  | PRO  | N-CA-CB  | -7.15 | 93.89       | 102.33   |
| 3   | B     | 96  | MET  | N-CA-C   | -7.13 | 103.50      | 111.28   |
| 2   | L     | 66  | MET  | CA-C-N   | -7.09 | 110.78      | 120.28   |
| 2   | L     | 66  | MET  | C-N-CA   | -7.09 | 110.78      | 120.28   |
| 3   | N     | 29  | LEU  | N-CA-C   | 6.97  | 118.53      | 111.07   |
| 2   | H     | 91  | SER  | N-CA-C   | -6.95 | 98.62       | 109.25   |
| 2   | H     | 314 | LEU  | N-CA-C   | -6.94 | 103.80      | 111.36   |
| 3   | B     | 157 | ARG  | CB-CA-C  | -6.93 | 96.04       | 110.17   |
| 2   | P     | 283 | ILE  | N-CA-C   | -6.85 | 103.63      | 110.62   |
| 1   | O     | 45  | GLN  | N-CA-C   | 6.84  | 120.97      | 111.74   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | K     | 176 | ILE  | N-CA-C  | 6.75  | 117.36      | 111.56   |
| 1   | A     | 176 | ILE  | CB-CA-C | -6.68 | 100.33      | 111.29   |
| 2   | H     | 85  | LEU  | N-CA-C  | -6.66 | 103.70      | 113.16   |
| 3   | J     | 274 | ARG  | CB-CA-C | -6.66 | 100.38      | 110.90   |
| 2   | P     | 303 | HIS  | N-CA-CB | -6.63 | 99.28       | 110.49   |
| 3   | B     | 94  | TYR  | N-CA-C  | 6.62  | 118.57      | 111.36   |
| 2   | L     | 252 | PRO  | CB-CA-C | -6.62 | 101.70      | 112.62   |
| 1   | K     | 88  | ARG  | N-CA-C  | 6.61  | 119.08      | 111.02   |
| 2   | L     | 90  | LYS  | N-CA-C  | -6.61 | 103.31      | 112.30   |
| 2   | H     | 318 | ASP  | CB-CA-C | 6.60  | 122.84      | 110.63   |
| 2   | H     | 21  | ILE  | CB-CA-C | -6.57 | 103.23      | 110.52   |
| 2   | D     | 65  | ILE  | CA-C-N  | -6.56 | 110.83      | 120.28   |
| 2   | D     | 65  | ILE  | C-N-CA  | -6.56 | 110.83      | 120.28   |
| 3   | J     | 53  | GLU  | N-CA-C  | 6.56  | 120.19      | 109.24   |
| 1   | O     | 181 | ASP  | CA-C-N  | -6.53 | 108.61      | 121.41   |
| 1   | O     | 181 | ASP  | C-N-CA  | -6.53 | 108.61      | 121.41   |
| 2   | P     | 36  | SER  | N-CA-C  | -6.53 | 104.16      | 111.28   |
| 2   | P     | 307 | THR  | N-CA-C  | -6.47 | 104.65      | 112.54   |
| 2   | L     | 61  | ILE  | CB-CA-C | -6.41 | 99.55       | 111.79   |
| 2   | P     | 37  | VAL  | N-CA-C  | -6.40 | 104.28      | 110.42   |
| 3   | N     | 257 | VAL  | CA-C-N  | -6.38 | 113.38      | 119.76   |
| 3   | N     | 257 | VAL  | C-N-CA  | -6.38 | 113.38      | 119.76   |
| 3   | N     | 53  | GLU  | N-CA-C  | 6.37  | 124.37      | 110.80   |
| 2   | P     | 98  | THR  | N-CA-C  | 6.36  | 117.88      | 111.07   |
| 3   | J     | 283 | ARG  | CA-C-N  | -6.34 | 111.28      | 122.07   |
| 3   | J     | 283 | ARG  | C-N-CA  | -6.34 | 111.28      | 122.07   |
| 1   | I     | 128 | GLY  | N-CA-C  | -6.34 | 105.15      | 112.50   |
| 3   | B     | 97  | ARG  | N-CA-C  | -6.29 | 104.34      | 111.07   |
| 2   | L     | 66  | MET  | N-CA-C  | -6.29 | 104.43      | 111.28   |
| 2   | H     | 70  | ARG  | N-CA-C  | 6.26  | 124.12      | 110.80   |
| 3   | J     | 77  | ILE  | CA-C-N  | -6.25 | 113.33      | 122.58   |
| 3   | J     | 77  | ILE  | C-N-CA  | -6.25 | 113.33      | 122.58   |
| 3   | N     | 64  | GLU  | N-CA-C  | -6.23 | 104.49      | 111.28   |
| 2   | D     | 28  | PRO  | CA-C-N  | -6.20 | 111.97      | 120.28   |
| 2   | D     | 28  | PRO  | C-N-CA  | -6.20 | 111.97      | 120.28   |
| 3   | J     | 61  | GLU  | CA-C-N  | -6.17 | 111.92      | 120.38   |
| 3   | J     | 61  | GLU  | C-N-CA  | -6.17 | 111.92      | 120.38   |
| 2   | L     | 92  | ARG  | N-CA-C  | -6.16 | 105.48      | 112.87   |
| 1   | K     | 134 | VAL  | N-CA-C  | -6.14 | 99.75       | 108.65   |
| 2   | D     | 70  | ARG  | N-CA-C  | 6.13  | 123.86      | 110.80   |
| 1   | K     | 270 | ALA  | N-CA-C  | 6.11  | 123.81      | 110.80   |
| 3   | B     | 63  | LEU  | N-CA-C  | -6.10 | 104.63      | 111.28   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | D     | 131 | THR  | N-CA-C  | -6.06 | 106.53      | 114.04   |
| 3   | J     | 262 | TYR  | CB-CA-C | -6.05 | 99.26       | 109.72   |
| 2   | H     | 342 | ARG  | N-CA-C  | -6.04 | 104.61      | 111.14   |
| 2   | P     | 39  | ARG  | N-CA-C  | -6.03 | 104.71      | 111.28   |
| 2   | H     | 70  | ARG  | CB-CA-C | -6.03 | 98.43       | 110.42   |
| 1   | O     | 133 | ILE  | N-CA-C  | 6.03  | 120.00      | 113.43   |
| 1   | C     | 124 | GLY  | N-CA-C  | -6.00 | 103.76      | 112.17   |
| 3   | B     | 56  | ASN  | N-CA-C  | -6.00 | 104.82      | 111.36   |
| 2   | P     | 44  | PRO  | N-CA-C  | 6.00  | 124.82      | 112.47   |
| 2   | D     | 133 | GLY  | N-CA-C  | -5.99 | 105.54      | 112.73   |
| 3   | N     | 263 | SER  | N-CA-C  | -5.99 | 98.05       | 110.80   |
| 3   | N     | 50  | HIS  | N-CA-C  | -5.96 | 104.78      | 111.28   |
| 2   | P     | 59  | GLU  | N-CA-C  | -5.95 | 104.79      | 111.28   |
| 2   | H     | 60  | ASP  | CA-C-N  | -5.95 | 111.27      | 121.97   |
| 2   | H     | 60  | ASP  | C-N-CA  | -5.95 | 111.27      | 121.97   |
| 1   | I     | 94  | TYR  | N-CA-C  | -5.94 | 106.67      | 114.04   |
| 3   | B     | 91  | LEU  | CB-CA-C | -5.92 | 102.76      | 112.06   |
| 2   | P     | 283 | ILE  | CB-CA-C | -5.92 | 104.14      | 112.14   |
| 2   | P     | 52  | VAL  | CB-CA-C | -5.89 | 102.46      | 110.42   |
| 2   | H     | 86  | PRO  | N-CA-C  | -5.88 | 103.53      | 110.70   |
| 3   | B     | 152 | LEU  | N-CA-C  | 5.88  | 118.79      | 110.50   |
| 2   | L     | 88  | SER  | N-CA-C  | -5.86 | 99.64       | 109.07   |
| 3   | F     | 65  | GLN  | N-CA-C  | -5.85 | 104.98      | 111.36   |
| 1   | G     | 10  | ILE  | CB-CA-C | -5.85 | 100.72      | 111.36   |
| 2   | L     | 90  | LYS  | CA-C-N  | -5.85 | 111.85      | 121.97   |
| 2   | L     | 90  | LYS  | C-N-CA  | -5.85 | 111.85      | 121.97   |
| 3   | N     | 193 | GLY  | CA-C-N  | -5.81 | 112.69      | 120.54   |
| 3   | N     | 193 | GLY  | C-N-CA  | -5.81 | 112.69      | 120.54   |
| 3   | B     | 51  | LEU  | CA-C-N  | -5.80 | 112.65      | 120.82   |
| 3   | B     | 51  | LEU  | C-N-CA  | -5.80 | 112.65      | 120.82   |
| 3   | N     | 87  | TYR  | N-CA-C  | 5.79  | 117.68      | 111.36   |
| 3   | N     | 20  | LEU  | CA-C-N  | 5.79  | 125.48      | 119.05   |
| 3   | N     | 20  | LEU  | C-N-CA  | 5.79  | 125.48      | 119.05   |
| 3   | J     | 283 | ARG  | CB-CA-C | 5.78  | 119.26      | 109.84   |
| 2   | P     | 48  | GLU  | N-CA-C  | -5.73 | 101.81      | 110.24   |
| 1   | O     | 135 | ASP  | N-CA-C  | -5.73 | 101.17      | 109.59   |
| 3   | J     | 60  | GLU  | N-CA-C  | -5.69 | 104.98      | 111.07   |
| 1   | I     | 129 | ILE  | CA-C-N  | -5.68 | 113.27      | 122.81   |
| 1   | I     | 129 | ILE  | C-N-CA  | -5.68 | 113.27      | 122.81   |
| 2   | P     | 54  | SER  | N-CA-C  | -5.67 | 104.47      | 111.33   |
| 2   | D     | 145 | GLY  | CA-C-N  | -5.67 | 115.11      | 122.99   |
| 2   | D     | 145 | GLY  | C-N-CA  | -5.67 | 115.11      | 122.99   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2   | P     | 100 | LEU  | N-CA-C   | 5.63  | 120.15      | 113.28   |
| 2   | P     | 7   | PRO  | CA-C-N   | -5.62 | 114.96      | 120.52   |
| 2   | P     | 7   | PRO  | C-N-CA   | -5.62 | 114.96      | 120.52   |
| 3   | N     | 192 | ASP  | N-CA-C   | -5.61 | 105.08      | 111.14   |
| 1   | E     | 108 | THR  | CB-CA-C  | 5.61  | 117.19      | 108.61   |
| 2   | H     | 55  | ASN  | N-CA-C   | -5.60 | 105.23      | 112.68   |
| 2   | D     | 9   | SER  | N-CA-C   | -5.60 | 101.76      | 110.10   |
| 3   | J     | 105 | PHE  | N-CA-C   | -5.59 | 106.45      | 113.72   |
| 3   | J     | 186 | ASN  | N-CA-C   | 5.56  | 117.34      | 111.28   |
| 2   | P     | 56  | ALA  | N-CA-C   | 5.53  | 119.06      | 111.54   |
| 2   | L     | 61  | ILE  | CA-C-N   | -5.53 | 110.98      | 121.54   |
| 2   | L     | 61  | ILE  | C-N-CA   | -5.53 | 110.98      | 121.54   |
| 2   | L     | 263 | VAL  | N-CA-CB  | -5.53 | 104.72      | 112.35   |
| 3   | F     | 66  | VAL  | N-CA-C   | 5.51  | 115.71      | 110.53   |
| 1   | O     | 134 | VAL  | N-CA-C   | -5.51 | 97.89       | 109.34   |
| 3   | N     | 273 | ALA  | N-CA-C   | -5.49 | 103.28      | 110.53   |
| 1   | I     | 136 | GLY  | CA-C-N   | -5.49 | 115.19      | 122.98   |
| 1   | I     | 136 | GLY  | C-N-CA   | -5.49 | 115.19      | 122.98   |
| 2   | D     | 148 | GLU  | CB-CG-CD | 5.47  | 121.91      | 112.60   |
| 3   | B     | 98  | LEU  | N-CA-C   | -5.47 | 105.39      | 111.36   |
| 3   | B     | 91  | LEU  | CA-C-O   | 5.44  | 128.58      | 122.27   |
| 1   | E     | 121 | ASN  | CA-C-N   | -5.44 | 115.05      | 121.90   |
| 1   | E     | 121 | ASN  | C-N-CA   | -5.44 | 115.05      | 121.90   |
| 2   | D     | 70  | ARG  | CB-CA-C  | -5.41 | 99.65       | 110.42   |
| 1   | I     | 93  | LEU  | N-CA-C   | -5.41 | 102.19      | 110.30   |
| 3   | F     | 81  | ILE  | O-C-N    | 5.39  | 127.19      | 121.91   |
| 3   | J     | 275 | HIS  | CB-CA-C  | -5.39 | 102.64      | 110.03   |
| 2   | P     | 283 | ILE  | CA-C-N   | -5.39 | 113.28      | 121.31   |
| 2   | P     | 283 | ILE  | C-N-CA   | -5.39 | 113.28      | 121.31   |
| 2   | P     | 55  | ASN  | N-CA-C   | -5.38 | 105.32      | 111.07   |
| 3   | B     | 283 | ARG  | N-CA-C   | -5.36 | 106.32      | 112.92   |
| 3   | B     | 153 | LYS  | N-CA-C   | -5.34 | 100.19      | 108.90   |
| 1   | E     | 225 | PRO  | CB-CA-C  | -5.34 | 102.75      | 111.56   |
| 3   | F     | 64  | GLU  | N-CA-C   | -5.33 | 105.37      | 111.07   |
| 1   | I     | 119 | ARG  | CA-C-N   | -5.31 | 115.13      | 122.30   |
| 1   | I     | 119 | ARG  | C-N-CA   | -5.31 | 115.13      | 122.30   |
| 3   | B     | 69  | SER  | N-CA-C   | -5.30 | 106.08      | 112.54   |
| 2   | P     | 92  | ARG  | N-CA-C   | -5.29 | 105.40      | 111.07   |
| 2   | P     | 95  | ILE  | N-CA-C   | -5.29 | 105.22      | 110.62   |
| 2   | L     | 254 | LEU  | CA-C-N   | -5.29 | 116.22      | 123.14   |
| 2   | L     | 254 | LEU  | C-N-CA   | -5.29 | 116.22      | 123.14   |
| 2   | P     | 6   | ILE  | CA-C-N   | -5.29 | 114.94      | 120.38   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2   | P     | 6   | ILE  | C-N-CA   | -5.29 | 114.94      | 120.38   |
| 2   | P     | 306 | ALA  | CB-CA-C  | -5.27 | 99.30       | 110.31   |
| 3   | F     | 48  | GLU  | CA-C-N   | -5.25 | 115.40      | 122.86   |
| 3   | F     | 48  | GLU  | C-N-CA   | -5.25 | 115.40      | 122.86   |
| 3   | N     | 258 | PRO  | N-CA-C   | -5.25 | 102.94      | 111.19   |
| 1   | I     | 133 | ILE  | N-CA-C   | -5.25 | 105.60      | 110.53   |
| 3   | J     | 89  | GLY  | CA-C-O   | -5.24 | 116.42      | 121.19   |
| 2   | D     | 139 | GLU  | CA-C-N   | -5.23 | 114.26      | 122.73   |
| 2   | D     | 139 | GLU  | C-N-CA   | -5.23 | 114.26      | 122.73   |
| 2   | L     | 142 | SER  | N-CA-C   | -5.22 | 105.59      | 111.28   |
| 3   | B     | 79  | GLY  | CA-C-N   | -5.21 | 113.57      | 122.33   |
| 3   | B     | 79  | GLY  | C-N-CA   | -5.21 | 113.57      | 122.33   |
| 1   | I     | 140 | SER  | CA-C-N   | -5.21 | 116.11      | 122.93   |
| 1   | I     | 140 | SER  | C-N-CA   | -5.21 | 116.11      | 122.93   |
| 3   | N     | 274 | ARG  | N-CA-C   | 5.21  | 121.90      | 110.80   |
| 2   | P     | 71  | ASN  | CA-C-N   | -5.19 | 113.63      | 122.56   |
| 2   | P     | 71  | ASN  | C-N-CA   | -5.19 | 113.63      | 122.56   |
| 3   | F     | 53  | GLU  | N-CA-C   | 5.18  | 116.84      | 108.08   |
| 1   | O     | 271 | GLY  | N-CA-C   | -5.17 | 104.52      | 112.85   |
| 2   | P     | 241 | VAL  | CB-CA-C  | -5.16 | 105.17      | 112.14   |
| 1   | A     | 94  | TYR  | N-CA-C   | -5.15 | 107.06      | 113.55   |
| 2   | L     | 267 | PHE  | CA-C-O   | -5.13 | 115.16      | 120.70   |
| 3   | B     | 158 | ALA  | N-CA-C   | -5.11 | 103.11      | 111.04   |
| 3   | B     | 52  | SER  | N-CA-C   | -5.09 | 102.51      | 110.10   |
| 1   | I     | 121 | ASN  | CA-CB-CG | 5.09  | 117.69      | 112.60   |
| 3   | B     | 280 | ALA  | N-CA-C   | -5.09 | 105.82      | 111.36   |
| 3   | N     | 62  | LYS  | N-CA-C   | -5.07 | 105.75      | 111.28   |
| 2   | L     | 248 | LEU  | CA-C-N   | -5.07 | 114.22      | 121.52   |
| 2   | L     | 248 | LEU  | C-N-CA   | -5.07 | 114.22      | 121.52   |
| 1   | M     | 52  | MET  | N-CA-C   | 5.05  | 116.67      | 109.14   |
| 2   | P     | 58  | GLU  | N-CA-C   | -5.04 | 105.79      | 111.28   |
| 3   | N     | 346 | VAL  | N-CA-C   | -5.02 | 107.94      | 112.96   |

There are no chirality outliers.

All (4) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 3   | B     | 59  | SER  | Mainchain |
| 1   | E     | 72  | LEU  | Mainchain |
| 3   | F     | 230 | PHE  | Peptide   |
| 2   | H     | 4   | GLN  | Peptide   |

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 2412  | 0        | 2284     | 116     | 0            |
| 1   | C     | 2389  | 0        | 2310     | 80      | 0            |
| 1   | E     | 2400  | 0        | 2277     | 125     | 0            |
| 1   | G     | 2444  | 0        | 2435     | 66      | 0            |
| 1   | I     | 2439  | 0        | 2329     | 138     | 0            |
| 1   | K     | 2480  | 0        | 2498     | 101     | 0            |
| 1   | M     | 2436  | 0        | 2329     | 128     | 0            |
| 1   | O     | 2454  | 0        | 2436     | 205     | 0            |
| 2   | D     | 2496  | 0        | 2451     | 170     | 0            |
| 2   | H     | 2555  | 0        | 2508     | 183     | 0            |
| 2   | L     | 2569  | 0        | 2526     | 240     | 0            |
| 2   | P     | 2539  | 0        | 2498     | 339     | 0            |
| 3   | B     | 2466  | 0        | 2365     | 188     | 1            |
| 3   | F     | 2400  | 0        | 2236     | 183     | 0            |
| 3   | J     | 2465  | 0        | 2376     | 202     | 1            |
| 3   | N     | 2407  | 0        | 2245     | 247     | 0            |
| All | All   | 39351 | 0        | 38103    | 2438    | 1            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 31.

All (2438) 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) |
|------------------|-----------------|--------------------------|-------------------|
| 3:N:29:LEU:CD1   | 3:N:288:PRO:HB3 | 1.24                     | 1.65              |
| 3:J:20:LEU:CB    | 3:J:78:ILE:HG21 | 1.20                     | 1.61              |
| 3:J:20:LEU:HB2   | 3:J:78:ILE:CG2  | 1.26                     | 1.61              |
| 2:P:138:LEU:HD23 | 1:M:131:HIS:CD2 | 1.15                     | 1.61              |
| 2:D:50:VAL:CG2   | 2:D:64:ALA:HB1  | 1.20                     | 1.60              |
| 3:N:30:MET:CE    | 3:N:291:MET:HB3 | 1.31                     | 1.55              |
| 3:F:254:ALA:HB1  | 3:F:273:ALA:CB  | 1.32                     | 1.52              |
| 2:P:138:LEU:CD2  | 1:M:131:HIS:CD2 | 1.92                     | 1.52              |
| 2:D:50:VAL:CG2   | 2:D:64:ALA:CB   | 1.85                     | 1.51              |
| 2:P:66:MET:CA    | 2:P:69:ARG:HG3  | 1.04                     | 1.50              |
| 3:N:29:LEU:HD11  | 3:N:288:PRO:CB  | 1.37                     | 1.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:P:66:MET:HA    | 2:P:69:ARG:CG    | 1.05                     | 1.49              |
| 3:N:30:MET:HE3   | 3:N:291:MET:SD   | 1.58                     | 1.44              |
| 2:L:253:GLY:O    | 2:L:288:ALA:CB   | 1.67                     | 1.43              |
| 1:O:175:ASN:ND2  | 1:O:204:TYR:CE1  | 1.82                     | 1.42              |
| 3:N:30:MET:CE    | 3:N:291:MET:CB   | 1.96                     | 1.42              |
| 1:O:173:LYS:NZ   | 2:P:239:ASN:CG   | 1.76                     | 1.40              |
| 2:P:233:MET:SD   | 2:P:241:VAL:HG21 | 1.63                     | 1.37              |
| 3:N:30:MET:HE3   | 3:N:291:MET:CE   | 1.55                     | 1.37              |
| 2:H:255:VAL:CB   | 2:H:270:ALA:CB   | 2.04                     | 1.36              |
| 3:N:30:MET:CE    | 3:N:291:MET:SD   | 2.14                     | 1.36              |
| 3:F:254:ALA:CB   | 3:F:273:ALA:HB3  | 1.56                     | 1.35              |
| 2:L:111:SER:HA   | 2:L:249:VAL:CG1  | 1.54                     | 1.35              |
| 2:D:17:THR:HG22  | 2:D:71:ASN:ND2   | 1.35                     | 1.35              |
| 2:P:21:ILE:HG23  | 2:P:52:VAL:CG1   | 1.54                     | 1.35              |
| 3:J:20:LEU:H     | 3:J:78:ILE:CG2   | 1.38                     | 1.35              |
| 3:J:20:LEU:CA    | 3:J:78:ILE:HG22  | 1.54                     | 1.35              |
| 2:P:138:LEU:HD23 | 1:M:131:HIS:NE2  | 1.34                     | 1.35              |
| 2:H:342:ARG:HE   | 3:N:305:GLU:CB   | 1.39                     | 1.34              |
| 2:P:21:ILE:CG2   | 2:P:52:VAL:CG1   | 2.05                     | 1.34              |
| 1:K:179:MET:HE3  | 2:L:139:GLU:CB   | 1.55                     | 1.33              |
| 3:N:30:MET:HE2   | 3:N:291:MET:CB   | 1.55                     | 1.32              |
| 2:H:342:ARG:NE   | 3:N:305:GLU:CB   | 1.90                     | 1.31              |
| 1:K:179:MET:CE   | 2:L:139:GLU:CB   | 2.08                     | 1.31              |
| 3:B:153:LYS:NZ   | 3:B:192:ASP:OD1  | 1.61                     | 1.31              |
| 2:H:259:ASN:ND2  | 2:H:268:GLU:OE1  | 1.64                     | 1.31              |
| 1:K:142:LYS:CD   | 2:L:135:TYR:CE2  | 2.13                     | 1.30              |
| 3:J:20:LEU:N     | 3:J:78:ILE:CG2   | 1.92                     | 1.30              |
| 2:P:129:GLU:CG   | 2:P:132:GLU:CB   | 2.08                     | 1.29              |
| 3:N:30:MET:CE    | 3:N:291:MET:CG   | 2.12                     | 1.28              |
| 3:B:81:ILE:HD11  | 3:B:95:ASP:CB    | 1.64                     | 1.27              |
| 3:F:92:ALA:HA    | 3:F:139:SER:CB   | 1.61                     | 1.26              |
| 3:B:28:GLU:OE2   | 3:B:282:GLY:HA2  | 1.34                     | 1.25              |
| 2:H:267:PHE:CZ   | 2:H:296:MET:HA   | 1.71                     | 1.25              |
| 2:H:252:PRO:HB3  | 2:H:271:THR:CB   | 1.66                     | 1.24              |
| 3:B:91:LEU:HD12  | 3:B:91:LEU:O     | 1.12                     | 1.23              |
| 3:J:20:LEU:CA    | 3:J:78:ILE:CG2   | 2.12                     | 1.23              |
| 2:P:129:GLU:CD   | 2:P:132:GLU:CB   | 2.06                     | 1.22              |
| 2:L:253:GLY:C    | 2:L:288:ALA:HB2  | 1.65                     | 1.22              |
| 1:O:175:ASN:ND2  | 1:O:204:TYR:CD1  | 2.08                     | 1.22              |
| 2:L:97:ARG:CD    | 2:L:130:ASN:OD1  | 1.86                     | 1.21              |
| 2:L:140:HIS:NE2  | 3:J:150:GLU:OE2  | 1.73                     | 1.21              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:B:93:SER:CB    | 3:B:96:MET:SD    | 2.29                     | 1.21              |
| 1:K:133:ILE:HG13 | 1:I:133:ILE:CD1  | 1.69                     | 1.21              |
| 2:D:148:GLU:OE2  | 3:B:150:GLU:OE1  | 1.58                     | 1.21              |
| 2:D:129:GLU:CD   | 2:D:132:GLU:H    | 1.48                     | 1.20              |
| 1:O:18:GLU:OE2   | 1:O:273:ASP:HA   | 1.39                     | 1.20              |
| 1:K:142:LYS:HD2  | 2:L:135:TYR:CZ   | 1.75                     | 1.20              |
| 1:K:177:MET:SD   | 2:L:135:TYR:HD2  | 1.64                     | 1.19              |
| 2:L:140:HIS:CD2  | 3:J:150:GLU:OE2  | 1.95                     | 1.19              |
| 2:D:17:THR:CG2   | 2:D:71:ASN:HD21  | 1.53                     | 1.19              |
| 1:K:142:LYS:HD3  | 2:L:135:TYR:CE2  | 1.77                     | 1.18              |
| 1:I:178:ARG:CB   | 3:J:91:LEU:HD12  | 1.71                     | 1.18              |
| 2:D:50:VAL:HG21  | 2:D:64:ALA:CB    | 1.56                     | 1.18              |
| 2:L:253:GLY:O    | 2:L:288:ALA:HB2  | 1.02                     | 1.18              |
| 3:J:20:LEU:N     | 3:J:78:ILE:HG22  | 1.53                     | 1.18              |
| 2:H:252:PRO:CB   | 2:H:271:THR:CB   | 2.22                     | 1.18              |
| 3:F:59:SER:CB    | 3:F:62:LYS:CB    | 2.22                     | 1.17              |
| 2:P:17:THR:O     | 2:P:71:ASN:ND2   | 1.76                     | 1.17              |
| 3:N:255:GLY:O    | 3:N:290:ALA:N    | 1.77                     | 1.17              |
| 1:K:214:GLN:NE2  | 2:L:250:GLY:O    | 1.78                     | 1.17              |
| 1:E:244:GLY:O    | 1:E:279:ALA:HB2  | 1.45                     | 1.16              |
| 1:M:178:ARG:HD3  | 3:N:86:GLU:HA    | 1.28                     | 1.16              |
| 2:L:111:SER:CA   | 2:L:249:VAL:CG1  | 2.24                     | 1.16              |
| 2:P:21:ILE:CG2   | 2:P:52:VAL:HG11  | 1.69                     | 1.15              |
| 3:N:104:LEU:HD23 | 3:N:263:SER:CB   | 1.75                     | 1.15              |
| 2:D:20:MET:O     | 2:D:49:GLU:HA    | 1.47                     | 1.15              |
| 2:L:111:SER:CA   | 2:L:249:VAL:HG12 | 1.75                     | 1.15              |
| 2:P:21:ILE:HG21  | 2:P:52:VAL:HG11  | 1.17                     | 1.15              |
| 3:B:300:ARG:HG3  | 3:B:308:SER:OG   | 1.47                     | 1.15              |
| 2:L:138:LEU:HA   | 1:I:131:HIS:CE1  | 1.82                     | 1.14              |
| 3:B:81:ILE:HD11  | 3:B:95:ASP:CA    | 1.78                     | 1.14              |
| 1:M:134:VAL:HG22 | 1:M:137:VAL:HB   | 1.14                     | 1.14              |
| 3:N:82:HIS:O     | 3:N:83:THR:HG22  | 1.46                     | 1.13              |
| 2:P:129:GLU:HG3  | 2:P:132:GLU:CB   | 1.72                     | 1.12              |
| 3:F:254:ALA:CB   | 3:F:273:ALA:CB   | 2.19                     | 1.12              |
| 2:L:9:SER:CB     | 2:L:70:ARG:O     | 1.98                     | 1.12              |
| 2:L:24:ASP:OD2   | 2:L:79:ILE:HA    | 1.45                     | 1.12              |
| 3:N:20:LEU:HB3   | 3:N:78:ILE:HG22  | 1.26                     | 1.12              |
| 2:D:19:THR:OG1   | 2:D:74:ALA:CB    | 1.98                     | 1.11              |
| 3:J:20:LEU:CB    | 3:J:78:ILE:CG2   | 1.93                     | 1.11              |
| 2:D:129:GLU:OE2  | 2:D:132:GLU:N    | 1.83                     | 1.11              |
| 1:O:175:ASN:ND2  | 1:O:204:TYR:CZ   | 1.95                     | 1.11              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 3:N:104:LEU:CD2 | 3:N:263:SER:HB2  | 1.79                     | 1.11              |
| 3:N:30:MET:HE1  | 3:N:291:MET:CB   | 1.68                     | 1.11              |
| 1:I:126:TYR:HD2 | 1:I:226:ASN:CG   | 1.59                     | 1.10              |
| 2:D:14:GLY:N    | 3:F:265:GLU:HA   | 1.66                     | 1.10              |
| 2:P:91:SER:HB3  | 2:P:94:ASN:CG    | 1.76                     | 1.10              |
| 1:M:178:ARG:HD3 | 3:N:86:GLU:CA    | 1.79                     | 1.10              |
| 2:H:267:PHE:CD2 | 2:H:296:MET:HG3  | 1.86                     | 1.10              |
| 3:F:284:ASN:O   | 3:F:335:CYS:HB3  | 1.51                     | 1.10              |
| 2:D:50:VAL:HG22 | 2:D:64:ALA:CB    | 1.77                     | 1.10              |
| 3:N:20:LEU:HD11 | 3:N:51:LEU:CA    | 1.82                     | 1.10              |
| 2:L:56:ALA:HA   | 2:L:92:ARG:NH2   | 1.67                     | 1.09              |
| 2:P:38:PHE:HA   | 2:P:41:ALA:HB2   | 1.35                     | 1.09              |
| 2:P:43:VAL:HG22 | 2:P:44:PRO:HG2   | 1.18                     | 1.09              |
| 3:N:20:LEU:CD1  | 3:N:51:LEU:HA    | 1.81                     | 1.09              |
| 1:O:142:LYS:HB2 | 2:P:135:TYR:OH   | 1.50                     | 1.09              |
| 3:N:26:GLY:HA2  | 3:N:29:LEU:HB3   | 1.16                     | 1.09              |
| 3:N:29:LEU:HD12 | 3:N:288:PRO:HB3  | 1.32                     | 1.09              |
| 3:N:103:ASP:C   | 3:N:263:SER:OG   | 1.96                     | 1.09              |
| 3:B:77:ILE:CG2  | 3:B:298:MET:SD   | 2.40                     | 1.08              |
| 3:J:264:ALA:O   | 2:P:13:GLY:N     | 1.86                     | 1.08              |
| 3:B:91:LEU:O    | 3:B:91:LEU:CD1   | 2.00                     | 1.08              |
| 2:H:324:THR:OG1 | 2:H:326:ASP:OD1  | 1.69                     | 1.08              |
| 3:J:20:LEU:H    | 3:J:78:ILE:HG23  | 1.08                     | 1.08              |
| 3:N:30:MET:HE3  | 3:N:291:MET:HE2  | 1.25                     | 1.08              |
| 2:L:97:ARG:HD3  | 2:L:130:ASN:OD1  | 0.90                     | 1.08              |
| 1:M:178:ARG:CD  | 3:N:86:GLU:HA    | 1.82                     | 1.08              |
| 1:K:142:LYS:HD2 | 2:L:135:TYR:OH   | 1.53                     | 1.07              |
| 2:P:140:HIS:HB2 | 1:M:129:ILE:HD13 | 1.10                     | 1.07              |
| 3:B:81:ILE:HD11 | 3:B:95:ASP:HB2   | 1.12                     | 1.07              |
| 3:F:63:LEU:O    | 3:F:67:LEU:N     | 1.87                     | 1.07              |
| 3:N:30:MET:HE1  | 3:N:291:MET:HB3  | 1.14                     | 1.07              |
| 2:D:19:THR:OG1  | 2:D:74:ALA:HB2   | 1.53                     | 1.07              |
| 2:L:253:GLY:O   | 2:L:288:ALA:CA   | 2.00                     | 1.07              |
| 3:J:15:PHE:HB3  | 3:J:16:PRO:HD3   | 1.36                     | 1.07              |
| 1:E:244:GLY:O   | 1:E:279:ALA:CB   | 2.02                     | 1.07              |
| 1:O:172:HIS:CD2 | 1:O:185:LEU:HD13 | 1.88                     | 1.07              |
| 1:O:315:THR:O   | 1:O:320:GLY:N    | 1.88                     | 1.07              |
| 1:I:43:ALA:HB3  | 1:I:80:HIS:HE1   | 1.16                     | 1.06              |
| 1:K:142:LYS:HD2 | 2:L:135:TYR:CE2  | 1.81                     | 1.06              |
| 3:J:20:LEU:C    | 3:J:78:ILE:HG22  | 1.79                     | 1.06              |
| 3:F:59:SER:CB   | 3:F:62:LYS:CA    | 2.32                     | 1.06              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 3:B:95:ASP:OD1  | 3:B:99:ARG:NH1   | 1.89                     | 1.05              |
| 2:H:255:VAL:CB  | 2:H:270:ALA:HB3  | 1.87                     | 1.05              |
| 1:E:175:ASN:HA  | 3:F:85:MET:HA    | 1.07                     | 1.05              |
| 1:I:43:ALA:CB   | 1:I:80:HIS:HE1   | 1.70                     | 1.05              |
| 3:N:20:LEU:CB   | 3:N:78:ILE:HG22  | 1.85                     | 1.05              |
| 1:K:125:GLU:OE2 | 2:L:135:TYR:OH   | 1.73                     | 1.04              |
| 2:L:61:ILE:CD1  | 2:L:64:ALA:HB3   | 1.87                     | 1.04              |
| 2:P:21:ILE:HG23 | 2:P:52:VAL:HG12  | 1.09                     | 1.04              |
| 1:K:177:MET:SD  | 2:L:135:TYR:CD2  | 2.50                     | 1.04              |
| 2:L:140:HIS:CE1 | 2:L:148:GLU:OE1  | 2.07                     | 1.04              |
| 2:H:61:ILE:O    | 2:H:64:ALA:HB3   | 1.55                     | 1.04              |
| 2:P:15:ARG:NH2  | 2:P:45:VAL:O     | 1.90                     | 1.04              |
| 3:N:21:PRO:CD   | 3:N:51:LEU:CB    | 2.35                     | 1.03              |
| 3:N:184:LYS:N   | 3:N:192:ASP:OD2  | 1.90                     | 1.03              |
| 3:N:29:LEU:HD11 | 3:N:288:PRO:CA   | 1.88                     | 1.03              |
| 3:F:62:LYS:O    | 3:F:66:VAL:N     | 1.91                     | 1.03              |
| 2:D:50:VAL:HG22 | 2:D:64:ALA:HB1   | 1.31                     | 1.02              |
| 2:L:111:SER:N   | 2:L:249:VAL:HG11 | 1.74                     | 1.02              |
| 1:M:134:VAL:CG2 | 1:M:137:VAL:HB   | 1.88                     | 1.02              |
| 2:L:64:ALA:O    | 2:L:68:ILE:HD12  | 1.59                     | 1.02              |
| 3:N:21:PRO:HD2  | 3:N:51:LEU:CB    | 1.88                     | 1.01              |
| 2:D:13:GLY:CA   | 3:F:265:GLU:HA   | 1.89                     | 1.01              |
| 1:O:18:GLU:OE2  | 1:O:273:ASP:CA   | 2.08                     | 1.01              |
| 2:D:138:LEU:CB  | 1:A:131:HIS:CE1  | 2.44                     | 1.01              |
| 3:B:81:ILE:CD1  | 3:B:95:ASP:HB2   | 1.89                     | 1.01              |
| 1:O:181:ASP:O   | 1:O:183:LEU:N    | 1.92                     | 1.01              |
| 1:I:80:HIS:CG   | 1:I:81:PRO:CD    | 2.44                     | 1.01              |
| 3:N:26:GLY:O    | 3:N:30:MET:N     | 1.91                     | 1.01              |
| 2:L:52:VAL:HG12 | 2:L:53:SER:H     | 1.26                     | 1.00              |
| 2:L:61:ILE:HD12 | 2:L:64:ALA:CB    | 1.91                     | 1.00              |
| 1:O:206:ASP:HB3 | 2:P:243:ASN:ND2  | 1.75                     | 1.00              |
| 3:B:96:MET:HA   | 3:B:99:ARG:HB2   | 1.41                     | 1.00              |
| 2:H:285:ASN:HA  | 2:H:324:THR:HG21 | 1.43                     | 1.00              |
| 1:I:126:TYR:CD2 | 1:I:226:ASN:CG   | 2.40                     | 1.00              |
| 1:O:173:LYS:NZ  | 2:P:239:ASN:OD1  | 1.93                     | 1.00              |
| 2:P:347:ILE:O   | 2:P:348:ASN:OD1  | 1.78                     | 0.99              |
| 3:B:95:ASP:O    | 3:B:99:ARG:N     | 1.94                     | 0.99              |
| 3:B:90:GLU:O    | 3:B:91:LEU:HG    | 1.60                     | 0.99              |
| 1:E:244:GLY:HA2 | 1:E:263:HIS:CB   | 1.92                     | 0.99              |
| 1:K:142:LYS:CD  | 2:L:135:TYR:HE2  | 1.72                     | 0.99              |
| 3:N:82:HIS:O    | 3:N:83:THR:CG2   | 2.11                     | 0.99              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:N:30:MET:HE2   | 3:N:291:MET:HB3  | 1.10                     | 0.99              |
| 1:O:172:HIS:HD2  | 1:O:185:LEU:HD13 | 1.18                     | 0.98              |
| 3:F:61:GLU:HB2   | 3:F:64:GLU:HG2   | 1.41                     | 0.98              |
| 1:I:126:TYR:HD2  | 1:I:226:ASN:ND2  | 1.62                     | 0.98              |
| 2:D:23:GLY:HA2   | 2:D:52:VAL:HG21  | 1.42                     | 0.98              |
| 2:D:50:VAL:CG2   | 2:D:64:ALA:HB2   | 1.88                     | 0.98              |
| 3:N:63:LEU:HD23  | 3:N:64:GLU:H     | 1.27                     | 0.98              |
| 2:L:142:SER:OG   | 3:J:150:GLU:OE2  | 1.82                     | 0.98              |
| 1:E:175:ASN:CA   | 3:F:85:MET:HA    | 1.94                     | 0.97              |
| 1:I:137:VAL:HG22 | 3:J:156:THR:HG22 | 1.46                     | 0.97              |
| 3:J:54:VAL:CB    | 3:J:88:LYS:NZ    | 2.27                     | 0.97              |
| 1:O:142:LYS:HD2  | 2:P:135:TYR:HE2  | 1.26                     | 0.97              |
| 1:O:173:LYS:HZ1  | 2:P:239:ASN:CG   | 1.63                     | 0.97              |
| 2:L:138:LEU:CA   | 1:I:131:HIS:CE1  | 2.46                     | 0.97              |
| 2:H:255:VAL:CB   | 2:H:270:ALA:HB2  | 1.94                     | 0.97              |
| 1:O:181:ASP:O    | 1:O:182:GLY:C    | 2.00                     | 0.97              |
| 1:O:175:ASN:ND2  | 1:O:204:TYR:CE2  | 2.31                     | 0.97              |
| 2:D:17:THR:HG22  | 2:D:71:ASN:HD21  | 0.90                     | 0.96              |
| 2:P:138:LEU:CD2  | 1:M:131:HIS:CG   | 2.47                     | 0.96              |
| 1:I:80:HIS:CG    | 1:I:81:PRO:HD2   | 2.00                     | 0.96              |
| 3:J:83:THR:OG1   | 3:J:84:PRO:HD3   | 1.66                     | 0.96              |
| 1:M:178:ARG:HD3  | 3:N:86:GLU:CB    | 1.95                     | 0.96              |
| 2:P:80:GLU:O     | 2:P:81:THR:HB    | 1.65                     | 0.96              |
| 2:P:35:LYS:O     | 2:P:39:ARG:N     | 1.98                     | 0.96              |
| 2:P:36:SER:HA    | 2:P:39:ARG:NH1   | 1.80                     | 0.96              |
| 2:P:66:MET:C     | 2:P:69:ARG:HG3   | 1.89                     | 0.96              |
| 3:F:131:GLU:OE2  | 3:F:133:THR:CG2  | 2.14                     | 0.96              |
| 2:L:50:VAL:HG21  | 2:L:64:ALA:HA    | 1.47                     | 0.96              |
| 1:E:243:LEU:HB3  | 1:E:262:VAL:HG23 | 1.49                     | 0.95              |
| 1:O:173:LYS:NZ   | 2:P:239:ASN:ND2  | 2.14                     | 0.95              |
| 2:P:33:HIS:O     | 2:P:37:VAL:HG23  | 1.64                     | 0.95              |
| 2:L:111:SER:HA   | 2:L:249:VAL:HG12 | 0.99                     | 0.95              |
| 2:P:66:MET:HA    | 2:P:69:ARG:CD    | 1.97                     | 0.95              |
| 3:J:91:LEU:O     | 3:J:139:SER:OG   | 1.84                     | 0.95              |
| 2:P:43:VAL:CG2   | 2:P:44:PRO:HG2   | 1.96                     | 0.95              |
| 1:M:179:MET:HG2  | 3:N:149:ILE:HG12 | 1.48                     | 0.95              |
| 3:N:184:LYS:C    | 3:N:192:ASP:OD2  | 2.10                     | 0.95              |
| 1:K:178:ARG:NH1  | 2:L:86:PRO:O     | 1.98                     | 0.95              |
| 3:J:15:PHE:HB3   | 3:J:16:PRO:CD    | 1.97                     | 0.95              |
| 3:J:75:VAL:HG22  | 3:J:267:ALA:HB3  | 1.49                     | 0.95              |
| 3:B:77:ILE:HG21  | 3:B:298:MET:CE   | 1.97                     | 0.95              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:173:LYS:HZ2  | 2:P:239:ASN:CG   | 1.58                     | 0.94              |
| 1:I:43:ALA:HB3   | 1:I:80:HIS:CE1   | 2.03                     | 0.94              |
| 2:P:43:VAL:HG22  | 2:P:44:PRO:CG    | 1.97                     | 0.94              |
| 1:E:88:ARG:HD3   | 1:E:122:THR:HG22 | 1.49                     | 0.94              |
| 1:E:88:ARG:NH1   | 1:E:122:THR:HB   | 1.83                     | 0.94              |
| 2:L:110:LYS:C    | 2:L:249:VAL:HG11 | 1.92                     | 0.94              |
| 2:P:152:ILE:HG13 | 1:M:133:ILE:HG23 | 1.47                     | 0.94              |
| 1:M:134:VAL:HG22 | 1:M:137:VAL:CB   | 1.96                     | 0.94              |
| 2:L:61:ILE:CD1   | 2:L:64:ALA:CB    | 2.46                     | 0.94              |
| 1:E:240:ILE:HD12 | 1:E:246:THR:CG2  | 1.98                     | 0.93              |
| 3:N:29:LEU:CD1   | 3:N:288:PRO:CB   | 2.16                     | 0.93              |
| 2:L:97:ARG:HD3   | 2:L:130:ASN:CG   | 1.92                     | 0.93              |
| 1:E:100:CYS:HB3  | 1:E:240:ILE:CG2  | 1.99                     | 0.93              |
| 1:O:131:HIS:O    | 1:O:138:VAL:CG2  | 2.16                     | 0.93              |
| 2:D:17:THR:CG2   | 2:D:71:ASN:ND2   | 2.21                     | 0.93              |
| 2:P:40:HIS:O     | 2:P:40:HIS:ND1   | 2.00                     | 0.93              |
| 1:O:269:ILE:HD11 | 1:O:274:MET:O    | 1.67                     | 0.93              |
| 3:N:104:LEU:HD23 | 3:N:263:SER:HB2  | 0.95                     | 0.93              |
| 3:N:255:GLY:O    | 3:N:290:ALA:HB2  | 1.67                     | 0.93              |
| 1:A:105:GLY:HA3  | 1:A:308:ILE:HG22 | 1.48                     | 0.93              |
| 3:F:63:LEU:HA    | 3:F:66:VAL:HB    | 1.48                     | 0.93              |
| 1:O:15:ILE:HG22  | 1:O:270:ALA:HA   | 1.48                     | 0.93              |
| 1:O:131:HIS:NE2  | 3:N:140:LEU:HA   | 1.84                     | 0.93              |
| 2:P:38:PHE:HA    | 2:P:41:ALA:CB    | 1.97                     | 0.93              |
| 3:N:23:ASP:OD2   | 3:N:54:VAL:CB    | 2.17                     | 0.93              |
| 3:F:131:GLU:OE2  | 3:F:133:THR:HG22 | 1.69                     | 0.93              |
| 2:L:74:ALA:O     | 2:L:266:VAL:HA   | 1.69                     | 0.93              |
| 2:P:233:MET:SD   | 2:P:241:VAL:CG2  | 2.56                     | 0.93              |
| 3:N:255:GLY:O    | 3:N:290:ALA:CA   | 2.17                     | 0.93              |
| 2:P:140:HIS:CE1  | 2:P:148:GLU:HB2  | 2.03                     | 0.93              |
| 1:O:15:ILE:CG2   | 1:O:270:ALA:HA   | 1.98                     | 0.93              |
| 3:N:79:GLY:HA2   | 3:N:291:MET:HE1  | 1.51                     | 0.92              |
| 2:P:52:VAL:O     | 2:P:52:VAL:HG13  | 1.68                     | 0.92              |
| 3:N:104:LEU:N    | 3:N:263:SER:OG   | 2.02                     | 0.92              |
| 2:L:50:VAL:HG21  | 2:L:64:ALA:CA    | 1.99                     | 0.92              |
| 2:D:14:GLY:H     | 3:F:265:GLU:HA   | 1.28                     | 0.92              |
| 2:D:13:GLY:C     | 3:F:265:GLU:HA   | 1.94                     | 0.91              |
| 1:O:269:ILE:CD1  | 1:O:274:MET:O    | 2.17                     | 0.91              |
| 3:N:20:LEU:HD11  | 3:N:51:LEU:HA    | 0.94                     | 0.91              |
| 1:O:313:SER:OG   | 1:O:330:GLU:OE1  | 1.87                     | 0.91              |
| 2:P:29:GLU:OE2   | 2:P:280:ASN:HA   | 1.70                     | 0.91              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:53:ILE:HG23  | 1:A:54:PRO:HD2   | 1.50                     | 0.91              |
| 2:H:267:PHE:CE2  | 2:H:296:MET:HG3  | 2.06                     | 0.91              |
| 1:O:132:VAL:HA   | 1:O:138:VAL:HG23 | 1.52                     | 0.91              |
| 3:N:30:MET:HE2   | 3:N:291:MET:CG   | 1.87                     | 0.91              |
| 2:P:20:MET:O     | 2:P:50:VAL:HG22  | 1.71                     | 0.90              |
| 3:N:255:GLY:O    | 3:N:290:ALA:CB   | 2.19                     | 0.90              |
| 3:N:26:GLY:CA    | 3:N:29:LEU:HB3   | 2.00                     | 0.90              |
| 1:I:80:HIS:CG    | 1:I:81:PRO:HD3   | 2.06                     | 0.90              |
| 2:P:135:TYR:CE1  | 2:P:151:LYS:HB2  | 2.07                     | 0.90              |
| 2:D:50:VAL:HG23  | 2:D:64:ALA:CB    | 2.02                     | 0.90              |
| 2:H:267:PHE:CE1  | 2:H:296:MET:HA   | 2.06                     | 0.90              |
| 2:H:342:ARG:CD   | 3:N:305:GLU:CB   | 2.49                     | 0.90              |
| 1:I:83:MET:HE2   | 1:I:83:MET:HA    | 1.52                     | 0.89              |
| 1:A:178:ARG:CB   | 3:B:91:LEU:HD21  | 2.02                     | 0.89              |
| 2:L:56:ALA:HA    | 2:L:92:ARG:HH22  | 1.30                     | 0.89              |
| 3:F:59:SER:CB    | 3:F:62:LYS:N     | 2.34                     | 0.89              |
| 1:E:100:CYS:CA   | 1:E:240:ILE:HG21 | 2.02                     | 0.89              |
| 2:P:90:LYS:CB    | 2:P:95:ILE:HD11  | 2.03                     | 0.89              |
| 3:J:60:GLU:O     | 3:J:63:LEU:HB3   | 1.73                     | 0.88              |
| 3:B:99:ARG:NH2   | 3:B:270:GLU:OE1  | 2.06                     | 0.88              |
| 1:I:130:GLU:O    | 1:I:131:HIS:CD2  | 2.27                     | 0.88              |
| 3:N:30:MET:HE2   | 3:N:291:MET:SD   | 1.96                     | 0.88              |
| 1:K:133:ILE:HG13 | 1:I:133:ILE:HD12 | 1.53                     | 0.88              |
| 2:L:111:SER:HA   | 2:L:249:VAL:HG11 | 1.55                     | 0.88              |
| 3:B:140:LEU:HB3  | 3:B:152:LEU:HD12 | 1.56                     | 0.87              |
| 3:F:53:GLU:HA    | 3:F:57:MET:O     | 1.73                     | 0.87              |
| 2:L:111:SER:CA   | 2:L:249:VAL:HG11 | 1.98                     | 0.87              |
| 1:I:126:TYR:CD2  | 1:I:226:ASN:ND2  | 2.42                     | 0.87              |
| 1:O:131:HIS:O    | 1:O:138:VAL:HG23 | 1.74                     | 0.87              |
| 3:N:19:MET:CE    | 3:N:48:GLU:OE2   | 2.22                     | 0.87              |
| 3:F:137:TYR:HD2  | 3:F:237:ASN:CG   | 1.83                     | 0.87              |
| 1:K:19:ILE:HB    | 1:K:277:PRO:HB3  | 1.55                     | 0.87              |
| 2:H:255:VAL:CB   | 2:H:270:ALA:HB1  | 2.03                     | 0.87              |
| 1:I:130:GLU:O    | 1:I:131:HIS:HD2  | 1.57                     | 0.87              |
| 3:N:277:PHE:O    | 3:N:280:ALA:HB2  | 1.72                     | 0.87              |
| 1:K:133:ILE:HG13 | 1:I:133:ILE:HD13 | 1.54                     | 0.87              |
| 1:M:43:ALA:CB    | 1:M:80:HIS:NE2   | 2.38                     | 0.87              |
| 2:H:61:ILE:O     | 2:H:64:ALA:CB    | 2.22                     | 0.87              |
| 2:P:139:GLU:CB   | 2:P:148:GLU:O    | 2.22                     | 0.87              |
| 3:F:19:MET:SD    | 3:F:30:MET:HB3   | 2.14                     | 0.87              |
| 3:J:20:LEU:HB2   | 3:J:78:ILE:CB    | 2.05                     | 0.86              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:P:138:LEU:HD21 | 1:M:131:HIS:CD2  | 2.10                     | 0.86              |
| 1:M:43:ALA:HB3   | 1:M:80:HIS:NE2   | 1.89                     | 0.86              |
| 2:D:140:HIS:HB3  | 1:A:129:ILE:HD12 | 1.57                     | 0.86              |
| 1:E:240:ILE:CD1  | 1:E:246:THR:HG21 | 2.06                     | 0.86              |
| 2:L:50:VAL:HG21  | 2:L:64:ALA:CB    | 2.05                     | 0.86              |
| 2:P:140:HIS:CB   | 1:M:129:ILE:HD13 | 2.02                     | 0.86              |
| 1:O:175:ASN:ND2  | 1:O:204:TYR:CG   | 2.44                     | 0.86              |
| 1:O:318:LEU:N    | 1:O:319:GLY:HA2  | 1.89                     | 0.86              |
| 2:P:91:SER:HB3   | 2:P:94:ASN:CB    | 2.04                     | 0.86              |
| 2:H:255:VAL:C    | 2:H:270:ALA:HB2  | 2.00                     | 0.86              |
| 1:O:173:LYS:HZ2  | 2:P:239:ASN:ND2  | 1.74                     | 0.86              |
| 1:E:83:MET:HE2   | 1:E:83:MET:HA    | 1.57                     | 0.86              |
| 1:I:80:HIS:CD2   | 1:I:81:PRO:HD3   | 2.10                     | 0.86              |
| 2:H:320:GLU:OE1  | 3:N:112:LYS:HE2  | 1.76                     | 0.86              |
| 2:P:150:LEU:HD11 | 1:M:131:HIS:ND1  | 1.91                     | 0.86              |
| 3:B:81:ILE:HD11  | 3:B:95:ASP:HA    | 1.57                     | 0.85              |
| 2:D:129:GLU:CD   | 2:D:132:GLU:N    | 2.29                     | 0.85              |
| 2:L:24:ASP:OD2   | 2:L:79:ILE:CA    | 2.25                     | 0.85              |
| 1:O:73:LYS:HD3   | 1:O:265:THR:CG2  | 2.06                     | 0.85              |
| 3:B:28:GLU:OE2   | 3:B:282:GLY:CA   | 2.22                     | 0.85              |
| 2:L:253:GLY:O    | 2:L:288:ALA:N    | 2.08                     | 0.85              |
| 1:C:19:ILE:HB    | 1:C:277:PRO:HB3  | 1.57                     | 0.85              |
| 1:K:179:MET:HE1  | 2:L:139:GLU:CB   | 2.07                     | 0.85              |
| 1:I:43:ALA:CB    | 1:I:80:HIS:CE1   | 2.58                     | 0.85              |
| 2:P:136:SER:O    | 2:P:137:SER:OG   | 1.94                     | 0.85              |
| 3:N:257:VAL:HG11 | 3:N:273:ALA:N    | 1.92                     | 0.85              |
| 2:P:21:ILE:HG21  | 2:P:52:VAL:CG1   | 1.85                     | 0.84              |
| 2:H:267:PHE:CE2  | 2:H:296:MET:CG   | 2.60                     | 0.84              |
| 2:H:317:MET:HE2  | 2:H:317:MET:HA   | 1.57                     | 0.84              |
| 1:O:73:LYS:CE    | 1:O:265:THR:OG1  | 2.25                     | 0.84              |
| 1:O:175:ASN:CG   | 1:O:204:TYR:CE1  | 2.55                     | 0.84              |
| 3:B:77:ILE:HG21  | 3:B:298:MET:SD   | 2.17                     | 0.84              |
| 1:M:178:ARG:NE   | 3:N:86:GLU:HA    | 1.91                     | 0.84              |
| 2:P:20:MET:O     | 2:P:50:VAL:CG2   | 2.25                     | 0.84              |
| 2:P:140:HIS:HB2  | 1:M:129:ILE:CD1  | 2.03                     | 0.84              |
| 3:N:257:VAL:CG1  | 3:N:273:ALA:N    | 2.40                     | 0.84              |
| 2:H:259:ASN:ND2  | 2:H:268:GLU:CD   | 2.35                     | 0.84              |
| 3:N:63:LEU:O     | 3:N:66:VAL:HB    | 1.78                     | 0.84              |
| 3:F:135:GLY:N    | 3:F:154:ILE:O    | 2.11                     | 0.84              |
| 2:P:133:GLY:HA2  | 2:P:235:ASN:H    | 1.42                     | 0.84              |
| 1:E:243:LEU:HD22 | 1:E:262:VAL:HG21 | 1.60                     | 0.83              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:126:TYR:HA   | 3:F:187:ILE:HG21 | 1.58                     | 0.83              |
| 1:I:80:HIS:ND1   | 1:I:81:PRO:HD2   | 1.93                     | 0.83              |
| 2:P:53:SER:O     | 2:P:56:ALA:HB2   | 1.79                     | 0.83              |
| 1:O:138:VAL:HG22 | 1:O:139:ALA:H    | 1.42                     | 0.83              |
| 2:L:61:ILE:HD11  | 2:L:64:ALA:HB3   | 1.61                     | 0.83              |
| 1:I:178:ARG:CB   | 3:J:91:LEU:CD1   | 2.57                     | 0.83              |
| 2:L:61:ILE:HD12  | 2:L:64:ALA:HB2   | 1.59                     | 0.83              |
| 3:J:75:VAL:HA    | 3:J:267:ALA:O    | 1.79                     | 0.83              |
| 3:N:20:LEU:CD1   | 3:N:51:LEU:CB    | 2.56                     | 0.83              |
| 1:G:206:ASP:OD1  | 2:H:239:ASN:HB3  | 1.79                     | 0.83              |
| 2:P:19:THR:HG21  | 2:P:68:ILE:HG12  | 1.60                     | 0.83              |
| 2:P:37:VAL:O     | 2:P:41:ALA:N     | 2.12                     | 0.83              |
| 2:D:13:GLY:HA2   | 3:F:265:GLU:HA   | 1.59                     | 0.82              |
| 3:B:96:MET:O     | 3:B:100:ARG:N    | 2.11                     | 0.82              |
| 3:N:184:LYS:CA   | 3:N:192:ASP:OD2  | 2.27                     | 0.82              |
| 3:N:20:LEU:HD12  | 3:N:51:LEU:CB    | 2.09                     | 0.82              |
| 3:J:254:ALA:CB   | 3:J:273:ALA:HB1  | 2.10                     | 0.82              |
| 3:F:70:MET:O     | 3:F:266:TYR:HE1  | 1.63                     | 0.82              |
| 1:K:299:ARG:HD3  | 1:K:338:LEU:HD13 | 1.59                     | 0.82              |
| 3:J:183:HIS:ND1  | 3:J:185:ALA:HB2  | 1.95                     | 0.82              |
| 3:J:20:LEU:CG    | 3:J:78:ILE:HG21  | 2.09                     | 0.82              |
| 1:O:18:GLU:CD    | 1:O:273:ASP:HA   | 2.04                     | 0.82              |
| 3:N:77:ILE:CG2   | 3:N:298:MET:SD   | 2.68                     | 0.81              |
| 3:J:184:LYS:C    | 3:J:192:ASP:OD2  | 2.23                     | 0.81              |
| 3:B:77:ILE:HG21  | 3:B:298:MET:HE1  | 1.60                     | 0.81              |
| 3:B:157:ARG:HG3  | 3:B:157:ARG:O    | 1.81                     | 0.81              |
| 3:B:299:LEU:HB2  | 3:B:308:SER:HB2  | 1.61                     | 0.81              |
| 2:L:40:HIS:NE2   | 2:L:344:ILE:CB   | 2.44                     | 0.81              |
| 1:I:175:ASN:HB2  | 3:J:84:PRO:HD2   | 1.60                     | 0.81              |
| 1:O:173:LYS:HZ3  | 2:P:239:ASN:CG   | 1.84                     | 0.81              |
| 2:P:53:SER:OG    | 2:P:54:SER:N     | 2.09                     | 0.81              |
| 3:N:82:HIS:C     | 3:N:83:THR:HG22  | 2.05                     | 0.81              |
| 2:L:61:ILE:O     | 2:L:62:ARG:C     | 2.21                     | 0.81              |
| 2:P:152:ILE:HG13 | 1:M:133:ILE:CG2  | 2.09                     | 0.81              |
| 1:E:88:ARG:HH11  | 1:E:122:THR:HB   | 1.42                     | 0.81              |
| 3:N:30:MET:CE    | 3:N:291:MET:HE2  | 2.08                     | 0.81              |
| 1:M:19:ILE:HB    | 1:M:277:PRO:HB3  | 1.63                     | 0.81              |
| 2:D:10:ALA:HB2   | 3:F:165:LYS:NZ   | 1.96                     | 0.81              |
| 3:F:236:PRO:HD2  | 3:F:239:TYR:HD2  | 1.46                     | 0.81              |
| 1:A:231:ILE:HA   | 3:B:217:ASP:HB3  | 1.60                     | 0.81              |
| 3:B:93:SER:O     | 3:B:96:MET:HG2   | 1.79                     | 0.81              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:N:20:LEU:CD1   | 3:N:51:LEU:CA    | 2.51                     | 0.81              |
| 2:D:129:GLU:OE2  | 2:D:131:THR:N    | 2.14                     | 0.81              |
| 3:N:24:GLY:O     | 3:N:27:PRO:HD2   | 1.79                     | 0.81              |
| 2:D:14:GLY:N     | 3:F:265:GLU:CA   | 2.44                     | 0.80              |
| 2:L:11:LYS:HD3   | 2:L:11:LYS:H     | 1.45                     | 0.80              |
| 2:D:148:GLU:CD   | 3:B:150:GLU:OE1  | 2.24                     | 0.80              |
| 1:E:307:THR:HG23 | 1:E:330:GLU:OE1  | 1.82                     | 0.80              |
| 2:L:61:ILE:HD12  | 2:L:64:ALA:HB3   | 1.54                     | 0.80              |
| 3:J:264:ALA:O    | 2:P:13:GLY:CA    | 2.29                     | 0.80              |
| 1:E:100:CYS:CB   | 1:E:240:ILE:HG21 | 2.11                     | 0.80              |
| 1:E:240:ILE:HD12 | 1:E:246:THR:HG22 | 1.61                     | 0.80              |
| 3:N:28:GLU:OE2   | 3:N:284:ASN:HA   | 1.80                     | 0.80              |
| 1:G:315:THR:O    | 1:G:319:GLY:HA2  | 1.81                     | 0.80              |
| 3:N:103:ASP:C    | 3:N:263:SER:HG   | 1.81                     | 0.80              |
| 3:B:94:TYR:O     | 3:B:98:LEU:N     | 2.11                     | 0.80              |
| 2:H:76:LYS:HZ2   | 2:H:268:GLU:CB   | 1.95                     | 0.80              |
| 2:L:90:LYS:O     | 2:L:91:SER:C     | 2.24                     | 0.80              |
| 1:I:146:GLU:HG3  | 1:I:187:LYS:HE3  | 1.63                     | 0.80              |
| 3:J:20:LEU:O     | 3:J:78:ILE:HG22  | 1.82                     | 0.80              |
| 2:D:14:GLY:H     | 3:F:265:GLU:CA   | 1.94                     | 0.80              |
| 3:F:15:PHE:HB3   | 3:F:16:PRO:HD3   | 1.63                     | 0.80              |
| 3:J:78:ILE:O     | 3:J:78:ILE:HD12  | 1.81                     | 0.80              |
| 2:D:138:LEU:CB   | 1:A:131:HIS:HE1  | 1.91                     | 0.80              |
| 3:F:61:GLU:O     | 3:F:64:GLU:N     | 2.14                     | 0.80              |
| 1:O:138:VAL:HG22 | 1:O:139:ALA:N    | 1.95                     | 0.80              |
| 3:N:255:GLY:C    | 3:N:290:ALA:HB2  | 2.05                     | 0.80              |
| 3:B:28:GLU:CD    | 3:B:282:GLY:HA2  | 2.07                     | 0.79              |
| 3:B:67:LEU:O     | 3:B:70:MET:N     | 2.14                     | 0.79              |
| 2:L:140:HIS:NE2  | 3:J:150:GLU:CD   | 2.40                     | 0.79              |
| 2:H:317:MET:HE2  | 2:H:317:MET:CA   | 2.11                     | 0.79              |
| 1:E:100:CYS:HB3  | 1:E:240:ILE:HG21 | 1.64                     | 0.79              |
| 3:F:19:MET:CE    | 3:F:48:GLU:OE1   | 2.30                     | 0.79              |
| 2:P:151:LYS:NZ   | 2:P:190:ASP:OD1  | 2.14                     | 0.79              |
| 2:H:113:PRO:HD2  | 2:H:314:LEU:HD13 | 1.62                     | 0.79              |
| 2:P:15:ARG:HG2   | 2:P:44:PRO:HD3   | 1.65                     | 0.79              |
| 2:H:61:ILE:O     | 2:H:64:ALA:N     | 2.16                     | 0.79              |
| 1:E:19:ILE:HB    | 1:E:277:PRO:HB3  | 1.64                     | 0.79              |
| 3:B:17:VAL:HG13  | 3:B:46:PHE:CE1   | 2.16                     | 0.79              |
| 2:H:285:ASN:CA   | 2:H:324:THR:HG21 | 2.13                     | 0.79              |
| 1:O:314:LEU:O    | 1:O:320:GLY:HA3  | 1.82                     | 0.79              |
| 2:P:58:GLU:O     | 2:P:61:ILE:HG22  | 1.82                     | 0.79              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:46:GLY:H     | 1:M:50:LYS:HA    | 1.46                     | 0.79              |
| 1:A:105:GLY:CA   | 1:A:308:ILE:HG22 | 2.12                     | 0.79              |
| 3:J:54:VAL:CB    | 3:J:88:LYS:HZ2   | 1.92                     | 0.79              |
| 1:O:73:LYS:HE3   | 1:O:265:THR:OG1  | 1.83                     | 0.79              |
| 1:O:181:ASP:O    | 1:O:184:PHE:N    | 2.16                     | 0.79              |
| 3:B:77:ILE:HG22  | 3:B:298:MET:SD   | 2.20                     | 0.78              |
| 3:B:81:ILE:CD1   | 3:B:95:ASP:CA    | 2.60                     | 0.78              |
| 1:M:180:SER:HA   | 3:N:149:ILE:HG21 | 1.65                     | 0.78              |
| 3:N:20:LEU:HB3   | 3:N:78:ILE:CG2   | 2.12                     | 0.78              |
| 1:K:142:LYS:CD   | 2:L:135:TYR:CZ   | 2.52                     | 0.78              |
| 2:L:148:GLU:OE2  | 3:J:142:HIS:NE2  | 2.17                     | 0.78              |
| 3:N:152:LEU:HD13 | 3:N:154:ILE:HD11 | 1.66                     | 0.78              |
| 2:D:148:GLU:OE2  | 3:B:150:GLU:CD   | 2.26                     | 0.78              |
| 3:N:63:LEU:HA    | 3:N:66:VAL:HB    | 1.65                     | 0.78              |
| 3:F:19:MET:O     | 3:F:48:GLU:HB2   | 1.84                     | 0.78              |
| 2:L:129:GLU:O    | 2:L:235:ASN:CB   | 2.31                     | 0.78              |
| 3:F:74:LYS:HA    | 3:F:266:TYR:HD1  | 1.48                     | 0.78              |
| 1:M:175:ASN:HB2  | 3:N:83:THR:HG21  | 1.64                     | 0.78              |
| 1:A:6:THR:HG23   | 1:A:35:GLN:HG2   | 1.64                     | 0.78              |
| 1:G:142:LYS:HB3  | 2:H:149:SER:HB3  | 1.63                     | 0.78              |
| 2:L:338:GLN:HA   | 2:L:341:ILE:HB   | 1.66                     | 0.78              |
| 1:I:125:GLU:OE2  | 1:I:142:LYS:NZ   | 2.16                     | 0.78              |
| 2:H:255:VAL:O    | 2:H:270:ALA:CB   | 2.32                     | 0.78              |
| 3:N:257:VAL:HG12 | 3:N:273:ALA:H    | 1.49                     | 0.78              |
| 2:P:140:HIS:HE1  | 2:P:148:GLU:CB   | 1.96                     | 0.78              |
| 2:H:347:ILE:HD12 | 2:H:347:ILE:O    | 1.83                     | 0.77              |
| 2:L:164:TYR:OH   | 2:L:260:TYR:CD2  | 2.37                     | 0.77              |
| 1:O:180:SER:OG   | 1:O:181:ASP:N    | 2.14                     | 0.77              |
| 2:P:138:LEU:CD2  | 1:M:131:HIS:NE2  | 2.24                     | 0.77              |
| 3:B:91:LEU:HD12  | 3:B:91:LEU:C     | 2.09                     | 0.77              |
| 1:M:43:ALA:HB3   | 1:M:80:HIS:CE1   | 2.19                     | 0.77              |
| 3:N:257:VAL:CG1  | 3:N:273:ALA:H    | 1.97                     | 0.77              |
| 1:E:83:MET:HA    | 1:E:83:MET:CE    | 2.13                     | 0.77              |
| 2:H:60:ASP:OD1   | 2:H:61:ILE:N     | 2.16                     | 0.77              |
| 2:L:138:LEU:CA   | 1:I:131:HIS:HE1  | 1.96                     | 0.77              |
| 1:O:175:ASN:ND2  | 1:O:204:TYR:CD2  | 2.52                     | 0.77              |
| 1:O:175:ASN:OD1  | 1:O:176:ILE:N    | 2.18                     | 0.77              |
| 1:E:96:ASN:HB3   | 1:E:119:ARG:HB3  | 1.65                     | 0.77              |
| 1:O:131:HIS:C    | 1:O:138:VAL:HG23 | 2.10                     | 0.77              |
| 2:P:233:MET:HE1  | 2:P:241:VAL:HG11 | 1.67                     | 0.77              |
| 1:A:175:ASN:O    | 3:B:91:LEU:HD13  | 1.84                     | 0.77              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:L:4:GLN:OE1    | 2:L:4:GLN:N      | 2.14                     | 0.77              |
| 1:O:131:HIS:NE2  | 3:N:140:LEU:CB   | 2.48                     | 0.77              |
| 3:B:96:MET:CA    | 3:B:99:ARG:HB2   | 2.15                     | 0.77              |
| 3:F:74:LYS:HA    | 3:F:266:TYR:CD1  | 2.20                     | 0.77              |
| 2:L:97:ARG:HA    | 2:L:102:LEU:HD12 | 1.65                     | 0.77              |
| 2:L:129:GLU:O    | 2:L:235:ASN:HB2  | 1.84                     | 0.77              |
| 1:O:131:HIS:NE2  | 3:N:140:LEU:CA   | 2.48                     | 0.77              |
| 3:N:29:LEU:HD11  | 3:N:288:PRO:HB3  | 0.77                     | 0.76              |
| 2:L:111:SER:N    | 2:L:249:VAL:CG1  | 2.45                     | 0.76              |
| 2:L:138:LEU:C    | 1:I:131:HIS:HE1  | 1.93                     | 0.76              |
| 3:J:104:LEU:CD1  | 3:J:268:VAL:HG21 | 2.15                     | 0.76              |
| 1:O:132:VAL:CA   | 1:O:138:VAL:HG23 | 2.16                     | 0.76              |
| 2:H:60:ASP:O     | 2:H:61:ILE:C     | 2.21                     | 0.76              |
| 1:O:129:ILE:HD13 | 3:N:142:HIS:HB2  | 1.67                     | 0.76              |
| 3:J:107:ASN:HB3  | 3:J:130:ARG:HB3  | 1.67                     | 0.76              |
| 2:L:33:HIS:HB3   | 2:L:337:ILE:HG12 | 1.66                     | 0.76              |
| 1:O:131:HIS:O    | 1:O:138:VAL:HG22 | 1.85                     | 0.76              |
| 2:P:61:ILE:O     | 2:P:65:ILE:HG13  | 1.86                     | 0.76              |
| 3:F:140:LEU:C    | 3:F:141:GLU:HG3  | 2.11                     | 0.76              |
| 1:I:85:LEU:O     | 1:I:88:ARG:N     | 2.17                     | 0.76              |
| 1:O:106:TYR:CE1  | 1:O:318:LEU:CD1  | 2.68                     | 0.76              |
| 2:H:323:HIS:ND1  | 2:H:327:ILE:HD11 | 1.99                     | 0.76              |
| 2:P:259:ASN:ND2  | 2:P:268:GLU:OE1  | 2.19                     | 0.76              |
| 3:N:77:ILE:HG21  | 3:N:298:MET:SD   | 2.26                     | 0.76              |
| 2:D:13:GLY:CA    | 3:F:265:GLU:CA   | 2.64                     | 0.76              |
| 1:O:19:ILE:HB    | 1:O:277:PRO:HB3  | 1.67                     | 0.75              |
| 1:A:4:VAL:HA     | 1:A:33:PRO:HB2   | 1.67                     | 0.75              |
| 3:N:113:SER:HA   | 3:N:251:VAL:HG13 | 1.67                     | 0.75              |
| 3:N:303:ASN:C    | 3:N:304:LEU:HD23 | 2.11                     | 0.75              |
| 3:F:64:GLU:HB2   | 3:F:65:GLN:NE2   | 2.01                     | 0.75              |
| 2:L:24:ASP:CG    | 2:L:79:ILE:HA    | 2.10                     | 0.75              |
| 1:O:18:GLU:OE2   | 1:O:273:ASP:N    | 2.19                     | 0.75              |
| 2:P:20:MET:HE1   | 2:P:35:LYS:HE2   | 1.68                     | 0.75              |
| 2:H:315:ALA:C    | 2:H:343:HIS:CE1  | 2.64                     | 0.75              |
| 1:O:86:LEU:O     | 1:O:90:THR:OG1   | 2.05                     | 0.75              |
| 2:P:255:VAL:HB   | 2:P:270:ALA:HB2  | 1.67                     | 0.75              |
| 1:A:15:ILE:HG22  | 1:A:270:ALA:HA   | 1.69                     | 0.75              |
| 3:J:136:GLU:OE1  | 3:J:136:GLU:N    | 2.20                     | 0.74              |
| 2:P:17:THR:C     | 2:P:71:ASN:ND2   | 2.45                     | 0.74              |
| 3:F:137:TYR:HD2  | 3:F:237:ASN:OD1  | 1.69                     | 0.74              |
| 3:N:63:LEU:HD23  | 3:N:64:GLU:N     | 2.02                     | 0.74              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:151:LYS:NZ   | 2:D:190:ASP:OD1  | 2.20                     | 0.74              |
| 3:F:131:GLU:OE2  | 3:F:133:THR:HG23 | 1.85                     | 0.74              |
| 3:F:206:TYR:HB3  | 3:F:209:ILE:HD13 | 1.68                     | 0.74              |
| 1:O:206:ASP:HB3  | 2:P:243:ASN:HD22 | 1.49                     | 0.74              |
| 2:P:66:MET:CB    | 2:P:69:ARG:HG3   | 2.13                     | 0.74              |
| 2:D:50:VAL:HG21  | 2:D:64:ALA:HB1   | 0.74                     | 0.74              |
| 2:H:255:VAL:O    | 2:H:270:ALA:N    | 2.20                     | 0.74              |
| 2:H:320:GLU:OE1  | 3:N:112:LYS:CE   | 2.35                     | 0.74              |
| 2:D:78:ASN:OD1   | 2:D:272:ARG:NH2  | 2.20                     | 0.74              |
| 2:H:76:LYS:NZ    | 2:H:268:GLU:HB3  | 2.02                     | 0.74              |
| 2:H:151:LYS:NZ   | 2:H:190:ASP:OD1  | 2.20                     | 0.74              |
| 3:F:104:LEU:HA   | 3:F:263:SER:CB   | 2.17                     | 0.74              |
| 3:F:143:GLU:CD   | 3:F:145:ALA:O    | 2.31                     | 0.74              |
| 3:F:17:VAL:O     | 3:F:47:GLN:N     | 2.21                     | 0.74              |
| 3:J:169:ASP:OD1  | 3:J:206:TYR:OH   | 2.06                     | 0.74              |
| 2:P:57:ASP:CB    | 2:P:60:ASP:HB2   | 2.18                     | 0.74              |
| 2:P:128:ARG:HH11 | 2:P:235:ASN:HB2  | 1.53                     | 0.74              |
| 3:F:137:TYR:CD2  | 3:F:237:ASN:OD1  | 2.41                     | 0.74              |
| 1:O:288:LEU:HB2  | 1:O:297:ALA:HB2  | 1.69                     | 0.74              |
| 2:H:62:ARG:HA    | 2:H:65:ILE:HD13  | 1.69                     | 0.73              |
| 3:J:49:HIS:O     | 3:J:50:HIS:C     | 2.25                     | 0.73              |
| 3:N:141:GLU:HG2  | 3:N:151:CYS:HB2  | 1.68                     | 0.73              |
| 2:D:17:THR:HG22  | 2:D:71:ASN:HD22  | 1.46                     | 0.73              |
| 3:F:70:MET:O     | 3:F:266:TYR:CE1  | 2.42                     | 0.73              |
| 1:A:93:LEU:HD11  | 1:A:258:ILE:HD12 | 1.70                     | 0.73              |
| 1:E:240:ILE:CD1  | 1:E:246:THR:CG2  | 2.66                     | 0.73              |
| 1:A:53:ILE:CG2   | 1:A:54:PRO:HD2   | 2.18                     | 0.73              |
| 3:F:59:SER:CB    | 3:F:62:LYS:H     | 2.00                     | 0.73              |
| 2:L:56:ALA:CA    | 2:L:92:ARG:HH22  | 2.02                     | 0.73              |
| 3:J:254:ALA:HA   | 3:J:273:ALA:HB2  | 1.69                     | 0.73              |
| 1:E:100:CYS:HB3  | 1:E:240:ILE:HG23 | 1.68                     | 0.73              |
| 3:J:49:HIS:CD2   | 3:J:66:VAL:HG22  | 2.23                     | 0.73              |
| 1:A:5:GLN:O      | 1:A:35:GLN:N     | 2.19                     | 0.73              |
| 3:B:93:SER:C     | 3:B:96:MET:SD    | 2.71                     | 0.73              |
| 3:J:83:THR:HG23  | 3:J:84:PRO:CD    | 2.18                     | 0.73              |
| 3:N:62:LYS:O     | 3:N:65:GLN:HB3   | 1.88                     | 0.73              |
| 2:D:23:GLY:HA2   | 2:D:52:VAL:CG2   | 2.18                     | 0.72              |
| 2:P:68:ILE:O     | 2:P:71:ASN:O     | 2.06                     | 0.72              |
| 3:B:97:ARG:HG2   | 3:B:97:ARG:HH11  | 1.53                     | 0.72              |
| 1:M:98:ARG:NH2   | 1:M:234:ASP:OD1  | 2.19                     | 0.72              |
| 1:C:53:ILE:HD11  | 1:C:58:LYS:HB2   | 1.69                     | 0.72              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:129:GLU:OE2  | 2:D:130:ASN:N    | 2.22                     | 0.72              |
| 3:B:94:TYR:O     | 3:B:97:ARG:HB3   | 1.90                     | 0.72              |
| 1:E:231:ILE:HA   | 3:F:217:ASP:HB3  | 1.69                     | 0.72              |
| 2:D:50:VAL:HG21  | 2:D:64:ALA:CA    | 2.19                     | 0.72              |
| 2:D:319:ASN:HD22 | 2:D:322:MET:HG2  | 1.54                     | 0.72              |
| 1:A:315:THR:OG1  | 1:A:318:LEU:HG   | 1.89                     | 0.72              |
| 2:H:346:VAL:HG13 | 2:H:350:ARG:HB2  | 1.69                     | 0.72              |
| 3:J:104:LEU:HA   | 3:J:263:SER:HB2  | 1.71                     | 0.72              |
| 1:A:140:SER:HB2  | 3:B:153:LYS:HB3  | 1.70                     | 0.72              |
| 1:O:134:VAL:HG23 | 1:O:136:GLY:O    | 1.89                     | 0.72              |
| 2:P:91:SER:HB3   | 2:P:94:ASN:HB3   | 1.70                     | 0.72              |
| 3:N:63:LEU:O     | 3:N:66:VAL:N     | 2.22                     | 0.72              |
| 2:P:129:GLU:CB   | 2:P:132:GLU:CB   | 2.67                     | 0.72              |
| 2:D:19:THR:OG1   | 2:D:74:ALA:CA    | 2.37                     | 0.72              |
| 2:D:27:GLY:O     | 2:D:31:MET:N     | 2.19                     | 0.72              |
| 3:B:157:ARG:CD   | 3:B:198:CYS:SG   | 2.78                     | 0.72              |
| 2:L:24:ASP:OD2   | 2:L:80:GLU:N     | 2.22                     | 0.72              |
| 1:M:15:ILE:HG22  | 1:M:270:ALA:HA   | 1.72                     | 0.72              |
| 2:P:20:MET:SD    | 2:P:47:PHE:HD2   | 2.13                     | 0.71              |
| 1:O:175:ASN:HB3  | 1:O:204:TYR:CE1  | 2.26                     | 0.71              |
| 3:B:81:ILE:CD1   | 3:B:95:ASP:HA    | 2.18                     | 0.71              |
| 1:E:93:LEU:O     | 1:E:121:ASN:HB3  | 1.90                     | 0.71              |
| 1:I:130:GLU:OE2  | 3:J:190:LEU:N    | 2.22                     | 0.71              |
| 2:P:17:THR:C     | 2:P:71:ASN:HD22  | 1.99                     | 0.71              |
| 2:L:138:LEU:HA   | 1:I:131:HIS:NE2  | 2.04                     | 0.71              |
| 2:P:43:VAL:HG21  | 2:P:305:TYR:CD2  | 2.25                     | 0.71              |
| 1:C:44:ILE:HD11  | 1:C:52:MET:HG3   | 1.72                     | 0.71              |
| 2:H:317:MET:HE2  | 2:H:317:MET:N    | 2.06                     | 0.71              |
| 1:E:6:THR:HA     | 1:E:35:GLN:HB3   | 1.72                     | 0.71              |
| 2:P:140:HIS:HE1  | 2:P:148:GLU:HB2  | 1.51                     | 0.71              |
| 2:P:140:HIS:CE1  | 2:P:148:GLU:CB   | 2.73                     | 0.71              |
| 2:D:140:HIS:CB   | 1:A:129:ILE:HD12 | 2.20                     | 0.71              |
| 2:H:91:SER:HB3   | 2:H:94:ASN:CB    | 2.21                     | 0.71              |
| 1:O:179:MET:O    | 2:P:147:VAL:HG11 | 1.90                     | 0.71              |
| 2:H:320:GLU:OE1  | 3:N:112:LYS:NZ   | 2.24                     | 0.71              |
| 3:F:62:LYS:O     | 3:F:66:VAL:HG23  | 1.90                     | 0.71              |
| 2:P:80:GLU:O     | 2:P:81:THR:CB    | 2.35                     | 0.71              |
| 1:A:109:PRO:O    | 3:B:120:ARG:NH1  | 2.22                     | 0.71              |
| 3:N:104:LEU:CA   | 3:N:263:SER:OG   | 2.39                     | 0.71              |
| 2:H:184:ASN:C    | 2:H:185:ILE:HD12 | 2.16                     | 0.70              |
| 1:O:289:ARG:NH2  | 1:O:301:GLU:OE1  | 2.23                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:74:THR:CB    | 1:E:75:PRO:CD    | 2.69                     | 0.70              |
| 3:F:59:SER:N     | 3:F:60:GLU:HA    | 2.07                     | 0.70              |
| 3:F:96:MET:O     | 3:F:99:ARG:HB2   | 1.91                     | 0.70              |
| 2:L:151:LYS:NZ   | 2:L:190:ASP:OD1  | 2.24                     | 0.70              |
| 2:P:150:LEU:CD1  | 1:M:131:HIS:ND1  | 2.54                     | 0.70              |
| 2:P:282:ASN:HB2  | 2:P:332:THR:OG1  | 1.92                     | 0.70              |
| 3:N:70:MET:HE1   | 3:N:75:VAL:C     | 2.16                     | 0.70              |
| 1:C:142:LYS:HD2  | 2:D:135:TYR:OH   | 1.91                     | 0.70              |
| 2:H:50:VAL:O     | 2:H:50:VAL:HG13  | 1.90                     | 0.70              |
| 3:F:283:ARG:O    | 3:F:284:ASN:ND2  | 2.24                     | 0.70              |
| 1:E:240:ILE:CG1  | 1:E:246:THR:HG21 | 2.21                     | 0.70              |
| 2:L:52:VAL:HG12  | 2:L:53:SER:N     | 2.01                     | 0.70              |
| 3:J:265:GLU:HA   | 2:P:14:GLY:N     | 2.07                     | 0.70              |
| 3:B:152:LEU:HB3  | 3:B:154:ILE:HD11 | 1.73                     | 0.70              |
| 3:B:16:PRO:HA    | 3:B:45:GLU:O     | 1.91                     | 0.70              |
| 1:K:178:ARG:HH12 | 2:L:86:PRO:C     | 2.00                     | 0.70              |
| 1:O:175:ASN:OD1  | 1:O:176:ILE:HG12 | 1.91                     | 0.70              |
| 2:P:36:SER:HA    | 2:P:39:ARG:HH12  | 1.53                     | 0.70              |
| 2:D:151:LYS:HE2  | 2:D:153:ILE:HD11 | 1.73                     | 0.70              |
| 2:H:297:LEU:HB2  | 2:H:306:ALA:HB2  | 1.73                     | 0.70              |
| 2:P:38:PHE:C     | 2:P:41:ALA:H     | 2.00                     | 0.70              |
| 3:N:19:MET:HE3   | 3:N:48:GLU:OE2   | 1.91                     | 0.70              |
| 2:H:267:PHE:CZ   | 2:H:296:MET:CA   | 2.65                     | 0.69              |
| 3:N:21:PRO:HD3   | 3:N:51:LEU:CB    | 2.19                     | 0.69              |
| 1:K:98:ARG:NH1   | 1:K:234:ASP:OD1  | 2.25                     | 0.69              |
| 1:K:142:LYS:CE   | 2:L:135:TYR:HE2  | 2.04                     | 0.69              |
| 1:I:230:ASP:OD2  | 3:J:184:LYS:NZ   | 2.24                     | 0.69              |
| 2:P:66:MET:O     | 2:P:69:ARG:HB2   | 1.91                     | 0.69              |
| 2:P:93:ASN:CG    | 2:P:97:ARG:HH21  | 2.01                     | 0.69              |
| 2:P:135:TYR:HE1  | 2:P:151:LYS:HB2  | 1.56                     | 0.69              |
| 2:D:295:MET:HA   | 2:D:298:ASP:HB2  | 1.72                     | 0.69              |
| 3:B:156:THR:OG1  | 3:B:159:LYS:HB2  | 1.92                     | 0.69              |
| 1:O:173:LYS:NZ   | 2:P:239:ASN:CB   | 2.56                     | 0.69              |
| 3:F:66:VAL:HG11  | 3:F:98:LEU:HD11  | 1.73                     | 0.69              |
| 2:P:94:ASN:HA    | 2:P:97:ARG:HG2   | 1.75                     | 0.69              |
| 2:D:129:GLU:CD   | 2:D:132:GLU:CB   | 2.66                     | 0.69              |
| 1:G:173:LYS:NZ   | 1:G:206:ASP:OD2  | 2.26                     | 0.69              |
| 1:O:269:ILE:HD12 | 1:O:274:MET:O    | 1.92                     | 0.69              |
| 3:B:90:GLU:O     | 3:B:91:LEU:CG    | 2.39                     | 0.69              |
| 3:B:90:GLU:C     | 3:B:91:LEU:HG    | 2.17                     | 0.69              |
| 2:H:76:LYS:HZ2   | 2:H:268:GLU:HB2  | 1.55                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:L:75:LEU:HD12  | 2:L:267:PHE:O    | 1.93                     | 0.69              |
| 1:O:181:ASP:C    | 1:O:183:LEU:N    | 2.50                     | 0.69              |
| 3:N:185:ALA:HA   | 3:N:192:ASP:CB   | 2.22                     | 0.69              |
| 1:C:30:ALA:O     | 1:C:299:ARG:NH1  | 2.25                     | 0.69              |
| 1:A:115:ILE:HD12 | 1:A:219:PHE:HB2  | 1.75                     | 0.69              |
| 2:L:20:MET:HB2   | 2:L:47:PHE:HD2   | 1.56                     | 0.69              |
| 2:L:57:ASP:CB    | 2:L:60:ASP:HA    | 2.22                     | 0.69              |
| 1:I:98:ARG:HD2   | 1:I:233:SER:HB2  | 1.72                     | 0.69              |
| 3:N:156:THR:O    | 3:N:157:ARG:C    | 2.27                     | 0.69              |
| 3:B:157:ARG:HD2  | 3:B:198:CYS:SG   | 2.32                     | 0.69              |
| 2:H:182:LYS:HE3  | 2:H:185:ILE:HD13 | 1.74                     | 0.69              |
| 1:E:240:ILE:HG13 | 1:E:246:THR:HG21 | 1.73                     | 0.69              |
| 3:F:140:LEU:O    | 3:F:141:GLU:HG3  | 1.93                     | 0.69              |
| 2:L:60:ASP:OD1   | 2:L:61:ILE:N     | 2.25                     | 0.69              |
| 2:L:254:LEU:HD21 | 2:L:285:ASN:HD21 | 1.56                     | 0.69              |
| 1:M:231:ILE:HA   | 3:N:217:ASP:HB3  | 1.75                     | 0.69              |
| 3:F:97:ARG:O     | 3:F:98:LEU:C     | 2.35                     | 0.69              |
| 3:F:110:HIS:O    | 3:F:257:VAL:HG13 | 1.92                     | 0.69              |
| 2:L:61:ILE:HD11  | 2:L:64:ALA:CB    | 2.21                     | 0.69              |
| 3:J:183:HIS:ND1  | 3:J:185:ALA:CB   | 2.55                     | 0.69              |
| 1:O:131:HIS:CE1  | 3:N:140:LEU:HA   | 2.28                     | 0.69              |
| 2:D:10:ALA:HB2   | 3:F:165:LYS:CE   | 2.22                     | 0.68              |
| 1:O:142:LYS:HB2  | 2:P:135:TYR:HH   | 1.55                     | 0.68              |
| 2:P:283:ILE:O    | 2:P:284:ALA:C    | 2.29                     | 0.68              |
| 1:A:146:GLU:HG3  | 1:A:187:LYS:HE3  | 1.74                     | 0.68              |
| 2:H:113:PRO:HB2  | 2:H:318:ASP:OD2  | 1.93                     | 0.68              |
| 3:F:153:LYS:NZ   | 3:F:192:ASP:OD1  | 2.25                     | 0.68              |
| 1:I:85:LEU:O     | 1:I:86:LEU:C     | 2.36                     | 0.68              |
| 2:H:255:VAL:O    | 2:H:270:ALA:HB2  | 1.93                     | 0.68              |
| 1:E:311:GLY:HA2  | 1:E:314:LEU:HD11 | 1.75                     | 0.68              |
| 3:F:92:ALA:CA    | 3:F:139:SER:CB   | 2.56                     | 0.68              |
| 3:J:83:THR:HG23  | 3:J:84:PRO:N     | 2.09                     | 0.68              |
| 2:P:237:TYR:O    | 2:P:241:VAL:HG23 | 1.94                     | 0.68              |
| 3:N:30:MET:O     | 3:N:33:VAL:N     | 2.25                     | 0.68              |
| 3:N:110:HIS:NE2  | 3:N:260:GLU:OE2  | 2.24                     | 0.68              |
| 1:I:83:MET:HE2   | 1:I:83:MET:CA    | 2.21                     | 0.68              |
| 1:O:174:ALA:HA   | 1:O:181:ASP:OD1  | 1.93                     | 0.68              |
| 3:F:143:GLU:CG   | 3:F:145:ALA:O    | 2.42                     | 0.68              |
| 1:K:142:LYS:HZ2  | 2:L:135:TYR:HE2  | 1.40                     | 0.68              |
| 2:L:73:VAL:HA    | 2:L:265:ALA:O    | 1.94                     | 0.68              |
| 2:H:21:ILE:HG13  | 2:H:50:VAL:CG1   | 2.24                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:175:ASN:HA   | 3:F:85:MET:CA    | 2.03                     | 0.68              |
| 2:L:50:VAL:HG21  | 2:L:64:ALA:HB2   | 1.76                     | 0.68              |
| 2:P:300:LEU:C    | 2:P:301:LYS:HG3  | 2.18                     | 0.68              |
| 2:D:19:THR:OG1   | 2:D:74:ALA:HA    | 1.94                     | 0.68              |
| 3:J:23:ASP:OD2   | 3:J:53:GLU:CB    | 2.42                     | 0.68              |
| 3:B:81:ILE:CG1   | 3:B:95:ASP:HB2   | 2.23                     | 0.67              |
| 2:L:111:SER:CB   | 2:L:249:VAL:HG12 | 2.24                     | 0.67              |
| 2:D:10:ALA:HB2   | 3:F:165:LYS:HE2  | 1.76                     | 0.67              |
| 2:P:36:SER:HA    | 2:P:39:ARG:HH11  | 1.59                     | 0.67              |
| 3:N:63:LEU:CA    | 3:N:66:VAL:HB    | 2.24                     | 0.67              |
| 3:B:17:VAL:HG13  | 3:B:46:PHE:CD1   | 2.29                     | 0.67              |
| 3:J:108:VAL:HG22 | 3:J:129:ILE:HG12 | 1.76                     | 0.67              |
| 3:J:265:GLU:O    | 2:P:13:GLY:C     | 2.37                     | 0.67              |
| 3:N:25:VAL:O     | 3:N:29:LEU:N     | 2.22                     | 0.67              |
| 2:H:342:ARG:HD3  | 3:N:305:GLU:CB   | 2.25                     | 0.67              |
| 1:I:130:GLU:OE1  | 3:J:191:GLY:N    | 2.28                     | 0.67              |
| 2:D:15:ARG:HG3   | 2:D:15:ARG:O     | 1.93                     | 0.67              |
| 2:H:76:LYS:NZ    | 2:H:268:GLU:CB   | 2.57                     | 0.67              |
| 1:O:73:LYS:HD3   | 1:O:265:THR:OG1  | 1.95                     | 0.67              |
| 1:K:142:LYS:NZ   | 2:L:135:TYR:HE2  | 1.91                     | 0.67              |
| 1:O:142:LYS:HB3  | 2:P:149:SER:HB2  | 1.77                     | 0.67              |
| 1:O:140:SER:HB2  | 2:P:151:LYS:HB3  | 1.76                     | 0.67              |
| 3:N:21:PRO:CD    | 3:N:22:GLY:H     | 2.08                     | 0.67              |
| 3:N:276:PRO:O    | 3:N:280:ALA:N    | 2.24                     | 0.67              |
| 2:L:164:TYR:OH   | 2:L:260:TYR:HD2  | 1.75                     | 0.66              |
| 2:P:57:ASP:CA    | 2:P:60:ASP:HB2   | 2.25                     | 0.66              |
| 3:N:288:PRO:HD2  | 3:N:289:THR:N    | 2.09                     | 0.66              |
| 1:A:44:ILE:HG12  | 1:A:52:MET:O     | 1.95                     | 0.66              |
| 3:F:299:LEU:HD23 | 3:F:302:LEU:HD12 | 1.77                     | 0.66              |
| 3:J:15:PHE:CB    | 3:J:16:PRO:CD    | 2.73                     | 0.66              |
| 1:O:142:LYS:HB2  | 2:P:135:TYR:CZ   | 2.31                     | 0.66              |
| 2:P:347:ILE:O    | 2:P:348:ASN:CG   | 2.38                     | 0.66              |
| 3:J:130:ARG:HG3  | 3:J:240:GLY:HA3  | 1.77                     | 0.66              |
| 1:M:134:VAL:CG2  | 1:M:137:VAL:CB   | 2.67                     | 0.66              |
| 3:N:61:GLU:HA    | 3:N:63:LEU:CD2   | 2.24                     | 0.66              |
| 3:B:94:TYR:HA    | 3:B:97:ARG:HB3   | 1.76                     | 0.66              |
| 1:I:120:GLU:OE1  | 1:I:122:THR:OG1  | 2.12                     | 0.66              |
| 2:P:133:GLY:O    | 2:P:134:GLU:CB   | 2.43                     | 0.66              |
| 2:P:137:SER:O    | 2:P:138:LEU:HB2  | 1.96                     | 0.66              |
| 1:G:214:GLN:O    | 2:H:118:ARG:NH2  | 2.23                     | 0.66              |
| 2:H:252:PRO:CA   | 2:H:271:THR:CB   | 2.73                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:41:VAL:HA    | 1:A:54:PRO:HG2   | 1.77                     | 0.66              |
| 3:N:30:MET:HE3   | 3:N:291:MET:CG   | 2.07                     | 0.66              |
| 3:J:131:GLU:OE1  | 3:J:237:ASN:ND2  | 2.28                     | 0.66              |
| 1:I:128:GLY:O    | 1:I:130:GLU:HG3  | 1.95                     | 0.66              |
| 3:J:54:VAL:CB    | 3:J:88:LYS:CE    | 2.74                     | 0.66              |
| 2:P:281:LYS:CB   | 2:P:283:ILE:HG12 | 2.26                     | 0.66              |
| 1:M:179:MET:HG2  | 3:N:149:ILE:CG1  | 2.24                     | 0.66              |
| 1:I:129:ILE:O    | 1:I:141:ILE:HB   | 1.95                     | 0.66              |
| 2:H:316:SER:HA   | 2:H:343:HIS:CE1  | 2.31                     | 0.66              |
| 1:E:313:SER:C    | 1:E:314:LEU:HD12 | 2.21                     | 0.66              |
| 1:I:115:ILE:HD12 | 1:I:219:PHE:HB2  | 1.78                     | 0.66              |
| 2:P:21:ILE:CG2   | 2:P:52:VAL:HG13  | 2.21                     | 0.66              |
| 2:P:61:ILE:HG23  | 2:P:62:ARG:N     | 2.10                     | 0.66              |
| 1:A:237:ALA:HB1  | 1:A:246:THR:HG21 | 1.77                     | 0.65              |
| 2:L:128:ARG:NH1  | 2:L:235:ASN:OD1  | 2.29                     | 0.65              |
| 3:N:21:PRO:HD2   | 3:N:22:GLY:H     | 1.61                     | 0.65              |
| 2:L:50:VAL:CG2   | 2:L:64:ALA:HB2   | 2.26                     | 0.65              |
| 2:L:14:GLY:H     | 3:N:265:GLU:HA   | 1.61                     | 0.65              |
| 2:L:130:ASN:O    | 2:L:130:ASN:ND2  | 2.27                     | 0.65              |
| 3:B:69:SER:O     | 3:B:73:ASN:ND2   | 2.29                     | 0.65              |
| 1:K:21:ALA:HA    | 1:K:24:MET:HE2   | 1.79                     | 0.65              |
| 2:P:140:HIS:H    | 2:P:140:HIS:HD1  | 1.45                     | 0.65              |
| 1:G:130:GLU:HB2  | 2:H:188:LEU:HD12 | 1.79                     | 0.65              |
| 3:J:86:GLU:HA    | 3:J:91:LEU:HD11  | 1.77                     | 0.65              |
| 1:E:238:GLY:HA3  | 3:F:224:VAL:CG2  | 2.26                     | 0.65              |
| 1:O:174:ALA:HB2  | 1:O:181:ASP:CG   | 2.22                     | 0.65              |
| 3:F:59:SER:CB    | 3:F:62:LYS:HA    | 2.24                     | 0.65              |
| 1:O:34:ILE:HG22  | 1:O:36:TRP:CE2   | 2.31                     | 0.65              |
| 2:P:150:LEU:HD11 | 1:M:131:HIS:CE1  | 2.32                     | 0.65              |
| 2:D:120:LYS:O    | 2:D:226:GLN:NE2  | 2.29                     | 0.65              |
| 2:H:255:VAL:C    | 2:H:270:ALA:CB   | 2.70                     | 0.64              |
| 1:M:178:ARG:HE   | 3:N:86:GLU:HA    | 1.59                     | 0.64              |
| 1:C:80:HIS:N     | 1:C:81:PRO:HD2   | 2.12                     | 0.64              |
| 2:H:107:ILE:HD11 | 2:H:126:ILE:HD12 | 1.78                     | 0.64              |
| 1:E:100:CYS:HA   | 1:E:240:ILE:HG21 | 1.77                     | 0.64              |
| 2:L:126:ILE:HG21 | 2:L:242:ASN:ND2  | 2.12                     | 0.64              |
| 1:I:129:ILE:CB   | 1:I:141:ILE:HB   | 2.27                     | 0.64              |
| 1:O:316:LYS:O    | 1:O:319:GLY:HA3  | 1.97                     | 0.64              |
| 2:P:20:MET:SD    | 2:P:47:PHE:CD2   | 2.90                     | 0.64              |
| 1:G:177:MET:HB3  | 1:G:180:SER:HB3  | 1.80                     | 0.64              |
| 3:J:104:LEU:HD13 | 3:J:268:VAL:CG2  | 2.26                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:J:254:ALA:CB   | 3:J:273:ALA:CB   | 2.75                     | 0.64              |
| 2:P:138:LEU:HD23 | 1:M:131:HIS:CE1  | 2.25                     | 0.64              |
| 3:F:127:VAL:HG21 | 3:F:170:TYR:HE2  | 1.63                     | 0.64              |
| 2:L:55:ASN:O     | 2:L:56:ALA:HB3   | 1.95                     | 0.64              |
| 3:J:254:ALA:HA   | 3:J:273:ALA:CB   | 2.27                     | 0.64              |
| 3:B:96:MET:HA    | 3:B:99:ARG:CB    | 2.24                     | 0.64              |
| 3:B:153:LYS:C    | 3:B:154:ILE:HD13 | 2.23                     | 0.64              |
| 1:C:129:ILE:HD13 | 3:B:142:HIS:HB2  | 1.79                     | 0.64              |
| 1:E:88:ARG:CZ    | 1:E:122:THR:HA   | 2.28                     | 0.64              |
| 3:F:143:GLU:OE2  | 3:F:145:ALA:O    | 2.15                     | 0.64              |
| 2:L:138:LEU:HB3  | 1:I:131:HIS:CE1  | 2.33                     | 0.64              |
| 1:O:44:ILE:HA    | 1:O:51:TRP:CZ3   | 2.33                     | 0.64              |
| 1:O:142:LYS:HD2  | 2:P:135:TYR:CE2  | 2.19                     | 0.64              |
| 2:P:90:LYS:CA    | 2:P:95:ILE:HD11  | 2.27                     | 0.64              |
| 1:C:157:PHE:HE2  | 1:C:192:ALA:HA   | 1.62                     | 0.64              |
| 3:J:254:ALA:HB1  | 3:J:273:ALA:HB1  | 1.80                     | 0.64              |
| 2:H:60:ASP:CG    | 2:H:61:ILE:N     | 2.56                     | 0.64              |
| 2:L:61:ILE:O     | 2:L:64:ALA:N     | 2.30                     | 0.64              |
| 1:I:83:MET:HA    | 1:I:83:MET:CE    | 2.21                     | 0.64              |
| 1:O:131:HIS:C    | 1:O:138:VAL:CG2  | 2.70                     | 0.64              |
| 3:B:140:LEU:HB2  | 3:B:152:LEU:HB2  | 1.80                     | 0.64              |
| 3:B:157:ARG:O    | 3:B:157:ARG:CG   | 2.44                     | 0.64              |
| 2:L:57:ASP:O     | 2:L:60:ASP:HA    | 1.97                     | 0.64              |
| 1:I:125:GLU:O    | 1:I:127:SER:O    | 2.16                     | 0.64              |
| 1:O:313:SER:O    | 1:O:327:PHE:HD2  | 1.81                     | 0.64              |
| 2:P:47:PHE:O     | 2:P:48:GLU:C     | 2.37                     | 0.64              |
| 1:M:41:VAL:HA    | 1:M:54:PRO:HG2   | 1.80                     | 0.64              |
| 1:A:103:ILE:CG2  | 1:A:308:ILE:HG21 | 2.28                     | 0.63              |
| 3:B:102:LEU:HB2  | 3:B:104:LEU:HG   | 1.80                     | 0.63              |
| 2:L:11:LYS:H     | 2:L:11:LYS:CD    | 2.11                     | 0.63              |
| 1:I:231:ILE:HA   | 3:J:217:ASP:HB3  | 1.78                     | 0.63              |
| 3:J:183:HIS:CE1  | 3:J:185:ALA:HB3  | 2.33                     | 0.63              |
| 2:P:270:ALA:O    | 2:P:272:ARG:NH1  | 2.31                     | 0.63              |
| 3:N:20:LEU:HB2   | 3:N:78:ILE:HG22  | 1.74                     | 0.63              |
| 3:N:185:ALA:CA   | 3:N:192:ASP:HB3  | 2.27                     | 0.63              |
| 1:I:11:PRO:HB2   | 1:I:17:PRO:HG3   | 1.78                     | 0.63              |
| 3:N:104:LEU:HA   | 3:N:263:SER:OG   | 1.96                     | 0.63              |
| 3:N:185:ALA:HB2  | 3:N:192:ASP:HB3  | 1.80                     | 0.63              |
| 1:K:179:MET:SD   | 2:L:139:GLU:CB   | 2.86                     | 0.63              |
| 2:L:50:VAL:HG13  | 2:L:50:VAL:O     | 1.97                     | 0.63              |
| 3:J:49:HIS:HD2   | 3:J:66:VAL:HG22  | 1.62                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:15:ILE:HG22  | 1:O:270:ALA:CA   | 2.25                     | 0.63              |
| 1:O:316:LYS:HA   | 1:O:320:GLY:O    | 1.98                     | 0.63              |
| 2:P:138:LEU:HB3  | 1:M:131:HIS:NE2  | 2.13                     | 0.63              |
| 1:M:45:GLN:HA    | 1:M:50:LYS:HA    | 1.81                     | 0.63              |
| 1:G:288:LEU:HD22 | 1:G:293:LEU:HD12 | 1.78                     | 0.63              |
| 3:F:67:LEU:HD23  | 3:F:67:LEU:C     | 2.23                     | 0.63              |
| 3:F:169:ASP:OD1  | 3:F:206:TYR:OH   | 2.11                     | 0.63              |
| 3:J:104:LEU:HD11 | 3:J:268:VAL:HG21 | 1.80                     | 0.63              |
| 2:P:66:MET:O     | 2:P:69:ARG:CB    | 2.47                     | 0.63              |
| 2:P:275:GLY:O    | 2:P:278:ILE:N    | 2.30                     | 0.63              |
| 2:H:9:SER:HB3    | 2:H:70:ARG:O     | 1.98                     | 0.63              |
| 1:O:106:TYR:CZ   | 1:O:318:LEU:HD11 | 2.34                     | 0.63              |
| 1:K:231:ILE:HG21 | 2:L:240:ILE:HD13 | 1.81                     | 0.63              |
| 3:J:54:VAL:CB    | 3:J:88:LYS:HZ1   | 2.08                     | 0.63              |
| 1:A:130:GLU:OE1  | 3:B:191:GLY:N    | 2.32                     | 0.63              |
| 2:H:313:VAL:O    | 2:H:317:MET:HG2  | 1.99                     | 0.63              |
| 2:P:152:ILE:CD1  | 1:M:133:ILE:HG21 | 2.29                     | 0.63              |
| 2:L:213:ILE:O    | 2:L:217:THR:OG1  | 2.15                     | 0.63              |
| 1:A:53:ILE:HG23  | 1:A:54:PRO:CD    | 2.25                     | 0.63              |
| 3:J:138:SER:C    | 3:J:140:LEU:HG   | 2.24                     | 0.62              |
| 2:H:133:GLY:HA3  | 2:H:235:ASN:H    | 1.63                     | 0.62              |
| 2:D:117:THR:OG1  | 2:D:119:HIS:O    | 2.15                     | 0.62              |
| 2:H:60:ASP:O     | 2:H:62:ARG:N     | 2.32                     | 0.62              |
| 2:H:76:LYS:NZ    | 2:H:268:GLU:OE2  | 2.26                     | 0.62              |
| 2:P:135:TYR:CE1  | 2:P:151:LYS:CB   | 2.82                     | 0.62              |
| 3:N:63:LEU:O     | 3:N:66:VAL:CB    | 2.47                     | 0.62              |
| 2:D:50:VAL:CG2   | 2:D:64:ALA:CA    | 2.75                     | 0.62              |
| 3:B:93:SER:O     | 3:B:96:MET:CG    | 2.47                     | 0.62              |
| 3:B:115:PRO:HB2  | 3:B:320:LYS:HB2  | 1.80                     | 0.62              |
| 3:F:58:ALA:O     | 3:F:59:SER:C     | 2.42                     | 0.62              |
| 1:K:99:PRO:HB3   | 1:K:116:VAL:HG22 | 1.80                     | 0.62              |
| 1:K:157:PHE:HE2  | 1:K:192:ALA:HA   | 1.65                     | 0.62              |
| 1:O:173:LYS:HZ2  | 2:P:239:ASN:CB   | 2.10                     | 0.62              |
| 1:O:173:LYS:HZ3  | 2:P:239:ASN:ND2  | 1.91                     | 0.62              |
| 2:P:86:PRO:N     | 2:P:87:PRO:HA    | 2.14                     | 0.62              |
| 2:L:15:ARG:NH1   | 2:L:46:ASP:HB2   | 2.14                     | 0.62              |
| 2:L:129:GLU:OE2  | 2:L:132:GLU:N    | 2.31                     | 0.62              |
| 1:I:126:TYR:CE2  | 1:I:226:ASN:OD1  | 2.52                     | 0.62              |
| 1:O:175:ASN:CB   | 1:O:204:TYR:CE1  | 2.82                     | 0.62              |
| 2:P:105:ASN:HB2  | 2:P:130:ASN:HD21 | 1.65                     | 0.62              |
| 1:A:289:ARG:NH2  | 1:A:301:GLU:OE1  | 2.32                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:315:THR:O    | 1:G:319:GLY:CA   | 2.47                     | 0.62              |
| 2:H:184:ASN:OD1  | 2:H:185:ILE:HD13 | 1.99                     | 0.62              |
| 2:L:14:GLY:N     | 3:N:265:GLU:HA   | 2.14                     | 0.62              |
| 2:L:66:MET:HA    | 2:L:69:ARG:HB2   | 1.81                     | 0.62              |
| 2:L:107:ILE:HG13 | 2:L:126:ILE:HB   | 1.81                     | 0.62              |
| 1:O:112:ASP:HB3  | 1:O:217:SER:HB3  | 1.80                     | 0.62              |
| 1:O:172:HIS:CE1  | 1:O:174:ALA:HB3  | 2.35                     | 0.62              |
| 2:P:35:LYS:NZ    | 2:P:49:GLU:OE2   | 2.29                     | 0.62              |
| 1:M:250:ASN:HB2  | 1:M:258:ILE:HB   | 1.81                     | 0.62              |
| 3:B:157:ARG:HG3  | 3:B:198:CYS:SG   | 2.40                     | 0.62              |
| 3:N:30:MET:O     | 3:N:33:VAL:HB    | 2.00                     | 0.62              |
| 2:D:50:VAL:HG22  | 2:D:64:ALA:HB2   | 1.63                     | 0.62              |
| 2:H:267:PHE:CD2  | 2:H:296:MET:CG   | 2.74                     | 0.62              |
| 2:L:56:ALA:HA    | 2:L:92:ARG:HH21  | 1.63                     | 0.62              |
| 2:L:60:ASP:OD1   | 2:L:61:ILE:HG22  | 2.00                     | 0.62              |
| 1:I:282:LEU:HA   | 1:I:285:VAL:HB   | 1.82                     | 0.62              |
| 1:E:118:ILE:HG21 | 1:E:156:ALA:HB2  | 1.80                     | 0.62              |
| 3:F:103:ASP:OD2  | 3:F:162:ARG:NH1  | 2.31                     | 0.62              |
| 1:O:73:LYS:CD    | 1:O:265:THR:OG1  | 2.47                     | 0.62              |
| 1:O:133:ILE:HG22 | 1:O:133:ILE:O    | 1.99                     | 0.62              |
| 2:P:66:MET:HA    | 2:P:69:ARG:HG2   | 1.58                     | 0.62              |
| 2:P:91:SER:N     | 2:P:94:ASN:OD1   | 2.31                     | 0.62              |
| 1:M:46:GLY:HA3   | 1:M:52:MET:HG2   | 1.81                     | 0.62              |
| 2:D:50:VAL:HG23  | 2:D:64:ALA:HB2   | 1.73                     | 0.62              |
| 1:O:73:LYS:HD3   | 1:O:265:THR:HG23 | 1.82                     | 0.62              |
| 3:N:83:THR:HG23  | 3:N:84:PRO:N     | 2.15                     | 0.62              |
| 1:C:281:LEU:O    | 1:C:285:VAL:N    | 2.28                     | 0.61              |
| 1:A:103:ILE:CG2  | 1:A:308:ILE:HD13 | 2.30                     | 0.61              |
| 3:B:19:MET:SD    | 3:B:30:MET:HB3   | 2.40                     | 0.61              |
| 2:H:267:PHE:CE1  | 2:H:296:MET:CA   | 2.80                     | 0.61              |
| 2:L:182:LYS:NZ   | 2:L:215:ASP:OD2  | 2.32                     | 0.61              |
| 2:P:39:ARG:HH11  | 2:P:39:ARG:HB3   | 1.65                     | 0.61              |
| 3:B:157:ARG:HA   | 3:B:160:SER:OG   | 2.00                     | 0.61              |
| 2:L:61:ILE:C     | 2:L:63:ASN:N     | 2.57                     | 0.61              |
| 1:O:106:TYR:CZ   | 1:O:318:LEU:CD1  | 2.83                     | 0.61              |
| 2:P:41:ALA:O     | 2:P:42:CYS:HB3   | 1.99                     | 0.61              |
| 2:D:104:ALA:HB3  | 2:D:260:TYR:HB2  | 1.81                     | 0.61              |
| 2:L:79:ILE:HD12  | 2:L:92:ARG:HB2   | 1.81                     | 0.61              |
| 1:M:80:HIS:HD2   | 1:M:81:PRO:HD2   | 1.64                     | 0.61              |
| 2:D:10:ALA:HB2   | 3:F:165:LYS:HZ3  | 1.66                     | 0.61              |
| 1:E:100:CYS:C    | 1:E:240:ILE:HG21 | 2.25                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:145:THR:O    | 1:E:149:SER:OG   | 2.14                     | 0.61              |
| 3:F:254:ALA:HB1  | 3:F:273:ALA:HB2  | 1.65                     | 0.61              |
| 3:J:20:LEU:CD2   | 3:J:78:ILE:HG21  | 2.31                     | 0.61              |
| 1:O:142:LYS:CD   | 2:P:135:TYR:HE2  | 2.06                     | 0.61              |
| 2:D:19:THR:HG1   | 2:D:74:ALA:HA    | 1.65                     | 0.61              |
| 2:D:22:PRO:HB2   | 2:D:28:PRO:HG3   | 1.83                     | 0.61              |
| 1:I:235:LEU:HD11 | 3:J:246:LEU:HD21 | 1.81                     | 0.61              |
| 2:P:94:ASN:OD1   | 2:P:95:ILE:N     | 2.34                     | 0.61              |
| 2:P:133:GLY:HA2  | 2:P:235:ASN:N    | 2.13                     | 0.61              |
| 2:P:279:ALA:C    | 2:P:280:ASN:HD22 | 2.09                     | 0.61              |
| 2:D:21:ILE:CB    | 2:D:50:VAL:CG1   | 2.79                     | 0.61              |
| 1:G:173:LYS:HE3  | 1:G:176:ILE:HG13 | 1.81                     | 0.61              |
| 1:I:98:ARG:NH1   | 1:I:234:ASP:OD1  | 2.33                     | 0.61              |
| 3:J:104:LEU:HD13 | 3:J:268:VAL:HG21 | 1.80                     | 0.61              |
| 2:P:90:LYS:HA    | 2:P:95:ILE:HD11  | 1.83                     | 0.61              |
| 2:P:281:LYS:CB   | 2:P:283:ILE:HD11 | 2.31                     | 0.61              |
| 1:C:10:ILE:HG12  | 1:C:41:VAL:HG11  | 1.83                     | 0.61              |
| 1:G:313:SER:OG   | 1:G:330:GLU:OE1  | 2.15                     | 0.61              |
| 2:H:113:PRO:HD2  | 2:H:314:LEU:CD1  | 2.31                     | 0.61              |
| 1:O:157:PHE:HE2  | 1:O:192:ALA:HA   | 1.66                     | 0.61              |
| 3:N:335:CYS:SG   | 3:N:336:HIS:N    | 2.73                     | 0.61              |
| 3:F:129:ILE:HD12 | 3:F:167:ALA:HA   | 1.82                     | 0.61              |
| 2:L:138:LEU:C    | 1:I:131:HIS:CE1  | 2.77                     | 0.61              |
| 1:I:138:VAL:HG11 | 3:J:191:GLY:HA2  | 1.82                     | 0.61              |
| 1:C:140:SER:HB2  | 2:D:151:LYS:HB3  | 1.82                     | 0.61              |
| 2:H:285:ASN:CB   | 2:H:324:THR:HG21 | 2.30                     | 0.61              |
| 1:O:318:LEU:N    | 1:O:318:LEU:HD22 | 2.15                     | 0.61              |
| 2:P:135:TYR:HE1  | 2:P:151:LYS:CB   | 2.13                     | 0.61              |
| 2:D:129:GLU:CD   | 2:D:130:ASN:H    | 2.08                     | 0.60              |
| 3:N:28:GLU:OE2   | 3:N:284:ASN:CA   | 2.49                     | 0.60              |
| 2:D:105:ASN:HB2  | 2:D:130:ASN:HD21 | 1.66                     | 0.60              |
| 1:E:15:ILE:HG22  | 1:E:270:ALA:HA   | 1.82                     | 0.60              |
| 3:N:61:GLU:HA    | 3:N:63:LEU:HD21  | 1.82                     | 0.60              |
| 3:B:97:ARG:HG2   | 3:B:97:ARG:NH1   | 2.16                     | 0.60              |
| 3:B:285:ILE:HG23 | 3:B:285:ILE:O    | 1.99                     | 0.60              |
| 2:H:61:ILE:O     | 2:H:64:ALA:CA    | 2.48                     | 0.60              |
| 2:H:346:VAL:HG12 | 2:H:346:VAL:O    | 2.01                     | 0.60              |
| 1:I:122:THR:OG1  | 1:I:123:GLU:N    | 2.33                     | 0.60              |
| 1:M:95:ALA:HB3   | 1:M:251:ILE:HB   | 1.82                     | 0.60              |
| 3:N:117:TYR:OH   | 3:N:328:ASP:O    | 2.19                     | 0.60              |
| 1:G:19:ILE:HB    | 1:G:277:PRO:HB3  | 1.83                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:P:91:SER:CB    | 2:P:94:ASN:HB3   | 2.31                     | 0.60              |
| 1:M:46:GLY:HA3   | 1:M:52:MET:CG    | 2.32                     | 0.60              |
| 3:B:99:ARG:HD3   | 3:B:104:LEU:HB2  | 1.83                     | 0.60              |
| 2:L:181:HIS:HE2  | 2:L:211:ASN:HB2  | 1.65                     | 0.60              |
| 2:P:300:LEU:C    | 2:P:301:LYS:CG   | 2.72                     | 0.60              |
| 2:P:300:LEU:O    | 2:P:301:LYS:HG3  | 2.01                     | 0.60              |
| 1:M:140:SER:HB2  | 3:N:153:LYS:HG2  | 1.83                     | 0.60              |
| 3:N:293:LEU:O    | 3:N:297:ASN:ND2  | 2.32                     | 0.60              |
| 2:H:180:VAL:HB   | 2:H:233:MET:HB3  | 1.84                     | 0.60              |
| 2:P:62:ARG:HA    | 2:P:65:ILE:HG13  | 1.84                     | 0.60              |
| 1:M:115:ILE:HD12 | 1:M:219:PHE:HB2  | 1.83                     | 0.60              |
| 3:N:63:LEU:C     | 3:N:66:VAL:HB    | 2.26                     | 0.60              |
| 1:E:330:GLU:HA   | 1:E:333:ARG:HG2  | 1.83                     | 0.60              |
| 1:I:126:TYR:CE1  | 3:J:187:ILE:HG21 | 2.37                     | 0.60              |
| 3:J:70:MET:HG3   | 3:J:102:LEU:HD11 | 1.82                     | 0.60              |
| 3:J:179:VAL:HG12 | 3:J:232:VAL:HB   | 1.84                     | 0.60              |
| 1:O:133:ILE:HG23 | 3:N:154:ILE:HG13 | 1.84                     | 0.60              |
| 1:M:93:LEU:HD11  | 1:M:258:ILE:HD12 | 1.83                     | 0.60              |
| 1:C:249:GLY:HA2  | 1:C:259:PHE:HA   | 1.83                     | 0.60              |
| 1:A:69:LYS:NZ    | 1:A:260:GLU:OE1  | 2.30                     | 0.60              |
| 1:K:91:PHE:HB3   | 1:K:256:VAL:HG11 | 1.83                     | 0.60              |
| 1:K:125:GLU:OE1  | 1:K:125:GLU:N    | 2.35                     | 0.60              |
| 3:N:193:GLY:O    | 3:N:194:LEU:C    | 2.39                     | 0.60              |
| 3:N:257:VAL:HG12 | 3:N:273:ALA:N    | 2.09                     | 0.60              |
| 3:N:279:GLN:O    | 3:N:281:VAL:N    | 2.30                     | 0.60              |
| 2:D:21:ILE:CB    | 2:D:50:VAL:HG12  | 2.31                     | 0.60              |
| 1:I:110:TYR:CE1  | 3:J:120:ARG:HD3  | 2.37                     | 0.60              |
| 2:L:138:LEU:CB   | 1:I:131:HIS:CE1  | 2.84                     | 0.60              |
| 1:K:224:MET:HE1  | 1:K:232:LEU:HD12 | 1.84                     | 0.59              |
| 2:L:57:ASP:C     | 2:L:60:ASP:HA    | 2.27                     | 0.59              |
| 3:J:61:GLU:O     | 3:J:62:LYS:C     | 2.44                     | 0.59              |
| 2:P:38:PHE:O     | 2:P:41:ALA:HB3   | 2.02                     | 0.59              |
| 2:D:13:GLY:HA2   | 3:F:265:GLU:CA   | 2.31                     | 0.59              |
| 2:H:323:HIS:ND1  | 2:H:327:ILE:CD1  | 2.65                     | 0.59              |
| 1:E:88:ARG:HD3   | 1:E:122:THR:CG2  | 2.28                     | 0.59              |
| 1:I:126:TYR:HE1  | 3:J:187:ILE:HG21 | 1.67                     | 0.59              |
| 3:J:49:HIS:CE1   | 3:J:69:SER:HG    | 2.20                     | 0.59              |
| 1:C:69:LYS:HD2   | 1:C:72:LEU:HD11  | 1.83                     | 0.59              |
| 3:B:142:HIS:NE2  | 3:B:150:GLU:OE1  | 2.35                     | 0.59              |
| 2:P:93:ASN:HD22  | 2:P:93:ASN:C     | 2.06                     | 0.59              |
| 2:P:152:ILE:CG1  | 1:M:133:ILE:HG23 | 2.28                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:N:61:GLU:C     | 3:N:63:LEU:HD23  | 2.27                     | 0.59              |
| 2:H:257:GLY:CA   | 2:H:268:GLU:O    | 2.51                     | 0.59              |
| 3:J:255:GLY:O    | 3:J:290:ALA:N    | 2.33                     | 0.59              |
| 3:N:154:ILE:HG22 | 3:N:155:VAL:N    | 2.15                     | 0.59              |
| 2:D:60:ASP:N     | 2:D:60:ASP:OD1   | 2.35                     | 0.59              |
| 2:H:112:LEU:HB2  | 2:H:115:VAL:HB   | 1.84                     | 0.59              |
| 1:O:98:ARG:CZ    | 1:O:233:SER:HB2  | 2.31                     | 0.59              |
| 2:P:127:VAL:HG12 | 2:P:161:ILE:HD11 | 1.83                     | 0.59              |
| 2:P:152:ILE:HD12 | 1:M:133:ILE:HG21 | 1.85                     | 0.59              |
| 1:E:178:ARG:CB   | 3:F:86:GLU:CB    | 2.81                     | 0.59              |
| 3:F:226:ASN:O    | 3:F:229:GLN:NE2  | 2.27                     | 0.59              |
| 1:I:103:ILE:HG22 | 1:I:105:GLY:H    | 1.67                     | 0.59              |
| 3:N:185:ALA:HA   | 3:N:192:ASP:HB2  | 1.83                     | 0.59              |
| 2:H:17:THR:O     | 2:H:71:ASN:ND2   | 2.36                     | 0.59              |
| 1:O:157:PHE:HE1  | 1:O:168:VAL:HG11 | 1.67                     | 0.59              |
| 3:N:104:LEU:HA   | 3:N:263:SER:CB   | 2.32                     | 0.59              |
| 2:H:76:LYS:HZ2   | 2:H:268:GLU:HB3  | 1.60                     | 0.59              |
| 1:E:238:GLY:HA3  | 3:F:224:VAL:HG21 | 1.85                     | 0.59              |
| 3:F:19:MET:HB3   | 3:F:48:GLU:CB    | 2.33                     | 0.59              |
| 3:F:42:VAL:HG12  | 3:F:44:VAL:HG22  | 1.85                     | 0.59              |
| 3:F:104:LEU:CA   | 3:F:263:SER:CB   | 2.81                     | 0.59              |
| 2:P:285:ASN:HA   | 2:P:324:THR:HG21 | 1.85                     | 0.59              |
| 1:M:161:ARG:NH1  | 1:M:195:CYS:SG   | 2.76                     | 0.59              |
| 1:O:133:ILE:O    | 1:O:134:VAL:HG13 | 2.03                     | 0.59              |
| 1:O:314:LEU:C    | 1:O:320:GLY:HA3  | 2.27                     | 0.59              |
| 1:A:145:THR:HG22 | 3:B:148:VAL:HG13 | 1.84                     | 0.59              |
| 1:E:100:CYS:CB   | 1:E:240:ILE:CG2  | 2.74                     | 0.59              |
| 1:E:183:LEU:HA   | 1:E:186:GLN:HG2  | 1.85                     | 0.58              |
| 1:O:73:LYS:HE2   | 1:O:265:THR:H    | 1.67                     | 0.58              |
| 1:M:132:VAL:HG23 | 1:M:132:VAL:O    | 2.03                     | 0.58              |
| 3:N:30:MET:HE1   | 3:N:291:MET:CA   | 2.31                     | 0.58              |
| 3:B:140:LEU:CB   | 3:B:152:LEU:HD12 | 2.31                     | 0.58              |
| 2:P:39:ARG:NH1   | 2:P:39:ARG:HB3   | 2.18                     | 0.58              |
| 2:D:17:THR:HG21  | 2:D:71:ASN:HD21  | 1.61                     | 0.58              |
| 1:A:129:ILE:HB   | 1:A:141:ILE:HB   | 1.85                     | 0.58              |
| 2:L:114:GLY:HA3  | 2:L:318:ASP:HA   | 1.85                     | 0.58              |
| 2:L:254:LEU:CD2  | 2:L:285:ASN:HD21 | 2.16                     | 0.58              |
| 1:I:132:VAL:O    | 1:I:132:VAL:HG12 | 2.04                     | 0.58              |
| 2:P:85:LEU:C     | 2:P:87:PRO:HA    | 2.29                     | 0.58              |
| 3:B:156:THR:HG21 | 3:B:159:LYS:HE3  | 1.84                     | 0.58              |
| 3:F:254:ALA:HB1  | 3:F:273:ALA:HB3  | 0.60                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:133:ILE:CG1  | 1:I:133:ILE:CD1  | 2.63                     | 0.58              |
| 2:L:78:ASN:OD1   | 2:L:272:ARG:NH2  | 2.37                     | 0.58              |
| 1:I:5:GLN:O      | 1:I:35:GLN:N     | 2.29                     | 0.58              |
| 1:I:125:GLU:CD   | 1:I:142:LYS:NZ   | 2.61                     | 0.58              |
| 1:M:91:PHE:CD2   | 1:M:256:VAL:HG11 | 2.38                     | 0.58              |
| 1:M:172:HIS:O    | 1:M:204:TYR:HA   | 2.03                     | 0.58              |
| 3:N:63:LEU:HD23  | 3:N:63:LEU:N     | 2.19                     | 0.58              |
| 1:A:53:ILE:CG2   | 1:A:54:PRO:CD    | 2.81                     | 0.58              |
| 1:E:9:LEU:HD23   | 1:E:38:GLU:HG2   | 1.85                     | 0.58              |
| 1:K:108:THR:HG21 | 1:K:240:ILE:HA   | 1.84                     | 0.58              |
| 1:K:142:LYS:HD2  | 2:L:135:TYR:HH   | 1.67                     | 0.58              |
| 2:L:56:ALA:CB    | 2:L:92:ARG:HH22  | 2.16                     | 0.58              |
| 2:P:57:ASP:O     | 2:P:60:ASP:HB2   | 2.03                     | 0.58              |
| 2:P:253:GLY:C    | 2:P:288:ALA:HB2  | 2.28                     | 0.58              |
| 1:C:171:VAL:HB   | 1:C:224:MET:HB3  | 1.84                     | 0.58              |
| 1:A:293:LEU:O    | 1:A:297:ALA:N    | 2.34                     | 0.58              |
| 1:I:126:TYR:CD2  | 1:I:226:ASN:OD1  | 2.55                     | 0.58              |
| 3:J:138:SER:O    | 3:J:140:LEU:HG   | 2.02                     | 0.58              |
| 1:O:276:ASN:HB2  | 1:O:315:THR:HG21 | 1.86                     | 0.58              |
| 2:P:22:PRO:HA    | 2:P:31:MET:HG3   | 1.84                     | 0.58              |
| 3:N:257:VAL:HG12 | 3:N:257:VAL:O    | 2.02                     | 0.58              |
| 1:E:146:GLU:N    | 3:F:147:GLY:O    | 2.36                     | 0.58              |
| 3:F:61:GLU:O     | 3:F:62:LYS:C     | 2.47                     | 0.58              |
| 3:F:62:LYS:C     | 3:F:66:VAL:HG23  | 2.28                     | 0.58              |
| 2:P:52:VAL:CG1   | 2:P:52:VAL:O     | 2.39                     | 0.58              |
| 3:N:28:GLU:OE2   | 3:N:284:ASN:CB   | 2.51                     | 0.58              |
| 3:N:70:MET:HG3   | 3:N:266:TYR:HD2  | 1.68                     | 0.58              |
| 2:H:107:ILE:HG12 | 2:H:126:ILE:HB   | 1.86                     | 0.58              |
| 1:K:242:GLY:O    | 1:K:246:THR:OG1  | 2.22                     | 0.58              |
| 1:G:209:CYS:HB3  | 2:H:244:VAL:HG23 | 1.86                     | 0.58              |
| 2:L:52:VAL:CG1   | 2:L:53:SER:H     | 2.09                     | 0.58              |
| 2:L:56:ALA:CA    | 2:L:92:ARG:NH2   | 2.55                     | 0.58              |
| 1:O:137:VAL:O    | 1:O:137:VAL:HG12 | 2.01                     | 0.58              |
| 2:P:9:SER:H      | 2:P:72:ARG:NH1   | 2.02                     | 0.58              |
| 2:P:98:THR:O     | 2:P:100:LEU:N    | 2.37                     | 0.58              |
| 3:N:63:LEU:O     | 3:N:66:VAL:CA    | 2.52                     | 0.58              |
| 3:N:89:GLY:O     | 3:N:90:GLU:CB    | 2.51                     | 0.58              |
| 1:A:103:ILE:HG22 | 1:A:308:ILE:HG21 | 1.86                     | 0.58              |
| 1:G:206:ASP:OD1  | 2:H:239:ASN:CB   | 2.51                     | 0.58              |
| 2:P:297:LEU:HB2  | 2:P:306:ALA:HB2  | 1.85                     | 0.58              |
| 1:M:288:LEU:HA   | 1:M:291:MET:HE2  | 1.85                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:B:108:VAL:HG22 | 3:B:129:ILE:HG12 | 1.86                     | 0.57              |
| 2:P:140:HIS:HD1  | 2:P:140:HIS:N    | 2.02                     | 0.57              |
| 3:B:17:VAL:CG1   | 3:B:46:PHE:CE1   | 2.87                     | 0.57              |
| 2:L:220:GLN:OE1  | 2:L:227:GLN:NE2  | 2.38                     | 0.57              |
| 3:J:138:SER:CB   | 3:J:140:LEU:HG   | 2.34                     | 0.57              |
| 3:J:173:LYS:HE2  | 2:P:15:ARG:NH1   | 2.18                     | 0.57              |
| 2:P:45:VAL:O     | 2:P:45:VAL:HG23  | 2.04                     | 0.57              |
| 2:D:9:SER:HB3    | 2:D:72:ARG:NE    | 2.19                     | 0.57              |
| 2:P:26:ILE:HG21  | 2:P:284:ALA:HB2  | 1.85                     | 0.57              |
| 1:M:77:ALA:HB3   | 1:M:80:HIS:HB2   | 1.86                     | 0.57              |
| 3:N:63:LEU:CD2   | 3:N:64:GLU:H     | 2.10                     | 0.57              |
| 3:B:275:HIS:CB   | 3:B:276:PRO:HD2  | 2.34                     | 0.57              |
| 1:K:86:LEU:O     | 1:K:90:THR:OG1   | 2.19                     | 0.57              |
| 3:J:60:GLU:O     | 3:J:63:LEU:CB    | 2.49                     | 0.57              |
| 2:P:107:ILE:HD11 | 2:P:242:ASN:HD22 | 1.69                     | 0.57              |
| 2:D:143:VAL:HG22 | 2:D:146:VAL:HB   | 1.86                     | 0.57              |
| 3:B:300:ARG:CG   | 3:B:308:SER:OG   | 2.39                     | 0.57              |
| 2:H:252:PRO:HB2  | 2:H:271:THR:CB   | 2.25                     | 0.57              |
| 1:I:142:LYS:HE2  | 1:I:177:MET:HE1  | 1.86                     | 0.57              |
| 1:O:138:VAL:CG2  | 1:O:139:ALA:N    | 2.67                     | 0.57              |
| 2:P:98:THR:O     | 2:P:99:SER:C     | 2.45                     | 0.57              |
| 1:A:244:GLY:C    | 1:A:279:ALA:HB2  | 2.29                     | 0.57              |
| 3:B:15:PHE:O     | 3:B:44:VAL:HA    | 2.04                     | 0.57              |
| 2:H:317:MET:HA   | 2:H:317:MET:CE   | 2.29                     | 0.57              |
| 3:F:185:ALA:HB2  | 3:F:192:ASP:HB2  | 1.85                     | 0.57              |
| 3:N:63:LEU:O     | 3:N:67:LEU:N     | 2.37                     | 0.57              |
| 3:N:315:VAL:HG22 | 3:N:342:ILE:HD12 | 1.86                     | 0.57              |
| 1:O:41:VAL:HA    | 1:O:54:PRO:HG2   | 1.87                     | 0.57              |
| 2:P:57:ASP:N     | 2:P:60:ASP:HB2   | 2.20                     | 0.57              |
| 1:M:175:ASN:CB   | 3:N:83:THR:HG21  | 2.35                     | 0.57              |
| 3:N:185:ALA:CB   | 3:N:192:ASP:HB3  | 2.35                     | 0.57              |
| 2:D:56:ALA:HB1   | 2:D:60:ASP:HB2   | 1.87                     | 0.57              |
| 1:E:69:LYS:HD2   | 1:E:72:LEU:HD11  | 1.87                     | 0.57              |
| 3:F:47:GLN:O     | 3:F:49:HIS:CD2   | 2.57                     | 0.57              |
| 1:I:210:LEU:HB2  | 3:J:245:ASN:HB3  | 1.86                     | 0.57              |
| 3:J:269:PHE:CZ   | 3:J:298:MET:HA   | 2.40                     | 0.57              |
| 1:O:174:ALA:N    | 1:O:181:ASP:OD2  | 2.37                     | 0.57              |
| 2:P:38:PHE:HB3   | 2:P:45:VAL:HG12  | 1.85                     | 0.57              |
| 3:B:17:VAL:O     | 3:B:46:PHE:HD1   | 1.87                     | 0.57              |
| 3:B:67:LEU:HA    | 3:B:70:MET:HB2   | 1.86                     | 0.57              |
| 3:B:155:VAL:O    | 3:B:155:VAL:HG13 | 2.05                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:P:282:ASN:CB   | 2:P:333:THR:HG23 | 2.29                     | 0.57              |
| 3:B:281:VAL:O    | 3:B:281:VAL:HG12 | 2.04                     | 0.56              |
| 2:H:59:GLU:O     | 2:H:62:ARG:HB2   | 2.05                     | 0.56              |
| 1:E:261:SER:HB3  | 1:E:280:LEU:HB2  | 1.86                     | 0.56              |
| 3:F:61:GLU:HB2   | 3:F:64:GLU:CG    | 2.26                     | 0.56              |
| 3:F:95:ASP:OD1   | 3:F:99:ARG:NH1   | 2.38                     | 0.56              |
| 1:E:126:TYR:HA   | 3:F:187:ILE:CG2  | 2.33                     | 0.56              |
| 1:E:299:ARG:HG2  | 1:E:338:LEU:HD13 | 1.87                     | 0.56              |
| 1:I:130:GLU:CD   | 3:J:190:LEU:HB2  | 2.30                     | 0.56              |
| 1:O:166:SER:OG   | 1:O:220:ASP:OD2  | 2.19                     | 0.56              |
| 2:P:129:GLU:OE2  | 2:P:130:ASN:N    | 2.37                     | 0.56              |
| 2:P:182:LYS:N    | 2:P:190:ASP:OD2  | 2.35                     | 0.56              |
| 1:M:118:ILE:HG22 | 1:M:152:ILE:HD11 | 1.87                     | 0.56              |
| 2:D:19:THR:HG21  | 2:D:68:ILE:HA    | 1.87                     | 0.56              |
| 2:D:114:GLY:HA2  | 2:D:318:ASP:HA   | 1.86                     | 0.56              |
| 1:A:125:GLU:HG2  | 1:A:142:LYS:HB2  | 1.87                     | 0.56              |
| 3:B:29:LEU:HB3   | 3:B:291:MET:HG3  | 1.87                     | 0.56              |
| 2:L:283:ILE:HD12 | 2:L:325:PRO:HG2  | 1.87                     | 0.56              |
| 1:O:91:PHE:HB3   | 1:O:256:VAL:HG11 | 1.86                     | 0.56              |
| 3:N:61:GLU:HA    | 3:N:61:GLU:OE1   | 2.06                     | 0.56              |
| 1:C:209:CYS:HB3  | 2:D:244:VAL:HG23 | 1.85                     | 0.56              |
| 2:H:312:ALA:O    | 2:H:315:ALA:N    | 2.38                     | 0.56              |
| 2:L:140:HIS:NE2  | 2:L:148:GLU:OE1  | 2.37                     | 0.56              |
| 3:J:20:LEU:N     | 3:J:78:ILE:HG23  | 1.83                     | 0.56              |
| 3:J:254:ALA:HB2  | 3:J:273:ALA:HB1  | 1.87                     | 0.56              |
| 2:L:140:HIS:NE2  | 2:L:142:SER:OG   | 2.39                     | 0.56              |
| 3:N:257:VAL:HG11 | 3:N:273:ALA:CA   | 2.36                     | 0.56              |
| 1:C:145:THR:HG22 | 2:D:146:VAL:HG22 | 1.86                     | 0.56              |
| 1:E:88:ARG:NH1   | 1:E:122:THR:CB   | 2.66                     | 0.56              |
| 1:E:225:PRO:HD2  | 1:E:228:TYR:HD2  | 1.69                     | 0.56              |
| 1:O:34:ILE:HG22  | 1:O:36:TRP:NE1   | 2.21                     | 0.56              |
| 2:P:152:ILE:CG1  | 1:M:133:ILE:CG2  | 2.82                     | 0.56              |
| 3:N:288:PRO:CD   | 3:N:289:THR:N    | 2.64                     | 0.56              |
| 2:D:33:HIS:ND1   | 2:D:337:ILE:HD13 | 2.21                     | 0.56              |
| 1:E:92:ASP:OD2   | 1:E:151:ARG:NH1  | 2.39                     | 0.56              |
| 2:L:64:ALA:C     | 2:L:68:ILE:HD12  | 2.29                     | 0.56              |
| 2:L:117:THR:OG1  | 2:L:119:HIS:O    | 2.23                     | 0.56              |
| 1:C:66:MET:HE3   | 1:C:287:MET:HG3  | 1.86                     | 0.56              |
| 1:G:120:GLU:OE2  | 1:G:122:THR:OG1  | 2.14                     | 0.56              |
| 2:L:51:HIS:C     | 2:L:52:VAL:HG23  | 2.29                     | 0.56              |
| 2:L:154:THR:OG1  | 2:L:157:LYS:HB2  | 2.06                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:224:MET:SD   | 1:O:232:LEU:HD12 | 2.46                     | 0.56              |
| 2:P:126:ILE:HG21 | 2:P:242:ASN:ND2  | 2.21                     | 0.56              |
| 3:B:141:GLU:HG3  | 3:B:151:CYS:SG   | 2.46                     | 0.56              |
| 2:H:139:GLU:HA   | 2:H:148:GLU:O    | 2.05                     | 0.56              |
| 1:E:83:MET:HE2   | 1:E:83:MET:CA    | 2.27                     | 0.56              |
| 3:J:134:GLU:OE2  | 3:J:156:THR:OG1  | 2.10                     | 0.56              |
| 2:P:281:LYS:CB   | 2:P:283:ILE:CG1  | 2.83                     | 0.56              |
| 3:N:127:VAL:HG13 | 3:N:232:VAL:HG13 | 1.87                     | 0.56              |
| 2:D:20:MET:O     | 2:D:49:GLU:CA    | 2.37                     | 0.56              |
| 3:B:67:LEU:O     | 3:B:71:LYS:N     | 2.39                     | 0.56              |
| 2:L:103:TYR:O    | 2:L:130:ASN:N    | 2.34                     | 0.56              |
| 1:I:43:ALA:HB1   | 1:I:80:HIS:CE1   | 2.41                     | 0.56              |
| 3:J:83:THR:HG23  | 3:J:84:PRO:HD2   | 1.88                     | 0.56              |
| 2:P:129:GLU:CD   | 2:P:130:ASN:H    | 2.13                     | 0.56              |
| 2:P:152:ILE:CD1  | 1:M:133:ILE:CG2  | 2.84                     | 0.56              |
| 3:J:113:SER:HA   | 3:J:251:VAL:HG13 | 1.86                     | 0.55              |
| 1:O:143:LEU:HD21 | 3:N:144:SER:O    | 2.06                     | 0.55              |
| 3:N:102:LEU:HB2  | 3:N:104:LEU:HG   | 1.86                     | 0.55              |
| 3:N:217:ASP:N    | 3:N:217:ASP:OD1  | 2.37                     | 0.55              |
| 2:L:110:LYS:HA   | 2:L:122:ILE:O    | 2.07                     | 0.55              |
| 1:O:181:ASP:N    | 1:O:181:ASP:OD1  | 2.35                     | 0.55              |
| 1:O:261:SER:HB3  | 1:O:280:LEU:HD13 | 1.88                     | 0.55              |
| 3:N:96:MET:O     | 3:N:100:ARG:N    | 2.39                     | 0.55              |
| 3:N:185:ALA:HA   | 3:N:192:ASP:HB3  | 1.85                     | 0.55              |
| 3:B:96:MET:SD    | 3:B:96:MET:N     | 2.66                     | 0.55              |
| 2:P:57:ASP:O     | 2:P:61:ILE:N     | 2.38                     | 0.55              |
| 2:P:300:LEU:O    | 2:P:301:LYS:CB   | 2.53                     | 0.55              |
| 1:K:157:PHE:HE1  | 1:K:168:VAL:HG11 | 1.72                     | 0.55              |
| 1:K:162:ASN:O    | 1:K:163:ASN:ND2  | 2.37                     | 0.55              |
| 1:K:315:THR:OG1  | 1:K:317:ASP:OD1  | 2.23                     | 0.55              |
| 2:L:285:ASN:HA   | 2:L:324:THR:HG21 | 1.89                     | 0.55              |
| 3:J:299:LEU:HB2  | 3:J:308:SER:HB2  | 1.88                     | 0.55              |
| 1:O:214:GLN:O    | 2:P:118:ARG:NH2  | 2.40                     | 0.55              |
| 2:P:138:LEU:CD2  | 1:M:131:HIS:CE1  | 2.87                     | 0.55              |
| 1:E:173:LYS:HG3  | 1:E:205:LEU:HB3  | 1.88                     | 0.55              |
| 2:P:62:ARG:O     | 2:P:65:ILE:HB    | 2.06                     | 0.55              |
| 3:N:77:ILE:HG21  | 3:N:298:MET:CE   | 2.37                     | 0.55              |
| 3:F:137:TYR:CD2  | 3:F:237:ASN:CG   | 2.75                     | 0.55              |
| 2:P:53:SER:O     | 2:P:56:ALA:CB    | 2.53                     | 0.55              |
| 3:N:136:GLU:OE1  | 3:N:136:GLU:N    | 2.39                     | 0.55              |
| 2:D:26:ILE:O     | 2:D:26:ILE:HG13  | 2.07                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:B:20:LEU:O     | 3:B:79:GLY:N     | 2.37                     | 0.55              |
| 2:H:117:THR:OG1  | 2:H:119:HIS:O    | 2.25                     | 0.55              |
| 1:I:15:ILE:HG22  | 1:I:270:ALA:HA   | 1.89                     | 0.55              |
| 3:J:138:SER:CB   | 3:J:140:LEU:CD1  | 2.85                     | 0.55              |
| 1:O:269:ILE:O    | 1:O:269:ILE:HG13 | 2.05                     | 0.55              |
| 2:P:57:ASP:CB    | 2:P:60:ASP:CB    | 2.85                     | 0.55              |
| 1:M:37:GLU:OE1   | 1:M:64:ASN:ND2   | 2.34                     | 0.55              |
| 1:M:69:LYS:NZ    | 1:M:260:GLU:OE1  | 2.33                     | 0.55              |
| 3:N:248:ALA:HB2  | 3:N:257:VAL:HG21 | 1.88                     | 0.55              |
| 2:D:33:HIS:CG    | 2:D:337:ILE:HD13 | 2.42                     | 0.55              |
| 3:B:96:MET:HE2   | 3:B:137:TYR:HD2  | 1.71                     | 0.55              |
| 1:K:115:ILE:HD11 | 1:K:216:PRO:O    | 2.07                     | 0.55              |
| 1:M:277:PRO:O    | 1:M:280:LEU:N    | 2.39                     | 0.55              |
| 1:A:288:LEU:HA   | 1:A:291:MET:HE2  | 1.89                     | 0.55              |
| 3:B:264:ALA:O    | 2:H:13:GLY:N     | 2.40                     | 0.55              |
| 1:G:119:ARG:HG3  | 1:G:229:GLY:HA3  | 1.89                     | 0.55              |
| 1:M:134:VAL:CG2  | 1:M:137:VAL:CG2  | 2.85                     | 0.55              |
| 3:N:30:MET:HE1   | 3:N:291:MET:CG   | 2.11                     | 0.55              |
| 3:N:52:SER:CB    | 3:N:81:ILE:HD12  | 2.37                     | 0.55              |
| 1:C:177:MET:SD   | 2:D:135:TYR:CE1  | 3.00                     | 0.55              |
| 2:D:129:GLU:CG   | 2:D:132:GLU:CB   | 2.85                     | 0.55              |
| 1:A:244:GLY:O    | 1:A:279:ALA:HB2  | 2.06                     | 0.55              |
| 1:G:315:THR:OG1  | 1:G:317:ASP:OD1  | 2.24                     | 0.55              |
| 1:M:119:ARG:HG3  | 1:M:229:GLY:HA3  | 1.88                     | 0.55              |
| 3:N:60:GLU:O     | 3:N:61:GLU:HB2   | 2.07                     | 0.55              |
| 3:N:70:MET:HG3   | 3:N:266:TYR:CD2  | 2.42                     | 0.55              |
| 1:A:69:LYS:HD2   | 1:A:72:LEU:HD11  | 1.88                     | 0.54              |
| 1:G:11:PRO:HB2   | 1:G:17:PRO:HG3   | 1.88                     | 0.54              |
| 1:K:125:GLU:CD   | 2:L:135:TYR:OH   | 2.46                     | 0.54              |
| 2:L:248:LEU:N    | 2:L:248:LEU:HD23 | 2.22                     | 0.54              |
| 2:L:347:ILE:O    | 2:L:348:ASN:C    | 2.48                     | 0.54              |
| 1:M:46:GLY:N     | 1:M:49:GLY:O     | 2.40                     | 0.54              |
| 1:E:99:PRO:HB3   | 1:E:116:VAL:HG22 | 1.89                     | 0.54              |
| 3:F:116:GLY:HA3  | 3:F:319:ILE:HG22 | 1.88                     | 0.54              |
| 1:I:315:THR:OG1  | 1:I:317:ASP:OD1  | 2.25                     | 0.54              |
| 1:M:137:VAL:O    | 1:M:137:VAL:HG12 | 2.06                     | 0.54              |
| 3:N:189:LYS:C    | 3:N:190:LEU:HD23 | 2.33                     | 0.54              |
| 2:P:40:HIS:HE1   | 2:P:346:VAL:CG2  | 2.20                     | 0.54              |
| 2:D:128:ARG:HB2  | 2:D:235:ASN:HA   | 1.88                     | 0.54              |
| 2:H:91:SER:CB    | 2:H:94:ASN:CB    | 2.86                     | 0.54              |
| 3:F:47:GLN:O     | 3:F:49:HIS:HD2   | 1.89                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:L:58:GLU:CB    | 2:L:59:GLU:CB    | 2.85                     | 0.54              |
| 2:P:243:ASN:O    | 2:P:246:ALA:HB3  | 2.06                     | 0.54              |
| 1:C:206:ASP:N    | 1:C:206:ASP:OD1  | 2.40                     | 0.54              |
| 2:D:93:ASN:OD1   | 2:D:97:ARG:NH2   | 2.33                     | 0.54              |
| 1:A:103:ILE:HG21 | 1:A:308:ILE:HD13 | 1.89                     | 0.54              |
| 3:B:75:VAL:HG22  | 3:B:267:ALA:HB3  | 1.90                     | 0.54              |
| 1:E:119:ARG:HG3  | 1:E:229:GLY:HA3  | 1.89                     | 0.54              |
| 2:L:61:ILE:O     | 2:L:63:ASN:N     | 2.40                     | 0.54              |
| 3:J:254:ALA:HB1  | 3:J:273:ALA:CB   | 2.35                     | 0.54              |
| 1:A:314:LEU:HD23 | 1:A:318:LEU:HB3  | 1.90                     | 0.54              |
| 2:L:129:GLU:OE1  | 2:L:157:LYS:HG2  | 2.08                     | 0.54              |
| 1:O:106:TYR:CE1  | 1:O:318:LEU:HD11 | 2.41                     | 0.54              |
| 2:P:68:ILE:HG23  | 2:P:74:ALA:HB2   | 1.89                     | 0.54              |
| 2:D:126:ILE:HD13 | 2:D:241:VAL:HG12 | 1.90                     | 0.54              |
| 3:B:335:CYS:SG   | 3:B:336:HIS:N    | 2.81                     | 0.54              |
| 2:H:257:GLY:N    | 2:H:268:GLU:O    | 2.41                     | 0.54              |
| 3:J:202:VAL:HA   | 3:J:205:LEU:HD12 | 1.90                     | 0.54              |
| 1:O:157:PHE:CE2  | 1:O:192:ALA:HA   | 2.43                     | 0.54              |
| 1:C:173:LYS:HD2  | 1:C:205:LEU:HD23 | 1.90                     | 0.54              |
| 1:A:7:VAL:CG2    | 1:A:34:ILE:HG23  | 2.37                     | 0.54              |
| 1:G:318:LEU:HB2  | 1:G:319:GLY:HA2  | 1.89                     | 0.54              |
| 2:H:255:VAL:CA   | 2:H:270:ALA:HB2  | 2.38                     | 0.54              |
| 1:E:93:LEU:HD11  | 1:E:258:ILE:HD12 | 1.89                     | 0.54              |
| 1:M:99:PRO:HD2   | 1:M:247:PRO:HG2  | 1.90                     | 0.54              |
| 1:A:49:GLY:HA3   | 1:A:51:TRP:CZ3   | 2.43                     | 0.54              |
| 2:H:129:GLU:OE2  | 2:H:131:THR:N    | 2.41                     | 0.54              |
| 2:H:182:LYS:HE3  | 2:H:185:ILE:CD1  | 2.38                     | 0.54              |
| 3:F:19:MET:HB3   | 3:F:48:GLU:HB2   | 1.90                     | 0.54              |
| 2:P:190:ASP:OD2  | 2:P:237:TYR:HE2  | 1.91                     | 0.54              |
| 2:P:282:ASN:HB3  | 2:P:333:THR:HG23 | 1.89                     | 0.54              |
| 1:M:11:PRO:HB2   | 1:M:17:PRO:HG3   | 1.88                     | 0.54              |
| 3:N:61:GLU:CA    | 3:N:63:LEU:CD2   | 2.85                     | 0.54              |
| 2:D:259:ASN:ND2  | 2:D:268:GLU:OE1  | 2.39                     | 0.54              |
| 1:K:53:ILE:HG22  | 1:K:86:LEU:HD13  | 1.90                     | 0.54              |
| 1:K:288:LEU:HD22 | 1:K:293:LEU:HD12 | 1.90                     | 0.54              |
| 2:P:98:THR:C     | 2:P:100:LEU:N    | 2.65                     | 0.54              |
| 3:B:30:MET:HE1   | 3:B:77:ILE:HG13  | 1.89                     | 0.53              |
| 1:G:110:TYR:CZ   | 2:H:118:ARG:HD2  | 2.43                     | 0.53              |
| 1:E:231:ILE:HG22 | 3:F:217:ASP:HB3  | 1.90                     | 0.53              |
| 3:J:153:LYS:HD3  | 3:J:188:MET:HE1  | 1.90                     | 0.53              |
| 1:M:46:GLY:CA    | 1:M:52:MET:CG    | 2.85                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:106:VAL:HG13 | 2:D:127:VAL:HG22 | 1.89                     | 0.53              |
| 3:F:61:GLU:C     | 3:F:63:LEU:N     | 2.64                     | 0.53              |
| 3:F:217:ASP:N    | 3:F:217:ASP:OD1  | 2.39                     | 0.53              |
| 2:L:194:LEU:HD21 | 2:L:198:ARG:HH11 | 1.73                     | 0.53              |
| 2:L:254:LEU:HD21 | 2:L:285:ASN:ND2  | 2.24                     | 0.53              |
| 1:I:331:ILE:O    | 1:I:335:VAL:HG13 | 2.07                     | 0.53              |
| 3:J:109:VAL:HG21 | 3:J:244:ASP:OD1  | 2.08                     | 0.53              |
| 3:J:184:LYS:N    | 3:J:192:ASP:OD2  | 2.38                     | 0.53              |
| 1:C:324:CYS:O    | 1:C:328:THR:OG1  | 2.19                     | 0.53              |
| 2:H:181:HIS:NE2  | 2:H:211:ASN:HB2  | 2.24                     | 0.53              |
| 1:E:26:ILE:HG12  | 1:E:332:CYS:SG   | 2.48                     | 0.53              |
| 3:F:25:VAL:HG13  | 3:F:281:VAL:O    | 2.09                     | 0.53              |
| 2:L:190:ASP:OD2  | 2:L:237:TYR:OH   | 2.25                     | 0.53              |
| 1:O:88:ARG:HD2   | 1:O:121:ASN:O    | 2.09                     | 0.53              |
| 1:M:229:GLY:O    | 1:M:233:SER:OG   | 2.23                     | 0.53              |
| 3:N:287:ASN:HB2  | 3:N:326:THR:OG1  | 2.07                     | 0.53              |
| 2:D:142:SER:OG   | 1:A:143:LEU:HD22 | 2.08                     | 0.53              |
| 2:L:143:VAL:HG22 | 2:L:144:ALA:N    | 2.24                     | 0.53              |
| 1:I:175:ASN:HB3  | 3:J:84:PRO:O     | 2.08                     | 0.53              |
| 3:J:283:ARG:O    | 3:J:285:ILE:HG22 | 2.08                     | 0.53              |
| 1:O:73:LYS:HD3   | 1:O:265:THR:HG21 | 1.89                     | 0.53              |
| 2:P:29:GLU:OE2   | 2:P:280:ASN:CA   | 2.52                     | 0.53              |
| 1:A:213:VAL:HG21 | 3:B:246:LEU:HD23 | 1.91                     | 0.53              |
| 1:K:26:ILE:HG12  | 1:K:332:CYS:SG   | 2.49                     | 0.53              |
| 1:O:34:ILE:CG2   | 1:O:36:TRP:CE2   | 2.92                     | 0.53              |
| 2:P:66:MET:CA    | 2:P:69:ARG:CG    | 1.99                     | 0.53              |
| 2:P:86:PRO:N     | 2:P:87:PRO:CA    | 2.71                     | 0.53              |
| 2:D:63:ASN:HB3   | 3:F:207:PRO:HG3  | 1.89                     | 0.53              |
| 2:H:129:GLU:CD   | 2:H:130:ASN:H    | 2.16                     | 0.53              |
| 2:H:213:ILE:O    | 2:H:217:THR:OG1  | 2.23                     | 0.53              |
| 3:F:102:LEU:O    | 3:F:263:SER:CB   | 2.56                     | 0.53              |
| 1:E:157:PHE:HE1  | 1:E:198:ILE:HB   | 1.74                     | 0.53              |
| 1:I:92:ASP:OD2   | 1:I:151:ARG:NH1  | 2.32                     | 0.53              |
| 2:P:35:LYS:HA    | 2:P:38:PHE:HB2   | 1.91                     | 0.53              |
| 2:P:93:ASN:CG    | 2:P:97:ARG:NH2   | 2.67                     | 0.53              |
| 3:N:19:MET:HE1   | 3:N:48:GLU:OE2   | 2.07                     | 0.53              |
| 3:N:119:THR:OG1  | 3:N:121:HIS:O    | 2.27                     | 0.53              |
| 3:N:299:LEU:HB2  | 3:N:308:SER:HB2  | 1.91                     | 0.53              |
| 3:B:105:PHE:O    | 3:B:131:GLU:HA   | 2.09                     | 0.53              |
| 2:H:96:LEU:N     | 2:H:96:LEU:HD23  | 2.23                     | 0.53              |
| 2:H:316:SER:HB3  | 2:H:340:VAL:HG22 | 1.91                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:150:LYS:O    | 1:K:154:GLU:HG3  | 2.08                     | 0.53              |
| 2:L:223:SER:OG   | 2:L:224:ARG:N    | 2.42                     | 0.53              |
| 2:L:253:GLY:CA   | 2:L:288:ALA:HB2  | 2.35                     | 0.53              |
| 3:J:138:SER:CB   | 3:J:140:LEU:HD12 | 2.38                     | 0.53              |
| 2:P:148:GLU:OE2  | 3:N:142:HIS:NE2  | 2.35                     | 0.53              |
| 3:B:217:ASP:OD1  | 3:B:217:ASP:N    | 2.40                     | 0.53              |
| 1:G:243:LEU:HB3  | 1:G:262:VAL:HG23 | 1.91                     | 0.53              |
| 3:F:19:MET:HG3   | 3:F:30:MET:HE3   | 1.90                     | 0.53              |
| 2:L:20:MET:HE1   | 2:L:35:LYS:HE3   | 1.91                     | 0.53              |
| 1:I:85:LEU:O     | 1:I:87:LEU:N     | 2.41                     | 0.53              |
| 1:O:145:THR:HG22 | 2:P:146:VAL:HG22 | 1.91                     | 0.53              |
| 2:P:129:GLU:OE2  | 2:P:131:THR:N    | 2.41                     | 0.53              |
| 2:P:319:ASN:ND2  | 2:P:322:MET:HG2  | 2.24                     | 0.53              |
| 1:A:80:HIS:CG    | 1:A:81:PRO:HD2   | 2.43                     | 0.53              |
| 2:L:90:LYS:O     | 2:L:92:ARG:N     | 2.42                     | 0.53              |
| 1:O:7:VAL:HG22   | 1:O:66:MET:HB2   | 1.91                     | 0.53              |
| 1:O:167:ASN:O    | 1:O:220:ASP:HB3  | 2.09                     | 0.53              |
| 2:P:6:ILE:HD12   | 2:P:7:PRO:HD2    | 1.91                     | 0.53              |
| 3:J:76:ALA:HB3   | 3:J:268:VAL:HG12 | 1.91                     | 0.52              |
| 1:O:132:VAL:HG23 | 1:O:132:VAL:O    | 2.09                     | 0.52              |
| 2:P:17:THR:HB    | 2:P:71:ASN:HD21  | 1.74                     | 0.52              |
| 2:P:150:LEU:CD1  | 1:M:131:HIS:CE1  | 2.92                     | 0.52              |
| 2:H:21:ILE:HG13  | 2:H:50:VAL:HG13  | 1.92                     | 0.52              |
| 3:F:25:VAL:HG21  | 3:F:286:ALA:CB   | 2.40                     | 0.52              |
| 1:M:98:ARG:NH1   | 1:M:233:SER:HB2  | 2.24                     | 0.52              |
| 1:E:235:LEU:HD21 | 3:F:246:LEU:HD11 | 1.91                     | 0.52              |
| 3:F:254:ALA:CB   | 3:F:273:ALA:HB2  | 2.29                     | 0.52              |
| 1:I:50:LYS:CB    | 1:I:80:HIS:CD2   | 2.92                     | 0.52              |
| 1:I:118:ILE:HG22 | 1:I:152:ILE:HD11 | 1.91                     | 0.52              |
| 3:J:20:LEU:O     | 3:J:78:ILE:CG2   | 2.54                     | 0.52              |
| 3:J:254:ALA:CA   | 3:J:273:ALA:CB   | 2.87                     | 0.52              |
| 1:O:175:ASN:HB3  | 1:O:204:TYR:HE1  | 1.74                     | 0.52              |
| 2:P:33:HIS:O     | 2:P:37:VAL:N     | 2.31                     | 0.52              |
| 2:P:57:ASP:O     | 2:P:60:ASP:N     | 2.43                     | 0.52              |
| 2:P:135:TYR:HD1  | 2:P:151:LYS:HA   | 1.73                     | 0.52              |
| 2:P:206:GLN:OE1  | 2:P:206:GLN:N    | 2.42                     | 0.52              |
| 3:N:257:VAL:CB   | 3:N:273:ALA:HB2  | 2.40                     | 0.52              |
| 3:B:15:PHE:HZ    | 2:H:350:ARG:N    | 2.07                     | 0.52              |
| 3:J:83:THR:CG2   | 3:J:84:PRO:CD    | 2.87                     | 0.52              |
| 3:J:83:THR:CB    | 3:J:84:PRO:HD3   | 2.39                     | 0.52              |
| 3:J:215:ILE:H    | 3:J:215:ILE:HD12 | 1.73                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:P:138:LEU:HD22 | 1:M:131:HIS:CG   | 2.38                     | 0.52              |
| 3:B:192:ASP:OD2  | 3:B:239:TYR:OH   | 2.23                     | 0.52              |
| 2:H:336:ALA:O    | 2:H:340:VAL:HG23 | 2.09                     | 0.52              |
| 1:I:125:GLU:OE2  | 1:I:142:LYS:HG3  | 2.09                     | 0.52              |
| 2:P:128:ARG:NE   | 2:P:242:ASN:OD1  | 2.43                     | 0.52              |
| 2:D:115:VAL:HG22 | 2:D:323:HIS:CE1  | 2.45                     | 0.52              |
| 2:H:312:ALA:O    | 2:H:315:ALA:HB3  | 2.10                     | 0.52              |
| 3:F:58:ALA:C     | 3:F:60:GLU:HA    | 2.35                     | 0.52              |
| 2:L:57:ASP:CB    | 2:L:60:ASP:C     | 2.83                     | 0.52              |
| 3:J:178:LYS:O    | 3:J:231:ASP:HB3  | 2.09                     | 0.52              |
| 2:P:9:SER:OG     | 2:P:10:ALA:N     | 2.42                     | 0.52              |
| 2:P:61:ILE:CG2   | 2:P:62:ARG:N     | 2.72                     | 0.52              |
| 1:M:178:ARG:CD   | 3:N:86:GLU:CB    | 2.80                     | 0.52              |
| 2:H:62:ARG:C     | 2:H:64:ALA:N     | 2.67                     | 0.52              |
| 3:J:183:HIS:CE1  | 3:J:185:ALA:CB   | 2.92                     | 0.52              |
| 1:O:34:ILE:HG21  | 1:O:36:TRP:CZ2   | 2.45                     | 0.52              |
| 1:O:137:VAL:HG11 | 1:M:134:VAL:HG11 | 1.92                     | 0.52              |
| 2:P:39:ARG:NH1   | 2:P:39:ARG:CB    | 2.73                     | 0.52              |
| 3:N:17:VAL:HG13  | 3:N:76:ALA:HA    | 1.91                     | 0.52              |
| 1:C:85:LEU:HD12  | 1:C:88:ARG:HD3   | 1.92                     | 0.52              |
| 2:P:66:MET:CB    | 2:P:69:ARG:CG    | 2.83                     | 0.52              |
| 3:N:52:SER:HB2   | 3:N:81:ILE:HD12  | 1.92                     | 0.52              |
| 3:F:103:ASP:C    | 3:F:263:SER:CB   | 2.82                     | 0.52              |
| 3:J:82:HIS:O     | 3:J:83:THR:HG22  | 2.09                     | 0.52              |
| 3:B:67:LEU:O     | 3:B:70:MET:CA    | 2.58                     | 0.52              |
| 3:B:95:ASP:OD1   | 3:B:99:ARG:CZ    | 2.58                     | 0.52              |
| 1:G:91:PHE:HB3   | 1:G:256:VAL:HG11 | 1.90                     | 0.52              |
| 1:I:68:LEU:HB2   | 1:I:287:MET:HE1  | 1.91                     | 0.52              |
| 1:I:125:GLU:OE1  | 1:I:142:LYS:NZ   | 2.43                     | 0.52              |
| 3:J:315:VAL:HA   | 3:J:342:ILE:HD11 | 1.91                     | 0.52              |
| 1:O:125:GLU:CD   | 1:O:125:GLU:H    | 2.15                     | 0.52              |
| 2:P:129:GLU:HB3  | 2:P:132:GLU:CB   | 2.40                     | 0.52              |
| 1:K:133:ILE:CG1  | 1:I:133:ILE:HD12 | 2.33                     | 0.51              |
| 3:J:96:MET:O     | 3:J:100:ARG:N    | 2.42                     | 0.51              |
| 1:O:208:VAL:O    | 1:O:212:MET:N    | 2.40                     | 0.51              |
| 1:A:95:ALA:HB3   | 1:A:251:ILE:HB   | 1.91                     | 0.51              |
| 2:H:256:ALA:HB2  | 2:H:291:LEU:HB3  | 1.92                     | 0.51              |
| 1:K:268:ASP:OD1  | 1:K:268:ASP:N    | 2.42                     | 0.51              |
| 2:L:197:CYS:O    | 2:L:201:ALA:N    | 2.42                     | 0.51              |
| 2:P:336:ALA:O    | 2:P:340:VAL:HG23 | 2.10                     | 0.51              |
| 3:N:21:PRO:CG    | 3:N:22:GLY:N     | 2.73                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:N:63:LEU:CD2   | 3:N:63:LEU:N     | 2.72                     | 0.51              |
| 1:C:21:ALA:HA    | 1:C:24:MET:HE2   | 1.91                     | 0.51              |
| 1:E:280:LEU:HD12 | 1:E:283:SER:HB2  | 1.92                     | 0.51              |
| 3:J:265:GLU:HA   | 2:P:14:GLY:CA    | 2.40                     | 0.51              |
| 1:O:138:VAL:CG2  | 1:O:139:ALA:H    | 2.16                     | 0.51              |
| 1:O:174:ALA:HA   | 1:O:181:ASP:CG   | 2.35                     | 0.51              |
| 2:P:66:MET:CB    | 2:P:69:ARG:HD3   | 2.41                     | 0.51              |
| 2:P:66:MET:O     | 2:P:70:ARG:N     | 2.43                     | 0.51              |
| 3:F:59:SER:N     | 3:F:60:GLU:CA    | 2.73                     | 0.51              |
| 3:F:248:ALA:HB1  | 3:F:254:ALA:HA   | 1.91                     | 0.51              |
| 1:I:80:HIS:CD2   | 1:I:81:PRO:CD    | 2.82                     | 0.51              |
| 3:J:49:HIS:NE2   | 3:J:69:SER:OG    | 2.43                     | 0.51              |
| 3:J:60:GLU:O     | 3:J:63:LEU:N     | 2.44                     | 0.51              |
| 2:D:28:PRO:O     | 2:D:32:LEU:HG    | 2.10                     | 0.51              |
| 1:A:173:LYS:NZ   | 1:A:206:ASP:OD2  | 2.44                     | 0.51              |
| 1:E:293:LEU:O    | 1:E:297:ALA:N    | 2.42                     | 0.51              |
| 3:F:140:LEU:O    | 3:F:141:GLU:CG   | 2.59                     | 0.51              |
| 1:I:288:LEU:HB3  | 1:I:293:LEU:HB2  | 1.91                     | 0.51              |
| 2:P:38:PHE:HA    | 2:P:41:ALA:HB3   | 1.90                     | 0.51              |
| 2:P:90:LYS:HA    | 2:P:95:ILE:CD1   | 2.41                     | 0.51              |
| 1:C:153:ALA:HB1  | 1:C:191:VAL:HG11 | 1.92                     | 0.51              |
| 3:F:122:ASN:O    | 3:F:228:TYR:OH   | 2.13                     | 0.51              |
| 3:F:179:VAL:HG12 | 3:F:232:VAL:HB   | 1.93                     | 0.51              |
| 1:K:15:ILE:HG22  | 1:K:270:ALA:HA   | 1.93                     | 0.51              |
| 2:L:55:ASN:O     | 2:L:56:ALA:CB    | 2.59                     | 0.51              |
| 1:I:68:LEU:HD12  | 1:I:259:PHE:O    | 2.10                     | 0.51              |
| 3:N:176:ARG:HD2  | 3:N:231:ASP:OD1  | 2.10                     | 0.51              |
| 1:A:227:LEU:O    | 1:A:231:ILE:HG12 | 2.11                     | 0.51              |
| 3:B:265:GLU:C    | 2:H:13:GLY:HA2   | 2.36                     | 0.51              |
| 3:B:265:GLU:CA   | 2:H:13:GLY:HA2   | 2.40                     | 0.51              |
| 3:B:271:THR:HG23 | 3:B:291:MET:HE3  | 1.93                     | 0.51              |
| 3:F:271:THR:HG22 | 3:F:291:MET:HG2  | 1.92                     | 0.51              |
| 1:K:308:ILE:HA   | 1:K:314:LEU:HD21 | 1.92                     | 0.51              |
| 1:I:137:VAL:O    | 1:I:137:VAL:HG12 | 2.11                     | 0.51              |
| 1:O:132:VAL:HG12 | 1:O:138:VAL:CG2  | 2.40                     | 0.51              |
| 1:M:46:GLY:HA2   | 1:M:52:MET:SD    | 2.50                     | 0.51              |
| 3:N:215:ILE:HD12 | 3:N:215:ILE:H    | 1.75                     | 0.51              |
| 1:C:206:ASP:HB3  | 2:D:239:ASN:HB3  | 1.93                     | 0.51              |
| 2:D:319:ASN:ND2  | 2:D:322:MET:HG2  | 2.25                     | 0.51              |
| 3:F:19:MET:CE    | 3:F:48:GLU:CD    | 2.83                     | 0.51              |
| 3:F:289:THR:O    | 3:F:293:LEU:HG   | 2.11                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:116:VAL:HG11 | 1:K:159:TYR:CE2  | 2.46                     | 0.51              |
| 1:O:134:VAL:CG2  | 1:O:137:VAL:HB   | 2.41                     | 0.51              |
| 1:O:318:LEU:N    | 1:O:318:LEU:CD2  | 2.74                     | 0.51              |
| 2:P:126:ILE:HG21 | 2:P:242:ASN:HD21 | 1.76                     | 0.51              |
| 2:D:140:HIS:CG   | 1:A:129:ILE:HG21 | 2.46                     | 0.51              |
| 1:G:129:ILE:HD13 | 3:F:142:HIS:HB2  | 1.93                     | 0.51              |
| 3:F:19:MET:HE3   | 3:F:48:GLU:CD    | 2.36                     | 0.51              |
| 3:F:214:MET:HG2  | 3:F:219:CYS:HB2  | 1.92                     | 0.51              |
| 2:P:38:PHE:O     | 2:P:41:ALA:N     | 2.43                     | 0.51              |
| 2:P:49:GLU:O     | 2:P:50:VAL:HG13  | 2.11                     | 0.51              |
| 2:P:90:LYS:HA    | 2:P:95:ILE:CG1   | 2.41                     | 0.51              |
| 2:P:94:ASN:O     | 2:P:97:ARG:HG2   | 2.11                     | 0.51              |
| 2:P:135:TYR:CE1  | 2:P:151:LYS:N    | 2.79                     | 0.51              |
| 1:M:265:THR:HG23 | 1:M:267:PRO:HD3  | 1.93                     | 0.51              |
| 3:B:157:ARG:CG   | 3:B:198:CYS:SG   | 2.98                     | 0.51              |
| 2:L:91:SER:O     | 2:L:91:SER:OG    | 2.29                     | 0.51              |
| 2:L:255:VAL:HB   | 2:L:270:ALA:CB   | 2.40                     | 0.51              |
| 3:J:165:LYS:HD2  | 2:P:7:PRO:HG3    | 1.93                     | 0.51              |
| 2:P:279:ALA:O    | 2:P:280:ASN:HB2  | 2.09                     | 0.51              |
| 2:D:30:LEU:O     | 2:D:34:VAL:HG23  | 2.10                     | 0.50              |
| 3:B:67:LEU:O     | 3:B:70:MET:HB2   | 2.11                     | 0.50              |
| 3:B:263:SER:O    | 2:H:13:GLY:N     | 2.44                     | 0.50              |
| 3:F:77:ILE:HG21  | 3:F:298:MET:HE1  | 1.93                     | 0.50              |
| 2:P:57:ASP:CB    | 2:P:60:ASP:CG    | 2.84                     | 0.50              |
| 1:C:9:LEU:HD12   | 1:C:10:ILE:H     | 1.77                     | 0.50              |
| 2:D:129:GLU:CD   | 2:D:131:THR:H    | 2.19                     | 0.50              |
| 1:A:177:MET:HE1  | 1:A:228:TYR:OH   | 2.12                     | 0.50              |
| 1:E:31:LYS:O     | 1:E:296:HIS:NE2  | 2.44                     | 0.50              |
| 1:O:180:SER:HG   | 1:O:181:ASP:H    | 1.52                     | 0.50              |
| 1:O:215:ASP:O    | 1:O:218:GLN:HG2  | 2.11                     | 0.50              |
| 2:P:275:GLY:O    | 2:P:278:ILE:HB   | 2.10                     | 0.50              |
| 3:N:21:PRO:CD    | 3:N:22:GLY:N     | 2.73                     | 0.50              |
| 3:N:73:ASN:C     | 3:N:75:VAL:H     | 2.19                     | 0.50              |
| 3:N:256:VAL:O    | 3:N:258:PRO:HD3  | 2.10                     | 0.50              |
| 1:O:299:ARG:HD3  | 1:O:338:LEU:HD22 | 1.93                     | 0.50              |
| 2:P:86:PRO:CB    | 2:P:87:PRO:C     | 2.84                     | 0.50              |
| 2:P:296:MET:HE2  | 2:P:297:LEU:HD23 | 1.94                     | 0.50              |
| 1:M:88:ARG:HA    | 1:M:93:LEU:HB2   | 1.92                     | 0.50              |
| 2:D:338:GLN:OE1  | 2:D:342:ARG:NH2  | 2.44                     | 0.50              |
| 2:H:255:VAL:CA   | 2:H:270:ALA:CB   | 2.84                     | 0.50              |
| 1:E:225:PRO:HD2  | 1:E:228:TYR:CD2  | 2.45                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:288:LEU:HD12 | 1:O:297:ALA:HA   | 1.94                     | 0.50              |
| 2:P:29:GLU:CD    | 2:P:280:ASN:HA   | 2.35                     | 0.50              |
| 2:P:281:LYS:CB   | 2:P:283:ILE:CD1  | 2.89                     | 0.50              |
| 1:E:173:LYS:HE2  | 3:F:137:TYR:OH   | 2.12                     | 0.50              |
| 3:F:220:CYS:HA   | 3:F:223:LEU:HD12 | 1.93                     | 0.50              |
| 1:I:50:LYS:CB    | 1:I:80:HIS:HD2   | 2.25                     | 0.50              |
| 3:J:54:VAL:CB    | 3:J:88:LYS:HE3   | 2.41                     | 0.50              |
| 3:J:60:GLU:O     | 3:J:64:GLU:N     | 2.41                     | 0.50              |
| 2:P:53:SER:O     | 2:P:56:ALA:N     | 2.44                     | 0.50              |
| 2:P:94:ASN:HA    | 2:P:97:ARG:CG    | 2.40                     | 0.50              |
| 1:C:15:ILE:HG22  | 1:C:270:ALA:HA   | 1.93                     | 0.50              |
| 1:C:15:ILE:HD12  | 1:C:275:ALA:HB1  | 1.93                     | 0.50              |
| 1:A:172:HIS:NE2  | 1:A:202:GLU:OE1  | 2.44                     | 0.50              |
| 2:H:316:SER:N    | 2:H:343:HIS:ND1  | 2.59                     | 0.50              |
| 1:E:99:PRO:HA    | 1:E:116:VAL:HA   | 1.93                     | 0.50              |
| 1:K:97:VAL:HG22  | 1:K:118:ILE:HG12 | 1.93                     | 0.50              |
| 1:K:130:GLU:OE1  | 2:L:189:GLY:N    | 2.35                     | 0.50              |
| 1:K:318:LEU:HB2  | 1:K:319:GLY:HA2  | 1.93                     | 0.50              |
| 3:J:160:SER:HG   | 3:J:198:CYS:HG   | 1.58                     | 0.50              |
| 3:J:180:THR:HG23 | 3:J:212:GLU:HB2  | 1.93                     | 0.50              |
| 1:O:118:ILE:HD13 | 1:O:156:ALA:HA   | 1.92                     | 0.50              |
| 3:N:63:LEU:CD2   | 3:N:64:GLU:N     | 2.73                     | 0.50              |
| 2:D:115:VAL:HG21 | 2:D:327:ILE:HD12 | 1.94                     | 0.50              |
| 2:D:336:ALA:HA   | 2:D:339:ASP:HB3  | 1.93                     | 0.50              |
| 1:G:32:ALA:O     | 1:G:34:ILE:N     | 2.45                     | 0.50              |
| 1:E:244:GLY:CA   | 1:E:263:HIS:CB   | 2.80                     | 0.50              |
| 1:E:303:ALA:HB1  | 1:E:334:ARG:HB3  | 1.92                     | 0.50              |
| 3:F:19:MET:SD    | 3:F:30:MET:CB    | 2.96                     | 0.50              |
| 2:L:24:ASP:OD2   | 2:L:79:ILE:C     | 2.53                     | 0.50              |
| 2:L:106:VAL:HG22 | 2:L:127:VAL:HG22 | 1.94                     | 0.50              |
| 2:L:298:ASP:OD1  | 2:L:303:HIS:ND1  | 2.45                     | 0.50              |
| 3:J:20:LEU:HB2   | 3:J:78:ILE:HG21  | 0.52                     | 0.50              |
| 3:J:83:THR:CB    | 3:J:84:PRO:CD    | 2.90                     | 0.50              |
| 3:B:180:THR:HG23 | 3:B:212:GLU:HB2  | 1.94                     | 0.50              |
| 3:B:219:CYS:O    | 3:B:223:LEU:HG   | 2.12                     | 0.50              |
| 3:B:300:ARG:HG3  | 3:B:308:SER:CB   | 2.37                     | 0.50              |
| 1:E:74:THR:CB    | 1:E:75:PRO:HD2   | 2.40                     | 0.50              |
| 1:E:240:ILE:CG1  | 1:E:246:THR:CG2  | 2.88                     | 0.50              |
| 3:F:19:MET:HE2   | 3:F:48:GLU:OE1   | 2.12                     | 0.50              |
| 1:K:119:ARG:HB2  | 1:K:229:GLY:HA3  | 1.94                     | 0.50              |
| 3:J:328:ASP:OD1  | 3:J:328:ASP:N    | 2.45                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:281:LEU:HD11 | 1:O:300:ILE:HG21 | 1.94                     | 0.50              |
| 1:M:125:GLU:HA   | 1:M:142:LYS:HA   | 1.93                     | 0.50              |
| 1:C:288:LEU:HD22 | 1:C:293:LEU:HD12 | 1.92                     | 0.50              |
| 1:G:56:GLU:O     | 1:G:60:SER:OG    | 2.25                     | 0.50              |
| 2:H:76:LYS:CE    | 2:H:268:GLU:HB3  | 2.42                     | 0.50              |
| 1:E:98:ARG:NH1   | 1:E:243:LEU:CD2  | 2.75                     | 0.50              |
| 2:P:233:MET:CE   | 2:P:241:VAL:HG21 | 2.40                     | 0.50              |
| 1:C:99:PRO:HA    | 1:C:116:VAL:HA   | 1.94                     | 0.49              |
| 1:C:106:TYR:HE2  | 1:C:241:GLY:HA3  | 1.77                     | 0.49              |
| 2:D:140:HIS:CE1  | 1:A:131:HIS:CD2  | 3.00                     | 0.49              |
| 1:A:127:SER:OG   | 1:A:129:ILE:HG12 | 2.12                     | 0.49              |
| 3:B:93:SER:O     | 3:B:96:MET:SD    | 2.70                     | 0.49              |
| 3:B:96:MET:HE2   | 3:B:137:TYR:CD2  | 2.47                     | 0.49              |
| 3:B:269:PHE:CZ   | 3:B:298:MET:HA   | 2.47                     | 0.49              |
| 1:E:174:ALA:O    | 1:E:178:ARG:HA   | 2.12                     | 0.49              |
| 2:L:342:ARG:C    | 2:L:344:ILE:H    | 2.19                     | 0.49              |
| 1:C:317:ASP:OD1  | 1:C:317:ASP:N    | 2.45                     | 0.49              |
| 2:D:65:ILE:O     | 2:D:66:MET:C     | 2.52                     | 0.49              |
| 3:B:141:GLU:CG   | 3:B:151:CYS:SG   | 3.00                     | 0.49              |
| 2:H:267:PHE:CE2  | 2:H:296:MET:HG2  | 2.44                     | 0.49              |
| 3:F:59:SER:CB    | 3:F:60:GLU:C     | 2.85                     | 0.49              |
| 3:J:70:MET:SD    | 3:J:76:ALA:HB2   | 2.52                     | 0.49              |
| 3:N:74:LYS:O     | 3:N:266:TYR:HA   | 2.12                     | 0.49              |
| 1:C:122:THR:OG1  | 1:C:123:GLU:N    | 2.43                     | 0.49              |
| 1:A:175:ASN:HB3  | 1:A:204:TYR:HE2  | 1.78                     | 0.49              |
| 1:K:206:ASP:N    | 1:K:206:ASP:OD1  | 2.46                     | 0.49              |
| 1:I:129:ILE:CB   | 1:I:141:ILE:CG2  | 2.90                     | 0.49              |
| 1:O:174:ALA:CA   | 1:O:181:ASP:CG   | 2.85                     | 0.49              |
| 1:O:229:GLY:O    | 1:O:233:SER:OG   | 2.18                     | 0.49              |
| 1:O:330:GLU:HA   | 1:O:333:ARG:HD3  | 1.94                     | 0.49              |
| 1:A:16:GLY:O     | 1:A:20:SER:OG    | 2.18                     | 0.49              |
| 3:B:74:LYS:O     | 3:B:266:TYR:HA   | 2.13                     | 0.49              |
| 1:E:83:MET:SD    | 1:E:83:MET:C     | 2.94                     | 0.49              |
| 1:K:9:LEU:HD12   | 1:K:10:ILE:H     | 1.77                     | 0.49              |
| 2:L:255:VAL:O    | 2:L:270:ALA:HB2  | 2.13                     | 0.49              |
| 1:O:171:VAL:HG13 | 1:O:208:VAL:HG21 | 1.94                     | 0.49              |
| 1:M:64:ASN:O     | 1:M:66:MET:N     | 2.40                     | 0.49              |
| 3:N:340:GLU:HA   | 3:N:343:CYS:HB2  | 1.93                     | 0.49              |
| 2:D:60:ASP:HA    | 2:D:63:ASN:OD1   | 2.12                     | 0.49              |
| 1:A:330:GLU:HA   | 1:A:333:ARG:HG2  | 1.94                     | 0.49              |
| 3:B:77:ILE:HG23  | 3:B:298:MET:SD   | 2.43                     | 0.49              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:G:66:MET:HE3  | 1:G:287:MET:HG3  | 1.94                     | 0.49              |
| 1:G:237:ALA:O   | 1:G:240:ILE:HG12 | 2.13                     | 0.49              |
| 2:H:181:HIS:HA  | 2:H:237:TYR:HE2  | 1.78                     | 0.49              |
| 1:E:235:LEU:HG  | 3:F:220:CYS:HB3  | 1.94                     | 0.49              |
| 3:F:326:THR:OG1 | 3:F:328:ASP:OD1  | 2.23                     | 0.49              |
| 2:L:140:HIS:HD2 | 3:J:150:GLU:OE2  | 1.81                     | 0.49              |
| 2:L:259:ASN:ND2 | 2:L:268:GLU:OE1  | 2.44                     | 0.49              |
| 3:J:136:GLU:O   | 3:J:138:SER:N    | 2.45                     | 0.49              |
| 1:M:8:THR:HA    | 1:M:37:GLU:HB3   | 1.95                     | 0.49              |
| 1:C:144:ILE:O   | 2:D:147:VAL:HG12 | 2.12                     | 0.49              |
| 2:D:19:THR:CB   | 2:D:74:ALA:HB2   | 2.42                     | 0.49              |
| 3:B:300:ARG:HB3 | 3:B:300:ARG:NH1  | 2.28                     | 0.49              |
| 1:E:130:GLU:HB2 | 3:F:190:LEU:HD12 | 1.95                     | 0.49              |
| 3:F:104:LEU:N   | 3:F:263:SER:CB   | 2.76                     | 0.49              |
| 1:K:53:ILE:HD13 | 1:K:90:THR:HG21  | 1.95                     | 0.49              |
| 2:L:30:LEU:O    | 2:L:34:VAL:HG23  | 2.12                     | 0.49              |
| 1:O:215:ASP:OD1 | 1:O:217:SER:OG   | 2.29                     | 0.49              |
| 2:D:163:GLU:OE1 | 2:D:203:ARG:NH2  | 2.45                     | 0.49              |
| 1:A:37:GLU:OE1  | 1:A:60:SER:OG    | 2.31                     | 0.49              |
| 2:H:33:HIS:HB3  | 2:H:337:ILE:HG12 | 1.95                     | 0.49              |
| 1:E:237:ALA:O   | 1:E:240:ILE:HG13 | 2.13                     | 0.49              |
| 1:K:41:VAL:HA   | 1:K:54:PRO:HG2   | 1.95                     | 0.49              |
| 2:L:58:GLU:N    | 2:L:59:GLU:C     | 2.71                     | 0.49              |
| 2:L:62:ARG:HA   | 2:L:65:ILE:CD1   | 2.43                     | 0.49              |
| 3:J:136:GLU:C   | 3:J:138:SER:H    | 2.21                     | 0.49              |
| 2:P:21:ILE:HD13 | 2:P:76:LYS:HB3   | 1.94                     | 0.49              |
| 2:P:43:VAL:CG2  | 2:P:44:PRO:CG    | 2.75                     | 0.49              |
| 2:P:76:LYS:NZ   | 2:P:268:GLU:OE2  | 2.39                     | 0.49              |
| 1:M:96:ASN:HB3  | 1:M:119:ARG:HB3  | 1.94                     | 0.49              |
| 1:A:7:VAL:CG2   | 1:A:34:ILE:HD12  | 2.42                     | 0.49              |
| 2:H:140:HIS:CD2 | 1:E:129:ILE:HG21 | 2.47                     | 0.49              |
| 1:K:287:MET:HG2 | 1:K:291:MET:HE2  | 1.94                     | 0.49              |
| 2:P:136:SER:C   | 2:P:137:SER:HG   | 2.07                     | 0.49              |
| 1:M:227:LEU:O   | 1:M:231:ILE:HG12 | 2.12                     | 0.49              |
| 1:M:228:TYR:HA  | 1:M:231:ILE:HD11 | 1.95                     | 0.49              |
| 2:D:286:PRO:O   | 2:D:290:LEU:HG   | 2.12                     | 0.49              |
| 3:B:165:LYS:HG3 | 2:H:12:TYR:OH    | 2.13                     | 0.49              |
| 3:B:199:CYS:O   | 3:B:203:ALA:N    | 2.36                     | 0.49              |
| 1:G:93:LEU:HD11 | 1:G:258:ILE:HD12 | 1.94                     | 0.49              |
| 2:L:52:VAL:HG22 | 2:L:61:ILE:HD13  | 1.94                     | 0.49              |
| 1:I:206:ASP:N   | 1:I:206:ASP:OD1  | 2.45                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:137:VAL:HG11 | 1:M:134:VAL:CG1  | 2.43                     | 0.49              |
| 1:O:278:THR:HG23 | 1:O:304:CYS:SG   | 2.52                     | 0.49              |
| 1:M:58:LYS:O     | 1:M:62:ASP:N     | 2.43                     | 0.49              |
| 3:N:25:VAL:HG12  | 3:N:29:LEU:HB2   | 1.95                     | 0.49              |
| 1:C:299:ARG:HD3  | 1:C:338:LEU:HD22 | 1.94                     | 0.49              |
| 1:A:228:TYR:N    | 1:A:228:TYR:CD1  | 2.81                     | 0.49              |
| 1:K:119:ARG:NH1  | 1:K:230:ASP:OD1  | 2.46                     | 0.49              |
| 2:L:4:GLN:H      | 2:L:4:GLN:CD     | 2.14                     | 0.49              |
| 2:L:124:ILE:HD11 | 2:L:228:PHE:HB2  | 1.95                     | 0.49              |
| 2:L:126:ILE:HG21 | 2:L:242:ASN:HD21 | 1.78                     | 0.49              |
| 2:P:319:ASN:HD22 | 2:P:322:MET:HG2  | 1.77                     | 0.49              |
| 3:N:63:LEU:HA    | 3:N:66:VAL:CB    | 2.39                     | 0.49              |
| 1:E:245:VAL:HA   | 1:E:279:ALA:HB2  | 1.95                     | 0.48              |
| 2:L:20:MET:HB2   | 2:L:47:PHE:CD2   | 2.43                     | 0.48              |
| 1:I:83:MET:C     | 1:I:83:MET:SD    | 2.95                     | 0.48              |
| 1:O:214:GLN:NE2  | 2:P:250:GLY:O    | 2.42                     | 0.48              |
| 2:P:91:SER:HB3   | 2:P:94:ASN:OD1   | 2.08                     | 0.48              |
| 3:F:63:LEU:CA    | 3:F:66:VAL:HB    | 2.33                     | 0.48              |
| 3:J:253:GLY:O    | 3:J:257:VAL:HG23 | 2.13                     | 0.48              |
| 2:P:18:VAL:O     | 2:P:47:PHE:HA    | 2.13                     | 0.48              |
| 2:P:117:THR:HG23 | 2:P:118:ARG:H    | 1.78                     | 0.48              |
| 2:P:194:LEU:O    | 2:P:198:ARG:HG3  | 2.13                     | 0.48              |
| 2:P:309:ILE:O    | 2:P:313:VAL:HG13 | 2.13                     | 0.48              |
| 3:N:17:VAL:O     | 3:N:46:PHE:HA    | 2.14                     | 0.48              |
| 3:N:288:PRO:HD2  | 3:N:289:THR:H    | 1.77                     | 0.48              |
| 2:H:316:SER:N    | 2:H:343:HIS:CE1  | 2.81                     | 0.48              |
| 2:H:323:HIS:CG   | 2:H:327:ILE:HD11 | 2.47                     | 0.48              |
| 3:F:236:PRO:HD2  | 3:F:239:TYR:CD2  | 2.37                     | 0.48              |
| 1:K:324:CYS:O    | 1:K:328:THR:OG1  | 2.27                     | 0.48              |
| 1:I:171:VAL:HG22 | 1:I:208:VAL:HG21 | 1.95                     | 0.48              |
| 2:P:140:HIS:N    | 2:P:140:HIS:ND1  | 2.59                     | 0.48              |
| 2:P:166:PHE:HB3  | 2:P:204:TYR:CD2  | 2.48                     | 0.48              |
| 3:N:180:THR:HB   | 3:N:233:LEU:HD13 | 1.95                     | 0.48              |
| 2:D:43:VAL:HG22  | 2:D:305:TYR:HD2  | 1.78                     | 0.48              |
| 2:D:261:GLY:N    | 2:D:264:TYR:O    | 2.47                     | 0.48              |
| 3:B:328:ASP:OD1  | 3:B:328:ASP:N    | 2.44                     | 0.48              |
| 1:G:26:ILE:HG12  | 1:G:332:CYS:SG   | 2.54                     | 0.48              |
| 1:K:332:CYS:HA   | 1:K:335:VAL:HG12 | 1.96                     | 0.48              |
| 1:I:25:LYS:O     | 1:I:29:ALA:N     | 2.47                     | 0.48              |
| 1:I:119:ARG:CZ   | 1:I:230:ASP:HB2  | 2.43                     | 0.48              |
| 2:H:253:GLY:O    | 2:H:285:ASN:ND2  | 2.46                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:L:51:HIS:C     | 2:L:52:VAL:CG2   | 2.85                     | 0.48              |
| 2:L:57:ASP:CB    | 2:L:60:ASP:CA    | 2.90                     | 0.48              |
| 2:L:143:VAL:CG2  | 2:L:144:ALA:H    | 2.27                     | 0.48              |
| 2:L:184:ASN:ND2  | 2:L:213:ILE:HD13 | 2.28                     | 0.48              |
| 1:O:231:ILE:HG21 | 2:P:240:ILE:HD13 | 1.96                     | 0.48              |
| 1:M:72:LEU:HD13  | 1:M:83:MET:HG2   | 1.94                     | 0.48              |
| 1:K:112:ASP:HB3  | 1:K:217:SER:HB3  | 1.94                     | 0.48              |
| 1:K:229:GLY:O    | 1:K:233:SER:OG   | 2.18                     | 0.48              |
| 1:K:315:THR:OG1  | 1:K:316:LYS:N    | 2.43                     | 0.48              |
| 1:I:155:PHE:CE2  | 1:I:251:ILE:HG13 | 2.47                     | 0.48              |
| 3:J:49:HIS:O     | 3:J:51:LEU:N     | 2.47                     | 0.48              |
| 1:A:21:ALA:HA    | 1:A:24:MET:SD    | 2.54                     | 0.48              |
| 3:B:77:ILE:HG13  | 3:B:77:ILE:O     | 2.12                     | 0.48              |
| 1:G:277:PRO:O    | 1:G:280:LEU:N    | 2.46                     | 0.48              |
| 2:L:15:ARG:HG2   | 2:L:44:PRO:HA    | 1.96                     | 0.48              |
| 1:I:106:TYR:CE2  | 1:I:318:LEU:HD22 | 2.49                     | 0.48              |
| 3:J:284:ASN:O    | 3:J:284:ASN:CG   | 2.56                     | 0.48              |
| 1:O:91:PHE:CB    | 1:O:256:VAL:HG11 | 2.44                     | 0.48              |
| 1:O:132:VAL:C    | 1:O:133:ILE:HD13 | 2.39                     | 0.48              |
| 2:P:20:MET:O     | 2:P:50:VAL:HG23  | 2.09                     | 0.48              |
| 2:P:213:ILE:O    | 2:P:217:THR:OG1  | 2.27                     | 0.48              |
| 2:D:10:ALA:CB    | 3:F:165:LYS:HE2  | 2.41                     | 0.48              |
| 2:D:111:SER:HB2  | 2:D:122:ILE:H    | 1.79                     | 0.48              |
| 2:H:62:ARG:O     | 2:H:63:ASN:C     | 2.54                     | 0.48              |
| 1:K:193:GLU:HA   | 1:K:196:LYS:HG2  | 1.94                     | 0.48              |
| 2:L:68:ILE:HD12  | 2:L:68:ILE:H     | 1.78                     | 0.48              |
| 2:L:140:HIS:CD2  | 3:J:150:GLU:CD   | 2.84                     | 0.48              |
| 3:J:92:ALA:O     | 3:J:93:SER:CB    | 2.62                     | 0.48              |
| 1:O:20:SER:O     | 1:O:24:MET:HG3   | 2.13                     | 0.48              |
| 1:O:132:VAL:N    | 1:O:138:VAL:HG23 | 2.28                     | 0.48              |
| 2:P:90:LYS:CB    | 2:P:95:ILE:CD1   | 2.86                     | 0.48              |
| 2:L:127:VAL:O    | 2:L:232:VAL:HA   | 2.14                     | 0.48              |
| 2:P:73:VAL:HG21  | 2:P:300:LEU:HD21 | 1.95                     | 0.48              |
| 1:E:243:LEU:HB3  | 1:E:262:VAL:CG2  | 2.33                     | 0.48              |
| 3:F:48:GLU:HG2   | 3:F:48:GLU:O     | 2.13                     | 0.48              |
| 1:I:30:ALA:HB1   | 1:I:299:ARG:HH21 | 1.79                     | 0.48              |
| 2:P:224:ARG:O    | 2:P:227:GLN:HG2  | 2.14                     | 0.48              |
| 1:C:88:ARG:HA    | 1:C:93:LEU:HB2   | 1.95                     | 0.47              |
| 1:C:225:PRO:HD2  | 1:C:228:TYR:CD2  | 2.49                     | 0.47              |
| 1:A:89:LYS:HE2   | 1:A:89:LYS:HB3   | 1.75                     | 0.47              |
| 3:B:93:SER:CA    | 3:B:96:MET:SD    | 3.01                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:130:GLU:C    | 1:G:131:HIS:HD1  | 2.22                     | 0.47              |
| 2:H:185:ILE:HD12 | 2:H:185:ILE:N    | 2.29                     | 0.47              |
| 1:O:116:VAL:HG11 | 1:O:159:TYR:CE2  | 2.49                     | 0.47              |
| 1:O:172:HIS:ND1  | 1:O:172:HIS:C    | 2.72                     | 0.47              |
| 1:M:178:ARG:CD   | 3:N:86:GLU:CA    | 2.59                     | 0.47              |
| 1:C:150:LYS:HB2  | 1:C:187:LYS:HE2  | 1.96                     | 0.47              |
| 1:A:34:ILE:HG22  | 1:A:34:ILE:O     | 2.13                     | 0.47              |
| 3:B:104:LEU:HD23 | 3:B:263:SER:HB3  | 1.95                     | 0.47              |
| 3:B:184:LYS:HD3  | 3:B:216:ILE:HG22 | 1.96                     | 0.47              |
| 1:E:98:ARG:HH12  | 1:E:243:LEU:HD21 | 1.79                     | 0.47              |
| 1:K:303:ALA:O    | 1:K:307:THR:OG1  | 2.29                     | 0.47              |
| 1:I:327:PHE:CE2  | 1:I:331:ILE:HD11 | 2.50                     | 0.47              |
| 3:J:69:SER:O     | 3:J:73:ASN:ND2   | 2.47                     | 0.47              |
| 3:N:214:MET:HG2  | 3:N:219:CYS:HB2  | 1.96                     | 0.47              |
| 2:D:14:GLY:H     | 3:F:265:GLU:CB   | 2.27                     | 0.47              |
| 3:F:202:VAL:HA   | 3:F:205:LEU:HD12 | 1.96                     | 0.47              |
| 3:J:284:ASN:OD1  | 3:J:335:CYS:N    | 2.39                     | 0.47              |
| 1:O:327:PHE:CE1  | 1:O:331:ILE:HD11 | 2.49                     | 0.47              |
| 1:M:8:THR:OG1    | 1:M:64:ASN:ND2   | 2.42                     | 0.47              |
| 3:N:33:VAL:HG22  | 3:N:292:LEU:HD23 | 1.97                     | 0.47              |
| 1:C:83:MET:HA    | 1:C:86:LEU:HB2   | 1.96                     | 0.47              |
| 1:A:281:LEU:HD11 | 1:A:300:ILE:HG21 | 1.95                     | 0.47              |
| 1:G:73:LYS:HG3   | 1:G:74:THR:H     | 1.79                     | 0.47              |
| 3:J:186:ASN:OD1  | 3:J:187:ILE:N    | 2.47                     | 0.47              |
| 3:N:102:LEU:HD12 | 3:N:104:LEU:HD11 | 1.96                     | 0.47              |
| 1:A:110:TYR:CE1  | 3:B:120:ARG:HD3  | 2.49                     | 0.47              |
| 3:B:94:TYR:HA    | 3:B:97:ARG:CB    | 2.44                     | 0.47              |
| 3:B:179:VAL:HG12 | 3:B:232:VAL:HB   | 1.97                     | 0.47              |
| 2:H:317:MET:CA   | 2:H:317:MET:CE   | 2.85                     | 0.47              |
| 2:L:61:ILE:HG23  | 2:L:62:ARG:N     | 2.29                     | 0.47              |
| 2:L:218:THR:HA   | 2:L:221:LEU:HD12 | 1.96                     | 0.47              |
| 3:J:93:SER:C     | 3:J:95:ASP:H     | 2.22                     | 0.47              |
| 2:P:79:ILE:HG21  | 2:P:92:ARG:CB    | 2.44                     | 0.47              |
| 3:N:131:GLU:OE2  | 3:N:133:THR:OG1  | 2.24                     | 0.47              |
| 2:D:62:ARG:O     | 2:D:66:MET:N     | 2.38                     | 0.47              |
| 2:D:66:MET:SD    | 3:F:205:LEU:HA   | 2.55                     | 0.47              |
| 2:D:253:GLY:O    | 2:D:287:THR:HB   | 2.15                     | 0.47              |
| 3:F:127:VAL:HG21 | 3:F:170:TYR:CE2  | 2.46                     | 0.47              |
| 2:L:143:VAL:CG2  | 2:L:144:ALA:N    | 2.77                     | 0.47              |
| 3:J:23:ASP:CG    | 3:J:53:GLU:CB    | 2.88                     | 0.47              |
| 1:O:168:VAL:O    | 1:O:200:PHE:HA   | 2.15                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:P:185:ILE:HG22 | 2:P:186:MET:HG3  | 1.97                     | 0.47              |
| 3:N:73:ASN:O     | 3:N:75:VAL:N     | 2.43                     | 0.47              |
| 2:D:338:GLN:HA   | 2:D:341:ILE:HD12 | 1.97                     | 0.47              |
| 1:A:148:ALA:O    | 1:A:152:ILE:HG22 | 2.15                     | 0.47              |
| 1:E:140:SER:HB2  | 3:F:153:LYS:HB3  | 1.96                     | 0.47              |
| 1:E:243:LEU:HD22 | 1:E:262:VAL:CG2  | 2.39                     | 0.47              |
| 1:K:9:LEU:HD13   | 1:K:68:LEU:HB3   | 1.96                     | 0.47              |
| 2:L:57:ASP:CB    | 2:L:61:ILE:N     | 2.78                     | 0.47              |
| 3:J:287:ASN:HB2  | 3:J:326:THR:OG1  | 2.15                     | 0.47              |
| 1:O:174:ALA:CB   | 1:O:181:ASP:CG   | 2.86                     | 0.47              |
| 1:O:284:ALA:O    | 1:O:288:LEU:HG   | 2.15                     | 0.47              |
| 2:P:135:TYR:CD1  | 2:P:151:LYS:HB2  | 2.49                     | 0.47              |
| 3:N:15:PHE:HB3   | 3:N:16:PRO:HD3   | 1.97                     | 0.47              |
| 3:N:21:PRO:CG    | 3:N:22:GLY:H     | 2.27                     | 0.47              |
| 2:D:27:GLY:N     | 2:D:28:PRO:CD    | 2.78                     | 0.47              |
| 1:A:99:PRO:HG2   | 1:A:247:PRO:HG2  | 1.97                     | 0.47              |
| 1:O:21:ALA:HA    | 1:O:24:MET:HE2   | 1.97                     | 0.47              |
| 1:O:267:PRO:HA   | 1:O:270:ALA:HB2  | 1.97                     | 0.47              |
| 1:C:73:LYS:HA    | 1:C:73:LYS:HD2   | 1.66                     | 0.47              |
| 1:A:231:ILE:HG22 | 3:B:217:ASP:HB3  | 1.97                     | 0.47              |
| 1:E:118:ILE:HG22 | 1:E:152:ILE:HD11 | 1.97                     | 0.47              |
| 1:E:186:GLN:O    | 1:E:190:GLU:HG3  | 2.14                     | 0.47              |
| 1:E:232:LEU:HA   | 1:E:235:LEU:HB2  | 1.96                     | 0.47              |
| 2:P:233:MET:CE   | 2:P:241:VAL:HG11 | 2.43                     | 0.47              |
| 1:M:61:MET:HE1   | 1:M:67:GLY:HA3   | 1.97                     | 0.47              |
| 2:D:323:HIS:HB2  | 2:D:329:GLY:HA3  | 1.96                     | 0.47              |
| 3:B:178:LYS:O    | 3:B:231:ASP:HB3  | 2.14                     | 0.47              |
| 1:K:64:ASN:O     | 1:K:66:MET:N     | 2.40                     | 0.47              |
| 3:N:119:THR:HG21 | 3:N:251:VAL:O    | 2.15                     | 0.47              |
| 1:C:99:PRO:HB3   | 1:C:116:VAL:HG22 | 1.96                     | 0.46              |
| 1:A:303:ALA:HB2  | 1:A:338:LEU:HD11 | 1.96                     | 0.46              |
| 1:G:122:THR:OG1  | 1:G:123:GLU:N    | 2.47                     | 0.46              |
| 2:L:58:GLU:CA    | 2:L:59:GLU:CB    | 2.93                     | 0.46              |
| 3:J:81:ILE:O     | 3:J:81:ILE:HG22  | 2.15                     | 0.46              |
| 2:P:57:ASP:C     | 2:P:60:ASP:HB2   | 2.40                     | 0.46              |
| 2:D:256:ALA:HB2  | 2:D:291:LEU:HB3  | 1.97                     | 0.46              |
| 1:A:181:ASP:OD1  | 1:A:181:ASP:N    | 2.48                     | 0.46              |
| 1:E:101:VAL:N    | 1:E:240:ILE:HG21 | 2.31                     | 0.46              |
| 2:L:35:LYS:NZ    | 2:L:49:GLU:OE2   | 2.31                     | 0.46              |
| 3:J:37:PHE:CD1   | 3:J:42:VAL:HG21  | 2.50                     | 0.46              |
| 3:J:88:LYS:HB3   | 3:J:89:GLY:H     | 1.40                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:125:GLU:CD   | 1:M:227:LEU:HD22 | 2.40                     | 0.46              |
| 1:A:118:ILE:HG22 | 1:A:152:ILE:HD11 | 1.98                     | 0.46              |
| 1:E:250:ASN:O    | 1:E:258:ILE:N    | 2.46                     | 0.46              |
| 1:K:64:ASN:C     | 1:K:66:MET:H     | 2.23                     | 0.46              |
| 1:M:83:MET:O     | 1:M:87:LEU:HG    | 2.16                     | 0.46              |
| 1:C:64:ASN:C     | 1:C:66:MET:H     | 2.24                     | 0.46              |
| 2:D:65:ILE:HD13  | 2:D:65:ILE:N     | 2.30                     | 0.46              |
| 3:F:143:GLU:HG2  | 3:F:145:ALA:O    | 2.15                     | 0.46              |
| 1:I:27:PHE:HZ    | 1:I:284:ALA:HB1  | 1.81                     | 0.46              |
| 1:I:80:HIS:CB    | 1:I:81:PRO:CD    | 2.86                     | 0.46              |
| 1:I:129:ILE:CB   | 1:I:141:ILE:CB   | 2.93                     | 0.46              |
| 1:I:129:ILE:CB   | 1:I:141:ILE:HG21 | 2.45                     | 0.46              |
| 1:O:106:TYR:CE2  | 1:O:318:LEU:HD11 | 2.50                     | 0.46              |
| 2:P:43:VAL:O     | 2:P:43:VAL:HG13  | 2.15                     | 0.46              |
| 1:C:41:VAL:HA    | 1:C:54:PRO:HG2   | 1.98                     | 0.46              |
| 2:D:245:CYS:HA   | 2:D:248:LEU:HB2  | 1.97                     | 0.46              |
| 2:D:311:LYS:HA   | 2:D:314:LEU:HG   | 1.97                     | 0.46              |
| 1:A:229:GLY:O    | 1:A:233:SER:OG   | 2.19                     | 0.46              |
| 1:G:281:LEU:HD11 | 1:G:300:ILE:HG21 | 1.98                     | 0.46              |
| 2:H:316:SER:CA   | 2:H:343:HIS:CE1  | 2.99                     | 0.46              |
| 1:K:201:ASN:OD1  | 1:K:201:ASN:N    | 2.49                     | 0.46              |
| 2:L:196:CYS:O    | 2:L:200:VAL:HG23 | 2.15                     | 0.46              |
| 3:J:18:THR:HB    | 3:J:76:ALA:HB2   | 1.98                     | 0.46              |
| 1:O:114:ASN:ND2  | 1:O:165:ARG:HH12 | 2.13                     | 0.46              |
| 3:N:178:LYS:O    | 3:N:231:ASP:HB3  | 2.15                     | 0.46              |
| 1:A:114:ASN:OD1  | 1:A:165:ARG:NH2  | 2.47                     | 0.46              |
| 1:A:133:ILE:HD11 | 1:A:139:ALA:HB3  | 1.97                     | 0.46              |
| 1:A:175:ASN:OD1  | 1:A:175:ASN:N    | 2.48                     | 0.46              |
| 1:O:114:ASN:OD1  | 1:O:165:ARG:NH2  | 2.40                     | 0.46              |
| 2:P:154:THR:OG1  | 2:P:157:LYS:HB2  | 2.16                     | 0.46              |
| 2:P:178:THR:O    | 2:P:231:MET:HA   | 2.15                     | 0.46              |
| 1:M:184:PHE:CD2  | 1:M:225:PRO:HG3  | 2.51                     | 0.46              |
| 3:N:235:MET:HE2  | 3:N:235:MET:HB3  | 1.84                     | 0.46              |
| 1:C:195:CYS:C    | 1:C:197:ASP:H    | 2.23                     | 0.46              |
| 2:D:213:ILE:O    | 2:D:217:THR:OG1  | 2.25                     | 0.46              |
| 2:H:114:GLY:HA3  | 2:H:318:ASP:HA   | 1.97                     | 0.46              |
| 1:E:146:GLU:HG3  | 1:E:187:LYS:HE3  | 1.97                     | 0.46              |
| 3:F:96:MET:O     | 3:F:99:ARG:N     | 2.49                     | 0.46              |
| 3:F:324:VAL:HG21 | 3:F:341:GLU:HG2  | 1.98                     | 0.46              |
| 2:L:18:VAL:HG13  | 2:L:74:ALA:HA    | 1.98                     | 0.46              |
| 3:J:37:PHE:CE1   | 3:J:299:LEU:HD11 | 2.50                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:J:80:LYS:HE3   | 3:J:99:ARG:HH22  | 1.81                     | 0.46              |
| 3:J:269:PHE:CE1  | 3:J:298:MET:HA   | 2.50                     | 0.46              |
| 1:O:114:ASN:CG   | 1:O:165:ARG:HH12 | 2.24                     | 0.46              |
| 2:P:107:ILE:HD11 | 2:P:126:ILE:HD12 | 1.98                     | 0.46              |
| 2:P:243:ASN:O    | 2:P:244:VAL:C    | 2.57                     | 0.46              |
| 1:C:201:ASN:OD1  | 1:C:201:ASN:N    | 2.48                     | 0.46              |
| 2:D:213:ILE:H    | 2:D:213:ILE:HG13 | 1.58                     | 0.46              |
| 2:H:60:ASP:C     | 2:H:62:ARG:N     | 2.72                     | 0.46              |
| 3:F:269:PHE:CZ   | 3:F:298:MET:HA   | 2.51                     | 0.46              |
| 1:K:9:LEU:HD22   | 1:K:36:TRP:CE3   | 2.51                     | 0.46              |
| 1:K:55:SER:HA    | 1:K:58:LYS:HB3   | 1.98                     | 0.46              |
| 1:I:175:ASN:CB   | 3:J:84:PRO:O     | 2.64                     | 0.46              |
| 1:I:180:SER:OG   | 1:I:181:ASP:N    | 2.48                     | 0.46              |
| 1:M:45:GLN:HA    | 1:M:50:LYS:CB    | 2.45                     | 0.46              |
| 3:N:185:ALA:N    | 3:N:192:ASP:OD2  | 2.49                     | 0.46              |
| 2:D:56:ALA:HB1   | 2:D:60:ASP:CB    | 2.45                     | 0.46              |
| 3:B:221:MET:O    | 3:B:224:VAL:HG22 | 2.15                     | 0.46              |
| 3:B:303:ASN:HB3  | 2:H:42:CYS:SG    | 2.56                     | 0.46              |
| 2:H:254:LEU:HD23 | 2:H:287:THR:HB   | 1.98                     | 0.46              |
| 3:J:119:THR:OG1  | 3:J:120:ARG:N    | 2.49                     | 0.46              |
| 2:P:35:LYS:O     | 2:P:38:PHE:N     | 2.49                     | 0.46              |
| 3:N:63:LEU:CD2   | 3:N:63:LEU:H     | 2.29                     | 0.46              |
| 1:C:177:MET:SD   | 2:D:135:TYR:HE1  | 2.39                     | 0.46              |
| 2:D:26:ILE:O     | 2:D:30:LEU:N     | 2.40                     | 0.46              |
| 2:D:62:ARG:HA    | 2:D:65:ILE:HG12  | 1.97                     | 0.46              |
| 2:D:282:ASN:C    | 2:D:333:THR:HG23 | 2.40                     | 0.46              |
| 3:F:108:VAL:HB   | 3:F:260:GLU:HB2  | 1.98                     | 0.46              |
| 2:L:255:VAL:HB   | 2:L:270:ALA:HB2  | 1.97                     | 0.46              |
| 3:J:136:GLU:C    | 3:J:138:SER:N    | 2.71                     | 0.46              |
| 3:J:177:GLY:N    | 3:J:231:ASP:OD2  | 2.35                     | 0.46              |
| 1:M:102:SER:OG   | 1:M:113:VAL:HG22 | 2.16                     | 0.46              |
| 3:N:257:VAL:HB   | 3:N:273:ALA:HB2  | 1.98                     | 0.46              |
| 1:C:95:ALA:HB3   | 1:C:251:ILE:HB   | 1.97                     | 0.45              |
| 3:B:93:SER:CB    | 3:B:96:MET:CE    | 2.92                     | 0.45              |
| 2:H:97:ARG:NH1   | 2:H:130:ASN:OD1  | 2.49                     | 0.45              |
| 1:E:83:MET:CE    | 1:E:83:MET:CA    | 2.85                     | 0.45              |
| 1:K:224:MET:SD   | 1:K:229:GLY:HA2  | 2.56                     | 0.45              |
| 1:I:110:TYR:HE1  | 3:J:120:ARG:HD3  | 1.81                     | 0.45              |
| 3:J:104:LEU:HD23 | 3:J:263:SER:HB3  | 1.99                     | 0.45              |
| 3:J:300:ARG:HG3  | 3:J:308:SER:OG   | 2.15                     | 0.45              |
| 2:P:96:LEU:O     | 2:P:96:LEU:HD22  | 2.16                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:P:220:GLN:OE1  | 2:P:227:GLN:NE2  | 2.49                     | 0.45              |
| 1:M:46:GLY:N     | 1:M:50:LYS:HA    | 2.21                     | 0.45              |
| 1:M:146:GLU:HB3  | 3:N:147:GLY:HA3  | 1.97                     | 0.45              |
| 3:N:303:ASN:O    | 3:N:304:LEU:HD23 | 2.14                     | 0.45              |
| 1:C:139:ALA:HA   | 2:D:151:LYS:O    | 2.15                     | 0.45              |
| 1:G:22:ALA:O     | 1:G:26:ILE:HG13  | 2.16                     | 0.45              |
| 2:H:76:LYS:HE3   | 2:H:268:GLU:HB3  | 1.98                     | 0.45              |
| 2:H:333:THR:O    | 2:H:337:ILE:HD12 | 2.17                     | 0.45              |
| 1:E:187:LYS:O    | 1:E:191:VAL:HG23 | 2.16                     | 0.45              |
| 3:F:60:GLU:C     | 3:F:62:LYS:N     | 2.71                     | 0.45              |
| 2:L:12:TYR:CZ    | 3:N:166:PHE:HA   | 2.51                     | 0.45              |
| 2:L:79:ILE:HD11  | 2:L:93:ASN:CA    | 2.45                     | 0.45              |
| 1:I:84:ASN:OD1   | 1:I:84:ASN:N     | 2.44                     | 0.45              |
| 1:O:91:PHE:HD2   | 1:O:93:LEU:HD21  | 1.82                     | 0.45              |
| 2:P:66:MET:CB    | 2:P:69:ARG:CD    | 2.94                     | 0.45              |
| 2:P:92:ARG:O     | 2:P:96:LEU:HB2   | 2.16                     | 0.45              |
| 1:M:236:CYS:HA   | 1:M:239:LEU:HG   | 1.98                     | 0.45              |
| 3:N:153:LYS:C    | 3:N:154:ILE:HD13 | 2.41                     | 0.45              |
| 1:A:141:ILE:HD13 | 3:B:152:LEU:HD23 | 1.97                     | 0.45              |
| 3:F:130:ARG:HG3  | 3:F:240:GLY:HA3  | 1.98                     | 0.45              |
| 3:F:184:LYS:HD3  | 3:F:216:ILE:HG22 | 1.98                     | 0.45              |
| 1:I:313:SER:HB2  | 1:I:330:GLU:OE1  | 2.17                     | 0.45              |
| 3:J:168:PHE:HB3  | 3:J:206:TYR:CD2  | 2.51                     | 0.45              |
| 2:P:33:HIS:C     | 2:P:37:VAL:HG23  | 2.36                     | 0.45              |
| 3:N:269:PHE:CZ   | 3:N:298:MET:HA   | 2.51                     | 0.45              |
| 1:C:157:PHE:CE2  | 1:C:192:ALA:HA   | 2.46                     | 0.45              |
| 2:D:344:ILE:HG22 | 2:D:346:VAL:HG23 | 1.97                     | 0.45              |
| 1:A:50:LYS:CB    | 1:A:80:HIS:CE1   | 3.00                     | 0.45              |
| 1:A:276:ASN:CG   | 1:A:278:THR:HG22 | 2.42                     | 0.45              |
| 1:K:310:ASP:CG   | 1:K:312:LYS:HE2  | 2.41                     | 0.45              |
| 2:L:140:HIS:NE2  | 2:L:148:GLU:CD   | 2.54                     | 0.45              |
| 3:J:112:LYS:HA   | 3:J:124:LEU:O    | 2.17                     | 0.45              |
| 3:J:265:GLU:O    | 2:P:13:GLY:O     | 2.34                     | 0.45              |
| 2:P:90:LYS:HA    | 2:P:95:ILE:HG13  | 1.97                     | 0.45              |
| 2:D:9:SER:HB3    | 2:D:72:ARG:CZ    | 2.47                     | 0.45              |
| 1:A:125:GLU:OE1  | 1:A:227:LEU:HD22 | 2.17                     | 0.45              |
| 3:B:95:ASP:O     | 3:B:99:ARG:HG2   | 2.17                     | 0.45              |
| 1:K:12:GLY:O     | 1:K:17:PRO:HD3   | 2.15                     | 0.45              |
| 2:L:129:GLU:HA   | 2:L:161:ILE:HD13 | 1.99                     | 0.45              |
| 3:J:111:VAL:HG23 | 3:J:126:LEU:HB2  | 1.99                     | 0.45              |
| 3:J:137:TYR:C    | 3:J:139:SER:N    | 2.73                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:119:ARG:HG3  | 1:O:229:GLY:HA3  | 1.97                     | 0.45              |
| 2:D:263:VAL:HG13 | 2:D:264:TYR:CD2  | 2.52                     | 0.45              |
| 3:F:104:LEU:O    | 3:F:132:GLN:NE2  | 2.45                     | 0.45              |
| 3:J:96:MET:O     | 3:J:100:ARG:HB2  | 2.16                     | 0.45              |
| 2:P:164:TYR:HE1  | 2:P:168:LEU:HD22 | 1.81                     | 0.45              |
| 2:P:298:ASP:OD1  | 2:P:303:HIS:CB   | 2.65                     | 0.45              |
| 1:M:45:GLN:HA    | 1:M:50:LYS:CA    | 2.46                     | 0.45              |
| 2:D:268:GLU:HB2  | 2:D:272:ARG:NH2  | 2.31                     | 0.45              |
| 3:B:96:MET:O     | 3:B:99:ARG:N     | 2.50                     | 0.45              |
| 2:H:129:GLU:OE1  | 2:H:157:LYS:HD3  | 2.16                     | 0.45              |
| 2:H:322:MET:N    | 2:H:322:MET:SD   | 2.89                     | 0.45              |
| 2:L:117:THR:OG1  | 2:L:118:ARG:N    | 2.46                     | 0.45              |
| 3:J:184:LYS:HG3  | 3:J:186:ASN:OD1  | 2.15                     | 0.45              |
| 1:O:175:ASN:HD22 | 1:O:204:TYR:CE2  | 1.75                     | 0.45              |
| 1:M:148:ALA:O    | 1:M:152:ILE:HG22 | 2.16                     | 0.45              |
| 1:M:235:LEU:HD12 | 3:N:220:CYS:HB3  | 1.99                     | 0.45              |
| 3:B:135:GLY:N    | 3:B:154:ILE:O    | 2.43                     | 0.45              |
| 3:B:291:MET:O    | 3:B:295:ALA:N    | 2.43                     | 0.45              |
| 3:B:340:GLU:O    | 3:B:344:ARG:N    | 2.40                     | 0.45              |
| 2:H:79:ILE:N     | 2:H:79:ILE:HD12  | 2.32                     | 0.45              |
| 1:E:324:CYS:O    | 1:E:328:THR:OG1  | 2.28                     | 0.45              |
| 3:J:77:ILE:HG21  | 3:J:298:MET:HE1  | 1.98                     | 0.45              |
| 1:O:97:VAL:HG22  | 1:O:118:ILE:HG12 | 1.99                     | 0.45              |
| 2:P:76:LYS:NZ    | 2:P:93:ASN:OD1   | 2.49                     | 0.45              |
| 2:P:300:LEU:O    | 2:P:301:LYS:CG   | 2.64                     | 0.45              |
| 3:N:16:PRO:HB2   | 3:N:73:ASN:OD1   | 2.16                     | 0.45              |
| 1:C:287:MET:HG2  | 1:C:291:MET:HE2  | 1.97                     | 0.45              |
| 1:A:301:GLU:HG2  | 1:A:305:PHE:CE2  | 2.52                     | 0.45              |
| 3:B:216:ILE:HD13 | 3:B:239:TYR:HB3  | 1.98                     | 0.45              |
| 2:H:62:ARG:O     | 2:H:64:ALA:N     | 2.50                     | 0.45              |
| 1:K:116:VAL:HG11 | 1:K:159:TYR:HE2  | 1.82                     | 0.45              |
| 1:I:27:PHE:CZ    | 1:I:284:ALA:HB1  | 2.51                     | 0.45              |
| 1:I:66:MET:SD    | 1:I:257:ALA:HB3  | 2.56                     | 0.45              |
| 1:I:134:VAL:HG22 | 1:I:137:VAL:HB   | 1.98                     | 0.45              |
| 3:J:49:HIS:NE2   | 3:J:69:SER:CB    | 2.80                     | 0.45              |
| 2:P:301:LYS:C    | 2:P:303:HIS:H    | 2.23                     | 0.45              |
| 1:C:80:HIS:N     | 1:C:81:PRO:CD    | 2.79                     | 0.45              |
| 1:C:98:ARG:NH1   | 1:C:234:ASP:OD1  | 2.50                     | 0.45              |
| 1:C:114:ASN:OD1  | 1:C:165:ARG:NH1  | 2.50                     | 0.45              |
| 3:B:37:PHE:CE1   | 3:B:299:LEU:HD11 | 2.52                     | 0.45              |
| 2:P:305:TYR:O    | 2:P:308:SER:HB3  | 2.17                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:80:HIS:CD2   | 1:M:81:PRO:HD2   | 2.50                     | 0.45              |
| 1:M:313:SER:O    | 1:M:314:LEU:HD12 | 2.17                     | 0.45              |
| 3:N:48:GLU:O     | 3:N:49:HIS:CD2   | 2.70                     | 0.45              |
| 3:B:86:GLU:H     | 3:B:91:LEU:HD22  | 1.82                     | 0.44              |
| 2:H:73:VAL:HG21  | 2:H:300:LEU:HD21 | 1.99                     | 0.44              |
| 3:F:107:ASN:HB3  | 3:F:130:ARG:HB3  | 2.00                     | 0.44              |
| 3:F:109:VAL:HG21 | 3:F:244:ASP:OD1  | 2.18                     | 0.44              |
| 1:I:128:GLY:O    | 1:I:130:GLU:CG   | 2.63                     | 0.44              |
| 1:O:277:PRO:O    | 1:O:280:LEU:N    | 2.50                     | 0.44              |
| 2:P:227:GLN:HG3  | 2:P:228:PHE:CD1  | 2.52                     | 0.44              |
| 1:M:231:ILE:HG13 | 1:M:232:LEU:H    | 1.82                     | 0.44              |
| 1:G:284:ALA:O    | 1:G:288:LEU:N    | 2.38                     | 0.44              |
| 1:E:8:THR:OG1    | 1:E:64:ASN:ND2   | 2.50                     | 0.44              |
| 1:E:74:THR:CB    | 1:E:75:PRO:HD3   | 2.46                     | 0.44              |
| 3:F:81:ILE:HG12  | 3:F:95:ASP:OD2   | 2.17                     | 0.44              |
| 3:F:298:MET:O    | 3:F:302:LEU:HG   | 2.17                     | 0.44              |
| 3:F:343:CYS:HA   | 3:F:346:VAL:HB   | 1.98                     | 0.44              |
| 2:L:62:ARG:HA    | 2:L:65:ILE:HD12  | 1.99                     | 0.44              |
| 2:L:111:SER:HB3  | 2:L:249:VAL:HG12 | 1.97                     | 0.44              |
| 1:O:73:LYS:HD3   | 1:O:265:THR:CB   | 2.45                     | 0.44              |
| 2:P:38:PHE:CZ    | 2:P:297:LEU:HD21 | 2.52                     | 0.44              |
| 2:P:313:VAL:HG12 | 2:P:340:VAL:HG11 | 1.99                     | 0.44              |
| 3:N:143:GLU:HA   | 3:N:149:ILE:HD12 | 1.98                     | 0.44              |
| 3:N:180:THR:HG23 | 3:N:212:GLU:HB3  | 1.98                     | 0.44              |
| 1:A:120:GLU:OE1  | 1:A:122:THR:N    | 2.49                     | 0.44              |
| 1:A:247:PRO:HD3  | 1:A:282:LEU:CD1  | 2.47                     | 0.44              |
| 3:B:78:ILE:HG12  | 3:B:270:GLU:HB3  | 1.99                     | 0.44              |
| 3:F:60:GLU:O     | 3:F:61:GLU:HG2   | 2.18                     | 0.44              |
| 1:K:318:LEU:H    | 1:K:319:GLY:HA3  | 1.83                     | 0.44              |
| 3:J:288:PRO:O    | 3:J:292:LEU:HG   | 2.16                     | 0.44              |
| 2:P:91:SER:O     | 2:P:94:ASN:OD1   | 2.35                     | 0.44              |
| 1:M:24:MET:HG2   | 1:M:36:TRP:CD2   | 2.52                     | 0.44              |
| 1:M:330:GLU:O    | 1:M:334:ARG:HB2  | 2.17                     | 0.44              |
| 1:G:27:PHE:CE2   | 1:G:288:LEU:HD21 | 2.53                     | 0.44              |
| 1:G:234:ASP:OD2  | 2:H:215:ASP:HB3  | 2.18                     | 0.44              |
| 1:E:335:VAL:HA   | 1:E:338:LEU:HD12 | 1.99                     | 0.44              |
| 1:K:142:LYS:HB3  | 2:L:149:SER:HB3  | 2.00                     | 0.44              |
| 2:L:140:HIS:O    | 2:L:140:HIS:CG   | 2.70                     | 0.44              |
| 1:I:88:ARG:HA    | 1:I:93:LEU:HB2   | 1.98                     | 0.44              |
| 3:J:83:THR:OG1   | 3:J:84:PRO:CD    | 2.52                     | 0.44              |
| 2:P:43:VAL:CG2   | 2:P:44:PRO:CD    | 2.96                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:P:141:GLU:O    | 2:P:142:SER:C    | 2.60                     | 0.44              |
| 1:A:53:ILE:HG22  | 1:A:54:PRO:N     | 2.33                     | 0.44              |
| 1:A:140:SER:HB2  | 3:B:153:LYS:HD3  | 2.00                     | 0.44              |
| 3:B:19:MET:HG3   | 3:B:30:MET:HE3   | 1.98                     | 0.44              |
| 3:B:91:LEU:CD1   | 3:B:91:LEU:C     | 2.81                     | 0.44              |
| 3:B:236:PRO:HD2  | 3:B:239:TYR:CD2  | 2.53                     | 0.44              |
| 1:G:94:TYR:CE2   | 1:G:151:ARG:HG2  | 2.53                     | 0.44              |
| 2:H:253:GLY:C    | 2:H:288:ALA:HB2  | 2.43                     | 0.44              |
| 2:P:94:ASN:CA    | 2:P:97:ARG:HG2   | 2.46                     | 0.44              |
| 3:N:82:HIS:O     | 3:N:83:THR:HG23  | 2.10                     | 0.44              |
| 1:A:7:VAL:HG23   | 1:A:34:ILE:HG23  | 2.00                     | 0.44              |
| 2:H:38:PHE:HD2   | 2:H:47:PHE:HE2   | 1.64                     | 0.44              |
| 1:E:98:ARG:HH12  | 1:E:243:LEU:CD2  | 2.31                     | 0.44              |
| 3:F:270:GLU:HG3  | 3:F:271:THR:O    | 2.18                     | 0.44              |
| 1:K:276:ASN:ND2  | 1:K:318:LEU:HD21 | 2.32                     | 0.44              |
| 1:A:160:ALA:HA   | 1:A:165:ARG:HG2  | 1.99                     | 0.44              |
| 1:A:166:SER:OG   | 1:A:220:ASP:OD2  | 2.33                     | 0.44              |
| 3:B:230:PHE:CD2  | 3:B:233:LEU:HD11 | 2.52                     | 0.44              |
| 3:F:60:GLU:C     | 3:F:61:GLU:CD    | 2.85                     | 0.44              |
| 1:K:133:ILE:HG21 | 1:I:133:ILE:HD12 | 1.99                     | 0.44              |
| 1:K:172:HIS:HE2  | 1:K:202:GLU:HG2  | 1.83                     | 0.44              |
| 2:L:4:GLN:N      | 2:L:4:GLN:CD     | 2.71                     | 0.44              |
| 2:L:115:VAL:HG12 | 2:L:117:THR:HG22 | 2.00                     | 0.44              |
| 2:L:300:LEU:HB2  | 2:L:302:LEU:HG   | 2.00                     | 0.44              |
| 2:P:33:HIS:O     | 2:P:37:VAL:CG2   | 2.52                     | 0.44              |
| 2:P:40:HIS:CE1   | 2:P:346:VAL:HG21 | 2.51                     | 0.44              |
| 3:N:95:ASP:O     | 3:N:98:LEU:HB3   | 2.17                     | 0.44              |
| 3:N:190:LEU:HD23 | 3:N:190:LEU:N    | 2.32                     | 0.44              |
| 2:D:27:GLY:O     | 2:D:31:MET:HG2   | 2.18                     | 0.44              |
| 2:H:285:ASN:HA   | 2:H:324:THR:CG2  | 2.31                     | 0.44              |
| 1:K:284:ALA:HA   | 1:K:287:MET:HE2  | 2.00                     | 0.44              |
| 1:I:330:GLU:HA   | 1:I:333:ARG:HG2  | 1.99                     | 0.44              |
| 3:J:83:THR:CG2   | 3:J:84:PRO:N     | 2.80                     | 0.44              |
| 1:O:38:GLU:O     | 1:O:39:ARG:HB2   | 2.17                     | 0.44              |
| 3:N:104:LEU:HA   | 3:N:263:SER:HA   | 2.00                     | 0.44              |
| 1:C:224:MET:SD   | 1:C:232:LEU:HD12 | 2.58                     | 0.44              |
| 1:A:68:LEU:HB2   | 1:A:287:MET:HE1  | 2.00                     | 0.44              |
| 1:A:146:GLU:N    | 3:B:147:GLY:O    | 2.39                     | 0.44              |
| 1:A:177:MET:HB2  | 1:A:177:MET:HE3  | 1.72                     | 0.44              |
| 3:B:25:VAL:HG11  | 3:B:286:ALA:HB2  | 2.00                     | 0.44              |
| 3:B:153:LYS:O    | 3:B:154:ILE:HD13 | 2.16                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:B:280:ALA:HB1  | 3:B:285:ILE:HG22 | 1.99                     | 0.44              |
| 2:H:50:VAL:HG21  | 2:H:64:ALA:HB1   | 2.00                     | 0.44              |
| 3:F:299:LEU:HB2  | 3:F:308:SER:HB2  | 1.99                     | 0.44              |
| 1:K:20:SER:O     | 1:K:24:MET:HG3   | 2.17                     | 0.44              |
| 2:L:18:VAL:HG13  | 2:L:73:VAL:O     | 2.17                     | 0.44              |
| 3:J:53:GLU:O     | 3:J:54:VAL:C     | 2.60                     | 0.44              |
| 1:O:204:TYR:O    | 1:O:208:VAL:HG23 | 2.18                     | 0.44              |
| 2:P:15:ARG:HH22  | 2:P:45:VAL:HG23  | 1.83                     | 0.44              |
| 1:M:119:ARG:CZ   | 1:M:230:ASP:HB2  | 2.47                     | 0.44              |
| 1:M:120:GLU:OE1  | 1:M:122:THR:N    | 2.49                     | 0.44              |
| 2:D:154:THR:OG1  | 2:D:157:LYS:HB2  | 2.18                     | 0.43              |
| 3:B:275:HIS:CB   | 3:B:276:PRO:CD   | 2.95                     | 0.43              |
| 1:G:123:GLU:CD   | 1:G:145:THR:H    | 2.26                     | 0.43              |
| 2:H:174:ARG:HA   | 2:H:174:ARG:HD2  | 1.81                     | 0.43              |
| 2:H:184:ASN:CG   | 2:H:185:ILE:HD13 | 2.43                     | 0.43              |
| 2:H:257:GLY:C    | 2:H:268:GLU:O    | 2.61                     | 0.43              |
| 1:E:22:ALA:O     | 1:E:26:ILE:HG13  | 2.17                     | 0.43              |
| 3:F:19:MET:HB3   | 3:F:48:GLU:HB3   | 1.98                     | 0.43              |
| 3:F:65:GLN:CD    | 3:F:65:GLN:N     | 2.73                     | 0.43              |
| 2:P:38:PHE:HD1   | 2:P:41:ALA:HB2   | 1.82                     | 0.43              |
| 1:C:175:ASN:OD1  | 1:C:176:ILE:HG12 | 2.18                     | 0.43              |
| 1:G:134:VAL:HG11 | 3:F:156:THR:HG21 | 2.00                     | 0.43              |
| 1:G:144:ILE:HD13 | 1:G:144:ILE:HA   | 1.91                     | 0.43              |
| 2:H:285:ASN:CG   | 2:H:324:THR:HG21 | 2.42                     | 0.43              |
| 3:F:74:LYS:O     | 3:F:266:TYR:HA   | 2.18                     | 0.43              |
| 1:K:167:ASN:O    | 1:K:220:ASP:HB3  | 2.19                     | 0.43              |
| 2:L:126:ILE:HD11 | 2:L:241:VAL:HG12 | 1.99                     | 0.43              |
| 1:O:234:ASP:OD2  | 2:P:215:ASP:HB3  | 2.18                     | 0.43              |
| 1:M:43:ALA:HB2   | 1:M:83:MET:HE1   | 1.99                     | 0.43              |
| 3:N:20:LEU:HD12  | 3:N:20:LEU:HA    | 1.74                     | 0.43              |
| 3:N:257:VAL:HG11 | 3:N:273:ALA:HB2  | 1.99                     | 0.43              |
| 2:D:129:GLU:OE1  | 2:D:132:GLU:N    | 2.47                     | 0.43              |
| 2:D:140:HIS:CD2  | 1:A:129:ILE:HG21 | 2.54                     | 0.43              |
| 2:D:155:LYS:O    | 2:D:159:LEU:HG   | 2.17                     | 0.43              |
| 1:G:315:THR:OG1  | 1:G:316:LYS:N    | 2.45                     | 0.43              |
| 2:H:62:ARG:O     | 2:H:65:ILE:N     | 2.51                     | 0.43              |
| 2:H:339:ASP:O    | 2:H:342:ARG:HB2  | 2.18                     | 0.43              |
| 3:F:19:MET:O     | 3:F:48:GLU:CB    | 2.62                     | 0.43              |
| 3:F:20:LEU:HD12  | 3:F:20:LEU:HA    | 1.69                     | 0.43              |
| 1:K:37:GLU:HG2   | 1:K:39:ARG:NH1   | 2.33                     | 0.43              |
| 2:L:254:LEU:CD2  | 2:L:285:ASN:ND2  | 2.79                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:100:CYS:HB3  | 1:O:240:ILE:HD13 | 2.00                     | 0.43              |
| 2:P:267:PHE:CZ   | 2:P:296:MET:HA   | 2.54                     | 0.43              |
| 1:C:86:LEU:O     | 1:C:90:THR:OG1   | 2.22                     | 0.43              |
| 2:D:21:ILE:CB    | 2:D:50:VAL:HG13  | 2.48                     | 0.43              |
| 1:A:168:VAL:O    | 1:A:200:PHE:HA   | 2.18                     | 0.43              |
| 3:B:255:GLY:O    | 3:B:289:THR:HB   | 2.17                     | 0.43              |
| 2:H:226:GLN:H    | 2:H:226:GLN:CD   | 2.27                     | 0.43              |
| 1:E:185:LEU:HD22 | 1:E:189:ARG:CZ   | 2.49                     | 0.43              |
| 3:F:15:PHE:HB3   | 3:F:16:PRO:CD    | 2.43                     | 0.43              |
| 1:I:81:PRO:HG2   | 1:I:86:LEU:HD11  | 2.00                     | 0.43              |
| 1:I:83:MET:SD    | 1:I:83:MET:O     | 2.76                     | 0.43              |
| 1:I:155:PHE:CZ   | 1:I:251:ILE:HG13 | 2.52                     | 0.43              |
| 1:O:268:ASP:OD1  | 1:O:268:ASP:N    | 2.50                     | 0.43              |
| 2:P:138:LEU:HB3  | 1:M:131:HIS:CE1  | 2.52                     | 0.43              |
| 2:D:151:LYS:O    | 2:D:152:ILE:HD13 | 2.19                     | 0.43              |
| 3:B:17:VAL:CG2   | 3:B:76:ALA:HA    | 2.48                     | 0.43              |
| 3:B:295:ALA:O    | 3:B:298:MET:HB3  | 2.18                     | 0.43              |
| 1:G:9:LEU:HG     | 1:G:10:ILE:N     | 2.34                     | 0.43              |
| 3:F:61:GLU:O     | 3:F:63:LEU:N     | 2.52                     | 0.43              |
| 1:K:276:ASN:CG   | 1:K:318:LEU:HD21 | 2.43                     | 0.43              |
| 2:L:61:ILE:O     | 2:L:61:ILE:HG13  | 2.18                     | 0.43              |
| 2:L:93:ASN:OD1   | 2:L:97:ARG:NH2   | 2.42                     | 0.43              |
| 1:I:124:GLY:C    | 1:I:126:TYR:N    | 2.76                     | 0.43              |
| 2:P:5:THR:C      | 2:P:6:ILE:CG2    | 2.91                     | 0.43              |
| 2:P:151:LYS:NZ   | 2:P:237:TYR:OH   | 2.52                     | 0.43              |
| 2:P:253:GLY:O    | 2:P:285:ASN:ND2  | 2.51                     | 0.43              |
| 1:C:142:LYS:CD   | 2:D:135:TYR:OH   | 2.65                     | 0.43              |
| 2:D:50:VAL:HG13  | 2:D:50:VAL:O     | 2.19                     | 0.43              |
| 1:A:159:TYR:O    | 1:A:163:ASN:ND2  | 2.48                     | 0.43              |
| 3:B:113:SER:HA   | 3:B:251:VAL:HG13 | 1.99                     | 0.43              |
| 1:G:206:ASP:CG   | 2:H:239:ASN:HB3  | 2.42                     | 0.43              |
| 1:E:98:ARG:CZ    | 1:E:233:SER:HB2  | 2.48                     | 0.43              |
| 1:I:64:ASN:C     | 1:I:66:MET:H     | 2.27                     | 0.43              |
| 2:P:62:ARG:HA    | 2:P:65:ILE:CG1   | 2.47                     | 0.43              |
| 3:N:271:THR:N    | 3:N:291:MET:HE3  | 2.34                     | 0.43              |
| 2:D:19:THR:OG1   | 2:D:74:ALA:HB1   | 2.05                     | 0.43              |
| 1:G:287:MET:O    | 1:G:291:MET:HG2  | 2.19                     | 0.43              |
| 1:E:5:GLN:O      | 1:E:35:GLN:N     | 2.48                     | 0.43              |
| 1:E:147:GLY:O    | 1:E:151:ARG:N    | 2.50                     | 0.43              |
| 1:E:294:PHE:HA   | 1:E:297:ALA:HB3  | 2.01                     | 0.43              |
| 3:F:48:GLU:O     | 3:F:48:GLU:CG    | 2.66                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:125:GLU:HG3  | 1:I:142:LYS:HB2  | 2.01                     | 0.43              |
| 1:O:315:THR:OG1  | 1:O:316:LYS:N    | 2.52                     | 0.43              |
| 2:P:93:ASN:C     | 2:P:93:ASN:ND2   | 2.76                     | 0.43              |
| 1:C:289:ARG:NH2  | 1:C:301:GLU:OE1  | 2.34                     | 0.43              |
| 3:B:189:LYS:O    | 3:B:193:GLY:HA3  | 2.19                     | 0.43              |
| 1:G:224:MET:SD   | 1:G:232:LEU:HD12 | 2.58                     | 0.43              |
| 1:G:268:ASP:N    | 1:G:268:ASP:OD1  | 2.52                     | 0.43              |
| 2:H:4:GLN:HB2    | 2:H:6:ILE:HG23   | 2.00                     | 0.43              |
| 1:E:174:ALA:HA   | 1:E:181:ASP:HB2  | 2.00                     | 0.43              |
| 3:F:58:ALA:C     | 3:F:60:GLU:CA    | 2.92                     | 0.43              |
| 1:I:125:GLU:HA   | 1:I:142:LYS:HA   | 2.00                     | 0.43              |
| 3:J:261:SER:HB2  | 3:J:268:VAL:HG23 | 2.00                     | 0.43              |
| 1:A:221:VAL:O    | 1:A:222:LEU:HD23 | 2.19                     | 0.43              |
| 1:A:302:ALA:O    | 1:A:306:ALA:N    | 2.49                     | 0.43              |
| 3:F:75:VAL:HG11  | 3:F:302:LEU:HD21 | 2.01                     | 0.43              |
| 1:O:165:ARG:HD3  | 1:O:165:ARG:HA   | 1.85                     | 0.43              |
| 2:P:21:ILE:HB    | 2:P:76:LYS:HB2   | 2.01                     | 0.43              |
| 2:P:184:ASN:OD1  | 2:P:184:ASN:N    | 2.52                     | 0.43              |
| 1:C:8:THR:OG1    | 1:C:64:ASN:ND2   | 2.42                     | 0.43              |
| 1:C:110:TYR:HD2  | 1:C:216:PRO:HG3  | 1.83                     | 0.43              |
| 2:D:13:GLY:C     | 3:F:265:GLU:CA   | 2.80                     | 0.43              |
| 1:A:303:ALA:HB1  | 1:A:334:ARG:HB3  | 2.01                     | 0.43              |
| 2:L:66:MET:O     | 2:L:67:ALA:C     | 2.58                     | 0.43              |
| 2:L:110:LYS:O    | 2:L:249:VAL:HG11 | 2.16                     | 0.43              |
| 2:L:184:ASN:OD1  | 2:L:185:ILE:N    | 2.52                     | 0.43              |
| 2:P:40:HIS:HE1   | 2:P:346:VAL:HG22 | 1.83                     | 0.43              |
| 2:P:66:MET:CA    | 2:P:69:ARG:CD    | 2.75                     | 0.43              |
| 2:D:337:ILE:O    | 2:D:341:ILE:HG13 | 2.19                     | 0.42              |
| 3:B:67:LEU:C     | 3:B:70:MET:H     | 2.26                     | 0.42              |
| 3:B:279:GLN:C    | 3:B:281:VAL:HG23 | 2.44                     | 0.42              |
| 1:G:289:ARG:NH2  | 1:G:301:GLU:OE1  | 2.51                     | 0.42              |
| 1:E:284:ALA:O    | 1:E:288:LEU:HG   | 2.19                     | 0.42              |
| 3:J:217:ASP:OD1  | 3:J:217:ASP:N    | 2.52                     | 0.42              |
| 2:P:135:TYR:CD1  | 2:P:151:LYS:HA   | 2.53                     | 0.42              |
| 2:P:190:ASP:OD2  | 2:P:237:TYR:CE2  | 2.71                     | 0.42              |
| 3:B:111:VAL:HG11 | 3:B:247:ALA:HB1  | 2.01                     | 0.42              |
| 3:B:265:GLU:HA   | 2:H:13:GLY:HA2   | 2.01                     | 0.42              |
| 3:B:336:HIS:HD2  | 3:B:340:GLU:OE2  | 2.02                     | 0.42              |
| 3:B:343:CYS:O    | 3:B:346:VAL:HG12 | 2.18                     | 0.42              |
| 2:L:42:CYS:HB3   | 3:N:303:ASN:HD22 | 1.84                     | 0.42              |
| 2:L:143:VAL:HG22 | 2:L:144:ALA:H    | 1.84                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:L:336:ALA:O    | 2:L:340:VAL:HG23 | 2.19                     | 0.42              |
| 3:J:23:ASP:OD1   | 3:J:53:GLU:CB    | 2.67                     | 0.42              |
| 3:J:104:LEU:CD1  | 3:J:268:VAL:CG2  | 2.88                     | 0.42              |
| 1:O:95:ALA:O     | 1:O:250:ASN:HA   | 2.19                     | 0.42              |
| 2:P:5:THR:C      | 2:P:6:ILE:HG22   | 2.44                     | 0.42              |
| 2:P:40:HIS:HE1   | 2:P:346:VAL:HG21 | 1.82                     | 0.42              |
| 3:N:262:TYR:N    | 3:N:262:TYR:CD1  | 2.87                     | 0.42              |
| 3:N:263:SER:O    | 3:N:264:ALA:C    | 2.61                     | 0.42              |
| 3:N:318:VAL:HG21 | 3:N:342:ILE:HD13 | 2.01                     | 0.42              |
| 2:D:246:ALA:O    | 2:D:251:GLY:N    | 2.52                     | 0.42              |
| 1:A:66:MET:HE1   | 1:A:290:HIS:CE1  | 2.55                     | 0.42              |
| 1:G:98:ARG:HE    | 1:G:98:ARG:HB2   | 1.51                     | 0.42              |
| 2:H:267:PHE:CE2  | 2:H:296:MET:HA   | 2.40                     | 0.42              |
| 1:K:168:VAL:HG22 | 1:K:221:VAL:HB   | 2.00                     | 0.42              |
| 3:J:235:MET:SD   | 3:J:243:ILE:HG13 | 2.59                     | 0.42              |
| 1:O:276:ASN:CG   | 1:O:315:THR:HG21 | 2.44                     | 0.42              |
| 1:O:282:LEU:HA   | 1:O:285:VAL:HB   | 2.02                     | 0.42              |
| 1:A:185:LEU:HD22 | 1:A:189:ARG:NH1  | 2.33                     | 0.42              |
| 3:B:96:MET:O     | 3:B:99:ARG:HB2   | 2.20                     | 0.42              |
| 3:F:19:MET:HE1   | 3:F:48:GLU:OE1   | 2.17                     | 0.42              |
| 3:F:180:THR:HG23 | 3:F:212:GLU:HB2  | 2.01                     | 0.42              |
| 3:F:235:MET:HB2  | 3:F:239:TYR:HB2  | 2.01                     | 0.42              |
| 1:K:126:TYR:CD2  | 2:L:185:ILE:HG12 | 2.55                     | 0.42              |
| 2:L:195:GLN:HA   | 2:L:198:ARG:HD2  | 2.02                     | 0.42              |
| 1:I:95:ALA:O     | 1:I:250:ASN:HA   | 2.20                     | 0.42              |
| 1:I:288:LEU:HB2  | 1:I:297:ALA:HB2  | 2.01                     | 0.42              |
| 3:J:86:GLU:CA    | 3:J:91:LEU:HD11  | 2.48                     | 0.42              |
| 3:J:307:HIS:O    | 3:J:311:ILE:HG13 | 2.20                     | 0.42              |
| 1:O:269:ILE:O    | 1:O:270:ALA:C    | 2.60                     | 0.42              |
| 2:P:5:THR:O      | 2:P:6:ILE:HG23   | 2.20                     | 0.42              |
| 2:P:135:TYR:CD1  | 2:P:151:LYS:CA   | 3.02                     | 0.42              |
| 1:C:13:ASP:O     | 1:C:71:PRO:HG2   | 2.19                     | 0.42              |
| 1:C:69:LYS:HE2   | 1:C:260:GLU:HB2  | 2.02                     | 0.42              |
| 2:D:140:HIS:ND1  | 1:A:131:HIS:NE2  | 2.61                     | 0.42              |
| 2:H:322:MET:HE3  | 2:H:339:ASP:HB2  | 2.01                     | 0.42              |
| 1:E:4:VAL:HA     | 1:E:33:PRO:HB2   | 2.00                     | 0.42              |
| 2:L:194:LEU:HD21 | 2:L:198:ARG:NH1  | 2.35                     | 0.42              |
| 1:I:91:PHE:HB2   | 1:I:93:LEU:HG    | 2.01                     | 0.42              |
| 1:I:210:LEU:HA   | 3:J:245:ASN:O    | 2.20                     | 0.42              |
| 3:J:49:HIS:CE1   | 3:J:69:SER:OG    | 2.73                     | 0.42              |
| 2:P:43:VAL:HG23  | 2:P:44:PRO:HD2   | 2.01                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:N:63:LEU:CG    | 3:N:64:GLU:N     | 2.82                     | 0.42              |
| 3:N:169:ASP:O    | 3:N:173:LYS:HB2  | 2.18                     | 0.42              |
| 1:C:108:THR:OG1  | 1:C:110:TYR:O    | 2.37                     | 0.42              |
| 2:D:107:ILE:HD11 | 2:D:242:ASN:ND2  | 2.34                     | 0.42              |
| 3:B:220:CYS:HA   | 3:B:223:LEU:HD12 | 2.00                     | 0.42              |
| 1:G:173:LYS:HD2  | 1:G:205:LEU:HD23 | 2.00                     | 0.42              |
| 1:G:285:VAL:HG11 | 1:G:301:GLU:HG3  | 2.01                     | 0.42              |
| 3:J:190:LEU:HD23 | 3:J:190:LEU:HA   | 1.85                     | 0.42              |
| 1:O:25:LYS:HG2   | 1:O:332:CYS:SG   | 2.60                     | 0.42              |
| 1:O:120:GLU:OE2  | 1:O:122:THR:OG1  | 2.27                     | 0.42              |
| 1:O:330:GLU:O    | 1:O:334:ARG:HG3  | 2.19                     | 0.42              |
| 2:P:304:SER:OG   | 2:P:305:TYR:N    | 2.52                     | 0.42              |
| 1:C:130:GLU:OE1  | 1:C:140:SER:OG   | 2.35                     | 0.42              |
| 1:C:234:ASP:O    | 2:D:219:MET:HB2  | 2.20                     | 0.42              |
| 1:A:247:PRO:HD3  | 1:A:282:LEU:HD12 | 2.00                     | 0.42              |
| 2:H:97:ARG:HB2   | 2:H:102:LEU:HB2  | 2.00                     | 0.42              |
| 2:H:185:ILE:CD1  | 2:H:185:ILE:N    | 2.81                     | 0.42              |
| 2:L:57:ASP:CB    | 2:L:59:GLU:O     | 2.68                     | 0.42              |
| 1:O:136:GLY:O    | 1:O:137:VAL:HB   | 2.20                     | 0.42              |
| 2:P:42:CYS:O     | 2:P:42:CYS:SG    | 2.77                     | 0.42              |
| 2:P:85:LEU:CB    | 2:P:87:PRO:HA    | 2.50                     | 0.42              |
| 2:D:64:ALA:O     | 2:D:67:ALA:HB3   | 2.19                     | 0.42              |
| 2:D:214:VAL:O    | 2:D:218:THR:HG23 | 2.19                     | 0.42              |
| 1:A:285:VAL:O    | 1:A:289:ARG:HG3  | 2.20                     | 0.42              |
| 3:B:105:PHE:CE2  | 3:B:162:ARG:HD3  | 2.55                     | 0.42              |
| 2:H:94:ASN:O     | 2:H:95:ILE:C     | 2.61                     | 0.42              |
| 2:H:267:PHE:HZ   | 2:H:299:HIS:HB3  | 1.85                     | 0.42              |
| 1:K:74:THR:O     | 1:K:74:THR:OG1   | 2.35                     | 0.42              |
| 2:L:66:MET:O     | 2:L:70:ARG:N     | 2.42                     | 0.42              |
| 2:L:73:VAL:HG22  | 2:L:265:ALA:HB3  | 2.01                     | 0.42              |
| 2:L:174:ARG:HB3  | 2:L:229:ASP:OD2  | 2.19                     | 0.42              |
| 1:I:81:PRO:CD    | 1:I:81:PRO:O     | 2.66                     | 0.42              |
| 1:I:285:VAL:O    | 1:I:289:ARG:HG3  | 2.19                     | 0.42              |
| 3:J:183:HIS:ND1  | 3:J:196:LEU:HD13 | 2.33                     | 0.42              |
| 3:J:235:MET:HG3  | 3:J:239:TYR:HB2  | 2.02                     | 0.42              |
| 1:O:250:ASN:C    | 1:O:251:ILE:HD12 | 2.45                     | 0.42              |
| 2:P:290:LEU:HD23 | 2:P:290:LEU:HA   | 1.88                     | 0.42              |
| 1:M:19:ILE:O     | 1:M:23:VAL:HG23  | 2.19                     | 0.42              |
| 1:M:231:ILE:HG22 | 3:N:217:ASP:HB3  | 2.01                     | 0.42              |
| 1:C:130:GLU:OE1  | 2:D:189:GLY:N    | 2.42                     | 0.42              |
| 1:C:247:PRO:HB3  | 1:C:282:LEU:HB3  | 2.02                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:92:ARG:O     | 2:D:95:ILE:HG22  | 2.20                     | 0.42              |
| 2:D:254:LEU:HD23 | 2:D:285:ASN:HD21 | 1.85                     | 0.42              |
| 1:A:123:GLU:HB2  | 1:A:124:GLY:H    | 1.62                     | 0.42              |
| 1:A:331:ILE:O    | 1:A:335:VAL:HG13 | 2.19                     | 0.42              |
| 3:B:136:GLU:OE1  | 3:B:153:LYS:HG3  | 2.20                     | 0.42              |
| 2:H:21:ILE:CG2   | 2:H:52:VAL:CB    | 2.98                     | 0.42              |
| 2:H:315:ALA:C    | 2:H:343:HIS:HE1  | 2.22                     | 0.42              |
| 1:E:240:ILE:HG13 | 1:E:246:THR:CG2  | 2.47                     | 0.42              |
| 3:F:37:PHE:CE1   | 3:F:299:LEU:HD11 | 2.55                     | 0.42              |
| 2:L:76:LYS:NZ    | 2:L:93:ASN:HD21  | 2.17                     | 0.42              |
| 2:L:140:HIS:NE2  | 3:J:150:GLU:OE1  | 2.52                     | 0.42              |
| 3:J:248:ALA:HA   | 3:J:257:VAL:HG21 | 2.02                     | 0.42              |
| 1:O:55:SER:HA    | 1:O:58:LYS:HB3   | 2.02                     | 0.42              |
| 1:O:318:LEU:HA   | 1:O:318:LEU:HD13 | 1.87                     | 0.42              |
| 2:P:88:SER:O     | 2:P:89:HIS:CB    | 2.66                     | 0.42              |
| 1:M:119:ARG:HD2  | 1:M:230:ASP:N    | 2.35                     | 0.42              |
| 3:N:156:THR:O    | 3:N:158:ALA:N    | 2.53                     | 0.42              |
| 3:N:260:GLU:OE1  | 3:N:262:TYR:HE1  | 2.03                     | 0.42              |
| 1:C:69:LYS:NZ    | 1:C:260:GLU:OE2  | 2.30                     | 0.42              |
| 2:D:97:ARG:HB2   | 2:D:102:LEU:HB2  | 2.01                     | 0.42              |
| 2:D:195:GLN:HA   | 2:D:198:ARG:HB2  | 2.02                     | 0.42              |
| 3:B:342:ILE:HD13 | 3:B:342:ILE:HA   | 1.85                     | 0.42              |
| 1:G:235:LEU:HD13 | 2:H:218:THR:HB   | 2.01                     | 0.42              |
| 1:G:239:LEU:HD23 | 2:H:222:VAL:HG21 | 2.02                     | 0.42              |
| 3:F:287:ASN:ND2  | 3:F:329:MET:SD   | 2.93                     | 0.42              |
| 1:K:22:ALA:O     | 1:K:26:ILE:HG13  | 2.19                     | 0.42              |
| 2:L:24:ASP:OD1   | 2:L:53:SER:HA    | 2.19                     | 0.42              |
| 2:L:112:LEU:HB2  | 2:L:115:VAL:HB   | 2.02                     | 0.42              |
| 2:L:316:SER:HB3  | 2:L:340:VAL:HG22 | 2.02                     | 0.42              |
| 1:I:167:ASN:O    | 1:I:220:ASP:HB3  | 2.19                     | 0.42              |
| 1:O:184:PHE:CE2  | 1:O:225:PRO:HD3  | 2.55                     | 0.42              |
| 1:O:293:LEU:HB3  | 1:O:296:HIS:HB2  | 2.01                     | 0.42              |
| 2:P:5:THR:O      | 2:P:6:ILE:CG2    | 2.68                     | 0.42              |
| 2:D:140:HIS:CE1  | 1:A:131:HIS:HD2  | 2.38                     | 0.41              |
| 2:D:140:HIS:NE2  | 2:D:148:GLU:OE1  | 2.53                     | 0.41              |
| 1:G:68:LEU:HB2   | 1:G:287:MET:HE1  | 2.02                     | 0.41              |
| 2:H:285:ASN:OD1  | 2:H:324:THR:HG21 | 2.20                     | 0.41              |
| 2:H:340:VAL:O    | 2:H:344:ILE:N    | 2.53                     | 0.41              |
| 3:F:135:GLY:CA   | 3:F:154:ILE:O    | 2.68                     | 0.41              |
| 2:L:152:ILE:HD12 | 1:I:133:ILE:HG23 | 2.01                     | 0.41              |
| 2:L:297:LEU:HD22 | 2:L:302:LEU:HD12 | 2.01                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:85:LEU:C     | 1:I:87:LEU:N     | 2.77                     | 0.41              |
| 1:O:98:ARG:HE    | 1:O:98:ARG:HB2   | 1.38                     | 0.41              |
| 2:P:284:ALA:O    | 2:P:333:THR:HG22 | 2.20                     | 0.41              |
| 1:M:167:ASN:O    | 1:M:220:ASP:HB3  | 2.20                     | 0.41              |
| 1:M:189:ARG:NH2  | 1:M:202:GLU:OE2  | 2.47                     | 0.41              |
| 2:D:129:GLU:HG3  | 2:D:132:GLU:CB   | 2.50                     | 0.41              |
| 3:B:78:ILE:O     | 3:B:78:ILE:HG13  | 2.13                     | 0.41              |
| 3:B:94:TYR:C     | 3:B:97:ARG:HB3   | 2.45                     | 0.41              |
| 3:B:182:VAL:CG1  | 3:B:216:ILE:HA   | 2.50                     | 0.41              |
| 1:G:225:PRO:HD2  | 1:G:228:TYR:CD2  | 2.55                     | 0.41              |
| 2:H:126:ILE:HG21 | 2:H:242:ASN:OD1  | 2.20                     | 0.41              |
| 1:E:172:HIS:O    | 1:E:205:LEU:N    | 2.52                     | 0.41              |
| 1:E:175:ASN:CB   | 3:F:85:MET:HA    | 2.48                     | 0.41              |
| 1:K:98:ARG:NE    | 1:K:233:SER:HB2  | 2.36                     | 0.41              |
| 1:K:120:GLU:HG2  | 1:K:152:ILE:HD13 | 2.02                     | 0.41              |
| 1:K:231:ILE:HG12 | 2:L:215:ASP:OD1  | 2.20                     | 0.41              |
| 2:L:65:ILE:O     | 2:L:69:ARG:N     | 2.35                     | 0.41              |
| 1:I:327:PHE:O    | 1:I:331:ILE:HG13 | 2.20                     | 0.41              |
| 3:J:287:ASN:OD1  | 3:J:289:THR:HB   | 2.21                     | 0.41              |
| 1:O:306:ALA:HA   | 1:O:309:LYS:HB3  | 2.02                     | 0.41              |
| 2:P:140:HIS:HB3  | 1:M:129:ILE:HG23 | 2.02                     | 0.41              |
| 2:P:300:LEU:O    | 2:P:301:LYS:HB2  | 2.19                     | 0.41              |
| 1:M:289:ARG:NH2  | 1:M:301:GLU:OE1  | 2.53                     | 0.41              |
| 1:C:281:LEU:HD12 | 1:C:284:ALA:HB3  | 2.03                     | 0.41              |
| 1:C:291:MET:HB2  | 1:C:293:LEU:HG   | 2.01                     | 0.41              |
| 2:D:65:ILE:O     | 2:D:69:ARG:N     | 2.50                     | 0.41              |
| 1:A:56:GLU:H     | 1:A:56:GLU:CD    | 2.28                     | 0.41              |
| 1:A:103:ILE:HG23 | 1:A:308:ILE:HD13 | 2.01                     | 0.41              |
| 2:H:252:PRO:HA   | 2:H:271:THR:CB   | 2.49                     | 0.41              |
| 1:K:73:LYS:HA    | 1:K:73:LYS:HD2   | 1.49                     | 0.41              |
| 2:L:57:ASP:C     | 2:L:59:GLU:C     | 2.88                     | 0.41              |
| 3:J:84:PRO:HD2   | 3:J:84:PRO:O     | 2.20                     | 0.41              |
| 1:O:133:ILE:CG2  | 3:N:154:ILE:HG13 | 2.49                     | 0.41              |
| 1:O:210:LEU:O    | 1:O:214:GLN:HG3  | 2.20                     | 0.41              |
| 1:O:213:VAL:HG11 | 2:P:244:VAL:HG13 | 2.02                     | 0.41              |
| 2:P:40:HIS:ND1   | 2:P:40:HIS:C     | 2.72                     | 0.41              |
| 2:P:326:ASP:OD1  | 2:P:327:ILE:HG23 | 2.20                     | 0.41              |
| 1:M:243:LEU:O    | 1:M:263:HIS:HB3  | 2.21                     | 0.41              |
| 3:N:256:VAL:O    | 3:N:258:PRO:CD   | 2.68                     | 0.41              |
| 1:G:145:THR:HG22 | 2:H:146:VAL:HG22 | 2.01                     | 0.41              |
| 1:E:11:PRO:HB3   | 1:E:17:PRO:HA    | 2.02                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:47:PRO:HD2   | 1:E:51:TRP:HE1   | 1.86                     | 0.41              |
| 1:E:158:GLU:O    | 1:E:162:ASN:HB2  | 2.20                     | 0.41              |
| 1:K:288:LEU:HD23 | 1:K:291:MET:HE3  | 2.03                     | 0.41              |
| 2:L:61:ILE:CD1   | 2:L:64:ALA:HB2   | 2.31                     | 0.41              |
| 2:L:256:ALA:HB2  | 2:L:291:LEU:HB3  | 2.02                     | 0.41              |
| 3:J:99:ARG:HD3   | 3:J:132:GLN:HG2  | 2.03                     | 0.41              |
| 1:O:157:PHE:CE1  | 1:O:168:VAL:HG11 | 2.52                     | 0.41              |
| 1:O:172:HIS:ND1  | 1:O:174:ALA:N    | 2.60                     | 0.41              |
| 1:O:201:ASN:OD1  | 1:O:201:ASN:N    | 2.52                     | 0.41              |
| 1:O:243:LEU:HB3  | 1:O:262:VAL:HG23 | 2.03                     | 0.41              |
| 3:N:125:ASP:O    | 3:N:126:LEU:HD23 | 2.20                     | 0.41              |
| 2:D:63:ASN:HB3   | 3:F:207:PRO:CG   | 2.49                     | 0.41              |
| 2:D:233:MET:HE1  | 2:D:241:VAL:HG11 | 2.01                     | 0.41              |
| 3:B:93:SER:CB    | 3:B:96:MET:CG    | 2.98                     | 0.41              |
| 1:G:314:LEU:HB2  | 1:G:320:GLY:H    | 1.85                     | 0.41              |
| 1:E:119:ARG:CZ   | 1:E:230:ASP:HB2  | 2.50                     | 0.41              |
| 3:F:207:PRO:C    | 3:F:209:ILE:H    | 2.28                     | 0.41              |
| 1:K:273:ASP:OD1  | 1:K:324:CYS:HB3  | 2.20                     | 0.41              |
| 2:L:43:VAL:HG22  | 2:L:305:TYR:HD2  | 1.85                     | 0.41              |
| 2:L:166:PHE:HD2  | 2:L:204:TYR:HB2  | 1.85                     | 0.41              |
| 3:J:184:LYS:CA   | 3:J:192:ASP:OD2  | 2.68                     | 0.41              |
| 1:O:160:ALA:HA   | 1:O:165:ARG:HB2  | 2.03                     | 0.41              |
| 2:P:135:TYR:HE1  | 2:P:151:LYS:N    | 2.19                     | 0.41              |
| 3:N:30:MET:CE    | 3:N:291:MET:CE   | 2.52                     | 0.41              |
| 3:N:304:LEU:HD23 | 3:N:304:LEU:N    | 2.34                     | 0.41              |
| 1:C:115:ILE:HD11 | 1:C:216:PRO:O    | 2.21                     | 0.41              |
| 2:D:15:ARG:NH1   | 2:D:46:ASP:OD2   | 2.53                     | 0.41              |
| 2:D:285:ASN:HA   | 2:D:324:THR:HG21 | 2.02                     | 0.41              |
| 2:H:237:TYR:N    | 2:H:237:TYR:CD1  | 2.87                     | 0.41              |
| 2:H:347:ILE:HD12 | 2:H:347:ILE:C    | 2.43                     | 0.41              |
| 1:E:86:LEU:O     | 1:E:90:THR:OG1   | 2.25                     | 0.41              |
| 1:I:120:GLU:OE2  | 1:I:120:GLU:C    | 2.63                     | 0.41              |
| 3:J:80:LYS:HD2   | 3:J:80:LYS:HA    | 1.90                     | 0.41              |
| 3:J:343:CYS:HA   | 3:J:346:VAL:HG12 | 2.03                     | 0.41              |
| 1:M:37:GLU:OE1   | 1:M:60:SER:OG    | 2.35                     | 0.41              |
| 3:N:259:GLY:HA3  | 3:N:272:GLY:CA   | 2.51                     | 0.41              |
| 1:C:88:ARG:HD2   | 1:C:121:ASN:O    | 2.20                     | 0.41              |
| 2:D:19:THR:HG23  | 2:D:71:ASN:HB2   | 2.01                     | 0.41              |
| 3:B:77:ILE:O     | 3:B:77:ILE:CG1   | 2.66                     | 0.41              |
| 3:B:96:MET:C     | 3:B:99:ARG:HB2   | 2.45                     | 0.41              |
| 3:F:312:ALA:O    | 3:F:316:LYS:HG3  | 2.20                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:225:PRO:HD2  | 1:K:228:TYR:CD2  | 2.56                     | 0.41              |
| 2:L:138:LEU:HD23 | 2:L:138:LEU:N    | 2.36                     | 0.41              |
| 2:L:176:LYS:O    | 2:L:229:ASP:HB3  | 2.20                     | 0.41              |
| 1:I:119:ARG:NH2  | 1:I:230:ASP:OD1  | 2.54                     | 0.41              |
| 3:J:29:LEU:O     | 3:J:33:VAL:HG23  | 2.20                     | 0.41              |
| 3:J:96:MET:HE2   | 3:J:137:TYR:HD2  | 1.86                     | 0.41              |
| 3:J:163:ILE:HD12 | 3:J:163:ILE:HA   | 1.93                     | 0.41              |
| 3:J:342:ILE:HA   | 3:J:342:ILE:HD13 | 1.75                     | 0.41              |
| 1:O:64:ASN:C     | 1:O:66:MET:H     | 2.29                     | 0.41              |
| 1:O:167:ASN:OD1  | 1:O:199:LYS:HB3  | 2.20                     | 0.41              |
| 1:M:127:SER:C    | 1:M:129:ILE:H    | 2.28                     | 0.41              |
| 3:N:248:ALA:CB   | 3:N:257:VAL:HG21 | 2.50                     | 0.41              |
| 2:H:20:MET:HB2   | 2:H:47:PHE:CD1   | 2.56                     | 0.41              |
| 3:J:108:VAL:HA   | 3:J:128:ILE:O    | 2.20                     | 0.41              |
| 3:J:153:LYS:CD   | 3:J:188:MET:HE1  | 2.50                     | 0.41              |
| 1:M:178:ARG:HG2  | 3:N:86:GLU:CB    | 2.51                     | 0.41              |
| 3:N:29:LEU:HD11  | 3:N:288:PRO:HA   | 1.93                     | 0.41              |
| 1:C:15:ILE:O     | 1:C:19:ILE:HG12  | 2.21                     | 0.41              |
| 1:C:143:LEU:HA   | 2:D:147:VAL:O    | 2.20                     | 0.41              |
| 1:C:195:CYS:C    | 1:C:197:ASP:N    | 2.79                     | 0.41              |
| 1:A:68:LEU:HD12  | 1:A:259:PHE:O    | 2.21                     | 0.41              |
| 1:A:108:THR:C    | 1:A:110:TYR:H    | 2.29                     | 0.41              |
| 1:A:130:GLU:CD   | 3:B:190:LEU:H    | 2.29                     | 0.41              |
| 3:B:111:VAL:CG2  | 3:B:126:LEU:HB2  | 2.51                     | 0.41              |
| 3:B:302:LEU:HD23 | 3:B:302:LEU:HA   | 1.85                     | 0.41              |
| 1:G:160:ALA:HA   | 1:G:165:ARG:HB2  | 2.02                     | 0.41              |
| 1:G:196:LYS:HE2  | 1:G:196:LYS:HB3  | 1.86                     | 0.41              |
| 1:G:285:VAL:HG13 | 1:G:297:ALA:HB1  | 2.02                     | 0.41              |
| 2:H:337:ILE:O    | 2:H:341:ILE:HG13 | 2.21                     | 0.41              |
| 1:E:15:ILE:HD13  | 1:E:266:ALA:HB3  | 2.03                     | 0.41              |
| 3:F:56:ASN:O     | 3:F:57:MET:CB    | 2.69                     | 0.41              |
| 2:L:195:GLN:O    | 2:L:195:GLN:HG2  | 2.21                     | 0.41              |
| 2:L:281:LYS:O    | 2:L:283:ILE:HG12 | 2.21                     | 0.41              |
| 1:I:187:LYS:HD3  | 1:I:187:LYS:HA   | 1.71                     | 0.41              |
| 3:J:37:PHE:C     | 3:J:39:ALA:H     | 2.29                     | 0.41              |
| 3:J:183:HIS:HD2  | 3:J:214:MET:O    | 2.03                     | 0.41              |
| 1:O:180:SER:OG   | 1:O:181:ASP:OD1  | 2.38                     | 0.41              |
| 2:P:137:SER:C    | 2:P:138:LEU:HD12 | 2.46                     | 0.41              |
| 3:N:182:VAL:HB   | 3:N:235:MET:HB3  | 2.02                     | 0.41              |
| 3:B:61:GLU:OE2   | 3:B:97:ARG:NH2   | 2.54                     | 0.41              |
| 3:B:81:ILE:HG13  | 3:B:81:ILE:O     | 2.21                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:B:87:TYR:O     | 3:B:91:LEU:HB3   | 2.21                     | 0.41              |
| 1:E:129:ILE:O    | 1:E:141:ILE:HB   | 2.21                     | 0.41              |
| 1:E:234:ASP:OD1  | 1:E:234:ASP:N    | 2.53                     | 0.41              |
| 2:L:74:ALA:O     | 2:L:266:VAL:CA   | 2.55                     | 0.41              |
| 2:L:323:HIS:CG   | 2:L:327:ILE:HD11 | 2.56                     | 0.41              |
| 2:L:344:ILE:O    | 2:L:345:ARG:CB   | 2.69                     | 0.41              |
| 1:I:125:GLU:O    | 1:I:126:TYR:C    | 2.63                     | 0.41              |
| 1:I:332:CYS:O    | 1:I:335:VAL:HG22 | 2.20                     | 0.41              |
| 3:J:15:PHE:O     | 3:J:44:VAL:HA    | 2.21                     | 0.41              |
| 1:O:11:PRO:HB2   | 1:O:17:PRO:HG3   | 2.03                     | 0.41              |
| 2:P:36:SER:CA    | 2:P:39:ARG:HH12  | 2.29                     | 0.41              |
| 2:P:66:MET:HB2   | 2:P:69:ARG:HD3   | 2.02                     | 0.41              |
| 1:M:53:ILE:CG2   | 1:M:86:LEU:HD13  | 2.51                     | 0.41              |
| 1:C:125:GLU:OE1  | 1:C:125:GLU:N    | 2.36                     | 0.40              |
| 1:A:123:GLU:CD   | 1:A:148:ALA:HB3  | 2.46                     | 0.40              |
| 3:B:37:PHE:CZ    | 3:B:299:LEU:HD21 | 2.56                     | 0.40              |
| 3:B:95:ASP:O     | 3:B:98:LEU:HB3   | 2.20                     | 0.40              |
| 3:B:235:MET:HE2  | 3:B:235:MET:HB3  | 1.90                     | 0.40              |
| 1:G:224:MET:SD   | 1:G:229:GLY:HA2  | 2.61                     | 0.40              |
| 2:H:124:ILE:HD11 | 2:H:228:PHE:HB2  | 2.03                     | 0.40              |
| 2:H:285:ASN:OD1  | 2:H:324:THR:CG2  | 2.69                     | 0.40              |
| 1:I:211:ASN:HB3  | 1:I:218:GLN:OE1  | 2.21                     | 0.40              |
| 1:O:16:GLY:O     | 1:O:20:SER:OG    | 2.23                     | 0.40              |
| 1:O:271:GLY:O    | 1:O:272:LYS:CB   | 2.70                     | 0.40              |
| 2:P:98:THR:C     | 2:P:100:LEU:H    | 2.28                     | 0.40              |
| 2:P:161:ILE:HA   | 2:P:161:ILE:HD12 | 1.85                     | 0.40              |
| 2:P:281:LYS:O    | 2:P:282:ASN:CB   | 2.69                     | 0.40              |
| 1:C:289:ARG:HH22 | 1:C:301:GLU:CD   | 2.25                     | 0.40              |
| 2:H:56:ALA:O     | 2:H:60:ASP:OD1   | 2.39                     | 0.40              |
| 2:H:95:ILE:O     | 2:H:96:LEU:C     | 2.63                     | 0.40              |
| 3:F:19:MET:O     | 3:F:48:GLU:HA    | 2.22                     | 0.40              |
| 3:F:60:GLU:O     | 3:F:61:GLU:CG    | 2.69                     | 0.40              |
| 1:I:15:ILE:HD12  | 1:I:275:ALA:HB1  | 2.01                     | 0.40              |
| 1:I:243:LEU:HB3  | 1:I:262:VAL:HG23 | 2.03                     | 0.40              |
| 3:J:60:GLU:O     | 3:J:63:LEU:CA    | 2.69                     | 0.40              |
| 2:P:40:HIS:CE1   | 2:P:346:VAL:CG2  | 3.02                     | 0.40              |
| 2:P:61:ILE:C     | 2:P:65:ILE:HG13  | 2.45                     | 0.40              |
| 2:P:135:TYR:CE1  | 2:P:151:LYS:CA   | 3.03                     | 0.40              |
| 1:M:308:ILE:HG12 | 1:M:327:PHE:HZ   | 1.86                     | 0.40              |
| 3:N:295:ALA:O    | 3:N:298:MET:HB3  | 2.20                     | 0.40              |
| 1:C:47:PRO:HG3   | 1:C:51:TRP:N     | 2.37                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:159:LEU:O    | 2:D:163:GLU:HG2  | 2.21                     | 0.40              |
| 1:A:15:ILE:HG23  | 1:A:265:THR:O    | 2.22                     | 0.40              |
| 3:B:176:ARG:HD2  | 3:B:231:ASP:OD1  | 2.21                     | 0.40              |
| 1:G:259:PHE:HE2  | 1:G:286:MET:HG2  | 1.86                     | 0.40              |
| 1:G:291:MET:HG2  | 1:G:291:MET:H    | 1.67                     | 0.40              |
| 1:E:89:LYS:HE2   | 1:E:89:LYS:HB3   | 1.83                     | 0.40              |
| 3:F:221:MET:O    | 3:F:224:VAL:HG22 | 2.21                     | 0.40              |
| 1:K:215:ASP:O    | 1:K:218:GLN:HG2  | 2.22                     | 0.40              |
| 3:J:239:TYR:HA   | 3:J:242:ILE:HG12 | 2.03                     | 0.40              |
| 2:P:34:VAL:HA    | 2:P:37:VAL:HG23  | 2.03                     | 0.40              |
| 1:M:183:LEU:HA   | 1:M:186:GLN:HG2  | 2.02                     | 0.40              |
| 3:N:19:MET:HE1   | 3:N:34:LYS:NZ    | 2.37                     | 0.40              |
| 3:N:198:CYS:O    | 3:N:201:GLU:HB2  | 2.21                     | 0.40              |
| 3:N:214:MET:HE3  | 3:N:214:MET:HB2  | 1.80                     | 0.40              |
| 1:C:123:GLU:CD   | 1:C:145:THR:H    | 2.29                     | 0.40              |
| 2:D:134:GLU:O    | 2:D:135:TYR:CB   | 2.69                     | 0.40              |
| 1:A:91:PHE:CD2   | 1:A:256:VAL:HG11 | 2.57                     | 0.40              |
| 1:A:205:LEU:HD22 | 1:A:228:TYR:CD2  | 2.56                     | 0.40              |
| 1:A:237:ALA:CB   | 1:A:246:THR:HG21 | 2.48                     | 0.40              |
| 3:B:184:LYS:HD2  | 3:B:186:ASN:OD1  | 2.21                     | 0.40              |
| 3:B:265:GLU:O    | 2:H:13:GLY:HA2   | 2.21                     | 0.40              |
| 1:G:281:LEU:HD11 | 1:G:300:ILE:CG2  | 2.51                     | 0.40              |
| 2:H:61:ILE:C     | 2:H:64:ALA:H     | 2.26                     | 0.40              |
| 2:H:84:ASN:O     | 2:H:87:PRO:CB    | 2.70                     | 0.40              |
| 2:H:281:LYS:O    | 2:H:283:ILE:HG12 | 2.22                     | 0.40              |
| 2:H:295:MET:HA   | 2:H:298:ASP:HB2  | 2.03                     | 0.40              |
| 2:H:316:SER:CB   | 2:H:340:VAL:HG22 | 2.51                     | 0.40              |
| 1:E:83:MET:SD    | 1:E:83:MET:O     | 2.79                     | 0.40              |
| 1:E:252:GLY:N    | 1:E:256:VAL:O    | 2.50                     | 0.40              |
| 2:L:125:LEU:HG   | 2:L:174:ARG:NH2  | 2.36                     | 0.40              |
| 1:I:158:GLU:O    | 1:I:162:ASN:N    | 2.44                     | 0.40              |
| 3:J:49:HIS:NE2   | 3:J:69:SER:HB2   | 2.37                     | 0.40              |
| 3:J:187:ILE:HD12 | 3:J:187:ILE:HA   | 1.89                     | 0.40              |
| 2:P:337:ILE:O    | 2:P:341:ILE:HG13 | 2.21                     | 0.40              |
| 3:N:239:TYR:N    | 3:N:239:TYR:CD1  | 2.88                     | 0.40              |
| 3:N:288:PRO:CD   | 3:N:289:THR:H    | 2.33                     | 0.40              |
| 1:C:66:MET:SD    | 1:C:257:ALA:HB3  | 2.62                     | 0.40              |
| 2:D:29:GLU:H     | 2:D:29:GLU:HG3   | 1.70                     | 0.40              |
| 1:A:53:ILE:CG2   | 1:A:54:PRO:N     | 2.84                     | 0.40              |
| 3:B:136:GLU:C    | 3:B:138:SER:H    | 2.29                     | 0.40              |
| 1:G:94:TYR:HA    | 1:G:122:THR:HG23 | 2.02                     | 0.40              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 2:H:217:THR:O   | 2:H:221:LEU:HG   | 2.22                     | 0.40              |
| 1:E:101:VAL:N   | 1:E:240:ILE:CG2  | 2.85                     | 0.40              |
| 1:E:236:CYS:O   | 1:E:240:ILE:HG12 | 2.22                     | 0.40              |
| 3:F:232:VAL:C   | 3:F:233:LEU:HD22 | 2.46                     | 0.40              |
| 1:I:124:GLY:C   | 1:I:126:TYR:H    | 2.29                     | 0.40              |
| 3:J:185:ALA:HA  | 3:J:192:ASP:HB2  | 2.03                     | 0.40              |
| 2:P:140:HIS:CD2 | 1:M:129:ILE:HG21 | 2.57                     | 0.40              |
| 3:N:184:LYS:HB3 | 3:N:239:TYR:OH   | 2.22                     | 0.40              |

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

| Atom-1        | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------|----------------------|--------------------------|-------------------|
| 3:B:282:GLY:O | 3:J:85:MET:CB[8_545] | 1.48                     | 0.72              |

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 1   | A     | 334/339 (98%) | 292 (87%) | 42 (13%) | 0        | 100         | 100 |
| 1   | C     | 322/339 (95%) | 276 (86%) | 46 (14%) | 0        | 100         | 100 |
| 1   | E     | 334/339 (98%) | 310 (93%) | 24 (7%)  | 0        | 100         | 100 |
| 1   | G     | 318/339 (94%) | 282 (89%) | 36 (11%) | 0        | 100         | 100 |
| 1   | I     | 334/339 (98%) | 291 (87%) | 42 (13%) | 1 (0%)   | 36          | 71  |
| 1   | K     | 321/339 (95%) | 292 (91%) | 29 (9%)  | 0        | 100         | 100 |
| 1   | M     | 334/339 (98%) | 292 (87%) | 42 (13%) | 0        | 100         | 100 |
| 1   | O     | 323/339 (95%) | 287 (89%) | 33 (10%) | 3 (1%)   | 14          | 50  |
| 2   | D     | 335/354 (95%) | 301 (90%) | 33 (10%) | 1 (0%)   | 36          | 71  |
| 2   | H     | 343/354 (97%) | 300 (88%) | 42 (12%) | 1 (0%)   | 36          | 71  |

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| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|-----------|----------|-------------|-----|
| 2   | L     | 345/354 (98%)   | 307 (89%)  | 34 (10%)  | 4 (1%)   | 10          | 43  |
| 2   | P     | 344/354 (97%)   | 296 (86%)  | 42 (12%)  | 6 (2%)   | 7           | 35  |
| 3   | B     | 333/352 (95%)   | 295 (89%)  | 38 (11%)  | 0        | 100         | 100 |
| 3   | F     | 333/352 (95%)   | 294 (88%)  | 37 (11%)  | 2 (1%)   | 21          | 59  |
| 3   | J     | 333/352 (95%)   | 285 (86%)  | 45 (14%)  | 3 (1%)   | 14          | 50  |
| 3   | N     | 332/352 (94%)   | 283 (85%)  | 39 (12%)  | 10 (3%)  | 3           | 22  |
| All | All   | 5318/5536 (96%) | 4683 (88%) | 604 (11%) | 31 (1%)  | 21          | 59  |

All (31) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | H     | 87  | PRO  |
| 3   | F     | 57  | MET  |
| 2   | L     | 85  | LEU  |
| 2   | L     | 87  | PRO  |
| 3   | J     | 84  | PRO  |
| 3   | J     | 281 | VAL  |
| 2   | P     | 44  | PRO  |
| 3   | N     | 83  | THR  |
| 3   | N     | 84  | PRO  |
| 2   | L     | 52  | VAL  |
| 3   | J     | 83  | THR  |
| 1   | O     | 44  | ILE  |
| 1   | O     | 182 | GLY  |
| 2   | P     | 139 | GLU  |
| 3   | N     | 53  | GLU  |
| 3   | N     | 90  | GLU  |
| 2   | D     | 138 | LEU  |
| 2   | P     | 137 | SER  |
| 3   | N     | 16  | PRO  |
| 3   | N     | 51  | LEU  |
| 3   | N     | 54  | VAL  |
| 3   | F     | 54  | VAL  |
| 2   | L     | 53  | SER  |
| 2   | P     | 6   | ILE  |
| 2   | P     | 53  | SER  |
| 3   | N     | 252 | GLY  |
| 3   | N     | 288 | PRO  |
| 1   | O     | 272 | LYS  |
| 2   | P     | 138 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | I     | 129 | ILE  |
| 3   | N     | 257 | VAL  |

### 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     | 241/276 (87%)   | 241 (100%)  | 0        | 100         | 100 |
| 1   | C     | 245/276 (89%)   | 245 (100%)  | 0        | 100         | 100 |
| 1   | E     | 239/276 (87%)   | 239 (100%)  | 0        | 100         | 100 |
| 1   | G     | 263/276 (95%)   | 263 (100%)  | 0        | 100         | 100 |
| 1   | I     | 249/276 (90%)   | 249 (100%)  | 0        | 100         | 100 |
| 1   | K     | 269/276 (98%)   | 269 (100%)  | 0        | 100         | 100 |
| 1   | M     | 248/276 (90%)   | 248 (100%)  | 0        | 100         | 100 |
| 1   | O     | 260/276 (94%)   | 260 (100%)  | 0        | 100         | 100 |
| 2   | D     | 259/299 (87%)   | 259 (100%)  | 0        | 100         | 100 |
| 2   | H     | 263/299 (88%)   | 263 (100%)  | 0        | 100         | 100 |
| 2   | L     | 265/299 (89%)   | 264 (100%)  | 1 (0%)   | 84          | 82  |
| 2   | P     | 261/299 (87%)   | 259 (99%)   | 2 (1%)   | 73          | 77  |
| 3   | B     | 247/296 (83%)   | 247 (100%)  | 0        | 100         | 100 |
| 3   | F     | 226/296 (76%)   | 226 (100%)  | 0        | 100         | 100 |
| 3   | J     | 246/296 (83%)   | 246 (100%)  | 0        | 100         | 100 |
| 3   | N     | 231/296 (78%)   | 231 (100%)  | 0        | 100         | 100 |
| All | All   | 4012/4588 (87%) | 4009 (100%) | 3 (0%)   | 88          | 88  |

All (3) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | L     | 24  | ASP  |
| 2   | P     | 62  | ARG  |
| 2   | P     | 140 | HIS  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 96  | ASN  |
| 1   | C     | 214 | GLN  |
| 2   | D     | 71  | ASN  |
| 2   | D     | 105 | ASN  |
| 2   | D     | 242 | ASN  |
| 1   | A     | 290 | HIS  |
| 1   | G     | 263 | HIS  |
| 1   | G     | 276 | ASN  |
| 2   | H     | 33  | HIS  |
| 2   | H     | 235 | ASN  |
| 2   | H     | 321 | ASN  |
| 1   | E     | 64  | ASN  |
| 1   | E     | 254 | ASN  |
| 3   | F     | 49  | HIS  |
| 3   | F     | 65  | GLN  |
| 3   | F     | 245 | ASN  |
| 1   | K     | 121 | ASN  |
| 1   | K     | 218 | GLN  |
| 2   | L     | 16  | HIS  |
| 2   | L     | 71  | ASN  |
| 2   | L     | 105 | ASN  |
| 2   | L     | 140 | HIS  |
| 2   | L     | 280 | ASN  |
| 1   | I     | 64  | ASN  |
| 1   | I     | 80  | HIS  |
| 1   | I     | 96  | ASN  |
| 1   | I     | 121 | ASN  |
| 1   | I     | 131 | HIS  |
| 1   | I     | 163 | ASN  |
| 1   | I     | 250 | ASN  |
| 3   | J     | 73  | ASN  |
| 3   | J     | 336 | HIS  |
| 1   | O     | 84  | ASN  |
| 2   | P     | 130 | ASN  |
| 2   | P     | 216 | ASN  |
| 2   | P     | 243 | ASN  |
| 2   | P     | 280 | ASN  |
| 2   | P     | 338 | GLN  |
| 2   | P     | 348 | ASN  |
| 1   | M     | 172 | HIS  |
| 3   | N     | 49  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | N     | 123 | ASN  |
| 3   | N     | 229 | GLN  |
| 3   | N     | 303 | ASN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 1   | A     | 336/339 (99%)   | 0.80   | 28 (8%) 17 21  | 44, 95, 154, 197      | 0     |
| 1   | C     | 328/339 (96%)   | 1.10   | 59 (17%) 3 8   | 77, 153, 193, 206     | 0     |
| 1   | E     | 336/339 (99%)   | 1.16   | 56 (16%) 4 9   | 125, 184, 217, 231    | 0     |
| 1   | G     | 324/339 (95%)   | 1.04   | 35 (10%) 11 15 | 108, 167, 200, 216    | 0     |
| 1   | I     | 336/339 (99%)   | 0.72   | 26 (7%) 19 22  | 36, 85, 145, 184      | 0     |
| 1   | K     | 327/339 (96%)   | 0.69   | 18 (5%) 30 29  | 35, 91, 134, 152      | 0     |
| 1   | M     | 336/339 (99%)   | 0.97   | 41 (12%) 8 13  | 54, 144, 180, 197     | 0     |
| 1   | O     | 329/339 (97%)   | 0.71   | 21 (6%) 25 27  | 46, 87, 142, 156      | 0     |
| 2   | D     | 339/354 (95%)   | 0.86   | 37 (10%) 10 15 | 76, 138, 164, 200     | 0     |
| 2   | H     | 347/354 (98%)   | 0.73   | 15 (4%) 40 35  | 64, 104, 138, 166     | 0     |
| 2   | L     | 347/354 (98%)   | 0.52   | 8 (2%) 61 48   | 30, 59, 99, 129       | 0     |
| 2   | P     | 346/354 (97%)   | 0.56   | 13 (3%) 44 37  | 45, 65, 102, 145      | 0     |
| 3   | B     | 335/352 (95%)   | 0.47   | 7 (2%) 63 50   | 40, 62, 78, 102       | 0     |
| 3   | F     | 335/352 (95%)   | 1.13   | 63 (18%) 3 8   | 125, 149, 169, 185    | 0     |
| 3   | J     | 335/352 (95%)   | 0.58   | 8 (2%) 59 47   | 33, 49, 75, 92        | 0     |
| 3   | N     | 334/352 (94%)   | 0.63   | 21 (6%) 26 27  | 54, 87, 142, 226      | 0     |
| All | All   | 5370/5536 (97%) | 0.79   | 456 (8%) 16 20 | 30, 106, 188, 231     | 0     |

All (456) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | E     | 243 | LEU  | 9.3  |
| 3   | F     | 254 | ALA  | 6.0  |
| 1   | O     | 37  | GLU  | 5.5  |
| 3   | J     | 50  | HIS  | 5.1  |
| 2   | H     | 131 | THR  | 5.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | E     | 244 | GLY  | 5.0  |
| 1   | E     | 337 | ASP  | 4.8  |
| 1   | I     | 3   | GLY  | 4.7  |
| 1   | E     | 246 | THR  | 4.7  |
| 1   | E     | 123 | GLU  | 4.6  |
| 3   | F     | 270 | GLU  | 4.3  |
| 1   | E     | 262 | VAL  | 4.3  |
| 3   | F     | 79  | GLY  | 4.3  |
| 3   | F     | 249 | GLY  | 4.3  |
| 3   | F     | 271 | THR  | 4.2  |
| 2   | L     | 59  | GLU  | 4.1  |
| 1   | C     | 294 | PHE  | 4.1  |
| 1   | E     | 112 | ASP  | 4.1  |
| 3   | F     | 170 | TYR  | 4.1  |
| 3   | F     | 248 | ALA  | 4.0  |
| 1   | C     | 266 | ALA  | 4.0  |
| 1   | E     | 125 | GLU  | 3.9  |
| 1   | M     | 45  | GLN  | 3.9  |
| 1   | M     | 151 | ARG  | 3.9  |
| 3   | F     | 50  | HIS  | 3.9  |
| 1   | A     | 275 | ALA  | 3.9  |
| 1   | M     | 337 | ASP  | 3.8  |
| 1   | E     | 104 | GLU  | 3.8  |
| 2   | D     | 116 | VAL  | 3.8  |
| 1   | M     | 83  | MET  | 3.7  |
| 1   | E     | 18  | GLU  | 3.7  |
| 3   | F     | 327 | SER  | 3.7  |
| 2   | D     | 21  | ILE  | 3.7  |
| 3   | F     | 330 | GLY  | 3.7  |
| 1   | A     | 312 | LYS  | 3.7  |
| 1   | E     | 327 | PHE  | 3.7  |
| 1   | M     | 240 | ILE  | 3.7  |
| 1   | E     | 274 | MET  | 3.6  |
| 3   | N     | 279 | GLN  | 3.6  |
| 3   | F     | 250 | LEU  | 3.6  |
| 1   | E     | 240 | ILE  | 3.6  |
| 3   | J     | 97  | ARG  | 3.5  |
| 3   | F     | 253 | GLY  | 3.5  |
| 1   | E     | 126 | TYR  | 3.5  |
| 1   | G     | 316 | LYS  | 3.5  |
| 1   | C     | 264 | GLY  | 3.4  |
| 1   | C     | 80  | HIS  | 3.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | L     | 58  | GLU  | 3.4  |
| 1   | G     | 25  | LYS  | 3.4  |
| 2   | P     | 88  | SER  | 3.4  |
| 3   | F     | 148 | VAL  | 3.4  |
| 3   | J     | 51  | LEU  | 3.4  |
| 2   | P     | 56  | ALA  | 3.4  |
| 1   | G     | 89  | LYS  | 3.4  |
| 1   | G     | 63  | LYS  | 3.3  |
| 2   | H     | 272 | ARG  | 3.3  |
| 3   | F     | 149 | ILE  | 3.3  |
| 1   | M     | 327 | PHE  | 3.3  |
| 3   | F     | 252 | GLY  | 3.3  |
| 1   | O     | 275 | ALA  | 3.3  |
| 1   | C     | 159 | TYR  | 3.3  |
| 3   | F     | 274 | ARG  | 3.3  |
| 1   | A     | 321 | ASN  | 3.3  |
| 1   | I     | 321 | ASN  | 3.2  |
| 1   | O     | 264 | GLY  | 3.2  |
| 1   | E     | 338 | LEU  | 3.2  |
| 1   | M     | 4   | VAL  | 3.2  |
| 2   | D     | 321 | ASN  | 3.2  |
| 2   | P     | 84  | ASN  | 3.2  |
| 1   | C     | 245 | VAL  | 3.2  |
| 1   | M     | 3   | GLY  | 3.2  |
| 1   | G     | 321 | ASN  | 3.2  |
| 1   | E     | 236 | CYS  | 3.2  |
| 1   | M     | 245 | VAL  | 3.2  |
| 3   | F     | 251 | VAL  | 3.2  |
| 2   | H     | 59  | GLU  | 3.1  |
| 3   | F     | 150 | GLU  | 3.1  |
| 3   | N     | 52  | SER  | 3.1  |
| 2   | H     | 55  | ASN  | 3.1  |
| 1   | E     | 310 | ASP  | 3.1  |
| 3   | N     | 276 | PRO  | 3.1  |
| 1   | C     | 37  | GLU  | 3.1  |
| 1   | C     | 31  | LYS  | 3.1  |
| 1   | A     | 264 | GLY  | 3.1  |
| 1   | I     | 49  | GLY  | 3.1  |
| 1   | C     | 40  | ASN  | 3.1  |
| 1   | A     | 274 | MET  | 3.1  |
| 1   | C     | 271 | GLY  | 3.1  |
| 3   | F     | 324 | VAL  | 3.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | E     | 193 | GLU  | 3.1  |
| 1   | O     | 271 | GLY  | 3.0  |
| 1   | M     | 295 | ASP  | 3.0  |
| 1   | C     | 316 | LYS  | 3.0  |
| 3   | F     | 262 | TYR  | 3.0  |
| 1   | G     | 241 | GLY  | 3.0  |
| 1   | C     | 117 | THR  | 3.0  |
| 2   | H     | 219 | MET  | 3.0  |
| 1   | I     | 29  | ALA  | 3.0  |
| 2   | D     | 335 | GLU  | 3.0  |
| 1   | M     | 323 | LYS  | 2.9  |
| 1   | O     | 317 | ASP  | 2.9  |
| 1   | I     | 15  | ILE  | 2.9  |
| 1   | I     | 104 | GLU  | 2.9  |
| 2   | D     | 16  | HIS  | 2.9  |
| 1   | K     | 254 | ASN  | 2.9  |
| 1   | K     | 241 | GLY  | 2.9  |
| 1   | E     | 289 | ARG  | 2.9  |
| 2   | P     | 83  | HIS  | 2.9  |
| 3   | F     | 323 | LYS  | 2.9  |
| 1   | C     | 27  | PHE  | 2.9  |
| 1   | G     | 33  | PRO  | 2.9  |
| 1   | G     | 296 | HIS  | 2.9  |
| 1   | K     | 313 | SER  | 2.9  |
| 1   | C     | 58  | LYS  | 2.9  |
| 1   | M     | 67  | GLY  | 2.9  |
| 3   | F     | 272 | GLY  | 2.9  |
| 2   | D     | 347 | ILE  | 2.8  |
| 3   | F     | 300 | ARG  | 2.8  |
| 3   | N     | 134 | GLU  | 2.8  |
| 1   | E     | 157 | PHE  | 2.8  |
| 2   | L     | 88  | SER  | 2.8  |
| 3   | N     | 257 | VAL  | 2.8  |
| 2   | D     | 348 | ASN  | 2.8  |
| 1   | C     | 193 | GLU  | 2.8  |
| 1   | O     | 306 | ALA  | 2.8  |
| 1   | C     | 15  | ILE  | 2.8  |
| 1   | E     | 242 | GLY  | 2.8  |
| 2   | P     | 135 | TYR  | 2.8  |
| 1   | M     | 336 | LYS  | 2.8  |
| 3   | F     | 307 | HIS  | 2.7  |
| 1   | G     | 271 | GLY  | 2.7  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | O     | 47  | PRO  | 2.7  |
| 1   | M     | 246 | THR  | 2.7  |
| 1   | M     | 178 | ARG  | 2.7  |
| 1   | O     | 336 | LYS  | 2.7  |
| 3   | F     | 283 | ARG  | 2.7  |
| 1   | I     | 255 | GLY  | 2.7  |
| 2   | D     | 257 | GLY  | 2.7  |
| 1   | G     | 275 | ALA  | 2.7  |
| 1   | C     | 5   | GLN  | 2.7  |
| 2   | D     | 352 | VAL  | 2.7  |
| 1   | I     | 295 | ASP  | 2.7  |
| 1   | K     | 323 | LYS  | 2.7  |
| 1   | A     | 280 | LEU  | 2.7  |
| 1   | A     | 307 | THR  | 2.7  |
| 1   | M     | 278 | THR  | 2.7  |
| 1   | E     | 142 | LYS  | 2.7  |
| 1   | E     | 189 | ARG  | 2.7  |
| 1   | E     | 194 | SER  | 2.7  |
| 1   | G     | 317 | ASP  | 2.6  |
| 3   | N     | 30  | MET  | 2.6  |
| 1   | C     | 38  | GLU  | 2.6  |
| 1   | C     | 244 | GLY  | 2.6  |
| 1   | I     | 188 | CYS  | 2.6  |
| 1   | K     | 38  | GLU  | 2.6  |
| 1   | M     | 313 | SER  | 2.6  |
| 1   | C     | 218 | GLN  | 2.6  |
| 3   | B     | 55  | GLN  | 2.6  |
| 3   | F     | 47  | GLN  | 2.6  |
| 2   | L     | 349 | GLY  | 2.6  |
| 2   | P     | 279 | ALA  | 2.6  |
| 1   | E     | 158 | GLU  | 2.6  |
| 1   | G     | 107 | LYS  | 2.6  |
| 1   | E     | 309 | LYS  | 2.6  |
| 3   | F     | 332 | TYR  | 2.6  |
| 3   | N     | 22  | GLY  | 2.6  |
| 3   | N     | 136 | GLU  | 2.6  |
| 2   | H     | 347 | ILE  | 2.6  |
| 1   | E     | 95  | ALA  | 2.6  |
| 2   | H     | 256 | ALA  | 2.6  |
| 1   | A     | 278 | THR  | 2.6  |
| 3   | F     | 113 | SER  | 2.6  |
| 1   | A     | 329 | GLU  | 2.6  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | K     | 316 | LYS  | 2.5  |
| 1   | E     | 38  | GLU  | 2.5  |
| 2   | D     | 113 | PRO  | 2.5  |
| 3   | F     | 84  | PRO  | 2.5  |
| 1   | C     | 272 | LYS  | 2.5  |
| 1   | C     | 9   | LEU  | 2.5  |
| 2   | D     | 334 | SER  | 2.5  |
| 3   | F     | 93  | SER  | 2.5  |
| 2   | P     | 349 | GLY  | 2.5  |
| 1   | G     | 69  | LYS  | 2.5  |
| 1   | G     | 81  | PRO  | 2.5  |
| 2   | H     | 86  | PRO  | 2.5  |
| 1   | E     | 36  | TRP  | 2.5  |
| 1   | G     | 292 | GLY  | 2.5  |
| 1   | K     | 274 | MET  | 2.5  |
| 1   | I     | 337 | ASP  | 2.5  |
| 3   | B     | 56  | ASN  | 2.5  |
| 1   | G     | 308 | ILE  | 2.5  |
| 1   | M     | 87  | LEU  | 2.5  |
| 2   | P     | 159 | LEU  | 2.5  |
| 1   | A     | 77  | ALA  | 2.5  |
| 3   | N     | 332 | TYR  | 2.5  |
| 1   | K     | 85  | LEU  | 2.5  |
| 1   | M     | 10  | ILE  | 2.5  |
| 2   | D     | 7   | PRO  | 2.5  |
| 3   | F     | 349 | LEU  | 2.5  |
| 1   | M     | 48  | GLY  | 2.5  |
| 1   | M     | 80  | HIS  | 2.5  |
| 1   | C     | 107 | LYS  | 2.5  |
| 1   | E     | 186 | GLN  | 2.5  |
| 1   | E     | 301 | GLU  | 2.5  |
| 3   | F     | 86  | GLU  | 2.5  |
| 2   | D     | 194 | LEU  | 2.5  |
| 1   | I     | 150 | LYS  | 2.5  |
| 2   | H     | 98  | THR  | 2.5  |
| 1   | M     | 299 | ARG  | 2.5  |
| 1   | M     | 321 | ASN  | 2.5  |
| 3   | F     | 39  | ALA  | 2.5  |
| 3   | N     | 254 | ALA  | 2.5  |
| 1   | C     | 309 | LYS  | 2.5  |
| 3   | F     | 173 | LYS  | 2.5  |
| 1   | G     | 338 | LEU  | 2.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 313 | SER  | 2.4  |
| 3   | F     | 143 | GLU  | 2.4  |
| 2   | D     | 252 | PRO  | 2.4  |
| 3   | F     | 80  | LYS  | 2.4  |
| 3   | F     | 92  | ALA  | 2.4  |
| 3   | N     | 50  | HIS  | 2.4  |
| 2   | D     | 88  | SER  | 2.4  |
| 1   | C     | 197 | ASP  | 2.4  |
| 1   | G     | 295 | ASP  | 2.4  |
| 2   | D     | 57  | ASP  | 2.4  |
| 1   | C     | 175 | ASN  | 2.4  |
| 1   | G     | 40  | ASN  | 2.4  |
| 3   | F     | 15  | PHE  | 2.4  |
| 1   | A     | 80  | HIS  | 2.4  |
| 1   | A     | 300 | ILE  | 2.4  |
| 1   | E     | 207 | THR  | 2.4  |
| 1   | M     | 47  | PRO  | 2.4  |
| 2   | L     | 137 | SER  | 2.4  |
| 1   | C     | 28  | ASP  | 2.4  |
| 1   | M     | 264 | GLY  | 2.4  |
| 1   | C     | 314 | LEU  | 2.4  |
| 1   | A     | 34  | ILE  | 2.4  |
| 1   | E     | 40  | ASN  | 2.4  |
| 1   | K     | 321 | ASN  | 2.4  |
| 1   | A     | 290 | HIS  | 2.4  |
| 2   | P     | 16  | HIS  | 2.4  |
| 1   | K     | 39  | ARG  | 2.4  |
| 2   | D     | 17  | THR  | 2.4  |
| 2   | D     | 234 | PRO  | 2.4  |
| 3   | F     | 208 | LYS  | 2.4  |
| 3   | F     | 163 | ILE  | 2.4  |
| 1   | C     | 96  | ASN  | 2.4  |
| 3   | N     | 291 | MET  | 2.4  |
| 3   | F     | 305 | GLU  | 2.4  |
| 1   | A     | 9   | LEU  | 2.4  |
| 2   | D     | 349 | GLY  | 2.4  |
| 3   | N     | 144 | SER  | 2.4  |
| 1   | C     | 51  | TRP  | 2.4  |
| 1   | A     | 76  | ILE  | 2.4  |
| 1   | G     | 28  | ASP  | 2.4  |
| 2   | D     | 69  | ARG  | 2.4  |
| 3   | F     | 288 | PRO  | 2.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | E     | 111 | THR  | 2.4  |
| 1   | E     | 202 | GLU  | 2.4  |
| 1   | A     | 322 | ALA  | 2.4  |
| 1   | O     | 295 | ASP  | 2.4  |
| 1   | G     | 314 | LEU  | 2.4  |
| 1   | M     | 296 | HIS  | 2.4  |
| 2   | L     | 83  | HIS  | 2.4  |
| 1   | E     | 145 | THR  | 2.3  |
| 2   | H     | 79  | ILE  | 2.3  |
| 1   | C     | 268 | ASP  | 2.3  |
| 1   | E     | 89  | LYS  | 2.3  |
| 1   | C     | 329 | GLU  | 2.3  |
| 1   | E     | 271 | GLY  | 2.3  |
| 1   | I     | 190 | GLU  | 2.3  |
| 2   | D     | 77  | GLY  | 2.3  |
| 3   | N     | 55  | GLN  | 2.3  |
| 1   | M     | 302 | ALA  | 2.3  |
| 1   | A     | 150 | LYS  | 2.3  |
| 1   | G     | 299 | ARG  | 2.3  |
| 1   | C     | 338 | LEU  | 2.3  |
| 1   | I     | 183 | LEU  | 2.3  |
| 1   | E     | 263 | HIS  | 2.3  |
| 3   | F     | 275 | HIS  | 2.3  |
| 1   | A     | 327 | PHE  | 2.3  |
| 2   | D     | 275 | GLY  | 2.3  |
| 1   | K     | 275 | ALA  | 2.3  |
| 1   | I     | 329 | GLU  | 2.3  |
| 1   | M     | 114 | ASN  | 2.3  |
| 2   | D     | 285 | ASN  | 2.3  |
| 1   | O     | 28  | ASP  | 2.3  |
| 1   | M     | 133 | ILE  | 2.3  |
| 1   | C     | 330 | GLU  | 2.3  |
| 2   | D     | 75  | LEU  | 2.3  |
| 3   | F     | 83  | THR  | 2.3  |
| 1   | K     | 11  | PRO  | 2.3  |
| 1   | M     | 241 | GLY  | 2.3  |
| 3   | N     | 307 | HIS  | 2.3  |
| 1   | C     | 275 | ALA  | 2.3  |
| 1   | M     | 148 | ALA  | 2.3  |
| 3   | B     | 92  | ALA  | 2.3  |
| 1   | A     | 282 | LEU  | 2.3  |
| 1   | G     | 38  | GLU  | 2.3  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | I     | 304 | CYS  | 2.3  |
| 3   | F     | 136 | GLU  | 2.3  |
| 3   | F     | 186 | ASN  | 2.3  |
| 1   | G     | 278 | THR  | 2.3  |
| 3   | F     | 166 | PHE  | 2.3  |
| 1   | M     | 78  | ALA  | 2.3  |
| 2   | P     | 254 | LEU  | 2.3  |
| 2   | D     | 231 | MET  | 2.3  |
| 2   | L     | 199 | GLU  | 2.3  |
| 1   | M     | 172 | HIS  | 2.3  |
| 1   | M     | 275 | ALA  | 2.3  |
| 2   | H     | 83  | HIS  | 2.3  |
| 1   | C     | 56  | GLU  | 2.2  |
| 1   | I     | 218 | GLN  | 2.3  |
| 3   | J     | 277 | PHE  | 2.2  |
| 1   | A     | 33  | PRO  | 2.2  |
| 1   | M     | 263 | HIS  | 2.2  |
| 3   | B     | 300 | ARG  | 2.2  |
| 1   | E     | 295 | ASP  | 2.2  |
| 1   | O     | 56  | GLU  | 2.2  |
| 1   | C     | 17  | PRO  | 2.2  |
| 1   | K     | 264 | GLY  | 2.2  |
| 1   | O     | 4   | VAL  | 2.2  |
| 1   | C     | 299 | ARG  | 2.2  |
| 2   | L     | 69  | ARG  | 2.2  |
| 3   | N     | 58  | ALA  | 2.2  |
| 3   | J     | 49  | HIS  | 2.2  |
| 1   | C     | 295 | ASP  | 2.2  |
| 1   | E     | 230 | ASP  | 2.2  |
| 3   | F     | 45  | GLU  | 2.2  |
| 3   | F     | 34  | LYS  | 2.2  |
| 3   | F     | 38  | LYS  | 2.2  |
| 2   | D     | 315 | ALA  | 2.2  |
| 2   | D     | 325 | PRO  | 2.2  |
| 3   | N     | 79  | GLY  | 2.2  |
| 1   | I     | 20  | SER  | 2.2  |
| 2   | H     | 142 | SER  | 2.2  |
| 1   | C     | 260 | GLU  | 2.2  |
| 1   | I     | 28  | ASP  | 2.2  |
| 2   | D     | 311 | LYS  | 2.2  |
| 3   | N     | 313 | ASP  | 2.2  |
| 1   | K     | 338 | LEU  | 2.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 29  | ALA  | 2.2  |
| 1   | E     | 52  | MET  | 2.2  |
| 1   | C     | 278 | THR  | 2.2  |
| 1   | A     | 313 | SER  | 2.2  |
| 1   | I     | 260 | GLU  | 2.2  |
| 1   | C     | 326 | ASP  | 2.2  |
| 3   | B     | 95  | ASP  | 2.2  |
| 1   | G     | 84  | ASN  | 2.2  |
| 1   | C     | 164 | HIS  | 2.2  |
| 1   | O     | 272 | LYS  | 2.2  |
| 2   | D     | 318 | ASP  | 2.2  |
| 1   | A     | 46  | GLY  | 2.2  |
| 1   | C     | 321 | ASN  | 2.2  |
| 1   | E     | 321 | ASN  | 2.2  |
| 1   | E     | 336 | LYS  | 2.2  |
| 2   | H     | 262 | HIS  | 2.2  |
| 1   | G     | 18  | GLU  | 2.2  |
| 1   | G     | 236 | CYS  | 2.2  |
| 1   | E     | 7   | VAL  | 2.2  |
| 2   | D     | 72  | ARG  | 2.2  |
| 1   | G     | 255 | GLY  | 2.1  |
| 1   | G     | 311 | GLY  | 2.1  |
| 1   | M     | 51  | TRP  | 2.2  |
| 1   | E     | 148 | ALA  | 2.1  |
| 2   | D     | 10  | ALA  | 2.1  |
| 2   | D     | 44  | PRO  | 2.1  |
| 1   | O     | 63  | LYS  | 2.1  |
| 1   | M     | 196 | LYS  | 2.1  |
| 3   | B     | 173 | LYS  | 2.1  |
| 3   | F     | 320 | LYS  | 2.1  |
| 1   | G     | 307 | THR  | 2.1  |
| 3   | J     | 83  | THR  | 2.1  |
| 1   | E     | 245 | VAL  | 2.1  |
| 1   | O     | 325 | SER  | 2.1  |
| 1   | O     | 334 | ARG  | 2.1  |
| 3   | F     | 35  | GLU  | 2.1  |
| 1   | I     | 237 | ALA  | 2.1  |
| 3   | N     | 278 | ALA  | 2.1  |
| 3   | N     | 282 | GLY  | 2.1  |
| 1   | E     | 93  | LEU  | 2.1  |
| 3   | F     | 174 | LYS  | 2.1  |
| 1   | C     | 169 | THR  | 2.1  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 2          | P            | 271        | THR         | 2.1         |
| 3          | F            | 49         | HIS         | 2.1         |
| 1          | K            | 88         | ARG         | 2.1         |
| 1          | M            | 104        | GLU         | 2.1         |
| 1          | O            | 86         | LEU         | 2.1         |
| 2          | D            | 294        | CYS         | 2.1         |
| 1          | E            | 220        | ASP         | 2.1         |
| 2          | D            | 55         | ASN         | 2.1         |
| 2          | H            | 322        | MET         | 2.1         |
| 3          | B            | 14         | SER         | 2.1         |
| 1          | A            | 78         | ALA         | 2.1         |
| 1          | G            | 253        | ALA         | 2.1         |
| 1          | I            | 78         | ALA         | 2.1         |
| 1          | M            | 77         | ALA         | 2.1         |
| 1          | M            | 298        | ALA         | 2.1         |
| 1          | G            | 268        | ASP         | 2.1         |
| 3          | F            | 75         | VAL         | 2.1         |
| 1          | C            | 167        | ASN         | 2.1         |
| 2          | D            | 235        | ASN         | 2.1         |
| 1          | G            | 21         | ALA         | 2.1         |
| 1          | M            | 303        | ALA         | 2.1         |
| 1          | G            | 154        | GLU         | 2.1         |
| 1          | E            | 143        | LEU         | 2.1         |
| 1          | I            | 182        | GLY         | 2.1         |
| 1          | E            | 269        | ILE         | 2.1         |
| 3          | F            | 28         | GLU         | 2.1         |
| 1          | O            | 161        | ARG         | 2.1         |
| 1          | K            | 336        | LYS         | 2.1         |
| 1          | I            | 79         | GLY         | 2.1         |
| 3          | F            | 259        | GLY         | 2.1         |
| 1          | C            | 26         | ILE         | 2.1         |
| 3          | F            | 134        | GLU         | 2.1         |
| 1          | C            | 168        | VAL         | 2.1         |
| 1          | C            | 262        | VAL         | 2.1         |
| 1          | O            | 245        | VAL         | 2.1         |
| 1          | O            | 274        | MET         | 2.1         |
| 3          | F            | 348        | ASP         | 2.1         |
| 1          | C            | 199        | LYS         | 2.1         |
| 3          | F            | 266        | TYR         | 2.1         |
| 1          | E            | 255        | GLY         | 2.1         |
| 1          | K            | 308        | ILE         | 2.1         |
| 1          | I            | 16         | GLY         | 2.1         |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | P     | 45  | VAL  | 2.1  |
| 2   | H     | 118 | ARG  | 2.0  |
| 1   | C     | 228 | TYR  | 2.0  |
| 1   | A     | 305 | PHE  | 2.0  |
| 1   | I     | 324 | CYS  | 2.0  |
| 1   | E     | 211 | ASN  | 2.0  |
| 3   | J     | 226 | ASN  | 2.0  |
| 1   | E     | 329 | GLU  | 2.0  |
| 3   | F     | 52  | SER  | 2.0  |
| 3   | F     | 261 | SER  | 2.0  |
| 1   | C     | 289 | ARG  | 2.0  |
| 3   | F     | 87  | TYR  | 2.0  |
| 1   | A     | 237 | ALA  | 2.0  |
| 1   | O     | 136 | GLY  | 2.0  |
| 1   | K     | 296 | HIS  | 2.0  |
| 1   | G     | 99  | PRO  | 2.0  |
| 1   | C     | 236 | CYS  | 2.0  |
| 1   | C     | 202 | GLU  | 2.0  |
| 1   | E     | 42  | THR  | 2.0  |
| 1   | I     | 45  | GLN  | 2.0  |
| 1   | E     | 165 | ARG  | 2.0  |
| 2   | D     | 345 | ARG  | 2.0  |
| 3   | J     | 90  | GLU  | 2.0  |
| 2   | P     | 136 | SER  | 2.0  |
| 1   | A     | 32  | ALA  | 2.0  |
| 2   | D     | 51  | HIS  | 2.0  |
| 1   | C     | 116 | VAL  | 2.0  |
| 1   | C     | 221 | VAL  | 2.0  |
| 3   | N     | 281 | VAL  | 2.0  |
| 1   | A     | 83  | MET  | 2.0  |
| 1   | C     | 155 | PHE  | 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.