



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:13 AM UTC

PDB ID : 5C0W / pdb\_00005c0w  
Title : Structure of a 12-subunit nuclear exosome complex bound to single-stranded RNA substrates  
Authors : Makino, D.L.; Conti, E.  
Deposited on : 2015-06-12  
Resolution : 4.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

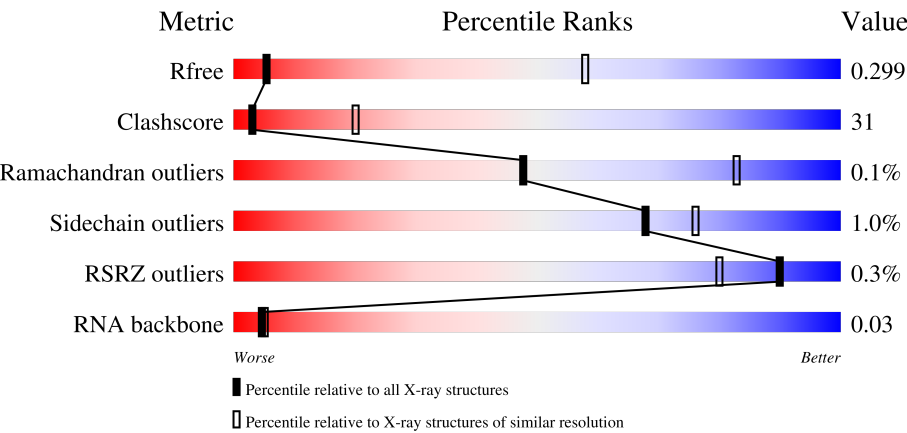
|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                             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

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.60 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.



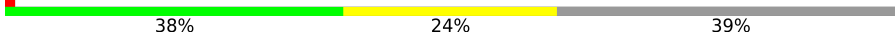
| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| R <sub>free</sub>     | 180053                      | 1007 (5.28-3.92)                                      |
| Clashscore            | 190562                      | 1022 (5.26-3.94)                                      |
| Ramachandran outliers | 187476                      | 1069 (5.30-3.90)                                      |
| Sidechain outliers    | 187428                      | 1051 (5.30-3.90)                                      |
| RSRZ outliers         | 180081                      | 1002 (5.28-3.92)                                      |
| RNA backbone          | 3983                        | 1041 (6.00-3.10)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain                            |
|-----|-------|--------|---------------------------------------------|
| 1   | A     | 305    | <div><div></div><div>58%39%..</div></div>   |
| 2   | B     | 248    | <div><div></div><div>61%36%..</div></div>   |
| 3   | C     | 394    | <div><div></div><div>47%33%.19%</div></div> |
| 4   | D     | 245    | <div><div></div><div>66%22%.9%</div></div>  |

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| Mol | Chain | Length | Quality of chain                                                                   |
|-----|-------|--------|------------------------------------------------------------------------------------|
| 5   | E     | 267    |  |
| 6   | F     | 250    |  |
| 7   | G     | 243    |  |
| 8   | H     | 361    |  |
| 9   | I     | 295    |  |
| 10  | J     | 1004   |  |
| 11  | K     | 695    |  |
| 12  | L     | 184    |  |
| 13  | N     | 18     |  |
| 13  | R     | 18     |  |

## 2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 31160 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 Exosome complex component RRP45.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 298      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2286  | 1434 | 389 | 446 | 17 |         |         |       |

- Molecule 2 is a protein called Exosome complex component SKI6.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2   | B     | 244      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1884  | 1176 | 339 | 360 | 9 |         |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| B     | -1      | GLY      | -      | expression tag | UNP P46948 |
| B     | 0       | HIS      | -      | expression tag | UNP P46948 |

- Molecule 3 is a protein called Exosome complex component RRP43.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 3   | C     | 321      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2431  | 1535 | 411 | 475 | 10 |         |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| C     | 102     | SER      | ALA    | conflict | UNP P25359 |
| C     | 363     | MET      | VAL    | conflict | UNP P25359 |

- Molecule 4 is a protein called Exosome complex component RRP46.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 4   | D     | 222      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1689  | 1062 | 284 | 333 | 10 |         |         |       |

There are 22 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| D     | -21     | GLY      | -      | expression tag | UNP P53256 |
| D     | -20     | HIS      | -      | expression tag | UNP P53256 |
| D     | -19     | GLY      | -      | expression tag | UNP P53256 |
| D     | -18     | ASN      | -      | expression tag | UNP P53256 |
| D     | -17     | ASN      | -      | expression tag | UNP P53256 |
| D     | -16     | LYS      | -      | expression tag | UNP P53256 |
| D     | -15     | GLU      | -      | expression tag | UNP P53256 |
| D     | -14     | PRO      | -      | expression tag | UNP P53256 |
| D     | -13     | ASN      | -      | expression tag | UNP P53256 |
| D     | -12     | THR      | -      | expression tag | UNP P53256 |
| D     | -11     | LYS      | -      | expression tag | UNP P53256 |
| D     | -10     | ASN      | -      | expression tag | UNP P53256 |
| D     | -9      | ARG      | -      | expression tag | UNP P53256 |
| D     | -8      | LEU      | -      | expression tag | UNP P53256 |
| D     | -7      | ASP      | -      | expression tag | UNP P53256 |
| D     | -6      | SER      | -      | expression tag | UNP P53256 |
| D     | -5      | ALA      | -      | expression tag | UNP P53256 |
| D     | -4      | GLU      | -      | expression tag | UNP P53256 |
| D     | -3      | LYS      | -      | expression tag | UNP P53256 |
| D     | -2      | LYS      | -      | expression tag | UNP P53256 |
| D     | -1      | LYS      | -      | expression tag | UNP P53256 |
| D     | 0       | LYS      | -      | expression tag | UNP P53256 |

- Molecule 5 is a protein called Exosome complex component RRP42.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 5   | E     | 266      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2046  | 1307 | 338 | 396 | 5 |         |         |       |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| E     | -1      | GLY      | -      | expression tag      | UNP Q12277 |
| E     | 0       | HIS      | -      | expression tag      | UNP Q12277 |
| E     | 138     | ILE      | VAL    | engineered mutation | UNP Q12277 |

- Molecule 6 is a protein called Exosome complex component MTR3.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 6   | F     | 213      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1627  | 1015 | 277 | 325 | 10 |         |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| F     | 75      | SER      | THR    | engineered mutation | UNP P48240 |
| F     | 161     | THR      | MET    | engineered mutation | UNP P48240 |

- Molecule 7 is a protein called Exosome complex component RRP40.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 7   | G     | 236      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1813  | 1158 | 298 | 347 | 10 |         |         |       |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| G     | -2      | GLY      | -      | expression tag | UNP Q08285 |
| G     | -1      | PRO      | -      | expression tag | UNP Q08285 |
| G     | 0       | HIS      | -      | expression tag | UNP Q08285 |

- Molecule 8 is a protein called Exosome complex component RRP4.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 8   | H     | 291      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2196  | 1375 | 384 | 425 | 12 |         |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| H     | -1      | ARG      | -      | expression tag | UNP P38792 |
| H     | 0       | SER      | -      | expression tag | UNP P38792 |

- Molecule 9 is a protein called Exosome complex component CSL4.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 9   | I     | 225      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1690  | 1057 | 300 | 326 | 7 |         |         |       |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| I     | -2      | GLY      | -      | expression tag | UNP P53859 |
| I     | -1      | PRO      | -      | expression tag | UNP P53859 |
| I     | 0       | HIS      | -      | expression tag | UNP P53859 |

- Molecule 10 is a protein called Exosome complex exonuclease DIS3.

| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 10  | J     | 970      | Total | C    | N    | O    | S  | 0       | 1       | 0     |
|     |       |          | 7645  | 4830 | 1334 | 1447 | 34 |         |         |       |

There are 5 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| J     | -2      | GLY      | -      | expression tag      | UNP Q08162 |
| J     | -1      | PRO      | -      | expression tag      | UNP Q08162 |
| J     | 0       | ALA      | -      | expression tag      | UNP Q08162 |
| J     | 171     | ASN      | ASP    | engineered mutation | UNP Q08162 |
| J     | 551     | ASN      | ASP    | engineered mutation | UNP Q08162 |

- Molecule 11 is a protein called Exosome complex exonuclease RRP6.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 11  | K     | 576      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4605  | 2924 | 784 | 884 | 13 |         |         |       |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| K     | -1      | GLY      | -      | expression tag      | UNP Q12149 |
| K     | 0       | ALA      | -      | expression tag      | UNP Q12149 |
| K     | 2       | ALA      | THR    | engineered mutation | UNP Q12149 |
| K     | 296     | ASN      | ASP    | engineered mutation | UNP Q12149 |

- Molecule 12 is a protein called Exosome complex protein LRP1.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 12  | L     | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 894   | 565 | 151 | 174 | 4 |         |         |       |

- Molecule 13 is a RNA chain called RNA synthetic.

| Mol | Chain | Residues | Atoms |     |    |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|----|---------|---------|-------|
| 13  | R     | 12       | Total | C   | N  | O  | P  | 0       | 0       | 0     |
|     |       |          | 224   | 100 | 40 | 72 | 12 |         |         |       |
| 13  | N     | 6        | Total | C   | N  | O  | P  | 0       | 0       | 0     |
|     |       |          | 128   | 58  | 24 | 40 | 6  |         |         |       |

- Molecule 14 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 14  | J     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 15 is ZINC ION (CCD ID: ZN) (formula: Zn).

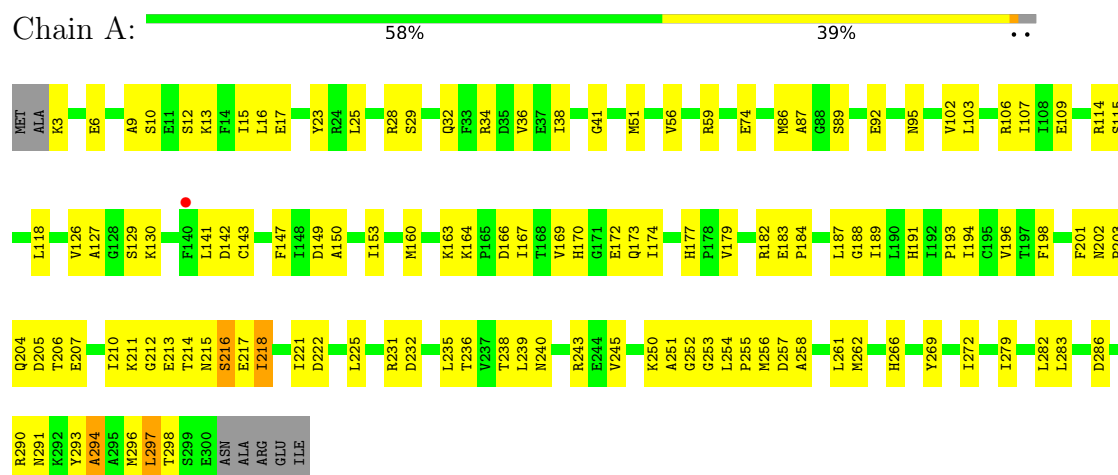
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 15  | J     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |



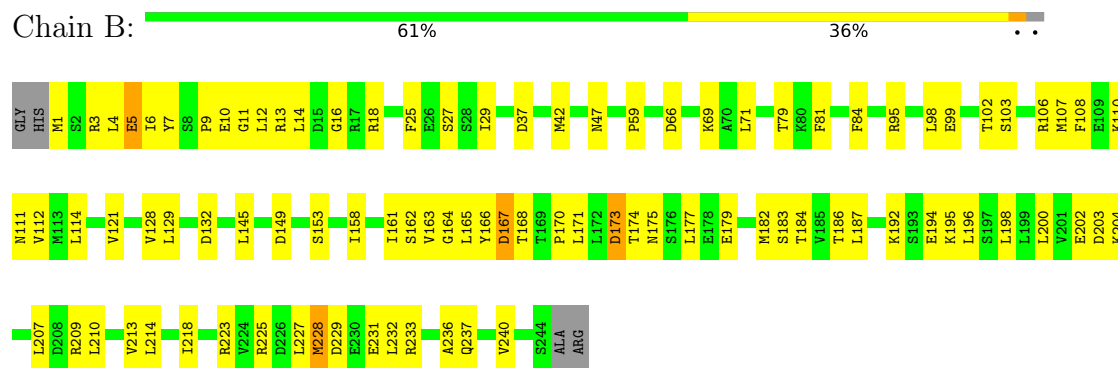
### 3 Residue-property plots

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

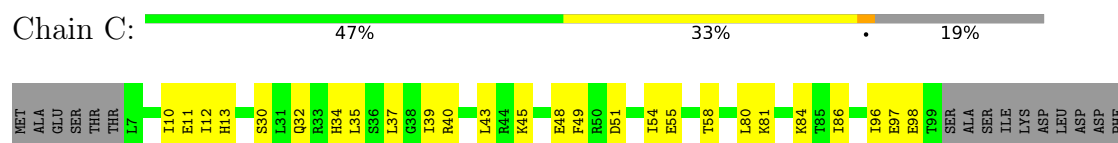
#### • Molecule 1: Exosome complex component RRP45

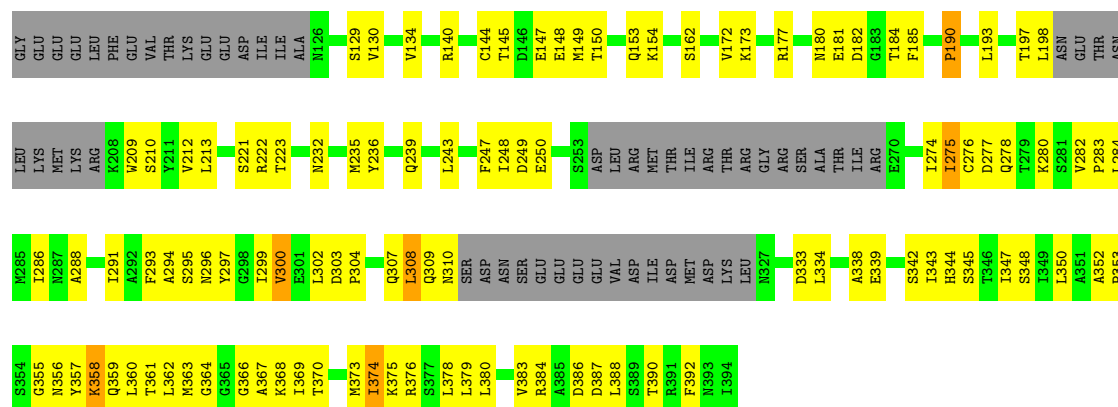


#### • Molecule 2: Exosome complex component SKI6



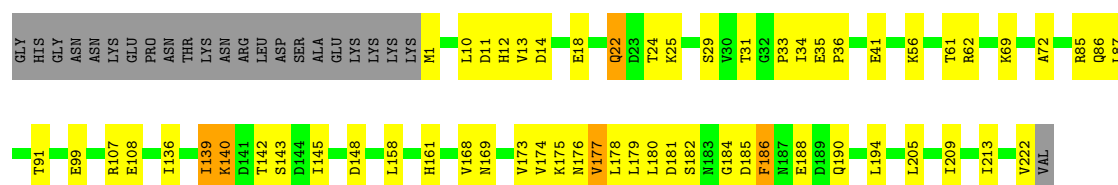
#### • Molecule 3: Exosome complex component RRP43





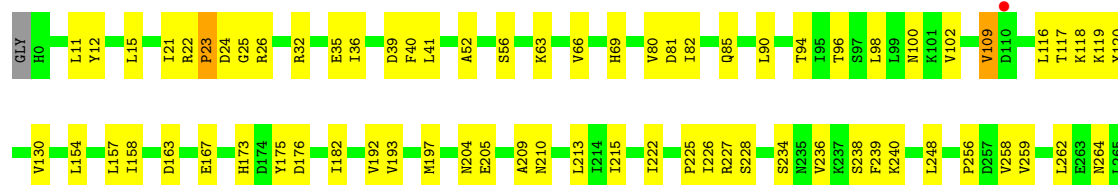
• Molecule 4: Exosome complex component RRP46

Chain D: 66% 22% 9%



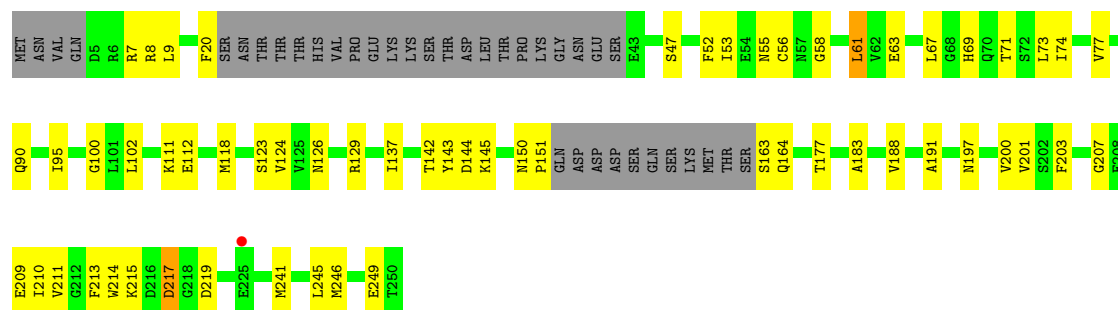
• Molecule 5: Exosome complex component RRP42

Chain E: 73% 26%



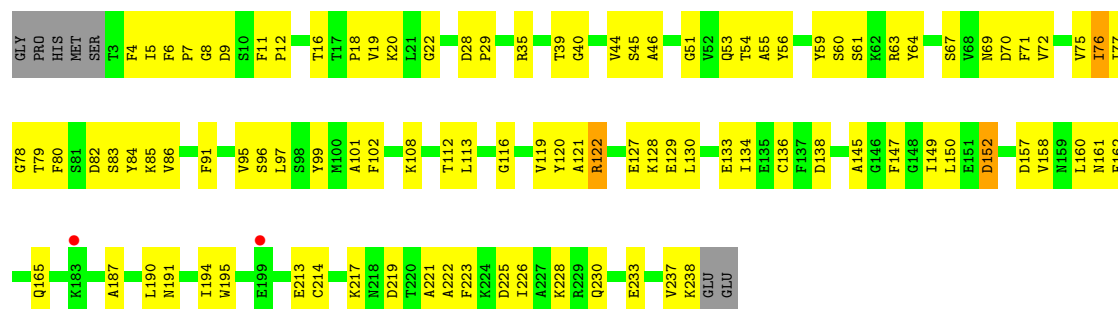
• Molecule 6: Exosome complex component MTR3

Chain F: 62% 23% 15%

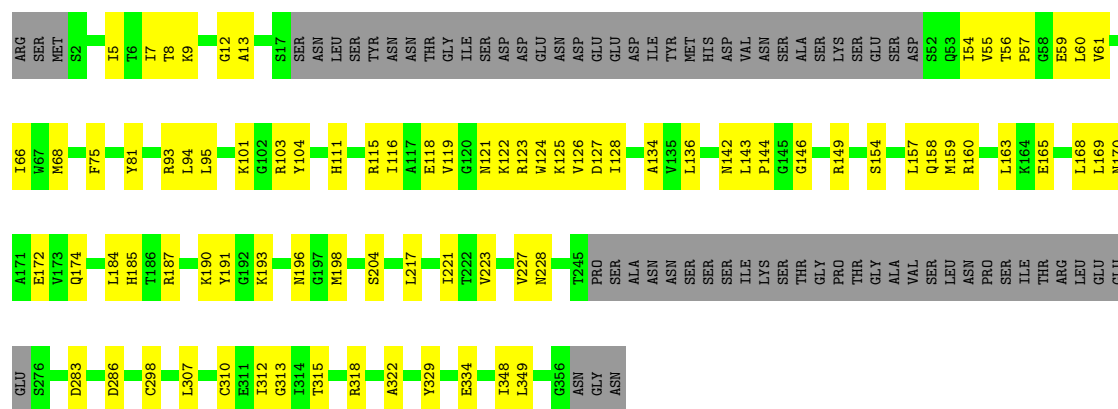


• Molecule 7: Exosome complex component RRP40

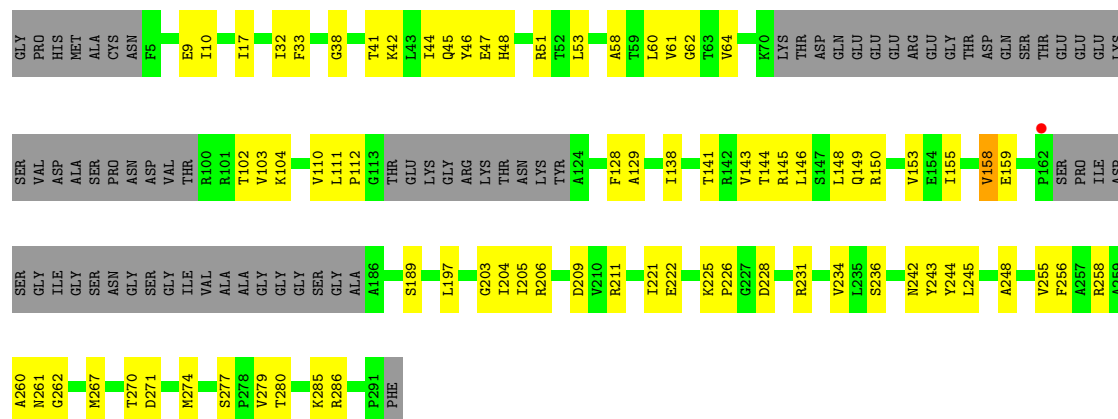
Chain G: 56% 40%



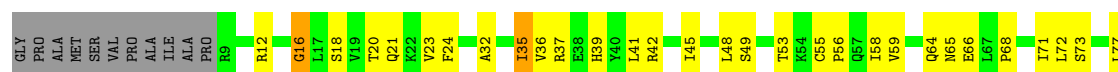
• Molecule 8: Exosome complex component RRP4

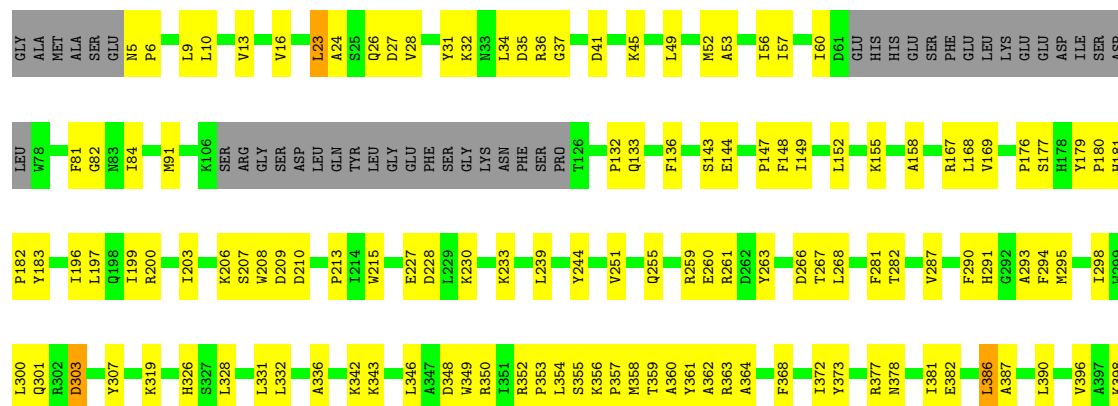


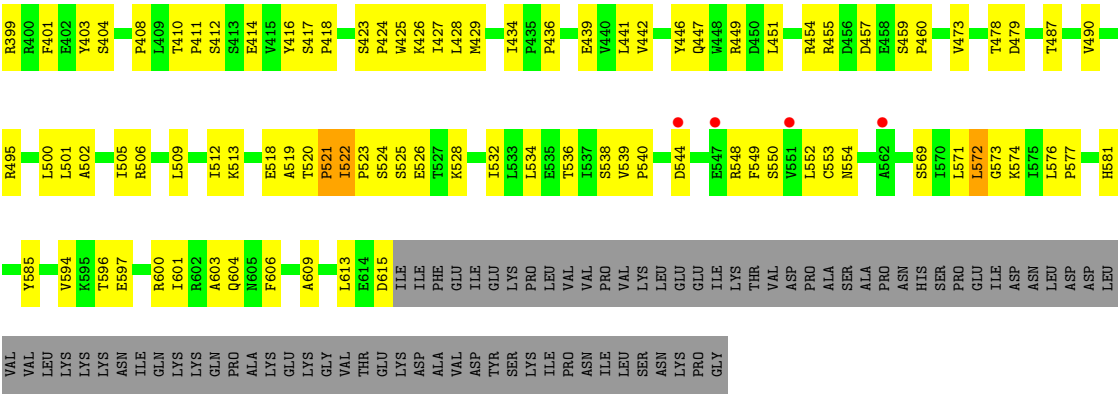
• Molecule 9: Exosome complex component CSL4



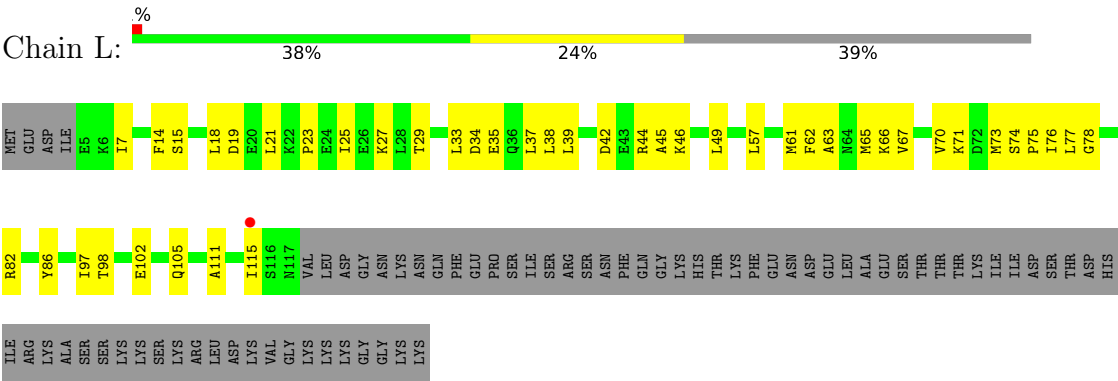
• Molecule 10: Exosome complex exonuclease DIS3



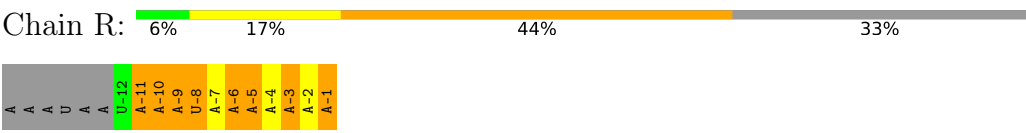




• Molecule 12: Exosome complex protein LRP1



• Molecule 13: RNA synthetic



• Molecule 13: RNA synthetic



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 32 2 1                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 195.38Å 195.38Å 463.65Å<br>90.00° 90.00° 120.00°            | Depositor        |
| Resolution (Å)                                                          | 59.09 – 4.60<br>59.09 – 4.60                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 69.5 (59.09-4.60)<br>69.5 (59.09-4.60)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.11                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.05 (at 4.65Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX                                                      | Depositor        |
| R, $R_{free}$                                                           | 0.271 , 0.284<br>0.297 , 0.299                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 2007 reflections (4.98%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 262.8                                                       | Xtriage          |
| Anisotropy                                                              | 0.302                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.31 , 563.4                                                | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.35$ , $\langle L^2 \rangle = 0.17$ | Xtriage          |
| Estimated twinning fraction                                             | 0.379 for -h,-k,l                                           | Xtriage          |
| Reported twinning fraction                                              | 0.510 for -h,-k,l                                           | Depositor        |
| Outliers                                                                | 0 of 40199 reflections                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.90                                                        | EDS              |
| Total number of atoms                                                   | 31160                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 341.0                                                       | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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

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

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     | 0.43         | 0/2321  | 0.81        | 8/3136 (0.3%)   |
| 2   | B     | 0.37         | 0/1907  | 0.76        | 1/2571 (0.0%)   |
| 3   | C     | 0.34         | 0/2465  | 0.76        | 2/3351 (0.1%)   |
| 4   | D     | 0.32         | 0/1707  | 0.77        | 4/2318 (0.2%)   |
| 5   | E     | 0.33         | 0/2086  | 0.71        | 2/2838 (0.1%)   |
| 6   | F     | 0.31         | 0/1650  | 0.70        | 2/2229 (0.1%)   |
| 7   | G     | 0.28         | 0/1850  | 0.79        | 2/2513 (0.1%)   |
| 8   | H     | 0.26         | 0/2229  | 0.72        | 1/3018 (0.0%)   |
| 9   | I     | 0.36         | 0/1714  | 0.73        | 2/2325 (0.1%)   |
| 10  | J     | 0.60         | 0/7797  | 0.91        | 11/10590 (0.1%) |
| 11  | K     | 0.52         | 0/4702  | 0.92        | 14/6392 (0.2%)  |
| 12  | L     | 0.46         | 0/903   | 0.88        | 1/1210 (0.1%)   |
| 13  | N     | 0.37         | 0/143   | 0.70        | 0/220           |
| 13  | R     | 0.48         | 0/251   | 0.96        | 1/388 (0.3%)    |
| All | All   | 0.45         | 0/31725 | 0.83        | 51/43099 (0.1%) |

There are no bond length outliers.

All (51) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|------|-------------|----------|
| 11  | K     | 303 | ASP  | N-CA-C    | 9.54 | 121.76      | 111.36   |
| 10  | J     | 272 | VAL  | N-CA-C    | 9.34 | 120.15      | 110.62   |
| 11  | K     | 342 | LYS  | N-CA-C    | 9.25 | 121.44      | 111.36   |
| 13  | R     | -8  | U    | P-O3'-C3' | 9.06 | 133.78      | 120.20   |
| 11  | K     | 28  | VAL  | N-CA-C    | 8.73 | 120.46      | 112.43   |
| 1   | A     | 298 | THR  | N-CA-C    | 8.57 | 122.00      | 110.35   |
| 11  | K     | 343 | LYS  | N-CA-C    | 8.21 | 120.23      | 111.28   |
| 10  | J     | 551 | ASN  | N-CA-C    | 6.83 | 118.73      | 111.28   |
| 11  | K     | 34  | LEU  | N-CA-C    | 6.75 | 118.29      | 111.07   |
| 9   | I     | 128 | PHE  | N-CA-C    | 6.68 | 120.63      | 111.54   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 216 | SER  | CB-CA-C | -6.35 | 109.26      | 116.63   |
| 4   | D     | 140 | LYS  | N-CA-C  | 6.31  | 118.16      | 111.28   |
| 1   | A     | 293 | TYR  | N-CA-C  | 6.22  | 120.64      | 111.87   |
| 10  | J     | 497 | LYS  | N-CA-C  | -6.21 | 103.82      | 111.33   |
| 9   | I     | 129 | ALA  | N-CA-C  | 6.01  | 117.83      | 111.28   |
| 1   | A     | 297 | LEU  | N-CA-C  | 6.00  | 117.83      | 111.28   |
| 11  | K     | 487 | THR  | CB-CA-C | -5.99 | 109.65      | 116.54   |
| 4   | D     | 186 | PHE  | N-CA-C  | 5.98  | 118.79      | 109.52   |
| 11  | K     | 526 | GLU  | N-CA-C  | 5.93  | 117.74      | 111.28   |
| 3   | C     | 275 | ILE  | N-CA-C  | 5.89  | 118.46      | 108.86   |
| 10  | J     | 725 | SER  | N-CA-C  | -5.88 | 104.87      | 111.28   |
| 11  | K     | 522 | ILE  | CB-CA-C | -5.83 | 108.17      | 114.35   |
| 12  | L     | 71  | LYS  | N-CA-C  | 5.78  | 117.58      | 111.28   |
| 6   | F     | 217 | ASP  | CB-CA-C | -5.74 | 109.97      | 116.63   |
| 1   | A     | 218 | ILE  | CB-CA-C | -5.70 | 104.07      | 110.96   |
| 11  | K     | 398 | LYS  | N-CA-C  | 5.68  | 117.47      | 111.28   |
| 7   | G     | 152 | ASP  | CB-CA-C | -5.63 | 110.10      | 116.63   |
| 5   | E     | 80  | VAL  | N-CA-C  | 5.60  | 116.01      | 108.17   |
| 10  | J     | 552 | ASP  | N-CA-C  | 5.59  | 117.68      | 109.24   |
| 6   | F     | 67  | LEU  | CB-CA-C | -5.57 | 110.17      | 116.63   |
| 8   | H     | 121 | ASN  | CB-CA-C | -5.54 | 110.20      | 116.63   |
| 10  | J     | 73  | SER  | O-C-N   | -5.48 | 116.29      | 122.97   |
| 2   | B     | 167 | ASP  | CB-CA-C | -5.44 | 110.29      | 116.54   |
| 7   | G     | 51  | GLY  | N-CA-C  | 5.38  | 122.74      | 115.32   |
| 3   | C     | 358 | LYS  | N-CA-C  | 5.35  | 117.19      | 111.36   |
| 4   | D     | 22  | GLN  | CB-CA-C | -5.35 | 110.39      | 116.54   |
| 10  | J     | 367 | ASP  | N-CA-C  | 5.29  | 117.05      | 111.28   |
| 1   | A     | 218 | ILE  | CA-C-N  | -5.26 | 114.60      | 122.39   |
| 1   | A     | 218 | ILE  | C-N-CA  | -5.26 | 114.60      | 122.39   |
| 1   | A     | 294 | ALA  | N-CA-C  | 5.23  | 116.98      | 111.28   |
| 10  | J     | 64  | GLN  | N-CA-C  | -5.21 | 102.57      | 110.28   |
| 4   | D     | 139 | ILE  | N-CA-C  | 5.20  | 116.71      | 109.80   |
| 10  | J     | 16  | GLY  | N-CA-C  | -5.19 | 108.09      | 115.30   |
| 5   | E     | 23  | PRO  | N-CA-C  | -5.18 | 106.33      | 113.53   |
| 11  | K     | 521 | PRO  | CA-C-N  | 5.15  | 123.48      | 120.24   |
| 11  | K     | 521 | PRO  | C-N-CA  | 5.15  | 123.48      | 120.24   |
| 11  | K     | 233 | LYS  | N-CA-C  | -5.11 | 107.08      | 113.72   |
| 10  | J     | 662 | ASP  | N-CA-C  | 5.09  | 116.91      | 111.36   |
| 10  | J     | 385 | LYS  | N-CA-C  | 5.08  | 118.60      | 111.74   |
| 11  | K     | 524 | SER  | N-CA-C  | 5.03  | 116.76      | 111.28   |
| 11  | K     | 519 | ALA  | N-CA-C  | 5.01  | 116.75      | 111.28   |

There are no chirality outliers.



There are no planarity outliers.

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 2286  | 0        | 2254     | 174     | 0            |
| 2   | B     | 1884  | 0        | 1923     | 215     | 0            |
| 3   | C     | 2431  | 0        | 2414     | 224     | 0            |
| 4   | D     | 1689  | 0        | 1733     | 124     | 0            |
| 5   | E     | 2046  | 0        | 2069     | 119     | 0            |
| 6   | F     | 1627  | 0        | 1577     | 61      | 0            |
| 7   | G     | 1813  | 0        | 1784     | 180     | 0            |
| 8   | H     | 2196  | 0        | 2158     | 145     | 0            |
| 9   | I     | 1690  | 0        | 1661     | 93      | 0            |
| 10  | J     | 7645  | 0        | 7573     | 581     | 1            |
| 11  | K     | 4605  | 0        | 4538     | 301     | 1            |
| 12  | L     | 894   | 0        | 917      | 58      | 0            |
| 13  | N     | 128   | 0        | 65       | 6       | 0            |
| 13  | R     | 224   | 0        | 113      | 25      | 0            |
| 14  | J     | 1     | 0        | 0        | 0       | 0            |
| 15  | J     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 31160 | 0        | 30779    | 1944    | 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 (1944) 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) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:16:GLY:HA2    | 10:J:152:PHE:CE1  | 1.44                     | 1.50              |
| 2:B:16:GLY:HA2    | 10:J:152:PHE:CD1  | 1.47                     | 1.49              |
| 10:J:630:LEU:HD11 | 10:J:680:LEU:CD2  | 1.47                     | 1.45              |
| 11:K:196:ILE:CG2  | 11:K:287:VAL:HG21 | 1.46                     | 1.44              |
| 10:J:630:LEU:CD1  | 10:J:680:LEU:HD21 | 1.44                     | 1.43              |
| 7:G:113:LEU:CD2   | 7:G:149:ILE:HG21  | 1.48                     | 1.41              |
| 11:K:5:ASN:HB3    | 11:K:6:PRO:CD     | 1.54                     | 1.35              |
| 11:K:52:MET:CE    | 12:L:25:ILE:HG13  | 1.56                     | 1.34              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:H:75:PHE:HZ     | 11:K:381:ILE:O    | 1.00                     | 1.28              |
| 11:K:196:ILE:HG21 | 11:K:287:VAL:CG2  | 1.65                     | 1.26              |
| 2:B:233:ARG:CD    | 8:H:54:ILE:HG21   | 1.65                     | 1.26              |
| 2:B:165:LEU:O     | 2:B:182:MET:CG    | 1.82                     | 1.26              |
| 2:B:233:ARG:HD2   | 8:H:54:ILE:CG2    | 1.63                     | 1.26              |
| 10:J:538:LEU:O    | 10:J:538:LEU:HD12 | 1.25                     | 1.25              |
| 8:H:174:GLN:HB2   | 8:H:185:HIS:CD2   | 1.71                     | 1.24              |
| 13:R:-3:A:O2'     | 13:R:-2:A:H5'     | 1.30                     | 1.24              |
| 2:B:233:ARG:CD    | 8:H:54:ILE:CG2    | 2.15                     | 1.24              |
| 8:H:75:PHE:CZ     | 11:K:381:ILE:O    | 1.89                     | 1.23              |
| 8:H:116:ILE:HD13  | 8:H:126:VAL:CG1   | 1.66                     | 1.23              |
| 10:J:345:PRO:HD3  | 10:J:423:PHE:CE2  | 1.72                     | 1.22              |
| 11:K:196:ILE:O    | 11:K:377:ARG:HD2  | 1.34                     | 1.22              |
| 10:J:842:PHE:CE1  | 10:J:858:LEU:HD12 | 1.72                     | 1.21              |
| 5:E:116:LEU:HD11  | 5:E:157:LEU:HB2   | 1.23                     | 1.20              |
| 10:J:24:PHE:CE1   | 10:J:35:ILE:HB    | 1.75                     | 1.20              |
| 8:H:157:LEU:HD12  | 8:H:158:GLN:HG3   | 1.21                     | 1.19              |
| 1:A:23:TYR:OH     | 7:G:238:LYS:HA    | 1.38                     | 1.19              |
| 10:J:42:ARG:HB2   | 10:J:152:PHE:O    | 1.40                     | 1.18              |
| 10:J:55:CYS:O     | 10:J:58:ILE:HG12  | 1.39                     | 1.18              |
| 10:J:738:VAL:CG1  | 10:J:858:LEU:HD11 | 1.75                     | 1.17              |
| 2:B:229:ASP:OD1   | 8:H:57:PRO:HD2    | 1.43                     | 1.17              |
| 2:B:165:LEU:O     | 2:B:182:MET:HG2   | 0.99                     | 1.17              |
| 10:J:552:ASP:HB3  | 10:J:570:ILE:HD13 | 1.22                     | 1.17              |
| 3:C:145:THR:CG2   | 3:C:147:GLU:HG2   | 1.73                     | 1.16              |
| 10:J:136:CYS:HA   | 10:J:145:PHE:HB2  | 1.26                     | 1.16              |
| 2:B:129:LEU:CD2   | 5:E:41:LEU:HD21   | 1.76                     | 1.16              |
| 10:J:94:VAL:O     | 10:J:98:ALA:HB3   | 1.44                     | 1.16              |
| 11:K:609:ALA:HA   | 11:K:613:LEU:HD12 | 1.27                     | 1.16              |
| 10:J:345:PRO:HD3  | 10:J:423:PHE:CZ   | 1.80                     | 1.16              |
| 10:J:630:LEU:CD1  | 10:J:680:LEU:CD2  | 2.11                     | 1.14              |
| 5:E:15:LEU:HD11   | 5:E:23:PRO:HD3    | 1.19                     | 1.14              |
| 8:H:126:VAL:CG2   | 8:H:134:ALA:HB3   | 1.78                     | 1.14              |
| 8:H:126:VAL:HG23  | 8:H:134:ALA:HB3   | 1.25                     | 1.14              |
| 10:J:738:VAL:HG13 | 10:J:858:LEU:HD11 | 1.23                     | 1.14              |
| 2:B:27:SER:HB2    | 2:B:231:GLU:HG2   | 1.20                     | 1.13              |
| 10:J:398:ARG:HD3  | 10:J:400:TRP:CD2  | 1.82                     | 1.13              |
| 10:J:624:PHE:CD2  | 10:J:842:PHE:HZ   | 1.67                     | 1.13              |
| 7:G:119:VAL:CG1   | 7:G:149:ILE:HG22  | 1.78                     | 1.13              |
| 8:H:119:VAL:HG22  | 8:H:124:TRP:CD1   | 1.82                     | 1.13              |
| 11:K:5:ASN:HB3    | 11:K:6:PRO:HD3    | 1.18                     | 1.12              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:J:222:ILE:HG13 | 10:J:235:ILE:HD11 | 1.29                     | 1.12              |
| 2:B:233:ARG:HD2   | 8:H:54:ILE:HG21   | 1.20                     | 1.12              |
| 3:C:35:LEU:HB3    | 3:C:302:LEU:CD2   | 1.80                     | 1.12              |
| 3:C:348:SER:HB2   | 3:C:361:THR:HB    | 1.26                     | 1.12              |
| 4:D:85:ARG:HH12   | 9:I:145:ARG:HA    | 0.95                     | 1.11              |
| 2:B:129:LEU:HD21  | 5:E:41:LEU:HD21   | 1.23                     | 1.11              |
| 10:J:48:LEU:HD13  | 10:J:146:ILE:HD11 | 1.23                     | 1.11              |
| 8:H:116:ILE:CD1   | 8:H:126:VAL:HG12  | 1.80                     | 1.10              |
| 11:K:196:ILE:CG2  | 11:K:287:VAL:CG2  | 2.26                     | 1.10              |
| 2:B:16:GLY:CA     | 10:J:152:PHE:CE1  | 2.34                     | 1.10              |
| 8:H:174:GLN:CB    | 8:H:185:HIS:HD2   | 1.64                     | 1.10              |
| 8:H:68:MET:HE3    | 8:H:94:LEU:HD13   | 1.25                     | 1.10              |
| 10:J:48:LEU:CD1   | 10:J:146:ILE:HD11 | 1.82                     | 1.09              |
| 10:J:435:ARG:O    | 10:J:464:LEU:HD12 | 1.48                     | 1.09              |
| 11:K:404:SER:HB2  | 11:K:418:PRO:HD2  | 1.14                     | 1.09              |
| 1:A:253:GLY:C     | 2:B:110:LYS:HG3   | 1.77                     | 1.09              |
| 5:E:158:ILE:HD11  | 5:E:173:HIS:HB2   | 1.20                     | 1.09              |
| 10:J:617:PRO:HA   | 10:J:648:SER:HB3  | 1.21                     | 1.09              |
| 3:C:145:THR:HG23  | 3:C:147:GLU:HG2   | 1.20                     | 1.09              |
| 10:J:45:ILE:HG22  | 10:J:148:PHE:CE1  | 1.87                     | 1.09              |
| 10:J:839:TYR:OH   | 13:R:-3:A:OP1     | 1.71                     | 1.09              |
| 2:B:81:PHE:HE1    | 2:B:129:LEU:HD12  | 1.15                     | 1.08              |
| 8:H:94:LEU:HD11   | 11:K:387:ALA:HB1  | 1.36                     | 1.08              |
| 11:K:5:ASN:CB     | 11:K:6:PRO:CD     | 2.32                     | 1.07              |
| 2:B:16:GLY:CA     | 10:J:152:PHE:CD1  | 2.36                     | 1.07              |
| 3:C:300:VAL:HG11  | 3:C:343:ILE:HG12  | 1.35                     | 1.07              |
| 4:D:34:ILE:HG22   | 7:G:91:PHE:O      | 1.52                     | 1.07              |
| 10:J:133:ARG:HB3  | 10:J:137:ARG:HH12 | 1.17                     | 1.07              |
| 7:G:69:ASN:OD1    | 7:G:122:ARG:NH1   | 1.88                     | 1.07              |
| 10:J:742:ILE:HG23 | 10:J:858:LEU:CD2  | 1.85                     | 1.06              |
| 2:B:164:GLY:O     | 2:B:171:LEU:N     | 1.85                     | 1.06              |
| 3:C:387:ASP:OD2   | 11:K:585:TYR:OH   | 1.73                     | 1.06              |
| 1:A:252:GLY:HA3   | 2:B:106:ARG:O     | 1.53                     | 1.06              |
| 4:D:85:ARG:HH12   | 9:I:145:ARG:CA    | 1.54                     | 1.06              |
| 10:J:552:ASP:HB3  | 10:J:570:ILE:CD1  | 1.86                     | 1.06              |
| 10:J:742:ILE:HD12 | 10:J:750:ALA:HB1  | 1.33                     | 1.06              |
| 3:C:295:SER:HB3   | 3:C:384:ARG:CD    | 1.84                     | 1.05              |
| 10:J:457:PRO:HG2  | 10:J:460:HIS:HD2  | 1.16                     | 1.05              |
| 7:G:113:LEU:CD2   | 7:G:149:ILE:CG2   | 2.34                     | 1.05              |
| 7:G:113:LEU:HD22  | 7:G:149:ILE:HG21  | 1.10                     | 1.05              |
| 10:J:133:ARG:HB3  | 10:J:137:ARG:NH1  | 1.71                     | 1.05              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:295:SER:HB3   | 3:C:384:ARG:HD3   | 1.37                     | 1.04              |
| 10:J:423:PHE:HE1  | 10:J:435:ARG:HG2  | 1.19                     | 1.04              |
| 10:J:742:ILE:HG23 | 10:J:858:LEU:HD23 | 1.35                     | 1.04              |
| 11:K:423:SER:HB2  | 11:K:426:LYS:HB2  | 1.04                     | 1.03              |
| 3:C:359:GLN:O     | 3:C:360:LEU:HD12  | 1.57                     | 1.03              |
| 10:J:539:ILE:HG23 | 10:J:553:ALA:HB1  | 1.41                     | 1.03              |
| 3:C:293:PHE:HB3   | 3:C:388:LEU:HD12  | 1.40                     | 1.03              |
| 10:J:135:LEU:HB3  | 10:J:145:PHE:CE2  | 1.93                     | 1.03              |
| 9:I:205:ILE:HG12  | 9:I:245:LEU:HB2   | 1.37                     | 1.03              |
| 8:H:118:GLU:OE2   | 8:H:125:LYS:HD2   | 1.59                     | 1.02              |
| 8:H:94:LEU:CD1    | 11:K:387:ALA:HB1  | 1.90                     | 1.02              |
| 7:G:119:VAL:HG12  | 7:G:149:ILE:HG22  | 1.03                     | 1.02              |
| 8:H:119:VAL:HG22  | 8:H:124:TRP:HD1   | 1.25                     | 1.02              |
| 8:H:157:LEU:CD1   | 8:H:158:GLN:HG3   | 1.89                     | 1.02              |
| 5:E:116:LEU:HD11  | 5:E:157:LEU:CB    | 1.87                     | 1.02              |
| 2:B:229:ASP:CG    | 8:H:57:PRO:HD2    | 1.83                     | 1.02              |
| 10:J:742:ILE:CG2  | 10:J:858:LEU:HD23 | 1.89                     | 1.02              |
| 10:J:701:VAL:HG23 | 10:J:716:GLU:O    | 1.58                     | 1.01              |
| 3:C:300:VAL:HG12  | 3:C:343:ILE:HG23  | 1.43                     | 1.01              |
| 11:K:196:ILE:HG22 | 11:K:373:TYR:OH   | 1.58                     | 1.01              |
| 2:B:10:GLU:HB2    | 10:J:149:HIS:NE2  | 1.75                     | 1.01              |
| 3:C:363:MET:SD    | 4:D:72:ALA:CB     | 2.49                     | 1.01              |
| 10:J:345:PRO:HB3  | 10:J:423:PHE:CE1  | 1.95                     | 1.01              |
| 10:J:842:PHE:CE1  | 10:J:858:LEU:CD1  | 2.42                     | 1.01              |
| 4:D:14:ASP:CG     | 7:G:63:ARG:HH21   | 1.67                     | 1.01              |
| 4:D:14:ASP:OD1    | 7:G:63:ARG:NH2    | 1.92                     | 1.01              |
| 7:G:113:LEU:HD21  | 7:G:149:ILE:CG2   | 1.90                     | 1.01              |
| 3:C:35:LEU:HB3    | 3:C:302:LEU:HD23  | 1.40                     | 1.01              |
| 3:C:363:MET:HE2   | 4:D:179:LEU:HD13  | 1.39                     | 1.01              |
| 7:G:77:ILE:HD11   | 7:G:85:LYS:HD3    | 1.39                     | 1.01              |
| 7:G:214:CYS:HA    | 7:G:223:PHE:CE1   | 1.96                     | 1.01              |
| 1:A:251:ALA:O     | 2:B:106:ARG:HB3   | 1.60                     | 1.00              |
| 7:G:6:PHE:N       | 7:G:9:ASP:OD2     | 1.93                     | 1.00              |
| 2:B:233:ARG:HD3   | 8:H:54:ILE:CG2    | 1.88                     | 1.00              |
| 10:J:143:LYS:HD3  | 10:J:145:PHE:CZ   | 1.96                     | 1.00              |
| 11:K:52:MET:HE3   | 12:L:25:ILE:HG13  | 1.40                     | 1.00              |
| 8:H:93:ARG:HD2    | 11:K:197:LEU:HD12 | 1.42                     | 1.00              |
| 10:J:842:PHE:HE1  | 10:J:858:LEU:HD12 | 1.23                     | 1.00              |
| 11:K:143:SER:O    | 11:K:144:GLU:HG2  | 1.59                     | 1.00              |
| 2:B:12:LEU:HD12   | 10:J:149:HIS:CG   | 1.97                     | 1.00              |
| 3:C:81:LYS:NZ     | 11:K:576:LEU:O    | 1.95                     | 1.00              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 8:H:55:VAL:HA    | 8:H:59:GLU:OE1    | 1.61                     | 0.99              |
| 11:K:423:SER:CB  | 11:K:426:LYS:HB2  | 1.91                     | 0.99              |
| 2:B:163:VAL:HG11 | 2:B:213:VAL:HG13  | 1.42                     | 0.99              |
| 1:A:23:TYR:HE1   | 7:G:237:VAL:HG12  | 1.24                     | 0.99              |
| 1:A:143:CYS:O    | 4:D:12:HIS:CE1    | 2.14                     | 0.99              |
| 7:G:150:LEU:HD13 | 7:G:195:TRP:CG    | 1.96                     | 0.98              |
| 11:K:423:SER:HB2 | 11:K:426:LYS:CB   | 1.93                     | 0.98              |
| 11:K:425:TRP:NE1 | 11:K:426:LYS:HG3  | 1.78                     | 0.98              |
| 11:K:404:SER:HB2 | 11:K:418:PRO:CD   | 1.93                     | 0.98              |
| 11:K:196:ILE:O   | 11:K:377:ARG:CD   | 2.11                     | 0.98              |
| 3:C:180:ASN:ND2  | 3:C:184:THR:HB    | 1.78                     | 0.98              |
| 11:K:5:ASN:HB3   | 11:K:6:PRO:HD2    | 1.45                     | 0.98              |
| 7:G:120:TYR:HD2  | 7:G:147:PHE:CD1   | 1.81                     | 0.98              |
| 2:B:10:GLU:HG2   | 10:J:149:HIS:CD2  | 1.97                     | 0.98              |
| 5:E:116:LEU:CD1  | 5:E:157:LEU:HD22  | 1.92                     | 0.98              |
| 7:G:113:LEU:HD21 | 7:G:149:ILE:HG21  | 1.39                     | 0.97              |
| 2:B:16:GLY:HA2   | 10:J:152:PHE:HE1  | 1.23                     | 0.97              |
| 2:B:225:ARG:NH2  | 8:H:57:PRO:O      | 1.98                     | 0.97              |
| 10:J:111:VAL:O   | 10:J:146:ILE:HG22 | 1.62                     | 0.97              |
| 4:D:1:MET:CE     | 4:D:205:LEU:HD22  | 1.95                     | 0.97              |
| 11:K:518:GLU:O   | 11:K:521:PRO:HD2  | 1.65                     | 0.97              |
| 1:A:210:ILE:HG22 | 1:A:212:GLY:N     | 1.80                     | 0.97              |
| 3:C:293:PHE:CB   | 3:C:388:LEU:HD12  | 1.95                     | 0.96              |
| 5:E:22:ARG:HB3   | 5:E:24:ASP:OD1    | 1.64                     | 0.96              |
| 2:B:107:MET:SD   | 2:B:198:LEU:HB2   | 2.04                     | 0.96              |
| 7:G:119:VAL:HG12 | 7:G:149:ILE:CG2   | 1.95                     | 0.96              |
| 10:J:538:LEU:O   | 10:J:538:LEU:CD1  | 2.13                     | 0.96              |
| 11:K:404:SER:CB  | 11:K:418:PRO:HD2  | 1.95                     | 0.96              |
| 5:E:158:ILE:CD1  | 5:E:173:HIS:HB2   | 1.96                     | 0.96              |
| 7:G:4:PHE:CE1    | 7:G:40:GLY:HA2    | 1.99                     | 0.96              |
| 7:G:80:PHE:CZ    | 7:G:85:LYS:HE2    | 2.01                     | 0.96              |
| 9:I:204:ILE:HG22 | 9:I:242:ASN:HB3   | 1.47                     | 0.96              |
| 5:E:158:ILE:HD11 | 5:E:173:HIS:CB    | 1.95                     | 0.96              |
| 11:K:57:ILE:HD12 | 11:K:84:ILE:HD12  | 1.48                     | 0.96              |
| 2:B:10:GLU:CD    | 10:J:149:HIS:HE2  | 1.73                     | 0.96              |
| 3:C:37:LEU:HD12  | 11:K:606:PHE:CD1  | 1.99                     | 0.96              |
| 8:H:123:ARG:HB2  | 8:H:136:LEU:O     | 1.66                     | 0.96              |
| 3:C:180:ASN:HD22 | 3:C:184:THR:HB    | 1.27                     | 0.95              |
| 2:B:81:PHE:CE1   | 2:B:129:LEU:HD12  | 2.00                     | 0.95              |
| 3:C:12:ILE:CD1   | 9:I:270:THR:HG22  | 1.95                     | 0.95              |
| 1:A:210:ILE:HG22 | 1:A:212:GLY:H     | 1.31                     | 0.95              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:J:800:TYR:CD2  | 10:J:917:TYR:CE2  | 2.53                     | 0.95              |
| 2:B:14:LEU:HD13   | 2:B:177:LEU:HD21  | 1.45                     | 0.95              |
| 2:B:163:VAL:HG11  | 2:B:213:VAL:CG1   | 1.96                     | 0.95              |
| 9:I:234:VAL:HG22  | 9:I:245:LEU:CD2   | 1.97                     | 0.95              |
| 2:B:9:PRO:HD2     | 10:J:133:ARG:NH2  | 1.82                     | 0.94              |
| 3:C:232:ASN:O     | 3:C:236:TYR:HD2   | 1.49                     | 0.94              |
| 11:K:196:ILE:HG21 | 11:K:287:VAL:HG21 | 0.99                     | 0.94              |
| 7:G:59:TYR:HE1    | 7:G:61:SER:HB2    | 1.32                     | 0.94              |
| 10:J:345:PRO:CD   | 10:J:423:PHE:CZ   | 2.48                     | 0.94              |
| 10:J:135:LEU:HB3  | 10:J:145:PHE:CD2  | 2.01                     | 0.94              |
| 10:J:259:TYR:CD1  | 10:J:393:VAL:HB   | 2.02                     | 0.94              |
| 11:K:361:TYR:OH   | 13:N:-12:U:O4     | 1.83                     | 0.94              |
| 3:C:302:LEU:HD12  | 3:C:302:LEU:O     | 1.66                     | 0.94              |
| 2:B:233:ARG:HD2   | 8:H:54:ILE:HG23   | 1.46                     | 0.94              |
| 3:C:37:LEU:HD12   | 11:K:606:PHE:CE1  | 2.02                     | 0.94              |
| 10:J:624:PHE:HD2  | 10:J:842:PHE:HZ   | 1.09                     | 0.94              |
| 3:C:357:TYR:O     | 4:D:184:GLY:O     | 1.85                     | 0.94              |
| 10:J:457:PRO:HG2  | 10:J:460:HIS:CD2  | 2.01                     | 0.94              |
| 10:J:800:TYR:CZ   | 10:J:931:PRO:HB3  | 2.03                     | 0.94              |
| 5:E:116:LEU:HD21  | 5:E:157:LEU:HD13  | 1.48                     | 0.93              |
| 12:L:102:GLU:O    | 12:L:105:GLN:HG2  | 1.67                     | 0.93              |
| 2:B:81:PHE:HE1    | 2:B:129:LEU:CD1   | 1.81                     | 0.93              |
| 11:K:401:PHE:HD1  | 11:K:416:TYR:CD2  | 1.86                     | 0.93              |
| 3:C:345:SER:HB3   | 3:C:369:ILE:HD11  | 1.48                     | 0.93              |
| 2:B:16:GLY:HA2    | 10:J:152:PHE:HD1  | 1.28                     | 0.93              |
| 3:C:367:ALA:O     | 4:D:176:ASN:ND2   | 2.01                     | 0.93              |
| 3:C:35:LEU:CB     | 3:C:302:LEU:CD2   | 2.47                     | 0.93              |
| 7:G:129:GLU:OE2   | 9:I:225:LYS:HE3   | 1.69                     | 0.93              |
| 10:J:423:PHE:CE1  | 10:J:435:ARG:HG2  | 2.03                     | 0.93              |
| 3:C:368:LYS:HG2   | 4:D:175:LYS:O     | 1.68                     | 0.93              |
| 10:J:804:LEU:HG   | 10:J:808:MET:HE2  | 1.51                     | 0.93              |
| 2:B:10:GLU:CG     | 10:J:149:HIS:CD2  | 2.52                     | 0.93              |
| 10:J:222:ILE:HG13 | 10:J:235:ILE:CD1  | 1.98                     | 0.93              |
| 11:K:331:LEU:HD13 | 11:K:372:ILE:HG21 | 1.50                     | 0.93              |
| 1:A:252:GLY:CA    | 2:B:107:MET:HA    | 1.99                     | 0.92              |
| 13:R:-3:A:HO2'    | 13:R:-2:A:H5'     | 1.30                     | 0.92              |
| 1:A:232:ASP:O     | 2:B:110:LYS:NZ    | 2.02                     | 0.92              |
| 2:B:12:LEU:HD13   | 10:J:152:PHE:CD2  | 2.03                     | 0.92              |
| 5:E:234:SER:HA    | 6:F:90:GLN:HE22   | 1.33                     | 0.92              |
| 7:G:77:ILE:HD11   | 7:G:85:LYS:CD     | 1.98                     | 0.92              |
| 11:K:60:ILE:HG21  | 11:K:84:ILE:HG23  | 1.48                     | 0.92              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:D:85:ARG:NH1    | 9:I:144:THR:O     | 2.01                     | 0.92              |
| 10:J:457:PRO:CG   | 10:J:460:HIS:HD2  | 1.81                     | 0.92              |
| 2:B:229:ASP:OD1   | 8:H:57:PRO:CD     | 2.16                     | 0.92              |
| 3:C:363:MET:CE    | 4:D:179:LEU:HD13  | 1.99                     | 0.92              |
| 4:D:161:HIS:HD2   | 4:D:182:SER:OG    | 1.53                     | 0.92              |
| 8:H:68:MET:SD     | 11:K:387:ALA:HA   | 2.08                     | 0.92              |
| 11:K:52:MET:HE1   | 12:L:25:ILE:HG13  | 1.50                     | 0.92              |
| 11:K:425:TRP:CD1  | 11:K:426:LYS:HG3  | 2.05                     | 0.91              |
| 8:H:174:GLN:HB2   | 8:H:185:HIS:HD2   | 0.78                     | 0.91              |
| 10:J:778:ILE:HG23 | 10:J:789:SER:OG   | 1.70                     | 0.91              |
| 8:H:116:ILE:HD13  | 8:H:126:VAL:HG12  | 0.92                     | 0.91              |
| 10:J:738:VAL:HG13 | 10:J:858:LEU:CD1  | 1.99                     | 0.91              |
| 5:E:116:LEU:CD1   | 5:E:157:LEU:HB2   | 2.00                     | 0.91              |
| 10:J:42:ARG:CB    | 10:J:152:PHE:O    | 2.18                     | 0.91              |
| 2:B:27:SER:CB     | 2:B:231:GLU:HG2   | 2.00                     | 0.91              |
| 11:K:196:ILE:HG22 | 11:K:287:VAL:HG21 | 1.53                     | 0.91              |
| 10:J:302:VAL:HG11 | 10:J:327:LYS:HD2  | 1.53                     | 0.91              |
| 11:K:505:ILE:O    | 11:K:509:LEU:HG   | 1.70                     | 0.91              |
| 2:B:10:GLU:HG2    | 10:J:149:HIS:HD2  | 1.35                     | 0.91              |
| 2:B:129:LEU:HD11  | 5:E:41:LEU:HD11   | 1.51                     | 0.91              |
| 7:G:60:SER:HA     | 7:G:161:ASN:OD1   | 1.68                     | 0.91              |
| 10:J:630:LEU:HD13 | 10:J:680:LEU:HD21 | 1.52                     | 0.91              |
| 1:A:126:VAL:HG13  | 1:A:129:SER:HB2   | 1.53                     | 0.90              |
| 3:C:145:THR:HG23  | 3:C:147:GLU:CG    | 2.00                     | 0.90              |
| 10:J:94:VAL:O     | 10:J:98:ALA:CB    | 2.19                     | 0.90              |
| 10:J:617:PRO:HA   | 10:J:648:SER:CB   | 2.02                     | 0.90              |
| 10:J:337:GLU:OE2  | 10:J:991:THR:HG21 | 1.71                     | 0.90              |
| 11:K:144:GLU:HB2  | 11:K:403:TYR:CD2  | 2.06                     | 0.90              |
| 5:E:262:LEU:HD13  | 8:H:7:ILE:HD13    | 1.53                     | 0.89              |
| 8:H:66:ILE:HD12   | 8:H:93:ARG:HH22   | 1.35                     | 0.89              |
| 7:G:130:LEU:HD22  | 9:I:221:ILE:HG12  | 1.54                     | 0.89              |
| 10:J:624:PHE:CD2  | 10:J:842:PHE:CZ   | 2.59                     | 0.89              |
| 11:K:609:ALA:CA   | 11:K:613:LEU:HD12 | 2.03                     | 0.89              |
| 2:B:108:PHE:CE1   | 2:B:158:ILE:HD12  | 2.08                     | 0.89              |
| 10:J:345:PRO:HD3  | 10:J:423:PHE:CD2  | 2.08                     | 0.89              |
| 1:A:143:CYS:O     | 4:D:12:HIS:ND1    | 2.05                     | 0.89              |
| 2:B:145:LEU:HG    | 2:B:228:MET:HE3   | 1.52                     | 0.89              |
| 7:G:59:TYR:O      | 7:G:161:ASN:ND2   | 2.06                     | 0.89              |
| 8:H:118:GLU:HG2   | 8:H:125:LYS:HB2   | 1.55                     | 0.89              |
| 10:J:808:MET:SD   | 10:J:919:ILE:HG12 | 2.13                     | 0.89              |
| 4:D:34:ILE:CG2    | 7:G:91:PHE:O      | 2.20                     | 0.88              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:D:85:ARG:NH1    | 9:I:145:ARG:CA    | 2.16                     | 0.88              |
| 11:K:573:GLY:O    | 11:K:577:PRO:HD2  | 1.72                     | 0.88              |
| 3:C:350:LEU:HG    | 3:C:359:GLN:HE21  | 1.37                     | 0.88              |
| 1:A:251:ALA:HB1   | 2:B:106:ARG:HB2   | 1.55                     | 0.88              |
| 3:C:232:ASN:O     | 3:C:236:TYR:CD2   | 2.26                     | 0.88              |
| 8:H:124:TRP:CE2   | 8:H:163:LEU:HB2   | 2.07                     | 0.88              |
| 9:I:255:VAL:HG23  | 9:I:256:PHE:H     | 1.37                     | 0.88              |
| 3:C:360:LEU:HD11  | 4:D:186:PHE:HE2   | 1.38                     | 0.88              |
| 3:C:145:THR:CG2   | 3:C:147:GLU:CG    | 2.52                     | 0.88              |
| 3:C:296:ASN:OD1   | 3:C:334:LEU:N     | 2.07                     | 0.87              |
| 10:J:71:ILE:O     | 10:J:144:ARG:HD3  | 1.74                     | 0.87              |
| 11:K:147:PRO:HB2  | 11:K:179:TYR:CE2  | 2.09                     | 0.87              |
| 2:B:12:LEU:HD13   | 10:J:152:PHE:CG   | 2.09                     | 0.87              |
| 6:F:102:LEU:HD11  | 6:F:143:TYR:HE1   | 1.38                     | 0.87              |
| 11:K:401:PHE:HD1  | 11:K:416:TYR:HD2  | 1.21                     | 0.87              |
| 8:H:116:ILE:CD1   | 8:H:126:VAL:CG1   | 2.46                     | 0.87              |
| 3:C:153:GLN:OE1   | 4:D:61:THR:OG1    | 1.92                     | 0.87              |
| 7:G:59:TYR:CE1    | 7:G:61:SER:HB2    | 2.10                     | 0.87              |
| 7:G:76:ILE:HD12   | 7:G:84:TYR:HB3    | 1.57                     | 0.87              |
| 11:K:52:MET:CE    | 12:L:25:ILE:CG1   | 2.50                     | 0.87              |
| 10:J:115:GLN:NE2  | 10:J:152:PHE:CE2  | 2.42                     | 0.86              |
| 8:H:94:LEU:HD11   | 11:K:387:ALA:CB   | 2.05                     | 0.86              |
| 8:H:94:LEU:CD1    | 11:K:387:ALA:CB   | 2.53                     | 0.86              |
| 10:J:136:CYS:CA   | 10:J:145:PHE:HB2  | 2.03                     | 0.86              |
| 5:E:35:GLU:HA     | 8:H:8:THR:HG22    | 1.58                     | 0.86              |
| 2:B:10:GLU:CB     | 10:J:149:HIS:CD2  | 2.59                     | 0.86              |
| 10:J:630:LEU:HD11 | 10:J:680:LEU:HD21 | 0.90                     | 0.86              |
| 10:J:742:ILE:CD1  | 10:J:750:ALA:HB1  | 2.06                     | 0.86              |
| 2:B:233:ARG:CD    | 8:H:54:ILE:HG23   | 2.01                     | 0.85              |
| 8:H:160:ARG:NH1   | 8:H:165:GLU:OE2   | 2.09                     | 0.85              |
| 1:A:177:HIS:ND1   | 1:A:182:ARG:HD2   | 1.90                     | 0.85              |
| 7:G:120:TYR:CD2   | 7:G:147:PHE:CD1   | 2.64                     | 0.85              |
| 13:R:-9:A:OP1     | 13:R:-9:A:C8      | 2.30                     | 0.85              |
| 4:D:85:ARG:NH1    | 9:I:145:ARG:HA    | 1.69                     | 0.85              |
| 11:K:509:LEU:O    | 11:K:512:ILE:HG12 | 1.76                     | 0.85              |
| 10:J:765:ILE:HG22 | 10:J:769:MET:HE2  | 1.56                     | 0.85              |
| 11:K:609:ALA:HA   | 11:K:613:LEU:CD1  | 2.06                     | 0.85              |
| 5:E:22:ARG:HG3    | 5:E:26:ARG:HB2    | 1.59                     | 0.85              |
| 9:I:44:ILE:HG22   | 9:I:45:GLN:N      | 1.91                     | 0.85              |
| 10:J:519:PRO:HA   | 10:J:522:VAL:HG22 | 1.59                     | 0.84              |
| 10:J:55:CYS:O     | 10:J:58:ILE:CG1   | 2.25                     | 0.84              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:K:60:ILE:HG13  | 11:K:84:ILE:HG21  | 1.59                     | 0.84              |
| 1:A:143:CYS:HB2   | 1:A:147:PHE:CZ    | 2.12                     | 0.84              |
| 3:C:297:TYR:CE1   | 3:C:380:LEU:HD23  | 2.11                     | 0.84              |
| 3:C:359:GLN:C     | 3:C:360:LEU:HD12  | 2.02                     | 0.84              |
| 2:B:13:ARG:NH1    | 2:B:171:LEU:HB3   | 1.92                     | 0.84              |
| 5:E:116:LEU:HD11  | 5:E:157:LEU:HD22  | 1.60                     | 0.84              |
| 10:J:539:ILE:HD11 | 10:J:569:HIS:NE2  | 1.93                     | 0.84              |
| 9:I:33:PHE:HE1    | 9:I:104:LYS:HD2   | 1.42                     | 0.84              |
| 1:A:253:GLY:HA2   | 2:B:110:LYS:HZ1   | 1.43                     | 0.84              |
| 1:A:253:GLY:O     | 2:B:110:LYS:HG3   | 1.76                     | 0.84              |
| 2:B:170:PRO:HG3   | 2:B:213:VAL:HG22  | 1.60                     | 0.84              |
| 1:A:23:TYR:CE1    | 7:G:237:VAL:HG12  | 2.11                     | 0.84              |
| 11:K:401:PHE:CD1  | 11:K:416:TYR:HD2  | 1.95                     | 0.84              |
| 8:H:68:MET:SD     | 11:K:390:LEU:HD12 | 2.17                     | 0.83              |
| 12:L:98:THR:O     | 12:L:102:GLU:HG3  | 1.77                     | 0.83              |
| 3:C:35:LEU:CB     | 3:C:302:LEU:HD22  | 2.06                     | 0.83              |
| 10:J:552:ASP:CB   | 10:J:570:ILE:HD13 | 2.06                     | 0.83              |
| 11:K:349:TRP:HZ2  | 11:K:361:TYR:CD2  | 1.95                     | 0.83              |
| 1:A:103:LEU:HG    | 2:B:102:THR:HG21  | 1.60                     | 0.83              |
| 10:J:800:TYR:HB3  | 10:J:917:TYR:OH   | 1.78                     | 0.83              |
| 7:G:136:CYS:O     | 7:G:147:PHE:HB2   | 1.77                     | 0.83              |
| 3:C:297:TYR:HE1   | 3:C:380:LEU:HD23  | 1.43                     | 0.83              |
| 6:F:102:LEU:CD1   | 6:F:143:TYR:CE1   | 2.62                     | 0.83              |
| 7:G:122:ARG:HD3   | 7:G:138:ASP:CG    | 2.03                     | 0.83              |
| 11:K:425:TRP:O    | 11:K:429:MET:HG3  | 1.77                     | 0.83              |
| 1:A:202:ASN:OD1   | 1:A:203:PRO:HD2   | 1.78                     | 0.82              |
| 10:J:45:ILE:CG2   | 10:J:148:PHE:CE1  | 2.61                     | 0.82              |
| 8:H:93:ARG:CD     | 11:K:197:LEU:HD12 | 2.09                     | 0.82              |
| 10:J:630:LEU:HD13 | 10:J:680:LEU:CD2  | 2.03                     | 0.82              |
| 10:J:930:VAL:O    | 10:J:934:GLY:HA2  | 1.80                     | 0.82              |
| 3:C:300:VAL:CG1   | 3:C:343:ILE:HG23  | 2.08                     | 0.82              |
| 2:B:177:LEU:HD22  | 10:J:37:ARG:HD2   | 1.60                     | 0.82              |
| 3:C:307:GLN:NE2   | 11:K:615:ASP:OD1  | 2.12                     | 0.82              |
| 3:C:374:ILE:O     | 3:C:378:LEU:HD13  | 1.80                     | 0.81              |
| 3:C:145:THR:HG21  | 3:C:147:GLU:OE2   | 1.79                     | 0.81              |
| 2:B:10:GLU:CB     | 10:J:149:HIS:NE2  | 2.42                     | 0.81              |
| 10:J:287:GLU:HG3  | 10:J:300:LEU:HD11 | 1.62                     | 0.81              |
| 10:J:723:THR:O    | 10:J:726:LEU:HB3  | 1.81                     | 0.81              |
| 8:H:126:VAL:HG23  | 8:H:134:ALA:CB    | 2.09                     | 0.81              |
| 8:H:204:SER:OG    | 8:H:228:ASN:O     | 1.99                     | 0.81              |
| 2:B:16:GLY:CA     | 10:J:152:PHE:HE1  | 1.83                     | 0.81              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:J:345:PRO:CB   | 10:J:423:PHE:CE1  | 2.63                     | 0.81              |
| 10:J:569:HIS:HD1  | 10:J:625:SER:HG   | 1.28                     | 0.81              |
| 6:F:102:LEU:HD11  | 6:F:143:TYR:CE1   | 2.15                     | 0.81              |
| 10:J:634:ALA:HB2  | 10:J:680:LEU:HG   | 1.60                     | 0.81              |
| 10:J:309:ARG:HG2  | 10:J:456:TRP:CD1  | 2.15                     | 0.80              |
| 5:E:256:PRO:HA    | 5:E:259:VAL:HG12  | 1.64                     | 0.80              |
| 11:K:336:ALA:HB1  | 11:K:368:PHE:CE1  | 2.16                     | 0.80              |
| 10:J:24:PHE:CZ    | 10:J:35:ILE:CG2   | 2.64                     | 0.80              |
| 11:K:401:PHE:CD1  | 11:K:416:TYR:CD2  | 2.68                     | 0.80              |
| 5:E:173:HIS:ND1   | 5:E:176:ASP:HB2   | 1.97                     | 0.80              |
| 10:J:701:VAL:HG21 | 10:J:715:VAL:CG1  | 2.12                     | 0.80              |
| 1:A:142:ASP:HB2   | 4:D:10:LEU:HD22   | 1.63                     | 0.80              |
| 2:B:25:PHE:CZ     | 2:B:42:MET:HE1    | 2.16                     | 0.80              |
| 9:I:204:ILE:CG2   | 9:I:242:ASN:HB3   | 2.12                     | 0.80              |
| 10:J:24:PHE:CZ    | 10:J:35:ILE:HB    | 2.16                     | 0.80              |
| 10:J:620:ASP:OD1  | 10:J:647:ARG:NE   | 2.15                     | 0.80              |
| 11:K:5:ASN:CB     | 11:K:6:PRO:HD2    | 2.05                     | 0.80              |
| 11:K:404:SER:OG   | 11:K:417:SER:HB2  | 1.82                     | 0.80              |
| 3:C:350:LEU:HB2   | 3:C:359:GLN:HG2   | 1.63                     | 0.80              |
| 4:D:161:HIS:CD2   | 4:D:182:SER:OG    | 2.34                     | 0.80              |
| 10:J:24:PHE:CE1   | 10:J:35:ILE:CB    | 2.63                     | 0.80              |
| 10:J:650:GLU:HG2  | 10:J:652:PHE:CZ   | 2.17                     | 0.80              |
| 11:K:455:ARG:HD2  | 12:L:34:ASP:OD1   | 1.82                     | 0.80              |
| 3:C:300:VAL:HG11  | 3:C:343:ILE:CG1   | 2.11                     | 0.79              |
| 11:K:290:PHE:HB3  | 11:K:293:ALA:HB2  | 1.63                     | 0.79              |
| 11:K:360:ALA:O    | 11:K:364:ALA:N    | 2.14                     | 0.79              |
| 10:J:630:LEU:CD1  | 10:J:680:LEU:HD23 | 2.09                     | 0.79              |
| 4:D:222:VAL:HG11  | 7:G:165:GLN:NE2   | 1.97                     | 0.79              |
| 9:I:255:VAL:HG23  | 9:I:256:PHE:N     | 1.98                     | 0.79              |
| 10:J:738:VAL:HG11 | 10:J:858:LEU:HD11 | 1.63                     | 0.79              |
| 10:J:845:PRO:HA   | 10:J:851:ASP:HB2  | 1.64                     | 0.79              |
| 2:B:25:PHE:CE2    | 2:B:42:MET:HE1    | 2.18                     | 0.79              |
| 2:B:111:ASN:ND2   | 2:B:158:ILE:HG13  | 1.98                     | 0.79              |
| 10:J:398:ARG:HD3  | 10:J:400:TRP:CE3  | 2.17                     | 0.79              |
| 3:C:293:PHE:HB3   | 3:C:388:LEU:CD1   | 2.12                     | 0.79              |
| 10:J:624:PHE:HD2  | 10:J:842:PHE:CZ   | 1.97                     | 0.79              |
| 5:E:116:LEU:CG    | 5:E:157:LEU:HD22  | 2.13                     | 0.79              |
| 1:A:143:CYS:HB2   | 1:A:147:PHE:HZ    | 1.44                     | 0.79              |
| 10:J:345:PRO:CD   | 10:J:423:PHE:CE2  | 2.63                     | 0.78              |
| 3:C:350:LEU:HD12  | 3:C:359:GLN:CD    | 2.07                     | 0.78              |
| 5:E:81:ASP:OD1    | 5:E:82:ILE:N      | 2.16                     | 0.78              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:H:315:THR:OG1   | 8:H:318:ARG:HG3   | 1.83                     | 0.78              |
| 11:K:520:THR:O    | 11:K:523:PRO:HD2  | 1.83                     | 0.78              |
| 12:L:33:LEU:HD12  | 12:L:34:ASP:N     | 1.97                     | 0.78              |
| 3:C:360:LEU:HD11  | 4:D:186:PHE:CE2   | 2.19                     | 0.78              |
| 7:G:76:ILE:HD12   | 7:G:84:TYR:CB     | 2.14                     | 0.78              |
| 11:K:144:GLU:HA   | 11:K:403:TYR:CE2  | 2.18                     | 0.78              |
| 12:L:65:MET:SD    | 12:L:70:VAL:HB    | 2.23                     | 0.78              |
| 2:B:5:GLU:O       | 2:B:14:LEU:HD11   | 1.84                     | 0.78              |
| 2:B:7:TYR:CZ      | 2:B:11:GLY:HA2    | 2.18                     | 0.78              |
| 5:E:22:ARG:CB     | 5:E:24:ASP:OD1    | 2.30                     | 0.78              |
| 10:J:222:ILE:CG1  | 10:J:235:ILE:HD11 | 2.13                     | 0.78              |
| 1:A:198:PHE:CE2   | 1:A:221:ILE:HG12  | 2.19                     | 0.78              |
| 10:J:149:HIS:HB3  | 10:J:152:PHE:HD2  | 1.49                     | 0.78              |
| 10:J:519:PRO:O    | 10:J:522:VAL:HG22 | 1.82                     | 0.78              |
| 8:H:93:ARG:HD2    | 11:K:197:LEU:CD1  | 2.13                     | 0.77              |
| 7:G:158:VAL:HG11  | 7:G:162:PHE:HD2   | 1.47                     | 0.77              |
| 2:B:108:PHE:CD1   | 2:B:158:ILE:HD12  | 2.19                     | 0.77              |
| 5:E:35:GLU:HG2    | 8:H:8:THR:HG21    | 1.65                     | 0.77              |
| 10:J:498:LYS:HE2  | 10:J:582:ALA:HB2  | 1.66                     | 0.77              |
| 2:B:10:GLU:OE2    | 10:J:149:HIS:NE2  | 2.14                     | 0.77              |
| 2:B:37:ASP:OD2    | 8:H:103:ARG:NH1   | 2.18                     | 0.77              |
| 3:C:350:LEU:CD1   | 3:C:359:GLN:NE2   | 2.47                     | 0.77              |
| 9:I:102:THR:HG22  | 9:I:103:VAL:N     | 1.98                     | 0.77              |
| 9:I:148:LEU:HD12  | 9:I:149:GLN:N     | 2.00                     | 0.77              |
| 3:C:96:ILE:HG22   | 3:C:210:SER:O     | 1.85                     | 0.77              |
| 10:J:539:ILE:HG23 | 10:J:553:ALA:CB   | 2.14                     | 0.77              |
| 7:G:80:PHE:HZ     | 7:G:85:LYS:HE2    | 1.49                     | 0.77              |
| 11:K:57:ILE:CD1   | 11:K:84:ILE:HD12  | 2.14                     | 0.76              |
| 10:J:844:SER:HB2  | 10:J:848:ARG:NH2  | 1.99                     | 0.76              |
| 1:A:114:ARG:NH1   | 2:B:202:GLU:OE1   | 2.10                     | 0.76              |
| 3:C:180:ASN:HB2   | 3:C:184:THR:H     | 1.51                     | 0.76              |
| 10:J:742:ILE:CG2  | 10:J:858:LEU:CD2  | 2.54                     | 0.76              |
| 1:A:86:MET:HG2    | 1:A:141:LEU:O     | 1.85                     | 0.76              |
| 5:E:116:LEU:HD11  | 5:E:157:LEU:CD2   | 2.15                     | 0.76              |
| 10:J:533:ASP:OD2  | 10:J:535:ARG:NH1  | 2.17                     | 0.76              |
| 10:J:802:ASN:OD1  | 10:J:806:ARG:NH2  | 2.16                     | 0.76              |
| 2:B:10:GLU:CG     | 10:J:149:HIS:NE2  | 2.48                     | 0.76              |
| 8:H:126:VAL:HG22  | 8:H:134:ALA:HB3   | 1.67                     | 0.76              |
| 10:J:345:PRO:HB3  | 10:J:423:PHE:HE1  | 1.46                     | 0.76              |
| 11:K:349:TRP:CZ2  | 11:K:361:TYR:CD2  | 2.73                     | 0.76              |
| 11:K:52:MET:HE3   | 12:L:25:ILE:CG1   | 2.11                     | 0.76              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:145:THR:HG21  | 3:C:147:GLU:HG2   | 1.67                     | 0.76              |
| 10:J:115:GLN:HB2  | 10:J:149:HIS:HA   | 1.66                     | 0.76              |
| 2:B:16:GLY:CA     | 10:J:152:PHE:HD1  | 1.88                     | 0.76              |
| 3:C:360:LEU:HB2   | 4:D:182:SER:HB2   | 1.68                     | 0.76              |
| 7:G:112:THR:O     | 7:G:112:THR:HG22  | 1.84                     | 0.76              |
| 10:J:569:HIS:ND1  | 10:J:625:SER:OG   | 2.19                     | 0.75              |
| 11:K:573:GLY:O    | 11:K:577:PRO:CD   | 2.33                     | 0.75              |
| 8:H:56:THR:N      | 8:H:59:GLU:OE1    | 2.17                     | 0.75              |
| 10:J:738:VAL:HG13 | 10:J:858:LEU:HD21 | 1.69                     | 0.75              |
| 3:C:350:LEU:HG    | 3:C:359:GLN:NE2   | 2.01                     | 0.75              |
| 10:J:919:ILE:O    | 10:J:919:ILE:HG22 | 1.85                     | 0.75              |
| 10:J:930:VAL:O    | 10:J:934:GLY:N    | 2.19                     | 0.75              |
| 4:D:34:ILE:CB     | 7:G:91:PHE:O      | 2.35                     | 0.75              |
| 1:A:256:MET:HE2   | 1:A:261:LEU:HG    | 1.69                     | 0.75              |
| 2:B:13:ARG:HD3    | 2:B:171:LEU:HD13  | 1.69                     | 0.75              |
| 2:B:29:ILE:HG13   | 2:B:232:LEU:CD1   | 2.16                     | 0.75              |
| 7:G:222:ALA:O     | 7:G:226:ILE:HG13  | 1.86                     | 0.75              |
| 1:A:252:GLY:HA2   | 2:B:107:MET:HA    | 1.68                     | 0.75              |
| 2:B:111:ASN:ND2   | 2:B:158:ILE:HD11  | 2.02                     | 0.75              |
| 3:C:357:TYR:O     | 4:D:185:ASP:HA    | 1.86                     | 0.75              |
| 11:K:228:ASP:OD2  | 11:K:263:TYR:OH   | 2.05                     | 0.75              |
| 5:E:116:LEU:HG    | 5:E:157:LEU:HD22  | 1.68                     | 0.75              |
| 10:J:345:PRO:HD3  | 10:J:423:PHE:CE1  | 2.20                     | 0.75              |
| 2:B:4:LEU:HD11    | 10:J:37:ARG:NH1   | 2.02                     | 0.75              |
| 10:J:345:PRO:HB3  | 10:J:435:ARG:HG2  | 1.68                     | 0.75              |
| 8:H:68:MET:CE     | 8:H:94:LEU:HD13   | 2.10                     | 0.75              |
| 5:E:116:LEU:HD11  | 5:E:157:LEU:CG    | 2.16                     | 0.74              |
| 9:I:44:ILE:CG2    | 9:I:45:GLN:H      | 1.99                     | 0.74              |
| 10:J:701:VAL:HB   | 10:J:932:LYS:O    | 1.86                     | 0.74              |
| 10:J:930:VAL:O    | 10:J:934:GLY:CA   | 2.35                     | 0.74              |
| 13:R:-4:A:O2'     | 13:R:-3:A:H5'     | 1.87                     | 0.74              |
| 2:B:29:ILE:HG13   | 2:B:232:LEU:HD13  | 1.67                     | 0.74              |
| 2:B:145:LEU:CG    | 2:B:228:MET:HE3   | 2.17                     | 0.74              |
| 9:I:44:ILE:HG22   | 9:I:45:GLN:H      | 1.51                     | 0.74              |
| 10:J:136:CYS:SG   | 10:J:145:PHE:HB3  | 2.27                     | 0.74              |
| 10:J:235:ILE:HG23 | 10:J:236:PRO:HD2  | 1.68                     | 0.74              |
| 11:K:539:VAL:N    | 11:K:540:PRO:CD   | 2.49                     | 0.74              |
| 5:E:234:SER:CA    | 6:F:90:GLN:HE22   | 2.01                     | 0.74              |
| 9:I:9:GLU:O       | 9:I:64:VAL:N      | 2.20                     | 0.74              |
| 10:J:755:HIS:HD2  | 10:J:833:GLY:H    | 1.36                     | 0.74              |
| 2:B:111:ASN:ND2   | 2:B:158:ILE:CD1   | 2.51                     | 0.74              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:J:765:ILE:CG2  | 10:J:769:MET:HE2  | 2.17                     | 0.73              |
| 2:B:10:GLU:CD     | 10:J:149:HIS:NE2  | 2.46                     | 0.73              |
| 3:C:300:VAL:CG1   | 3:C:343:ILE:HG12  | 2.15                     | 0.73              |
| 8:H:157:LEU:HD12  | 8:H:158:GLN:CG    | 2.13                     | 0.73              |
| 11:K:319:LYS:HA   | 11:K:326:HIS:HE1  | 1.52                     | 0.73              |
| 1:A:253:GLY:HA2   | 2:B:110:LYS:NZ    | 2.02                     | 0.73              |
| 10:J:566:VAL:HG13 | 10:J:677:LEU:HD21 | 1.69                     | 0.73              |
| 11:K:147:PRO:HB2  | 11:K:179:TYR:CD2  | 2.23                     | 0.73              |
| 3:C:363:MET:SD    | 4:D:72:ALA:HB1    | 2.25                     | 0.73              |
| 10:J:815:ALA:HB2  | 13:R:-6:A:H5"     | 1.70                     | 0.73              |
| 11:K:349:TRP:CZ2  | 11:K:361:TYR:HD2  | 2.06                     | 0.73              |
| 10:J:519:PRO:HA   | 10:J:522:VAL:CG2  | 2.19                     | 0.73              |
| 10:J:48:LEU:HD13  | 10:J:146:ILE:CD1  | 2.12                     | 0.73              |
| 10:J:143:LYS:HD3  | 10:J:145:PHE:HZ   | 1.54                     | 0.73              |
| 10:J:316:VAL:HG22 | 10:J:395:ILE:HD12 | 1.69                     | 0.73              |
| 4:D:145:ILE:HD12  | 4:D:145:ILE:O     | 1.87                     | 0.73              |
| 10:J:127:PRO:HD2  | 10:J:344:ASN:OD1  | 1.87                     | 0.73              |
| 10:J:551:ASN:OD1  | 10:J:844:SER:HA   | 1.89                     | 0.73              |
| 9:I:44:ILE:CG2    | 9:I:45:GLN:N      | 2.52                     | 0.73              |
| 9:I:234:VAL:HG22  | 9:I:245:LEU:HD21  | 1.69                     | 0.73              |
| 10:J:65:ASN:O     | 10:J:66:GLU:HG2   | 1.89                     | 0.73              |
| 10:J:315:GLN:O    | 10:J:395:ILE:HG23 | 1.88                     | 0.73              |
| 3:C:12:ILE:HD13   | 9:I:270:THR:HG22  | 1.70                     | 0.72              |
| 7:G:150:LEU:HD13  | 7:G:195:TRP:CD2   | 2.24                     | 0.72              |
| 5:E:22:ARG:HG3    | 5:E:26:ARG:CB     | 2.19                     | 0.72              |
| 1:A:183:GLU:HG3   | 1:A:184:PRO:HD2   | 1.70                     | 0.72              |
| 4:D:33:PRO:HB2    | 4:D:86:GLN:HG2    | 1.70                     | 0.72              |
| 7:G:213:GLU:OE1   | 7:G:226:ILE:HG23  | 1.89                     | 0.72              |
| 11:K:447:GLN:O    | 11:K:451:LEU:HG   | 1.90                     | 0.72              |
| 1:A:245:VAL:HG23  | 2:B:207:LEU:HD13  | 1.71                     | 0.72              |
| 2:B:10:GLU:CG     | 10:J:149:HIS:HE2  | 2.03                     | 0.72              |
| 11:K:49:LEU:HD11  | 12:L:14:PHE:HZ    | 1.54                     | 0.72              |
| 3:C:35:LEU:HB2    | 3:C:302:LEU:HD22  | 1.71                     | 0.72              |
| 11:K:41:ASP:O     | 11:K:45:LYS:HG2   | 1.89                     | 0.72              |
| 11:K:298:ILE:HG23 | 11:K:401:PHE:HB2  | 1.70                     | 0.72              |
| 11:K:425:TRP:NE1  | 11:K:426:LYS:CG   | 2.52                     | 0.72              |
| 5:E:11:LEU:HD11   | 5:E:204:ASN:HB2   | 1.71                     | 0.72              |
| 2:B:129:LEU:CG    | 5:E:41:LEU:HD21   | 2.18                     | 0.72              |
| 1:A:214:THR:HG22  | 1:A:215:ASN:N     | 2.05                     | 0.72              |
| 6:F:197:ASN:ND2   | 6:F:219:ASP:OD1   | 2.23                     | 0.72              |
| 11:K:332:LEU:HD22 | 11:K:368:PHE:CD2  | 2.25                     | 0.72              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:L:19:ASP:O     | 12:L:23:PRO:HD3   | 1.90                     | 0.72              |
| 11:K:144:GLU:HB2  | 11:K:403:TYR:CG   | 2.24                     | 0.71              |
| 1:A:23:TYR:HH     | 7:G:238:LYS:HA    | 1.51                     | 0.71              |
| 1:A:252:GLY:HA3   | 2:B:106:ARG:C     | 2.14                     | 0.71              |
| 1:A:253:GLY:C     | 2:B:110:LYS:CG    | 2.61                     | 0.71              |
| 3:C:232:ASN:HD21  | 3:C:294:ALA:H     | 1.38                     | 0.71              |
| 3:C:293:PHE:CD2   | 3:C:388:LEU:HD13  | 2.26                     | 0.71              |
| 7:G:76:ILE:CD1    | 7:G:84:TYR:HB3    | 2.19                     | 0.71              |
| 11:K:449:ARG:HD2  | 11:K:460:PRO:O    | 1.90                     | 0.71              |
| 11:K:538:SER:HB3  | 11:K:540:PRO:HD2  | 1.71                     | 0.71              |
| 7:G:59:TYR:HE1    | 7:G:61:SER:CB     | 2.03                     | 0.71              |
| 12:L:66:LYS:HE2   | 12:L:73:MET:HE2   | 1.72                     | 0.71              |
| 7:G:122:ARG:HD3   | 7:G:138:ASP:OD2   | 1.89                     | 0.71              |
| 10:J:981:VAL:HG23 | 10:J:999:LEU:O    | 1.90                     | 0.71              |
| 1:A:214:THR:CG2   | 1:A:215:ASN:N     | 2.54                     | 0.71              |
| 7:G:129:GLU:HB2   | 9:I:226:PRO:HG2   | 1.70                     | 0.71              |
| 2:B:13:ARG:HD3    | 2:B:171:LEU:HD22  | 1.71                     | 0.71              |
| 3:C:363:MET:HE2   | 4:D:179:LEU:CD1   | 2.18                     | 0.71              |
| 3:C:288:ALA:HA    | 3:C:291:ILE:HD12  | 1.71                     | 0.71              |
| 7:G:120:TYR:CE2   | 7:G:147:PHE:CE1   | 2.78                     | 0.71              |
| 10:J:436:ILE:HG22 | 10:J:465:GLY:C    | 2.15                     | 0.71              |
| 10:J:805:VAL:HA   | 10:J:808:MET:HE3  | 1.71                     | 0.71              |
| 1:A:216:SER:OG    | 1:A:217:GLU:OE1   | 2.08                     | 0.71              |
| 7:G:120:TYR:HD2   | 7:G:147:PHE:HD1   | 1.37                     | 0.71              |
| 1:A:201:PHE:HB2   | 1:A:218:ILE:CB    | 2.21                     | 0.71              |
| 2:B:10:GLU:HB2    | 10:J:149:HIS:CD2  | 2.23                     | 0.71              |
| 3:C:197:THR:O     | 3:C:198:LEU:C     | 2.34                     | 0.71              |
| 5:E:66:VAL:CG2    | 10:J:32:ALA:HB3   | 2.21                     | 0.71              |
| 10:J:458:THR:HG23 | 10:J:459:THR:HG23 | 1.72                     | 0.71              |
| 13:R:-3:A:O2'     | 13:R:-2:A:C5'     | 2.25                     | 0.71              |
| 10:J:56:PRO:O     | 10:J:59:VAL:HG12  | 1.91                     | 0.70              |
| 10:J:765:ILE:HG22 | 10:J:769:MET:CE   | 2.21                     | 0.70              |
| 10:J:800:TYR:HD2  | 10:J:917:TYR:CE2  | 2.08                     | 0.70              |
| 10:J:946:GLU:HG3  | 10:J:965:THR:HG23 | 1.73                     | 0.70              |
| 5:E:35:GLU:HA     | 8:H:8:THR:CG2     | 2.20                     | 0.70              |
| 9:I:205:ILE:HG12  | 9:I:245:LEU:CB    | 2.19                     | 0.70              |
| 13:R:-3:A:C2'     | 13:R:-2:A:H5'     | 2.20                     | 0.70              |
| 3:C:294:ALA:O     | 3:C:384:ARG:NE    | 2.24                     | 0.70              |
| 11:K:60:ILE:HG21  | 11:K:84:ILE:CG2   | 2.21                     | 0.70              |
| 2:B:145:LEU:CD2   | 2:B:228:MET:HE3   | 2.21                     | 0.70              |
| 2:B:165:LEU:HA    | 2:B:170:PRO:HA    | 1.72                     | 0.70              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:362:LEU:HB2   | 4:D:180:LEU:HB3   | 1.72                     | 0.70              |
| 3:C:375:LYS:HE2   | 4:D:188:GLU:OE2   | 1.90                     | 0.70              |
| 7:G:59:TYR:CE1    | 7:G:61:SER:CB     | 2.74                     | 0.70              |
| 8:H:116:ILE:HD11  | 8:H:163:LEU:HD13  | 1.72                     | 0.70              |
| 3:C:35:LEU:CB     | 3:C:302:LEU:HD23  | 2.14                     | 0.70              |
| 3:C:308:LEU:HD12  | 3:C:309:GLN:N     | 2.07                     | 0.70              |
| 6:F:102:LEU:HD13  | 6:F:143:TYR:CD1   | 2.26                     | 0.70              |
| 7:G:120:TYR:CD2   | 7:G:147:PHE:CE1   | 2.79                     | 0.70              |
| 11:K:6:PRO:O      | 11:K:10:LEU:HG    | 1.92                     | 0.70              |
| 11:K:133:GLN:NE2  | 11:K:457:ASP:OD2  | 2.25                     | 0.70              |
| 7:G:6:PHE:O       | 7:G:9:ASP:CG      | 2.34                     | 0.70              |
| 2:B:111:ASN:ND2   | 2:B:158:ILE:CG1   | 2.55                     | 0.69              |
| 3:C:43:LEU:HD13   | 11:K:603:ALA:HB2  | 1.74                     | 0.69              |
| 1:A:214:THR:HG22  | 1:A:216:SER:H     | 1.56                     | 0.69              |
| 8:H:126:VAL:CG2   | 8:H:134:ALA:CB    | 2.66                     | 0.69              |
| 11:K:57:ILE:HG23  | 11:K:84:ILE:HD11  | 1.72                     | 0.69              |
| 11:K:332:LEU:CD2  | 11:K:368:PHE:CD2  | 2.75                     | 0.69              |
| 13:R:-9:A:OP1     | 13:R:-9:A:H8      | 1.75                     | 0.69              |
| 4:D:145:ILE:HB    | 4:D:194:LEU:HD13  | 1.71                     | 0.69              |
| 10:J:603:MET:HE2  | 10:J:846:ILE:O    | 1.93                     | 0.69              |
| 1:A:253:GLY:O     | 2:B:110:LYS:CG    | 2.41                     | 0.69              |
| 10:J:345:PRO:CD   | 10:J:423:PHE:CE1  | 2.74                     | 0.69              |
| 3:C:180:ASN:HD22  | 3:C:184:THR:CB    | 2.03                     | 0.69              |
| 3:C:275:ILE:HG22  | 3:C:276:CYS:O     | 1.92                     | 0.69              |
| 10:J:708:GLU:HB2  | 10:J:711:ASP:HB2  | 1.75                     | 0.69              |
| 10:J:742:ILE:HG23 | 10:J:858:LEU:HD21 | 1.70                     | 0.69              |
| 11:K:442:VAL:HG22 | 11:K:473:VAL:HG21 | 1.73                     | 0.69              |
| 3:C:239:GLN:HB3   | 3:C:392:PHE:CE1   | 2.28                     | 0.69              |
| 7:G:113:LEU:HD22  | 7:G:149:ILE:CG2   | 2.05                     | 0.69              |
| 1:A:87:ALA:HA     | 1:A:142:ASP:HA    | 1.73                     | 0.69              |
| 1:A:210:ILE:CG2   | 1:A:212:GLY:H     | 2.03                     | 0.69              |
| 8:H:193:LYS:NZ    | 8:H:283:ASP:OD1   | 2.22                     | 0.69              |
| 10:J:18:SER:HB2   | 10:J:41:LEU:HB2   | 1.74                     | 0.69              |
| 12:L:74:SER:N     | 12:L:75:PRO:HD2   | 2.07                     | 0.69              |
| 5:E:82:ILE:HG12   | 5:E:130:VAL:HB    | 1.75                     | 0.69              |
| 10:J:617:PRO:CA   | 10:J:648:SER:HB3  | 2.11                     | 0.69              |
| 3:C:293:PHE:CG    | 3:C:388:LEU:HD12  | 2.28                     | 0.69              |
| 10:J:808:MET:HG2  | 10:J:919:ILE:HD13 | 1.75                     | 0.69              |
| 6:F:150:ASN:O     | 6:F:151:PRO:C     | 2.36                     | 0.68              |
| 10:J:136:CYS:HA   | 10:J:145:PHE:CB   | 2.14                     | 0.68              |
| 10:J:538:LEU:HD13 | 10:J:670:LEU:HG   | 1.75                     | 0.68              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:K:251:VAL:HG23 | 11:K:303:ASP:OD2  | 1.92                     | 0.68              |
| 10:J:135:LEU:HB3  | 10:J:145:PHE:CZ   | 2.28                     | 0.68              |
| 7:G:233:GLU:O     | 7:G:237:VAL:HG23  | 1.93                     | 0.68              |
| 10:J:519:PRO:C    | 10:J:522:VAL:HG22 | 2.19                     | 0.68              |
| 11:K:434:ILE:HG21 | 11:K:442:VAL:HG21 | 1.75                     | 0.68              |
| 3:C:12:ILE:HD11   | 9:I:270:THR:HG22  | 1.75                     | 0.68              |
| 10:J:343:ASP:O    | 10:J:423:PHE:HE2  | 1.76                     | 0.68              |
| 11:K:244:TYR:O    | 11:K:459:SER:OG   | 2.09                     | 0.68              |
| 11:K:425:TRP:CD1  | 11:K:426:LYS:CG   | 2.77                     | 0.68              |
| 3:C:145:THR:HG21  | 3:C:147:GLU:CG    | 2.23                     | 0.68              |
| 8:H:126:VAL:HG21  | 8:H:184:LEU:HD12  | 1.74                     | 0.68              |
| 10:J:573:VAL:CG2  | 10:J:846:ILE:HG13 | 2.24                     | 0.68              |
| 2:B:81:PHE:CE1    | 2:B:129:LEU:CD1   | 2.70                     | 0.68              |
| 1:A:143:CYS:CB    | 1:A:147:PHE:CZ    | 2.76                     | 0.68              |
| 2:B:10:GLU:HB2    | 10:J:149:HIS:HE2  | 1.56                     | 0.68              |
| 3:C:386:ASP:O     | 3:C:390:THR:HG23  | 1.93                     | 0.68              |
| 5:E:15:LEU:CD1    | 5:E:23:PRO:HD3    | 2.12                     | 0.68              |
| 1:A:109:GLU:HG3   | 2:B:95:ARG:HH12   | 1.59                     | 0.68              |
| 10:J:97:GLN:OE1   | 10:J:197:ASN:ND2  | 2.26                     | 0.68              |
| 11:K:155:LYS:HG2  | 11:K:158:ALA:HB2  | 1.75                     | 0.68              |
| 6:F:100:GLY:HA3   | 6:F:142:THR:HA    | 1.74                     | 0.68              |
| 10:J:919:ILE:O    | 10:J:920:LYS:HG3  | 1.94                     | 0.68              |
| 11:K:349:TRP:HZ2  | 11:K:361:TYR:CE2  | 2.12                     | 0.68              |
| 2:B:183:SER:OG    | 2:B:203:ASP:CB    | 2.42                     | 0.68              |
| 3:C:297:TYR:OH    | 3:C:380:LEU:HB3   | 1.93                     | 0.67              |
| 6:F:71:THR:OG1    | 6:F:144:ASP:OD1   | 2.04                     | 0.67              |
| 5:E:15:LEU:HD21   | 5:E:205:GLU:HG2   | 1.76                     | 0.67              |
| 9:I:236:SER:HB2   | 9:I:244:TYR:HD2   | 1.59                     | 0.67              |
| 10:J:910:ASN:O    | 10:J:911:GLU:HB2  | 1.94                     | 0.67              |
| 3:C:184:THR:HG22  | 3:C:185:PHE:N     | 2.10                     | 0.67              |
| 5:E:35:GLU:HG2    | 8:H:8:THR:CG2     | 2.25                     | 0.67              |
| 6:F:102:LEU:HD13  | 6:F:143:TYR:CE1   | 2.28                     | 0.67              |
| 10:J:24:PHE:CZ    | 10:J:35:ILE:HG22  | 2.29                     | 0.67              |
| 12:L:102:GLU:O    | 12:L:105:GLN:CG   | 2.41                     | 0.67              |
| 9:I:143:VAL:HA    | 9:I:153:VAL:HG12  | 1.77                     | 0.67              |
| 10:J:345:PRO:HG3  | 10:J:423:PHE:CD1  | 2.29                     | 0.67              |
| 10:J:345:PRO:CG   | 10:J:423:PHE:CE1  | 2.78                     | 0.67              |
| 1:A:36:VAL:HG22   | 1:A:51:MET:HG2    | 1.75                     | 0.67              |
| 3:C:348:SER:HB2   | 3:C:361:THR:CB    | 2.16                     | 0.67              |
| 11:K:454:ARG:O    | 12:L:38:LEU:CD1   | 2.43                     | 0.67              |
| 7:G:4:PHE:HD2     | 7:G:6:PHE:CZ      | 2.12                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:J:272:VAL:HG12 | 10:J:273:LEU:HG   | 1.77                     | 0.67              |
| 2:B:27:SER:HB2    | 2:B:231:GLU:CG    | 2.13                     | 0.67              |
| 8:H:123:ARG:CB    | 8:H:136:LEU:O     | 2.42                     | 0.67              |
| 10:J:636:ILE:HD11 | 10:J:733:LEU:HD11 | 1.77                     | 0.67              |
| 11:K:56:ILE:HG21  | 12:L:57:LEU:HD13  | 1.76                     | 0.67              |
| 9:I:267:MET:HG2   | 9:I:277:SER:HB3   | 1.76                     | 0.67              |
| 10:J:315:GLN:OE1  | 10:J:397:ARG:HB3  | 1.94                     | 0.67              |
| 11:K:167:ARG:C    | 11:K:168:LEU:HD12 | 2.20                     | 0.67              |
| 11:K:549:PHE:O    | 11:K:553:CYS:CB   | 2.43                     | 0.67              |
| 3:C:309:GLN:O     | 3:C:310:ASN:C     | 2.36                     | 0.66              |
| 2:B:79:THR:OG1    | 2:B:81:PHE:CE2    | 2.48                     | 0.66              |
| 7:G:83:SER:HB2    | 7:G:97:LEU:O      | 1.95                     | 0.66              |
| 10:J:871:HIS:HA   | 10:J:877:MET:SD   | 2.35                     | 0.66              |
| 10:J:919:ILE:O    | 10:J:919:ILE:CG2  | 2.43                     | 0.66              |
| 10:J:929:LEU:HD13 | 10:J:936:GLU:HG3  | 1.78                     | 0.66              |
| 10:J:518:ASP:O    | 10:J:522:VAL:HG13 | 1.94                     | 0.66              |
| 8:H:55:VAL:CA     | 8:H:59:GLU:OE1    | 2.41                     | 0.66              |
| 1:A:130:LYS:NZ    | 1:A:172:GLU:O     | 2.27                     | 0.66              |
| 1:A:253:GLY:CA    | 2:B:110:LYS:CG    | 2.73                     | 0.66              |
| 2:B:229:ASP:OD1   | 8:H:57:PRO:CG     | 2.42                     | 0.66              |
| 7:G:158:VAL:HG21  | 7:G:194:ILE:HD12  | 1.76                     | 0.66              |
| 10:J:519:PRO:O    | 10:J:522:VAL:CG2  | 2.43                     | 0.66              |
| 10:J:903:VAL:CG1  | 10:J:907:MET:HE3  | 2.26                     | 0.66              |
| 11:K:147:PRO:HB2  | 11:K:179:TYR:HE2  | 1.60                     | 0.66              |
| 10:J:222:ILE:HG21 | 10:J:235:ILE:HD12 | 1.77                     | 0.66              |
| 1:A:251:ALA:CB    | 2:B:106:ARG:HB2   | 2.24                     | 0.66              |
| 2:B:183:SER:OG    | 2:B:203:ASP:HB3   | 1.96                     | 0.66              |
| 10:J:633:SER:HB3  | 10:J:635:ASN:HD21 | 1.59                     | 0.66              |
| 11:K:427:ILE:HG22 | 11:K:428:LEU:HD23 | 1.77                     | 0.66              |
| 11:K:539:VAL:N    | 11:K:540:PRO:HD2  | 2.11                     | 0.66              |
| 7:G:213:GLU:OE2   | 7:G:230:GLN:NE2   | 2.29                     | 0.66              |
| 1:A:253:GLY:CA    | 2:B:110:LYS:HG3   | 2.26                     | 0.66              |
| 10:J:316:VAL:HG11 | 10:J:392:VAL:HG22 | 1.78                     | 0.66              |
| 5:E:256:PRO:HA    | 5:E:259:VAL:CG1   | 2.26                     | 0.66              |
| 8:H:118:GLU:CG    | 8:H:125:LYS:HB2   | 2.26                     | 0.66              |
| 5:E:26:ARG:NH1    | 5:E:32:ARG:HG3    | 2.12                     | 0.65              |
| 9:I:102:THR:HG22  | 9:I:103:VAL:H     | 1.60                     | 0.65              |
| 4:D:136:ILE:HD13  | 4:D:194:LEU:HD11  | 1.77                     | 0.65              |
| 7:G:136:CYS:O     | 7:G:147:PHE:CB    | 2.45                     | 0.65              |
| 1:A:201:PHE:HB2   | 1:A:218:ILE:HB    | 1.76                     | 0.65              |
| 3:C:357:TYR:O     | 4:D:185:ASP:CA    | 2.44                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:K:181:HIS:CE1  | 11:K:307:TYR:CD1  | 2.84                     | 0.65              |
| 1:A:166:ASP:OD2   | 10:J:493:ARG:NH2  | 2.30                     | 0.65              |
| 1:A:194:ILE:O     | 1:A:238:THR:HG23  | 1.95                     | 0.65              |
| 10:J:734:ALA:O    | 10:J:738:VAL:HG23 | 1.97                     | 0.65              |
| 1:A:205:ASP:OD2   | 1:A:205:ASP:C     | 2.40                     | 0.65              |
| 1:A:205:ASP:OD2   | 1:A:206:THR:N     | 2.30                     | 0.65              |
| 4:D:14:ASP:CG     | 7:G:63:ARG:NH2    | 2.49                     | 0.65              |
| 10:J:222:ILE:HG21 | 10:J:235:ILE:CD1  | 2.26                     | 0.65              |
| 10:J:742:ILE:HD12 | 10:J:750:ALA:CB   | 2.21                     | 0.65              |
| 2:B:13:ARG:O      | 10:J:152:PHE:CZ   | 2.50                     | 0.65              |
| 10:J:641:PHE:O    | 10:J:642:MET:HG3  | 1.97                     | 0.65              |
| 10:J:694:LEU:CD1  | 10:J:783:SER:HB2  | 2.27                     | 0.65              |
| 1:A:142:ASP:OD1   | 1:A:143:CYS:N     | 2.30                     | 0.65              |
| 4:D:174:VAL:O     | 4:D:174:VAL:HG13  | 1.96                     | 0.65              |
| 6:F:215:LYS:NZ    | 6:F:217:ASP:O     | 2.30                     | 0.65              |
| 10:J:519:PRO:CA   | 10:J:522:VAL:HG22 | 2.25                     | 0.65              |
| 11:K:57:ILE:HD12  | 11:K:84:ILE:CD1   | 2.25                     | 0.65              |
| 1:A:240:ASN:CA    | 1:A:272:ILE:HD13  | 2.27                     | 0.64              |
| 10:J:24:PHE:CZ    | 10:J:35:ILE:CB    | 2.80                     | 0.64              |
| 10:J:65:ASN:O     | 10:J:66:GLU:CG    | 2.44                     | 0.64              |
| 10:J:755:HIS:CD2  | 10:J:833:GLY:H    | 2.13                     | 0.64              |
| 2:B:170:PRO:CG    | 2:B:213:VAL:HG22  | 2.26                     | 0.64              |
| 3:C:363:MET:CE    | 4:D:179:LEU:CD1   | 2.72                     | 0.64              |
| 10:J:503:LEU:HD21 | 10:J:605:PRO:HG2  | 1.79                     | 0.64              |
| 10:J:663:ASP:OD1  | 10:J:664:LYS:N    | 2.30                     | 0.64              |
| 11:K:56:ILE:O     | 11:K:60:ILE:HG12  | 1.97                     | 0.64              |
| 1:A:89:SER:CB     | 7:G:91:PHE:CE1    | 2.80                     | 0.64              |
| 10:J:731:MET:SD   | 13:R:-2:A:OP1     | 2.56                     | 0.64              |
| 11:K:381:ILE:HG12 | 11:K:386:LEU:HD23 | 1.79                     | 0.64              |
| 10:J:901:TYR:O    | 10:J:905:GLN:HG3  | 1.98                     | 0.64              |
| 11:K:331:LEU:HD13 | 11:K:372:ILE:CG2  | 2.26                     | 0.64              |
| 1:A:183:GLU:CG    | 1:A:184:PRO:HD2   | 2.28                     | 0.64              |
| 1:A:251:ALA:C     | 2:B:106:ARG:HB3   | 2.22                     | 0.64              |
| 2:B:129:LEU:HD21  | 5:E:41:LEU:CD2    | 2.16                     | 0.64              |
| 1:A:59:ARG:NH1    | 4:D:56:LYS:HE2    | 2.13                     | 0.64              |
| 11:K:423:SER:O    | 11:K:427:ILE:HG13 | 1.98                     | 0.64              |
| 1:A:89:SER:HB2    | 7:G:91:PHE:CZ     | 2.32                     | 0.64              |
| 10:J:126:TYR:N    | 10:J:344:ASN:OD1  | 2.30                     | 0.64              |
| 10:J:630:LEU:HD13 | 10:J:634:ALA:HA   | 1.80                     | 0.64              |
| 3:C:86:ILE:HG21   | 11:K:576:LEU:HD22 | 1.78                     | 0.64              |
| 10:J:21:GLN:HG3   | 10:J:36:VAL:CG1   | 2.28                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:J:701:VAL:HG21 | 10:J:715:VAL:HG13 | 1.80                     | 0.64              |
| 9:I:255:VAL:CG2   | 9:I:256:PHE:H     | 2.11                     | 0.64              |
| 10:J:549:ASP:OD1  | 10:J:600:ARG:NH1  | 2.30                     | 0.63              |
| 10:J:115:GLN:OE1  | 10:J:152:PHE:CD2  | 2.51                     | 0.63              |
| 10:J:800:TYR:OH   | 10:J:931:PRO:HA   | 1.98                     | 0.63              |
| 10:J:774:LYS:HB3  | 10:J:776:MET:HE3  | 1.80                     | 0.63              |
| 11:K:53:ALA:O     | 11:K:57:ILE:HG12  | 1.98                     | 0.63              |
| 4:D:13:VAL:HG11   | 4:D:29:SER:HB2    | 1.80                     | 0.63              |
| 5:E:264:ASN:O     | 8:H:9:LYS:HE3     | 1.97                     | 0.63              |
| 5:E:11:LEU:CD1    | 5:E:204:ASN:HB2   | 2.28                     | 0.63              |
| 10:J:399:SER:O    | 10:J:403:TYR:OH   | 2.15                     | 0.63              |
| 10:J:804:LEU:HG   | 10:J:808:MET:CE   | 2.26                     | 0.63              |
| 10:J:842:PHE:CD1  | 10:J:858:LEU:HD12 | 2.32                     | 0.63              |
| 1:A:36:VAL:CG2    | 1:A:51:MET:HE2    | 2.28                     | 0.63              |
| 1:A:106:ARG:HG2   | 2:B:99:GLU:CB     | 2.29                     | 0.63              |
| 3:C:10:ILE:HD12   | 3:C:12:ILE:HD12   | 1.81                     | 0.63              |
| 10:J:300:LEU:O    | 10:J:389:THR:HA   | 1.98                     | 0.63              |
| 11:K:501:LEU:O    | 11:K:505:ILE:HG12 | 1.99                     | 0.63              |
| 1:A:102:VAL:HG11  | 2:B:98:LEU:HB3    | 1.80                     | 0.63              |
| 2:B:167:ASP:CG    | 2:B:168:THR:H     | 2.05                     | 0.63              |
| 5:E:158:ILE:CG1   | 5:E:173:HIS:HB2   | 2.28                     | 0.63              |
| 10:J:555:HIS:CE1  | 10:J:567:GLY:HA3  | 2.34                     | 0.63              |
| 1:A:201:PHE:HB2   | 1:A:218:ILE:HG21  | 1.80                     | 0.63              |
| 2:B:12:LEU:HD12   | 10:J:149:HIS:CB   | 2.29                     | 0.63              |
| 2:B:14:LEU:CD1    | 2:B:177:LEU:HD21  | 2.23                     | 0.63              |
| 3:C:362:LEU:O     | 4:D:179:LEU:HD12  | 1.98                     | 0.63              |
| 5:E:109:VAL:HG13  | 5:E:182:ILE:HD11  | 1.81                     | 0.63              |
| 1:A:225:LEU:CD2   | 4:D:12:HIS:CD2    | 2.82                     | 0.63              |
| 2:B:111:ASN:HD22  | 2:B:158:ILE:CD1   | 2.12                     | 0.63              |
| 3:C:235:MET:O     | 3:C:239:GLN:HG2   | 1.98                     | 0.63              |
| 5:E:66:VAL:HG21   | 10:J:32:ALA:HB3   | 1.81                     | 0.63              |
| 11:K:60:ILE:CG2   | 11:K:84:ILE:HG23  | 2.26                     | 0.63              |
| 2:B:237:GLN:OE1   | 2:B:237:GLN:HA    | 1.98                     | 0.62              |
| 3:C:345:SER:CB    | 3:C:369:ILE:HD11  | 2.25                     | 0.62              |
| 4:D:36:PRO:HB3    | 4:D:87:LEU:HB2    | 1.80                     | 0.62              |
| 5:E:226:ILE:HB    | 6:F:215:LYS:HB3   | 1.80                     | 0.62              |
| 10:J:149:HIS:HB3  | 10:J:152:PHE:CD2  | 2.33                     | 0.62              |
| 10:J:538:LEU:HB2  | 10:J:670:LEU:HD12 | 1.81                     | 0.62              |
| 6:F:200:VAL:HB    | 6:F:214:TRP:HB3   | 1.81                     | 0.62              |
| 10:J:807:ILE:HD13 | 10:J:929:LEU:HD21 | 1.81                     | 0.62              |
| 11:K:149:ILE:O    | 11:K:149:ILE:HG13 | 1.98                     | 0.62              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 3:C:190:PRO:CG     | 3:C:193:LEU:HD12  | 2.28                     | 0.62              |
| 10:J:72:LEU:HD11   | 10:J:146:ILE:HG21 | 1.80                     | 0.62              |
| 10:J:661:ILE:HG23  | 10:J:675:ARG:HG2  | 1.80                     | 0.62              |
| 11:K:213:PRO:HG3   | 11:K:359:THR:CG2  | 2.29                     | 0.62              |
| 11:K:550:SER:O     | 11:K:554:ASN:HB2  | 1.99                     | 0.62              |
| 2:B:165:LEU:HD21   | 2:B:209:ARG:HG3   | 1.81                     | 0.62              |
| 8:H:154:SER:O      | 8:H:157:LEU:HG    | 2.00                     | 0.62              |
| 7:G:29:PRO:HB3     | 9:I:260:ALA:HB2   | 1.82                     | 0.62              |
| 8:H:313:GLY:O      | 8:H:318:ARG:HD2   | 2.00                     | 0.62              |
| 10:J:112[B]:ILE:HA | 10:J:146:ILE:HG23 | 1.81                     | 0.62              |
| 10:J:694:LEU:HD11  | 10:J:783:SER:HB2  | 1.81                     | 0.62              |
| 10:J:701:VAL:HG22  | 10:J:702:LYS:N    | 2.13                     | 0.62              |
| 10:J:706:ASP:OD1   | 10:J:707:SER:N    | 2.30                     | 0.62              |
| 11:K:144:GLU:OE2   | 11:K:454:ARG:NH1  | 2.33                     | 0.62              |
| 1:A:201:PHE:HB2    | 1:A:218:ILE:CG2   | 2.29                     | 0.62              |
| 10:J:676:ALA:O     | 10:J:680:LEU:HD13 | 2.00                     | 0.62              |
| 3:C:363:MET:SD     | 4:D:72:ALA:HB3    | 2.40                     | 0.62              |
| 8:H:329:TYR:HB3    | 8:H:334:GLU:OE1   | 1.99                     | 0.62              |
| 10:J:112[A]:ILE:HA | 10:J:146:ILE:HG23 | 1.81                     | 0.62              |
| 10:J:345:PRO:N     | 10:J:423:PHE:CZ   | 2.66                     | 0.62              |
| 10:J:573:VAL:HG21  | 10:J:846:ILE:HG13 | 1.82                     | 0.62              |
| 4:D:161:HIS:CD2    | 4:D:182:SER:CB    | 2.83                     | 0.62              |
| 11:K:550:SER:O     | 11:K:554:ASN:CB   | 2.48                     | 0.62              |
| 4:D:222:VAL:CG1    | 7:G:165:GLN:NE2   | 2.63                     | 0.62              |
| 5:E:238:SER:HB3    | 6:F:211:VAL:CG1   | 2.30                     | 0.62              |
| 10:J:24:PHE:HZ     | 10:J:35:ILE:CG2   | 2.13                     | 0.62              |
| 11:K:196:ILE:HG21  | 11:K:287:VAL:HG22 | 1.73                     | 0.62              |
| 11:K:319:LYS:HA    | 11:K:326:HIS:CE1  | 2.32                     | 0.62              |
| 11:K:404:SER:CB    | 11:K:417:SER:HB2  | 2.29                     | 0.62              |
| 8:H:94:LEU:HD13    | 11:K:387:ALA:HB1  | 1.76                     | 0.61              |
| 10:J:738:VAL:HG13  | 10:J:858:LEU:CD2  | 2.30                     | 0.61              |
| 3:C:277:ASP:OD2    | 3:C:280:LYS:HB2   | 1.99                     | 0.61              |
| 6:F:126:ASN:ND2    | 9:I:42:LYS:HZ3    | 1.98                     | 0.61              |
| 8:H:94:LEU:HD13    | 11:K:387:ALA:CB   | 2.27                     | 0.61              |
| 10:J:72:LEU:HD21   | 10:J:146:ILE:CG2  | 2.30                     | 0.61              |
| 1:A:89:SER:HB2     | 7:G:91:PHE:CE1    | 2.34                     | 0.61              |
| 8:H:111:HIS:O      | 8:H:227:VAL:HG23  | 1.99                     | 0.61              |
| 10:J:499:VAL:HG22  | 10:J:583:LEU:HA   | 1.82                     | 0.61              |
| 2:B:223:ARG:O      | 2:B:227:LEU:HG    | 1.98                     | 0.61              |
| 4:D:222:VAL:HG11   | 7:G:165:GLN:HE22  | 1.65                     | 0.61              |
| 3:C:379:LEU:O      | 3:C:383:VAL:HG23  | 2.00                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:H:56:THR:O      | 8:H:59:GLU:HB2    | 2.01                     | 0.61              |
| 10:J:288:GLY:O    | 10:J:300:LEU:HD12 | 2.01                     | 0.61              |
| 10:J:706:ASP:CG   | 10:J:707:SER:H    | 2.07                     | 0.61              |
| 3:C:249:ASP:O     | 3:C:250:GLU:C     | 2.40                     | 0.61              |
| 10:J:573:VAL:CG2  | 10:J:846:ILE:CG1  | 2.78                     | 0.61              |
| 7:G:158:VAL:HG11  | 7:G:162:PHE:CD2   | 2.31                     | 0.61              |
| 9:I:102:THR:CG2   | 9:I:103:VAL:N     | 2.63                     | 0.61              |
| 9:I:258:ARG:HB2   | 9:I:262:GLY:HA2   | 1.83                     | 0.61              |
| 10:J:633:SER:HB3  | 10:J:635:ASN:ND2  | 2.15                     | 0.61              |
| 10:J:800:TYR:CD2  | 10:J:917:TYR:CZ   | 2.87                     | 0.61              |
| 2:B:10:GLU:CB     | 10:J:149:HIS:HE2  | 2.11                     | 0.61              |
| 10:J:81:ALA:HB1   | 10:J:82:PRO:HA    | 1.83                     | 0.61              |
| 10:J:259:TYR:CG   | 10:J:393:VAL:HB   | 2.35                     | 0.61              |
| 11:K:549:PHE:O    | 11:K:553:CYS:HB3  | 2.00                     | 0.61              |
| 3:C:352:ALA:HB3   | 3:C:356:ASN:O     | 2.01                     | 0.61              |
| 4:D:34:ILE:HG21   | 7:G:91:PHE:HB3    | 1.81                     | 0.61              |
| 10:J:663:ASP:O    | 10:J:664:LYS:HB3  | 2.01                     | 0.61              |
| 11:K:251:VAL:O    | 11:K:267:THR:OG1  | 2.19                     | 0.61              |
| 2:B:16:GLY:N      | 10:J:152:PHE:HE1  | 1.99                     | 0.61              |
| 3:C:350:LEU:CG    | 3:C:359:GLN:NE2   | 2.63                     | 0.61              |
| 7:G:136:CYS:O     | 7:G:147:PHE:HD2   | 1.83                     | 0.61              |
| 1:A:291:ASN:HB2   | 1:A:294:ALA:HB2   | 1.83                     | 0.60              |
| 2:B:236:ALA:O     | 2:B:240:VAL:HG23  | 2.01                     | 0.60              |
| 3:C:303:ASP:N     | 3:C:304:PRO:CD    | 2.63                     | 0.60              |
| 5:E:22:ARG:HB2    | 5:E:26:ARG:H      | 1.66                     | 0.60              |
| 5:E:238:SER:HB3   | 6:F:211:VAL:HG13  | 1.83                     | 0.60              |
| 10:J:842:PHE:CD1  | 10:J:858:LEU:CD1  | 2.83                     | 0.60              |
| 7:G:120:TYR:CE2   | 7:G:147:PHE:HE1   | 2.19                     | 0.60              |
| 11:K:196:ILE:HG13 | 11:K:197:LEU:HG   | 1.81                     | 0.60              |
| 5:E:193:VAL:O     | 5:E:193:VAL:HG23  | 1.99                     | 0.60              |
| 8:H:56:THR:O      | 8:H:59:GLU:CB     | 2.50                     | 0.60              |
| 8:H:123:ARG:N     | 8:H:159:MET:HE1   | 2.17                     | 0.60              |
| 10:J:919:ILE:O    | 10:J:920:LYS:CG   | 2.49                     | 0.60              |
| 11:K:52:MET:O     | 11:K:56:ILE:HG13  | 2.02                     | 0.60              |
| 1:A:169:VAL:HG23  | 1:A:174:ILE:HG22  | 1.84                     | 0.60              |
| 2:B:164:GLY:O     | 2:B:170:PRO:HA    | 2.01                     | 0.60              |
| 6:F:56:CYS:HB2    | 6:F:77:VAL:O      | 2.00                     | 0.60              |
| 11:K:197:LEU:HD21 | 11:K:390:LEU:HD11 | 1.82                     | 0.60              |
| 11:K:356:LYS:HB3  | 11:K:357:PRO:HD3  | 1.82                     | 0.60              |
| 2:B:177:LEU:HD22  | 10:J:37:ARG:CD    | 2.31                     | 0.60              |
| 5:E:39:ASP:O      | 8:H:12:GLY:HA2    | 2.02                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:E:94:THR:HG23   | 6:F:112:GLU:HG3   | 1.84                     | 0.60              |
| 10:J:981:VAL:CG2  | 10:J:999:LEU:O    | 2.49                     | 0.60              |
| 3:C:282:VAL:HG23  | 3:C:283:PRO:HD2   | 1.82                     | 0.60              |
| 7:G:67:SER:OG     | 7:G:70:ASP:CG     | 2.44                     | 0.60              |
| 10:J:316:VAL:HG22 | 10:J:395:ILE:CD1  | 2.31                     | 0.60              |
| 3:C:299:ILE:HB    | 3:C:345:SER:HB2   | 1.81                     | 0.60              |
| 8:H:68:MET:CE     | 11:K:387:ALA:HA   | 2.32                     | 0.60              |
| 10:J:553:ALA:C    | 10:J:554:LEU:HD12 | 2.27                     | 0.60              |
| 3:C:145:THR:HG21  | 3:C:147:GLU:CD    | 2.25                     | 0.60              |
| 3:C:173:LYS:HG3   | 3:C:173:LYS:O     | 2.02                     | 0.60              |
| 4:D:34:ILE:CG2    | 7:G:91:PHE:HB3    | 2.32                     | 0.60              |
| 10:J:103:GLU:HG2  | 10:J:135:LEU:HD11 | 1.83                     | 0.60              |
| 11:K:424:PRO:HB2  | 11:K:446:TYR:CZ   | 2.36                     | 0.60              |
| 2:B:84:PHE:CE2    | 10:J:36:VAL:O     | 2.55                     | 0.59              |
| 3:C:150:THR:O     | 3:C:154:LYS:HG3   | 2.02                     | 0.59              |
| 4:D:169:ASN:HA    | 7:G:8:GLY:O       | 2.03                     | 0.59              |
| 5:E:256:PRO:CA    | 5:E:259:VAL:HG12  | 2.32                     | 0.59              |
| 7:G:128:LYS:HE3   | 9:I:261:ASN:OD1   | 2.02                     | 0.59              |
| 10:J:844:SER:HB2  | 10:J:848:ARG:HH21 | 1.65                     | 0.59              |
| 3:C:190:PRO:HG3   | 3:C:193:LEU:HD12  | 1.84                     | 0.59              |
| 3:C:308:LEU:HD12  | 3:C:309:GLN:H     | 1.67                     | 0.59              |
| 5:E:256:PRO:O     | 5:E:259:VAL:HG12  | 2.01                     | 0.59              |
| 9:I:48:HIS:CE1    | 11:K:552:LEU:HD12 | 2.37                     | 0.59              |
| 9:I:64:VAL:HG22   | 9:I:110:VAL:HG22  | 1.84                     | 0.59              |
| 11:K:434:ILE:CG2  | 11:K:473:VAL:HG11 | 2.32                     | 0.59              |
| 10:J:800:TYR:HD2  | 10:J:917:TYR:CZ   | 2.20                     | 0.59              |
| 10:J:941:LEU:HA   | 10:J:944:LEU:HD12 | 1.84                     | 0.59              |
| 1:A:3:LYS:NZ      | 4:D:35:GLU:O      | 2.35                     | 0.59              |
| 3:C:248:ILE:HD12  | 3:C:274:ILE:HG12  | 1.85                     | 0.59              |
| 3:C:360:LEU:N     | 4:D:182:SER:O     | 2.34                     | 0.59              |
| 3:C:363:MET:HA    | 4:D:178:LEU:O     | 2.02                     | 0.59              |
| 7:G:120:TYR:HE2   | 7:G:147:PHE:HE1   | 1.49                     | 0.59              |
| 9:I:48:HIS:ND1    | 11:K:552:LEU:HD12 | 2.18                     | 0.59              |
| 10:J:539:ILE:CG1  | 10:J:569:HIS:CD2  | 2.84                     | 0.59              |
| 10:J:630:LEU:CD2  | 10:J:680:LEU:HD23 | 2.32                     | 0.59              |
| 1:A:169:VAL:C     | 1:A:170:HIS:HD1   | 2.10                     | 0.59              |
| 2:B:84:PHE:CZ     | 10:J:36:VAL:O     | 2.55                     | 0.59              |
| 11:K:255:GLN:HG2  | 11:K:362:ALA:O    | 2.03                     | 0.59              |
| 2:B:225:ARG:NH2   | 2:B:229:ASP:OD2   | 2.35                     | 0.59              |
| 5:E:12:TYR:OH     | 5:E:210:ASN:OD1   | 2.16                     | 0.59              |
| 12:L:42:ASP:OD2   | 12:L:44:ARG:HB3   | 2.01                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:L:82:ARG:O     | 12:L:86:TYR:HD2   | 1.85                     | 0.59              |
| 1:A:86:MET:HE3    | 4:D:91:THR:HG22   | 1.85                     | 0.59              |
| 10:J:282:GLU:O    | 10:J:283:TYR:CD1  | 2.56                     | 0.59              |
| 2:B:111:ASN:HD21  | 2:B:158:ILE:HG13  | 1.68                     | 0.59              |
| 3:C:288:ALA:HA    | 3:C:291:ILE:CD1   | 2.32                     | 0.59              |
| 3:C:363:MET:SD    | 4:D:72:ALA:HB2    | 2.40                     | 0.59              |
| 10:J:115:GLN:NE2  | 10:J:152:PHE:HE2  | 1.98                     | 0.59              |
| 2:B:112:VAL:HG13  | 2:B:153:SER:O     | 2.03                     | 0.58              |
| 3:C:282:VAL:CG2   | 3:C:283:PRO:HD2   | 2.33                     | 0.58              |
| 7:G:4:PHE:CD2     | 7:G:6:PHE:CZ      | 2.91                     | 0.58              |
| 7:G:22:GLY:HA3    | 7:G:55:ALA:O      | 2.03                     | 0.58              |
| 7:G:237:VAL:O     | 7:G:238:LYS:C     | 2.45                     | 0.58              |
| 11:K:424:PRO:O    | 11:K:428:LEU:HG   | 2.03                     | 0.58              |
| 1:A:253:GLY:CA    | 2:B:110:LYS:HG2   | 2.33                     | 0.58              |
| 1:A:253:GLY:N     | 2:B:110:LYS:HG2   | 2.19                     | 0.58              |
| 8:H:172:GLU:HB3   | 8:H:185:HIS:CE1   | 2.38                     | 0.58              |
| 11:K:301:GLN:HG2  | 11:K:307:TYR:CE1  | 2.38                     | 0.58              |
| 1:A:36:VAL:HG21   | 1:A:51:MET:HE2    | 1.86                     | 0.58              |
| 12:L:102:GLU:C    | 12:L:105:GLN:HG2  | 2.28                     | 0.58              |
| 5:E:193:VAL:HG12  | 5:E:209:ALA:HA    | 1.85                     | 0.58              |
| 7:G:113:LEU:HD21  | 7:G:149:ILE:HG12  | 1.84                     | 0.58              |
| 9:I:102:THR:CG2   | 9:I:103:VAL:H     | 2.15                     | 0.58              |
| 4:D:1:MET:HE1     | 4:D:205:LEU:HD22  | 1.80                     | 0.58              |
| 3:C:180:ASN:HB2   | 3:C:184:THR:N     | 2.17                     | 0.58              |
| 3:C:345:SER:HB3   | 3:C:369:ILE:CD1   | 2.28                     | 0.58              |
| 6:F:47:SER:HB2    | 6:F:63:GLU:HB2    | 1.85                     | 0.58              |
| 11:K:144:GLU:HB2  | 11:K:403:TYR:CE2  | 2.37                     | 0.58              |
| 11:K:348:ASP:CG   | 11:K:350:ARG:HB2  | 2.28                     | 0.58              |
| 7:G:136:CYS:O     | 7:G:147:PHE:CD2   | 2.56                     | 0.58              |
| 11:K:346:LEU:HD12 | 11:K:346:LEU:N    | 2.18                     | 0.58              |
| 12:L:74:SER:N     | 12:L:75:PRO:CD    | 2.66                     | 0.58              |
| 1:A:59:ARG:NH1    | 4:D:56:LYS:CE     | 2.66                     | 0.58              |
| 7:G:219:ASP:HB2   | 7:G:222:ALA:HB3   | 1.86                     | 0.58              |
| 8:H:122:LYS:HA    | 8:H:159:MET:SD    | 2.42                     | 0.58              |
| 10:J:800:TYR:CE2  | 10:J:931:PRO:HB3  | 2.38                     | 0.58              |
| 11:K:381:ILE:HG13 | 11:K:386:LEU:HD22 | 1.84                     | 0.58              |
| 7:G:217:LYS:HG3   | 7:G:226:ILE:HD11  | 1.85                     | 0.58              |
| 11:K:52:MET:HE2   | 12:L:25:ILE:HG13  | 1.72                     | 0.58              |
| 11:K:168:LEU:HD12 | 11:K:168:LEU:N    | 2.18                     | 0.58              |
| 12:L:66:LYS:CE    | 12:L:73:MET:HE2   | 2.33                     | 0.58              |
| 7:G:7:PRO:HD3     | 7:G:39:THR:HG22   | 1.86                     | 0.58              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 10:J:634:ALA:CB   | 10:J:680:LEU:HG  | 2.33                     | 0.58              |
| 2:B:18:ARG:HG3    | 10:J:42:ARG:NH2  | 2.19                     | 0.57              |
| 2:B:175:ASN:O     | 2:B:179:GLU:HG3  | 2.04                     | 0.57              |
| 3:C:350:LEU:CD1   | 3:C:359:GLN:CD   | 2.73                     | 0.57              |
| 7:G:150:LEU:HD13  | 7:G:195:TRP:CD1  | 2.37                     | 0.57              |
| 10:J:600:ARG:HH21 | 10:J:606:MET:HE3 | 1.69                     | 0.57              |
| 10:J:225:LEU:CD2  | 10:J:231:ILE:CD1 | 2.83                     | 0.57              |
| 11:K:355:SER:HB2  | 11:K:358:MET:HG3 | 1.84                     | 0.57              |
| 1:A:163:LYS:HB3   | 1:A:184:PRO:HB2  | 1.85                     | 0.57              |
| 8:H:217:LEU:HD13  | 8:H:221:ILE:HD12 | 1.87                     | 0.57              |
| 10:J:398:ARG:HD3  | 10:J:400:TRP:CG  | 2.39                     | 0.57              |
| 10:J:498:LYS:HG2  | 10:J:582:ALA:CB  | 2.34                     | 0.57              |
| 5:E:262:LEU:HD13  | 8:H:7:ILE:CD1    | 2.30                     | 0.57              |
| 7:G:217:LYS:HB2   | 7:G:223:PHE:HE1  | 1.68                     | 0.57              |
| 8:H:124:TRP:CE3   | 8:H:136:LEU:HD23 | 2.39                     | 0.57              |
| 10:J:21:GLN:HG3   | 10:J:36:VAL:HG11 | 1.86                     | 0.57              |
| 10:J:53:THR:O     | 10:J:56:PRO:HD2  | 2.05                     | 0.57              |
| 10:J:115:GLN:CD   | 10:J:152:PHE:CE2 | 2.82                     | 0.57              |
| 2:B:107:MET:SD    | 2:B:198:LEU:CB   | 2.87                     | 0.57              |
| 7:G:150:LEU:HD22  | 7:G:195:TRP:CE3  | 2.39                     | 0.57              |
| 4:D:33:PRO:HD2    | 7:G:63:ARG:HG2   | 1.87                     | 0.57              |
| 10:J:104:ASN:O    | 10:J:143:LYS:NZ  | 2.23                     | 0.57              |
| 10:J:617:PRO:O    | 10:J:618:TYR:HB2 | 2.04                     | 0.57              |
| 2:B:111:ASN:CG    | 2:B:158:ILE:HD11 | 2.29                     | 0.57              |
| 7:G:76:ILE:HD13   | 7:G:86:VAL:HB    | 1.86                     | 0.57              |
| 11:K:91:MET:CE    | 11:K:455:ARG:NH2 | 2.68                     | 0.57              |
| 3:C:32:GLN:HB3    | 3:C:304:PRO:HG2  | 1.87                     | 0.57              |
| 3:C:348:SER:CB    | 3:C:361:THR:HB   | 2.18                     | 0.57              |
| 10:J:701:VAL:CG2  | 10:J:716:GLU:O   | 2.45                     | 0.57              |
| 3:C:293:PHE:CD2   | 3:C:388:LEU:CD1  | 2.87                     | 0.57              |
| 13:R:-2:A:H2'     | 13:R:-1:A:C5'    | 2.34                     | 0.57              |
| 1:A:6:GLU:HG2     | 7:G:77:ILE:HG21  | 1.86                     | 0.56              |
| 10:J:255:PHE:HD2  | 10:J:458:THR:O   | 1.88                     | 0.56              |
| 11:K:16:VAL:HG21  | 12:L:21:LEU:HD22 | 1.86                     | 0.56              |
| 1:A:245:VAL:HG23  | 2:B:207:LEU:CD1  | 2.35                     | 0.56              |
| 11:K:196:ILE:CG2  | 11:K:373:TYR:OH  | 2.45                     | 0.56              |
| 1:A:240:ASN:C     | 1:A:272:ILE:CD1  | 2.77                     | 0.56              |
| 2:B:4:LEU:HD11    | 10:J:37:ARG:HH12 | 1.68                     | 0.56              |
| 3:C:239:GLN:HB3   | 3:C:392:PHE:HE1  | 1.71                     | 0.56              |
| 5:E:158:ILE:HD11  | 5:E:173:HIS:CA   | 2.35                     | 0.56              |
| 5:E:256:PRO:C     | 5:E:259:VAL:HG12 | 2.31                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:G:44:VAL:HG12   | 7:G:55:ALA:HB2    | 1.87                     | 0.56              |
| 10:J:225:LEU:HD22 | 10:J:231:ILE:HD11 | 1.86                     | 0.56              |
| 10:J:400:TRP:CZ2  | 10:J:453:ILE:HG21 | 2.40                     | 0.56              |
| 10:J:800:TYR:CZ   | 10:J:931:PRO:CB   | 2.83                     | 0.56              |
| 11:K:144:GLU:HA   | 11:K:403:TYR:CZ   | 2.40                     | 0.56              |
| 7:G:99:TYR:O      | 7:G:102:PHE:HD1   | 1.88                     | 0.56              |
| 12:L:19:ASP:O     | 12:L:23:PRO:CD    | 2.53                     | 0.56              |
| 2:B:183:SER:OG    | 2:B:203:ASP:HB2   | 2.05                     | 0.56              |
| 8:H:124:TRP:NE1   | 8:H:163:LEU:HB2   | 2.20                     | 0.56              |
| 10:J:573:VAL:HG21 | 10:J:846:ILE:CG1  | 2.35                     | 0.56              |
| 7:G:71:PHE:O      | 7:G:190:LEU:N     | 2.26                     | 0.56              |
| 8:H:104:TYR:CD1   | 8:H:204:SER:HB3   | 2.41                     | 0.56              |
| 1:A:179:VAL:HG23  | 1:A:184:PRO:HD3   | 1.86                     | 0.56              |
| 10:J:65:ASN:O     | 10:J:66:GLU:CD    | 2.49                     | 0.56              |
| 10:J:484:LEU:CD2  | 10:J:596:LEU:HD22 | 2.35                     | 0.56              |
| 11:K:597:GLU:O    | 11:K:601:ILE:HG13 | 2.05                     | 0.56              |
| 1:A:296:MET:HE1   | 10:J:508:HIS:NE2  | 2.21                     | 0.56              |
| 3:C:295:SER:HB3   | 3:C:384:ARG:HD2   | 1.79                     | 0.56              |
| 7:G:113:LEU:HD21  | 7:G:149:ILE:HG23  | 1.81                     | 0.56              |
| 7:G:150:LEU:HD22  | 7:G:195:TRP:CZ3   | 2.41                     | 0.56              |
| 7:G:223:PHE:HD1   | 7:G:226:ILE:HD12  | 1.71                     | 0.56              |
| 9:I:255:VAL:CG2   | 9:I:256:PHE:N     | 2.68                     | 0.56              |
| 10:J:135:LEU:C    | 10:J:145:PHE:CD2  | 2.84                     | 0.56              |
| 10:J:567:GLY:HA3  | 10:J:627:ILE:HG13 | 1.87                     | 0.56              |
| 10:J:45:ILE:HG22  | 10:J:148:PHE:HE1  | 1.61                     | 0.56              |
| 12:L:62:PHE:CZ    | 12:L:66:LYS:HE3   | 2.41                     | 0.56              |
| 3:C:153:GLN:HB2   | 4:D:61:THR:HB     | 1.88                     | 0.56              |
| 10:J:282:GLU:OE2  | 10:J:811:ARG:NH2  | 2.38                     | 0.56              |
| 11:K:410:THR:HG23 | 11:K:411:PRO:HD2  | 1.88                     | 0.56              |
| 11:K:532:ILE:O    | 11:K:536:THR:HG23 | 2.06                     | 0.56              |
| 4:D:136:ILE:HG21  | 4:D:194:LEU:HD11  | 1.87                     | 0.55              |
| 10:J:401:ARG:NH1  | 10:J:403:TYR:CE1  | 2.75                     | 0.55              |
| 3:C:363:MET:HG2   | 4:D:179:LEU:HD13  | 1.88                     | 0.55              |
| 5:E:90:LEU:CD2    | 6:F:118:MET:HE1   | 2.36                     | 0.55              |
| 11:K:91:MET:HE3   | 11:K:455:ARG:NH2  | 2.21                     | 0.55              |
| 1:A:23:TYR:OH     | 7:G:238:LYS:CA    | 2.33                     | 0.55              |
| 2:B:13:ARG:O      | 10:J:152:PHE:CE1  | 2.60                     | 0.55              |
| 2:B:79:THR:HG22   | 2:B:128:VAL:O     | 2.06                     | 0.55              |
| 3:C:363:MET:CG    | 4:D:179:LEU:HD13  | 2.36                     | 0.55              |
| 5:E:90:LEU:HD12   | 6:F:111:LYS:HB3   | 1.87                     | 0.55              |
| 7:G:113:LEU:CD2   | 7:G:149:ILE:HG12  | 2.36                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:I:10:ILE:HG13   | 9:I:62:GLY:O      | 2.06                     | 0.55              |
| 10:J:267:GLY:CA   | 10:J:272:VAL:HB   | 2.36                     | 0.55              |
| 11:K:490:VAL:HG13 | 11:K:495:ARG:HH21 | 1.71                     | 0.55              |
| 11:K:596:THR:O    | 11:K:600:ARG:HG3  | 2.06                     | 0.55              |
| 1:A:205:ASP:OD2   | 1:A:207:GLU:N     | 2.35                     | 0.55              |
| 2:B:168:THR:HA    | 2:B:209:ARG:CZ    | 2.37                     | 0.55              |
| 5:E:116:LEU:CD1   | 5:E:157:LEU:CD2   | 2.73                     | 0.55              |
| 11:K:502:ALA:O    | 11:K:506:ARG:HG3  | 2.07                     | 0.55              |
| 7:G:4:PHE:HD2     | 7:G:6:PHE:CE1     | 2.23                     | 0.55              |
| 7:G:75:VAL:C      | 7:G:86:VAL:HG23   | 2.31                     | 0.55              |
| 9:I:228:ASP:OD2   | 9:I:286:ARG:NE    | 2.32                     | 0.55              |
| 2:B:164:GLY:O     | 2:B:170:PRO:CA    | 2.53                     | 0.55              |
| 3:C:181:GLU:O     | 3:C:182:ASP:HB2   | 2.07                     | 0.55              |
| 11:K:60:ILE:HG21  | 11:K:84:ILE:HG12  | 1.88                     | 0.55              |
| 11:K:410:THR:HG22 | 11:K:412:SER:H    | 1.72                     | 0.55              |
| 1:A:143:CYS:SG    | 1:A:147:PHE:CZ    | 2.99                     | 0.55              |
| 1:A:214:THR:CG2   | 1:A:215:ASN:H     | 2.18                     | 0.55              |
| 1:A:252:GLY:N     | 2:B:107:MET:HA    | 2.21                     | 0.55              |
| 5:E:90:LEU:HD21   | 6:F:118:MET:HE1   | 1.88                     | 0.55              |
| 5:E:96:THR:O      | 5:E:100:ASN:ND2   | 2.36                     | 0.55              |
| 9:I:47:GLU:HA     | 9:I:51:ARG:O      | 2.07                     | 0.55              |
| 10:J:952:ALA:HB3  | 10:J:961:THR:HB   | 1.89                     | 0.55              |
| 9:I:206:ARG:NE    | 9:I:209:ASP:OD2   | 2.40                     | 0.55              |
| 2:B:3:ARG:HB3     | 10:J:123:ASN:OD1  | 2.07                     | 0.55              |
| 2:B:13:ARG:CD     | 2:B:171:LEU:HD13  | 2.35                     | 0.55              |
| 3:C:300:VAL:CG1   | 3:C:343:ILE:CG2   | 2.84                     | 0.55              |
| 5:E:258:VAL:HG13  | 8:H:5:ILE:HG21    | 1.89                     | 0.55              |
| 7:G:122:ARG:HG2   | 7:G:138:ASP:HB2   | 1.89                     | 0.55              |
| 10:J:135:LEU:O    | 10:J:145:PHE:CD2  | 2.60                     | 0.55              |
| 11:K:207:SER:O    | 11:K:210:ASP:HB2  | 2.07                     | 0.55              |
| 3:C:86:ILE:HD13   | 11:K:576:LEU:HD22 | 1.89                     | 0.55              |
| 3:C:299:ILE:HB    | 3:C:345:SER:CB    | 2.36                     | 0.55              |
| 6:F:102:LEU:CD1   | 6:F:143:TYR:CD1   | 2.89                     | 0.55              |
| 10:J:278:ILE:HG23 | 10:J:278:ILE:O    | 2.06                     | 0.55              |
| 2:B:163:VAL:CG1   | 2:B:213:VAL:HG13  | 2.27                     | 0.54              |
| 3:C:275:ILE:CG2   | 3:C:276:CYS:N     | 2.70                     | 0.54              |
| 7:G:219:ASP:O     | 7:G:223:PHE:CG    | 2.60                     | 0.54              |
| 9:I:279:VAL:HG23  | 9:I:280:THR:N     | 2.22                     | 0.54              |
| 10:J:552:ASP:HA   | 10:J:615:LEU:HD12 | 1.89                     | 0.54              |
| 1:A:240:ASN:C     | 1:A:272:ILE:HD13  | 2.31                     | 0.54              |
| 7:G:46:ALA:HB2    | 7:G:53:GLN:HE22   | 1.72                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:K:144:GLU:CA   | 11:K:403:TYR:CE2  | 2.90                     | 0.54              |
| 2:B:14:LEU:HD13   | 2:B:177:LEU:CD2   | 2.29                     | 0.54              |
| 2:B:164:GLY:HA3   | 2:B:174:THR:CG2   | 2.37                     | 0.54              |
| 3:C:184:THR:CG2   | 3:C:185:PHE:N     | 2.70                     | 0.54              |
| 1:A:164:LYS:HD3   | 1:A:187:LEU:CD2   | 2.38                     | 0.54              |
| 1:A:164:LYS:HD3   | 1:A:187:LEU:HD21  | 1.89                     | 0.54              |
| 3:C:98:GLU:HG3    | 3:C:210:SER:HB2   | 1.89                     | 0.54              |
| 3:C:172:VAL:HB    | 3:C:209:TRP:O     | 2.08                     | 0.54              |
| 4:D:107:ARG:NH2   | 4:D:148:ASP:OD1   | 2.41                     | 0.54              |
| 8:H:60:LEU:HD13   | 8:H:81:TYR:CE2    | 2.42                     | 0.54              |
| 8:H:94:LEU:CD1    | 11:K:387:ALA:HB2  | 2.36                     | 0.54              |
| 10:J:400:TRP:CZ3  | 10:J:453:ILE:HG22 | 2.42                     | 0.54              |
| 10:J:498:LYS:O    | 10:J:501:GLU:HG2  | 2.08                     | 0.54              |
| 3:C:12:ILE:HG22   | 3:C:13:HIS:N      | 2.22                     | 0.54              |
| 7:G:108:LYS:NZ    | 13:N:-12:U:OP2    | 2.28                     | 0.54              |
| 7:G:129:GLU:OE2   | 9:I:225:LYS:CE    | 2.49                     | 0.54              |
| 10:J:45:ILE:CG2   | 10:J:148:PHE:CZ   | 2.91                     | 0.54              |
| 10:J:907:MET:HE2  | 10:J:914:GLU:OE1  | 2.08                     | 0.54              |
| 10:J:961:THR:HG23 | 10:J:972:ASP:OD1  | 2.08                     | 0.54              |
| 5:E:192:VAL:HG22  | 5:E:197:MET:HE3   | 1.90                     | 0.54              |
| 7:G:7:PRO:CD      | 7:G:39:THR:HG22   | 2.38                     | 0.54              |
| 7:G:16:THR:O      | 7:G:18:PRO:HD3    | 2.08                     | 0.54              |
| 7:G:96:SER:HB3    | 7:G:133:GLU:HG2   | 1.90                     | 0.54              |
| 1:A:188:GLY:C     | 1:A:189:ILE:HD12  | 2.33                     | 0.54              |
| 4:D:1:MET:HE3     | 4:D:205:LEU:HD22  | 1.85                     | 0.54              |
| 6:F:129:ARG:HH21  | 9:I:42:LYS:HD3    | 1.73                     | 0.54              |
| 1:A:6:GLU:HG2     | 7:G:77:ILE:CG2    | 2.37                     | 0.54              |
| 4:D:145:ILE:HD13  | 4:D:194:LEU:HD12  | 1.89                     | 0.54              |
| 9:I:32:ILE:HG21   | 11:K:534:LEU:HD13 | 1.90                     | 0.54              |
| 9:I:60:LEU:O      | 9:I:110:VAL:HG11  | 2.08                     | 0.54              |
| 10:J:126:TYR:OH   | 10:J:413:ASP:HB2  | 2.08                     | 0.54              |
| 10:J:135:LEU:HD13 | 10:J:145:PHE:CZ   | 2.43                     | 0.54              |
| 3:C:300:VAL:CG1   | 3:C:343:ILE:CG1   | 2.82                     | 0.54              |
| 3:C:357:TYR:H     | 4:D:185:ASP:HB2   | 1.73                     | 0.54              |
| 6:F:61:LEU:HD23   | 6:F:74:ILE:HG12   | 1.88                     | 0.54              |
| 9:I:138:ILE:HG21  | 9:I:231:ARG:HE    | 1.72                     | 0.54              |
| 10:J:55:CYS:N     | 10:J:56:PRO:CD    | 2.70                     | 0.54              |
| 11:K:349:TRP:CH2  | 11:K:361:TYR:HD2  | 2.26                     | 0.54              |
| 3:C:97:GLU:HG2    | 3:C:209:TRP:CD1   | 2.43                     | 0.53              |
| 5:E:23:PRO:O      | 8:H:298:CYS:SG    | 2.66                     | 0.53              |
| 7:G:158:VAL:CG1   | 7:G:162:PHE:CD2   | 2.90                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:I:211:ARG:NH2   | 9:I:248:ALA:O     | 2.41                     | 0.53              |
| 10:J:525:ASP:C    | 10:J:525:ASP:OD1  | 2.50                     | 0.53              |
| 11:K:291:HIS:CD2  | 11:K:328:LEU:HB2  | 2.43                     | 0.53              |
| 11:K:442:VAL:HG22 | 11:K:473:VAL:CG2  | 2.36                     | 0.53              |
| 10:J:568:VAL:O    | 10:J:625:SER:HA   | 2.08                     | 0.53              |
| 11:K:57:ILE:CD1   | 11:K:84:ILE:CD1   | 2.84                     | 0.53              |
| 11:K:356:LYS:N    | 11:K:357:PRO:CD   | 2.71                     | 0.53              |
| 2:B:12:LEU:CD1    | 10:J:149:HIS:CB   | 2.86                     | 0.53              |
| 3:C:299:ILE:N     | 3:C:345:SER:O     | 2.38                     | 0.53              |
| 3:C:378:LEU:CD2   | 4:D:186:PHE:HE1   | 2.22                     | 0.53              |
| 10:J:225:LEU:CD2  | 10:J:231:ILE:HD11 | 2.38                     | 0.53              |
| 8:H:142:ASN:OD1   | 8:H:187:ARG:HA    | 2.08                     | 0.53              |
| 10:J:769:MET:HG2  | 10:J:958:TYR:CZ   | 2.43                     | 0.53              |
| 10:J:778:ILE:HA   | 10:J:789:SER:HB2  | 1.89                     | 0.53              |
| 2:B:233:ARG:HD3   | 8:H:54:ILE:HG22   | 1.88                     | 0.53              |
| 10:J:425:ILE:HD12 | 10:J:425:ILE:N    | 2.22                     | 0.53              |
| 2:B:149:ASP:OD1   | 8:H:101:LYS:HD3   | 2.08                     | 0.53              |
| 3:C:162:SER:HB2   | 3:C:358:LYS:HD2   | 1.90                     | 0.53              |
| 7:G:76:ILE:CD1    | 7:G:84:TYR:CB     | 2.84                     | 0.53              |
| 7:G:214:CYS:CA    | 7:G:223:PHE:CE1   | 2.84                     | 0.53              |
| 10:J:398:ARG:CD   | 10:J:400:TRP:CE3  | 2.91                     | 0.53              |
| 10:J:451:ILE:HG22 | 10:J:467:PHE:HA   | 1.91                     | 0.53              |
| 10:J:628:TRP:CZ2  | 10:J:733:LEU:HD23 | 2.42                     | 0.53              |
| 11:K:332:LEU:HD21 | 11:K:368:PHE:CD2  | 2.42                     | 0.53              |
| 11:K:522:ILE:N    | 11:K:523:PRO:CD   | 2.72                     | 0.53              |
| 2:B:192:LYS:O     | 2:B:192:LYS:HG2   | 2.09                     | 0.53              |
| 6:F:150:ASN:HB3   | 6:F:151:PRO:HD2   | 1.91                     | 0.53              |
| 7:G:80:PHE:HZ     | 7:G:85:LYS:CE     | 2.17                     | 0.53              |
| 12:L:73:MET:C     | 12:L:75:PRO:HD2   | 2.34                     | 0.53              |
| 2:B:107:MET:CE    | 2:B:198:LEU:HB2   | 2.38                     | 0.53              |
| 6:F:126:ASN:HD21  | 9:I:42:LYS:NZ     | 2.07                     | 0.53              |
| 10:J:48:LEU:CD1   | 10:J:146:ILE:CD1  | 2.73                     | 0.53              |
| 10:J:127:PRO:CD   | 10:J:344:ASN:OD1  | 2.56                     | 0.53              |
| 10:J:135:LEU:HD13 | 10:J:145:PHE:CE1  | 2.44                     | 0.53              |
| 10:J:628:TRP:CE2  | 10:J:733:LEU:HD23 | 2.43                     | 0.53              |
| 1:A:253:GLY:O     | 2:B:110:LYS:CB    | 2.57                     | 0.53              |
| 2:B:12:LEU:CD1    | 10:J:152:PHE:CD2  | 2.85                     | 0.53              |
| 4:D:34:ILE:HB     | 7:G:91:PHE:O      | 2.09                     | 0.53              |
| 4:D:205:LEU:O     | 4:D:209:ILE:HG13  | 2.10                     | 0.53              |
| 10:J:135:LEU:O    | 10:J:145:PHE:HD2  | 1.92                     | 0.53              |
| 11:K:381:ILE:CG1  | 11:K:386:LEU:HD23 | 2.39                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:162:SER:CA    | 3:C:358:LYS:HD2   | 2.39                     | 0.52              |
| 3:C:162:SER:CB    | 3:C:358:LYS:HD2   | 2.38                     | 0.52              |
| 10:J:873:ASP:O    | 10:J:877:MET:HG2  | 2.09                     | 0.52              |
| 11:K:352:ARG:HA   | 11:K:353:PRO:C    | 2.34                     | 0.52              |
| 1:A:153:ILE:HG23  | 1:A:279:ILE:HD11  | 1.90                     | 0.52              |
| 2:B:111:ASN:CB    | 2:B:158:ILE:HD11  | 2.38                     | 0.52              |
| 9:I:17:ILE:HD11   | 9:I:58:ALA:HB2    | 1.91                     | 0.52              |
| 10:J:72:LEU:HD21  | 10:J:146:ILE:HG21 | 1.91                     | 0.52              |
| 10:J:600:ARG:NH2  | 10:J:606:MET:HE3  | 2.23                     | 0.52              |
| 11:K:52:MET:HE3   | 12:L:25:ILE:CB    | 2.39                     | 0.52              |
| 1:A:225:LEU:HD23  | 4:D:12:HIS:CD2    | 2.45                     | 0.52              |
| 6:F:126:ASN:ND2   | 9:I:42:LYS:NZ     | 2.57                     | 0.52              |
| 7:G:79:THR:OG1    | 7:G:99:TYR:OH     | 2.24                     | 0.52              |
| 10:J:991:THR:HG22 | 10:J:993:LYS:H    | 1.74                     | 0.52              |
| 11:K:45:LYS:HZ2   | 12:L:15:SER:HB3   | 1.73                     | 0.52              |
| 11:K:544:ASP:O    | 11:K:548:ARG:HG3  | 2.09                     | 0.52              |
| 12:L:62:PHE:HA    | 12:L:76:ILE:HG12  | 1.90                     | 0.52              |
| 2:B:129:LEU:HG    | 5:E:41:LEU:HD21   | 1.91                     | 0.52              |
| 3:C:293:PHE:CG    | 3:C:388:LEU:CD1   | 2.93                     | 0.52              |
| 5:E:227:ARG:HD2   | 6:F:214:TRP:CE3   | 2.45                     | 0.52              |
| 8:H:93:ARG:CD     | 11:K:197:LEU:CD1  | 2.83                     | 0.52              |
| 10:J:345:PRO:CG   | 10:J:423:PHE:CD1  | 2.91                     | 0.52              |
| 10:J:689:LEU:O    | 10:J:784:LYS:HE2  | 2.10                     | 0.52              |
| 10:J:751:MET:HE2  | 10:J:853:VAL:HG11 | 1.91                     | 0.52              |
| 10:J:902:TYR:HA   | 10:J:905:GLN:HE21 | 1.74                     | 0.52              |
| 6:F:246:MET:HE1   | 9:I:10:ILE:HD13   | 1.89                     | 0.52              |
| 7:G:4:PHE:CE1     | 7:G:40:GLY:CA     | 2.83                     | 0.52              |
| 7:G:28:ASP:OD2    | 7:G:35:ARG:NH1    | 2.43                     | 0.52              |
| 11:K:360:ALA:HA   | 11:K:363:ARG:HB3  | 1.91                     | 0.52              |
| 1:A:198:PHE:CE2   | 1:A:221:ILE:CG1   | 2.93                     | 0.52              |
| 3:C:10:ILE:CD1    | 3:C:12:ILE:HD12   | 2.40                     | 0.52              |
| 10:J:225:LEU:HD23 | 10:J:231:ILE:CD1  | 2.40                     | 0.52              |
| 1:A:15:ILE:HG12   | 1:A:25:LEU:HD11   | 1.92                     | 0.52              |
| 7:G:122:ARG:HG3   | 7:G:122:ARG:O     | 2.09                     | 0.52              |
| 8:H:322:ALA:HB2   | 8:H:348:ILE:HD11  | 1.91                     | 0.52              |
| 10:J:762:ASN:ND2  | 10:J:812:CYS:O    | 2.41                     | 0.52              |
| 1:A:89:SER:C      | 7:G:91:PHE:CZ     | 2.88                     | 0.52              |
| 5:E:264:ASN:HB2   | 8:H:9:LYS:HE3     | 1.91                     | 0.52              |
| 10:J:299:VAL:HG23 | 10:J:388:PRO:O    | 2.10                     | 0.52              |
| 10:J:800:TYR:CB   | 10:J:917:TYR:OH   | 2.54                     | 0.52              |
| 12:L:73:MET:HE3   | 12:L:76:ILE:HG21  | 1.90                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:E:22:ARG:HB2    | 5:E:26:ARG:N      | 2.24                     | 0.52              |
| 5:E:66:VAL:HG22   | 10:J:32:ALA:HB3   | 1.92                     | 0.52              |
| 8:H:157:LEU:HD12  | 8:H:157:LEU:C     | 2.35                     | 0.52              |
| 9:I:234:VAL:HG22  | 9:I:245:LEU:HD23  | 1.85                     | 0.52              |
| 10:J:368:LYS:O    | 10:J:372:LEU:N    | 2.37                     | 0.52              |
| 3:C:239:GLN:CB    | 3:C:392:PHE:CE1   | 2.93                     | 0.51              |
| 8:H:123:ARG:CA    | 8:H:159:MET:HE1   | 2.40                     | 0.51              |
| 10:J:77:LEU:HD22  | 10:J:109:PHE:HE2  | 1.75                     | 0.51              |
| 10:J:165:THR:HG22 | 10:J:167:ASN:H    | 1.75                     | 0.51              |
| 10:J:566:VAL:CG1  | 10:J:677:LEU:HD21 | 2.38                     | 0.51              |
| 11:K:336:ALA:CB   | 11:K:368:PHE:CE1  | 2.90                     | 0.51              |
| 12:L:33:LEU:HD12  | 12:L:33:LEU:C     | 2.34                     | 0.51              |
| 1:A:294:ALA:HA    | 1:A:297:LEU:HD12  | 1.92                     | 0.51              |
| 2:B:6:ILE:HG21    | 2:B:166:TYR:CD1   | 2.45                     | 0.51              |
| 2:B:167:ASP:CG    | 2:B:168:THR:N     | 2.69                     | 0.51              |
| 10:J:889:ARG:NH1  | 13:R:-6:A:OP1     | 2.43                     | 0.51              |
| 11:K:348:ASP:OD1  | 11:K:350:ARG:HB2  | 2.11                     | 0.51              |
| 2:B:13:ARG:O      | 10:J:152:PHE:HZ   | 1.92                     | 0.51              |
| 2:B:170:PRO:HB3   | 2:B:213:VAL:HG22  | 1.93                     | 0.51              |
| 7:G:20:LYS:HB3    | 7:G:54:THR:HG22   | 1.91                     | 0.51              |
| 10:J:93:ASN:O     | 10:J:97:GLN:HG2   | 2.10                     | 0.51              |
| 11:K:168:LEU:N    | 11:K:168:LEU:CD1  | 2.73                     | 0.51              |
| 1:A:240:ASN:O     | 1:A:272:ILE:HD11  | 2.11                     | 0.51              |
| 2:B:29:ILE:HD11   | 2:B:145:LEU:HD22  | 1.93                     | 0.51              |
| 9:I:271:ASP:HB3   | 9:I:274:MET:HB3   | 1.93                     | 0.51              |
| 10:J:71:ILE:O     | 10:J:144:ARG:CD   | 2.52                     | 0.51              |
| 10:J:769:MET:HG2  | 10:J:958:TYR:CE2  | 2.44                     | 0.51              |
| 11:K:346:LEU:N    | 11:K:346:LEU:CD1  | 2.73                     | 0.51              |
| 13:R:-3:A:H2'     | 13:R:-2:A:C8      | 2.46                     | 0.51              |
| 8:H:174:GLN:CB    | 8:H:185:HIS:CD2   | 2.55                     | 0.51              |
| 11:K:144:GLU:CB   | 11:K:403:TYR:CE2  | 2.93                     | 0.51              |
| 7:G:122:ARG:CD    | 7:G:138:ASP:CG    | 2.80                     | 0.51              |
| 9:I:148:LEU:HD12  | 9:I:149:GLN:HB2   | 1.91                     | 0.51              |
| 10:J:345:PRO:HB3  | 10:J:435:ARG:CG   | 2.40                     | 0.51              |
| 10:J:516:LEU:HD22 | 10:J:528:LEU:HD11 | 1.93                     | 0.51              |
| 11:K:500:LEU:HD23 | 11:K:500:LEU:C    | 2.35                     | 0.51              |
| 2:B:1:MET:HE2     | 10:J:347:ILE:O    | 2.11                     | 0.51              |
| 2:B:129:LEU:HG    | 5:E:41:LEU:CD2    | 2.41                     | 0.51              |
| 3:C:350:LEU:HD11  | 3:C:359:GLN:NE2   | 2.24                     | 0.51              |
| 5:E:158:ILE:HG13  | 5:E:173:HIS:N     | 2.25                     | 0.51              |
| 10:J:344:ASN:HA   | 10:J:423:PHE:CE2  | 2.46                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:J:368:LYS:O    | 10:J:372:LEU:HB2  | 2.11                     | 0.51              |
| 10:J:910:ASN:O    | 10:J:911:GLU:CB   | 2.58                     | 0.51              |
| 11:K:386:LEU:O    | 11:K:386:LEU:HD12 | 2.11                     | 0.51              |
| 2:B:4:LEU:CD1     | 10:J:37:ARG:NH1   | 2.72                     | 0.51              |
| 10:J:225:LEU:HD22 | 10:J:231:ILE:CD1  | 2.41                     | 0.51              |
| 1:A:251:ALA:CB    | 2:B:106:ARG:CB    | 2.89                     | 0.51              |
| 2:B:59:PRO:HG3    | 2:B:121:VAL:HG23  | 1.93                     | 0.51              |
| 2:B:229:ASP:OD1   | 8:H:57:PRO:HG2    | 2.09                     | 0.51              |
| 9:I:203:GLY:HA2   | 9:I:243:TYR:H     | 1.76                     | 0.51              |
| 10:J:21:GLN:CG    | 10:J:36:VAL:HG11  | 2.41                     | 0.51              |
| 10:J:345:PRO:HD3  | 10:J:423:PHE:CG   | 2.45                     | 0.51              |
| 10:J:426:LEU:HD12 | 10:J:431:LEU:CD1  | 2.40                     | 0.51              |
| 2:B:5:GLU:O       | 2:B:14:LEU:CD1    | 2.57                     | 0.51              |
| 2:B:161:ILE:HG13  | 2:B:162:SER:N     | 2.26                     | 0.51              |
| 2:B:194:GLU:OE1   | 2:B:218:ILE:HD13  | 2.11                     | 0.51              |
| 6:F:63:GLU:OE1    | 11:K:572:LEU:HB2  | 2.11                     | 0.51              |
| 7:G:187:ALA:HB3   | 7:G:195:TRP:HB3   | 1.93                     | 0.51              |
| 8:H:125:LYS:HA    | 8:H:134:ALA:O     | 2.11                     | 0.51              |
| 10:J:287:GLU:HG3  | 10:J:300:LEU:CD1  | 2.35                     | 0.51              |
| 3:C:147:GLU:HG3   | 3:C:148:GLU:N     | 2.25                     | 0.50              |
| 4:D:22:GLN:HG3    | 4:D:107:ARG:NH2   | 2.26                     | 0.50              |
| 10:J:144:ARG:HG3  | 10:J:144:ARG:HH21 | 1.74                     | 0.50              |
| 10:J:773:ARG:O    | 10:J:773:ARG:HD3  | 2.11                     | 0.50              |
| 3:C:30:SER:O      | 3:C:34:HIS:ND1    | 2.38                     | 0.50              |
| 5:E:240:LYS:HD3   | 6:F:209:GLU:HG2   | 1.93                     | 0.50              |
| 7:G:59:TYR:C      | 7:G:161:ASN:HD21  | 2.10                     | 0.50              |
| 10:J:143:LYS:HD3  | 10:J:145:PHE:CE2  | 2.41                     | 0.50              |
| 10:J:759:PRO:HD3  | 10:J:814:MET:SD   | 2.50                     | 0.50              |
| 3:C:177:ARG:HD2   | 3:C:247:PHE:CE1   | 2.46                     | 0.50              |
| 9:I:33:PHE:CE1    | 9:I:104:LYS:HD2   | 2.33                     | 0.50              |
| 10:J:398:ARG:HG3  | 10:J:398:ARG:NH1  | 2.25                     | 0.50              |
| 10:J:404:VAL:HG22 | 10:J:450:VAL:HG22 | 1.92                     | 0.50              |
| 11:K:434:ILE:HG23 | 11:K:473:VAL:HG11 | 1.93                     | 0.50              |
| 11:K:454:ARG:O    | 12:L:38:LEU:HD13  | 2.11                     | 0.50              |
| 11:K:512:ILE:HG13 | 11:K:513:LYS:N    | 2.25                     | 0.50              |
| 1:A:142:ASP:OD2   | 4:D:11:ASP:N      | 2.41                     | 0.50              |
| 2:B:170:PRO:CB    | 2:B:213:VAL:HG22  | 2.41                     | 0.50              |
| 5:E:116:LEU:HG    | 5:E:117:THR:HG23  | 1.94                     | 0.50              |
| 7:G:29:PRO:HB3    | 9:I:260:ALA:CB    | 2.41                     | 0.50              |
| 10:J:111:VAL:O    | 10:J:146:ILE:CG2  | 2.49                     | 0.50              |
| 10:J:701:VAL:CG2  | 10:J:715:VAL:HG13 | 2.41                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:K:49:LEU:CD2   | 12:L:18:LEU:HD21  | 2.41                     | 0.50              |
| 11:K:81:PHE:CE1   | 12:L:61:MET:HG3   | 2.45                     | 0.50              |
| 1:A:204:GLN:O     | 1:A:204:GLN:HG2   | 2.11                     | 0.50              |
| 2:B:13:ARG:HD3    | 2:B:171:LEU:CD2   | 2.41                     | 0.50              |
| 9:I:149:GLN:O     | 9:I:150:ARG:HG3   | 2.12                     | 0.50              |
| 10:J:45:ILE:HG13  | 10:J:153:SER:HB2  | 1.92                     | 0.50              |
| 3:C:243:LEU:HD11  | 3:C:284:LEU:HD13  | 1.93                     | 0.50              |
| 7:G:112:THR:O     | 7:G:112:THR:CG2   | 2.54                     | 0.50              |
| 10:J:65:ASN:O     | 10:J:66:GLU:OE2   | 2.30                     | 0.50              |
| 10:J:311:PHE:HE1  | 10:J:456:TRP:CE3  | 2.30                     | 0.50              |
| 10:J:534:LEU:HG   | 10:J:644:SER:HB2  | 1.93                     | 0.50              |
| 1:A:89:SER:HB3    | 7:G:91:PHE:CE1    | 2.47                     | 0.50              |
| 4:D:34:ILE:HA     | 7:G:91:PHE:O      | 2.12                     | 0.50              |
| 7:G:76:ILE:HD12   | 7:G:84:TYR:CG     | 2.47                     | 0.50              |
| 10:J:570:ILE:HD12 | 10:J:843:THR:O    | 2.12                     | 0.50              |
| 10:J:754:ARG:NH1  | 10:J:817:GLN:OE1  | 2.43                     | 0.50              |
| 11:K:381:ILE:CG1  | 11:K:386:LEU:CD2  | 2.90                     | 0.50              |
| 1:A:74:GLU:OE1    | 10:J:439:ARG:NH1  | 2.41                     | 0.50              |
| 7:G:95:VAL:HG11   | 7:G:134:ILE:HG23  | 1.93                     | 0.50              |
| 7:G:127:GLU:HB2   | 7:G:130:LEU:HB3   | 1.93                     | 0.50              |
| 10:J:347:ILE:N    | 10:J:421:ASN:OD1  | 2.44                     | 0.50              |
| 10:J:402:GLN:NE2  | 10:J:468:VAL:HG11 | 2.26                     | 0.50              |
| 12:L:82:ARG:O     | 12:L:86:TYR:CD2   | 2.65                     | 0.50              |
| 1:A:38:ILE:CD1    | 1:A:279:ILE:HG12  | 2.42                     | 0.50              |
| 3:C:239:GLN:OE1   | 3:C:291:ILE:HD13  | 2.12                     | 0.50              |
| 3:C:369:ILE:HB    | 4:D:177:VAL:CG1   | 2.41                     | 0.50              |
| 1:A:115:SER:O     | 2:B:204:LYS:HE3   | 2.11                     | 0.49              |
| 3:C:297:TYR:CZ    | 3:C:380:LEU:HB3   | 2.46                     | 0.49              |
| 8:H:116:ILE:HD13  | 8:H:126:VAL:HG11  | 1.82                     | 0.49              |
| 10:J:24:PHE:HZ    | 10:J:35:ILE:HG22  | 1.76                     | 0.49              |
| 10:J:398:ARG:HG3  | 10:J:398:ARG:HH11 | 1.76                     | 0.49              |
| 11:K:331:LEU:HB3  | 11:K:372:ILE:CD1  | 2.42                     | 0.49              |
| 5:E:158:ILE:CD1   | 5:E:173:HIS:CA    | 2.90                     | 0.49              |
| 7:G:7:PRO:HD3     | 7:G:39:THR:CG2    | 2.42                     | 0.49              |
| 10:J:725:SER:O    | 10:J:729:GLU:HG2  | 2.12                     | 0.49              |
| 12:L:35:GLU:O     | 12:L:39:LEU:HG    | 2.12                     | 0.49              |
| 1:A:210:ILE:O     | 1:A:213:GLU:O     | 2.30                     | 0.49              |
| 5:E:197:MET:HE1   | 5:E:213:LEU:HD12  | 1.93                     | 0.49              |
| 11:K:441:LEU:HD11 | 11:K:505:ILE:HD13 | 1.95                     | 0.49              |
| 1:A:103:LEU:O     | 1:A:107:ILE:HG12  | 2.12                     | 0.49              |
| 1:A:160:MET:O     | 1:A:283:LEU:HD11  | 2.12                     | 0.49              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:A:250:LYS:HE3    | 2:B:196:LEU:O     | 2.13                     | 0.49              |
| 2:B:1:MET:CE       | 10:J:347:ILE:O    | 2.60                     | 0.49              |
| 5:E:22:ARG:HG3     | 5:E:26:ARG:CA     | 2.42                     | 0.49              |
| 10:J:45:ILE:HG21   | 10:J:148:PHE:CZ   | 2.47                     | 0.49              |
| 10:J:630:LEU:HD11  | 10:J:680:LEU:HD22 | 1.73                     | 0.49              |
| 11:K:143:SER:O     | 11:K:144:GLU:CG   | 2.46                     | 0.49              |
| 12:L:45:ALA:O      | 12:L:49:LEU:HD13  | 2.12                     | 0.49              |
| 4:D:85:ARG:HE      | 9:I:145:ARG:NE    | 2.05                     | 0.49              |
| 7:G:77:ILE:HG13    | 7:G:78:GLY:N      | 2.28                     | 0.49              |
| 8:H:68:MET:HG2     | 11:K:387:ALA:HB2  | 1.93                     | 0.49              |
| 9:I:60:LEU:HD21    | 9:I:112:PRO:HG3   | 1.93                     | 0.49              |
| 10:J:457:PRO:CG    | 10:J:460:HIS:CD2  | 2.74                     | 0.49              |
| 10:J:778:ILE:HA    | 10:J:789:SER:CB   | 2.43                     | 0.49              |
| 11:K:23:LEU:HD12   | 11:K:23:LEU:O     | 2.13                     | 0.49              |
| 1:A:286:ASP:O      | 1:A:290:ARG:HG2   | 2.13                     | 0.49              |
| 7:G:213:GLU:O      | 7:G:217:LYS:HG2   | 2.12                     | 0.49              |
| 8:H:116:ILE:HD11   | 8:H:169:LEU:HD21  | 1.94                     | 0.49              |
| 10:J:135:LEU:HB3   | 10:J:145:PHE:CG   | 2.44                     | 0.49              |
| 11:K:5:ASN:CB      | 11:K:6:PRO:HD3    | 2.10                     | 0.49              |
| 11:K:180:PRO:O     | 11:K:181:HIS:C    | 2.56                     | 0.49              |
| 11:K:298:ILE:HG21  | 11:K:416:TYR:CE2  | 2.47                     | 0.49              |
| 11:K:381:ILE:HG13  | 11:K:386:LEU:CD2  | 2.43                     | 0.49              |
| 2:B:229:ASP:HB3    | 8:H:56:THR:HB     | 1.95                     | 0.49              |
| 3:C:275:ILE:HG22   | 3:C:276:CYS:N     | 2.28                     | 0.49              |
| 4:D:140:LYS:HA     | 4:D:158:LEU:HG    | 1.93                     | 0.49              |
| 10:J:398:ARG:HD3   | 10:J:400:TRP:CE2  | 2.44                     | 0.49              |
| 10:J:701:VAL:CG2   | 10:J:702:LYS:N    | 2.76                     | 0.49              |
| 3:C:49:PHE:CD2     | 3:C:333:ASP:HB2   | 2.47                     | 0.49              |
| 7:G:157:ASP:C      | 7:G:158:VAL:HG23  | 2.38                     | 0.49              |
| 8:H:115:ARG:HB2    | 8:H:168:LEU:HD23  | 1.94                     | 0.49              |
| 10:J:112[A]:ILE:HA | 10:J:146:ILE:CG2  | 2.43                     | 0.49              |
| 10:J:112[B]:ILE:HA | 10:J:146:ILE:CG2  | 2.43                     | 0.49              |
| 10:J:728:GLU:HG3   | 13:R:-3:A:C4'     | 2.42                     | 0.49              |
| 10:J:800:TYR:CE2   | 10:J:917:TYR:CE2  | 3.01                     | 0.49              |
| 11:K:239:LEU:HD21  | 11:K:300:LEU:HD21 | 1.93                     | 0.49              |
| 11:K:424:PRO:HB3   | 11:K:446:TYR:OH   | 2.12                     | 0.49              |
| 13:N:-11:A:C2'     | 13:N:-10:A:OP2    | 2.60                     | 0.49              |
| 3:C:345:SER:HA     | 3:C:364:GLY:HA2   | 1.93                     | 0.49              |
| 7:G:101:ALA:O      | 7:G:136:CYS:HB2   | 2.13                     | 0.49              |
| 8:H:115:ARG:HB2    | 8:H:168:LEU:CD2   | 2.42                     | 0.49              |
| 10:J:480:GLU:HG3   | 10:J:901:TYR:CE1  | 2.48                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:J:618:TYR:N    | 10:J:648:SER:O    | 2.41                     | 0.49              |
| 10:J:920:LYS:HB2  | 10:J:927:VAL:HB   | 1.95                     | 0.49              |
| 3:C:277:ASP:OD1   | 3:C:277:ASP:O     | 2.30                     | 0.48              |
| 8:H:307:LEU:HD21  | 8:H:348:ILE:HD12  | 1.95                     | 0.48              |
| 10:J:397:ARG:HG2  | 10:J:398:ARG:N    | 2.25                     | 0.48              |
| 10:J:484:LEU:HD23 | 10:J:596:LEU:HD22 | 1.94                     | 0.48              |
| 10:J:539:ILE:HG12 | 10:J:569:HIS:CD2  | 2.48                     | 0.48              |
| 11:K:298:ILE:HG21 | 11:K:416:TYR:CD2  | 2.47                     | 0.48              |
| 7:G:11:PHE:CD1    | 7:G:12:PRO:HD2    | 2.48                     | 0.48              |
| 8:H:68:MET:HE3    | 11:K:387:ALA:HA   | 1.93                     | 0.48              |
| 10:J:708:GLU:HG3  | 10:J:711:ASP:OD2  | 2.13                     | 0.48              |
| 11:K:31:TYR:O     | 11:K:32:LYS:C     | 2.52                     | 0.48              |
| 12:L:63:ALA:O     | 12:L:67:VAL:HG23  | 2.12                     | 0.48              |
| 12:L:65:MET:SD    | 12:L:70:VAL:CB    | 2.98                     | 0.48              |
| 1:A:89:SER:OG     | 4:D:31:THR:HG21   | 2.13                     | 0.48              |
| 3:C:296:ASN:O     | 3:C:333:ASP:N     | 2.38                     | 0.48              |
| 10:J:158:VAL:O    | 10:J:169:ARG:NH1  | 2.47                     | 0.48              |
| 10:J:400:TRP:CE2  | 10:J:453:ILE:HG21 | 2.47                     | 0.48              |
| 10:J:742:ILE:HG22 | 10:J:858:LEU:HD23 | 1.88                     | 0.48              |
| 11:K:294:PHE:CZ   | 11:K:295:MET:HG3  | 2.49                     | 0.48              |
| 13:R:-2:A:H2'     | 13:R:-1:A:H5''    | 1.94                     | 0.48              |
| 13:N:-11:A:H8     | 13:N:-11:A:O5'    | 1.97                     | 0.48              |
| 1:A:109:GLU:CG    | 2:B:95:ARG:HH12   | 2.25                     | 0.48              |
| 6:F:95:ILE:HG12   | 6:F:137:ILE:HB    | 1.95                     | 0.48              |
| 10:J:316:VAL:HG13 | 10:J:392:VAL:HG13 | 1.94                     | 0.48              |
| 10:J:990:ILE:HD12 | 10:J:990:ILE:N    | 2.29                     | 0.48              |
| 11:K:147:PRO:O    | 11:K:179:TYR:CE2  | 2.66                     | 0.48              |
| 11:K:208:TRP:CE3  | 11:K:209:ASP:HB2  | 2.48                     | 0.48              |
| 11:K:331:LEU:CD1  | 11:K:372:ILE:HG21 | 2.33                     | 0.48              |
| 11:K:455:ARG:HH21 | 12:L:37:LEU:HD13  | 1.79                     | 0.48              |
| 12:L:73:MET:CE    | 12:L:76:ILE:HG21  | 2.44                     | 0.48              |
| 12:L:76:ILE:HG23  | 12:L:77:LEU:N     | 2.28                     | 0.48              |
| 2:B:13:ARG:HD3    | 2:B:171:LEU:CD1   | 2.39                     | 0.48              |
| 2:B:164:GLY:O     | 2:B:170:PRO:C     | 2.54                     | 0.48              |
| 3:C:378:LEU:CD2   | 4:D:186:PHE:CE1   | 2.96                     | 0.48              |
| 4:D:85:ARG:NH1    | 9:I:144:THR:C     | 2.71                     | 0.48              |
| 7:G:221:ALA:O     | 7:G:225:ASP:OD2   | 2.32                     | 0.48              |
| 11:K:410:THR:HG22 | 11:K:412:SER:N    | 2.29                     | 0.48              |
| 1:A:23:TYR:CE1    | 7:G:237:VAL:CG1   | 2.91                     | 0.48              |
| 1:A:126:VAL:CG1   | 1:A:129:SER:HB2   | 2.36                     | 0.48              |
| 3:C:147:GLU:HG3   | 3:C:148:GLU:HG3   | 1.96                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:221:SER:HA    | 6:F:55:ASN:HB2    | 1.95                     | 0.48              |
| 3:C:299:ILE:O     | 3:C:343:ILE:HG23  | 2.13                     | 0.48              |
| 9:I:141:THR:HG22  | 9:I:155:ILE:HA    | 1.95                     | 0.48              |
| 10:J:760:SER:HA   | 10:J:780:LEU:CD1  | 2.43                     | 0.48              |
| 3:C:45:LYS:HB2    | 3:C:48:GLU:HG3    | 1.95                     | 0.48              |
| 3:C:162:SER:HA    | 3:C:358:LYS:HD2   | 1.94                     | 0.48              |
| 3:C:239:GLN:CB    | 3:C:392:PHE:HE1   | 2.27                     | 0.48              |
| 11:K:200:ARG:HH22 | 11:K:203:ILE:HD11 | 1.79                     | 0.48              |
| 11:K:355:SER:HB3  | 11:K:357:PRO:HD2  | 1.96                     | 0.48              |
| 3:C:302:LEU:HD12  | 3:C:302:LEU:C     | 2.35                     | 0.48              |
| 5:E:22:ARG:HB2    | 5:E:25:GLY:H      | 1.78                     | 0.48              |
| 8:H:310:CYS:HB2   | 8:H:312:ILE:HG12  | 1.96                     | 0.48              |
| 9:I:244:TYR:O     | 9:I:245:LEU:HD23  | 2.13                     | 0.48              |
| 10:J:426:LEU:HD12 | 10:J:431:LEU:HD12 | 1.96                     | 0.48              |
| 1:A:12:SER:O      | 1:A:16:LEU:HG     | 2.14                     | 0.48              |
| 5:E:11:LEU:HD22   | 5:E:23:PRO:HG3    | 1.96                     | 0.48              |
| 6:F:188:VAL:HG13  | 9:I:44:ILE:HD13   | 1.96                     | 0.48              |
| 8:H:124:TRP:HE3   | 8:H:136:LEU:HD23  | 1.79                     | 0.48              |
| 10:J:841:HIS:HB3  | 10:J:851:ASP:OD1  | 2.13                     | 0.48              |
| 2:B:13:ARG:NH1    | 2:B:171:LEU:CB    | 2.73                     | 0.48              |
| 5:E:158:ILE:HG13  | 5:E:173:HIS:H     | 1.78                     | 0.48              |
| 3:C:58:THR:HB     | 11:K:571:LEU:HD13 | 1.96                     | 0.47              |
| 3:C:363:MET:HE1   | 4:D:69:LYS:HA     | 1.96                     | 0.47              |
| 4:D:69:LYS:NZ     | 4:D:181:ASP:OD2   | 2.42                     | 0.47              |
| 9:I:38:GLY:H      | 9:I:41:THR:HG1    | 1.60                     | 0.47              |
| 11:K:35:ASP:OD1   | 11:K:36:ARG:N     | 2.46                     | 0.47              |
| 11:K:281:PHE:HB3  | 11:K:307:TYR:O    | 2.13                     | 0.47              |
| 11:K:436:PRO:HA   | 11:K:439:GLU:HB2  | 1.94                     | 0.47              |
| 12:L:78:GLY:O     | 12:L:82:ARG:HG3   | 2.14                     | 0.47              |
| 3:C:369:ILE:HB    | 4:D:177:VAL:HG12  | 1.96                     | 0.47              |
| 6:F:69:HIS:ND1    | 6:F:145:LYS:O     | 2.43                     | 0.47              |
| 7:G:6:PHE:O       | 7:G:9:ASP:OD2     | 2.31                     | 0.47              |
| 8:H:172:GLU:OE1   | 8:H:185:HIS:CE1   | 2.67                     | 0.47              |
| 10:J:20:THR:HG23  | 10:J:39:HIS:HB3   | 1.96                     | 0.47              |
| 10:J:347:ILE:HD11 | 10:J:464:LEU:CD1  | 2.44                     | 0.47              |
| 10:J:869:LEU:C    | 10:J:869:LEU:HD12 | 2.39                     | 0.47              |
| 10:J:903:VAL:HG13 | 10:J:907:MET:HE3  | 1.95                     | 0.47              |
| 11:K:294:PHE:CZ   | 11:K:295:MET:HE2  | 2.49                     | 0.47              |
| 11:K:348:ASP:OD2  | 11:K:350:ARG:NE   | 2.36                     | 0.47              |
| 11:K:352:ARG:HB3  | 11:K:353:PRO:HA   | 1.96                     | 0.47              |
| 1:A:13:LYS:O      | 1:A:17:GLU:HG3    | 2.15                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:216:SER:OG    | 1:A:217:GLU:N     | 2.45                     | 0.47              |
| 3:C:40:ARG:NH2    | 3:C:339:GLU:OE1   | 2.43                     | 0.47              |
| 3:C:239:GLN:CD    | 3:C:291:ILE:HD13  | 2.39                     | 0.47              |
| 4:D:14:ASP:OD2    | 7:G:63:ARG:NH2    | 2.47                     | 0.47              |
| 5:E:66:VAL:HG21   | 10:J:32:ALA:CB    | 2.42                     | 0.47              |
| 11:K:520:THR:N    | 11:K:521:PRO:CD   | 2.77                     | 0.47              |
| 1:A:169:VAL:C     | 1:A:170:HIS:ND1   | 2.72                     | 0.47              |
| 1:A:191:HIS:CE1   | 1:A:193:PRO:HG3   | 2.50                     | 0.47              |
| 2:B:69:LYS:HB2    | 2:B:114:LEU:O     | 2.14                     | 0.47              |
| 5:E:258:VAL:HA    | 8:H:5:ILE:HG22    | 1.96                     | 0.47              |
| 10:J:345:PRO:HD3  | 10:J:423:PHE:CD1  | 2.49                     | 0.47              |
| 10:J:553:ALA:O    | 10:J:554:LEU:HD12 | 2.15                     | 0.47              |
| 10:J:901:TYR:O    | 10:J:905:GLN:CG   | 2.60                     | 0.47              |
| 1:A:225:LEU:HD22  | 4:D:12:HIS:CD2    | 2.48                     | 0.47              |
| 3:C:357:TYR:O     | 4:D:184:GLY:C     | 2.54                     | 0.47              |
| 4:D:22:GLN:HG3    | 4:D:107:ARG:HH22  | 1.80                     | 0.47              |
| 10:J:48:LEU:HD12  | 10:J:146:ILE:HD11 | 1.86                     | 0.47              |
| 10:J:135:LEU:HD22 | 10:J:145:PHE:CZ   | 2.50                     | 0.47              |
| 11:K:9:LEU:O      | 11:K:13:VAL:HG23  | 2.15                     | 0.47              |
| 11:K:49:LEU:HD21  | 12:L:18:LEU:HD21  | 1.96                     | 0.47              |
| 3:C:239:GLN:OE1   | 3:C:291:ILE:CD1   | 2.63                     | 0.47              |
| 8:H:126:VAL:HG21  | 8:H:184:LEU:CD1   | 2.41                     | 0.47              |
| 10:J:235:ILE:CG2  | 10:J:236:PRO:HD2  | 2.42                     | 0.47              |
| 10:J:574:THR:HG22 | 10:J:852:VAL:HG13 | 1.96                     | 0.47              |
| 11:K:60:ILE:HG13  | 11:K:84:ILE:CG2   | 2.38                     | 0.47              |
| 11:K:147:PRO:O    | 11:K:148:PHE:C    | 2.56                     | 0.47              |
| 11:K:349:TRP:CZ2  | 11:K:361:TYR:CE2  | 2.97                     | 0.47              |
| 1:A:225:LEU:CD2   | 4:D:12:HIS:NE2    | 2.78                     | 0.47              |
| 5:E:175:TYR:HE1   | 10:J:166:ILE:HD13 | 1.80                     | 0.47              |
| 7:G:97:LEU:HD13   | 7:G:134:ILE:HG13  | 1.97                     | 0.47              |
| 9:I:46:TYR:O      | 9:I:53:LEU:HB3    | 2.14                     | 0.47              |
| 10:J:309:ARG:HG2  | 10:J:456:TRP:CG   | 2.50                     | 0.47              |
| 10:J:409:PRO:HA   | 10:J:445:LEU:HD11 | 1.96                     | 0.47              |
| 10:J:641:PHE:C    | 10:J:642:MET:HG3  | 2.40                     | 0.47              |
| 3:C:40:ARG:NE     | 3:C:339:GLU:OE2   | 2.32                     | 0.47              |
| 3:C:172:VAL:HB    | 3:C:209:TRP:HB2   | 1.97                     | 0.47              |
| 7:G:82:ASP:C      | 7:G:99:TYR:CD2    | 2.92                     | 0.47              |
| 8:H:104:TYR:OH    | 8:H:227:VAL:HG12  | 2.15                     | 0.47              |
| 10:J:573:VAL:CG2  | 10:J:846:ILE:HG12 | 2.45                     | 0.47              |
| 10:J:664:LYS:HG2  | 10:J:664:LYS:O    | 2.15                     | 0.47              |
| 11:K:206:LYS:HE2  | 11:K:259:ARG:O    | 2.14                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:K:424:PRO:CB   | 11:K:446:TYR:OH   | 2.63                     | 0.47              |
| 12:L:42:ASP:O     | 12:L:46:LYS:HG3   | 2.14                     | 0.47              |
| 1:A:36:VAL:HG22   | 1:A:51:MET:HE2    | 1.96                     | 0.47              |
| 1:A:196:VAL:HG12  | 1:A:198:PHE:CE1   | 2.49                     | 0.47              |
| 1:A:240:ASN:HA    | 1:A:272:ILE:HD13  | 1.96                     | 0.47              |
| 2:B:9:PRO:HD2     | 10:J:133:ARG:HH22 | 1.76                     | 0.47              |
| 3:C:232:ASN:HD22  | 3:C:232:ASN:N     | 2.12                     | 0.47              |
| 4:D:85:ARG:HH12   | 9:I:144:THR:C     | 2.22                     | 0.47              |
| 12:L:57:LEU:O     | 12:L:61:MET:HG2   | 2.14                     | 0.47              |
| 12:L:111:ALA:O    | 12:L:115:ILE:HG12 | 2.15                     | 0.47              |
| 3:C:278:GLN:NE2   | 6:F:20:PHE:O      | 2.40                     | 0.46              |
| 3:C:362:LEU:O     | 3:C:363:MET:HG3   | 2.16                     | 0.46              |
| 9:I:222:GLU:HB3   | 9:I:285:LYS:HD3   | 1.97                     | 0.46              |
| 10:J:706:ASP:CG   | 10:J:707:SER:N    | 2.72                     | 0.46              |
| 10:J:738:VAL:HG13 | 10:J:858:LEU:CG   | 2.45                     | 0.46              |
| 2:B:71:LEU:HB2    | 2:B:121:VAL:HG22  | 1.97                     | 0.46              |
| 3:C:11:GLU:C      | 3:C:12:ILE:HG13   | 2.40                     | 0.46              |
| 7:G:119:VAL:HA    | 7:G:149:ILE:HA    | 1.97                     | 0.46              |
| 10:J:12:ARG:NH2   | 10:J:16:GLY:O     | 2.48                     | 0.46              |
| 11:K:215:TRP:CZ3  | 11:K:354:LEU:HD12 | 2.50                     | 0.46              |
| 11:K:434:ILE:HG21 | 11:K:473:VAL:HG11 | 1.96                     | 0.46              |
| 2:B:18:ARG:HG3    | 10:J:42:ARG:CZ    | 2.46                     | 0.46              |
| 3:C:12:ILE:CG2    | 3:C:13:HIS:N      | 2.77                     | 0.46              |
| 8:H:217:LEU:HD11  | 8:H:223:VAL:HG12  | 1.96                     | 0.46              |
| 10:J:626:VAL:O    | 10:J:626:VAL:HG13 | 2.16                     | 0.46              |
| 10:J:771:ASN:O    | 10:J:775:ASN:HA   | 2.16                     | 0.46              |
| 11:K:332:LEU:CD2  | 11:K:368:PHE:CG   | 2.98                     | 0.46              |
| 11:K:539:VAL:HB   | 11:K:540:PRO:HD3  | 1.97                     | 0.46              |
| 11:K:569:SER:HB2  | 11:K:574:LYS:HG3  | 1.96                     | 0.46              |
| 1:A:92:GLU:HB2    | 1:A:95:ASN:HB2    | 1.95                     | 0.46              |
| 1:A:257:ASP:OD1   | 1:A:258:ALA:N     | 2.47                     | 0.46              |
| 3:C:299:ILE:C     | 3:C:300:VAL:CG1   | 2.89                     | 0.46              |
| 4:D:36:PRO:HG2    | 4:D:41:GLU:HG2    | 1.96                     | 0.46              |
| 6:F:124:VAL:HG21  | 6:F:191:ALA:HB2   | 1.97                     | 0.46              |
| 10:J:365:ILE:CG2  | 10:J:366:SER:N    | 2.79                     | 0.46              |
| 11:K:27:ASP:OD1   | 11:K:27:ASP:O     | 2.33                     | 0.46              |
| 4:D:145:ILE:O     | 4:D:145:ILE:CD1   | 2.59                     | 0.46              |
| 8:H:66:ILE:HD12   | 8:H:93:ARG:NH2    | 2.16                     | 0.46              |
| 10:J:140:ASP:C    | 10:J:142:HIS:H    | 2.23                     | 0.46              |
| 2:B:112:VAL:HB    | 2:B:114:LEU:HG    | 1.97                     | 0.46              |
| 2:B:164:GLY:HA3   | 2:B:174:THR:HG21  | 1.98                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:210:LEU:HG    | 2:B:214:LEU:HD13  | 1.98                     | 0.46              |
| 3:C:43:LEU:HD13   | 11:K:603:ALA:CB   | 2.43                     | 0.46              |
| 5:E:215:ILE:HD13  | 5:E:248:LEU:HD23  | 1.98                     | 0.46              |
| 5:E:236:VAL:HG12  | 6:F:123:SER:OG    | 2.16                     | 0.46              |
| 5:E:256:PRO:O     | 5:E:259:VAL:CG1   | 2.63                     | 0.46              |
| 9:I:159:GLU:OE1   | 9:I:231:ARG:NH2   | 2.49                     | 0.46              |
| 9:I:279:VAL:HG23  | 9:I:280:THR:H     | 1.81                     | 0.46              |
| 10:J:987:MET:HE3  | 10:J:994:ARG:HD3  | 1.98                     | 0.46              |
| 11:K:609:ALA:CB   | 11:K:613:LEU:HD12 | 2.46                     | 0.46              |
| 1:A:214:THR:HG23  | 1:A:215:ASN:H     | 1.81                     | 0.46              |
| 5:E:24:ASP:OD1    | 5:E:24:ASP:N      | 2.46                     | 0.46              |
| 10:J:255:PHE:HB3  | 10:J:308:ASN:OD1  | 2.16                     | 0.46              |
| 10:J:382:ARG:HG2  | 10:J:382:ARG:O    | 2.15                     | 0.46              |
| 10:J:401:ARG:HG3  | 10:J:402:GLN:O    | 2.15                     | 0.46              |
| 10:J:435:ARG:HD3  | 10:J:462:TYR:HB2  | 1.97                     | 0.46              |
| 2:B:129:LEU:HD11  | 5:E:41:LEU:CD1    | 2.35                     | 0.46              |
| 5:E:40:PHE:HB3    | 8:H:13:ALA:C      | 2.41                     | 0.46              |
| 5:E:163:ASP:HA    | 5:E:167:GLU:HA    | 1.97                     | 0.46              |
| 8:H:196:ASN:OD1   | 8:H:286:ASP:N     | 2.39                     | 0.46              |
| 10:J:276:GLY:HA3  | 10:J:290:VAL:HG13 | 1.98                     | 0.46              |
| 10:J:327:LYS:C    | 10:J:387:GLN:H    | 2.22                     | 0.46              |
| 10:J:568:VAL:HG23 | 10:J:628:TRP:HZ3  | 1.80                     | 0.46              |
| 10:J:916:GLY:O    | 10:J:979:VAL:HG22 | 2.15                     | 0.46              |
| 11:K:136:PHE:CZ   | 11:K:268:LEU:O    | 2.69                     | 0.46              |
| 2:B:14:LEU:CD1    | 2:B:177:LEU:CD2   | 2.90                     | 0.46              |
| 2:B:166:TYR:O     | 2:B:167:ASP:C     | 2.58                     | 0.46              |
| 6:F:245:LEU:O     | 6:F:249:GLU:CB    | 2.64                     | 0.46              |
| 8:H:116:ILE:HA    | 8:H:126:VAL:HG12  | 1.98                     | 0.46              |
| 10:J:302:VAL:HG12 | 10:J:389:THR:HG21 | 1.98                     | 0.46              |
| 10:J:318:VAL:HB   | 10:J:390:ALA:HB1  | 1.97                     | 0.46              |
| 10:J:539:ILE:HD12 | 10:J:555:HIS:HB3  | 1.96                     | 0.46              |
| 10:J:628:TRP:CE2  | 10:J:733:LEU:CD2  | 2.99                     | 0.46              |
| 10:J:641:PHE:O    | 10:J:642:MET:CG   | 2.63                     | 0.46              |
| 10:J:728:GLU:O    | 10:J:732:LEU:HG   | 2.15                     | 0.46              |
| 1:A:252:GLY:CA    | 2:B:107:MET:CA    | 2.85                     | 0.46              |
| 5:E:69:HIS:NE2    | 5:E:118:LYS:O     | 2.48                     | 0.46              |
| 8:H:104:TYR:OH    | 8:H:227:VAL:CG1   | 2.64                     | 0.46              |
| 9:I:10:ILE:HG13   | 9:I:62:GLY:C      | 2.41                     | 0.46              |
| 10:J:77:LEU:HD22  | 10:J:109:PHE:CE2  | 2.51                     | 0.46              |
| 10:J:701:VAL:HG21 | 10:J:715:VAL:HG12 | 1.95                     | 0.46              |
| 11:K:144:GLU:O    | 11:K:144:GLU:HG3  | 2.15                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:144:CYS:SG    | 6:F:8:ARG:NE      | 2.89                     | 0.45              |
| 3:C:344:HIS:HB2   | 3:C:366:GLY:N     | 2.31                     | 0.45              |
| 4:D:143:SER:HB3   | 4:D:190:GLN:HE22  | 1.81                     | 0.45              |
| 7:G:4:PHE:HE1     | 7:G:40:GLY:HA2    | 1.71                     | 0.45              |
| 10:J:774:LYS:HB3  | 10:J:776:MET:CE   | 2.45                     | 0.45              |
| 11:K:525:SER:O    | 11:K:528:LYS:HB2  | 2.16                     | 0.45              |
| 1:A:118:LEU:HD12  | 1:A:188:GLY:O     | 2.16                     | 0.45              |
| 1:A:240:ASN:O     | 1:A:272:ILE:CD1   | 2.64                     | 0.45              |
| 3:C:362:LEU:CB    | 4:D:180:LEU:HB3   | 2.44                     | 0.45              |
| 4:D:34:ILE:CA     | 7:G:91:PHE:O      | 2.64                     | 0.45              |
| 5:E:23:PRO:HB3    | 8:H:198:MET:SD    | 2.56                     | 0.45              |
| 9:I:158:VAL:HG13  | 9:I:189:SER:HB2   | 1.98                     | 0.45              |
| 10:J:539:ILE:CD1  | 10:J:555:HIS:HB3  | 2.47                     | 0.45              |
| 11:K:155:LYS:NZ   | 11:K:182:PRO:O    | 2.36                     | 0.45              |
| 11:K:196:ILE:O    | 11:K:377:ARG:CG   | 2.63                     | 0.45              |
| 1:A:239:LEU:HB2   | 1:A:272:ILE:HG12  | 1.98                     | 0.45              |
| 1:A:253:GLY:HA2   | 2:B:110:LYS:CG    | 2.46                     | 0.45              |
| 3:C:363:MET:HG2   | 4:D:179:LEU:CD1   | 2.46                     | 0.45              |
| 10:J:534:LEU:HB2  | 10:J:646:ILE:HG22 | 1.99                     | 0.45              |
| 11:K:207:SER:O    | 11:K:210:ASP:CB   | 2.64                     | 0.45              |
| 11:K:208:TRP:O    | 11:K:209:ASP:CB   | 2.64                     | 0.45              |
| 1:A:253:GLY:H     | 2:B:110:LYS:HG2   | 1.81                     | 0.45              |
| 2:B:163:VAL:O     | 2:B:184:THR:HA    | 2.16                     | 0.45              |
| 7:G:82:ASP:C      | 7:G:99:TYR:CE2    | 2.95                     | 0.45              |
| 7:G:102:PHE:CE2   | 7:G:136:CYS:SG    | 2.96                     | 0.45              |
| 10:J:49:SER:HA    | 10:J:72:LEU:HB2   | 1.97                     | 0.45              |
| 10:J:432:PRO:HG3  | 10:J:456:TRP:CH2  | 2.51                     | 0.45              |
| 10:J:488:HIS:CE1  | 10:J:894:ALA:HA   | 2.51                     | 0.45              |
| 10:J:538:LEU:HD13 | 10:J:670:LEU:CG   | 2.45                     | 0.45              |
| 11:K:355:SER:O    | 11:K:358:MET:HB2  | 2.16                     | 0.45              |
| 1:A:34:ARG:NE     | 1:A:222:ASP:OD2   | 2.33                     | 0.45              |
| 10:J:634:ALA:HB2  | 10:J:680:LEU:CG   | 2.38                     | 0.45              |
| 10:J:825:SER:OG   | 10:J:827:PRO:HD2  | 2.16                     | 0.45              |
| 10:J:844:SER:C    | 10:J:851:ASP:OD2  | 2.59                     | 0.45              |
| 10:J:919:ILE:C    | 10:J:920:LYS:HG3  | 2.41                     | 0.45              |
| 11:K:143:SER:C    | 11:K:144:GLU:HG2  | 2.38                     | 0.45              |
| 11:K:346:LEU:CD1  | 11:K:346:LEU:H    | 2.29                     | 0.45              |
| 11:K:355:SER:HB2  | 11:K:358:MET:CG   | 2.46                     | 0.45              |
| 11:K:538:SER:C    | 11:K:540:PRO:HD2  | 2.42                     | 0.45              |
| 1:A:10:SER:HB3    | 7:G:152:ASP:O     | 2.17                     | 0.45              |
| 3:C:239:GLN:NE2   | 3:C:291:ILE:HD13  | 2.31                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:E:119:LYS:HE2   | 5:E:120:TYR:CZ    | 2.52                     | 0.45              |
| 8:H:115:ARG:O     | 8:H:127:ASP:N     | 2.49                     | 0.45              |
| 9:I:205:ILE:HG23  | 9:I:245:LEU:O     | 2.16                     | 0.45              |
| 10:J:255:PHE:O    | 10:J:458:THR:OG1  | 2.33                     | 0.45              |
| 10:J:328:ALA:N    | 10:J:386:ILE:HA   | 2.31                     | 0.45              |
| 10:J:731:MET:CG   | 13:R:-2:A:OP1     | 2.64                     | 0.45              |
| 6:F:241:MET:O     | 6:F:245:LEU:HG    | 2.16                     | 0.45              |
| 7:G:76:ILE:HG21   | 7:G:84:TYR:CD1    | 2.52                     | 0.45              |
| 9:I:150:ARG:HG2   | 9:I:206:ARG:HA    | 1.99                     | 0.45              |
| 10:J:375:LYS:O    | 10:J:379:ILE:HG12 | 2.17                     | 0.45              |
| 10:J:496:SER:O    | 10:J:499:VAL:N    | 2.47                     | 0.45              |
| 10:J:538:LEU:HD13 | 10:J:670:LEU:CD1  | 2.47                     | 0.45              |
| 3:C:300:VAL:HG12  | 3:C:343:ILE:CG2   | 2.30                     | 0.45              |
| 3:C:338:ALA:O     | 3:C:342:SER:OG    | 2.30                     | 0.45              |
| 3:C:368:LYS:HA    | 4:D:176:ASN:CG    | 2.42                     | 0.45              |
| 4:D:1:MET:HE2     | 4:D:205:LEU:HD22  | 1.93                     | 0.45              |
| 6:F:126:ASN:OD1   | 9:I:42:LYS:NZ     | 2.50                     | 0.45              |
| 8:H:204:SER:OG    | 8:H:228:ASN:C     | 2.59                     | 0.45              |
| 9:I:48:HIS:CG     | 11:K:552:LEU:HD12 | 2.52                     | 0.45              |
| 10:J:135:LEU:HD22 | 10:J:145:PHE:CE2  | 2.51                     | 0.45              |
| 10:J:573:VAL:HB   | 10:J:845:PRO:HB2  | 1.98                     | 0.45              |
| 5:E:234:SER:CB    | 6:F:90:GLN:HE22   | 2.30                     | 0.45              |
| 7:G:225:ASP:O     | 7:G:228:LYS:HB3   | 2.17                     | 0.45              |
| 11:K:227:GLU:HA   | 11:K:230:LYS:HD3  | 1.99                     | 0.45              |
| 2:B:162:SER:OG    | 2:B:173:ASP:HA    | 2.17                     | 0.45              |
| 3:C:347:ILE:HG12  | 3:C:362:LEU:HG    | 1.97                     | 0.45              |
| 10:J:327:LYS:O    | 10:J:387:GLN:N    | 2.34                     | 0.45              |
| 3:C:11:GLU:O      | 3:C:12:ILE:HG13   | 2.17                     | 0.44              |
| 10:J:275:GLN:OE1  | 10:J:275:GLN:N    | 2.50                     | 0.44              |
| 10:J:630:LEU:HD12 | 10:J:631:ASP:O    | 2.17                     | 0.44              |
| 1:A:225:LEU:HD23  | 4:D:12:HIS:NE2    | 2.31                     | 0.44              |
| 3:C:172:VAL:N     | 3:C:209:TRP:O     | 2.42                     | 0.44              |
| 5:E:240:LYS:NZ    | 6:F:209:GLU:OE2   | 2.49                     | 0.44              |
| 7:G:219:ASP:N     | 7:G:223:PHE:CZ    | 2.86                     | 0.44              |
| 10:J:135:LEU:CB   | 10:J:145:PHE:CD2  | 2.89                     | 0.44              |
| 10:J:335:ASP:OD2  | 10:J:940:ARG:NH2  | 2.49                     | 0.44              |
| 5:E:98:LEU:O      | 5:E:102:VAL:HG23  | 2.16                     | 0.44              |
| 5:E:264:ASN:HB2   | 8:H:9:LYS:CE      | 2.48                     | 0.44              |
| 6:F:58:GLY:HA3    | 6:F:183:ALA:HB2   | 1.99                     | 0.44              |
| 6:F:177:THR:HG21  | 6:F:191:ALA:H     | 1.83                     | 0.44              |
| 10:J:533:ASP:CG   | 10:J:535:ARG:HE   | 2.26                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:K:200:ARG:NH2  | 11:K:203:ILE:HD11 | 2.32                     | 0.44              |
| 1:A:291:ASN:CB    | 1:A:294:ALA:HB2   | 2.47                     | 0.44              |
| 2:B:161:ILE:CG2   | 2:B:187:LEU:HB2   | 2.48                     | 0.44              |
| 5:E:90:LEU:HD21   | 6:F:118:MET:CE    | 2.47                     | 0.44              |
| 10:J:543:ASP:HB3  | 10:J:547:CYS:SG   | 2.57                     | 0.44              |
| 11:K:378:ASN:O    | 11:K:382:GLU:HG3  | 2.17                     | 0.44              |
| 11:K:518:GLU:O    | 11:K:521:PRO:CD   | 2.52                     | 0.44              |
| 1:A:198:PHE:CD2   | 1:A:221:ILE:HG12  | 2.52                     | 0.44              |
| 3:C:55:GLU:HB3    | 3:C:58:THR:HG21   | 1.99                     | 0.44              |
| 6:F:163:SER:OG    | 6:F:164:GLN:N     | 2.51                     | 0.44              |
| 10:J:634:ALA:HB2  | 10:J:680:LEU:HA   | 1.99                     | 0.44              |
| 12:L:44:ARG:HD2   | 12:L:44:ARG:O     | 2.18                     | 0.44              |
| 3:C:363:MET:CG    | 4:D:179:LEU:CD1   | 2.95                     | 0.44              |
| 7:G:59:TYR:O      | 7:G:161:ASN:CG    | 2.59                     | 0.44              |
| 7:G:214:CYS:SG    | 7:G:223:PHE:CD1   | 3.04                     | 0.44              |
| 8:H:312:ILE:HD12  | 8:H:349:LEU:HD21  | 1.99                     | 0.44              |
| 10:J:365:ILE:HG22 | 10:J:366:SER:N    | 2.33                     | 0.44              |
| 10:J:435:ARG:O    | 10:J:464:LEU:CD1  | 2.41                     | 0.44              |
| 10:J:539:ILE:HG13 | 10:J:569:HIS:CD2  | 2.53                     | 0.44              |
| 1:A:196:VAL:CG1   | 1:A:198:PHE:CE1   | 3.01                     | 0.44              |
| 1:A:210:ILE:HG22  | 1:A:211:LYS:N     | 2.32                     | 0.44              |
| 3:C:378:LEU:HG    | 4:D:186:PHE:HZ    | 1.81                     | 0.44              |
| 4:D:222:VAL:HG11  | 7:G:165:GLN:CD    | 2.42                     | 0.44              |
| 10:J:842:PHE:O    | 10:J:855:HIS:HE1  | 2.00                     | 0.44              |
| 13:R:-3:A:C2'     | 13:R:-2:A:C5'     | 2.92                     | 0.44              |
| 1:A:245:VAL:CG2   | 2:B:207:LEU:HD13  | 2.45                     | 0.44              |
| 3:C:378:LEU:HG    | 4:D:186:PHE:CZ    | 2.52                     | 0.44              |
| 5:E:22:ARG:HG3    | 5:E:26:ARG:C      | 2.43                     | 0.44              |
| 9:I:270:THR:OG1   | 9:I:271:ASP:N     | 2.50                     | 0.44              |
| 10:J:65:ASN:C     | 10:J:66:GLU:HG2   | 2.43                     | 0.44              |
| 10:J:901:TYR:CE2  | 10:J:905:GLN:NE2  | 2.86                     | 0.44              |
| 10:J:939:ILE:HG22 | 10:J:944:LEU:HG   | 1.99                     | 0.44              |
| 11:K:5:ASN:HB2    | 11:K:6:PRO:HD2    | 1.93                     | 0.44              |
| 11:K:24:ALA:HB2   | 12:L:66:LYS:HB3   | 2.00                     | 0.44              |
| 12:L:73:MET:HE3   | 12:L:76:ILE:CG2   | 2.48                     | 0.44              |
| 13:R:-5:A:O2'     | 13:R:-4:A:H5'     | 2.18                     | 0.44              |
| 1:A:89:SER:HB2    | 7:G:91:PHE:CE2    | 2.52                     | 0.44              |
| 1:A:210:ILE:CG2   | 1:A:211:LYS:N     | 2.79                     | 0.44              |
| 1:A:258:ALA:O     | 1:A:262:MET:HG2   | 2.18                     | 0.44              |
| 3:C:35:LEU:HB2    | 3:C:302:LEU:CD2   | 2.33                     | 0.44              |
| 3:C:378:LEU:HD23  | 4:D:186:PHE:HE1   | 1.81                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:E:167:GLU:O     | 5:E:167:GLU:HG2   | 2.17                     | 0.44              |
| 5:E:234:SER:HA    | 6:F:90:GLN:NE2    | 2.15                     | 0.44              |
| 7:G:6:PHE:CA      | 7:G:9:ASP:OD2     | 2.65                     | 0.44              |
| 8:H:170:ASN:HB2   | 8:H:191:TYR:HA    | 2.00                     | 0.44              |
| 10:J:488:HIS:NE2  | 10:J:894:ALA:HA   | 2.33                     | 0.44              |
| 10:J:566:VAL:CG1  | 10:J:677:LEU:CD2  | 2.96                     | 0.44              |
| 10:J:697:ALA:HB2  | 10:J:806:ARG:HD3  | 1.99                     | 0.44              |
| 10:J:727:VAL:O    | 10:J:731:MET:HG2  | 2.18                     | 0.44              |
| 11:K:57:ILE:HG23  | 11:K:84:ILE:CD1   | 2.45                     | 0.44              |
| 3:C:172:VAL:CB    | 3:C:209:TRP:O     | 2.66                     | 0.43              |
| 5:E:52:ALA:HB3    | 5:E:56:SER:HB2    | 1.99                     | 0.43              |
| 10:J:539:ILE:CG2  | 10:J:553:ALA:CB   | 2.92                     | 0.43              |
| 11:K:183:TYR:CZ   | 11:K:282:THR:HG21 | 2.53                     | 0.43              |
| 13:R:-4:A:H2'     | 13:R:-3:A:C8      | 2.52                     | 0.43              |
| 8:H:190:LYS:HE3   | 8:H:191:TYR:CZ    | 2.53                     | 0.43              |
| 10:J:23:VAL:HA    | 10:J:36:VAL:HG22  | 2.00                     | 0.43              |
| 10:J:23:VAL:HG13  | 10:J:23:VAL:O     | 2.18                     | 0.43              |
| 10:J:306:ASN:ND2  | 10:J:321:LEU:HD11 | 2.33                     | 0.43              |
| 10:J:311:PHE:CE1  | 10:J:456:TRP:CZ3  | 3.05                     | 0.43              |
| 10:J:496:SER:O    | 10:J:497:LYS:C    | 2.61                     | 0.43              |
| 10:J:496:SER:O    | 10:J:499:VAL:HB   | 2.17                     | 0.43              |
| 10:J:738:VAL:HG21 | 10:J:842:PHE:CG   | 2.53                     | 0.43              |
| 10:J:778:ILE:CG2  | 10:J:789:SER:OG   | 2.56                     | 0.43              |
| 4:D:169:ASN:CA    | 7:G:8:GLY:O       | 2.66                     | 0.43              |
| 7:G:72:VAL:HG12   | 7:G:191:ASN:HB3   | 2.00                     | 0.43              |
| 10:J:400:TRP:CZ3  | 10:J:453:ILE:CG2  | 3.01                     | 0.43              |
| 10:J:551:ASN:HB2  | 13:R:-1:A:P       | 2.59                     | 0.43              |
| 11:K:132:PRO:CG   | 11:K:268:LEU:HD13 | 2.47                     | 0.43              |
| 11:K:266:ASP:OD2  | 11:K:352:ARG:NH1  | 2.51                     | 0.43              |
| 11:K:401:PHE:CD1  | 11:K:416:TYR:CE2  | 3.05                     | 0.43              |
| 1:A:149:ASP:O     | 1:A:153:ILE:HG13  | 2.19                     | 0.43              |
| 1:A:194:ILE:O     | 1:A:238:THR:HA    | 2.18                     | 0.43              |
| 2:B:84:PHE:O      | 5:E:63:LYS:NZ     | 2.37                     | 0.43              |
| 3:C:300:VAL:HG11  | 3:C:343:ILE:CD1   | 2.47                     | 0.43              |
| 7:G:76:ILE:CD1    | 7:G:86:VAL:HB     | 2.49                     | 0.43              |
| 10:J:394:TYR:O    | 10:J:395:ILE:HD13 | 2.19                     | 0.43              |
| 10:J:630:LEU:HD12 | 10:J:630:LEU:C    | 2.44                     | 0.43              |
| 11:K:410:THR:CG2  | 11:K:412:SER:OG   | 2.66                     | 0.43              |
| 11:K:479:ASP:OD1  | 11:K:479:ASP:N    | 2.50                     | 0.43              |
| 2:B:165:LEU:O     | 2:B:182:MET:HG3   | 2.00                     | 0.43              |
| 7:G:158:VAL:CG1   | 7:G:162:PHE:HD2   | 2.19                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:J:134:THR:OG1  | 10:J:137:ARG:NH2  | 2.51                     | 0.43              |
| 11:K:35:ASP:OD1   | 11:K:37:GLY:N     | 2.42                     | 0.43              |
| 11:K:199:ILE:HG23 | 11:K:378:ASN:CG   | 2.43                     | 0.43              |
| 11:K:424:PRO:CB   | 11:K:446:TYR:CZ   | 3.02                     | 0.43              |
| 1:A:28:ARG:NH1    | 1:A:34:ARG:HD3    | 2.33                     | 0.43              |
| 1:A:126:VAL:HG12  | 1:A:130:LYS:HB2   | 2.00                     | 0.43              |
| 3:C:299:ILE:O     | 3:C:300:VAL:HG12  | 2.19                     | 0.43              |
| 4:D:61:THR:OG1    | 6:F:9:LEU:HD21    | 2.19                     | 0.43              |
| 4:D:174:VAL:O     | 4:D:174:VAL:CG1   | 2.66                     | 0.43              |
| 8:H:160:ARG:NH1   | 8:H:165:GLU:CD    | 2.75                     | 0.43              |
| 10:J:400:TRP:CH2  | 10:J:453:ILE:HG21 | 2.52                     | 0.43              |
| 10:J:401:ARG:CZ   | 10:J:403:TYR:CE1  | 3.02                     | 0.43              |
| 10:J:692:GLY:HA2  | 10:J:784:LYS:HG3  | 2.01                     | 0.43              |
| 11:K:169:VAL:O    | 11:K:177:SER:OG   | 2.24                     | 0.43              |
| 11:K:176:PRO:HG3  | 11:K:408:PRO:CD   | 2.49                     | 0.43              |
| 11:K:206:LYS:HD3  | 11:K:206:LYS:HA   | 1.74                     | 0.43              |
| 1:A:250:LYS:CE    | 2:B:196:LEU:O     | 2.67                     | 0.43              |
| 5:E:21:ILE:HG22   | 5:E:22:ARG:O      | 2.19                     | 0.43              |
| 7:G:120:TYR:O     | 7:G:147:PHE:HB3   | 2.19                     | 0.43              |
| 11:K:26:GLN:OE1   | 12:L:7:ILE:HG12   | 2.17                     | 0.43              |
| 1:A:38:ILE:HB     | 1:A:282:LEU:HD13  | 2.00                     | 0.43              |
| 3:C:368:LYS:HA    | 4:D:176:ASN:OD1   | 2.19                     | 0.43              |
| 4:D:18:GLU:OE2    | 4:D:25:LYS:HD2    | 2.19                     | 0.43              |
| 4:D:85:ARG:NH2    | 9:I:146:LEU:H     | 2.16                     | 0.43              |
| 4:D:99:GLU:OE2    | 4:D:108:GLU:HG3   | 2.18                     | 0.43              |
| 7:G:217:LYS:HG3   | 7:G:226:ILE:CD1   | 2.49                     | 0.43              |
| 10:J:345:PRO:HG3  | 10:J:422:VAL:C    | 2.44                     | 0.43              |
| 11:K:356:LYS:N    | 11:K:357:PRO:HD2  | 2.33                     | 0.43              |
| 5:E:82:ILE:HB     | 5:E:85:GLN:HB2    | 2.00                     | 0.43              |
| 5:E:82:ILE:HG23   | 5:E:130:VAL:O     | 2.19                     | 0.43              |
| 10:J:928:VAL:O    | 10:J:936:GLU:HA   | 2.18                     | 0.43              |
| 11:K:399:ARG:CB   | 11:K:414:GLU:HA   | 2.49                     | 0.43              |
| 1:A:107:ILE:HG21  | 1:A:236:THR:HG21  | 2.00                     | 0.43              |
| 1:A:243:ARG:HG2   | 1:A:269:TYR:OH    | 2.19                     | 0.43              |
| 2:B:233:ARG:HD3   | 8:H:54:ILE:HG21   | 1.63                     | 0.43              |
| 3:C:357:TYR:O     | 4:D:185:ASP:HB3   | 2.19                     | 0.43              |
| 10:J:136:CYS:CA   | 10:J:145:PHE:CB   | 2.85                     | 0.43              |
| 1:A:202:ASN:CG    | 1:A:203:PRO:HD2   | 2.41                     | 0.42              |
| 1:A:256:MET:O     | 2:B:195:LYS:HA    | 2.17                     | 0.42              |
| 2:B:7:TYR:OH      | 2:B:11:GLY:HA2    | 2.18                     | 0.42              |
| 5:E:173:HIS:CE1   | 5:E:176:ASP:HB2   | 2.54                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:G:219:ASP:O     | 7:G:223:PHE:CD2   | 2.72                     | 0.42              |
| 10:J:133:ARG:CB   | 10:J:137:ARG:HH12 | 2.07                     | 0.42              |
| 10:J:346:ASP:HA   | 10:J:421:ASN:OD1  | 2.18                     | 0.42              |
| 10:J:926:ILE:O    | 10:J:938:LEU:HD12 | 2.19                     | 0.42              |
| 11:K:294:PHE:CE2  | 11:K:295:MET:HE2  | 2.53                     | 0.42              |
| 1:A:164:LYS:NZ    | 1:A:187:LEU:HD23  | 2.34                     | 0.42              |
| 3:C:10:ILE:O      | 3:C:10:ILE:HG13   | 2.19                     | 0.42              |
| 6:F:203:PHE:HB3   | 6:F:207:GLY:HA2   | 2.02                     | 0.42              |
| 7:G:158:VAL:CG1   | 7:G:162:PHE:HB3   | 2.49                     | 0.42              |
| 8:H:8:THR:HG23    | 8:H:8:THR:O       | 2.18                     | 0.42              |
| 9:I:148:LEU:HD12  | 9:I:148:LEU:C     | 2.42                     | 0.42              |
| 10:J:113:VAL:HG11 | 10:J:132:LEU:HD21 | 2.02                     | 0.42              |
| 10:J:395:ILE:CG2  | 10:J:397:ARG:O    | 2.67                     | 0.42              |
| 10:J:484:LEU:HD12 | 10:J:488:HIS:CE1  | 2.54                     | 0.42              |
| 10:J:516:LEU:CD2  | 10:J:528:LEU:HD11 | 2.48                     | 0.42              |
| 10:J:701:VAL:HG22 | 10:J:702:LYS:H    | 1.83                     | 0.42              |
| 11:K:359:THR:O    | 11:K:363:ARG:N    | 2.39                     | 0.42              |
| 13:N:-13:A:N3     | 13:N:-13:A:H2'    | 2.34                     | 0.42              |
| 5:E:15:LEU:HD21   | 5:E:205:GLU:CG    | 2.48                     | 0.42              |
| 5:E:15:LEU:HD12   | 5:E:21:ILE:O      | 2.19                     | 0.42              |
| 7:G:130:LEU:HD12  | 9:I:146:LEU:O     | 2.20                     | 0.42              |
| 8:H:101:LYS:HE2   | 8:H:101:LYS:HB3   | 1.90                     | 0.42              |
| 10:J:278:ILE:O    | 10:J:278:ILE:CG2  | 2.66                     | 0.42              |
| 10:J:551:ASN:HB2  | 13:R:-1:A:OP1     | 2.19                     | 0.42              |
| 10:J:804:LEU:HD13 | 10:J:917:TYR:HB2  | 2.00                     | 0.42              |
| 11:K:213:PRO:HG3  | 11:K:359:THR:HG21 | 1.99                     | 0.42              |
| 7:G:67:SER:OG     | 7:G:70:ASP:OD2    | 2.37                     | 0.42              |
| 11:K:332:LEU:HD21 | 11:K:368:PHE:HB2  | 2.01                     | 0.42              |
| 7:G:113:LEU:CD1   | 7:G:149:ILE:CG2   | 2.98                     | 0.42              |
| 10:J:652:PHE:HD1  | 10:J:656:GLN:OE1  | 2.03                     | 0.42              |
| 10:J:728:GLU:HG3  | 13:R:-3:A:O4'     | 2.20                     | 0.42              |
| 11:K:348:ASP:C    | 11:K:350:ARG:H    | 2.26                     | 0.42              |
| 2:B:12:LEU:HD12   | 10:J:149:HIS:ND1  | 2.30                     | 0.42              |
| 2:B:66:ASP:HB3    | 2:B:69:LYS:O      | 2.19                     | 0.42              |
| 3:C:369:ILE:HG22  | 3:C:374:ILE:HD11  | 2.01                     | 0.42              |
| 5:E:239:PHE:O     | 6:F:210:ILE:N     | 2.48                     | 0.42              |
| 8:H:146:GLY:O     | 8:H:149:ARG:N     | 2.51                     | 0.42              |
| 8:H:172:GLU:CD    | 11:K:411:PRO:HG3  | 2.44                     | 0.42              |
| 11:K:522:ILE:HB   | 11:K:523:PRO:HD3  | 2.01                     | 0.42              |
| 1:A:194:ILE:CG2   | 1:A:272:ILE:HG22  | 2.50                     | 0.42              |
| 1:A:201:PHE:CE2   | 1:A:231:ARG:HA    | 2.54                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:254:LEU:HD12  | 1:A:255:PRO:HD2   | 2.02                     | 0.42              |
| 1:A:262:MET:HE3   | 1:A:266:HIS:HE1   | 1.85                     | 0.42              |
| 2:B:186:THR:HB    | 2:B:200:LEU:HB3   | 2.02                     | 0.42              |
| 3:C:147:GLU:CG    | 3:C:148:GLU:N     | 2.83                     | 0.42              |
| 4:D:139:ILE:HB    | 4:D:142:THR:OG1   | 2.20                     | 0.42              |
| 9:I:149:GLN:O     | 9:I:150:ARG:CG    | 2.67                     | 0.42              |
| 10:J:48:LEU:CB    | 10:J:146:ILE:HD11 | 2.50                     | 0.42              |
| 10:J:254:THR:HG22 | 10:J:255:PHE:N    | 2.34                     | 0.42              |
| 10:J:527:LEU:HD13 | 10:J:864:TYR:CE1  | 2.55                     | 0.42              |
| 10:J:543:ASP:OD2  | 10:J:550:ILE:HG23 | 2.19                     | 0.42              |
| 10:J:567:GLY:HA2  | 10:J:627:ILE:HA   | 2.02                     | 0.42              |
| 10:J:844:SER:N    | 10:J:851:ASP:OD2  | 2.52                     | 0.42              |
| 3:C:222:ARG:HG2   | 3:C:223:THR:N     | 2.34                     | 0.42              |
| 3:C:376:ARG:HG3   | 3:C:380:LEU:HD13  | 2.01                     | 0.42              |
| 7:G:6:PHE:HB3     | 7:G:7:PRO:HD2     | 2.01                     | 0.42              |
| 7:G:53:GLN:HG3    | 7:G:54:THR:N      | 2.34                     | 0.42              |
| 7:G:86:VAL:HG11   | 7:G:134:ILE:HD11  | 2.02                     | 0.42              |
| 9:I:204:ILE:HG23  | 9:I:204:ILE:O     | 2.19                     | 0.42              |
| 10:J:596:LEU:HD22 | 10:J:898:SER:HB2  | 2.01                     | 0.42              |
| 11:K:81:PHE:CD1   | 12:L:61:MET:HG3   | 2.55                     | 0.42              |
| 1:A:9:ALA:CB      | 7:G:116:GLY:O     | 2.68                     | 0.42              |
| 2:B:9:PRO:HG2     | 10:J:133:ARG:CZ   | 2.48                     | 0.42              |
| 2:B:106:ARG:HA    | 2:B:106:ARG:HD3   | 1.67                     | 0.42              |
| 3:C:303:ASP:N     | 3:C:304:PRO:HD3   | 2.35                     | 0.42              |
| 3:C:370:THR:H     | 3:C:373:MET:HE2   | 1.85                     | 0.42              |
| 5:E:228:SER:OG    | 6:F:213:PHE:N     | 2.46                     | 0.42              |
| 10:J:105:PRO:HA   | 10:J:143:LYS:HZ3  | 1.85                     | 0.42              |
| 10:J:723:THR:O    | 10:J:726:LEU:CB   | 2.62                     | 0.42              |
| 11:K:572:LEU:HD13 | 11:K:576:LEU:HD11 | 2.02                     | 0.42              |
| 1:A:41:GLY:O      | 1:A:290:ARG:NH1   | 2.45                     | 0.42              |
| 10:J:397:ARG:CG   | 10:J:398:ARG:N    | 2.83                     | 0.42              |
| 10:J:618:TYR:CE1  | 10:J:649:ARG:O    | 2.73                     | 0.42              |
| 10:J:652:PHE:HB3  | 10:J:653:SER:O    | 2.20                     | 0.42              |
| 10:J:763:PHE:O    | 10:J:767:ASN:HB2  | 2.20                     | 0.42              |
| 11:K:196:ILE:HG23 | 11:K:287:VAL:CG2  | 2.39                     | 0.42              |
| 3:C:51:ASP:CG     | 11:K:581:HIS:ND1  | 2.78                     | 0.41              |
| 3:C:378:LEU:HD21  | 4:D:186:PHE:CE1   | 2.55                     | 0.41              |
| 5:E:158:ILE:CD1   | 5:E:173:HIS:HA    | 2.50                     | 0.41              |
| 6:F:53:ILE:HG22   | 6:F:55:ASN:H      | 1.84                     | 0.41              |
| 8:H:61:VAL:HG11   | 8:H:95:LEU:HD21   | 2.02                     | 0.41              |
| 8:H:124:TRP:CZ2   | 8:H:163:LEU:HB2   | 2.53                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:J:368:LYS:O    | 10:J:372:LEU:CB   | 2.68                     | 0.41              |
| 11:K:336:ALA:HB2  | 11:K:368:PHE:CD1  | 2.54                     | 0.41              |
| 2:B:47:ASN:OD1    | 2:B:132:ASP:N     | 2.52                     | 0.41              |
| 3:C:54:ILE:HG22   | 3:C:80:LEU:HD13   | 2.01                     | 0.41              |
| 3:C:84:LYS:HE3    | 3:C:223:THR:HG21  | 2.02                     | 0.41              |
| 10:J:276:GLY:HA3  | 10:J:290:VAL:CG1  | 2.51                     | 0.41              |
| 10:J:549:ASP:CG   | 13:R:-1:A:HO3'    | 2.28                     | 0.41              |
| 10:J:738:VAL:CG1  | 10:J:858:LEU:HD21 | 2.46                     | 0.41              |
| 11:K:260:GLU:O    | 11:K:261:ARG:HD2  | 2.19                     | 0.41              |
| 3:C:232:ASN:ND2   | 3:C:294:ALA:H     | 2.13                     | 0.41              |
| 3:C:357:TYR:O     | 4:D:185:ASP:CB    | 2.68                     | 0.41              |
| 10:J:554:LEU:HG   | 10:J:568:VAL:HG22 | 2.02                     | 0.41              |
| 10:J:714:GLU:HG2  | 10:J:715:VAL:N    | 2.35                     | 0.41              |
| 11:K:176:PRO:HG3  | 11:K:408:PRO:HD2  | 2.03                     | 0.41              |
| 11:K:478:THR:HG22 | 11:K:509:LEU:HD11 | 2.03                     | 0.41              |
| 1:A:235:LEU:HD13  | 1:A:250:LYS:HB2   | 2.03                     | 0.41              |
| 2:B:37:ASP:CG     | 8:H:103:ARG:HH11  | 2.28                     | 0.41              |
| 7:G:64:TYR:HA     | 7:G:160:LEU:HD11  | 2.01                     | 0.41              |
| 7:G:127:GLU:HG3   | 9:I:221:ILE:HD13  | 2.03                     | 0.41              |
| 10:J:126:TYR:N    | 10:J:127:PRO:HD2  | 2.35                     | 0.41              |
| 10:J:630:LEU:HD21 | 10:J:680:LEU:HD23 | 2.02                     | 0.41              |
| 10:J:946:GLU:CG   | 10:J:965:THR:HG23 | 2.46                     | 0.41              |
| 1:A:194:ILE:C     | 1:A:238:THR:HG23  | 2.45                     | 0.41              |
| 3:C:140:ARG:HD2   | 9:I:197:LEU:HD11  | 2.02                     | 0.41              |
| 3:C:375:LYS:O     | 3:C:379:LEU:HG    | 2.20                     | 0.41              |
| 4:D:62:ARG:NH2    | 4:D:108:GLU:OE2   | 2.50                     | 0.41              |
| 5:E:102:VAL:HG22  | 5:E:225:PRO:HD2   | 2.01                     | 0.41              |
| 5:E:173:HIS:CE1   | 5:E:176:ASP:CG    | 2.99                     | 0.41              |
| 6:F:126:ASN:CG    | 9:I:42:LYS:HZ3    | 2.28                     | 0.41              |
| 10:J:401:ARG:NH1  | 10:J:403:TYR:HE1  | 2.18                     | 0.41              |
| 10:J:500:LEU:HA   | 10:J:503:LEU:HD12 | 2.01                     | 0.41              |
| 10:J:738:VAL:HG11 | 10:J:842:PHE:CD1  | 2.55                     | 0.41              |
| 10:J:889:ARG:HG2  | 10:J:893:PHE:CZ   | 2.56                     | 0.41              |
| 11:K:410:THR:HG21 | 11:K:412:SER:OG   | 2.20                     | 0.41              |
| 4:D:139:ILE:HD13  | 4:D:139:ILE:N     | 2.34                     | 0.41              |
| 5:E:11:LEU:HD23   | 5:E:11:LEU:HA     | 1.85                     | 0.41              |
| 7:G:45:SER:O      | 7:G:53:GLN:OE1    | 2.38                     | 0.41              |
| 8:H:56:THR:O      | 8:H:59:GLU:HB3    | 2.20                     | 0.41              |
| 8:H:124:TRP:HZ2   | 8:H:159:MET:O     | 2.03                     | 0.41              |
| 8:H:143:LEU:HB3   | 8:H:144:PRO:HD2   | 2.01                     | 0.41              |
| 8:H:172:GLU:OE1   | 8:H:185:HIS:HE1   | 2.02                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:H:204:SER:HG    | 8:H:228:ASN:C     | 2.28                     | 0.41              |
| 10:J:58:ILE:HG13  | 10:J:59:VAL:N     | 2.34                     | 0.41              |
| 10:J:347:ILE:HD11 | 10:J:464:LEU:HD11 | 2.01                     | 0.41              |
| 10:J:407:LEU:HD23 | 10:J:424:VAL:HG22 | 2.03                     | 0.41              |
| 11:K:423:SER:HB2  | 11:K:426:LYS:CG   | 2.48                     | 0.41              |
| 1:A:250:LYS:HE2   | 1:A:256:MET:HG2   | 2.02                     | 0.41              |
| 2:B:5:GLU:O       | 2:B:14:LEU:HD21   | 2.20                     | 0.41              |
| 2:B:167:ASP:OD1   | 2:B:168:THR:N     | 2.53                     | 0.41              |
| 2:B:233:ARG:NE    | 8:H:54:ILE:HG21   | 2.29                     | 0.41              |
| 4:D:209:ILE:O     | 4:D:213:ILE:HG13  | 2.20                     | 0.41              |
| 7:G:145:ALA:HB1   | 7:G:147:PHE:CD2   | 2.55                     | 0.41              |
| 8:H:128:ILE:HG13  | 8:H:134:ALA:HB2   | 2.02                     | 0.41              |
| 8:H:136:LEU:HD12  | 8:H:184:LEU:O     | 2.21                     | 0.41              |
| 10:J:126:TYR:OH   | 10:J:413:ASP:CB   | 2.69                     | 0.41              |
| 10:J:484:LEU:CD1  | 10:J:488:HIS:CE1  | 3.03                     | 0.41              |
| 10:J:757:ALA:O    | 10:J:814:MET:SD   | 2.79                     | 0.41              |
| 10:J:808:MET:SD   | 10:J:919:ILE:CG1  | 2.97                     | 0.41              |
| 10:J:930:VAL:CG1  | 10:J:931:PRO:HD2  | 2.51                     | 0.41              |
| 11:K:45:LYS:NZ    | 12:L:15:SER:HB3   | 2.35                     | 0.41              |
| 11:K:144:GLU:CB   | 11:K:403:TYR:CZ   | 3.03                     | 0.41              |
| 11:K:181:HIS:ND1  | 11:K:182:PRO:N    | 2.69                     | 0.41              |
| 11:K:549:PHE:O    | 11:K:553:CYS:HB2  | 2.20                     | 0.41              |
| 3:C:129:SER:OG    | 3:C:130:VAL:N     | 2.54                     | 0.41              |
| 10:J:290:VAL:O    | 10:J:290:VAL:HG12 | 2.20                     | 0.41              |
| 10:J:624:PHE:CD1  | 10:J:643:LYS:HG2  | 2.56                     | 0.41              |
| 11:K:294:PHE:HA   | 11:K:396:VAL:HG13 | 2.02                     | 0.41              |
| 1:A:103:LEU:HG    | 2:B:102:THR:CG2   | 2.41                     | 0.41              |
| 1:A:169:VAL:HG23  | 1:A:174:ILE:CG2   | 2.49                     | 0.41              |
| 2:B:25:PHE:CE1    | 2:B:27:SER:OG     | 2.74                     | 0.41              |
| 2:B:103:SER:O     | 2:B:107:MET:HG3   | 2.21                     | 0.41              |
| 2:B:107:MET:CE    | 2:B:198:LEU:CB    | 2.98                     | 0.41              |
| 2:B:164:GLY:CA    | 2:B:174:THR:HG21  | 2.51                     | 0.41              |
| 3:C:278:GLN:HG3   | 6:F:20:PHE:HB3    | 2.03                     | 0.41              |
| 3:C:352:ALA:HA    | 3:C:353:PRO:HD3   | 1.97                     | 0.41              |
| 6:F:126:ASN:CG    | 9:I:42:LYS:NZ     | 2.79                     | 0.41              |
| 7:G:22:GLY:HA3    | 7:G:56:TYR:HB3    | 2.02                     | 0.41              |
| 7:G:121:ALA:CB    | 7:G:134:ILE:HD12  | 2.50                     | 0.41              |
| 8:H:124:TRP:CZ2   | 8:H:159:MET:HB3   | 2.56                     | 0.41              |
| 10:J:319:GLU:O    | 10:J:390:ALA:HB1  | 2.21                     | 0.41              |
| 10:J:426:LEU:HD12 | 10:J:431:LEU:CB   | 2.51                     | 0.41              |
| 10:J:663:ASP:O    | 10:J:664:LYS:CB   | 2.66                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:L:23:PRO:O     | 12:L:27:LYS:HG3   | 2.21                     | 0.41              |
| 12:L:62:PHE:CZ    | 12:L:66:LYS:CE    | 3.04                     | 0.41              |
| 1:A:127:ALA:HB3   | 10:J:454:ASP:OD2  | 2.21                     | 0.41              |
| 3:C:130:VAL:HG12  | 3:C:213:LEU:HB2   | 2.03                     | 0.41              |
| 3:C:353:PRO:C     | 3:C:355:GLY:N     | 2.77                     | 0.41              |
| 4:D:143:SER:O     | 4:D:190:GLN:NE2   | 2.53                     | 0.41              |
| 5:E:119:LYS:O     | 5:E:119:LYS:HG3   | 2.21                     | 0.41              |
| 10:J:645:VAL:O    | 10:J:645:VAL:HG13 | 2.20                     | 0.41              |
| 10:J:715:VAL:HG21 | 10:J:906:VAL:HG11 | 2.03                     | 0.41              |
| 13:N:-11:A:H2'    | 13:N:-10:A:OP2    | 2.20                     | 0.41              |
| 1:A:3:LYS:HD3     | 7:G:91:PHE:CE1    | 2.55                     | 0.40              |
| 1:A:56:VAL:HG21   | 1:A:150:ALA:HB1   | 2.04                     | 0.40              |
| 4:D:145:ILE:O     | 4:D:145:ILE:CG1   | 2.69                     | 0.40              |
| 10:J:165:THR:HG22 | 10:J:166:ILE:N    | 2.36                     | 0.40              |
| 10:J:738:VAL:HG21 | 10:J:842:PHE:CD2  | 2.55                     | 0.40              |
| 10:J:807:ILE:HG21 | 10:J:929:LEU:HD21 | 2.02                     | 0.40              |
| 11:K:290:PHE:CB   | 11:K:293:ALA:HB2  | 2.41                     | 0.40              |
| 11:K:601:ILE:HA   | 11:K:604:GLN:HG2  | 2.02                     | 0.40              |
| 3:C:39:ILE:HD12   | 3:C:39:ILE:HA     | 1.90                     | 0.40              |
| 4:D:168:VAL:HG23  | 4:D:173:VAL:HB    | 2.03                     | 0.40              |
| 6:F:52:PHE:CE2    | 6:F:61:LEU:HB2    | 2.56                     | 0.40              |
| 7:G:5:ILE:O       | 7:G:5:ILE:HG23    | 2.21                     | 0.40              |
| 8:H:54:ILE:O      | 8:H:59:GLU:OE2    | 2.38                     | 0.40              |
| 9:I:111:LEU:HA    | 9:I:112:PRO:HD3   | 1.88                     | 0.40              |
| 10:J:71:ILE:CG2   | 10:J:144:ARG:HB3  | 2.51                     | 0.40              |
| 10:J:991:THR:HG22 | 10:J:993:LYS:HB2  | 2.04                     | 0.40              |
| 11:K:360:ALA:O    | 11:K:364:ALA:CB   | 2.69                     | 0.40              |
| 11:K:423:SER:O    | 11:K:427:ILE:CG1  | 2.68                     | 0.40              |
| 12:L:25:ILE:O     | 12:L:29:THR:HG23  | 2.21                     | 0.40              |
| 12:L:76:ILE:CG2   | 12:L:77:LEU:N     | 2.84                     | 0.40              |
| 13:R:-11:A:H2'    | 13:R:-10:A:C1'    | 2.52                     | 0.40              |
| 3:C:149:MET:HE2   | 6:F:7:ARG:HG3     | 2.04                     | 0.40              |
| 3:C:360:LEU:CD1   | 4:D:186:PHE:CE2   | 2.99                     | 0.40              |
| 4:D:24:THR:OG1    | 4:D:107:ARG:NH1   | 2.54                     | 0.40              |
| 10:J:148:PHE:CE2  | 10:J:150:ASN:HA   | 2.57                     | 0.40              |
| 10:J:624:PHE:CE2  | 10:J:842:PHE:CZ   | 3.08                     | 0.40              |
| 10:J:731:MET:HG3  | 13:R:-2:A:OP1     | 2.22                     | 0.40              |
| 10:J:854:ALA:O    | 10:J:858:LEU:HG   | 2.22                     | 0.40              |
| 1:A:56:VAL:CG2    | 1:A:150:ALA:HB1   | 2.51                     | 0.40              |
| 1:A:89:SER:C      | 7:G:91:PHE:CE1    | 3.00                     | 0.40              |
| 3:C:359:GLN:HA    | 4:D:182:SER:O     | 2.22                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:J:72:LEU:HD21  | 10:J:146:ILE:HG22 | 2.03                     | 0.40              |
| 10:J:287:GLU:CG   | 10:J:300:LEU:HD11 | 2.44                     | 0.40              |
| 1:A:29:SER:HB2    | 1:A:32:GLN:HB2    | 2.04                     | 0.40              |
| 2:B:165:LEU:HD11  | 2:B:209:ARG:HD2   | 2.02                     | 0.40              |
| 5:E:36:ILE:O      | 8:H:9:LYS:HA      | 2.20                     | 0.40              |
| 10:J:20:THR:OG1   | 10:J:21:GLN:N     | 2.54                     | 0.40              |
| 10:J:136:CYS:N    | 10:J:145:PHE:HB2  | 2.36                     | 0.40              |
| 10:J:626:VAL:HA   | 10:J:640:ASN:O    | 2.21                     | 0.40              |
| 11:K:152:LEU:HD12 | 11:K:152:LEU:HA   | 1.79                     | 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) |
|------------------|----------------------|--------------------------|-------------------|
| 10:J:872:ARG:NH2 | 11:K:82:GLY:O[2_544] | 2.14                     | 0.06              |

## 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     | 296/305 (97%) | 290 (98%) | 6 (2%)  | 0        | 100         | 100 |
| 2   | B     | 242/248 (98%) | 236 (98%) | 5 (2%)  | 1 (0%)   | 30          | 67  |
| 3   | C     | 311/394 (79%) | 299 (96%) | 11 (4%) | 1 (0%)   | 36          | 71  |
| 4   | D     | 220/245 (90%) | 214 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 5   | E     | 264/267 (99%) | 248 (94%) | 16 (6%) | 0        | 100         | 100 |
| 6   | F     | 207/250 (83%) | 201 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 7   | G     | 234/243 (96%) | 230 (98%) | 4 (2%)  | 0        | 100         | 100 |
| 8   | H     | 285/361 (79%) | 278 (98%) | 7 (2%)  | 0        | 100         | 100 |
| 9   | I     | 217/295 (74%) | 206 (95%) | 11 (5%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 10  | J     | 965/1004 (96%)  | 939 (97%)  | 25 (3%)  | 1 (0%)   | 48          | 83  |
| 11  | K     | 570/695 (82%)   | 549 (96%)  | 21 (4%)  | 0        | 100         | 100 |
| 12  | L     | 111/184 (60%)   | 111 (100%) | 0        | 0        | 100         | 100 |
| All | All   | 3922/4491 (87%) | 3801 (97%) | 118 (3%) | 3 (0%)   | 48          | 83  |

All (3) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 190 | PRO  |
| 2   | B     | 173 | ASP  |
| 10  | J     | 68  | PRO  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 1   | A     | 253/266 (95%)   | 251 (99%)  | 2 (1%)   | 73          | 77  |
| 2   | B     | 210/219 (96%)   | 208 (99%)  | 2 (1%)   | 68          | 76  |
| 3   | C     | 266/350 (76%)   | 260 (98%)  | 6 (2%)   | 44          | 63  |
| 4   | D     | 194/216 (90%)   | 193 (100%) | 1 (0%)   | 81          | 81  |
| 5   | E     | 238/241 (99%)   | 235 (99%)  | 3 (1%)   | 61          | 72  |
| 6   | F     | 178/219 (81%)   | 175 (98%)  | 3 (2%)   | 53          | 67  |
| 7   | G     | 200/211 (95%)   | 197 (98%)  | 3 (2%)   | 57          | 70  |
| 8   | H     | 237/313 (76%)   | 237 (100%) | 0        | 100         | 100 |
| 9   | I     | 177/242 (73%)   | 175 (99%)  | 2 (1%)   | 65          | 74  |
| 10  | J     | 845/902 (94%)   | 837 (99%)  | 8 (1%)   | 70          | 76  |
| 11  | K     | 514/636 (81%)   | 510 (99%)  | 4 (1%)   | 73          | 77  |
| 12  | L     | 99/168 (59%)    | 98 (99%)   | 1 (1%)   | 68          | 76  |
| All | All   | 3411/3983 (86%) | 3376 (99%) | 35 (1%)  | 68          | 76  |

All (35) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 167 | ILE  |
| 1   | A     | 173 | GLN  |
| 2   | B     | 5   | GLU  |
| 2   | B     | 228 | MET  |
| 3   | C     | 134 | VAL  |
| 3   | C     | 212 | VAL  |
| 3   | C     | 286 | ILE  |
| 3   | C     | 300 | VAL  |
| 3   | C     | 308 | LEU  |
| 3   | C     | 374 | ILE  |
| 4   | D     | 177 | VAL  |
| 5   | E     | 109 | VAL  |
| 5   | E     | 154 | LEU  |
| 5   | E     | 222 | ILE  |
| 6   | F     | 61  | LEU  |
| 6   | F     | 73  | LEU  |
| 6   | F     | 201 | VAL  |
| 7   | G     | 19  | VAL  |
| 7   | G     | 76  | ILE  |
| 7   | G     | 122 | ARG  |
| 9   | I     | 61  | VAL  |
| 9   | I     | 158 | VAL  |
| 10  | J     | 35  | ILE  |
| 10  | J     | 176 | LYS  |
| 10  | J     | 213 | ILE  |
| 10  | J     | 290 | VAL  |
| 10  | J     | 299 | VAL  |
| 10  | J     | 539 | ILE  |
| 10  | J     | 905 | GLN  |
| 10  | J     | 969 | LYS  |
| 11  | K     | 23  | LEU  |
| 11  | K     | 386 | LEU  |
| 11  | K     | 572 | LEU  |
| 11  | K     | 594 | VAL  |
| 12  | L     | 97  | ILE  |

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

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 191 | HIS  |
| 2   | B     | 77  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 101 | GLN  |
| 2   | B     | 111 | ASN  |
| 2   | B     | 115 | ASN  |
| 2   | B     | 127 | HIS  |
| 3   | C     | 180 | ASN  |
| 3   | C     | 232 | ASN  |
| 3   | C     | 359 | GLN  |
| 4   | D     | 12  | HIS  |
| 4   | D     | 161 | HIS  |
| 4   | D     | 190 | GLN  |
| 5   | E     | 183 | ASN  |
| 6   | F     | 90  | GLN  |
| 6   | F     | 108 | ASN  |
| 6   | F     | 126 | ASN  |
| 6   | F     | 247 | ASN  |
| 7   | G     | 218 | ASN  |
| 8   | H     | 121 | ASN  |
| 8   | H     | 158 | GLN  |
| 8   | H     | 185 | HIS  |
| 8   | H     | 238 | GLN  |
| 9   | I     | 233 | GLN  |
| 9   | I     | 242 | ASN  |
| 10  | J     | 39  | HIS  |
| 10  | J     | 97  | GLN  |
| 10  | J     | 167 | ASN  |
| 10  | J     | 171 | ASN  |
| 10  | J     | 197 | ASN  |
| 10  | J     | 306 | ASN  |
| 10  | J     | 460 | HIS  |
| 10  | J     | 635 | ASN  |
| 10  | J     | 755 | HIS  |
| 10  | J     | 767 | ASN  |
| 10  | J     | 855 | HIS  |
| 10  | J     | 905 | GLN  |
| 10  | J     | 949 | ASN  |
| 11  | K     | 94  | HIS  |
| 11  | K     | 175 | ASN  |
| 11  | K     | 231 | ASN  |
| 11  | K     | 337 | ASN  |
| 11  | K     | 516 | ASN  |
| 12  | L     | 36  | GLN  |
| 12  | L     | 92  | GLN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed    | Backbone Outliers | Pucker Outliers |
|-----|-------|-------------|-------------------|-----------------|
| 13  | N     | 5/18 (27%)  | 5 (100%)          | 0               |
| 13  | R     | 11/18 (61%) | 9 (81%)           | 0               |
| All | All   | 16/36 (44%) | 14 (87%)          | 0               |

All (14) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13  | R     | -11 | A    |
| 13  | R     | -10 | A    |
| 13  | R     | -9  | A    |
| 13  | R     | -8  | U    |
| 13  | R     | -7  | A    |
| 13  | R     | -6  | A    |
| 13  | R     | -5  | A    |
| 13  | R     | -3  | A    |
| 13  | R     | -1  | A    |
| 13  | N     | -12 | U    |
| 13  | N     | -11 | A    |
| 13  | N     | -10 | A    |
| 13  | N     | -9  | A    |
| 13  | N     | -8  | U    |

There are no RNA pucker outliers to report.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9  |
|-----|-------|-----------------|--------|---------------|-----------------------|--------|
| 1   | A     | 298/305 (97%)   | -0.62  | 1 (0%) 90 80  | 281, 296, 335, 355    | 0      |
| 2   | B     | 244/248 (98%)   | -0.72  | 0 100 100     | 294, 316, 360, 410    | 0      |
| 3   | C     | 321/394 (81%)   | -0.70  | 0 100 100     | 291, 331, 352, 375    | 0      |
| 4   | D     | 222/245 (90%)   | -0.69  | 0 100 100     | 288, 303, 338, 355    | 0      |
| 5   | E     | 266/267 (99%)   | -0.68  | 1 (0%) 88 77  | 285, 307, 399, 449    | 0      |
| 6   | F     | 213/250 (85%)   | -0.46  | 1 (0%) 87 75  | 324, 370, 391, 403    | 0      |
| 7   | G     | 236/243 (97%)   | -0.41  | 2 (0%) 82 68  | 292, 359, 394, 405    | 0      |
| 8   | H     | 291/361 (80%)   | -0.59  | 0 100 100     | 292, 338, 371, 394    | 0      |
| 9   | I     | 225/295 (76%)   | -0.25  | 1 (0%) 88 77  | 340, 374, 433, 442    | 0      |
| 10  | J     | 970/1004 (96%)  | -0.60  | 2 (0%) 91 82  | 203, 334, 407, 450    | 1 (0%) |
| 11  | K     | 576/695 (82%)   | -0.54  | 4 (0%) 84 70  | 288, 349, 416, 459    | 0      |
| 12  | L     | 113/184 (61%)   | -0.27  | 1 (0%) 81 66  | 297, 366, 456, 482    | 0      |
| 13  | N     | 6/18 (33%)      | -0.81  | 0 100 100     | 338, 376, 392, 414    | 0      |
| 13  | R     | 12/18 (66%)     | -0.64  | 0 100 100     | 313, 328, 418, 422    | 0      |
| All | All   | 3993/4527 (88%) | -0.57  | 13 (0%) 90 80 | 203, 338, 408, 482    | 1 (0%) |

All (13) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 11  | K     | 551 | VAL  | 4.6  |
| 11  | K     | 547 | GLU  | 4.0  |
| 11  | K     | 544 | ASP  | 3.4  |
| 5   | E     | 110 | ASP  | 3.0  |
| 7   | G     | 199 | GLU  | 2.8  |
| 1   | A     | 140 | PHE  | 2.6  |
| 11  | K     | 562 | ALA  | 2.6  |
| 9   | I     | 162 | PRO  | 2.6  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 10  | J     | 972 | ASP  | 2.5  |
| 7   | G     | 183 | LYS  | 2.2  |
| 12  | L     | 115 | ILE  | 2.2  |
| 10  | J     | 382 | ARG  | 2.1  |
| 6   | F     | 225 | GLU  | 2.1  |

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 14  | MG   | J     | 1101 | 1/1   | 0.99 | 0.04 | 320,320,320,320             | 0     |
| 15  | ZN   | J     | 1102 | 1/1   | 0.99 | 0.04 | 353,353,353,353             | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.