



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:39 PM UTC

PDB ID : 3HOV / pdb\_00003hov  
Title : Complete RNA polymerase II elongation complex II  
Authors : Sydow, J.F.; Brueckner, F.; Cheung, A.C.M.; Damsma, G.E.; Dengl, S.;  
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Deposited on : 2009-06-03  
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

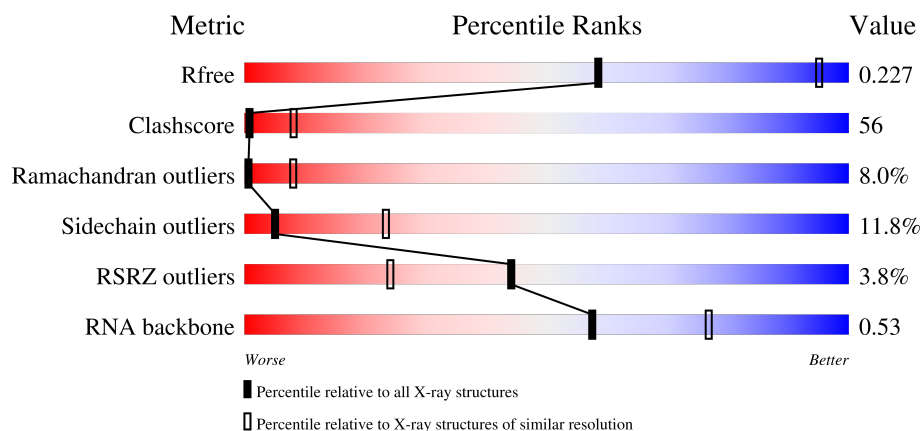
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 1085 (3.54-3.46)                                      |
| Clashscore            | 190562                      | 1140 (3.54-3.46)                                      |
| Ramachandran outliers | 187476                      | 1113 (3.54-3.46)                                      |
| Sidechain outliers    | 187428                      | 1114 (3.54-3.46)                                      |
| RSRZ outliers         | 180081                      | 1084 (3.54-3.46)                                      |
| RNA backbone          | 3983                        | 1010 (3.98-3.02)                                      |

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     | 1733   |                  |
| 2   | B     | 1224   |                  |
| 3   | C     | 318    |                  |
| 4   | D     | 221    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 5   | E     | 215    |                  |
| 6   | F     | 155    |                  |
| 7   | G     | 171    |                  |
| 8   | H     | 146    |                  |
| 9   | I     | 122    |                  |
| 10  | J     | 70     |                  |
| 11  | K     | 120    |                  |
| 12  | L     | 70     |                  |
| 13  | T     | 26     |                  |
| 14  | N     | 13     |                  |
| 15  | P     | 17     |                  |

## 2 Entry composition [i](#)

There are 17 unique types of molecules in this entry. The entry contains 31777 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 DNA-directed RNA polymerase II subunit RPB1.

| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 1   | A     | 1416     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 11143 | 7021 | 1949 | 2111 | 62 |         |         |       |

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 2   | B     | 1104     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 8779  | 5560 | 1537 | 1627 | 55 |         |         |       |

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 3   | C     | 266      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2095  | 1317 | 348 | 417 | 13 |         |         |       |

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 4   | D     | 178      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1434  | 887 | 257 | 288 | 2 |         |         |       |

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 5   | E     | 214      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1752  | 1111 | 309 | 321 | 11 |         |         |       |

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6   | F     | 87       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 705   | 451 | 119 | 132 | 3 |         |         |       |

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 7   | G     | 171      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1340  | 861 | 222 | 249 | 8 |         |         |       |

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8   | H     | 134      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1076  | 677 | 182 | 213 | 4 |         |         |       |

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

| Mol | Chain | Residues | Atoms |     |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 9   | I     | 119      | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 971   | 596 | 179 | 186 | 10 |         |         |       |

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 10  | J     | 65       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 532   | 339 | 93 | 94 | 6 |         |         |       |

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 11  | K     | 114      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 919   | 590 | 156 | 171 | 2 |         |         |       |

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 12  | L     | 46       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 363   | 224 | 72 | 63 | 4 |         |         |       |

- Molecule 13 is a DNA chain called 5'-D(\*AP\*GP\*CP\*TP\*CP\*AP\*A\*GP\*TP\*AP\*GP\*TP\*TP\*AP\*TP\*GP\*CP\*CP\*(BRU)P\*GP\*GP\*TP\*CP\*AP\*TP\*T)-3'.

| Mol | Chain | Residues | Atoms |    |     |    |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|-----|----|-----|----|---------|---------|-------|
| 13  | T     | 17       | Total | Br | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 347   | 1  | 166 | 61 | 103 | 16 |         |         |       |

- Molecule 14 is a DNA chain called 5'-D(\*T\*AP\*CP\*TP\*AP\*CP\*TP\*TP\*GP\*AP\*GP\*CP\*T)-3'.

| Mol | Chain | Residues | Atoms |    |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|---------|-------|
| 14  | N     | 5        | Total | C  | N  | O  | P | 0       | 0       | 0     |
|     |       |          | 97    | 48 | 18 | 27 | 4 |         |         |       |

- Molecule 15 is a RNA chain called 5'-R(\*UP\*GP\*CP\*AP\*UP\*UP\*UP\*CP\*GP\*AP\*CP\*CP\*AP\*GP\*GP\*CP\*A)-3'.

| Mol | Chain | Residues | Atoms |    |    |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|----|---------|---------|-------|
| 15  | P     | 10       | Total | C  | N  | O  | P  | 0       | 0       | 0     |
|     |       |          | 215   | 96 | 42 | 67 | 10 |         |         |       |

- Molecule 16 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 16  | A     | 2        | Total | Zn | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 16  | B     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 16  | C     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 16  | I     | 2        | Total | Zn | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 16  | J     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 16  | L     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

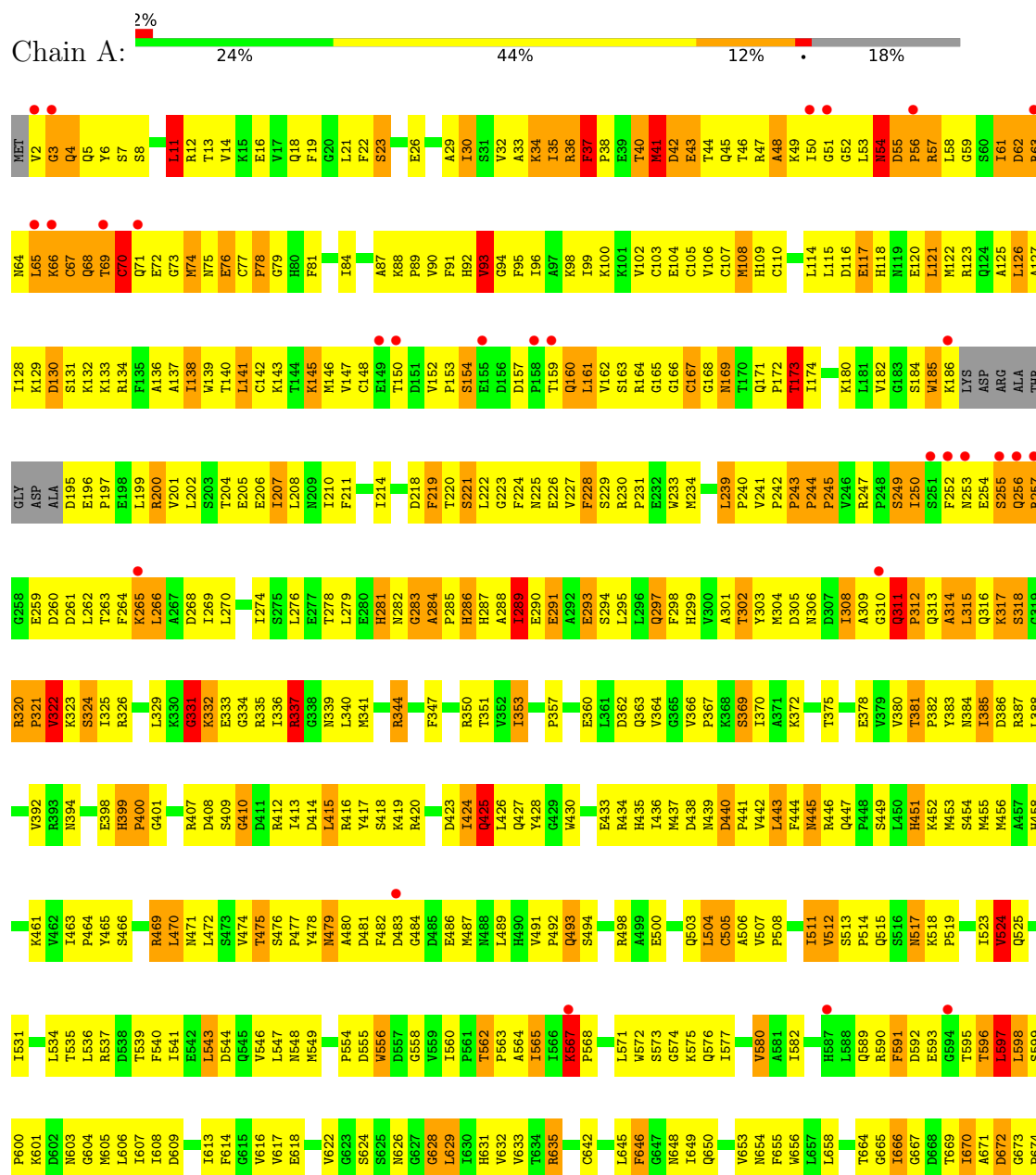
- Molecule 17 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 17  | A     | 1        | Total | Mg | 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.

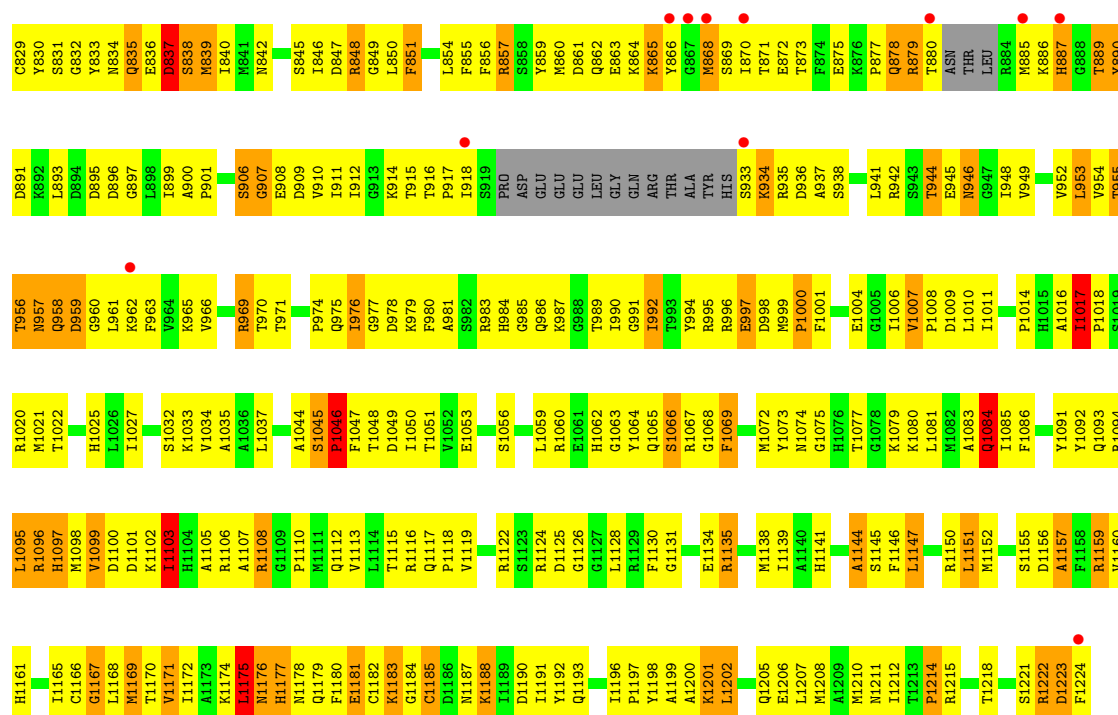
- Molecule 1: DNA-directed RNA polymerase II subunit RPB1



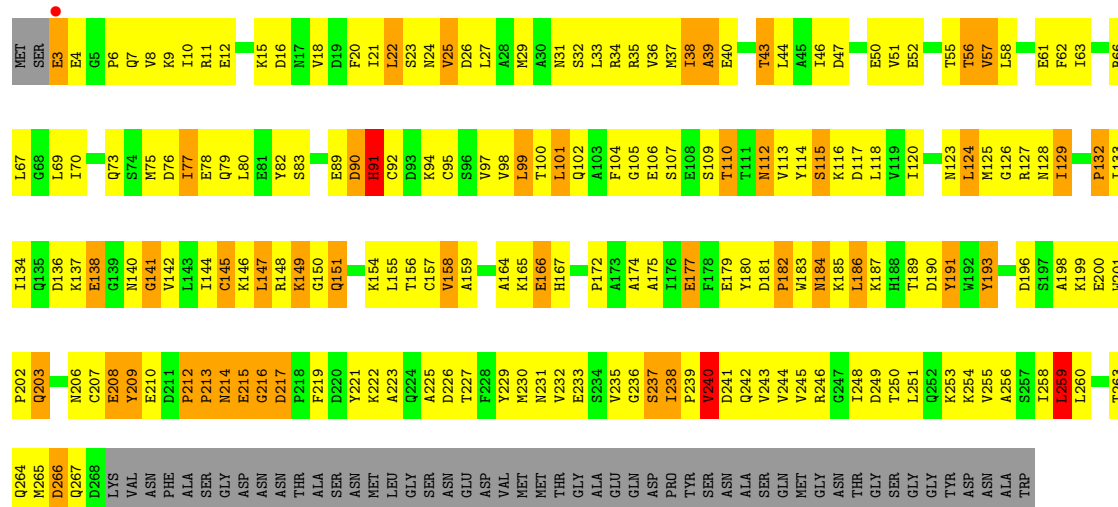


Chain B:  5% 23% 51% 15% 10%

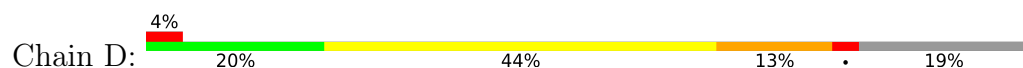


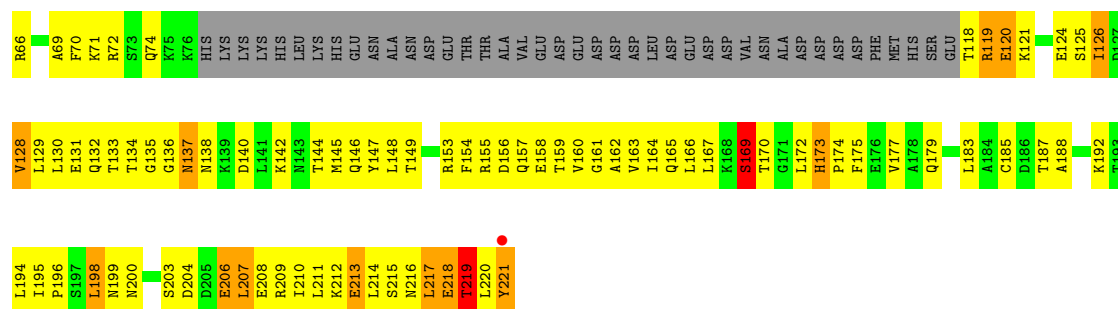


• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

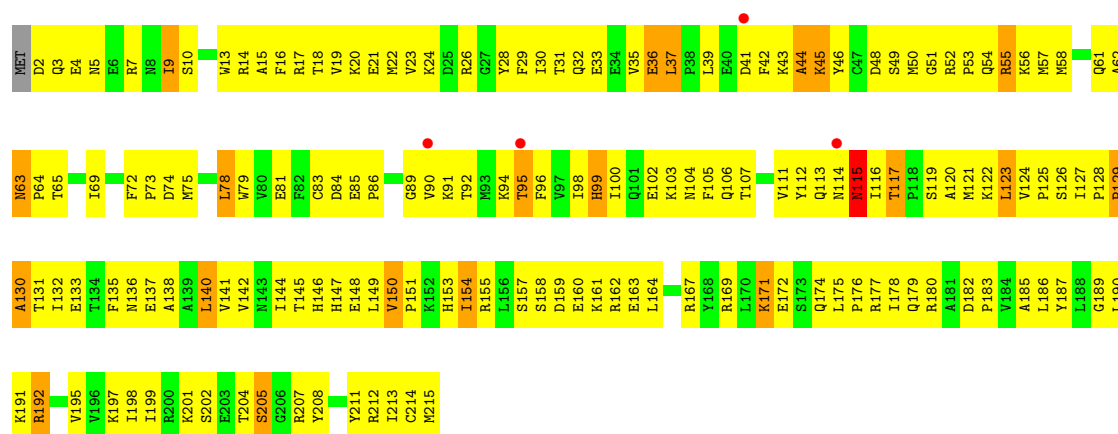


• Molecule 4: DNA-directed RNA polymerase II subunit RPB4

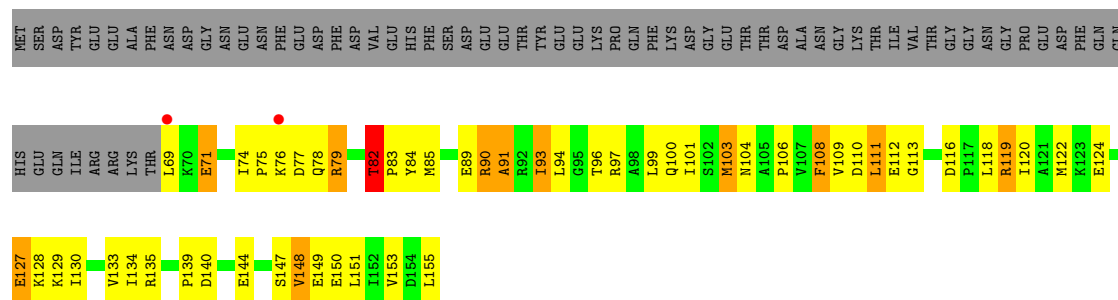
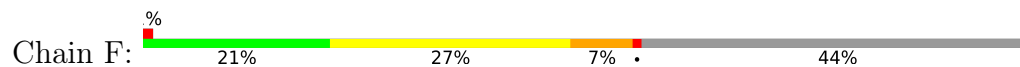




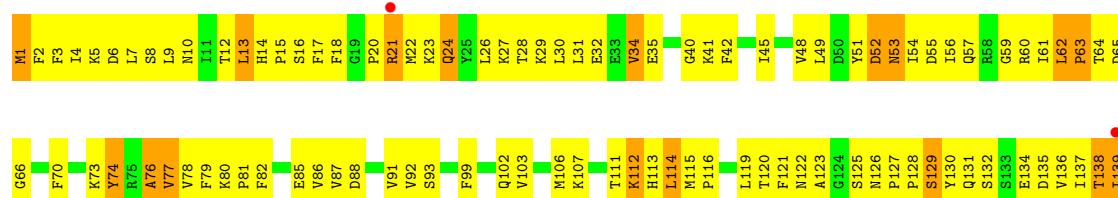
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1



• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

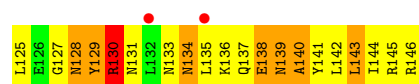
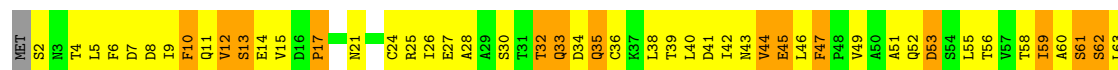
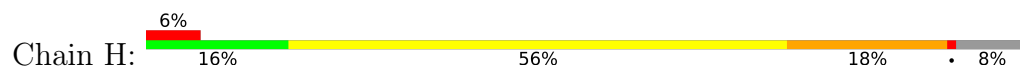


• Molecule 7: DNA-directed RNA polymerase II subunit RPB7

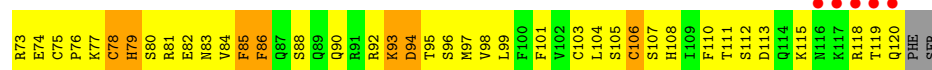




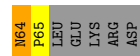
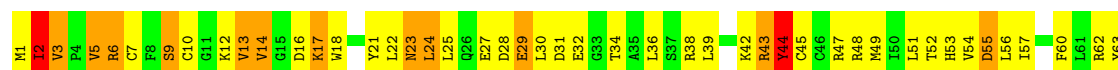
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



- Molecule 9: DNA-directed RNA polymerase II subunit RPB9



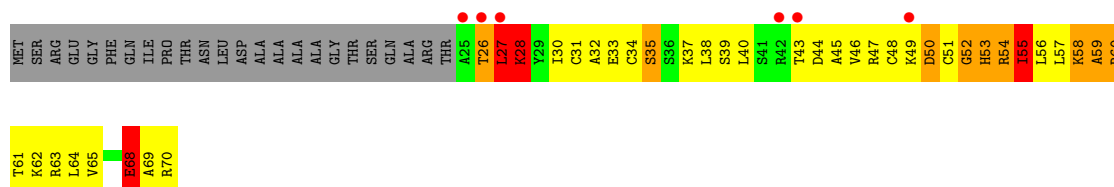
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5



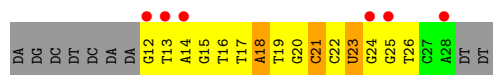
- Molecule 11: DNA-directed RNA polymerase II subunit RPB11



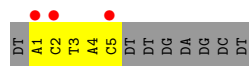
- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4



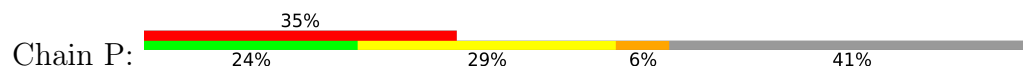
- Molecule 13: 5'-D(\*AP\*GP\*CP\*TP\*CP\*AP\*A\*GP\*TP\*AP\*GP\*TP\*TP\*AP\*TP\*GP\*CP\*CP\*(BRU)P\*GP\*GP\*TP\*CP\*AP\*TP\*T)-3'



- Molecule 14: 5'-D(\*T\*AP\*CP\*TP\*AP\*CP\*TP\*TP\*GP\*AP\*GP\*CP\*T)-3'



- Molecule 15: 5'-R(\*UP\*GP\*CP\*AP\*UP\*UP\*UP\*CP\*GP\*AP\*CP\*CP\*AP\*GP\*GP\*CP\*A)-3'



## 4 Data and refinement statistics

| Property                                                                | Value                                                                         | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------------------------|------------------|
| Space group                                                             | C 2 2 21                                                                      | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 222.25Å 393.38Å 283.09Å<br>90.00° 90.00° 90.00°                               | Depositor        |
| Resolution (Å)                                                          | 50.00 – 3.50<br>50.00 – 3.50                                                  | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.9 (50.00-3.50)<br>99.9 (50.00-3.50)                                        | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                                               | Depositor        |
| $R_{sym}$                                                               | 0.10                                                                          | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 3.76 (at 3.48Å)                                                               | Xtriage          |
| Refinement program                                                      | CNS 1.2                                                                       | Depositor        |
| R, $R_{free}$                                                           | 0.210 , 0.226<br>0.212 , 0.227                                                | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 4056 reflections (2.61%)                                                      | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 85.9                                                                          | Xtriage          |
| Anisotropy                                                              | 0.056                                                                         | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.33 , 98.6                                                                   | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$                   | Xtriage          |
| Estimated twinning fraction                                             | 0.017 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l<br>0.024 for 1/2*h+1/2*k,3/2*h-1/2*k,-l | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.91                                                                          | EDS              |
| Total number of atoms                                                   | 31777                                                                         | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 82.0                                                                          | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.92% 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, BRU, 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     | 0.62         | 1/11342 (0.0%) | 1.14        | 97/15337 (0.6%)  |
| 2   | B     | 0.58         | 0/8948         | 1.10        | 66/12062 (0.5%)  |
| 3   | C     | 0.59         | 0/2133         | 1.12        | 12/2891 (0.4%)   |
| 4   | D     | 0.56         | 0/1444         | 1.17        | 20/1935 (1.0%)   |
| 5   | E     | 0.53         | 0/1788         | 1.09        | 9/2406 (0.4%)    |
| 6   | F     | 0.69         | 0/717          | 1.31        | 9/967 (0.9%)     |
| 7   | G     | 0.58         | 0/1368         | 1.18        | 10/1844 (0.5%)   |
| 8   | H     | 0.47         | 0/1094         | 1.02        | 5/1481 (0.3%)    |
| 9   | I     | 0.52         | 0/989          | 1.09        | 5/1331 (0.4%)    |
| 10  | J     | 0.61         | 0/541          | 1.13        | 5/727 (0.7%)     |
| 11  | K     | 0.56         | 0/937          | 0.97        | 2/1265 (0.2%)    |
| 12  | L     | 0.60         | 0/365          | 1.14        | 3/485 (0.6%)     |
| 13  | T     | 0.37         | 0/365          | 0.87        | 0/560            |
| 14  | N     | 0.37         | 0/108          | 0.72        | 0/164            |
| 15  | P     | 0.38         | 0/240          | 0.81        | 1/372 (0.3%)     |
| All | All   | 0.59         | 1/32379 (0.0%) | 1.11        | 244/43827 (0.6%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 2   | B     | 0                   | 1                   |
| 8   | H     | 0                   | 1                   |
| 13  | T     | 0                   | 3                   |
| All | All   | 0                   | 5                   |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | A     | 55  | ASP  | CA-C  | -5.93 | 1.45        | 1.52     |

All (244) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|--------|-------------|----------|
| 6   | F     | 71   | GLU  | N-CA-C | -13.24 | 96.48       | 113.17   |
| 2   | B     | 427  | ASP  | N-CA-C | -12.54 | 100.33      | 114.62   |
| 1   | A     | 3    | GLY  | N-CA-C | -11.71 | 97.99       | 115.32   |
| 2   | B     | 1185 | CYS  | N-CA-C | -11.67 | 99.74       | 114.56   |
| 5   | E     | 171  | LYS  | N-CA-C | -11.54 | 95.65       | 110.53   |
| 5   | E     | 5    | ASN  | N-CA-C | -11.39 | 99.39       | 113.97   |
| 3   | C     | 39   | ALA  | N-CA-C | 11.36  | 128.24      | 112.45   |
| 4   | D     | 26   | THR  | N-CA-C | -10.99 | 98.12       | 112.41   |
| 7   | G     | 62   | LEU  | CA-C-N | -10.36 | 106.89      | 119.84   |
| 7   | G     | 62   | LEU  | C-N-CA | -10.36 | 106.89      | 119.84   |
| 2   | B     | 296  | GLU  | N-CA-C | -9.80  | 100.87      | 113.12   |
| 7   | G     | 65   | ASP  | N-CA-C | -9.42  | 96.52       | 110.46   |
| 2   | B     | 363  | HIS  | N-CA-C | -9.39  | 97.40       | 110.35   |
| 1   | A     | 511  | ILE  | N-CA-C | 9.04   | 119.63      | 110.23   |
| 1   | A     | 117  | GLU  | N-CA-C | -8.78  | 102.48      | 113.01   |
| 4   | D     | 31   | GLN  | N-CA-C | -8.72  | 101.24      | 112.23   |
| 1   | A     | 629  | LEU  | N-CA-C | -8.50  | 101.93      | 111.71   |
| 1   | A     | 56   | PRO  | N-CA-C | -8.32  | 95.34       | 112.47   |
| 4   | D     | 38   | ILE  | N-CA-C | 8.30   | 120.83      | 108.54   |
| 2   | B     | 428  | ILE  | N-CA-C | -8.24  | 102.39      | 110.72   |
| 12  | L     | 68   | GLU  | N-CA-C | -8.12  | 97.78       | 109.96   |
| 7   | G     | 34   | VAL  | N-CA-C | 8.11   | 118.54      | 111.56   |
| 4   | D     | 188  | ALA  | N-CA-C | -8.04  | 102.46      | 111.71   |
| 10  | J     | 5    | VAL  | N-CA-C | -7.99  | 99.27       | 109.58   |
| 1   | A     | 466  | SER  | N-CA-C | 7.96   | 121.79      | 112.72   |
| 1   | A     | 40   | THR  | N-CA-C | -7.86  | 102.31      | 111.03   |
| 2   | B     | 473  | MET  | N-CA-C | -7.83  | 103.45      | 113.16   |
| 1   | A     | 1162 | VAL  | N-CA-C | -7.77  | 103.86      | 112.80   |
| 1   | A     | 710  | LEU  | N-CA-C | -7.77  | 102.14      | 111.69   |
| 4   | D     | 41   | GLN  | N-CA-C | -7.71  | 103.86      | 112.57   |
| 1   | A     | 311  | GLN  | N-CA-C | 7.71   | 126.84      | 109.81   |
| 2   | B     | 807  | ARG  | N-CA-C | -7.68  | 102.91      | 111.82   |
| 1   | A     | 266  | LEU  | N-CA-C | -7.64  | 102.29      | 111.69   |
| 2   | B     | 851  | PHE  | N-CA-C | 7.63   | 122.17      | 112.86   |
| 1   | A     | 998  | LEU  | N-CA-C | 7.59   | 120.75      | 109.59   |
| 4   | D     | 24   | ALA  | N-CA-C | 7.58   | 118.70      | 108.23   |
| 2   | B     | 934  | LYS  | N-CA-C | 7.45   | 121.60      | 107.75   |
| 9   | I     | 85   | PHE  | N-CA-C | 7.43   | 120.61      | 110.35   |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2   | B     | 1177 | HIS  | N-CA-C  | -7.43 | 103.29      | 112.88   |
| 2   | B     | 976  | ILE  | N-CA-C  | 7.43  | 117.51      | 110.53   |
| 4   | D     | 72   | ARG  | N-CA-C  | -7.38 | 103.53      | 112.54   |
| 1   | A     | 1256 | GLU  | N-CA-C  | 7.28  | 119.11      | 111.03   |
| 1   | A     | 23   | SER  | N-CA-C  | -7.22 | 100.97      | 110.07   |
| 7   | G     | 64   | THR  | N-CA-C  | -7.18 | 103.64      | 113.18   |
| 1   | A     | 1311 | VAL  | N-CA-C  | 7.14  | 118.11      | 108.11   |
| 1   | A     | 1005 | GLU  | N-CA-C  | 7.13  | 118.70      | 111.07   |
| 1   | A     | 440  | ASP  | N-CA-C  | -7.10 | 100.70      | 109.65   |
| 1   | A     | 4    | GLN  | N-CA-C  | 7.10  | 125.93      | 110.80   |
| 2   | B     | 1066 | SER  | N-CA-C  | 7.09  | 120.05      | 111.82   |
| 2   | B     | 1009 | ASP  | N-CA-C  | -7.03 | 105.24      | 113.88   |
| 4   | D     | 8    | PHE  | N-CA-C  | 6.99  | 125.69      | 110.80   |
| 1   | A     | 30   | ILE  | CB-CA-C | -6.96 | 103.06      | 111.97   |
| 1   | A     | 1104 | ILE  | N-CA-C  | 6.94  | 117.44      | 110.23   |
| 2   | B     | 66   | ASP  | N-CA-C  | -6.90 | 103.25      | 113.61   |
| 9   | I     | 68   | LEU  | CA-C-N  | 6.86  | 126.78      | 119.85   |
| 9   | I     | 68   | LEU  | C-N-CA  | 6.86  | 126.78      | 119.85   |
| 6   | F     | 82   | THR  | CA-C-N  | 6.84  | 126.55      | 119.64   |
| 6   | F     | 82   | THR  | C-N-CA  | 6.84  | 126.55      | 119.64   |
| 1   | A     | 1403 | GLU  | N-CA-C  | 6.84  | 125.37      | 110.80   |
| 1   | A     | 987  | VAL  | N-CA-C  | 6.81  | 117.51      | 110.36   |
| 1   | A     | 281  | HIS  | N-CA-C  | -6.79 | 104.61      | 113.17   |
| 2   | B     | 526  | GLU  | N-CA-C  | 6.77  | 120.70      | 108.17   |
| 3   | C     | 40   | GLU  | N-CA-C  | 6.73  | 121.16      | 112.41   |
| 3   | C     | 112  | ASN  | N-CA-C  | 6.73  | 119.70      | 108.73   |
| 1   | A     | 78   | PRO  | N-CA-C  | -6.70 | 98.68       | 112.47   |
| 2   | B     | 1184 | GLY  | N-CA-C  | -6.69 | 106.73      | 114.69   |
| 6   | F     | 108  | PHE  | N-CA-C  | 6.67  | 120.33      | 112.72   |
| 2   | B     | 628  | THR  | N-CA-C  | -6.66 | 104.29      | 112.88   |
| 4   | D     | 51   | ASN  | N-CA-C  | -6.66 | 100.67      | 110.52   |
| 2   | B     | 41   | LYS  | N-CA-C  | 6.56  | 119.76      | 111.69   |
| 1   | A     | 1404 | GLU  | N-CA-C  | 6.55  | 121.11      | 111.87   |
| 2   | B     | 1101 | ASP  | N-CA-C  | -6.55 | 105.20      | 113.72   |
| 5   | E     | 63   | ASN  | N-CA-C  | 6.55  | 120.49      | 109.09   |
| 10  | J     | 9    | SER  | N-CA-C  | 6.55  | 118.11      | 110.97   |
| 1   | A     | 1163 | ILE  | CA-C-N  | 6.53  | 125.76      | 118.97   |
| 1   | A     | 1163 | ILE  | C-N-CA  | 6.53  | 125.76      | 118.97   |
| 1   | A     | 242  | PRO  | CA-C-N  | 6.50  | 127.08      | 120.38   |
| 1   | A     | 242  | PRO  | C-N-CA  | 6.50  | 127.08      | 120.38   |
| 1   | A     | 173  | THR  | N-CA-C  | -6.49 | 100.06      | 109.59   |
| 1   | A     | 1389 | PHE  | N-CA-C  | 6.45  | 118.85      | 111.11   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 15  | P     | 1    | C    | N1-C1'-C2' | 6.45  | 121.67      | 112.00   |
| 5   | E     | 205  | SER  | N-CA-C     | 6.45  | 120.45      | 112.59   |
| 1   | A     | 886  | ILE  | N-CA-C     | 6.44  | 116.93      | 110.23   |
| 3   | C     | 200  | GLU  | N-CA-C     | 6.41  | 118.35      | 111.36   |
| 1   | A     | 1451 | VAL  | N-CA-C     | -6.41 | 106.73      | 112.12   |
| 4   | D     | 12   | ARG  | N-CA-C     | 6.40  | 119.65      | 110.24   |
| 2   | B     | 555  | ILE  | N-CA-C     | -6.33 | 104.16      | 110.30   |
| 2   | B     | 681  | TRP  | N-CA-C     | -6.33 | 102.92      | 112.04   |
| 1   | A     | 55   | ASP  | N-CA-CB    | 6.33  | 121.63      | 110.37   |
| 7   | G     | 76   | ALA  | N-CA-C     | 6.31  | 117.81      | 108.60   |
| 3   | C     | 91   | HIS  | N-CA-C     | 6.30  | 118.12      | 108.42   |
| 1   | A     | 398  | GLU  | N-CA-C     | -6.29 | 102.22      | 110.53   |
| 1   | A     | 1421 | CYS  | N-CA-C     | -6.22 | 103.59      | 111.92   |
| 2   | B     | 99   | LYS  | N-CA-C     | -6.21 | 101.52      | 110.08   |
| 4   | D     | 209  | ARG  | N-CA-C     | -6.20 | 104.15      | 111.03   |
| 1   | A     | 289  | ILE  | N-CA-C     | -6.17 | 105.05      | 111.58   |
| 1   | A     | 293  | GLU  | N-CA-C     | -6.16 | 104.12      | 111.69   |
| 2   | B     | 838  | SER  | N-CA-C     | -6.15 | 99.98       | 109.52   |
| 2   | B     | 395  | GLN  | N-CA-C     | -6.15 | 102.38      | 110.43   |
| 2   | B     | 292  | ILE  | N-CA-C     | 6.15  | 122.16      | 108.88   |
| 2   | B     | 1045 | SER  | CA-C-N     | 6.06  | 127.41      | 119.84   |
| 2   | B     | 1045 | SER  | C-N-CA     | 6.06  | 127.41      | 119.84   |
| 1   | A     | 37   | PHE  | CA-C-N     | -6.05 | 114.66      | 120.83   |
| 1   | A     | 37   | PHE  | C-N-CA     | -6.05 | 114.66      | 120.83   |
| 1   | A     | 228  | PHE  | N-CA-C     | 6.03  | 120.77      | 113.41   |
| 2   | B     | 1099 | VAL  | N-CA-C     | 6.00  | 116.66      | 110.36   |
| 1   | A     | 539  | THR  | N-CA-C     | 6.00  | 117.79      | 109.15   |
| 1   | A     | 513  | SER  | N-CA-C     | 6.00  | 117.62      | 110.07   |
| 10  | J     | 44   | TYR  | N-CA-C     | 5.95  | 119.37      | 111.75   |
| 1   | A     | 513  | SER  | CA-C-N     | 5.95  | 125.57      | 119.56   |
| 1   | A     | 513  | SER  | C-N-CA     | 5.95  | 125.57      | 119.56   |
| 3   | C     | 259  | LEU  | N-CA-C     | -5.93 | 104.44      | 111.03   |
| 1   | A     | 320  | ARG  | CA-C-N     | 5.92  | 127.25      | 119.84   |
| 1   | A     | 320  | ARG  | C-N-CA     | 5.92  | 127.25      | 119.84   |
| 1   | A     | 505  | CYS  | N-CA-C     | 5.91  | 119.74      | 111.30   |
| 1   | A     | 331  | GLY  | N-CA-C     | 5.90  | 127.17      | 113.18   |
| 1   | A     | 11   | LEU  | N-CA-C     | 5.89  | 118.13      | 108.52   |
| 1   | A     | 227  | VAL  | CB-CA-C    | -5.89 | 104.78      | 111.55   |
| 9   | I     | 52   | ILE  | N-CA-C     | 5.87  | 115.98      | 108.12   |
| 1   | A     | 524  | VAL  | N-CA-C     | 5.86  | 115.97      | 108.82   |
| 1   | A     | 337  | ARG  | N-CA-C     | 5.86  | 118.44      | 111.71   |
| 1   | A     | 966  | ASN  | N-CA-C     | -5.85 | 104.98      | 111.36   |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | A     | 1169 | ILE  | N-CA-C  | 5.85  | 121.51      | 109.34   |
| 8   | H     | 34   | ASP  | N-CA-C  | -5.84 | 106.78      | 112.97   |
| 1   | A     | 861  | GLY  | N-CA-C  | -5.82 | 107.28      | 115.32   |
| 2   | B     | 829  | CYS  | N-CA-C  | -5.82 | 100.18      | 109.96   |
| 1   | A     | 1395 | GLY  | N-CA-C  | 5.82  | 118.62      | 111.93   |
| 2   | B     | 1201 | LYS  | N-CA-C  | -5.80 | 104.96      | 111.28   |
| 2   | B     | 650  | GLU  | N-CA-C  | 5.74  | 117.83      | 108.76   |
| 1   | A     | 239  | LEU  | N-CA-C  | 5.74  | 119.02      | 108.69   |
| 2   | B     | 498  | THR  | N-CA-C  | 5.71  | 118.72      | 109.40   |
| 1   | A     | 143  | LYS  | N-CA-C  | -5.71 | 104.66      | 111.69   |
| 2   | B     | 208  | SER  | N-CA-C  | 5.71  | 118.73      | 110.28   |
| 8   | H     | 130  | ARG  | N-CA-C  | -5.71 | 105.44      | 113.20   |
| 6   | F     | 148  | VAL  | N-CA-C  | -5.68 | 104.83      | 110.62   |
| 1   | A     | 646  | PHE  | N-CA-C  | -5.67 | 105.00      | 111.07   |
| 2   | B     | 1188 | LYS  | N-CA-C  | -5.67 | 105.77      | 114.16   |
| 2   | B     | 1084 | GLN  | N-CA-C  | -5.67 | 100.47      | 109.59   |
| 5   | E     | 55   | ARG  | N-CA-C  | 5.66  | 117.44      | 111.28   |
| 1   | A     | 108  | MET  | N-CA-C  | -5.65 | 103.46      | 110.41   |
| 2   | B     | 570  | VAL  | CA-C-N  | 5.65  | 125.11      | 119.24   |
| 2   | B     | 570  | VAL  | C-N-CA  | 5.65  | 125.11      | 119.24   |
| 1   | A     | 875  | ALA  | N-CA-C  | 5.65  | 119.68      | 112.34   |
| 7   | G     | 52   | ASP  | N-CA-C  | 5.64  | 117.42      | 111.28   |
| 2   | B     | 837  | ASP  | N-CA-C  | 5.63  | 119.47      | 111.92   |
| 2   | B     | 736  | THR  | N-CA-C  | -5.63 | 106.23      | 114.39   |
| 8   | H     | 35   | GLN  | N-CA-C  | -5.63 | 106.34      | 113.43   |
| 2   | B     | 513  | GLN  | N-CA-C  | 5.60  | 117.92      | 110.53   |
| 1   | A     | 567  | LYS  | CA-C-N  | -5.59 | 113.16      | 118.97   |
| 1   | A     | 567  | LYS  | C-N-CA  | -5.59 | 113.16      | 118.97   |
| 2   | B     | 1135 | ARG  | N-CA-C  | -5.58 | 105.11      | 111.14   |
| 1   | A     | 425  | GLN  | N-CA-C  | -5.57 | 99.33       | 108.41   |
| 2   | B     | 1130 | PHE  | N-CA-C  | -5.55 | 98.19       | 108.24   |
| 4   | D     | 7    | THR  | N-CA-C  | 5.55  | 116.64      | 107.20   |
| 2   | B     | 649  | LYS  | N-CA-C  | -5.54 | 101.51      | 110.32   |
| 6   | F     | 127  | GLU  | N-CA-C  | -5.54 | 105.21      | 112.41   |
| 4   | D     | 137  | ASN  | N-CA-C  | -5.53 | 105.31      | 113.61   |
| 2   | B     | 542  | MET  | N-CA-C  | 5.53  | 118.07      | 111.71   |
| 6   | F     | 74   | ILE  | CA-C-N  | 5.51  | 125.51      | 119.89   |
| 6   | F     | 74   | ILE  | C-N-CA  | 5.51  | 125.51      | 119.89   |
| 1   | A     | 1424 | VAL  | CB-CA-C | -5.51 | 104.83      | 111.88   |
| 2   | B     | 748  | ILE  | N-CA-C  | -5.50 | 104.86      | 112.50   |
| 2   | B     | 423  | LYS  | N-CA-C  | -5.50 | 105.31      | 112.23   |
| 4   | D     | 169  | SER  | N-CA-C  | -5.49 | 107.59      | 114.56   |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 7   | G     | 129  | SER  | N-CA-C  | 5.49  | 116.60      | 108.86   |
| 1   | A     | 847  | ASP  | N-CA-C  | 5.49  | 120.95      | 113.37   |
| 3   | C     | 191  | TYR  | N-CA-C  | 5.47  | 118.29      | 110.24   |
| 5   | E     | 63   | ASN  | CA-C-N  | 5.47  | 126.67      | 119.84   |
| 5   | E     | 63   | ASN  | C-N-CA  | 5.47  | 126.67      | 119.84   |
| 2   | B     | 102  | VAL  | CB-CA-C | -5.47 | 105.25      | 111.59   |
| 12  | L     | 58   | LYS  | N-CA-C  | 5.46  | 119.09      | 111.56   |
| 2   | B     | 606  | LYS  | N-CA-C  | -5.45 | 107.17      | 113.88   |
| 2   | B     | 814  | PHE  | N-CA-C  | 5.44  | 116.89      | 111.07   |
| 1   | A     | 362  | ASP  | N-CA-C  | 5.43  | 119.02      | 112.93   |
| 1   | A     | 1405 | THR  | N-CA-C  | 5.42  | 122.35      | 110.80   |
| 1   | A     | 827  | THR  | N-CA-C  | -5.42 | 105.45      | 111.36   |
| 1   | A     | 3    | GLY  | CA-C-N  | 5.42  | 131.89      | 121.54   |
| 1   | A     | 3    | GLY  | C-N-CA  | 5.42  | 131.89      | 121.54   |
| 6   | F     | 91   | ALA  | N-CA-C  | -5.41 | 105.29      | 111.07   |
| 1   | A     | 174  | ILE  | N-CA-C  | 5.40  | 116.76      | 108.71   |
| 11  | K     | 68   | PHE  | N-CA-C  | 5.38  | 117.18      | 108.41   |
| 1   | A     | 54   | ASN  | CA-C-N  | 5.37  | 134.90      | 121.80   |
| 1   | A     | 54   | ASN  | C-N-CA  | 5.37  | 134.90      | 121.80   |
| 11  | K     | 55   | LYS  | N-CA-C  | -5.37 | 106.32      | 112.92   |
| 7   | G     | 40   | GLY  | N-CA-C  | -5.37 | 107.67      | 114.16   |
| 2   | B     | 901  | PRO  | N-CA-C  | 5.36  | 120.89      | 113.98   |
| 9   | I     | 10   | CYS  | N-CA-C  | 5.35  | 118.89      | 111.55   |
| 4   | D     | 70   | PHE  | N-CA-C  | -5.35 | 105.99      | 113.37   |
| 1   | A     | 1064 | VAL  | N-CA-C  | 5.34  | 120.46      | 109.34   |
| 1   | A     | 454  | SER  | N-CA-C  | -5.34 | 106.77      | 113.28   |
| 4   | D     | 54   | GLU  | N-CA-C  | -5.32 | 105.59      | 111.71   |
| 2   | B     | 603  | LEU  | N-CA-C  | -5.30 | 105.08      | 112.45   |
| 3   | C     | 193  | TYR  | N-CA-C  | 5.30  | 115.35      | 107.88   |
| 1   | A     | 291  | GLU  | N-CA-C  | -5.29 | 106.33      | 112.89   |
| 3   | C     | 203  | GLN  | N-CA-C  | -5.28 | 101.92      | 110.32   |
| 2   | B     | 832  | GLY  | N-CA-C  | -5.28 | 107.51      | 115.32   |
| 2   | B     | 39   | ARG  | N-CA-C  | -5.27 | 104.78      | 111.11   |
| 2   | B     | 629  | ASP  | N-CA-C  | 5.27  | 117.73      | 110.35   |
| 1   | A     | 564  | ALA  | N-CA-C  | -5.26 | 105.66      | 111.71   |
| 1   | A     | 683  | ILE  | N-CA-C  | -5.26 | 105.48      | 110.42   |
| 3   | C     | 38   | ILE  | CB-CA-C | -5.26 | 105.13      | 112.02   |
| 2   | B     | 1000 | PRO  | N-CA-C  | -5.25 | 102.91      | 111.68   |
| 5   | E     | 117  | THR  | N-CA-C  | 5.24  | 116.01      | 109.57   |
| 2   | B     | 35   | SER  | N-CA-C  | -5.24 | 105.47      | 111.07   |
| 1   | A     | 74   | MET  | N-CA-C  | 5.22  | 121.92      | 110.80   |
| 1   | A     | 1444 | MET  | N-CA-C  | 5.22  | 117.75      | 109.50   |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2   | B     | 693  | ILE  | N-CA-C  | 5.21  | 115.12      | 107.15   |
| 2   | B     | 896  | ASP  | N-CA-C  | -5.21 | 106.90      | 113.20   |
| 2   | B     | 510  | LYS  | N-CA-C  | 5.21  | 121.32      | 109.81   |
| 8   | H     | 45   | GLU  | N-CA-C  | -5.21 | 106.99      | 113.55   |
| 3   | C     | 212  | PRO  | CA-C-N  | 5.20  | 126.34      | 119.84   |
| 3   | C     | 212  | PRO  | C-N-CA  | 5.20  | 126.34      | 119.84   |
| 2   | B     | 825  | VAL  | N-CA-C  | 5.20  | 116.45      | 108.71   |
| 4   | D     | 29   | LEU  | N-CA-C  | -5.19 | 103.07      | 110.59   |
| 1   | A     | 1376 | THR  | N-CA-C  | 5.17  | 119.71      | 113.41   |
| 8   | H     | 13   | SER  | N-CA-C  | -5.17 | 105.54      | 111.07   |
| 1   | A     | 1339 | LEU  | N-CA-C  | 5.16  | 119.55      | 113.16   |
| 10  | J     | 5    | VAL  | CB-CA-C | -5.14 | 103.44      | 111.26   |
| 1   | A     | 366  | VAL  | N-CA-C  | 5.14  | 113.59      | 107.73   |
| 1   | A     | 243  | PRO  | CA-C-N  | 5.14  | 125.67      | 120.38   |
| 1   | A     | 243  | PRO  | C-N-CA  | 5.14  | 125.67      | 120.38   |
| 10  | J     | 3    | VAL  | N-CA-C  | 5.14  | 114.61      | 108.96   |
| 1   | A     | 321  | PRO  | N-CA-C  | 5.13  | 123.05      | 112.47   |
| 1   | A     | 582  | ILE  | CA-C-N  | 5.13  | 126.26      | 119.84   |
| 1   | A     | 582  | ILE  | C-N-CA  | 5.13  | 126.26      | 119.84   |
| 1   | A     | 890  | ASP  | N-CA-C  | -5.13 | 105.81      | 111.71   |
| 12  | L     | 52   | GLY  | N-CA-C  | -5.13 | 106.58      | 112.73   |
| 2   | B     | 1144 | ALA  | N-CA-C  | 5.12  | 117.26      | 111.02   |
| 2   | B     | 981  | ALA  | N-CA-C  | 5.10  | 116.27      | 108.52   |
| 2   | B     | 112  | LEU  | N-CA-C  | 5.08  | 116.84      | 110.24   |
| 5   | E     | 122  | LYS  | N-CA-C  | -5.08 | 107.11      | 113.15   |
| 1   | A     | 580  | VAL  | N-CA-C  | -5.07 | 105.45      | 112.50   |
| 1   | A     | 1207 | LEU  | N-CA-C  | 5.06  | 117.08      | 109.23   |
| 2   | B     | 574  | SER  | CA-C-N  | 5.06  | 126.17      | 119.84   |
| 2   | B     | 574  | SER  | C-N-CA  | 5.06  | 126.17      | 119.84   |
| 1   | A     | 1209 | MET  | N-CA-C  | -5.05 | 105.77      | 111.28   |
| 4   | D     | 217  | LEU  | N-CA-C  | -5.05 | 105.77      | 112.34   |
| 7   | G     | 138  | THR  | N-CA-C  | 5.05  | 115.82      | 108.14   |
| 2   | B     | 890  | TYR  | N-CA-C  | -5.03 | 107.31      | 113.50   |
| 1   | A     | 1403 | GLU  | CA-C-N  | -5.03 | 114.60      | 122.79   |
| 1   | A     | 1403 | GLU  | C-N-CA  | -5.03 | 114.60      | 122.79   |
| 4   | D     | 173  | HIS  | CA-C-N  | 5.01  | 125.03      | 119.32   |
| 4   | D     | 173  | HIS  | C-N-CA  | 5.01  | 125.03      | 119.32   |
| 1   | A     | 81   | PHE  | N-CA-C  | 5.00  | 117.16      | 110.35   |

There are no chirality outliers.

All (5) planarity outliers are listed below:

| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 2   | B     | 1192 | TYR  | Sidechain |
| 8   | H     | 102  | TYR  | Sidechain |
| 13  | T     | 18   | DA   | Sidechain |
| 13  | T     | 19   | DT   | Sidechain |
| 13  | T     | 21   | DC   | Sidechain |

## 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     | 11143 | 0        | 11217    | 1289    | 0            |
| 2   | B     | 8779  | 0        | 8808     | 1125    | 0            |
| 3   | C     | 2095  | 0        | 2051     | 273     | 0            |
| 4   | D     | 1434  | 0        | 1460     | 167     | 0            |
| 5   | E     | 1752  | 0        | 1776     | 208     | 0            |
| 6   | F     | 705   | 0        | 731      | 79      | 0            |
| 7   | G     | 1340  | 0        | 1357     | 140     | 0            |
| 8   | H     | 1076  | 0        | 1046     | 165     | 0            |
| 9   | I     | 971   | 0        | 929      | 123     | 0            |
| 10  | J     | 532   | 0        | 542      | 79      | 0            |
| 11  | K     | 919   | 0        | 929      | 90      | 0            |
| 12  | L     | 363   | 0        | 388      | 85      | 0            |
| 13  | T     | 347   | 0        | 192      | 20      | 0            |
| 14  | N     | 97    | 0        | 58       | 6       | 0            |
| 15  | P     | 215   | 0        | 111      | 6       | 0            |
| 16  | A     | 2     | 0        | 0        | 0       | 0            |
| 16  | B     | 1     | 0        | 0        | 0       | 0            |
| 16  | C     | 1     | 0        | 0        | 0       | 0            |
| 16  | I     | 2     | 0        | 0        | 0       | 0            |
| 16  | J     | 1     | 0        | 0        | 0       | 0            |
| 16  | L     | 1     | 0        | 0        | 0       | 0            |
| 17  | A     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 31777 | 0        | 31595    | 3563    | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 56.

All (3563) 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:559:SER:HA    | 2:B:563:MET:HB3  | 1.20                     | 1.18              |
| 2:B:583:ASN:HD21  | 2:B:628:THR:HG22 | 1.08                     | 1.17              |
| 2:B:622:LYS:HE2   | 9:I:59:VAL:HG22  | 1.28                     | 1.14              |
| 2:B:261:ARG:HH11  | 2:B:261:ARG:HB3  | 1.12                     | 1.13              |
| 2:B:1072:MET:HE3  | 2:B:1085:ILE:HB  | 1.23                     | 1.12              |
| 1:A:53:LEU:HD23   | 1:A:54:ASN:N     | 1.65                     | 1.12              |
| 1:A:567:LYS:HB3   | 8:H:96:VAL:H     | 1.06                     | 1.11              |
| 1:A:53:LEU:HD23   | 1:A:54:ASN:H     | 0.97                     | 1.10              |
| 1:A:901:LEU:H     | 1:A:926:GLN:NE2  | 1.47                     | 1.10              |
| 3:C:57:VAL:HG11   | 10:J:60:PHE:HB3  | 1.21                     | 1.10              |
| 5:E:124:VAL:HG13  | 5:E:132:ILE:HB   | 1.30                     | 1.07              |
| 8:H:4:THR:HA      | 8:H:60:ALA:HB2   | 1.30                     | 1.07              |
| 1:A:34:LYS:HE3    | 1:A:57:ARG:HH12  | 1.13                     | 1.06              |
| 2:B:278:GLN:HG2   | 2:B:279:ASP:H    | 1.14                     | 1.06              |
| 2:B:577:ALA:HB1   | 2:B:589:VAL:HG11 | 1.37                     | 1.05              |
| 9:I:93:LYS:H      | 9:I:93:LYS:HD3   | 1.22                     | 1.04              |
| 5:E:94:LYS:HE2    | 5:E:98:ILE:HD11  | 1.35                     | 1.04              |
| 1:A:41:MET:HB3    | 1:A:49:LYS:HA    | 1.40                     | 1.03              |
| 1:A:1161:THR:HG22 | 1:A:1163:ILE:H   | 1.21                     | 1.03              |
| 2:B:770:GLN:OE1   | 2:B:983:ARG:HA   | 1.58                     | 1.01              |
| 2:B:430:ARG:HB3   | 2:B:430:ARG:HH11 | 1.25                     | 1.01              |
| 2:B:510:LYS:CG    | 2:B:511:PRO:HD3  | 1.91                     | 1.01              |
| 12:L:26:THR:HG22  | 12:L:27:LEU:H    | 1.22                     | 1.01              |
| 1:A:49:LYS:HZ3    | 1:A:61:ILE:HG13  | 1.25                     | 1.00              |
| 1:A:1385:THR:HG23 | 1:A:1387:HIS:H   | 1.24                     | 1.00              |
| 2:B:579:ARG:HB2   | 2:B:586:TRP:HE1  | 1.25                     | 1.00              |
| 3:C:177:GLU:HG3   | 3:C:231:ASN:HB3  | 1.42                     | 1.00              |
| 1:A:353:ILE:HG21  | 1:A:487:MET:HG3  | 1.43                     | 0.99              |
| 5:E:56:LYS:HE2    | 5:E:84:ASP:HB2   | 1.45                     | 0.99              |
| 2:B:120:ARG:HH12  | 12:L:54:ARG:HH11 | 1.08                     | 0.98              |
| 2:B:114:PRO:HG3   | 2:B:181:LEU:HD11 | 1.46                     | 0.98              |
| 1:A:902:LEU:HG    | 1:A:926:GLN:HG3  | 1.46                     | 0.98              |
| 1:A:66:LYS:HZ3    | 1:A:68:GLN:H     | 1.07                     | 0.98              |
| 2:B:217:ARG:HE    | 2:B:405:ARG:HB2  | 1.26                     | 0.98              |
| 8:H:95:TYR:HE2    | 8:H:97:MET:HG3   | 1.25                     | 0.98              |
| 2:B:510:LYS:HG3   | 2:B:511:PRO:HD3  | 0.99                     | 0.98              |
| 1:A:308:ILE:HG22  | 1:A:309:ALA:H    | 1.26                     | 0.98              |
| 12:L:55:ILE:HG12  | 12:L:56:LEU:H    | 1.27                     | 0.97              |
| 1:A:108:MET:HA    | 1:A:210:ILE:HD13 | 1.40                     | 0.97              |
| 1:A:34:LYS:CE     | 1:A:57:ARG:HH12  | 1.76                     | 0.97              |
| 12:L:38:LEU:HD11  | 12:L:49:LYS:HE2  | 1.47                     | 0.97              |
| 1:A:407:ARG:HD2   | 1:A:413:ILE:HD11 | 1.42                     | 0.97              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:445:ASN:HB2   | 1:A:455:MET:HG2   | 1.45                     | 0.97              |
| 1:A:779:PHE:CE1   | 1:A:785:PRO:HD3   | 2.00                     | 0.96              |
| 4:D:118:THR:HB    | 4:D:121:LYS:HB2   | 1.44                     | 0.96              |
| 11:K:47:ARG:HB3   | 11:K:47:ARG:HH11  | 1.30                     | 0.96              |
| 2:B:508:LEU:N     | 14:N:1:DA:HO5'    | 1.61                     | 0.96              |
| 8:H:82:PRO:C      | 8:H:84:ALA:H      | 1.73                     | 0.96              |
| 1:A:90:VAL:HB     | 1:A:297:GLN:NE2   | 1.80                     | 0.96              |
| 10:J:64:ASN:HB3   | 10:J:65:PRO:CD    | 1.95                     | 0.96              |
| 10:J:16:ASP:OD1   | 10:J:17:LYS:HD2   | 1.66                     | 0.96              |
| 1:A:567:LYS:HB3   | 8:H:96:VAL:N      | 1.80                     | 0.95              |
| 1:A:779:PHE:HE1   | 1:A:785:PRO:HD3   | 1.31                     | 0.95              |
| 9:I:111:THR:HG22  | 9:I:112:SER:H     | 1.30                     | 0.95              |
| 1:A:399:HIS:HB3   | 1:A:400:PRO:HD3   | 1.48                     | 0.95              |
| 2:B:911:ILE:HD11  | 2:B:941:LEU:HD13  | 1.49                     | 0.95              |
| 1:A:688:LYS:HD2   | 1:A:691:LEU:HD23  | 1.46                     | 0.95              |
| 2:B:510:LYS:HG3   | 2:B:511:PRO:CD    | 1.95                     | 0.94              |
| 2:B:999:MET:HG3   | 2:B:1000:PRO:HD2  | 1.48                     | 0.94              |
| 2:B:1065:GLN:HE21 | 2:B:1067:ARG:N    | 1.65                     | 0.94              |
| 1:A:351:THR:HG22  | 2:B:1103:ILE:HA   | 1.47                     | 0.94              |
| 1:A:14:VAL:H      | 1:A:1432:GLN:HE22 | 1.03                     | 0.94              |
| 8:H:40:LEU:HD13   | 8:H:123:MET:HE3   | 1.49                     | 0.94              |
| 11:K:58:PHE:HB3   | 11:K:76:GLN:HB3   | 1.50                     | 0.94              |
| 2:B:751:VAL:HG13  | 2:B:812:LEU:HD22  | 1.49                     | 0.93              |
| 5:E:114:ASN:O     | 5:E:115:ASN:HB3   | 1.66                     | 0.93              |
| 9:I:50:THR:HG22   | 9:I:51:ASN:H      | 1.33                     | 0.93              |
| 1:A:541:ILE:HD13  | 1:A:549:MET:HE1   | 1.48                     | 0.93              |
| 1:A:244:PRO:HB2   | 1:A:245:PRO:HD3   | 1.51                     | 0.93              |
| 10:J:5:VAL:HG12   | 10:J:6:ARG:HG3    | 1.48                     | 0.93              |
| 1:A:754:SER:H     | 1:A:757:ASN:HD22  | 1.10                     | 0.93              |
| 1:A:41:MET:CB     | 1:A:49:LYS:HA     | 1.99                     | 0.92              |
| 1:A:567:LYS:HZ1   | 8:H:43:ASN:HB3    | 1.35                     | 0.92              |
| 1:A:858:ASN:ND2   | 1:A:860:LEU:H     | 1.66                     | 0.92              |
| 2:B:261:ARG:HB3   | 2:B:261:ARG:NH1   | 1.83                     | 0.92              |
| 1:A:903:ASN:HD22  | 1:A:904:THR:N     | 1.67                     | 0.92              |
| 1:A:830:LYS:O     | 1:A:834:THR:HB    | 1.70                     | 0.92              |
| 10:J:3:VAL:HG21   | 10:J:18:TRP:HB2   | 1.50                     | 0.92              |
| 1:A:34:LYS:HZ2    | 1:A:57:ARG:HH22   | 1.12                     | 0.92              |
| 3:C:56:THR:HG21   | 3:C:145:CYS:SG    | 2.10                     | 0.92              |
| 1:A:741:ASN:HD22  | 1:A:744:LYS:H     | 1.18                     | 0.92              |
| 2:B:710:LEU:HA    | 2:B:733:HIS:HB3   | 1.49                     | 0.92              |
| 4:D:155:ARG:HD3   | 4:D:221:TYR:HE1   | 1.34                     | 0.91              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:1065:GLN:NE2  | 2:B:1067:ARG:H    | 1.68                     | 0.91              |
| 13:T:24:DG:H2''   | 13:T:25:DG:H5'    | 1.52                     | 0.91              |
| 2:B:579:ARG:HB2   | 2:B:586:TRP:NE1   | 1.85                     | 0.91              |
| 6:F:93:ILE:HD11   | 6:F:134:ILE:HD11  | 1.53                     | 0.91              |
| 2:B:603:LEU:HD13  | 2:B:608:ASP:HB2   | 1.50                     | 0.91              |
| 1:A:855:THR:HG21  | 1:A:857:ARG:HE    | 1.33                     | 0.91              |
| 9:I:111:THR:HG22  | 9:I:113:ASP:H     | 1.32                     | 0.91              |
| 1:A:517:ASN:HD22  | 1:A:1364:ASN:HD22 | 1.04                     | 0.90              |
| 8:H:59:ILE:HG22   | 8:H:60:ALA:H      | 1.36                     | 0.90              |
| 1:A:315:LEU:HD23  | 1:A:315:LEU:H     | 1.36                     | 0.90              |
| 1:A:1116:LEU:N    | 1:A:1308:THR:HG22 | 1.86                     | 0.90              |
| 1:A:1420:ASP:HB3  | 1:A:1422:ARG:HG3  | 1.51                     | 0.90              |
| 2:B:996:ARG:HH12  | 3:C:174:ALA:HA    | 1.36                     | 0.90              |
| 6:F:103:MET:CE    | 7:G:66:GLY:H      | 1.82                     | 0.90              |
| 2:B:879:ARG:H     | 2:B:879:ARG:CZ    | 1.83                     | 0.90              |
| 2:B:806:THR:HG22  | 2:B:808:ALA:H     | 1.34                     | 0.90              |
| 2:B:789:MET:HE2   | 2:B:953:LEU:HD22  | 1.53                     | 0.90              |
| 1:A:1387:HIS:O    | 1:A:1391:ARG:HG3  | 1.72                     | 0.90              |
| 5:E:22:MET:HE3    | 5:E:26:ARG:NE     | 1.87                     | 0.90              |
| 7:G:34:VAL:HG11   | 7:G:74:TYR:HE1    | 1.37                     | 0.90              |
| 1:A:344:ARG:HB3   | 1:A:344:ARG:HH11  | 1.36                     | 0.89              |
| 1:A:913:LEU:HD12  | 1:A:914:GLU:H     | 1.38                     | 0.89              |
| 2:B:637:LEU:HD12  | 2:B:693:ILE:HD12  | 1.55                     | 0.89              |
| 1:A:66:LYS:NZ     | 1:A:68:GLN:H      | 1.71                     | 0.89              |
| 1:A:1385:THR:HG22 | 1:A:1388:GLY:H    | 1.35                     | 0.89              |
| 2:B:120:ARG:NH1   | 12:L:54:ARG:HH11  | 1.70                     | 0.89              |
| 2:B:36:ALA:HA     | 2:B:39:ARG:HD2    | 1.54                     | 0.89              |
| 2:B:744:HIS:HD2   | 2:B:745:PRO:HD2   | 1.37                     | 0.89              |
| 2:B:766:ARG:NH2   | 2:B:1020:ARG:HH11 | 1.70                     | 0.89              |
| 4:D:154:PHE:CD1   | 4:D:163:VAL:HG21  | 2.08                     | 0.88              |
| 10:J:1:MET:H1     | 10:J:57:ILE:H     | 1.21                     | 0.88              |
| 1:A:381:THR:HG22  | 1:A:383:TYR:H     | 1.36                     | 0.88              |
| 2:B:102:VAL:HG23  | 2:B:112:LEU:HB2   | 1.53                     | 0.88              |
| 2:B:516:ASN:HD22  | 2:B:516:ASN:N     | 1.70                     | 0.88              |
| 8:H:130:ARG:HH11  | 8:H:130:ARG:HB2   | 1.38                     | 0.88              |
| 2:B:766:ARG:HH22  | 2:B:1020:ARG:HH11 | 1.18                     | 0.88              |
| 2:B:642:ASP:HA    | 2:B:649:LYS:HA    | 1.54                     | 0.88              |
| 5:E:78:LEU:HB2    | 5:E:107:THR:HB    | 1.53                     | 0.88              |
| 1:A:87:ALA:HB3    | 1:A:276:LEU:HD23  | 1.56                     | 0.88              |
| 2:B:542:MET:HG2   | 2:B:747:MET:HE3   | 1.55                     | 0.88              |
| 8:H:89:LEU:C      | 8:H:91:ASP:H      | 1.81                     | 0.88              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:567:LYS:HD2   | 1:A:568:PRO:HD2  | 1.54                     | 0.88              |
| 1:A:901:LEU:H     | 1:A:926:GLN:HE21 | 1.20                     | 0.88              |
| 2:B:168:GLY:H     | 2:B:450:ALA:HB1  | 1.38                     | 0.88              |
| 2:B:706:GLN:HE22  | 2:B:730:ARG:HD3  | 1.38                     | 0.88              |
| 1:A:671:ALA:HB3   | 1:A:676:MET:HE2  | 1.57                     | 0.87              |
| 1:A:61:ILE:HG22   | 1:A:62:ASP:H     | 1.40                     | 0.87              |
| 1:A:534:LEU:O     | 1:A:574:GLY:HA3  | 1.73                     | 0.87              |
| 1:A:768:GLN:HG2   | 1:A:816:HIS:HA   | 1.57                     | 0.87              |
| 2:B:778:MET:HE1   | 2:B:1094:ARG:HD3 | 1.57                     | 0.86              |
| 9:I:111:THR:HG22  | 9:I:112:SER:N    | 1.86                     | 0.86              |
| 5:E:22:MET:HE3    | 5:E:26:ARG:HE    | 1.38                     | 0.86              |
| 1:A:107:CYS:HA    | 1:A:171:GLN:NE2  | 1.90                     | 0.86              |
| 1:A:288:ALA:HA    | 1:A:291:GLU:CD   | 2.01                     | 0.86              |
| 8:H:24:CYS:HB2    | 8:H:44:VAL:HG21  | 1.58                     | 0.86              |
| 2:B:469:GLN:O     | 2:B:472:ALA:HB3  | 1.74                     | 0.86              |
| 2:B:800:GLN:HB3   | 10:J:52:THR:CG2  | 2.05                     | 0.86              |
| 7:G:1:MET:HE1     | 7:G:79:PHE:HA    | 1.58                     | 0.86              |
| 12:L:28:LYS:HE3   | 12:L:39:SER:OG   | 1.75                     | 0.86              |
| 2:B:1065:GLN:HE21 | 2:B:1067:ARG:H   | 0.87                     | 0.85              |
| 2:B:1187:ASN:HD21 | 2:B:1190:ASP:HB3 | 1.41                     | 0.85              |
| 4:D:130:LEU:HD13  | 4:D:142:LYS:HG2  | 1.58                     | 0.85              |
| 1:A:40:THR:HG22   | 1:A:41:MET:HG3   | 1.59                     | 0.85              |
| 13:T:16:DT:H5'    | 13:T:16:DT:H6    | 1.41                     | 0.85              |
| 1:A:853:ASP:OD1   | 1:A:855:THR:HB   | 1.74                     | 0.85              |
| 2:B:243:ALA:HA    | 2:B:250:PHE:O    | 1.76                     | 0.85              |
| 4:D:12:ARG:HG2    | 4:D:12:ARG:HH11  | 1.42                     | 0.85              |
| 5:E:153:HIS:O     | 5:E:154:ILE:HG13 | 1.76                     | 0.85              |
| 1:A:855:THR:HG23  | 1:A:857:ARG:HG3  | 1.57                     | 0.84              |
| 1:A:1364:ASN:OD1  | 1:A:1366:ARG:HG2 | 1.77                     | 0.84              |
| 13:T:13:DT:H2''   | 13:T:14:DA:OP2   | 1.77                     | 0.84              |
| 7:G:128:PRO:O     | 7:G:138:THR:HG23 | 1.77                     | 0.84              |
| 2:B:616:ILE:HG13  | 2:B:697:GLU:HG3  | 1.59                     | 0.84              |
| 3:C:50:GLU:OE1    | 12:L:64:LEU:HD22 | 1.76                     | 0.84              |
| 1:A:567:LYS:CG    | 1:A:568:PRO:HD2  | 2.07                     | 0.84              |
| 5:E:198:ILE:HD11  | 5:E:212:ARG:HG3  | 1.60                     | 0.84              |
| 6:F:103:MET:HE2   | 7:G:66:GLY:H     | 1.41                     | 0.84              |
| 1:A:315:LEU:HD23  | 1:A:315:LEU:N    | 1.92                     | 0.84              |
| 1:A:265:LYS:N     | 1:A:265:LYS:HE3  | 1.92                     | 0.84              |
| 1:A:316:GLN:HG2   | 1:A:317:LYS:HG2  | 1.60                     | 0.84              |
| 3:C:115:SER:HB3   | 3:C:141:GLY:O    | 1.78                     | 0.84              |
| 3:C:123:ASN:ND2   | 3:C:125:MET:HG3  | 1.92                     | 0.84              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:822:GLU:HG3  | 2:B:513:GLN:HE21  | 1.43                     | 0.84              |
| 1:A:444:PHE:CE2  | 1:A:487:MET:HE3   | 2.13                     | 0.84              |
| 3:C:47:ASP:HA    | 12:L:69:ALA:HB3   | 1.58                     | 0.84              |
| 8:H:42:ILE:HG23  | 8:H:95:TYR:HE1    | 1.42                     | 0.84              |
| 10:J:1:MET:N     | 10:J:57:ILE:H     | 1.76                     | 0.84              |
| 2:B:879:ARG:H    | 2:B:879:ARG:NH1   | 1.76                     | 0.83              |
| 3:C:73:GLN:NE2   | 3:C:75:MET:HB2    | 1.93                     | 0.83              |
| 4:D:14:ARG:HH22  | 4:D:16:LYS:HZ3    | 1.24                     | 0.83              |
| 8:H:95:TYR:CE2   | 8:H:97:MET:HG3    | 2.13                     | 0.83              |
| 5:E:197:LYS:HE2  | 5:E:199:ILE:HD11  | 1.60                     | 0.83              |
| 2:B:705:MET:H    | 2:B:710:LEU:HD12  | 1.43                     | 0.83              |
| 8:H:59:ILE:HG22  | 8:H:60:ALA:N      | 1.93                     | 0.83              |
| 2:B:521:LEU:HD22 | 2:B:633:VAL:HG12  | 1.59                     | 0.83              |
| 2:B:531:GLN:HG2  | 2:B:532:ALA:H     | 1.44                     | 0.83              |
| 1:A:596:THR:O    | 1:A:598:LEU:N     | 2.12                     | 0.83              |
| 1:A:629:LEU:O    | 1:A:633:VAL:HG23  | 1.79                     | 0.83              |
| 2:B:583:ASN:ND2  | 2:B:628:THR:HG22  | 1.91                     | 0.83              |
| 1:A:63:ARG:HA    | 1:A:74:MET:HE2    | 1.60                     | 0.83              |
| 1:A:567:LYS:CB   | 8:H:95:TYR:HA     | 2.09                     | 0.83              |
| 9:I:6:PHE:HB3    | 9:I:12:ASN:O      | 1.78                     | 0.83              |
| 1:A:567:LYS:HB2  | 1:A:568:PRO:CD    | 2.09                     | 0.82              |
| 1:A:858:ASN:C    | 1:A:858:ASN:HD22  | 1.84                     | 0.82              |
| 12:L:40:LEU:HD13 | 12:L:44:ASP:HB3   | 1.60                     | 0.82              |
| 1:A:43:GLU:HG3   | 1:A:46:THR:HB     | 1.59                     | 0.82              |
| 1:A:875:ALA:HB2  | 1:A:1366:ARG:HD2  | 1.59                     | 0.82              |
| 2:B:56:ASP:HB3   | 2:B:57:TYR:CD1    | 2.14                     | 0.82              |
| 2:B:879:ARG:HH22 | 2:B:885:MET:HE2   | 1.44                     | 0.82              |
| 12:L:32:ALA:CB   | 12:L:55:ILE:HG13  | 2.09                     | 0.82              |
| 2:B:429:PHE:HA   | 2:B:432:MET:HE3   | 1.61                     | 0.82              |
| 5:E:16:PHE:CZ    | 5:E:20:LYS:HE2    | 2.15                     | 0.82              |
| 1:A:34:LYS:HZ2   | 1:A:57:ARG:NH2    | 1.77                     | 0.82              |
| 1:A:1127:ASP:OD2 | 1:A:1130:GLN:HB2  | 1.79                     | 0.82              |
| 2:B:744:HIS:CD2  | 2:B:745:PRO:HD2   | 2.14                     | 0.82              |
| 15:P:3:A:H2'     | 15:P:4:C:C6       | 2.14                     | 0.82              |
| 1:A:256:GLN:O    | 1:A:257:ARG:HB2   | 1.79                     | 0.82              |
| 1:A:567:LYS:HD3  | 8:H:95:TYR:CD2    | 2.14                     | 0.82              |
| 1:A:372:LYS:HA   | 1:A:435:HIS:HD1   | 1.44                     | 0.82              |
| 1:A:1116:LEU:H   | 1:A:1308:THR:HG22 | 1.44                     | 0.82              |
| 2:B:169:ARG:HB2  | 2:B:454:THR:HG23  | 1.59                     | 0.82              |
| 1:A:55:ASP:C     | 1:A:57:ARG:H      | 1.87                     | 0.82              |
| 2:B:846:ILE:HG23 | 2:B:974:PRO:HG2   | 1.60                     | 0.82              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:G:122:ASN:ND2   | 7:G:125:SER:HB3   | 1.95                     | 0.82              |
| 12:L:55:ILE:HD13  | 12:L:55:ILE:H     | 1.44                     | 0.82              |
| 1:A:93:VAL:HG22   | 1:A:301:ALA:HA    | 1.60                     | 0.81              |
| 9:I:50:THR:CG2    | 9:I:52:ILE:HG12   | 2.10                     | 0.81              |
| 1:A:503:GLN:HE21  | 6:F:90:ARG:NH2    | 1.78                     | 0.81              |
| 1:A:239:LEU:HD12  | 1:A:240:PRO:HD2   | 1.61                     | 0.81              |
| 2:B:705:MET:HA    | 2:B:705:MET:HE3   | 1.61                     | 0.81              |
| 3:C:112:ASN:HB3   | 3:C:114:TYR:CE1   | 2.15                     | 0.81              |
| 1:A:353:ILE:HG21  | 1:A:487:MET:CG    | 2.10                     | 0.81              |
| 2:B:172:ILE:HD13  | 2:B:178:ASN:HD22  | 1.44                     | 0.81              |
| 5:E:147:HIS:HB3   | 5:E:150:VAL:HG23  | 1.61                     | 0.81              |
| 1:A:567:LYS:CD    | 1:A:568:PRO:HD2   | 2.10                     | 0.81              |
| 4:D:154:PHE:CE1   | 4:D:163:VAL:HG21  | 2.15                     | 0.81              |
| 1:A:710:LEU:H     | 1:A:710:LEU:HD12  | 1.44                     | 0.81              |
| 7:G:34:VAL:HG11   | 7:G:74:TYR:CE1    | 2.15                     | 0.81              |
| 1:A:866:PHE:O     | 1:A:867:ILE:HD12  | 1.78                     | 0.81              |
| 1:A:1110:ASN:HD22 | 1:A:1110:ASN:N    | 1.78                     | 0.81              |
| 2:B:622:LYS:HE2   | 9:I:59:VAL:CG2    | 2.09                     | 0.81              |
| 2:B:995:ARG:HH12  | 3:C:165:LYS:HG2   | 1.45                     | 0.81              |
| 1:A:34:LYS:HE3    | 1:A:57:ARG:NH1    | 1.96                     | 0.81              |
| 1:A:55:ASP:N      | 1:A:56:PRO:HD3    | 1.96                     | 0.81              |
| 2:B:56:ASP:HB3    | 2:B:57:TYR:HD1    | 1.45                     | 0.81              |
| 2:B:465:ASN:HD22  | 2:B:465:ASN:N     | 1.78                     | 0.81              |
| 7:G:112:LYS:HA    | 7:G:115:MET:HE3   | 1.63                     | 0.81              |
| 2:B:278:GLN:HG2   | 2:B:279:ASP:N     | 1.93                     | 0.80              |
| 7:G:26:LEU:HD12   | 7:G:56:ILE:HD11   | 1.63                     | 0.80              |
| 12:L:30:ILE:O     | 12:L:56:LEU:HA    | 1.80                     | 0.80              |
| 1:A:754:SER:N     | 1:A:757:ASN:HD22  | 1.78                     | 0.80              |
| 1:A:767:GLN:NE2   | 1:A:774:ARG:HB3   | 1.96                     | 0.80              |
| 2:B:579:ARG:HG2   | 2:B:579:ARG:HH11  | 1.46                     | 0.80              |
| 12:L:47:ARG:HB2   | 12:L:47:ARG:HH11  | 1.46                     | 0.80              |
| 6:F:130:ILE:HB    | 6:F:148:VAL:HG21  | 1.60                     | 0.80              |
| 1:A:709:THR:HG22  | 1:A:710:LEU:H     | 1.44                     | 0.80              |
| 1:A:901:LEU:HA    | 1:A:907:THR:OG1   | 1.81                     | 0.80              |
| 1:A:1259:MET:HA   | 1:A:1262:LYS:HD2  | 1.61                     | 0.80              |
| 2:B:1004:GLU:HG3  | 10:J:42:LYS:HZ1   | 1.46                     | 0.80              |
| 3:C:7:GLN:HE21    | 11:K:104:ASN:ND2  | 1.77                     | 0.80              |
| 3:C:238:ILE:HG22  | 3:C:243:VAL:HG23  | 1.64                     | 0.80              |
| 1:A:541:ILE:HG22  | 1:A:546:VAL:HG23  | 1.63                     | 0.80              |
| 2:B:916:THR:HB    | 2:B:935:ARG:HD2   | 1.64                     | 0.80              |
| 1:A:1409:LEU:HD13 | 2:B:1207:LEU:HD11 | 1.63                     | 0.80              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:C:148:ARG:H     | 3:C:151:GLN:HG3  | 1.45                     | 0.80              |
| 1:A:595:THR:O     | 1:A:596:THR:HG23 | 1.80                     | 0.80              |
| 11:K:57:LEU:HB2   | 11:K:76:GLN:HG2  | 1.61                     | 0.80              |
| 1:A:66:LYS:HD3    | 1:A:67:CYS:N     | 1.97                     | 0.80              |
| 2:B:597:MET:HA    | 2:B:597:MET:HE3  | 1.62                     | 0.80              |
| 1:A:738:LYS:HG3   | 1:A:740:LEU:HG   | 1.61                     | 0.80              |
| 2:B:744:HIS:HD2   | 2:B:745:PRO:CD   | 1.93                     | 0.80              |
| 2:B:999:MET:HA    | 2:B:999:MET:HE3  | 1.63                     | 0.80              |
| 8:H:58:THR:HG22   | 8:H:59:ILE:H     | 1.48                     | 0.80              |
| 10:J:63:TYR:O     | 10:J:64:ASN:HB2  | 1.79                     | 0.79              |
| 1:A:392:VAL:HG13  | 1:A:415:LEU:HD11 | 1.65                     | 0.79              |
| 3:C:66:ARG:NH1    | 10:J:2:ILE:HG21  | 1.98                     | 0.79              |
| 6:F:111:LEU:HD12  | 6:F:111:LEU:H    | 1.45                     | 0.79              |
| 8:H:130:ARG:HB2   | 8:H:130:ARG:NH1  | 1.96                     | 0.79              |
| 1:A:1081:LEU:HD11 | 1:A:1098:VAL:H   | 1.47                     | 0.79              |
| 4:D:159:THR:O     | 4:D:163:VAL:HG23 | 1.82                     | 0.79              |
| 1:A:416:ARG:HH11  | 1:A:417:TYR:HE1  | 1.29                     | 0.79              |
| 5:E:9:ILE:HD11    | 5:E:53:PRO:HD3   | 1.65                     | 0.79              |
| 5:E:19:VAL:O      | 5:E:23:VAL:HG23  | 1.82                     | 0.79              |
| 9:I:111:THR:CG2   | 9:I:112:SER:H    | 1.95                     | 0.79              |
| 3:C:8:VAL:O       | 3:C:9:LYS:HG3    | 1.83                     | 0.79              |
| 1:A:683:ILE:HD13  | 1:A:801:GLU:HG3  | 1.65                     | 0.79              |
| 2:B:294:ASP:O     | 2:B:296:GLU:N    | 2.14                     | 0.79              |
| 1:A:372:LYS:HA    | 1:A:435:HIS:ND1  | 1.98                     | 0.79              |
| 1:A:53:LEU:CD2    | 1:A:54:ASN:H     | 1.88                     | 0.79              |
| 1:A:567:LYS:NZ    | 8:H:43:ASN:HB3   | 1.98                     | 0.79              |
| 2:B:1138:MET:HE2  | 2:B:1146:PHE:CD2 | 2.18                     | 0.79              |
| 1:A:1121:GLU:HG2  | 1:A:1122:PRO:HD2 | 1.65                     | 0.78              |
| 8:H:130:ARG:HD3   | 8:H:130:ARG:N    | 1.97                     | 0.78              |
| 10:J:57:ILE:HA    | 10:J:60:PHE:HD2  | 1.48                     | 0.78              |
| 1:A:503:GLN:NE2   | 6:F:90:ARG:NH2   | 2.32                     | 0.78              |
| 2:B:583:ASN:HD21  | 2:B:628:THR:CG2  | 1.94                     | 0.78              |
| 2:B:917:PRO:O     | 2:B:918:ILE:HG13 | 1.83                     | 0.78              |
| 1:A:829:VAL:HG21  | 2:B:508:LEU:HD13 | 1.64                     | 0.78              |
| 1:A:1015:VAL:HG12 | 1:A:1019:CYS:SG  | 2.22                     | 0.78              |
| 2:B:766:ARG:HH21  | 2:B:1020:ARG:CD  | 1.96                     | 0.78              |
| 9:I:50:THR:HG22   | 9:I:51:ASN:N     | 1.99                     | 0.78              |
| 2:B:25:ILE:CG2    | 2:B:658:ILE:HD12 | 2.13                     | 0.78              |
| 7:G:7:LEU:HB2     | 7:G:74:TYR:CE2   | 2.19                     | 0.78              |
| 12:L:47:ARG:HG2   | 12:L:48:CYS:H    | 1.47                     | 0.78              |
| 1:A:225:ASN:HD22  | 1:A:228:PHE:H    | 1.32                     | 0.78              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1323:ASP:OD1  | 1:A:1325:THR:HG22 | 1.84                     | 0.78              |
| 7:G:138:THR:HG22  | 7:G:139:ILE:N     | 1.99                     | 0.78              |
| 8:H:95:TYR:HE2    | 8:H:97:MET:CG     | 1.97                     | 0.78              |
| 2:B:25:ILE:HG21   | 2:B:658:ILE:HD12  | 1.65                     | 0.78              |
| 2:B:65:GLU:OE1    | 2:B:418:LYS:HE3   | 1.84                     | 0.78              |
| 2:B:289:LEU:HD13  | 2:B:375:ALA:HB2   | 1.64                     | 0.78              |
| 2:B:241:ARG:HG2   | 2:B:253:THR:CG2   | 2.13                     | 0.77              |
| 5:E:84:ASP:O      | 5:E:86:PRO:HD3    | 1.84                     | 0.77              |
| 4:D:71:LYS:HA     | 4:D:74:GLN:HB2    | 1.66                     | 0.77              |
| 9:I:7:CYS:HB3     | 9:I:14:LEU:HD21   | 1.64                     | 0.77              |
| 1:A:687:LYS:O     | 1:A:690:VAL:HG12  | 1.83                     | 0.77              |
| 2:B:102:VAL:HG22  | 2:B:112:LEU:HD22  | 1.66                     | 0.77              |
| 2:B:815:ARG:HB2   | 2:B:815:ARG:HH11  | 1.50                     | 0.77              |
| 4:D:14:ARG:HB3    | 4:D:14:ARG:HH11   | 1.48                     | 0.77              |
| 1:A:1161:THR:HG22 | 1:A:1163:ILE:N    | 1.99                     | 0.77              |
| 1:A:1224:LEU:HD11 | 1:A:1240:CYS:HB3  | 1.65                     | 0.77              |
| 2:B:613:VAL:HG22  | 2:B:628:THR:HA    | 1.67                     | 0.77              |
| 2:B:796:LEU:HD21  | 2:B:821:GLN:HE21  | 1.50                     | 0.77              |
| 3:C:11:ARG:HD3    | 3:C:209:TYR:CE2   | 2.20                     | 0.77              |
| 1:A:783:THR:HG21  | 1:A:796:SER:O     | 1.85                     | 0.77              |
| 1:A:961:ARG:HG2   | 1:A:965:GLN:HE21  | 1.49                     | 0.77              |
| 9:I:105:SER:O     | 9:I:106:CYS:HB3   | 1.83                     | 0.77              |
| 1:A:770:VAL:HG12  | 1:A:771:GLU:HG3   | 1.66                     | 0.77              |
| 2:B:221:ASN:OD1   | 2:B:242:SER:HA    | 1.84                     | 0.77              |
| 1:A:1329:THR:HG22 | 1:A:1331:SER:N    | 2.00                     | 0.77              |
| 2:B:102:VAL:CG2   | 2:B:112:LEU:HB2   | 2.13                     | 0.77              |
| 2:B:309:GLN:CD    | 9:I:52:ILE:HD11   | 2.08                     | 0.77              |
| 8:H:127:GLY:O     | 8:H:128:ASN:HB2   | 1.83                     | 0.77              |
| 1:A:66:LYS:HZ3    | 1:A:68:GLN:N      | 1.83                     | 0.77              |
| 6:F:69:LEU:HB3    | 6:F:71:GLU:OE1    | 1.84                     | 0.77              |
| 8:H:17:PRO:HB3    | 8:H:24:CYS:SG     | 2.25                     | 0.76              |
| 11:K:65:HIS:CD2   | 11:K:67:PHE:H     | 2.02                     | 0.76              |
| 12:L:32:ALA:HB2   | 12:L:55:ILE:HG13  | 1.67                     | 0.76              |
| 1:A:934:LYS:O     | 1:A:937:VAL:HG12  | 1.85                     | 0.76              |
| 1:A:981:LEU:HD21  | 1:A:1039:LYS:HA   | 1.66                     | 0.76              |
| 1:A:14:VAL:N      | 1:A:1432:GLN:HE22 | 1.83                     | 0.76              |
| 7:G:126:ASN:HD22  | 7:G:127:PRO:HA    | 1.51                     | 0.76              |
| 1:A:250:ILE:O     | 1:A:250:ILE:HG22  | 1.84                     | 0.76              |
| 1:A:122:MET:HA    | 1:A:141:LEU:HD11  | 1.66                     | 0.76              |
| 1:A:1112:LYS:O    | 1:A:1114:PRO:HD3  | 1.85                     | 0.76              |
| 2:B:995:ARG:NH1   | 3:C:165:LYS:HG2   | 2.00                     | 0.76              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:167:HIS:CD2   | 12:L:70:ARG:HB3   | 2.21                     | 0.76              |
| 1:A:157:ASP:OD2   | 1:A:159:THR:HB    | 1.85                     | 0.76              |
| 1:A:332:LYS:C     | 1:A:334:GLY:H     | 1.93                     | 0.76              |
| 1:A:567:LYS:CB    | 1:A:568:PRO:HD2   | 2.15                     | 0.76              |
| 9:I:26:LEU:HD23   | 9:I:37:GLU:HA     | 1.68                     | 0.76              |
| 2:B:745:PRO:O     | 2:B:748:ILE:HG12  | 1.86                     | 0.75              |
| 1:A:297:GLN:HA    | 1:A:297:GLN:HE21  | 1.49                     | 0.75              |
| 1:A:567:LYS:HB2   | 8:H:95:TYR:HA     | 1.64                     | 0.75              |
| 4:D:162:ALA:HA    | 4:D:165:GLN:HE21  | 1.49                     | 0.75              |
| 1:A:567:LYS:HB2   | 1:A:568:PRO:HD2   | 1.65                     | 0.75              |
| 1:A:1259:MET:HE3  | 1:A:1263:ILE:HG13 | 1.67                     | 0.75              |
| 1:A:697:ALA:HB2   | 1:A:702:LEU:HD11  | 1.69                     | 0.75              |
| 1:A:1329:THR:HG22 | 1:A:1331:SER:H    | 1.51                     | 0.75              |
| 7:G:14:HIS:CD2    | 7:G:16:SER:H      | 2.04                     | 0.75              |
| 2:B:473:MET:HE3   | 2:B:474:SER:HA    | 1.66                     | 0.75              |
| 9:I:111:THR:HG22  | 9:I:113:ASP:N     | 2.01                     | 0.75              |
| 2:B:707:PRO:HG2   | 2:B:708:GLU:H     | 1.51                     | 0.75              |
| 2:B:758:PHE:CE2   | 2:B:1044:ALA:HA   | 2.21                     | 0.75              |
| 5:E:112:TYR:O     | 5:E:137:GLU:HG3   | 1.86                     | 0.75              |
| 8:H:55:LEU:HD22   | 8:H:144:ILE:HG22  | 1.68                     | 0.75              |
| 12:L:53:HIS:HB3   | 12:L:55:ILE:CD1   | 2.16                     | 0.75              |
| 2:B:644:GLU:OE2   | 2:B:646:LEU:HB3   | 1.86                     | 0.75              |
| 4:D:155:ARG:HD3   | 4:D:221:TYR:CE1   | 2.21                     | 0.75              |
| 9:I:80:SER:OG     | 9:I:105:SER:HB2   | 1.87                     | 0.75              |
| 1:A:69:THR:O      | 1:A:71:GLN:N      | 2.20                     | 0.74              |
| 1:A:381:THR:HG23  | 1:A:382:PRO:HD2   | 1.66                     | 0.74              |
| 2:B:483:LEU:HD11  | 2:B:491:THR:HG23  | 1.69                     | 0.74              |
| 7:G:15:PRO:HA     | 7:G:18:PHE:CD1    | 2.22                     | 0.74              |
| 1:A:172:PRO:HB3   | 1:A:185:TRP:CE2   | 2.21                     | 0.74              |
| 1:A:1433:MET:HE1  | 7:G:63:PRO:HB2    | 1.69                     | 0.74              |
| 1:A:1189:SER:O    | 1:A:1241:ARG:HD3  | 1.86                     | 0.74              |
| 5:E:23:VAL:O      | 5:E:28:TYR:HB2    | 1.87                     | 0.74              |
| 2:B:880:THR:HB    | 2:B:934:LYS:HD2   | 1.68                     | 0.74              |
| 3:C:120:ILE:HG21  | 3:C:124:LEU:HD11  | 1.69                     | 0.74              |
| 12:L:47:ARG:HB2   | 12:L:47:ARG:NH1   | 2.02                     | 0.74              |
| 1:A:416:ARG:NH1   | 1:A:417:TYR:HE1   | 1.84                     | 0.74              |
| 1:A:973:ILE:HD13  | 1:A:1037:LEU:HA   | 1.69                     | 0.74              |
| 4:D:12:ARG:HG2    | 4:D:12:ARG:NH1    | 1.99                     | 0.74              |
| 1:A:288:ALA:HA    | 1:A:291:GLU:OE1   | 1.87                     | 0.74              |
| 1:A:714:PHE:HB2   | 9:I:97:MET:HE1    | 1.68                     | 0.74              |
| 2:B:824:ILE:HG12  | 10:J:48:ARG:HH12  | 1.52                     | 0.74              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:B:800:GLN:HB3   | 10:J:52:THR:HG21 | 1.69                     | 0.74              |
| 10:J:44:TYR:H     | 10:J:44:TYR:HD2  | 1.35                     | 0.74              |
| 1:A:1118:VAL:HG23 | 1:A:1306:LEU:HB2 | 1.69                     | 0.74              |
| 2:B:890:TYR:O     | 2:B:893:LEU:HB2  | 1.88                     | 0.74              |
| 3:C:165:LYS:O     | 11:K:6:ARG:NH1   | 2.21                     | 0.74              |
| 5:E:15:ALA:O      | 5:E:19:VAL:HG23  | 1.87                     | 0.74              |
| 1:A:672:ASP:HB3   | 1:A:736:ASN:OD1  | 1.87                     | 0.73              |
| 2:B:427:ASP:HA    | 2:B:430:ARG:HD2  | 1.70                     | 0.73              |
| 3:C:147:LEU:HB2   | 3:C:151:GLN:HB2  | 1.69                     | 0.73              |
| 1:A:901:LEU:N     | 1:A:926:GLN:NE2  | 2.31                     | 0.73              |
| 1:A:1444:MET:CG   | 7:G:60:ARG:HA    | 2.18                     | 0.73              |
| 2:B:39:ARG:HH21   | 2:B:665:GLU:HG2  | 1.53                     | 0.73              |
| 2:B:732:SER:HB2   | 2:B:734:HIS:CE1  | 2.23                     | 0.73              |
| 6:F:82:THR:HG23   | 6:F:84:TYR:H     | 1.52                     | 0.73              |
| 7:G:45:ILE:HA     | 7:G:78:VAL:HG12  | 1.70                     | 0.73              |
| 1:A:1308:THR:HG23 | 1:A:1309:ASP:N   | 2.01                     | 0.73              |
| 2:B:37:PHE:HE1    | 2:B:41:LYS:HD3   | 1.53                     | 0.73              |
| 2:B:969:ARG:HD2   | 3:C:61:GLU:OE2   | 1.87                     | 0.73              |
| 7:G:126:ASN:HD22  | 7:G:127:PRO:CA   | 1.99                     | 0.73              |
| 1:A:21:LEU:HD11   | 1:A:1414:ALA:HA  | 1.70                     | 0.73              |
| 1:A:446:ARG:HB2   | 1:A:487:MET:SD   | 2.28                     | 0.73              |
| 2:B:39:ARG:HH21   | 2:B:665:GLU:CG   | 2.01                     | 0.73              |
| 1:A:122:MET:HA    | 1:A:141:LEU:CD1  | 2.18                     | 0.73              |
| 1:A:722:LEU:HD21  | 1:A:794:PRO:HB3  | 1.70                     | 0.73              |
| 1:A:1006:ILE:HD11 | 5:E:163:GLU:HG3  | 1.69                     | 0.73              |
| 7:G:139:ILE:HG23  | 7:G:140:LYS:N    | 2.01                     | 0.73              |
| 1:A:2:VAL:HG22    | 1:A:3:GLY:H      | 1.53                     | 0.73              |
| 1:A:369:SER:HB3   | 11:K:2:ASN:OD1   | 1.88                     | 0.73              |
| 2:B:292:ILE:HD11  | 2:B:327:ARG:H    | 1.53                     | 0.73              |
| 7:G:139:ILE:HG23  | 7:G:140:LYS:H    | 1.53                     | 0.73              |
| 1:A:567:LYS:CB    | 8:H:96:VAL:H     | 1.96                     | 0.73              |
| 1:A:571:LEU:HD22  | 8:H:46:LEU:HD11  | 1.70                     | 0.73              |
| 1:A:913:LEU:HD12  | 1:A:914:GLU:N    | 2.04                     | 0.73              |
| 2:B:294:ASP:C     | 2:B:296:GLU:H    | 1.96                     | 0.73              |
| 2:B:547:VAL:HG12  | 2:B:612:GLU:OE2  | 1.88                     | 0.73              |
| 1:A:433:GLU:OE1   | 2:B:1108:ARG:NH2 | 2.22                     | 0.73              |
| 2:B:805:THR:HG22  | 2:B:806:THR:H    | 1.51                     | 0.73              |
| 2:B:859:TYR:CZ    | 2:B:941:LEU:HD12 | 2.23                     | 0.73              |
| 3:C:66:ARG:NH2    | 10:J:3:VAL:O     | 2.22                     | 0.73              |
| 13:T:15:DG:C2'    | 13:T:16:DT:H71   | 2.19                     | 0.73              |
| 1:A:518:LYS:HE2   | 1:A:624:SER:O    | 1.89                     | 0.73              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:D:66:ARG:HD2   | 4:D:133:THR:HB    | 1.70                     | 0.73              |
| 1:A:12:ARG:HD2   | 2:B:1218:THR:HB   | 1.70                     | 0.72              |
| 1:A:675:THR:O    | 1:A:679:ILE:HG13  | 1.88                     | 0.72              |
| 1:A:879:GLU:O    | 1:A:955:PRO:HA    | 1.89                     | 0.72              |
| 1:A:1141:THR:CG2 | 1:A:1205:LYS:HD3  | 2.19                     | 0.72              |
| 2:B:273:LEU:HB2  | 2:B:276:ILE:HD12  | 1.69                     | 0.72              |
| 2:B:652:LYS:HB3  | 2:B:689:LEU:HD23  | 1.68                     | 0.72              |
| 2:B:800:GLN:HB3  | 10:J:52:THR:HG22  | 1.69                     | 0.72              |
| 6:F:77:ASP:O     | 6:F:78:GLN:HB2    | 1.90                     | 0.72              |
| 10:J:30:LEU:HD11 | 10:J:38:ARG:HH11  | 1.55                     | 0.72              |
| 2:B:834:ASN:HB3  | 2:B:840:ILE:HG13  | 1.72                     | 0.72              |
| 5:E:44:ALA:O     | 5:E:45:LYS:HB2    | 1.89                     | 0.72              |
| 7:G:13:LEU:HD22  | 7:G:17:PHE:HB2    | 1.72                     | 0.72              |
| 7:G:112:LYS:HA   | 7:G:115:MET:CE    | 2.19                     | 0.72              |
| 1:A:265:LYS:HE3  | 1:A:265:LYS:CA    | 2.19                     | 0.72              |
| 1:A:709:THR:HG22 | 1:A:710:LEU:N     | 2.04                     | 0.72              |
| 2:B:364:ILE:O    | 2:B:365:THR:HB    | 1.89                     | 0.72              |
| 2:B:642:ASP:HB3  | 2:B:649:LYS:HD2   | 1.71                     | 0.72              |
| 2:B:658:ILE:HG22 | 2:B:662:MET:HE2   | 1.69                     | 0.72              |
| 3:C:183:TRP:CZ2  | 3:C:207:CYS:HB3   | 2.24                     | 0.72              |
| 1:A:40:THR:HG23  | 1:A:54:ASN:HD21   | 1.54                     | 0.72              |
| 10:J:3:VAL:HG21  | 10:J:18:TRP:CB    | 2.19                     | 0.72              |
| 10:J:64:ASN:HB3  | 10:J:65:PRO:HD3   | 1.69                     | 0.72              |
| 1:A:249:SER:O    | 1:A:250:ILE:HG13  | 1.90                     | 0.72              |
| 2:B:193:LYS:NZ   | 12:L:32:ALA:HB1   | 2.05                     | 0.72              |
| 4:D:156:ASP:HB2  | 4:D:159:THR:HG23  | 1.70                     | 0.72              |
| 1:A:855:THR:HG21 | 1:A:857:ARG:NE    | 2.03                     | 0.72              |
| 1:A:1158:PRO:O   | 1:A:1159:ARG:HG3  | 1.89                     | 0.72              |
| 3:C:114:TYR:CD2  | 3:C:140:ASN:HB3   | 2.24                     | 0.72              |
| 1:A:56:PRO:O     | 1:A:57:ARG:NE     | 2.23                     | 0.72              |
| 1:A:903:ASN:ND2  | 1:A:905:ASP:H     | 1.87                     | 0.72              |
| 1:A:1118:VAL:CG2 | 1:A:1306:LEU:HB2  | 2.20                     | 0.72              |
| 2:B:35:SER:HA    | 2:B:811:TYR:HE2   | 1.55                     | 0.72              |
| 1:A:1223:ASP:HA  | 1:A:1243:VAL:HG22 | 1.72                     | 0.72              |
| 2:B:549:THR:HG22 | 2:B:550:ASP:H     | 1.55                     | 0.72              |
| 2:B:953:LEU:HD23 | 2:B:953:LEU:O     | 1.88                     | 0.72              |
| 1:A:61:ILE:HG22  | 1:A:62:ASP:N      | 2.04                     | 0.71              |
| 1:A:107:CYS:HA   | 1:A:171:GLN:HE22  | 1.53                     | 0.71              |
| 1:A:534:LEU:O    | 1:A:534:LEU:HG    | 1.90                     | 0.71              |
| 7:G:115:MET:HE1  | 7:G:130:TYR:CE2   | 2.25                     | 0.71              |
| 1:A:535:THR:CG2  | 1:A:616:VAL:HA    | 2.19                     | 0.71              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:646:PHE:O    | 1:A:650:GLN:HG3   | 1.90                     | 0.71              |
| 10:J:1:MET:H1    | 10:J:57:ILE:N     | 1.87                     | 0.71              |
| 5:E:4:GLU:HB3    | 5:E:7:ARG:HE      | 1.54                     | 0.71              |
| 1:A:899:VAL:HB   | 1:A:929:LEU:HD12  | 1.73                     | 0.71              |
| 2:B:638:PHE:HD2  | 2:B:690:VAL:HG12  | 1.54                     | 0.71              |
| 2:B:654:ARG:HH11 | 2:B:654:ARG:HG3   | 1.55                     | 0.71              |
| 2:B:798:TYR:HE2  | 3:C:62:PHE:CZ     | 2.08                     | 0.71              |
| 12:L:26:THR:HG22 | 12:L:27:LEU:N     | 2.00                     | 0.71              |
| 3:C:128:ASN:O    | 3:C:129:ILE:HG13  | 1.89                     | 0.71              |
| 1:A:870:GLU:HG2  | 5:E:208:TYR:CG    | 2.25                     | 0.71              |
| 1:A:1210:GLY:O   | 1:A:1214:GLU:HG2  | 1.91                     | 0.71              |
| 2:B:1016:ALA:O   | 2:B:1020:ARG:HG3  | 1.90                     | 0.71              |
| 3:C:57:VAL:HG11  | 10:J:60:PHE:CB    | 2.12                     | 0.71              |
| 3:C:183:TRP:O    | 3:C:185:LYS:N     | 2.24                     | 0.71              |
| 6:F:96:THR:O     | 6:F:100:GLN:HG3   | 1.89                     | 0.71              |
| 7:G:88:ASP:HB3   | 7:G:144:ARG:HA    | 1.73                     | 0.71              |
| 9:I:76:PRO:HD2   | 9:I:108:HIS:HD2   | 1.56                     | 0.71              |
| 1:A:62:ASP:O     | 1:A:63:ARG:C      | 2.33                     | 0.71              |
| 1:A:858:ASN:HD22 | 1:A:860:LEU:H     | 1.39                     | 0.71              |
| 1:A:868:TYR:CD2  | 1:A:1058:VAL:HG21 | 2.26                     | 0.71              |
| 8:H:82:PRO:C     | 8:H:84:ALA:N      | 2.46                     | 0.71              |
| 12:L:38:LEU:CD1  | 12:L:49:LYS:HE2   | 2.20                     | 0.71              |
| 1:A:590:ARG:O    | 1:A:591:PHE:HB2   | 1.91                     | 0.71              |
| 1:A:1202:MET:HE1 | 1:A:1212:VAL:HG21 | 1.72                     | 0.71              |
| 4:D:14:ARG:HB3   | 4:D:14:ARG:NH1    | 2.05                     | 0.71              |
| 11:K:36:GLU:OE2  | 11:K:70:ARG:HD3   | 1.91                     | 0.71              |
| 1:A:438:ASP:O    | 1:A:439:ASN:HB2   | 1.91                     | 0.70              |
| 2:B:165:VAL:HG11 | 2:B:448:ILE:HD13  | 1.71                     | 0.70              |
| 2:B:244:LEU:HD21 | 2:B:366:GLN:HE21  | 1.55                     | 0.70              |
| 2:B:706:GLN:NE2  | 2:B:730:ARG:HD3   | 2.05                     | 0.70              |
| 4:D:175:PHE:HZ   | 7:G:85:GLU:HG3    | 1.55                     | 0.70              |
| 5:E:14:ARG:HH21  | 5:E:141:VAL:HG12  | 1.54                     | 0.70              |
| 1:A:93:VAL:CG2   | 1:A:301:ALA:HA    | 2.20                     | 0.70              |
| 1:A:367:PRO:HG2  | 1:A:370:ILE:HD12  | 1.71                     | 0.70              |
| 1:A:399:HIS:O    | 1:A:401:GLY:N     | 2.24                     | 0.70              |
| 1:A:1258:HIS:O   | 1:A:1262:LYS:HE3  | 1.90                     | 0.70              |
| 2:B:345:LYS:HE3  | 2:B:349:ILE:HD11  | 1.73                     | 0.70              |
| 2:B:589:VAL:HG12 | 2:B:590:HIS:H     | 1.55                     | 0.70              |
| 2:B:603:LEU:HD12 | 2:B:609:ILE:HG12  | 1.74                     | 0.70              |
| 2:B:615:MET:HB3  | 2:B:626:ILE:HG12  | 1.74                     | 0.70              |
| 2:B:1063:GLY:O   | 3:C:202:PRO:HG2   | 1.91                     | 0.70              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:42:ASP:O      | 1:A:44:THR:N      | 2.24                     | 0.70              |
| 1:A:335:ARG:HH12  | 2:B:1206:GLU:CD   | 1.99                     | 0.70              |
| 1:A:517:ASN:ND2   | 1:A:1364:ASN:HD22 | 1.86                     | 0.70              |
| 1:A:722:LEU:H     | 1:A:722:LEU:HD12  | 1.56                     | 0.70              |
| 1:A:1121:GLU:CG   | 1:A:1122:PRO:HD2  | 2.21                     | 0.70              |
| 2:B:553:PRO:O     | 2:B:557:PHE:HB2   | 1.92                     | 0.70              |
| 2:B:766:ARG:HH21  | 2:B:1020:ARG:HD3  | 1.56                     | 0.70              |
| 3:C:32:SER:O      | 3:C:36:VAL:HG23   | 1.91                     | 0.70              |
| 9:I:93:LYS:H      | 9:I:93:LYS:CD     | 1.99                     | 0.70              |
| 2:B:570:VAL:HG21  | 2:B:573:GLN:CD    | 2.16                     | 0.70              |
| 2:B:1201:LYS:HE2  | 2:B:1205:GLN:CD   | 2.17                     | 0.70              |
| 1:A:512:VAL:HA    | 1:A:519:PRO:HA    | 1.73                     | 0.70              |
| 1:A:705:LYS:HB2   | 1:A:708:MET:HE3   | 1.72                     | 0.70              |
| 5:E:117:THR:HG22  | 5:E:119:SER:H     | 1.56                     | 0.70              |
| 8:H:104:PHE:CZ    | 8:H:136:LYS:HA    | 2.26                     | 0.70              |
| 1:A:284:ALA:O     | 1:A:286:HIS:N     | 2.23                     | 0.70              |
| 1:A:310:GLY:O     | 1:A:312:PRO:HD2   | 1.91                     | 0.70              |
| 2:B:363:HIS:O     | 2:B:364:ILE:HB    | 1.92                     | 0.70              |
| 5:E:204:THR:HG23  | 5:E:205:SER:N     | 2.06                     | 0.70              |
| 6:F:69:LEU:HB3    | 6:F:71:GLU:CD     | 2.16                     | 0.70              |
| 8:H:42:ILE:HG23   | 8:H:95:TYR:CE1    | 2.26                     | 0.70              |
| 2:B:758:PHE:CE1   | 2:B:1027:ILE:HG22 | 2.27                     | 0.70              |
| 7:G:26:LEU:HD12   | 7:G:56:ILE:CD1    | 2.22                     | 0.70              |
| 11:K:21:ILE:HG12  | 11:K:33:ILE:HG12  | 1.73                     | 0.70              |
| 1:A:1223:ASP:HA   | 1:A:1243:VAL:CG2  | 2.22                     | 0.70              |
| 2:B:373:ARG:HA    | 2:B:566:LEU:HD23  | 1.73                     | 0.70              |
| 2:B:737:THR:HG21  | 9:I:66:PRO:HA     | 1.72                     | 0.70              |
| 2:B:863:GLU:OE2   | 2:B:873:THR:HA    | 1.91                     | 0.70              |
| 5:E:176:PRO:O     | 5:E:212:ARG:HA    | 1.92                     | 0.70              |
| 2:B:393:LYS:HA    | 2:B:393:LYS:HE3   | 1.74                     | 0.69              |
| 2:B:847:ASP:C     | 2:B:849:GLY:H     | 2.00                     | 0.69              |
| 2:B:944:THR:HG21  | 2:B:1122:ARG:NH2  | 2.06                     | 0.69              |
| 1:A:1385:THR:HG23 | 1:A:1387:HIS:N    | 2.04                     | 0.69              |
| 3:C:147:LEU:N     | 3:C:147:LEU:HD23  | 2.08                     | 0.69              |
| 7:G:116:PRO:HG2   | 7:G:119:LEU:HB2   | 1.74                     | 0.69              |
| 2:B:807:ARG:NH1   | 2:B:807:ARG:HB3   | 2.07                     | 0.69              |
| 3:C:244:VAL:O     | 3:C:248:ILE:HG13  | 1.91                     | 0.69              |
| 2:B:168:GLY:HA2   | 2:B:454:THR:OG1   | 1.93                     | 0.69              |
| 2:B:378:LEU:O     | 2:B:382:ILE:HG13  | 1.92                     | 0.69              |
| 2:B:563:MET:HE1   | 2:B:580:VAL:HB    | 1.73                     | 0.69              |
| 1:A:93:VAL:HG13   | 1:A:301:ALA:HB1   | 1.74                     | 0.69              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B:653:VAL:HG23 | 2:B:689:LEU:HB3   | 1.72                     | 0.69              |
| 3:C:203:GLN:HG2  | 3:C:207:CYS:SG    | 2.33                     | 0.69              |
| 5:E:79:TRP:HE1   | 5:E:81:GLU:HB2    | 1.58                     | 0.69              |
| 5:E:180:ARG:HB2  | 5:E:215:MET:OXT   | 1.92                     | 0.69              |
| 12:L:34:CYS:HB3  | 12:L:51:CYS:SG    | 2.32                     | 0.69              |
| 1:A:107:CYS:SG   | 1:A:148:CYS:HB2   | 2.33                     | 0.69              |
| 3:C:208:GLU:O    | 3:C:210:GLU:N     | 2.25                     | 0.69              |
| 2:B:295:GLY:N    | 2:B:298:LEU:HD23  | 2.08                     | 0.69              |
| 2:B:405:ARG:NE   | 2:B:629:ASP:OD2   | 2.22                     | 0.69              |
| 4:D:134:THR:HG22 | 4:D:135:GLY:N     | 2.08                     | 0.69              |
| 6:F:111:LEU:HD12 | 6:F:111:LEU:N     | 2.07                     | 0.69              |
| 12:L:61:THR:HG22 | 12:L:63:ARG:HG3   | 1.75                     | 0.69              |
| 12:L:61:THR:CG2  | 12:L:63:ARG:HG3   | 2.23                     | 0.69              |
| 1:A:11:LEU:O     | 1:A:11:LEU:HD23   | 1.93                     | 0.69              |
| 1:A:563:PRO:HG3  | 1:A:572:TRP:CZ2   | 2.27                     | 0.69              |
| 1:A:709:THR:HG21 | 1:A:711:ARG:HG3   | 1.75                     | 0.69              |
| 2:B:562:GLY:HA3  | 2:B:590:HIS:ND1   | 2.08                     | 0.69              |
| 2:B:710:LEU:CA   | 2:B:733:HIS:HB3   | 2.22                     | 0.69              |
| 2:B:873:THR:O    | 2:B:914:LYS:HA    | 1.93                     | 0.69              |
| 3:C:51:VAL:HG22  | 3:C:155:LEU:HD22  | 1.74                     | 0.69              |
| 7:G:1:MET:SD     | 7:G:79:PHE:CD1    | 2.86                     | 0.69              |
| 11:K:113:THR:O   | 11:K:114:LEU:HB2  | 1.93                     | 0.69              |
| 13:T:15:DG:H2''  | 13:T:16:DT:H71    | 1.75                     | 0.69              |
| 1:A:407:ARG:HG2  | 1:A:430:TRP:CZ2   | 2.28                     | 0.69              |
| 1:A:1444:MET:HE1 | 6:F:135:ARG:HB2   | 1.75                     | 0.69              |
| 2:B:282:ILE:HD12 | 2:B:382:ILE:HD13  | 1.75                     | 0.69              |
| 2:B:345:LYS:O    | 2:B:347:LYS:HG2   | 1.91                     | 0.69              |
| 2:B:365:THR:HG21 | 2:B:370:PHE:CG    | 2.28                     | 0.69              |
| 2:B:579:ARG:HA   | 2:B:589:VAL:HG13  | 1.74                     | 0.69              |
| 2:B:778:MET:CE   | 2:B:1094:ARG:HD3  | 2.22                     | 0.69              |
| 2:B:1004:GLU:HG3 | 10:J:42:LYS:NZ    | 2.07                     | 0.69              |
| 9:I:65:ASP:HB3   | 9:I:68:LEU:HD12   | 1.75                     | 0.69              |
| 10:J:12:LYS:O    | 10:J:14:VAL:HG23  | 1.92                     | 0.69              |
| 1:A:67:CYS:C     | 1:A:68:GLN:HG3    | 2.17                     | 0.69              |
| 11:K:45:LEU:HG   | 11:K:94:ILE:HD13  | 1.74                     | 0.69              |
| 12:L:47:ARG:CG   | 12:L:48:CYS:H     | 2.06                     | 0.69              |
| 15:P:1:C:O2      | 15:P:1:C:H2'      | 1.92                     | 0.68              |
| 1:A:186:LYS:NZ   | 1:A:197:PRO:HD3   | 2.07                     | 0.68              |
| 1:A:883:LEU:HD11 | 1:A:1017:LEU:HD11 | 1.75                     | 0.68              |
| 1:A:1150:SER:HB3 | 1:A:1195:LEU:HD23 | 1.73                     | 0.68              |
| 1:A:1202:MET:HE1 | 1:A:1212:VAL:CG2  | 2.22                     | 0.68              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:244:LEU:HD21  | 2:B:366:GLN:NE2   | 2.08                     | 0.68              |
| 2:B:470:LYS:C     | 2:B:472:ALA:N     | 2.52                     | 0.68              |
| 1:A:93:VAL:HG23   | 1:A:304:MET:HE3   | 1.76                     | 0.68              |
| 1:A:451:HIS:CD2   | 1:A:1074:GLU:HG3  | 2.28                     | 0.68              |
| 1:A:503:GLN:HE21  | 6:F:90:ARG:HH21   | 1.41                     | 0.68              |
| 1:A:822:GLU:HG3   | 2:B:513:GLN:NE2   | 2.08                     | 0.68              |
| 1:A:1214:GLU:O    | 1:A:1218:GLN:HG2  | 1.93                     | 0.68              |
| 5:E:117:THR:HB    | 5:E:120:ALA:HB2   | 1.74                     | 0.68              |
| 1:A:381:THR:HG22  | 1:A:383:TYR:N     | 2.08                     | 0.68              |
| 1:A:860:LEU:HD11  | 1:A:1393:ASN:HB2  | 1.76                     | 0.68              |
| 1:A:868:TYR:HD2   | 1:A:1058:VAL:HG21 | 1.59                     | 0.68              |
| 1:A:1208:THR:HG22 | 1:A:1210:GLY:H    | 1.57                     | 0.68              |
| 2:B:295:GLY:H     | 2:B:298:LEU:HD23  | 1.58                     | 0.68              |
| 2:B:642:ASP:CA    | 2:B:649:LYS:HG3   | 2.23                     | 0.68              |
| 7:G:139:ILE:HD13  | 7:G:140:LYS:HE3   | 1.74                     | 0.68              |
| 9:I:61:ASP:C      | 9:I:63:GLY:H      | 2.02                     | 0.68              |
| 1:A:308:ILE:HG22  | 1:A:309:ALA:N     | 2.06                     | 0.68              |
| 2:B:1169:MET:HE1  | 2:B:1201:LYS:HA   | 1.76                     | 0.68              |
| 5:E:78:LEU:HB2    | 5:E:107:THR:CB    | 2.24                     | 0.68              |
| 1:A:567:LYS:CB    | 1:A:568:PRO:CD    | 2.72                     | 0.68              |
| 11:K:47:ARG:HB3   | 11:K:47:ARG:NH1   | 2.06                     | 0.68              |
| 2:B:273:LEU:CB    | 2:B:276:ILE:HD12  | 2.24                     | 0.68              |
| 2:B:558:LEU:HD21  | 2:B:600:LEU:HD11  | 1.76                     | 0.68              |
| 1:A:37:PHE:N      | 1:A:37:PHE:CD1    | 2.59                     | 0.68              |
| 1:A:903:ASN:HD22  | 1:A:903:ASN:C     | 2.00                     | 0.68              |
| 2:B:875:GLU:O     | 2:B:877:PRO:HD3   | 1.93                     | 0.68              |
| 4:D:208:GLU:O     | 4:D:212:LYS:HG3   | 1.92                     | 0.68              |
| 6:F:69:LEU:O      | 6:F:71:GLU:HG3    | 1.94                     | 0.68              |
| 2:B:345:LYS:HG2   | 2:B:346:GLU:H     | 1.58                     | 0.67              |
| 1:A:1291:VAL:HG22 | 1:A:1292:PRO:HD2  | 1.76                     | 0.67              |
| 2:B:259:TYR:HD1   | 2:B:259:TYR:H     | 1.43                     | 0.67              |
| 2:B:705:MET:N     | 2:B:710:LEU:HD12  | 2.09                     | 0.67              |
| 11:K:55:LYS:HB3   | 11:K:81:TYR:HD1   | 1.59                     | 0.67              |
| 4:D:7:THR:O       | 4:D:9:GLN:N       | 2.27                     | 0.67              |
| 5:E:29:PHE:O      | 5:E:30:ILE:HG13   | 1.94                     | 0.67              |
| 5:E:117:THR:HB    | 5:E:120:ALA:CB    | 2.24                     | 0.67              |
| 8:H:135:LEU:HB2   | 8:H:137:GLN:HE21  | 1.58                     | 0.67              |
| 1:A:11:LEU:HB2    | 2:B:1193:GLN:HG3  | 1.75                     | 0.67              |
| 1:A:34:LYS:HG2    | 1:A:57:ARG:HH22   | 1.59                     | 0.67              |
| 1:A:414:ASP:OD1   | 1:A:416:ARG:HG2   | 1.93                     | 0.67              |
| 2:B:293:PRO:HD2   | 2:B:296:GLU:OE1   | 1.94                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:33:LEU:HG     | 3:C:37:MET:HE2    | 1.76                     | 0.67              |
| 9:I:50:THR:HG22   | 9:I:52:ILE:H      | 1.59                     | 0.67              |
| 1:A:672:ASP:OD1   | 1:A:674:PRO:HD2   | 1.95                     | 0.67              |
| 2:B:241:ARG:HG2   | 2:B:253:THR:HG22  | 1.77                     | 0.67              |
| 2:B:559:SER:CA    | 2:B:563:MET:HB3   | 2.12                     | 0.67              |
| 5:E:171:LYS:HG2   | 5:E:174:GLN:CD    | 2.19                     | 0.67              |
| 1:A:1144:LYS:HB2  | 1:A:1268:LEU:O    | 1.93                     | 0.67              |
| 2:B:613:VAL:HG13  | 2:B:627:PHE:O     | 1.95                     | 0.67              |
| 9:I:62:ILE:HD11   | 9:I:86:PHE:HE2    | 1.57                     | 0.67              |
| 1:A:500:GLU:OE2   | 1:A:1438:THR:HG21 | 1.95                     | 0.67              |
| 1:A:567:LYS:HB3   | 8:H:95:TYR:HA     | 1.76                     | 0.67              |
| 1:A:684:ALA:O     | 1:A:687:LYS:HB2   | 1.94                     | 0.67              |
| 2:B:287:ARG:HG2   | 2:B:292:ILE:HA    | 1.77                     | 0.67              |
| 2:B:291:ILE:HD13  | 2:B:300:HIS:CD2   | 2.30                     | 0.67              |
| 3:C:133:ILE:CD1   | 3:C:237:SER:HA    | 2.25                     | 0.67              |
| 1:A:75:ASN:HD22   | 2:B:1116:ARG:NH1  | 1.92                     | 0.67              |
| 2:B:659:ALA:HA    | 2:B:662:MET:HE3   | 1.76                     | 0.67              |
| 6:F:147:SER:OG    | 6:F:150:GLU:HG3   | 1.94                     | 0.67              |
| 7:G:18:PHE:HA     | 7:G:22:MET:HE3    | 1.77                     | 0.67              |
| 1:A:167:CYS:HB2   | 1:A:169:ASN:ND2   | 2.10                     | 0.67              |
| 1:A:1095:THR:CG2  | 1:A:1112:LYS:HD2  | 2.24                     | 0.67              |
| 1:A:1242:VAL:HG12 | 1:A:1243:VAL:N    | 2.09                     | 0.67              |
| 2:B:34:ILE:HG12   | 2:B:542:MET:HE1   | 1.77                     | 0.67              |
| 2:B:288:ALA:HB1   | 2:B:331:LEU:HD12  | 1.75                     | 0.67              |
| 2:B:526:GLU:HG3   | 2:B:771:SER:HB3   | 1.77                     | 0.67              |
| 2:B:577:ALA:CB    | 2:B:589:VAL:HG11  | 2.20                     | 0.67              |
| 5:E:100:ILE:HG23  | 5:E:105:PHE:HB2   | 1.77                     | 0.67              |
| 1:A:145:LYS:HA    | 1:A:145:LYS:HE3   | 1.77                     | 0.67              |
| 2:B:649:LYS:HD3   | 2:B:736:THR:O     | 1.95                     | 0.67              |
| 8:H:25:ARG:HH22   | 8:H:122:LEU:HD12  | 1.60                     | 0.67              |
| 1:A:1141:THR:HG23 | 1:A:1205:LYS:HD3  | 1.76                     | 0.66              |
| 2:B:33:VAL:HG21   | 2:B:638:PHE:HZ    | 1.59                     | 0.66              |
| 6:F:82:THR:HG23   | 6:F:84:TYR:N      | 2.10                     | 0.66              |
| 8:H:11:GLN:HA     | 8:H:53:ASP:O      | 1.95                     | 0.66              |
| 8:H:14:GLU:HG2    | 8:H:15:VAL:N      | 2.09                     | 0.66              |
| 10:J:64:ASN:HB3   | 10:J:65:PRO:HD2   | 1.78                     | 0.66              |
| 11:K:63:VAL:HG23  | 11:K:63:VAL:O     | 1.96                     | 0.66              |
| 1:A:87:ALA:CB     | 1:A:276:LEU:HD23  | 2.24                     | 0.66              |
| 1:A:266:LEU:HD21  | 1:A:303:TYR:CE1   | 2.30                     | 0.66              |
| 2:B:430:ARG:HH11  | 2:B:430:ARG:CB    | 2.04                     | 0.66              |
| 2:B:644:GLU:HB3   | 2:B:648:HIS:O     | 1.94                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:807:ARG:HB3   | 2:B:807:ARG:HH11  | 1.61                     | 0.66              |
| 8:H:100:THR:HG23  | 8:H:138:GLU:HA    | 1.77                     | 0.66              |
| 10:J:64:ASN:HD22  | 10:J:65:PRO:HD3   | 1.60                     | 0.66              |
| 1:A:184:SER:CB    | 1:A:199:LEU:HD23  | 2.26                     | 0.66              |
| 1:A:1444:MET:HG3  | 7:G:60:ARG:HA     | 1.76                     | 0.66              |
| 2:B:308:TRP:CH2   | 9:I:45:ARG:HG2    | 2.29                     | 0.66              |
| 2:B:345:LYS:CG    | 2:B:346:GLU:H     | 2.07                     | 0.66              |
| 3:C:10:ILE:HG22   | 3:C:11:ARG:O      | 1.96                     | 0.66              |
| 12:L:26:THR:CG2   | 12:L:27:LEU:H     | 2.03                     | 0.66              |
| 1:A:1094:VAL:HG13 | 1:A:1113:THR:CG2  | 2.26                     | 0.66              |
| 2:B:277:LYS:HE2   | 2:B:336:ARG:C     | 2.21                     | 0.66              |
| 5:E:116:ILE:HB    | 5:E:121:MET:HE2   | 1.76                     | 0.66              |
| 1:A:1148:ILE:HD11 | 1:A:1198:ASP:HA   | 1.77                     | 0.66              |
| 2:B:865:LYS:HG2   | 2:B:961:LEU:HD21  | 1.78                     | 0.66              |
| 6:F:109:VAL:HG12  | 6:F:110:ASP:N     | 2.10                     | 0.66              |
| 2:B:273:LEU:HD21  | 2:B:360:PHE:CD1   | 2.31                     | 0.66              |
| 2:B:428:ILE:HG22  | 2:B:432:MET:HE2   | 1.77                     | 0.66              |
| 10:J:48:ARG:HE    | 10:J:49:MET:CE    | 2.08                     | 0.66              |
| 1:A:399:HIS:CB    | 1:A:400:PRO:HD3   | 2.24                     | 0.66              |
| 1:A:541:ILE:HD13  | 1:A:549:MET:CE    | 2.23                     | 0.66              |
| 11:K:49:GLU:HG3   | 11:K:94:ILE:HG13  | 1.78                     | 0.66              |
| 1:A:72:GLU:HB3    | 1:A:76:GLU:HG2    | 1.78                     | 0.66              |
| 1:A:1353:TYR:C    | 1:A:1353:TYR:CD2  | 2.73                     | 0.66              |
| 1:A:1445:ILE:H    | 1:A:1445:ILE:HD12 | 1.60                     | 0.66              |
| 4:D:4:SER:O       | 4:D:5:THR:HB      | 1.95                     | 0.66              |
| 2:B:57:TYR:HD1    | 2:B:57:TYR:N      | 1.93                     | 0.66              |
| 2:B:172:ILE:CD1   | 2:B:178:ASN:HD22  | 2.09                     | 0.66              |
| 4:D:18:VAL:O      | 4:D:19:GLU:HB2    | 1.94                     | 0.66              |
| 10:J:1:MET:N      | 10:J:56:LEU:N     | 2.43                     | 0.66              |
| 1:A:745:GLN:HA    | 1:A:748:MET:HE3   | 1.78                     | 0.66              |
| 2:B:313:MET:SD    | 2:B:390:LEU:HD21  | 2.35                     | 0.66              |
| 2:B:842:ASN:ND2   | 2:B:845:SER:OG    | 2.29                     | 0.66              |
| 2:B:953:LEU:HD21  | 2:B:965:LYS:HB2   | 1.77                     | 0.66              |
| 2:B:1181:GLU:HA   | 2:B:1187:ASN:O    | 1.96                     | 0.66              |
| 4:D:134:THR:HG22  | 4:D:135:GLY:H     | 1.61                     | 0.66              |
| 1:A:110:CYS:HB3   | 1:A:167:CYS:SG    | 2.36                     | 0.65              |
| 1:A:388:LEU:O     | 1:A:392:VAL:HG23  | 1.96                     | 0.65              |
| 1:A:741:ASN:ND2   | 1:A:744:LYS:H     | 1.93                     | 0.65              |
| 2:B:357:GLN:O     | 2:B:366:GLN:HA    | 1.96                     | 0.65              |
| 3:C:148:ARG:N     | 3:C:151:GLN:HG3   | 2.11                     | 0.65              |
| 3:C:189:THR:HG22  | 3:C:190:ASP:N     | 2.11                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:F:99:LEU:O      | 6:F:103:MET:HG2   | 1.97                     | 0.65              |
| 1:A:1102:LYS:O    | 1:A:1106:ASN:ND2  | 2.29                     | 0.65              |
| 2:B:402:GLY:HA2   | 2:B:695:ALA:HB3   | 1.75                     | 0.65              |
| 2:B:422:LYS:O     | 2:B:426:LYS:HG2   | 1.96                     | 0.65              |
| 2:B:473:MET:HE3   | 2:B:474:SER:CA    | 2.26                     | 0.65              |
| 3:C:189:THR:HG22  | 3:C:190:ASP:H     | 1.62                     | 0.65              |
| 7:G:53:ASN:HD22   | 7:G:53:ASN:N      | 1.94                     | 0.65              |
| 8:H:143:LEU:HD12  | 8:H:143:LEU:N     | 2.11                     | 0.65              |
| 1:A:425:GLN:OE1   | 1:A:425:GLN:N     | 2.30                     | 0.65              |
| 1:A:828:ALA:HB1   | 2:B:530:GLY:HA2   | 1.78                     | 0.65              |
| 2:B:483:LEU:HD11  | 2:B:491:THR:CG2   | 2.27                     | 0.65              |
| 5:E:128:PRO:HA    | 5:E:129:PRO:C     | 2.21                     | 0.65              |
| 2:B:763:GLN:HG2   | 2:B:765:PRO:HD2   | 1.78                     | 0.65              |
| 2:B:798:TYR:HE2   | 3:C:62:PHE:CE2    | 2.14                     | 0.65              |
| 3:C:6:PRO:HB2     | 3:C:25:VAL:HG22   | 1.77                     | 0.65              |
| 4:D:220:LEU:HG    | 4:D:221:TYR:H     | 1.60                     | 0.65              |
| 5:E:111:VAL:HG12  | 5:E:137:GLU:HG2   | 1.77                     | 0.65              |
| 12:L:49:LYS:O     | 12:L:50:ASP:HB2   | 1.95                     | 0.65              |
| 1:A:184:SER:HB3   | 1:A:199:LEU:HD23  | 1.79                     | 0.65              |
| 1:A:1342:GLU:HG3  | 5:E:198:ILE:HG21  | 1.77                     | 0.65              |
| 8:H:130:ARG:HH11  | 8:H:130:ARG:CB    | 2.07                     | 0.65              |
| 1:A:873:MET:C     | 1:A:1058:VAL:HG23 | 2.21                     | 0.65              |
| 1:A:889:SER:HB3   | 1:A:1297:GLU:HG3  | 1.78                     | 0.65              |
| 2:B:1147:LEU:HD22 | 2:B:1151:LEU:HD22 | 1.78                     | 0.65              |
| 2:B:1202:LEU:O    | 2:B:1206:GLU:HG3  | 1.97                     | 0.65              |
| 1:A:102:VAL:CG1   | 1:A:211:PHE:HE1   | 2.10                     | 0.65              |
| 1:A:316:GLN:HG2   | 1:A:317:LYS:N     | 2.10                     | 0.65              |
| 1:A:353:ILE:HD12  | 1:A:470:LEU:HD21  | 1.78                     | 0.65              |
| 1:A:562:THR:HB    | 8:H:98:TYR:HD2    | 1.62                     | 0.65              |
| 1:A:1386:ARG:HB2  | 1:A:1403:GLU:HG3  | 1.77                     | 0.65              |
| 3:C:73:GLN:HE21   | 3:C:75:MET:HB2    | 1.62                     | 0.65              |
| 3:C:104:PHE:HE2   | 3:C:150:GLY:HA2   | 1.62                     | 0.65              |
| 1:A:869:GLY:O     | 5:E:204:THR:HG21  | 1.97                     | 0.65              |
| 1:A:1155:ASP:OD2  | 1:A:1161:THR:HG23 | 1.97                     | 0.65              |
| 2:B:60:GLN:O      | 2:B:63:ILE:HG22   | 1.97                     | 0.65              |
| 1:A:134:ARG:HD2   | 1:A:221:SER:O     | 1.97                     | 0.65              |
| 1:A:1041:ALA:O    | 1:A:1045:VAL:HG23 | 1.97                     | 0.65              |
| 2:B:217:ARG:HD2   | 2:B:217:ARG:C     | 2.22                     | 0.65              |
| 2:B:351:TYR:CE1   | 2:B:355:ILE:HD11  | 2.32                     | 0.65              |
| 2:B:418:LYS:HE2   | 2:B:422:LYS:NZ    | 2.12                     | 0.65              |
| 2:B:240:ILE:CG2   | 2:B:254:LEU:HB3   | 2.27                     | 0.65              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B:792:MET:HG2  | 2:B:855:PHE:HE1   | 1.62                     | 0.65              |
| 2:B:1147:LEU:CD2 | 2:B:1151:LEU:HD22 | 2.27                     | 0.65              |
| 4:D:71:LYS:HG2   | 4:D:74:GLN:HG3    | 1.78                     | 0.65              |
| 11:K:12:LEU:HD23 | 11:K:16:GLU:O     | 1.97                     | 0.65              |
| 1:A:7:SER:OG     | 2:B:1161:HIS:HE1  | 1.79                     | 0.64              |
| 1:A:207:ILE:HG22 | 1:A:211:PHE:CE2   | 2.32                     | 0.64              |
| 1:A:886:ILE:HG23 | 1:A:887:GLY:N     | 2.12                     | 0.64              |
| 2:B:859:TYR:OH   | 2:B:941:LEU:HD12  | 1.96                     | 0.64              |
| 2:B:1084:GLN:HG2 | 3:C:201:TRP:CZ2   | 2.32                     | 0.64              |
| 2:B:1084:GLN:N   | 2:B:1084:GLN:NE2  | 2.44                     | 0.64              |
| 3:C:124:LEU:O    | 3:C:127:ARG:HG2   | 1.97                     | 0.64              |
| 7:G:139:ILE:HG23 | 7:G:140:LYS:HG3   | 1.78                     | 0.64              |
| 1:A:1101:LEU:HB2 | 1:A:1355:VAL:HG11 | 1.78                     | 0.64              |
| 2:B:189:LEU:O    | 2:B:192:LEU:N     | 2.29                     | 0.64              |
| 2:B:226:PHE:HA   | 2:B:395:GLN:HG3   | 1.78                     | 0.64              |
| 3:C:73:GLN:HE21  | 3:C:75:MET:H      | 1.44                     | 0.64              |
| 6:F:89:GLU:OE2   | 6:F:134:ILE:HG21  | 1.97                     | 0.64              |
| 1:A:960:ILE:O    | 1:A:963:ILE:HG22  | 1.97                     | 0.64              |
| 1:A:977:LYS:HB3  | 1:A:978:PRO:HD2   | 1.79                     | 0.64              |
| 4:D:220:LEU:CG   | 4:D:221:TYR:H     | 2.10                     | 0.64              |
| 1:A:382:PRO:HD3  | 1:A:428:TYR:CD2   | 2.33                     | 0.64              |
| 1:A:596:THR:C    | 1:A:598:LEU:H     | 2.04                     | 0.64              |
| 1:A:896:ARG:HD3  | 1:A:897:TYR:CE1   | 2.33                     | 0.64              |
| 2:B:120:ARG:NH1  | 12:L:54:ARG:HD2   | 2.12                     | 0.64              |
| 2:B:705:MET:H    | 2:B:710:LEU:CD1   | 2.11                     | 0.64              |
| 3:C:69:LEU:N     | 3:C:69:LEU:HD12   | 2.12                     | 0.64              |
| 3:C:177:GLU:CG   | 3:C:231:ASN:HB3   | 2.25                     | 0.64              |
| 1:A:34:LYS:HG3   | 1:A:36:ARG:HH22   | 1.62                     | 0.64              |
| 1:A:535:THR:HG21 | 1:A:617:VAL:H     | 1.62                     | 0.64              |
| 1:A:49:LYS:HE2   | 1:A:61:ILE:HD12   | 1.78                     | 0.64              |
| 1:A:854:ASN:HD22 | 1:A:1000:LEU:HD23 | 1.63                     | 0.64              |
| 1:A:1150:SER:HB3 | 1:A:1195:LEU:CD2  | 2.28                     | 0.64              |
| 2:B:638:PHE:CD2  | 2:B:690:VAL:HG12  | 2.32                     | 0.64              |
| 2:B:1072:MET:HE3 | 2:B:1085:ILE:CB   | 2.15                     | 0.64              |
| 1:A:1215:ARG:NH1 | 1:A:1272:THR:O    | 2.31                     | 0.64              |
| 2:B:562:GLY:HA3  | 2:B:590:HIS:CE1   | 2.33                     | 0.64              |
| 2:B:1183:LYS:O   | 2:B:1183:LYS:HE3  | 1.97                     | 0.64              |
| 1:A:463:ILE:HB   | 1:A:464:PRO:HD2   | 1.78                     | 0.64              |
| 2:B:29:ASP:HB3   | 2:B:658:ILE:HD13  | 1.80                     | 0.64              |
| 2:B:185:THR:H    | 2:B:188:ASP:HB2   | 1.63                     | 0.64              |
| 2:B:359:GLU:O    | 2:B:362:PRO:HD3   | 1.98                     | 0.64              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B:954:VAL:O    | 12:L:55:ILE:O     | 2.15                     | 0.64              |
| 4:D:29:LEU:HD22  | 4:D:29:LEU:N      | 2.12                     | 0.64              |
| 5:E:79:TRP:HB2   | 5:E:105:PHE:CE1   | 2.32                     | 0.64              |
| 12:L:32:ALA:HB3  | 12:L:55:ILE:HG13  | 1.79                     | 0.64              |
| 1:A:68:GLN:OE1   | 1:A:68:GLN:O      | 2.15                     | 0.64              |
| 1:A:129:LYS:O    | 1:A:130:ASP:CB    | 2.46                     | 0.64              |
| 2:B:549:THR:HB   | 2:B:628:THR:OG1   | 1.96                     | 0.64              |
| 2:B:737:THR:CG2  | 9:I:66:PRO:HA     | 2.28                     | 0.64              |
| 8:H:8:ASP:OD2    | 8:H:9:ILE:N       | 2.30                     | 0.64              |
| 8:H:84:ALA:HA    | 8:H:87:ARG:HD2    | 1.80                     | 0.64              |
| 1:A:14:VAL:H     | 1:A:1432:GLN:NE2  | 1.87                     | 0.64              |
| 1:A:321:PRO:O    | 1:A:322:VAL:HB    | 1.97                     | 0.64              |
| 2:B:955:THR:CG2  | 2:B:956:THR:N     | 2.59                     | 0.64              |
| 5:E:179:GLN:O    | 5:E:182:ASP:HB2   | 1.98                     | 0.64              |
| 1:A:351:THR:CG2  | 2:B:1103:ILE:HA   | 2.27                     | 0.63              |
| 2:B:620:ARG:NH1  | 9:I:68:LEU:HD21   | 2.13                     | 0.63              |
| 3:C:138:GLU:OE1  | 3:C:138:GLU:N     | 2.31                     | 0.63              |
| 7:G:15:PRO:HA    | 7:G:18:PHE:CE1    | 2.33                     | 0.63              |
| 1:A:265:LYS:HE3  | 1:A:265:LYS:HA    | 1.79                     | 0.63              |
| 1:A:287:HIS:HA   | 1:A:290:GLU:HG2   | 1.80                     | 0.63              |
| 2:B:273:LEU:HD21 | 2:B:360:PHE:HD1   | 1.63                     | 0.63              |
| 2:B:811:TYR:N    | 2:B:811:TYR:CD1   | 2.65                     | 0.63              |
| 10:J:14:VAL:O    | 10:J:14:VAL:HG12  | 1.97                     | 0.63              |
| 11:K:55:LYS:HB3  | 11:K:81:TYR:CD1   | 2.32                     | 0.63              |
| 1:A:340:LEU:HD13 | 1:A:1429:ILE:HG23 | 1.80                     | 0.63              |
| 1:A:555:ASP:O    | 1:A:556:TRP:C     | 2.40                     | 0.63              |
| 2:B:115:GLN:HG2  | 2:B:193:LYS:HB2   | 1.81                     | 0.63              |
| 2:B:244:LEU:HD11 | 2:B:366:GLN:HE22  | 1.63                     | 0.63              |
| 2:B:425:THR:HA   | 2:B:428:ILE:HD12  | 1.81                     | 0.63              |
| 2:B:879:ARG:CZ   | 2:B:879:ARG:N     | 2.59                     | 0.63              |
| 3:C:18:VAL:HG12  | 3:C:18:VAL:O      | 1.97                     | 0.63              |
| 3:C:238:ILE:HG23 | 3:C:242:GLN:HB2   | 1.80                     | 0.63              |
| 9:I:8:ARG:HG3    | 9:I:34:TYR:CE1    | 2.33                     | 0.63              |
| 5:E:120:ALA:O    | 5:E:123:LEU:HG    | 1.98                     | 0.63              |
| 9:I:7:CYS:SG     | 9:I:8:ARG:O       | 2.56                     | 0.63              |
| 1:A:601:LYS:HD3  | 1:A:603:ASN:HD21  | 1.63                     | 0.63              |
| 1:A:1420:ASP:O   | 1:A:1421:CYS:HB2  | 1.98                     | 0.63              |
| 2:B:1201:LYS:HE2 | 2:B:1205:GLN:OE1  | 1.97                     | 0.63              |
| 3:C:36:VAL:HG21  | 3:C:251:LEU:HB2   | 1.79                     | 0.63              |
| 15:P:5:C:O2'     | 15:P:6:A:H5'      | 1.99                     | 0.63              |
| 1:A:108:MET:HA   | 1:A:210:ILE:CD1   | 2.23                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:284:ILE:HD13  | 2:B:333:PHE:CD2   | 2.34                     | 0.63              |
| 2:B:307:ASP:OD2   | 2:B:310:MET:HB2   | 1.99                     | 0.63              |
| 5:E:37:LEU:CD1    | 5:E:41:ASP:HB2    | 2.29                     | 0.63              |
| 5:E:111:VAL:CG1   | 5:E:137:GLU:HG2   | 2.29                     | 0.63              |
| 7:G:13:LEU:CD2    | 7:G:17:PHE:HB2    | 2.29                     | 0.63              |
| 1:A:1235:LYS:HG2  | 1:A:1237:ILE:HD11 | 1.79                     | 0.63              |
| 1:A:1241:ARG:O    | 1:A:1242:VAL:HB   | 1.98                     | 0.63              |
| 4:D:207:LEU:HD12  | 4:D:207:LEU:O     | 1.99                     | 0.63              |
| 8:H:81:PRO:CB     | 8:H:82:PRO:HD2    | 2.28                     | 0.63              |
| 8:H:130:ARG:HD3   | 8:H:130:ARG:H     | 1.63                     | 0.63              |
| 1:A:106:VAL:HG12  | 1:A:107:CYS:N     | 2.13                     | 0.63              |
| 1:A:973:ILE:HD11  | 1:A:1041:ALA:CB   | 2.29                     | 0.63              |
| 1:A:1438:THR:HB   | 2:B:1144:ALA:HB3  | 1.81                     | 0.63              |
| 2:B:589:VAL:HG12  | 2:B:590:HIS:N     | 2.14                     | 0.63              |
| 3:C:39:ALA:HA     | 3:C:164:ALA:HB3   | 1.80                     | 0.63              |
| 1:A:567:LYS:HD3   | 8:H:95:TYR:CG     | 2.33                     | 0.63              |
| 1:A:1107:VAL:HG12 | 1:A:1107:VAL:O    | 1.99                     | 0.63              |
| 1:A:1450:LEU:O    | 1:A:1450:LEU:HG   | 1.98                     | 0.63              |
| 2:B:108:VAL:HG23  | 2:B:109:THR:N     | 2.14                     | 0.63              |
| 2:B:839:MET:HE1   | 2:B:980:PHE:HB2   | 1.81                     | 0.63              |
| 6:F:119:ARG:HH11  | 6:F:119:ARG:HG3   | 1.64                     | 0.63              |
| 1:A:416:ARG:HG3   | 1:A:417:TYR:CE1   | 2.34                     | 0.62              |
| 1:A:1187:GLN:HG3  | 1:A:1188:GLN:H    | 1.64                     | 0.62              |
| 2:B:345:LYS:CE    | 2:B:349:ILE:HD11  | 2.29                     | 0.62              |
| 3:C:123:ASN:HD21  | 3:C:125:MET:HG3   | 1.61                     | 0.62              |
| 4:D:39:ASN:ND2    | 4:D:41:GLN:HB2    | 2.14                     | 0.62              |
| 4:D:71:LYS:HA     | 4:D:74:GLN:CB     | 2.29                     | 0.62              |
| 5:E:48:ASP:CG     | 5:E:49:SER:H      | 2.06                     | 0.62              |
| 5:E:135:PHE:HD2   | 5:E:140:LEU:HD21  | 1.64                     | 0.62              |
| 8:H:82:PRO:O      | 8:H:84:ALA:N      | 2.31                     | 0.62              |
| 1:A:98:LYS:O      | 1:A:102:VAL:HG23  | 1.99                     | 0.62              |
| 1:A:698:GLN:HA    | 9:I:97:MET:O      | 1.99                     | 0.62              |
| 1:A:1241:ARG:O    | 1:A:1242:VAL:CB   | 2.48                     | 0.62              |
| 1:A:1315:GLU:C    | 1:A:1317:MET:H    | 2.08                     | 0.62              |
| 2:B:29:ASP:HB3    | 2:B:658:ILE:CD1   | 2.29                     | 0.62              |
| 2:B:70:ILE:H      | 2:B:429:PHE:HE1   | 1.46                     | 0.62              |
| 2:B:955:THR:OG1   | 12:L:55:ILE:HA    | 1.99                     | 0.62              |
| 12:L:30:ILE:HG22  | 12:L:31:CYS:N     | 2.14                     | 0.62              |
| 2:B:334:ILE:HG22  | 2:B:334:ILE:O     | 1.99                     | 0.62              |
| 2:B:498:THR:HG22  | 2:B:537:LYS:H     | 1.63                     | 0.62              |
| 2:B:579:ARG:HG2   | 2:B:579:ARG:NH1   | 2.10                     | 0.62              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B:766:ARG:HH21 | 2:B:1020:ARG:HD2  | 1.64                     | 0.62              |
| 2:B:1174:LYS:O   | 2:B:1176:ASN:N    | 2.31                     | 0.62              |
| 8:H:139:ASN:O    | 8:H:140:ALA:CB    | 2.46                     | 0.62              |
| 1:A:472:LEU:O    | 1:A:475:THR:HB    | 1.99                     | 0.62              |
| 2:B:465:ASN:N    | 2:B:465:ASN:ND2   | 2.47                     | 0.62              |
| 2:B:515:HIS:CD2  | 2:B:517:THR:HG23  | 2.35                     | 0.62              |
| 2:B:846:ILE:CG2  | 2:B:974:PRO:HG2   | 2.27                     | 0.62              |
| 2:B:955:THR:HG22 | 2:B:956:THR:O     | 1.98                     | 0.62              |
| 2:B:1224:PHE:CE1 | 5:E:171:LYS:HG3   | 2.34                     | 0.62              |
| 4:D:33:PHE:CE1   | 7:G:80:LYS:HD3    | 2.35                     | 0.62              |
| 6:F:79:ARG:HG2   | 6:F:144:GLU:HB3   | 1.80                     | 0.62              |
| 1:A:70:CYS:O     | 1:A:72:GLU:HG2    | 1.99                     | 0.62              |
| 1:A:1317:MET:HE1 | 1:A:1339:LEU:HD21 | 1.82                     | 0.62              |
| 1:A:1345:ARG:HG2 | 1:A:1372:VAL:CG1  | 2.29                     | 0.62              |
| 2:B:916:THR:HB   | 2:B:935:ARG:CD    | 2.30                     | 0.62              |
| 8:H:38:LEU:HD13  | 8:H:125:LEU:CD1   | 2.30                     | 0.62              |
| 2:B:351:TYR:O    | 2:B:355:ILE:HG13  | 1.99                     | 0.62              |
| 2:B:635:ARG:NH2  | 2:B:742:GLU:OE2   | 2.31                     | 0.62              |
| 2:B:642:ASP:HB3  | 2:B:649:LYS:CD    | 2.29                     | 0.62              |
| 2:B:911:ILE:CG2  | 2:B:966:VAL:HG11  | 2.30                     | 0.62              |
| 1:A:153:PRO:HB3  | 1:A:161:LEU:HD22  | 1.81                     | 0.62              |
| 1:A:185:TRP:CH2  | 1:A:200:ARG:HG2   | 2.34                     | 0.62              |
| 1:A:503:GLN:NE2  | 6:F:90:ARG:HH21   | 1.93                     | 0.62              |
| 2:B:240:ILE:HG23 | 2:B:254:LEU:HB3   | 1.82                     | 0.62              |
| 2:B:516:ASN:HD22 | 2:B:516:ASN:H     | 1.48                     | 0.62              |
| 3:C:133:ILE:HD11 | 3:C:237:SER:HA    | 1.82                     | 0.62              |
| 7:G:138:THR:HG22 | 7:G:139:ILE:H     | 1.64                     | 0.62              |
| 1:A:264:PHE:HB3  | 1:A:265:LYS:HZ1   | 1.65                     | 0.62              |
| 1:A:794:PRO:HG2  | 1:A:795:GLU:OE2   | 1.99                     | 0.62              |
| 2:B:53:GLN:HG2   | 2:B:547:VAL:HG22  | 1.80                     | 0.62              |
| 2:B:769:TYR:CD1  | 2:B:987:LYS:NZ    | 2.67                     | 0.62              |
| 3:C:18:VAL:HG23  | 3:C:240:VAL:HB    | 1.82                     | 0.62              |
| 9:I:50:THR:HG21  | 9:I:52:ILE:HG12   | 1.81                     | 0.62              |
| 1:A:62:ASP:O     | 1:A:64:ASN:HB2    | 2.00                     | 0.62              |
| 1:A:148:CYS:HB3  | 1:A:167:CYS:O     | 2.00                     | 0.62              |
| 1:A:332:LYS:C    | 1:A:334:GLY:N     | 2.57                     | 0.62              |
| 1:A:993:LEU:HD22 | 1:A:1046:LEU:HD22 | 1.80                     | 0.62              |
| 1:A:1130:GLN:O   | 1:A:1134:ILE:HG13 | 2.00                     | 0.62              |
| 1:A:1149:ALA:HB2 | 9:I:47:GLU:HA     | 1.81                     | 0.62              |
| 2:B:305:VAL:O    | 2:B:305:VAL:HG12  | 2.00                     | 0.62              |
| 11:K:108:GLU:O   | 11:K:112:GLN:HG2  | 2.00                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:L:39:SER:O     | 12:L:40:LEU:HG    | 2.00                     | 0.62              |
| 12:L:58:LYS:O     | 12:L:59:ALA:O     | 2.18                     | 0.62              |
| 1:A:35:ILE:HA     | 1:A:52:GLY:O      | 1.99                     | 0.62              |
| 2:B:957:ASN:ND2   | 2:B:961:LEU:HB2   | 2.14                     | 0.62              |
| 2:B:1177:HIS:CB   | 2:B:1179:GLN:HE21 | 2.12                     | 0.62              |
| 5:E:153:HIS:O     | 5:E:154:ILE:CG1   | 2.47                     | 0.62              |
| 9:I:50:THR:CG2    | 9:I:51:ASN:H      | 2.09                     | 0.62              |
| 1:A:34:LYS:NZ     | 1:A:57:ARG:HH12   | 1.98                     | 0.61              |
| 1:A:129:LYS:O     | 1:A:130:ASP:HB2   | 2.00                     | 0.61              |
| 1:A:821:ARG:HB2   | 1:A:821:ARG:HH11  | 1.65                     | 0.61              |
| 1:A:1120:LEU:HD22 | 1:A:1125:ALA:HA   | 1.81                     | 0.61              |
| 1:A:1191:TRP:HZ3  | 9:I:43:VAL:HG21   | 1.64                     | 0.61              |
| 2:B:98:THR:O      | 2:B:126:SER:HB2   | 2.00                     | 0.61              |
| 2:B:234:ILE:HG12  | 2:B:257:LYS:HG2   | 1.82                     | 0.61              |
| 2:B:806:THR:HG21  | 2:B:808:ALA:HB3   | 1.80                     | 0.61              |
| 4:D:146:GLN:HA    | 4:D:149:THR:HG22  | 1.82                     | 0.61              |
| 8:H:55:LEU:HD22   | 8:H:144:ILE:CG2   | 2.30                     | 0.61              |
| 8:H:106:GLU:C     | 8:H:108:SER:H     | 2.08                     | 0.61              |
| 1:A:427:GLN:HG3   | 1:A:430:TRP:CZ2   | 2.35                     | 0.61              |
| 2:B:57:TYR:CD1    | 2:B:57:TYR:N      | 2.64                     | 0.61              |
| 2:B:277:LYS:CG    | 2:B:336:ARG:HG2   | 2.31                     | 0.61              |
| 2:B:701:ILE:HD11  | 2:B:703:ILE:HD11  | 1.83                     | 0.61              |
| 2:B:865:LYS:HB2   | 2:B:961:LEU:HD11  | 1.81                     | 0.61              |
| 3:C:43:THR:CG2    | 3:C:44:LEU:N      | 2.63                     | 0.61              |
| 1:A:50:ILE:C      | 1:A:52:GLY:H      | 2.09                     | 0.61              |
| 1:A:382:PRO:HB3   | 1:A:428:TYR:HE2   | 1.66                     | 0.61              |
| 1:A:469:ARG:NH2   | 2:B:991:GLY:O     | 2.34                     | 0.61              |
| 1:A:907:THR:HG23  | 1:A:908:LEU:N     | 2.16                     | 0.61              |
| 1:A:1312:ASN:HD21 | 1:A:1315:GLU:HG3  | 1.65                     | 0.61              |
| 2:B:35:SER:O      | 2:B:39:ARG:HG3    | 2.01                     | 0.61              |
| 2:B:1095:LEU:H    | 2:B:1095:LEU:HD12 | 1.65                     | 0.61              |
| 8:H:127:GLY:O     | 8:H:128:ASN:CB    | 2.47                     | 0.61              |
| 1:A:252:PHE:O     | 1:A:256:GLN:NE2   | 2.33                     | 0.61              |
| 1:A:317:LYS:O     | 1:A:318:SER:CB    | 2.47                     | 0.61              |
| 1:A:1242:VAL:CG1  | 1:A:1243:VAL:N    | 2.63                     | 0.61              |
| 2:B:508:LEU:HB3   | 14:N:1:DA:O3'     | 2.01                     | 0.61              |
| 2:B:996:ARG:NH1   | 3:C:174:ALA:HA    | 2.13                     | 0.61              |
| 8:H:32:THR:HG22   | 8:H:33:GLN:OE1    | 2.01                     | 0.61              |
| 1:A:311:GLN:O     | 1:A:312:PRO:C     | 2.41                     | 0.61              |
| 1:A:535:THR:HG21  | 1:A:617:VAL:N     | 2.16                     | 0.61              |
| 1:A:568:PRO:HB2   | 3:C:221:TYR:CZ    | 2.35                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:590:ARG:HG2   | 1:A:590:ARG:HH11  | 1.65                     | 0.61              |
| 1:A:698:GLN:NE2   | 9:I:99:LEU:HD11   | 2.16                     | 0.61              |
| 1:A:1341:ILE:HG23 | 1:A:1342:GLU:N    | 2.14                     | 0.61              |
| 2:B:642:ASP:HA    | 2:B:649:LYS:HG3   | 1.81                     | 0.61              |
| 5:E:124:VAL:CG1   | 5:E:132:ILE:HB    | 2.20                     | 0.61              |
| 8:H:4:THR:HG22    | 8:H:5:LEU:N       | 2.15                     | 0.61              |
| 10:J:30:LEU:HD22  | 10:J:34:THR:HG21  | 1.83                     | 0.61              |
| 10:J:44:TYR:HA    | 10:J:47:ARG:HB2   | 1.83                     | 0.61              |
| 11:K:82:ASP:OD1   | 11:K:84:LYS:N     | 2.34                     | 0.61              |
| 1:A:1225:PHE:CE2  | 1:A:1227:ILE:HD11 | 2.36                     | 0.61              |
| 2:B:899:ILE:HG21  | 2:B:949:VAL:HG21  | 1.83                     | 0.61              |
| 4:D:146:GLN:O     | 4:D:149:THR:HG22  | 1.99                     | 0.61              |
| 5:E:39:LEU:HG     | 5:E:43:LYS:HE3    | 1.82                     | 0.61              |
| 9:I:74:GLU:HB3    | 9:I:81:ARG:CD     | 2.30                     | 0.61              |
| 1:A:150:THR:HG23  | 1:A:166:GLY:HA2   | 1.83                     | 0.61              |
| 1:A:285:PRO:HG2   | 1:A:288:ALA:HB3   | 1.81                     | 0.61              |
| 1:A:1387:HIS:HA   | 1:A:1391:ARG:HE   | 1.66                     | 0.61              |
| 2:B:114:PRO:HG2   | 2:B:115:GLN:H     | 1.65                     | 0.61              |
| 3:C:251:LEU:O     | 3:C:255:VAL:HG23  | 2.00                     | 0.61              |
| 8:H:63:LEU:HD11   | 8:H:141:TYR:CE2   | 2.36                     | 0.61              |
| 9:I:73:ARG:HH12   | 9:I:112:SER:HB3   | 1.64                     | 0.61              |
| 1:A:75:ASN:HD22   | 2:B:1116:ARG:HH12 | 1.47                     | 0.61              |
| 1:A:331:GLY:O     | 1:A:332:LYS:O     | 2.18                     | 0.61              |
| 1:A:399:HIS:HB3   | 1:A:400:PRO:CD    | 2.28                     | 0.61              |
| 1:A:591:PHE:HA    | 1:A:595:THR:HG21  | 1.82                     | 0.61              |
| 1:A:1076:ALA:HA   | 1:A:1079:MET:HE2  | 1.81                     | 0.61              |
| 3:C:181:ASP:OD1   | 3:C:186:LEU:HD13  | 2.01                     | 0.61              |
| 3:C:221:TYR:CE1   | 3:C:222:LYS:HG3   | 2.35                     | 0.61              |
| 10:J:23:ASN:C     | 10:J:25:LEU:H     | 2.09                     | 0.61              |
| 1:A:84:ILE:CD1    | 1:A:270:LEU:HD13  | 2.31                     | 0.61              |
| 4:D:35:LEU:H      | 4:D:35:LEU:HD12   | 1.64                     | 0.61              |
| 5:E:32:GLN:HG3    | 5:E:36:GLU:OE2    | 2.00                     | 0.61              |
| 6:F:83:PRO:HD2    | 6:F:84:TYR:HD1    | 1.65                     | 0.61              |
| 6:F:93:ILE:CD1    | 6:F:134:ILE:HD11  | 2.30                     | 0.61              |
| 10:J:24:LEU:O     | 10:J:30:LEU:HB2   | 2.01                     | 0.61              |
| 1:A:78:PRO:HA     | 2:B:1201:LYS:HZ1  | 1.65                     | 0.61              |
| 2:B:50:SER:OG     | 2:B:411:PRO:HD3   | 2.01                     | 0.61              |
| 2:B:611:PRO:HB3   | 2:B:685:LEU:HD11  | 1.83                     | 0.61              |
| 2:B:824:ILE:HG12  | 10:J:48:ARG:NH1   | 2.15                     | 0.61              |
| 2:B:1096:ARG:HG3  | 2:B:1097:HIS:H    | 1.66                     | 0.61              |
| 4:D:13:ARG:C      | 4:D:15:LEU:H      | 2.08                     | 0.61              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 7:G:115:MET:HB3  | 7:G:116:PRO:HD2   | 1.81                     | 0.61              |
| 13:T:23:BRU:H6   | 13:T:23:BRU:H5''  | 1.83                     | 0.61              |
| 1:A:244:PRO:HB2  | 1:A:245:PRO:CD    | 2.27                     | 0.60              |
| 1:A:710:LEU:HD12 | 1:A:710:LEU:N     | 2.15                     | 0.60              |
| 2:B:39:ARG:NH2   | 2:B:665:GLU:HG2   | 2.15                     | 0.60              |
| 2:B:100:PRO:HD2  | 2:B:180:TYR:CE1   | 2.36                     | 0.60              |
| 2:B:277:LYS:HG3  | 2:B:336:ARG:HG2   | 1.83                     | 0.60              |
| 2:B:957:ASN:O    | 2:B:959:ASP:N     | 2.33                     | 0.60              |
| 5:E:78:LEU:CB    | 5:E:107:THR:HB    | 2.28                     | 0.60              |
| 6:F:109:VAL:HG13 | 6:F:127:GLU:OE1   | 2.01                     | 0.60              |
| 10:J:30:LEU:HD11 | 10:J:38:ARG:NH1   | 2.15                     | 0.60              |
| 1:A:108:MET:O    | 1:A:109:HIS:HB3   | 2.01                     | 0.60              |
| 1:A:172:PRO:HD3  | 1:A:185:TRP:NE1   | 2.16                     | 0.60              |
| 1:A:420:ARG:O    | 1:A:424:ILE:HG13  | 2.01                     | 0.60              |
| 1:A:853:ASP:O    | 1:A:854:ASN:HB2   | 2.00                     | 0.60              |
| 2:B:839:MET:HE3  | 2:B:1010:LEU:CD2  | 2.30                     | 0.60              |
| 2:B:842:ASN:O    | 2:B:846:ILE:HG13  | 2.01                     | 0.60              |
| 5:E:99:HIS:CE1   | 5:E:103:LYS:HG3   | 2.36                     | 0.60              |
| 7:G:126:ASN:HD22 | 7:G:127:PRO:N     | 1.99                     | 0.60              |
| 1:A:49:LYS:HZ3   | 1:A:61:ILE:CG1    | 2.10                     | 0.60              |
| 1:A:384:ASN:OD1  | 1:A:388:LEU:HD12  | 2.00                     | 0.60              |
| 2:B:172:ILE:HD13 | 2:B:178:ASN:ND2   | 2.15                     | 0.60              |
| 2:B:756:ILE:O    | 2:B:759:PRO:HD3   | 2.01                     | 0.60              |
| 2:B:1182:CYS:O   | 2:B:1182:CYS:SG   | 2.59                     | 0.60              |
| 3:C:104:PHE:HD2  | 3:C:105:GLY:N     | 1.99                     | 0.60              |
| 7:G:35:GLU:HG2   | 7:G:48:VAL:HG23   | 1.81                     | 0.60              |
| 2:B:552:MET:HA   | 2:B:552:MET:HE3   | 1.83                     | 0.60              |
| 4:D:8:PHE:CE1    | 4:D:37:GLN:HB2    | 2.37                     | 0.60              |
| 6:F:118:LEU:O    | 6:F:122:MET:HG3   | 2.01                     | 0.60              |
| 1:A:401:GLY:C    | 1:A:435:HIS:HD2   | 2.09                     | 0.60              |
| 1:A:1004:ASN:ND2 | 5:E:167:ARG:HD2   | 2.15                     | 0.60              |
| 2:B:120:ARG:HH12 | 12:L:54:ARG:NH1   | 1.90                     | 0.60              |
| 2:B:653:VAL:CG2  | 2:B:689:LEU:HB3   | 2.31                     | 0.60              |
| 3:C:183:TRP:O    | 3:C:185:LYS:HG3   | 2.01                     | 0.60              |
| 1:A:117:GLU:H    | 1:A:117:GLU:CD    | 2.09                     | 0.60              |
| 1:A:185:TRP:HE3  | 1:A:185:TRP:H     | 1.50                     | 0.60              |
| 1:A:714:PHE:CB   | 9:I:97:MET:HE1    | 2.30                     | 0.60              |
| 1:A:981:LEU:CD2  | 1:A:1039:LYS:HA   | 2.29                     | 0.60              |
| 1:A:1340:GLY:HA2 | 5:E:183:PRO:HD2   | 1.81                     | 0.60              |
| 2:B:1085:ILE:N   | 2:B:1085:ILE:HD12 | 2.16                     | 0.60              |
| 7:G:21:ARG:HD2   | 7:G:24:GLN:HB3    | 1.83                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:79:GLY:HA3    | 1:A:243:PRO:HG3   | 1.82                     | 0.60              |
| 1:A:96:ILE:HA     | 1:A:99:ILE:HD12   | 1.84                     | 0.60              |
| 1:A:107:CYS:HB2   | 1:A:114:LEU:HD21  | 1.82                     | 0.60              |
| 1:A:323:LYS:H     | 1:A:323:LYS:HD2   | 1.67                     | 0.60              |
| 1:A:1339:LEU:HD13 | 5:E:147:HIS:CD2   | 2.37                     | 0.60              |
| 2:B:345:LYS:HG2   | 2:B:346:GLU:N     | 2.16                     | 0.60              |
| 1:A:335:ARG:NH1   | 2:B:1202:LEU:HD13 | 2.17                     | 0.60              |
| 1:A:1109:LYS:C    | 1:A:1110:ASN:HD22 | 2.10                     | 0.60              |
| 2:B:192:LEU:O     | 2:B:193:LYS:HB2   | 2.01                     | 0.60              |
| 2:B:464:GLY:O     | 2:B:477:ALA:HA    | 2.02                     | 0.60              |
| 2:B:542:MET:HG2   | 2:B:747:MET:CE    | 2.31                     | 0.60              |
| 4:D:14:ARG:O      | 4:D:16:LYS:N      | 2.32                     | 0.60              |
| 1:A:1118:VAL:O    | 1:A:1305:VAL:HG13 | 2.02                     | 0.60              |
| 2:B:69:LEU:HB3    | 2:B:429:PHE:CE1   | 2.36                     | 0.60              |
| 2:B:247:GLY:C     | 2:B:249:ARG:H     | 2.10                     | 0.60              |
| 3:C:243:VAL:O     | 3:C:243:VAL:HG12  | 2.00                     | 0.60              |
| 1:A:42:ASP:HA     | 1:A:46:THR:O      | 2.02                     | 0.60              |
| 1:A:265:LYS:O     | 1:A:269:ILE:HG13  | 2.02                     | 0.60              |
| 1:A:711:ARG:HH21  | 9:I:97:MET:HG2    | 1.66                     | 0.60              |
| 1:A:1167:GLU:O    | 1:A:1170:ILE:HD12 | 2.02                     | 0.60              |
| 2:B:292:ILE:HD11  | 2:B:327:ARG:N     | 2.16                     | 0.60              |
| 2:B:327:ARG:NH2   | 2:B:371:GLU:HG2   | 2.17                     | 0.60              |
| 2:B:787:VAL:O     | 2:B:787:VAL:HG12  | 2.01                     | 0.60              |
| 11:K:21:ILE:CG2   | 11:K:31:VAL:HG11  | 2.31                     | 0.60              |
| 1:A:65:LEU:O      | 1:A:66:LYS:C      | 2.44                     | 0.59              |
| 1:A:535:THR:HG21  | 1:A:616:VAL:HA    | 1.82                     | 0.59              |
| 2:B:64:CYS:HA     | 2:B:67:SER:OG     | 2.02                     | 0.59              |
| 2:B:313:MET:HE2   | 2:B:390:LEU:HD11  | 1.81                     | 0.59              |
| 2:B:637:LEU:CD2   | 2:B:742:GLU:HA    | 2.32                     | 0.59              |
| 2:B:797:TYR:O     | 10:J:1:MET:HG2    | 2.01                     | 0.59              |
| 2:B:806:THR:CG2   | 2:B:808:ALA:HB3   | 2.31                     | 0.59              |
| 3:C:263:THR:O     | 3:C:266:ASP:HB2   | 2.02                     | 0.59              |
| 4:D:52:LEU:O      | 4:D:54:GLU:N      | 2.34                     | 0.59              |
| 1:A:998:LEU:HD12  | 1:A:998:LEU:N     | 2.17                     | 0.59              |
| 1:A:1114:PRO:O    | 1:A:1311:VAL:HG23 | 2.02                     | 0.59              |
| 2:B:418:LYS:HG2   | 2:B:422:LYS:HE3   | 1.83                     | 0.59              |
| 3:C:177:GLU:HG3   | 3:C:231:ASN:HD22  | 1.64                     | 0.59              |
| 5:E:212:ARG:HG3   | 5:E:212:ARG:HH11  | 1.66                     | 0.59              |
| 7:G:27:LYS:O      | 7:G:31:LEU:HG     | 2.02                     | 0.59              |
| 11:K:31:VAL:HG12  | 11:K:32:VAL:N     | 2.15                     | 0.59              |
| 1:A:7:SER:HB3     | 2:B:1193:GLN:HE22 | 1.67                     | 0.59              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:626:ASN:O    | 1:A:631:HIS:CD2   | 2.55                     | 0.59              |
| 2:B:291:ILE:HD13 | 2:B:300:HIS:NE2   | 2.17                     | 0.59              |
| 2:B:616:ILE:HD12 | 2:B:616:ILE:N     | 2.17                     | 0.59              |
| 2:B:708:GLU:HG3  | 2:B:709:ASP:H     | 1.65                     | 0.59              |
| 4:D:7:THR:O      | 4:D:7:THR:HG23    | 2.02                     | 0.59              |
| 7:G:119:LEU:HD13 | 7:G:132:SER:HB2   | 1.83                     | 0.59              |
| 12:L:53:HIS:O    | 12:L:55:ILE:HD13  | 2.02                     | 0.59              |
| 12:L:55:ILE:HG12 | 12:L:56:LEU:N     | 2.02                     | 0.59              |
| 1:A:809:THR:OG1  | 1:A:812:GLU:HG3   | 2.02                     | 0.59              |
| 2:B:303:TYR:CD2  | 2:B:303:TYR:N     | 2.70                     | 0.59              |
| 2:B:531:GLN:HG2  | 2:B:532:ALA:N     | 2.15                     | 0.59              |
| 2:B:916:THR:HB   | 2:B:935:ARG:CG    | 2.33                     | 0.59              |
| 3:C:124:LEU:HD21 | 3:C:129:ILE:O     | 2.03                     | 0.59              |
| 4:D:154:PHE:HE1  | 4:D:163:VAL:HG11  | 1.66                     | 0.59              |
| 8:H:84:ALA:HB1   | 8:H:87:ARG:HB2    | 1.84                     | 0.59              |
| 8:H:123:MET:HE1  | 8:H:142:LEU:HD11  | 1.82                     | 0.59              |
| 12:L:27:LEU:HD13 | 12:L:37:LYS:HD2   | 1.85                     | 0.59              |
| 2:B:1177:HIS:HB3 | 2:B:1179:GLN:HE21 | 1.66                     | 0.59              |
| 10:J:57:ILE:HA   | 10:J:60:PHE:CD2   | 2.34                     | 0.59              |
| 1:A:100:LYS:HE2  | 1:A:104:GLU:OE2   | 2.02                     | 0.59              |
| 1:A:381:THR:HG23 | 1:A:382:PRO:CD    | 2.32                     | 0.59              |
| 1:A:728:LYS:HA   | 1:A:731:ARG:NH1   | 2.18                     | 0.59              |
| 1:A:1267:MET:HA  | 1:A:1271:ILE:HD12 | 1.83                     | 0.59              |
| 1:A:1342:GLU:CG  | 5:E:198:ILE:HD13  | 2.32                     | 0.59              |
| 2:B:815:ARG:HB2  | 2:B:815:ARG:NH1   | 2.16                     | 0.59              |
| 5:E:124:VAL:HA   | 5:E:132:ILE:HD12  | 1.84                     | 0.59              |
| 8:H:89:LEU:C     | 8:H:91:ASP:N      | 2.52                     | 0.59              |
| 1:A:850:VAL:HG21 | 1:A:1058:VAL:HG11 | 1.84                     | 0.59              |
| 1:A:857:ARG:NH1  | 6:F:139:PRO:HB2   | 2.17                     | 0.59              |
| 1:A:986:ILE:O    | 1:A:990:VAL:HG23  | 2.03                     | 0.59              |
| 1:A:1063:MET:SD  | 1:A:1436:ILE:HB   | 2.42                     | 0.59              |
| 1:A:1293:SER:HB2 | 1:A:1299:VAL:HG21 | 1.85                     | 0.59              |
| 2:B:39:ARG:HG2   | 2:B:39:ARG:NH1    | 2.17                     | 0.59              |
| 2:B:467:GLY:CA   | 2:B:475:SER:HB3   | 2.33                     | 0.59              |
| 2:B:807:ARG:HG2  | 2:B:1045:SER:OG   | 2.03                     | 0.59              |
| 3:C:35:ARG:NH1   | 11:K:41:THR:H     | 2.01                     | 0.59              |
| 1:A:67:CYS:O     | 1:A:68:GLN:HG3    | 2.03                     | 0.59              |
| 1:A:89:PRO:C     | 1:A:204:THR:HG21  | 2.28                     | 0.59              |
| 1:A:598:LEU:O    | 1:A:599:SER:C     | 2.46                     | 0.59              |
| 1:A:679:ILE:HG23 | 1:A:729:ALA:HB1   | 1.85                     | 0.59              |
| 1:A:836:TYR:CE2  | 1:A:840:ARG:HD2   | 2.37                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1348:LEU:O    | 1:A:1352:VAL:HG23 | 2.03                     | 0.59              |
| 2:B:313:MET:HE3   | 2:B:386:LEU:HD22  | 1.83                     | 0.59              |
| 2:B:642:ASP:O     | 2:B:644:GLU:N     | 2.28                     | 0.59              |
| 2:B:860:MET:HG2   | 2:B:861:ASP:H     | 1.67                     | 0.59              |
| 2:B:911:ILE:HD11  | 2:B:941:LEU:CD1   | 2.29                     | 0.59              |
| 8:H:25:ARG:NH2    | 8:H:122:LEU:HD12  | 2.16                     | 0.59              |
| 8:H:139:ASN:O     | 8:H:140:ALA:HB2   | 2.02                     | 0.59              |
| 1:A:41:MET:HB2    | 1:A:48:ALA:O      | 2.03                     | 0.59              |
| 1:A:311:GLN:O     | 1:A:313:GLN:N     | 2.36                     | 0.59              |
| 1:A:694:THR:O     | 1:A:698:GLN:HG3   | 2.03                     | 0.59              |
| 1:A:728:LYS:O     | 1:A:732:LEU:HG    | 2.02                     | 0.59              |
| 1:A:768:GLN:CG    | 1:A:816:HIS:HA    | 2.30                     | 0.59              |
| 1:A:1444:MET:HG2  | 7:G:60:ARG:HA     | 1.84                     | 0.59              |
| 2:B:129:PHE:HD2   | 2:B:166:PHE:HA    | 1.67                     | 0.59              |
| 1:A:23:SER:HB3    | 1:A:233:TRP:CZ2   | 2.38                     | 0.59              |
| 1:A:486:GLU:OE1   | 2:B:1102:LYS:HD3  | 2.03                     | 0.59              |
| 1:A:1206:ASP:HB3  | 1:A:1274:ARG:HH22 | 1.67                     | 0.59              |
| 1:A:1208:THR:HG22 | 1:A:1210:GLY:N    | 2.18                     | 0.59              |
| 2:B:48:LEU:HD23   | 2:B:173:MET:SD    | 2.43                     | 0.59              |
| 2:B:806:THR:HG22  | 2:B:808:ALA:N     | 2.12                     | 0.59              |
| 2:B:868:MET:O     | 2:B:870:ILE:HG13  | 2.03                     | 0.59              |
| 3:C:114:TYR:CD2   | 3:C:140:ASN:CB    | 2.86                     | 0.59              |
| 1:A:565:ILE:HD13  | 1:A:567:LYS:HE2   | 1.84                     | 0.58              |
| 1:A:774:ARG:NH2   | 1:A:797:LYS:HB2   | 2.18                     | 0.58              |
| 1:A:1110:ASN:N    | 1:A:1110:ASN:ND2  | 2.50                     | 0.58              |
| 2:B:811:TYR:H     | 2:B:811:TYR:HD1   | 1.51                     | 0.58              |
| 4:D:138:ASN:HD21  | 7:G:35:GLU:HB3    | 1.67                     | 0.58              |
| 11:K:93:SER:O     | 11:K:97:LYS:HG3   | 2.03                     | 0.58              |
| 12:L:68:GLU:H     | 12:L:68:GLU:CD    | 2.11                     | 0.58              |
| 1:A:344:ARG:HB3   | 1:A:344:ARG:NH1   | 2.11                     | 0.58              |
| 1:A:915:SER:O     | 1:A:919:ILE:HB    | 2.02                     | 0.58              |
| 1:A:1259:MET:HE3  | 1:A:1263:ILE:CG1  | 2.32                     | 0.58              |
| 2:B:794:ASN:C     | 2:B:795:ILE:HD12  | 2.27                     | 0.58              |
| 2:B:1065:GLN:NE2  | 2:B:1067:ARG:HG2  | 2.18                     | 0.58              |
| 1:A:828:ALA:CB    | 2:B:530:GLY:HA2   | 2.32                     | 0.58              |
| 1:A:1029:ARG:HH11 | 1:A:1029:ARG:HG3  | 1.68                     | 0.58              |
| 1:A:1081:LEU:HD11 | 1:A:1098:VAL:N    | 2.18                     | 0.58              |
| 1:A:1158:PRO:C    | 1:A:1159:ARG:HG3  | 2.28                     | 0.58              |
| 2:B:766:ARG:HH22  | 2:B:1020:ARG:NH1  | 1.96                     | 0.58              |
| 2:B:899:ILE:CG2   | 2:B:949:VAL:HG21  | 2.33                     | 0.58              |
| 4:D:12:ARG:NH1    | 4:D:14:ARG:HA     | 2.18                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:E:136:ASN:OD1   | 5:E:138:ALA:N     | 2.37                     | 0.58              |
| 1:A:182:VAL:CG2   | 1:A:201:VAL:HG22  | 2.33                     | 0.58              |
| 1:A:854:ASN:ND2   | 1:A:1000:LEU:HD23 | 2.18                     | 0.58              |
| 1:A:1293:SER:OG   | 1:A:1294:PRO:HD2  | 2.04                     | 0.58              |
| 2:B:531:GLN:CG    | 2:B:532:ALA:H     | 2.11                     | 0.58              |
| 2:B:708:GLU:O     | 2:B:710:LEU:N     | 2.36                     | 0.58              |
| 3:C:167:HIS:NE2   | 12:L:70:ARG:HB3   | 2.18                     | 0.58              |
| 3:C:209:TYR:HD1   | 3:C:209:TYR:H     | 1.49                     | 0.58              |
| 5:E:94:LYS:CE     | 5:E:98:ILE:HD11   | 2.23                     | 0.58              |
| 7:G:138:THR:CG2   | 7:G:139:ILE:N     | 2.66                     | 0.58              |
| 8:H:4:THR:HA      | 8:H:60:ALA:CB     | 2.20                     | 0.58              |
| 8:H:128:ASN:ND2   | 8:H:131:ASN:OD1   | 2.36                     | 0.58              |
| 10:J:53:HIS:CD2   | 10:J:54:VAL:N     | 2.72                     | 0.58              |
| 1:A:697:ALA:CB    | 1:A:702:LEU:HD11  | 2.34                     | 0.58              |
| 1:A:718:VAL:O     | 1:A:721:PHE:HB2   | 2.03                     | 0.58              |
| 2:B:792:MET:HA    | 2:B:856:PHE:O     | 2.02                     | 0.58              |
| 2:B:847:ASP:C     | 2:B:849:GLY:N     | 2.62                     | 0.58              |
| 2:B:978:ASP:OD2   | 2:B:1098:MET:HG2  | 2.04                     | 0.58              |
| 4:D:216:ASN:C     | 4:D:218:GLU:N     | 2.59                     | 0.58              |
| 5:E:26:ARG:O      | 5:E:75:MET:HE1    | 2.03                     | 0.58              |
| 11:K:21:ILE:HG23  | 11:K:31:VAL:HG11  | 1.84                     | 0.58              |
| 1:A:132:LYS:HE3   | 1:A:1411:GLU:HG3  | 1.85                     | 0.58              |
| 1:A:535:THR:HG22  | 1:A:616:VAL:HA    | 1.85                     | 0.58              |
| 1:A:600:PRO:HA    | 8:H:25:ARG:NH1    | 2.19                     | 0.58              |
| 1:A:606:LEU:HG    | 1:A:613:ILE:HD12  | 1.86                     | 0.58              |
| 1:A:718:VAL:O     | 1:A:722:LEU:HD12  | 2.02                     | 0.58              |
| 1:A:1094:VAL:HG13 | 1:A:1113:THR:HG21 | 1.86                     | 0.58              |
| 1:A:1152:ILE:HD13 | 1:A:1260:LEU:HD23 | 1.86                     | 0.58              |
| 1:A:1236:LEU:C    | 1:A:1237:ILE:HD12 | 2.29                     | 0.58              |
| 2:B:449:ASN:C     | 2:B:451:LYS:H     | 2.11                     | 0.58              |
| 2:B:468:GLU:OE1   | 2:B:470:LYS:HE3   | 2.03                     | 0.58              |
| 2:B:603:LEU:HB3   | 2:B:609:ILE:HD11  | 1.85                     | 0.58              |
| 2:B:792:MET:HE2   | 2:B:857:ARG:NH2   | 2.19                     | 0.58              |
| 2:B:863:GLU:O     | 2:B:961:LEU:HD13  | 2.02                     | 0.58              |
| 2:B:1180:PHE:HB3  | 2:B:1191:ILE:HD13 | 1.84                     | 0.58              |
| 3:C:73:GLN:HE21   | 3:C:75:MET:CB     | 2.16                     | 0.58              |
| 4:D:5:THR:O       | 4:D:5:THR:HG23    | 2.04                     | 0.58              |
| 5:E:121:MET:C     | 5:E:123:LEU:H     | 2.12                     | 0.58              |
| 5:E:177:ARG:HD3   | 5:E:215:MET:SD    | 2.43                     | 0.58              |
| 6:F:109:VAL:HG12  | 6:F:110:ASP:H     | 1.66                     | 0.58              |
| 6:F:111:LEU:C     | 6:F:113:GLY:H     | 2.10                     | 0.58              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 8:H:84:ALA:CA     | 8:H:87:ARG:HD2   | 2.32                     | 0.58              |
| 11:K:45:LEU:HG    | 11:K:94:ILE:CD1  | 2.34                     | 0.58              |
| 1:A:12:ARG:HD2    | 2:B:1218:THR:CB  | 2.34                     | 0.58              |
| 1:A:341:MET:HE3   | 2:B:1135:ARG:NH1 | 2.19                     | 0.58              |
| 1:A:573:SER:O     | 1:A:576:GLN:HB2  | 2.03                     | 0.58              |
| 1:A:1353:TYR:C    | 1:A:1353:TYR:HD2 | 2.11                     | 0.58              |
| 2:B:558:LEU:HD22  | 2:B:596:LEU:HD21 | 1.85                     | 0.58              |
| 3:C:76:ASP:OD2    | 3:C:128:ASN:N    | 2.36                     | 0.58              |
| 7:G:52:ASP:C      | 7:G:53:ASN:HD22  | 2.12                     | 0.58              |
| 1:A:35:ILE:CD1    | 1:A:241:VAL:HG11 | 2.34                     | 0.58              |
| 1:A:698:GLN:O     | 9:I:98:VAL:HG13  | 2.03                     | 0.58              |
| 2:B:778:MET:HE1   | 2:B:1094:ARG:CD  | 2.31                     | 0.58              |
| 2:B:1152:MET:CE   | 2:B:1157:ALA:HA  | 2.34                     | 0.58              |
| 8:H:145:ARG:O     | 8:H:146:ARG:HB2  | 2.03                     | 0.58              |
| 1:A:1111:MET:HE2  | 1:A:1113:THR:O   | 2.04                     | 0.58              |
| 2:B:251:ILE:O     | 2:B:251:ILE:HG22 | 2.02                     | 0.58              |
| 2:B:508:LEU:O     | 2:B:509:ALA:HB3  | 2.04                     | 0.58              |
| 3:C:166:GLU:HG3   | 11:K:10:PHE:HZ   | 1.68                     | 0.58              |
| 1:A:41:MET:O      | 1:A:42:ASP:O     | 2.22                     | 0.58              |
| 1:A:55:ASP:CG     | 1:A:55:ASP:O     | 2.45                     | 0.58              |
| 2:B:245:GLU:C     | 2:B:246:LYS:HG3  | 2.29                     | 0.58              |
| 2:B:278:GLN:CG    | 2:B:279:ASP:H    | 2.00                     | 0.58              |
| 3:C:226:ASP:O     | 3:C:227:THR:HB   | 2.02                     | 0.58              |
| 7:G:27:LYS:HE2    | 7:G:54:ILE:HB    | 1.84                     | 0.58              |
| 10:J:44:TYR:CD2   | 10:J:44:TYR:N    | 2.72                     | 0.58              |
| 1:A:866:PHE:C     | 1:A:867:ILE:HD12 | 2.28                     | 0.57              |
| 1:A:1135:ARG:HG2  | 1:A:1136:SER:N   | 2.19                     | 0.57              |
| 2:B:205:ILE:N     | 2:B:205:ILE:HD12 | 2.19                     | 0.57              |
| 2:B:1177:HIS:HB2  | 2:B:1179:GLN:NE2 | 2.19                     | 0.57              |
| 1:A:66:LYS:O      | 1:A:67:CYS:HB2   | 2.04                     | 0.57              |
| 1:A:205:GLU:H     | 1:A:205:GLU:CD   | 2.12                     | 0.57              |
| 1:A:699:ALA:HB3   | 1:A:701:LEU:HG   | 1.86                     | 0.57              |
| 1:A:922:ASP:OD1   | 1:A:924:LYS:HB2  | 2.04                     | 0.57              |
| 1:A:1237:ILE:HG22 | 1:A:1238:ILE:N   | 2.19                     | 0.57              |
| 2:B:637:LEU:HD21  | 2:B:742:GLU:HA   | 1.86                     | 0.57              |
| 2:B:842:ASN:ND2   | 2:B:845:SER:H    | 2.01                     | 0.57              |
| 2:B:998:ASP:OD1   | 3:C:35:ARG:NH2   | 2.36                     | 0.57              |
| 5:E:42:PHE:HE1    | 5:E:58:MET:HE3   | 1.69                     | 0.57              |
| 6:F:97:ARG:HH21   | 6:F:108:PHE:HE1  | 1.52                     | 0.57              |
| 9:I:82:GLU:HB3    | 9:I:104:LEU:HD12 | 1.85                     | 0.57              |
| 12:L:33:GLU:H     | 12:L:33:GLU:CD   | 2.11                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1120:LEU:O   | 1:A:1323:ASP:HB2 | 2.04                     | 0.57              |
| 1:A:1293:SER:HB2 | 1:A:1299:VAL:CG2 | 2.34                     | 0.57              |
| 2:B:307:ASP:OD2  | 2:B:310:MET:HE3  | 2.04                     | 0.57              |
| 6:F:97:ARG:O     | 6:F:101:ILE:HG13 | 2.05                     | 0.57              |
| 12:L:52:GLY:O    | 12:L:53:HIS:C    | 2.48                     | 0.57              |
| 1:A:16:GLU:OE1   | 4:D:13:ARG:NH2   | 2.38                     | 0.57              |
| 1:A:666:ILE:HD12 | 1:A:666:ILE:N    | 2.19                     | 0.57              |
| 1:A:1259:MET:HA  | 1:A:1262:LYS:CD  | 2.31                     | 0.57              |
| 2:B:168:GLY:N    | 2:B:450:ALA:HB1  | 2.16                     | 0.57              |
| 2:B:292:ILE:HD13 | 2:B:326:ASP:HA   | 1.87                     | 0.57              |
| 2:B:377:PHE:CD2  | 2:B:381:MET:HE2  | 2.39                     | 0.57              |
| 3:C:89:GLU:O     | 3:C:90:ASP:HB3   | 2.05                     | 0.57              |
| 4:D:130:LEU:C    | 4:D:132:GLN:H    | 2.13                     | 0.57              |
| 11:K:88:LYS:O    | 11:K:91:CYS:HB2  | 2.03                     | 0.57              |
| 1:A:19:PHE:O     | 1:A:1416:ALA:HA  | 2.04                     | 0.57              |
| 1:A:35:ILE:HG22  | 1:A:35:ILE:O     | 2.02                     | 0.57              |
| 1:A:117:GLU:HA   | 1:A:123:ARG:HG3  | 1.85                     | 0.57              |
| 1:A:182:VAL:HG22 | 1:A:201:VAL:HG22 | 1.87                     | 0.57              |
| 1:A:285:PRO:O    | 1:A:287:HIS:N    | 2.37                     | 0.57              |
| 1:A:316:GLN:NE2  | 1:A:317:LYS:HE2  | 2.19                     | 0.57              |
| 1:A:979:SER:OG   | 1:A:980:ASP:N    | 2.37                     | 0.57              |
| 1:A:1280:GLU:O   | 1:A:1281:ARG:C   | 2.48                     | 0.57              |
| 2:B:582:VAL:HG23 | 2:B:626:ILE:HB   | 1.85                     | 0.57              |
| 6:F:77:ASP:O     | 6:F:78:GLN:CB    | 2.51                     | 0.57              |
| 7:G:106:MET:HG2  | 7:G:107:LYS:N    | 2.19                     | 0.57              |
| 9:I:55:THR:HG22  | 9:I:58:VAL:HG21  | 1.85                     | 0.57              |
| 1:A:313:GLN:O    | 1:A:314:ALA:C    | 2.46                     | 0.57              |
| 1:A:360:GLU:HB2  | 1:A:363:GLN:HG3  | 1.85                     | 0.57              |
| 1:A:444:PHE:CE2  | 1:A:487:MET:CE   | 2.87                     | 0.57              |
| 1:A:744:LYS:HG2  | 1:A:748:MET:HE2  | 1.86                     | 0.57              |
| 2:B:1166:CYS:O   | 2:B:1168:LEU:N   | 2.36                     | 0.57              |
| 3:C:113:VAL:HG23 | 3:C:147:LEU:HD21 | 1.85                     | 0.57              |
| 4:D:71:LYS:HA    | 4:D:74:GLN:CG    | 2.34                     | 0.57              |
| 4:D:128:VAL:HG12 | 4:D:129:LEU:N    | 2.20                     | 0.57              |
| 12:L:49:LYS:O    | 12:L:50:ASP:CB   | 2.52                     | 0.57              |
| 1:A:164:ARG:HG3  | 1:A:165:GLY:H    | 1.68                     | 0.57              |
| 1:A:387:ARG:HH11 | 1:A:437:MET:HE1  | 1.69                     | 0.57              |
| 1:A:907:THR:CG2  | 1:A:908:LEU:N    | 2.68                     | 0.57              |
| 2:B:185:THR:O    | 2:B:186:GLU:C    | 2.47                     | 0.57              |
| 3:C:8:VAL:C      | 3:C:9:LYS:HG3    | 2.29                     | 0.57              |
| 5:E:178:ILE:HG22 | 5:E:213:ILE:O    | 2.05                     | 0.57              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 12:L:60:ARG:HG2   | 12:L:61:THR:H    | 1.69                     | 0.57              |
| 1:A:106:VAL:HG21  | 1:A:214:ILE:CD1  | 2.33                     | 0.57              |
| 1:A:335:ARG:NH1   | 2:B:1206:GLU:CD  | 2.63                     | 0.57              |
| 1:A:897:TYR:HB3   | 1:A:936:LEU:HD12 | 1.85                     | 0.57              |
| 1:A:961:ARG:HG2   | 1:A:965:GLN:NE2  | 2.17                     | 0.57              |
| 2:B:229:ALA:HB1   | 2:B:231:PRO:HD2  | 1.87                     | 0.57              |
| 2:B:351:TYR:CZ    | 2:B:355:ILE:HD11 | 2.40                     | 0.57              |
| 2:B:794:ASN:O     | 2:B:795:ILE:HD12 | 2.05                     | 0.57              |
| 2:B:1099:VAL:HG13 | 2:B:1100:ASP:N   | 2.20                     | 0.57              |
| 3:C:39:ALA:O      | 3:C:164:ALA:HB3  | 2.05                     | 0.57              |
| 3:C:241:ASP:O     | 3:C:245:VAL:HG23 | 2.05                     | 0.57              |
| 4:D:210:ILE:O     | 4:D:214:LEU:HD23 | 2.05                     | 0.57              |
| 8:H:11:GLN:C      | 8:H:28:ALA:HB1   | 2.29                     | 0.57              |
| 8:H:24:CYS:HB2    | 8:H:44:VAL:CG2   | 2.31                     | 0.57              |
| 9:I:61:ASP:O      | 9:I:63:GLY:N     | 2.38                     | 0.57              |
| 14:N:2:DC:H1'     | 14:N:3:DT:H5'    | 1.86                     | 0.57              |
| 1:A:973:ILE:HD11  | 1:A:1041:ALA:HB2 | 1.87                     | 0.57              |
| 2:B:211:VAL:O     | 2:B:480:SER:HA   | 2.05                     | 0.57              |
| 1:A:268:ASP:HB3   | 1:A:299:HIS:ND1  | 2.20                     | 0.57              |
| 1:A:416:ARG:NH1   | 1:A:417:TYR:CE1  | 2.71                     | 0.57              |
| 1:A:896:ARG:NH2   | 1:A:1030:ARG:NH2 | 2.53                     | 0.57              |
| 2:B:276:ILE:HA    | 2:B:336:ARG:O    | 2.05                     | 0.57              |
| 3:C:33:LEU:O      | 3:C:37:MET:HG3   | 2.05                     | 0.57              |
| 3:C:148:ARG:HD3   | 3:C:149:LYS:HG3  | 1.85                     | 0.57              |
| 8:H:40:LEU:CD1    | 8:H:123:MET:HE3  | 2.30                     | 0.57              |
| 1:A:949:ASP:OD1   | 1:A:951:GLU:HB2  | 2.05                     | 0.56              |
| 1:A:1139:GLU:O    | 1:A:1139:GLU:HG2 | 2.05                     | 0.56              |
| 2:B:25:ILE:HD13   | 2:B:653:VAL:HG12 | 1.87                     | 0.56              |
| 3:C:215:GLU:O     | 3:C:216:GLY:C    | 2.47                     | 0.56              |
| 5:E:28:TYR:CE1    | 5:E:78:LEU:HD13  | 2.40                     | 0.56              |
| 5:E:89:GLY:C      | 5:E:91:LYS:H     | 2.13                     | 0.56              |
| 8:H:56:THR:HB     | 8:H:145:ARG:HG2  | 1.86                     | 0.56              |
| 1:A:443:LEU:HD12  | 2:B:1146:PHE:CZ  | 2.40                     | 0.56              |
| 1:A:903:ASN:ND2   | 1:A:903:ASN:C    | 2.63                     | 0.56              |
| 2:B:20:ASP:C      | 2:B:22:SER:H     | 2.13                     | 0.56              |
| 2:B:731:VAL:HG12  | 2:B:734:HIS:NE2  | 2.20                     | 0.56              |
| 3:C:36:VAL:HG21   | 3:C:251:LEU:HD13 | 1.87                     | 0.56              |
| 4:D:185:CYS:O     | 4:D:211:LEU:HD22 | 2.04                     | 0.56              |
| 1:A:7:SER:HB3     | 2:B:1193:GLN:NE2 | 2.20                     | 0.56              |
| 1:A:37:PHE:N      | 1:A:37:PHE:HD1   | 2.02                     | 0.56              |
| 1:A:332:LYS:O     | 1:A:334:GLY:N    | 2.38                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1200:ALA:HA   | 1:A:1203:ASN:HD22 | 1.70                     | 0.56              |
| 2:B:418:LYS:HE2   | 2:B:422:LYS:HZ2   | 1.70                     | 0.56              |
| 2:B:878:GLN:O     | 2:B:879:ARG:C     | 2.48                     | 0.56              |
| 4:D:25:ALA:HB1    | 4:D:196:PRO:HG2   | 1.86                     | 0.56              |
| 4:D:155:ARG:CD    | 4:D:221:TYR:HE1   | 2.11                     | 0.56              |
| 8:H:58:THR:HG22   | 8:H:59:ILE:N      | 2.18                     | 0.56              |
| 9:I:74:GLU:HB3    | 9:I:81:ARG:HD2    | 1.88                     | 0.56              |
| 12:L:34:CYS:O     | 12:L:34:CYS:SG    | 2.64                     | 0.56              |
| 1:A:57:ARG:O      | 1:A:68:GLN:HG2    | 2.06                     | 0.56              |
| 1:A:720:ARG:HG2   | 1:A:720:ARG:O     | 2.04                     | 0.56              |
| 2:B:39:ARG:HG2    | 2:B:39:ARG:HH11   | 1.70                     | 0.56              |
| 4:D:32:GLU:OE1    | 7:G:41:LYS:HE2    | 2.05                     | 0.56              |
| 7:G:1:MET:C       | 7:G:1:MET:HE2     | 2.30                     | 0.56              |
| 1:A:351:THR:HG22  | 2:B:1103:ILE:CA   | 2.27                     | 0.56              |
| 1:A:635:ARG:HH11  | 1:A:635:ARG:HA    | 1.69                     | 0.56              |
| 1:A:824:LEU:O     | 1:A:827:THR:HG22  | 2.06                     | 0.56              |
| 1:A:964:ILE:O     | 1:A:967:ALA:HB3   | 2.04                     | 0.56              |
| 1:A:1445:ILE:HD12 | 1:A:1445:ILE:N    | 2.21                     | 0.56              |
| 2:B:53:GLN:HG2    | 2:B:547:VAL:CG2   | 2.36                     | 0.56              |
| 2:B:303:TYR:N     | 2:B:303:TYR:HD2   | 2.03                     | 0.56              |
| 4:D:126:ILE:HD13  | 4:D:145:MET:HE3   | 1.87                     | 0.56              |
| 1:A:34:LYS:HG3    | 1:A:36:ARG:NH2    | 2.19                     | 0.56              |
| 1:A:224:PHE:CE2   | 1:A:234:MET:HE2   | 2.41                     | 0.56              |
| 1:A:315:LEU:N     | 1:A:315:LEU:CD2   | 2.64                     | 0.56              |
| 1:A:321:PRO:O     | 1:A:322:VAL:CB    | 2.53                     | 0.56              |
| 2:B:68:THR:HG22   | 2:B:91:SER:HA     | 1.87                     | 0.56              |
| 2:B:238:ALA:HB3   | 2:B:256:VAL:HB    | 1.88                     | 0.56              |
| 2:B:758:PHE:HE1   | 2:B:1027:ILE:HG22 | 1.67                     | 0.56              |
| 2:B:1084:GLN:NE2  | 2:B:1084:GLN:H    | 2.03                     | 0.56              |
| 3:C:253:LYS:O     | 3:C:256:ALA:HB3   | 2.06                     | 0.56              |
| 4:D:51:ASN:O      | 4:D:52:LEU:O      | 2.24                     | 0.56              |
| 5:E:198:ILE:CD1   | 5:E:212:ARG:HG3   | 2.34                     | 0.56              |
| 11:K:65:HIS:HD2   | 11:K:67:PHE:H     | 1.51                     | 0.56              |
| 1:A:370:ILE:HG12  | 2:B:1105:ALA:HB2  | 1.88                     | 0.56              |
| 2:B:245:GLU:O     | 2:B:246:LYS:HG3   | 2.05                     | 0.56              |
| 2:B:274:PRO:CG    | 2:B:359:GLU:HB3   | 2.36                     | 0.56              |
| 2:B:557:PHE:CZ    | 2:B:603:LEU:HD11  | 2.41                     | 0.56              |
| 2:B:601:ARG:O     | 2:B:605:ARG:HG3   | 2.06                     | 0.56              |
| 2:B:1096:ARG:CG   | 2:B:1097:HIS:N    | 2.69                     | 0.56              |
| 3:C:51:VAL:HG22   | 3:C:155:LEU:CD2   | 2.36                     | 0.56              |
| 5:E:69:ILE:H      | 5:E:69:ILE:HD12   | 1.71                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:E:69:ILE:HD12   | 5:E:69:ILE:N      | 2.21                     | 0.56              |
| 5:E:94:LYS:O      | 5:E:98:ILE:HG13   | 2.05                     | 0.56              |
| 5:E:157:SER:OG    | 5:E:160:GLU:HG3   | 2.06                     | 0.56              |
| 1:A:929:LEU:HD21  | 1:A:983:ILE:HG23  | 1.88                     | 0.56              |
| 1:A:1011:GLN:HE22 | 1:A:1015:VAL:HG21 | 1.71                     | 0.56              |
| 2:B:20:ASP:O      | 2:B:22:SER:N      | 2.29                     | 0.56              |
| 2:B:360:PHE:CZ    | 2:B:361:LEU:HD13  | 2.41                     | 0.56              |
| 2:B:604:ARG:C     | 2:B:606:LYS:H     | 2.11                     | 0.56              |
| 2:B:868:MET:HE3   | 2:B:868:MET:HA    | 1.87                     | 0.56              |
| 2:B:969:ARG:NH1   | 3:C:61:GLU:OE1    | 2.38                     | 0.56              |
| 2:B:1116:ARG:HG3  | 2:B:1198:TYR:CG   | 2.41                     | 0.56              |
| 3:C:112:ASN:HB3   | 3:C:114:TYR:HE1   | 1.66                     | 0.56              |
| 3:C:177:GLU:HG3   | 3:C:231:ASN:CB    | 2.26                     | 0.56              |
| 7:G:1:MET:O       | 7:G:2:PHE:C       | 2.48                     | 0.56              |
| 11:K:47:ARG:HD3   | 11:K:59:ALA:O     | 2.06                     | 0.56              |
| 13:T:18:DA:H3'    | 13:T:18:DA:OP1    | 2.06                     | 0.56              |
| 1:A:11:LEU:HB2    | 2:B:1193:GLN:CG   | 2.36                     | 0.56              |
| 1:A:470:LEU:N     | 1:A:470:LEU:HD23  | 2.20                     | 0.56              |
| 1:A:741:ASN:HD22  | 1:A:744:LYS:N     | 1.96                     | 0.56              |
| 1:A:825:ILE:O     | 1:A:829:VAL:HG23  | 2.06                     | 0.56              |
| 1:A:1205:LYS:O    | 1:A:1207:LEU:HG   | 2.06                     | 0.56              |
| 2:B:167:ILE:HD12  | 2:B:167:ILE:N     | 2.21                     | 0.56              |
| 2:B:345:LYS:CG    | 2:B:346:GLU:N     | 2.69                     | 0.56              |
| 2:B:575:PRO:HG2   | 2:B:576:ASP:H     | 1.69                     | 0.56              |
| 2:B:640:VAL:HG23  | 2:B:740:HIS:HA    | 1.87                     | 0.56              |
| 2:B:977:GLY:HA3   | 2:B:1099:VAL:HB   | 1.87                     | 0.56              |
| 1:A:53:LEU:CD2    | 1:A:54:ASN:N      | 2.55                     | 0.56              |
| 1:A:186:LYS:HZ3   | 1:A:197:PRO:HD3   | 1.69                     | 0.56              |
| 1:A:230:ARG:HG3   | 1:A:233:TRP:CZ3   | 2.41                     | 0.56              |
| 1:A:1170:ILE:HD12 | 1:A:1170:ILE:H    | 1.71                     | 0.56              |
| 2:B:102:VAL:HG21  | 2:B:112:LEU:HD13  | 1.88                     | 0.56              |
| 2:B:637:LEU:HD12  | 2:B:693:ILE:CD1   | 2.32                     | 0.56              |
| 2:B:731:VAL:HG12  | 2:B:732:SER:N     | 2.21                     | 0.56              |
| 2:B:935:ARG:HG3   | 2:B:935:ARG:O     | 2.05                     | 0.56              |
| 2:B:1177:HIS:CB   | 2:B:1179:GLN:NE2  | 2.69                     | 0.56              |
| 3:C:99:LEU:N      | 3:C:99:LEU:CD2    | 2.68                     | 0.56              |
| 4:D:59:ILE:HG21   | 4:D:145:MET:SD    | 2.46                     | 0.56              |
| 1:A:41:MET:HB2    | 1:A:49:LYS:HA     | 1.84                     | 0.55              |
| 1:A:62:ASP:O      | 1:A:64:ASN:N      | 2.39                     | 0.55              |
| 1:A:909:ASP:OD1   | 1:A:911:SER:N     | 2.37                     | 0.55              |
| 1:A:1116:LEU:C    | 1:A:1116:LEU:HD12 | 2.31                     | 0.55              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:B:47:GLN:O      | 2:B:173:MET:HE1  | 2.06                     | 0.55              |
| 2:B:614:SER:C     | 2:B:615:MET:HG3  | 2.31                     | 0.55              |
| 2:B:654:ARG:H     | 2:B:657:HIS:HD2  | 1.53                     | 0.55              |
| 2:B:1224:PHE:CZ   | 5:E:171:LYS:HG3  | 2.39                     | 0.55              |
| 4:D:4:SER:O       | 4:D:5:THR:CB     | 2.54                     | 0.55              |
| 6:F:89:GLU:O      | 6:F:93:ILE:HD12  | 2.05                     | 0.55              |
| 12:L:38:LEU:O     | 12:L:39:SER:HB3  | 2.06                     | 0.55              |
| 1:A:90:VAL:HB     | 1:A:297:GLN:HE21 | 1.68                     | 0.55              |
| 1:A:482:PHE:C     | 1:A:484:GLY:H    | 2.15                     | 0.55              |
| 1:A:1006:ILE:CD1  | 5:E:163:GLU:HG3  | 2.36                     | 0.55              |
| 2:B:273:LEU:CD2   | 2:B:360:PHE:HD1  | 2.19                     | 0.55              |
| 2:B:644:GLU:C     | 2:B:646:LEU:H    | 2.13                     | 0.55              |
| 2:B:999:MET:HE2   | 2:B:1011:ILE:CD1 | 2.37                     | 0.55              |
| 3:C:29:MET:HE1    | 11:K:97:LYS:HD2  | 1.88                     | 0.55              |
| 4:D:173:HIS:O     | 4:D:177:VAL:HG23 | 2.06                     | 0.55              |
| 5:E:42:PHE:CE1    | 5:E:58:MET:HE3   | 2.41                     | 0.55              |
| 10:J:23:ASN:O     | 10:J:25:LEU:N    | 2.40                     | 0.55              |
| 1:A:264:PHE:C     | 1:A:265:LYS:HE3  | 2.30                     | 0.55              |
| 1:A:427:GLN:HG3   | 1:A:430:TRP:CE2  | 2.40                     | 0.55              |
| 2:B:68:THR:HA     | 2:B:90:ILE:O     | 2.07                     | 0.55              |
| 2:B:209:GLU:OE2   | 2:B:485:ARG:NE   | 2.34                     | 0.55              |
| 2:B:309:GLN:HG3   | 9:I:52:ILE:CD1   | 2.37                     | 0.55              |
| 2:B:383:ASN:O     | 2:B:387:LEU:HD13 | 2.06                     | 0.55              |
| 2:B:560:GLU:O     | 2:B:561:TRP:CD1  | 2.59                     | 0.55              |
| 3:C:196:ASP:CG    | 3:C:199:LYS:HD3  | 2.32                     | 0.55              |
| 4:D:153:ARG:C     | 4:D:154:PHE:CD2  | 2.85                     | 0.55              |
| 5:E:98:ILE:HG22   | 5:E:102:GLU:HG3  | 1.88                     | 0.55              |
| 9:I:34:TYR:CD2    | 9:I:35:VAL:N     | 2.74                     | 0.55              |
| 1:A:562:THR:HB    | 8:H:98:TYR:CD2   | 2.42                     | 0.55              |
| 2:B:427:ASP:HA    | 2:B:430:ARG:CD   | 2.36                     | 0.55              |
| 2:B:916:THR:O     | 2:B:935:ARG:HG2  | 2.07                     | 0.55              |
| 5:E:2:ASP:O       | 5:E:3:GLN:HG2    | 2.06                     | 0.55              |
| 5:E:129:PRO:O     | 5:E:130:ALA:C    | 2.48                     | 0.55              |
| 6:F:111:LEU:H     | 6:F:111:LEU:CD1  | 2.16                     | 0.55              |
| 1:A:709:THR:CG2   | 1:A:711:ARG:HG3  | 2.35                     | 0.55              |
| 2:B:1113:VAL:HG23 | 15:P:1:C:H4'     | 1.88                     | 0.55              |
| 4:D:12:ARG:HH12   | 4:D:14:ARG:HA    | 1.71                     | 0.55              |
| 5:E:46:TYR:CD2    | 5:E:58:MET:HG2   | 2.41                     | 0.55              |
| 7:G:1:MET:HE3     | 7:G:80:LYS:H     | 1.70                     | 0.55              |
| 1:A:598:LEU:HA    | 8:H:122:LEU:HD13 | 1.87                     | 0.55              |
| 1:A:1277:GLU:C    | 1:A:1279:ILE:H   | 2.15                     | 0.55              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B:97:VAL:O     | 2:B:97:VAL:HG13   | 2.06                     | 0.55              |
| 2:B:101:MET:HB3  | 2:B:109:THR:HG22  | 1.87                     | 0.55              |
| 2:B:459:TYR:CZ   | 2:B:469:GLN:HG3   | 2.42                     | 0.55              |
| 2:B:1096:ARG:HG3 | 2:B:1097:HIS:N    | 2.21                     | 0.55              |
| 4:D:69:ALA:C     | 4:D:71:LYS:H      | 2.12                     | 0.55              |
| 8:H:123:MET:HE1  | 8:H:142:LEU:CD1   | 2.37                     | 0.55              |
| 1:A:7:SER:OG     | 2:B:1161:HIS:CE1  | 2.59                     | 0.55              |
| 1:A:172:PRO:HB3  | 1:A:185:TRP:CD2   | 2.41                     | 0.55              |
| 1:A:446:ARG:HG2  | 1:A:446:ARG:HH11  | 1.71                     | 0.55              |
| 1:A:886:ILE:HG23 | 1:A:887:GLY:H     | 1.72                     | 0.55              |
| 1:A:982:THR:HB   | 1:A:985:ASP:H     | 1.72                     | 0.55              |
| 2:B:640:VAL:O    | 2:B:641:GLU:C     | 2.50                     | 0.55              |
| 2:B:654:ARG:H    | 2:B:657:HIS:CD2   | 2.25                     | 0.55              |
| 2:B:1103:ILE:O   | 2:B:1122:ARG:NH1  | 2.40                     | 0.55              |
| 2:B:1115:THR:O   | 2:B:1116:ARG:HB2  | 2.06                     | 0.55              |
| 3:C:99:LEU:N     | 3:C:99:LEU:HD22   | 2.21                     | 0.55              |
| 8:H:61:SER:O     | 8:H:62:SER:HB2    | 2.07                     | 0.55              |
| 8:H:84:ALA:CB    | 8:H:87:ARG:HD2    | 2.37                     | 0.55              |
| 8:H:101:ALA:HB2  | 8:H:116:TYR:CE2   | 2.42                     | 0.55              |
| 8:H:106:GLU:HG2  | 8:H:112:ILE:CD1   | 2.37                     | 0.55              |
| 1:A:120:GLU:HG3  | 1:A:123:ARG:NH2   | 2.22                     | 0.55              |
| 1:A:714:PHE:O    | 1:A:718:VAL:HG23  | 2.07                     | 0.55              |
| 1:A:1011:GLN:NE2 | 1:A:1015:VAL:HG21 | 2.21                     | 0.55              |
| 1:A:1433:MET:CE  | 7:G:63:PRO:HB2    | 2.36                     | 0.55              |
| 2:B:361:LEU:O    | 2:B:363:HIS:O     | 2.25                     | 0.55              |
| 2:B:652:LYS:HD2  | 2:B:688:GLY:O     | 2.07                     | 0.55              |
| 2:B:1017:ILE:HB  | 2:B:1018:PRO:HD3  | 1.89                     | 0.55              |
| 4:D:219:THR:HG22 | 4:D:220:LEU:O     | 2.07                     | 0.55              |
| 9:I:74:GLU:HB3   | 9:I:81:ARG:NE     | 2.22                     | 0.55              |
| 1:A:693:VAL:HG21 | 1:A:721:PHE:HE1   | 1.70                     | 0.55              |
| 2:B:333:PHE:O    | 2:B:334:ILE:HG13  | 2.07                     | 0.55              |
| 2:B:370:PHE:HD2  | 2:B:373:ARG:HD3   | 1.72                     | 0.55              |
| 2:B:1004:GLU:CG  | 10:J:42:LYS:NZ    | 2.70                     | 0.55              |
| 3:C:80:LEU:HD11  | 3:C:95:CYS:CA     | 2.37                     | 0.55              |
| 4:D:12:ARG:HH11  | 4:D:12:ARG:CG     | 2.15                     | 0.55              |
| 4:D:213:GLU:OE1  | 4:D:213:GLU:HA    | 2.07                     | 0.55              |
| 1:A:1436:ILE:O   | 1:A:1437:GLY:C    | 2.50                     | 0.55              |
| 2:B:254:LEU:HD23 | 2:B:381:MET:HE1   | 1.89                     | 0.55              |
| 3:C:112:ASN:CB   | 3:C:114:TYR:HE1   | 2.19                     | 0.55              |
| 8:H:130:ARG:HB3  | 8:H:134:ASN:H     | 1.72                     | 0.55              |
| 12:L:38:LEU:HG   | 12:L:39:SER:H     | 1.72                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:381:THR:HG21  | 1:A:383:TYR:CD1   | 2.42                     | 0.54              |
| 1:A:512:VAL:O     | 1:A:512:VAL:CG1   | 2.56                     | 0.54              |
| 1:A:596:THR:C     | 1:A:598:LEU:N     | 2.62                     | 0.54              |
| 1:A:1161:THR:CG2  | 1:A:1163:ILE:H    | 2.08                     | 0.54              |
| 2:B:185:THR:O     | 2:B:188:ASP:N     | 2.40                     | 0.54              |
| 2:B:434:ARG:O     | 2:B:436:VAL:HG23  | 2.07                     | 0.54              |
| 2:B:590:HIS:NE2   | 2:B:592:ASN:O     | 2.39                     | 0.54              |
| 2:B:792:MET:HG2   | 2:B:855:PHE:CE1   | 2.41                     | 0.54              |
| 2:B:855:PHE:HZ    | 2:B:857:ARG:HH12  | 1.54                     | 0.54              |
| 4:D:120:GLU:OE1   | 4:D:120:GLU:O     | 2.25                     | 0.54              |
| 7:G:21:ARG:HD2    | 7:G:24:GLN:CB     | 2.37                     | 0.54              |
| 7:G:49:LEU:HG     | 7:G:76:ALA:HA     | 1.88                     | 0.54              |
| 8:H:26:ILE:HG22   | 8:H:40:LEU:O      | 2.07                     | 0.54              |
| 9:I:82:GLU:HB3    | 9:I:104:LEU:CG    | 2.37                     | 0.54              |
| 10:J:9:SER:HB2    | 10:J:45:CYS:HB2   | 1.89                     | 0.54              |
| 1:A:154:SER:HB3   | 1:A:162:VAL:HG21  | 1.88                     | 0.54              |
| 1:A:645:LEU:HD11  | 1:A:649:ILE:HD11  | 1.89                     | 0.54              |
| 1:A:1445:ILE:H    | 1:A:1445:ILE:CD1  | 2.18                     | 0.54              |
| 2:B:93:GLY:O      | 2:B:130:VAL:HG13  | 2.07                     | 0.54              |
| 2:B:108:VAL:HG23  | 2:B:109:THR:H     | 1.70                     | 0.54              |
| 2:B:427:ASP:HA    | 2:B:430:ARG:HG3   | 1.89                     | 0.54              |
| 2:B:637:LEU:HD22  | 2:B:741:CYS:O     | 2.07                     | 0.54              |
| 3:C:91:HIS:C      | 3:C:91:HIS:CD2    | 2.85                     | 0.54              |
| 3:C:123:ASN:CG    | 3:C:125:MET:H     | 2.16                     | 0.54              |
| 8:H:59:ILE:O      | 8:H:60:ALA:HB3    | 2.07                     | 0.54              |
| 8:H:89:LEU:HB2    | 8:H:91:ASP:CG     | 2.32                     | 0.54              |
| 11:K:47:ARG:O     | 11:K:47:ARG:HD2   | 2.08                     | 0.54              |
| 1:A:1349:TYR:C    | 1:A:1349:TYR:CD2  | 2.85                     | 0.54              |
| 1:A:1437:GLY:O    | 1:A:1439:GLY:N    | 2.40                     | 0.54              |
| 2:B:313:MET:CE    | 2:B:386:LEU:HD22  | 2.37                     | 0.54              |
| 5:E:3:GLN:NE2     | 5:E:52:ARG:HH12   | 2.05                     | 0.54              |
| 8:H:12:VAL:CG1    | 8:H:26:ILE:HD11   | 2.37                     | 0.54              |
| 1:A:710:LEU:H     | 1:A:710:LEU:CD1   | 2.17                     | 0.54              |
| 1:A:903:ASN:HD22  | 1:A:904:THR:H     | 1.51                     | 0.54              |
| 1:A:1118:VAL:HG12 | 1:A:1327:ILE:HG13 | 1.88                     | 0.54              |
| 2:B:519:TRP:C     | 2:B:519:TRP:CD1   | 2.85                     | 0.54              |
| 2:B:906:SER:O     | 2:B:907:GLY:C     | 2.50                     | 0.54              |
| 6:F:69:LEU:HD13   | 6:F:71:GLU:OE1    | 2.06                     | 0.54              |
| 7:G:87:VAL:CG2    | 7:G:103:VAL:HG21  | 2.36                     | 0.54              |
| 10:J:23:ASN:C     | 10:J:25:LEU:N     | 2.62                     | 0.54              |
| 10:J:27:GLU:C     | 10:J:29:GLU:H     | 2.15                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:102:VAL:HG13  | 1:A:222:LEU:HD13  | 1.89                     | 0.54              |
| 1:A:107:CYS:HB2   | 1:A:114:LEU:CD2   | 2.37                     | 0.54              |
| 1:A:219:PHE:HE1   | 1:A:230:ARG:HE    | 1.54                     | 0.54              |
| 1:A:269:ILE:HG12  | 1:A:299:HIS:HB3   | 1.90                     | 0.54              |
| 1:A:382:PRO:HD3   | 1:A:428:TYR:HD2   | 1.71                     | 0.54              |
| 1:A:443:LEU:HD12  | 2:B:1146:PHE:CE2  | 2.43                     | 0.54              |
| 1:A:524:VAL:HG12  | 1:A:525:GLN:H     | 1.73                     | 0.54              |
| 1:A:984:LYS:HG2   | 1:A:988:LEU:HD12  | 1.89                     | 0.54              |
| 1:A:1312:ASN:ND2  | 1:A:1315:GLU:HB2  | 2.22                     | 0.54              |
| 2:B:315:LYS:N     | 2:B:316:PRO:HD2   | 2.22                     | 0.54              |
| 2:B:686:ASN:C     | 2:B:688:GLY:H     | 2.15                     | 0.54              |
| 3:C:75:MET:HB3    | 3:C:128:ASN:HB3   | 1.90                     | 0.54              |
| 3:C:265:MET:HE1   | 11:K:19:LEU:HB2   | 1.88                     | 0.54              |
| 4:D:71:LYS:CA     | 4:D:74:GLN:HB2    | 2.36                     | 0.54              |
| 5:E:207:ARG:HB3   | 5:E:207:ARG:HH11  | 1.73                     | 0.54              |
| 1:A:332:LYS:HG2   | 1:A:333:GLU:HG2   | 1.90                     | 0.54              |
| 1:A:1173:HIS:CD2  | 1:A:1227:ILE:HG23 | 2.42                     | 0.54              |
| 1:A:1424:VAL:HG11 | 2:B:1139:ILE:HD13 | 1.89                     | 0.54              |
| 2:B:423:LYS:O     | 2:B:427:ASP:HB2   | 2.08                     | 0.54              |
| 2:B:620:ARG:HH12  | 9:I:68:LEU:HD21   | 1.71                     | 0.54              |
| 2:B:789:MET:HE3   | 2:B:965:LYS:HB3   | 1.90                     | 0.54              |
| 3:C:229:TYR:N     | 3:C:229:TYR:CD1   | 2.75                     | 0.54              |
| 5:E:78:LEU:HA     | 5:E:107:THR:HB    | 1.88                     | 0.54              |
| 8:H:109:LYS:HG2   | 8:H:110:ASP:OD1   | 2.07                     | 0.54              |
| 1:A:41:MET:O      | 1:A:42:ASP:C      | 2.50                     | 0.54              |
| 1:A:427:GLN:O     | 1:A:428:TYR:C     | 2.50                     | 0.54              |
| 1:A:709:THR:HB    | 1:A:712:GLU:H     | 1.71                     | 0.54              |
| 1:A:1219:THR:HG21 | 1:A:1271:ILE:HD11 | 1.89                     | 0.54              |
| 2:B:639:ILE:CG2   | 2:B:641:GLU:HG2   | 2.38                     | 0.54              |
| 2:B:875:GLU:O     | 2:B:877:PRO:CD    | 2.55                     | 0.54              |
| 3:C:31:ASN:O      | 3:C:34:ARG:HB3    | 2.07                     | 0.54              |
| 3:C:73:GLN:NE2    | 3:C:75:MET:H      | 2.06                     | 0.54              |
| 4:D:118:THR:HG22  | 4:D:118:THR:O     | 2.07                     | 0.54              |
| 5:E:144:ILE:HD13  | 5:E:183:PRO:HB3   | 1.90                     | 0.54              |
| 10:J:36:LEU:HD11  | 10:J:51:LEU:HB2   | 1.89                     | 0.54              |
| 1:A:500:GLU:O     | 1:A:504:LEU:HB2   | 2.08                     | 0.54              |
| 1:A:673:GLY:O     | 1:A:676:MET:HB2   | 2.08                     | 0.54              |
| 1:A:1349:TYR:O    | 1:A:1350:LYS:C    | 2.51                     | 0.54              |
| 1:A:1397:LEU:HB2  | 1:A:1426:GLU:OE1  | 2.08                     | 0.54              |
| 2:B:390:LEU:O     | 2:B:392:ARG:HG3   | 2.08                     | 0.54              |
| 2:B:658:ILE:CG2   | 2:B:662:MET:HE2   | 2.38                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:862:GLN:HG2   | 2:B:963:PHE:HD1   | 1.72                     | 0.54              |
| 2:B:871:THR:HG22  | 2:B:872:GLU:O     | 2.08                     | 0.54              |
| 5:E:144:ILE:HG13  | 5:E:145:THR:H     | 1.72                     | 0.54              |
| 7:G:9:LEU:HD12    | 7:G:10:ASN:N      | 2.22                     | 0.54              |
| 9:I:73:ARG:HD2    | 9:I:101:PHE:CE2   | 2.43                     | 0.54              |
| 1:A:597:LEU:HD12  | 1:A:597:LEU:N     | 2.23                     | 0.54              |
| 1:A:1161:THR:HG22 | 1:A:1162:VAL:N    | 2.22                     | 0.54              |
| 2:B:258:LEU:HG    | 2:B:258:LEU:O     | 2.07                     | 0.54              |
| 2:B:282:ILE:CD1   | 2:B:382:ILE:HD13  | 2.38                     | 0.54              |
| 2:B:361:LEU:HD21  | 2:B:377:PHE:HD2   | 1.73                     | 0.54              |
| 2:B:707:PRO:HG2   | 2:B:708:GLU:N     | 2.22                     | 0.54              |
| 3:C:80:LEU:HD11   | 3:C:95:CYS:HA     | 1.90                     | 0.54              |
| 6:F:90:ARG:HD3    | 6:F:155:LEU:HD13  | 1.89                     | 0.54              |
| 7:G:51:TYR:C      | 7:G:51:TYR:CD2    | 2.86                     | 0.54              |
| 12:L:58:LYS:O     | 12:L:58:LYS:HG2   | 2.08                     | 0.54              |
| 1:A:600:PRO:HG2   | 1:A:601:LYS:H     | 1.72                     | 0.54              |
| 1:A:919:ILE:HD13  | 1:A:983:ILE:HD12  | 1.88                     | 0.54              |
| 2:B:241:ARG:HG2   | 2:B:253:THR:HG21  | 1.90                     | 0.54              |
| 4:D:14:ARG:NH2    | 4:D:16:LYS:HD2    | 2.23                     | 0.54              |
| 8:H:84:ALA:HB2    | 8:H:87:ARG:HD2    | 1.90                     | 0.54              |
| 9:I:62:ILE:HD11   | 9:I:86:PHE:CE2    | 2.41                     | 0.54              |
| 1:A:95:PHE:O      | 1:A:96:ILE:C      | 2.51                     | 0.53              |
| 1:A:122:MET:HE3   | 1:A:126:LEU:HD21  | 1.88                     | 0.53              |
| 1:A:152:VAL:HG13  | 1:A:153:PRO:HD2   | 1.89                     | 0.53              |
| 1:A:879:GLU:OE1   | 1:A:962:ARG:NH2   | 2.41                     | 0.53              |
| 1:A:1155:ASP:CG   | 1:A:1162:VAL:HG23 | 2.33                     | 0.53              |
| 1:A:1171:GLN:HA   | 1:A:1174:PHE:CD1  | 2.43                     | 0.53              |
| 1:A:1241:ARG:O    | 1:A:1242:VAL:HG23 | 2.08                     | 0.53              |
| 2:B:244:LEU:HD11  | 2:B:366:GLN:NE2   | 2.23                     | 0.53              |
| 2:B:289:LEU:CD1   | 2:B:375:ALA:HB2   | 2.36                     | 0.53              |
| 2:B:521:LEU:HB3   | 2:B:633:VAL:HG11  | 1.90                     | 0.53              |
| 3:C:208:GLU:C     | 3:C:210:GLU:H     | 2.15                     | 0.53              |
| 5:E:90:VAL:HA     | 5:E:120:ALA:HB2   | 1.91                     | 0.53              |
| 11:K:65:HIS:HD2   | 11:K:67:PHE:N     | 2.05                     | 0.53              |
| 1:A:34:LYS:NZ     | 1:A:57:ARG:NH1    | 2.57                     | 0.53              |
| 1:A:168:GLY:O     | 1:A:169:ASN:C     | 2.51                     | 0.53              |
| 1:A:1098:VAL:N    | 1:A:1099:PRO:HD2  | 2.23                     | 0.53              |
| 1:A:1199:ARG:HG3  | 1:A:1236:LEU:HD11 | 1.89                     | 0.53              |
| 2:B:110:HIS:HB2   | 12:L:54:ARG:NH2   | 2.23                     | 0.53              |
| 2:B:171:PRO:HD2   | 2:B:457:LEU:HD13  | 1.91                     | 0.53              |
| 2:B:399:ASP:OD2   | 2:B:510:LYS:HB2   | 2.07                     | 0.53              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B:797:TYR:HE1  | 2:B:854:LEU:HD23  | 1.73                     | 0.53              |
| 2:B:889:THR:HG23 | 2:B:891:ASP:H     | 1.72                     | 0.53              |
| 2:B:1124:ARG:O   | 2:B:1125:ASP:HB3  | 2.07                     | 0.53              |
| 2:B:1181:GLU:OE2 | 2:B:1188:LYS:HE3  | 2.07                     | 0.53              |
| 3:C:35:ARG:HH12  | 11:K:41:THR:H     | 1.54                     | 0.53              |
| 3:C:63:ILE:HA    | 3:C:66:ARG:HG3    | 1.90                     | 0.53              |
| 3:C:80:LEU:CD1   | 3:C:95:CYS:HA     | 2.39                     | 0.53              |
| 3:C:107:SER:C    | 3:C:109:SER:H     | 2.17                     | 0.53              |
| 5:E:64:PRO:HB2   | 5:E:69:ILE:HD11   | 1.89                     | 0.53              |
| 7:G:111:THR:CG2  | 7:G:114:LEU:HD13  | 2.37                     | 0.53              |
| 12:L:47:ARG:HG3  | 12:L:52:GLY:O     | 2.09                     | 0.53              |
| 1:A:508:PRO:O    | 1:A:511:ILE:HG13  | 2.09                     | 0.53              |
| 1:A:898:ARG:HD2  | 1:A:899:VAL:H     | 1.73                     | 0.53              |
| 1:A:967:ALA:HA   | 1:A:1044:TRP:CZ3  | 2.43                     | 0.53              |
| 2:B:25:ILE:HG22  | 2:B:658:ILE:HD12  | 1.90                     | 0.53              |
| 2:B:129:PHE:HA   | 2:B:165:VAL:O     | 2.08                     | 0.53              |
| 2:B:360:PHE:HE2  | 2:B:374:LYS:HB3   | 1.73                     | 0.53              |
| 2:B:361:LEU:HD21 | 2:B:377:PHE:CD2   | 2.43                     | 0.53              |
| 2:B:855:PHE:HZ   | 2:B:857:ARG:NH1   | 2.05                     | 0.53              |
| 3:C:44:LEU:HD21  | 3:C:159:ALA:CB    | 2.38                     | 0.53              |
| 4:D:35:LEU:HD12  | 4:D:35:LEU:N      | 2.23                     | 0.53              |
| 7:G:1:MET:SD     | 7:G:2:PHE:N       | 2.82                     | 0.53              |
| 1:A:22:PHE:HE2   | 1:A:30:ILE:HD11   | 1.74                     | 0.53              |
| 1:A:102:VAL:HB   | 1:A:211:PHE:CE1   | 2.43                     | 0.53              |
| 1:A:115:LEU:HD12 | 1:A:142:CYS:HB3   | 1.91                     | 0.53              |
| 1:A:264:PHE:HB3  | 1:A:265:LYS:NZ    | 2.23                     | 0.53              |
| 1:A:903:ASN:ND2  | 1:A:904:THR:N     | 2.49                     | 0.53              |
| 2:B:90:ILE:HD12  | 2:B:432:MET:SD    | 2.49                     | 0.53              |
| 2:B:237:VAL:HG22 | 2:B:257:LYS:HA    | 1.90                     | 0.53              |
| 2:B:622:LYS:NZ   | 9:I:59:VAL:HG13   | 2.24                     | 0.53              |
| 2:B:770:GLN:HG2  | 2:B:983:ARG:O     | 2.07                     | 0.53              |
| 2:B:801:LYS:O    | 10:J:52:THR:HG23  | 2.08                     | 0.53              |
| 3:C:8:VAL:HG12   | 3:C:9:LYS:N       | 2.22                     | 0.53              |
| 4:D:144:THR:HG22 | 4:D:148:LEU:HD12  | 1.89                     | 0.53              |
| 6:F:94:LEU:HD22  | 6:F:122:MET:HG2   | 1.90                     | 0.53              |
| 11:K:47:ARG:HH11 | 11:K:47:ARG:CB    | 2.13                     | 0.53              |
| 1:A:75:ASN:ND2   | 2:B:1116:ARG:HH12 | 2.06                     | 0.53              |
| 1:A:1147:THR:HB  | 9:I:48:LEU:HD12   | 1.91                     | 0.53              |
| 2:B:582:VAL:CG2  | 2:B:626:ILE:HB    | 2.38                     | 0.53              |
| 5:E:144:ILE:HG13 | 5:E:145:THR:N     | 2.23                     | 0.53              |
| 5:E:204:THR:CG2  | 5:E:205:SER:N     | 2.71                     | 0.53              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 7:G:87:VAL:HG23   | 7:G:103:VAL:HG21 | 1.88                     | 0.53              |
| 1:A:49:LYS:NZ     | 1:A:61:ILE:HG13  | 2.10                     | 0.53              |
| 1:A:605:MET:HE2   | 1:A:607:ILE:CG1  | 2.38                     | 0.53              |
| 1:A:1173:HIS:O    | 1:A:1174:PHE:CD2 | 2.61                     | 0.53              |
| 1:A:1206:ASP:O    | 1:A:1274:ARG:CZ  | 2.56                     | 0.53              |
| 2:B:126:SER:OG    | 2:B:172:ILE:HD11 | 2.08                     | 0.53              |
| 2:B:661:LEU:HD23  | 2:B:679:TYR:O    | 2.08                     | 0.53              |
| 3:C:23:SER:O      | 3:C:24:ASN:HB3   | 2.08                     | 0.53              |
| 3:C:166:GLU:C     | 11:K:6:ARG:NH1   | 2.67                     | 0.53              |
| 3:C:179:GLU:HG2   | 3:C:180:TYR:N    | 2.24                     | 0.53              |
| 5:E:124:VAL:HB    | 5:E:125:PRO:HD3  | 1.90                     | 0.53              |
| 5:E:164:LEU:HD21  | 5:E:211:TYR:CG   | 2.44                     | 0.53              |
| 9:I:17:ARG:HG2    | 9:I:28:GLU:HG2   | 1.90                     | 0.53              |
| 9:I:111:THR:HG21  | 9:I:113:ASP:HB2  | 1.91                     | 0.53              |
| 1:A:195:ASP:O     | 1:A:196:GLU:HB3  | 2.09                     | 0.53              |
| 1:A:332:LYS:O     | 1:A:333:GLU:HB2  | 2.08                     | 0.53              |
| 1:A:399:HIS:CB    | 1:A:400:PRO:CD   | 2.86                     | 0.53              |
| 1:A:500:GLU:OE2   | 2:B:1145:SER:HB2 | 2.09                     | 0.53              |
| 1:A:1148:ILE:HG12 | 1:A:1198:ASP:HB2 | 1.90                     | 0.53              |
| 2:B:26:THR:O      | 2:B:29:ASP:HB2   | 2.07                     | 0.53              |
| 2:B:579:ARG:CA    | 2:B:589:VAL:HG13 | 2.38                     | 0.53              |
| 2:B:996:ARG:NH2   | 3:C:175:ALA:H    | 2.05                     | 0.53              |
| 3:C:238:ILE:HD11  | 3:C:246:ARG:NH1  | 2.23                     | 0.53              |
| 7:G:14:HIS:HD2    | 7:G:16:SER:H     | 1.50                     | 0.53              |
| 8:H:12:VAL:HA     | 8:H:28:ALA:HB2   | 1.91                     | 0.53              |
| 11:K:107:THR:HG22 | 11:K:108:GLU:N   | 2.23                     | 0.53              |
| 1:A:79:GLY:HA3    | 1:A:243:PRO:CG   | 2.39                     | 0.53              |
| 1:A:297:GLN:HE21  | 1:A:297:GLN:CA   | 2.20                     | 0.53              |
| 1:A:689:LYS:O     | 1:A:693:VAL:HG23 | 2.08                     | 0.53              |
| 1:A:1116:LEU:N    | 1:A:1308:THR:CG2 | 2.68                     | 0.53              |
| 1:A:1143:LEU:HD12 | 1:A:1143:LEU:O   | 2.08                     | 0.53              |
| 2:B:758:PHE:CE1   | 2:B:1027:ILE:CG2 | 2.91                     | 0.53              |
| 2:B:785:TYR:CD1   | 2:B:786:ASN:N    | 2.77                     | 0.53              |
| 7:G:9:LEU:HD12    | 7:G:10:ASN:H     | 1.74                     | 0.53              |
| 7:G:150:CYS:C     | 7:G:151:ILE:HG13 | 2.34                     | 0.53              |
| 8:H:4:THR:HG22    | 8:H:6:PHE:H      | 1.74                     | 0.53              |
| 9:I:73:ARG:HH12   | 9:I:112:SER:CB   | 2.21                     | 0.53              |
| 1:A:317:LYS:O     | 1:A:318:SER:HB3  | 2.09                     | 0.53              |
| 1:A:709:THR:HB    | 1:A:712:GLU:HG3  | 1.91                     | 0.53              |
| 1:A:898:ARG:HD2   | 1:A:899:VAL:N    | 2.23                     | 0.53              |
| 1:A:905:ASP:O     | 1:A:906:HIS:ND1  | 2.42                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:779:GLY:O     | 2:B:795:ILE:HA    | 2.08                     | 0.53              |
| 2:B:955:THR:HG23  | 2:B:956:THR:H     | 1.74                     | 0.53              |
| 2:B:983:ARG:HD2   | 2:B:1091:TYR:HB3  | 1.89                     | 0.53              |
| 2:B:1072:MET:CE   | 2:B:1085:ILE:HB   | 2.16                     | 0.53              |
| 2:B:1116:ARG:HG3  | 2:B:1198:TYR:CD2  | 2.43                     | 0.53              |
| 4:D:47:LEU:HD13   | 4:D:48:ILE:N      | 2.24                     | 0.53              |
| 8:H:106:GLU:HA    | 8:H:112:ILE:HD12  | 1.91                     | 0.53              |
| 11:K:50:LEU:HD11  | 11:K:75:ILE:CD1   | 2.39                     | 0.53              |
| 12:L:59:ALA:O     | 12:L:60:ARG:O     | 2.27                     | 0.53              |
| 2:B:405:ARG:NE    | 2:B:632:ARG:HG2   | 2.23                     | 0.53              |
| 2:B:1152:MET:HE3  | 2:B:1157:ALA:CB   | 2.39                     | 0.53              |
| 3:C:144:ILE:HG22  | 3:C:145:CYS:HB3   | 1.91                     | 0.53              |
| 5:E:56:LYS:NZ     | 5:E:84:ASP:H      | 2.07                     | 0.53              |
| 9:I:92:ARG:HD2    | 9:I:94:ASP:OD2    | 2.08                     | 0.53              |
| 1:A:278:THR:O     | 1:A:278:THR:HG22  | 2.09                     | 0.52              |
| 1:A:1149:ALA:CB   | 9:I:47:GLU:HA     | 2.38                     | 0.52              |
| 1:A:1170:ILE:HG22 | 1:A:1174:PHE:CZ   | 2.44                     | 0.52              |
| 1:A:1293:SER:OG   | 1:A:1295:THR:HG23 | 2.08                     | 0.52              |
| 2:B:431:TYR:CG    | 2:B:447:ALA:HB2   | 2.45                     | 0.52              |
| 2:B:641:GLU:C     | 2:B:643:ASP:H     | 2.17                     | 0.52              |
| 2:B:866:TYR:CG    | 2:B:870:ILE:HB    | 2.44                     | 0.52              |
| 2:B:879:ARG:NH2   | 2:B:885:MET:HE2   | 2.21                     | 0.52              |
| 2:B:936:ASP:OD1   | 2:B:937:ALA:N     | 2.41                     | 0.52              |
| 1:A:167:CYS:HB2   | 1:A:169:ASN:HD21  | 1.72                     | 0.52              |
| 1:A:250:ILE:O     | 1:A:250:ILE:CG2   | 2.56                     | 0.52              |
| 1:A:1333:ILE:O    | 1:A:1337:GLU:HG3  | 2.09                     | 0.52              |
| 2:B:508:LEU:N     | 2:B:512:ARG:HE    | 2.07                     | 0.52              |
| 2:B:848:ARG:HH22  | 2:B:996:ARG:HD3   | 1.74                     | 0.52              |
| 2:B:971:THR:OG1   | 3:C:61:GLU:HG3    | 2.08                     | 0.52              |
| 4:D:220:LEU:HD23  | 4:D:221:TYR:N     | 2.25                     | 0.52              |
| 7:G:121:PHE:HB2   | 7:G:130:TYR:CE2   | 2.44                     | 0.52              |
| 1:A:281:HIS:C     | 1:A:282:ASN:HD22  | 2.16                     | 0.52              |
| 1:A:335:ARG:NH1   | 2:B:1206:GLU:OE1  | 2.42                     | 0.52              |
| 1:A:593:GLU:C     | 1:A:595:THR:H     | 2.16                     | 0.52              |
| 1:A:1187:GLN:NE2  | 1:A:1188:GLN:HE21 | 2.07                     | 0.52              |
| 2:B:526:GLU:OE1   | 2:B:752:ALA:HB3   | 2.09                     | 0.52              |
| 2:B:789:MET:HE2   | 2:B:953:LEU:CD2   | 2.31                     | 0.52              |
| 2:B:816:GLU:O     | 2:B:817:LEU:HD23  | 2.09                     | 0.52              |
| 3:C:213:PRO:O     | 3:C:214:ASN:HB3   | 2.10                     | 0.52              |
| 5:E:17:ARG:O      | 5:E:21:GLU:HG3    | 2.09                     | 0.52              |
| 5:E:61:GLN:HG2    | 5:E:62:ALA:N      | 2.25                     | 0.52              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:E:185:ALA:O    | 5:E:190:LEU:HG    | 2.08                     | 0.52              |
| 9:I:88:SER:C     | 9:I:90:GLN:H      | 2.17                     | 0.52              |
| 11:K:18:LYS:NZ   | 11:K:38:GLU:HG2   | 2.23                     | 0.52              |
| 1:A:818:MET:HE3  | 2:B:514:LEU:O     | 2.10                     | 0.52              |
| 2:B:657:HIS:CE1  | 2:B:689:LEU:HD11  | 2.44                     | 0.52              |
| 2:B:980:PHE:CE2  | 2:B:1094:ARG:HG3  | 2.44                     | 0.52              |
| 7:G:139:ILE:CG2  | 7:G:140:LYS:H     | 2.21                     | 0.52              |
| 1:A:63:ARG:CA    | 1:A:74:MET:HE2    | 2.34                     | 0.52              |
| 1:A:434:ARG:NH2  | 1:A:440:ASP:OD1   | 2.43                     | 0.52              |
| 1:A:853:ASP:OD1  | 1:A:855:THR:CB    | 2.52                     | 0.52              |
| 3:C:67:LEU:HD11  | 3:C:155:LEU:CD1   | 2.40                     | 0.52              |
| 4:D:203:SER:OG   | 4:D:206:GLU:HB2   | 2.09                     | 0.52              |
| 7:G:51:TYR:O     | 7:G:54:ILE:HG13   | 2.09                     | 0.52              |
| 11:K:57:LEU:HB2  | 11:K:76:GLN:CG    | 2.36                     | 0.52              |
| 1:A:84:ILE:HD11  | 1:A:270:LEU:HD13  | 1.92                     | 0.52              |
| 1:A:901:LEU:N    | 1:A:926:GLN:HE21  | 1.99                     | 0.52              |
| 1:A:1365:TYR:CE2 | 1:A:1369:ALA:HB2  | 2.44                     | 0.52              |
| 2:B:44:VAL:O     | 2:B:45:SER:C      | 2.53                     | 0.52              |
| 2:B:101:MET:HE3  | 2:B:169:ARG:HH22  | 1.75                     | 0.52              |
| 2:B:176:SER:O    | 2:B:182:SER:HB3   | 2.09                     | 0.52              |
| 2:B:906:SER:HA   | 2:B:946:ASN:HB2   | 1.92                     | 0.52              |
| 2:B:1033:LYS:HD3 | 2:B:1059:LEU:HD11 | 1.92                     | 0.52              |
| 4:D:7:THR:HG21   | 4:D:32:GLU:CD     | 2.35                     | 0.52              |
| 4:D:40:HIS:CE1   | 7:G:7:LEU:O       | 2.63                     | 0.52              |
| 4:D:216:ASN:C    | 4:D:218:GLU:H     | 2.17                     | 0.52              |
| 13:T:24:DG:H2''  | 13:T:25:DG:C5'    | 2.34                     | 0.52              |
| 1:A:598:LEU:CD1  | 8:H:124:ARG:HB2   | 2.40                     | 0.52              |
| 1:A:720:ARG:O    | 1:A:724:GLU:HB3   | 2.09                     | 0.52              |
| 1:A:821:ARG:HB2  | 1:A:821:ARG:NH1   | 2.25                     | 0.52              |
| 1:A:829:VAL:HG21 | 2:B:508:LEU:CD1   | 2.37                     | 0.52              |
| 2:B:288:ALA:CB   | 2:B:331:LEU:HD12  | 2.40                     | 0.52              |
| 2:B:336:ARG:HH11 | 2:B:336:ARG:HG3   | 1.75                     | 0.52              |
| 2:B:619:ILE:HD12 | 9:I:65:ASP:HB2    | 1.91                     | 0.52              |
| 2:B:639:ILE:HG22 | 2:B:641:GLU:HG2   | 1.92                     | 0.52              |
| 3:C:6:PRO:CG     | 11:K:101:LEU:HD12 | 2.40                     | 0.52              |
| 5:E:55:ARG:HG3   | 5:E:55:ARG:HH11   | 1.74                     | 0.52              |
| 5:E:112:TYR:C    | 5:E:112:TYR:CD1   | 2.88                     | 0.52              |
| 6:F:94:LEU:HD21  | 6:F:122:MET:HA    | 1.92                     | 0.52              |
| 1:A:858:ASN:ND2  | 1:A:858:ASN:C     | 2.55                     | 0.52              |
| 1:A:901:LEU:HD22 | 1:A:919:ILE:HG23  | 1.91                     | 0.52              |
| 1:A:1030:ARG:HG2 | 1:A:1034:GLU:OE2  | 2.10                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:254:LEU:HD12  | 2:B:272:THR:O     | 2.10                     | 0.52              |
| 2:B:300:HIS:O     | 2:B:303:TYR:HE2   | 1.93                     | 0.52              |
| 2:B:712:PRO:O     | 2:B:733:HIS:NE2   | 2.43                     | 0.52              |
| 2:B:911:ILE:HG21  | 2:B:966:VAL:HG11  | 1.90                     | 0.52              |
| 2:B:997:GLU:HG2   | 3:C:39:ALA:HB2    | 1.91                     | 0.52              |
| 2:B:1096:ARG:O    | 2:B:1097:HIS:CB   | 2.57                     | 0.52              |
| 2:B:1115:THR:HG22 | 2:B:1117:GLN:HG3  | 1.92                     | 0.52              |
| 3:C:254:LYS:HE2   | 11:K:42:LEU:HD13  | 1.92                     | 0.52              |
| 6:F:76:LYS:O      | 6:F:79:ARG:HD3    | 2.09                     | 0.52              |
| 6:F:111:LEU:C     | 6:F:113:GLY:N     | 2.68                     | 0.52              |
| 9:I:44:TYR:CD1    | 9:I:45:ARG:N      | 2.78                     | 0.52              |
| 9:I:78:CYS:SG     | 9:I:105:SER:O     | 2.65                     | 0.52              |
| 1:A:22:PHE:CE2    | 1:A:30:ILE:HD11   | 2.45                     | 0.52              |
| 1:A:182:VAL:HG22  | 1:A:201:VAL:HA    | 1.91                     | 0.52              |
| 1:A:412:ARG:CZ    | 2:B:1108:ARG:NH1  | 2.73                     | 0.52              |
| 1:A:711:ARG:O     | 1:A:714:PHE:HB3   | 2.10                     | 0.52              |
| 1:A:1100:ARG:O    | 1:A:1103:GLU:HB3  | 2.09                     | 0.52              |
| 1:A:1454:MET:O    | 1:A:1454:MET:HG3  | 2.09                     | 0.52              |
| 2:B:301:ILE:HG21  | 2:B:314:LEU:HD11  | 1.92                     | 0.52              |
| 2:B:614:SER:HB2   | 2:B:697:GLU:OE1   | 2.10                     | 0.52              |
| 2:B:620:ARG:CZ    | 9:I:68:LEU:HD21   | 2.40                     | 0.52              |
| 2:B:708:GLU:O     | 2:B:709:ASP:C     | 2.53                     | 0.52              |
| 3:C:22:LEU:HD11   | 11:K:101:LEU:HD21 | 1.92                     | 0.52              |
| 1:A:442:VAL:CG2   | 1:A:489:LEU:HD11  | 2.40                     | 0.52              |
| 1:A:628:GLY:O     | 1:A:632:VAL:HG23  | 2.10                     | 0.52              |
| 1:A:687:LYS:HE2   | 1:A:795:GLU:OE2   | 2.10                     | 0.52              |
| 1:A:999:VAL:HG12  | 1:A:1000:LEU:HG   | 1.90                     | 0.52              |
| 1:A:1100:ARG:NH2  | 1:A:1351:GLU:CG   | 2.73                     | 0.52              |
| 1:A:1227:ILE:HG22 | 1:A:1228:TRP:H    | 1.75                     | 0.52              |
| 1:A:1291:VAL:HG22 | 1:A:1292:PRO:CD   | 2.40                     | 0.52              |
| 2:B:199:MET:HE2   | 2:B:492:LEU:HD23  | 1.91                     | 0.52              |
| 2:B:234:ILE:HG21  | 2:B:237:VAL:HG23  | 1.90                     | 0.52              |
| 2:B:622:LYS:HZ3   | 9:I:59:VAL:HG13   | 1.75                     | 0.52              |
| 2:B:1115:THR:HG22 | 2:B:1117:GLN:CG   | 2.40                     | 0.52              |
| 5:E:182:ASP:HB3   | 5:E:185:ALA:HB2   | 1.92                     | 0.52              |
| 6:F:90:ARG:HG3    | 6:F:91:ALA:N      | 2.25                     | 0.52              |
| 6:F:103:MET:HE2   | 7:G:66:GLY:N      | 2.18                     | 0.52              |
| 7:G:138:THR:O     | 7:G:140:LYS:N     | 2.43                     | 0.52              |
| 9:I:59:VAL:C      | 9:I:61:ASP:H      | 2.18                     | 0.52              |
| 1:A:44:THR:O      | 1:A:45:GLN:HB2    | 2.09                     | 0.51              |
| 1:A:512:VAL:O     | 1:A:512:VAL:HG12  | 2.09                     | 0.51              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:786:HIS:N    | 1:A:786:HIS:CD2   | 2.76                     | 0.51              |
| 1:A:1124:HIS:HB2 | 1:A:1130:GLN:HG2  | 1.92                     | 0.51              |
| 2:B:101:MET:HB3  | 2:B:109:THR:CG2   | 2.40                     | 0.51              |
| 2:B:1033:LYS:O   | 2:B:1037:LEU:HG   | 2.10                     | 0.51              |
| 3:C:3:GLU:HG2    | 3:C:4:GLU:HG3     | 1.92                     | 0.51              |
| 3:C:113:VAL:CG2  | 3:C:147:LEU:HD21  | 2.39                     | 0.51              |
| 4:D:14:ARG:C     | 4:D:16:LYS:H      | 2.18                     | 0.51              |
| 7:G:115:MET:O    | 7:G:164:LYS:HD3   | 2.10                     | 0.51              |
| 8:H:89:LEU:O     | 8:H:91:ASP:N      | 2.42                     | 0.51              |
| 12:L:38:LEU:HG   | 12:L:39:SER:N     | 2.25                     | 0.51              |
| 1:A:367:PRO:HB3  | 1:A:465:TYR:O     | 2.10                     | 0.51              |
| 1:A:609:ASP:HB2  | 1:A:969:GLN:HE22  | 1.75                     | 0.51              |
| 2:B:331:LEU:O    | 2:B:334:ILE:HB    | 2.10                     | 0.51              |
| 2:B:847:ASP:O    | 2:B:849:GLY:N     | 2.42                     | 0.51              |
| 2:B:860:MET:HG2  | 2:B:861:ASP:N     | 2.25                     | 0.51              |
| 2:B:975:GLN:HG2  | 2:B:976:ILE:H     | 1.74                     | 0.51              |
| 2:B:1084:GLN:H   | 2:B:1084:GLN:HE21 | 1.58                     | 0.51              |
| 3:C:18:VAL:CG2   | 3:C:240:VAL:HB    | 2.39                     | 0.51              |
| 3:C:35:ARG:NH1   | 11:K:41:THR:N     | 2.58                     | 0.51              |
| 3:C:242:GLN:C    | 3:C:244:VAL:H     | 2.17                     | 0.51              |
| 3:C:258:ILE:HD12 | 3:C:258:ILE:N     | 2.25                     | 0.51              |
| 4:D:29:LEU:HD12  | 7:G:82:PHE:CE2    | 2.44                     | 0.51              |
| 7:G:1:MET:SD     | 7:G:79:PHE:CE1    | 3.03                     | 0.51              |
| 1:A:744:LYS:CG   | 1:A:748:MET:HE2   | 2.39                     | 0.51              |
| 1:A:899:VAL:CG2  | 1:A:908:LEU:HD21  | 2.40                     | 0.51              |
| 1:A:1094:VAL:HA  | 1:A:1113:THR:HG21 | 1.92                     | 0.51              |
| 1:A:1166:ASP:HA  | 1:A:1169:ILE:HD12 | 1.92                     | 0.51              |
| 1:A:1229:SER:HB2 | 1:A:1233:ASP:OD2  | 2.11                     | 0.51              |
| 2:B:203:PHE:N    | 2:B:203:PHE:CD1   | 2.78                     | 0.51              |
| 2:B:796:LEU:HD21 | 2:B:821:GLN:NE2   | 2.21                     | 0.51              |
| 4:D:220:LEU:HD23 | 4:D:221:TYR:C     | 2.36                     | 0.51              |
| 8:H:76:THR:O     | 8:H:77:ARG:HB2    | 2.10                     | 0.51              |
| 8:H:104:PHE:CZ   | 8:H:136:LYS:HG3   | 2.45                     | 0.51              |
| 13:T:16:DT:H5'   | 13:T:16:DT:C6     | 2.32                     | 0.51              |
| 1:A:883:LEU:CD2  | 1:A:1021:LEU:HB2  | 2.40                     | 0.51              |
| 1:A:925:LEU:HD13 | 1:A:983:ILE:CG2   | 2.41                     | 0.51              |
| 2:B:259:TYR:N    | 2:B:259:TYR:CD1   | 2.79                     | 0.51              |
| 2:B:435:THR:C    | 2:B:437:GLU:H     | 2.16                     | 0.51              |
| 2:B:654:ARG:HG3  | 2:B:654:ARG:NH1   | 2.24                     | 0.51              |
| 2:B:991:GLY:O    | 2:B:992:ILE:HB    | 2.09                     | 0.51              |
| 3:C:133:ILE:HD12 | 3:C:237:SER:HA    | 1.92                     | 0.51              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:C:235:VAL:HG21 | 10:J:6:ARG:NH2    | 2.25                     | 0.51              |
| 4:D:192:LYS:HD2  | 4:D:199:ASN:HA    | 1.91                     | 0.51              |
| 5:E:65:THR:O     | 5:E:69:ILE:HD12   | 2.11                     | 0.51              |
| 7:G:139:ILE:CG2  | 7:G:140:LYS:N     | 2.71                     | 0.51              |
| 1:A:252:PHE:HB2  | 1:A:256:GLN:CD    | 2.35                     | 0.51              |
| 1:A:446:ARG:HD3  | 1:A:480:ALA:HB2   | 1.92                     | 0.51              |
| 1:A:554:PRO:HD2  | 1:A:648:ASN:OD1   | 2.10                     | 0.51              |
| 1:A:671:ALA:CB   | 1:A:676:MET:HE2   | 2.35                     | 0.51              |
| 1:A:1120:LEU:C   | 1:A:1120:LEU:HD12 | 2.36                     | 0.51              |
| 2:B:96:TYR:N     | 2:B:129:PHE:O     | 2.33                     | 0.51              |
| 2:B:120:ARG:HG2  | 2:B:955:THR:HG21  | 1.92                     | 0.51              |
| 2:B:324:ILE:HG22 | 2:B:324:ILE:O     | 2.10                     | 0.51              |
| 2:B:579:ARG:HD2  | 2:B:586:TRP:CZ2   | 2.45                     | 0.51              |
| 3:C:92:CYS:SG    | 3:C:94:LYS:HB2    | 2.50                     | 0.51              |
| 3:C:133:ILE:HD12 | 3:C:237:SER:N     | 2.26                     | 0.51              |
| 4:D:134:THR:CG2  | 4:D:135:GLY:N     | 2.74                     | 0.51              |
| 8:H:123:MET:HG2  | 8:H:124:ARG:N     | 2.24                     | 0.51              |
| 1:A:436:ILE:HD11 | 1:A:491:VAL:HG11  | 1.91                     | 0.51              |
| 1:A:1112:LYS:O   | 1:A:1114:PRO:CD   | 2.57                     | 0.51              |
| 1:A:1365:TYR:C   | 1:A:1365:TYR:CD2  | 2.89                     | 0.51              |
| 2:B:226:PHE:HA   | 2:B:395:GLN:CG    | 2.41                     | 0.51              |
| 2:B:336:ARG:HG3  | 2:B:336:ARG:NH1   | 2.26                     | 0.51              |
| 2:B:430:ARG:HB3  | 2:B:430:ARG:NH1   | 2.10                     | 0.51              |
| 2:B:557:PHE:CE1  | 2:B:603:LEU:HD11  | 2.46                     | 0.51              |
| 2:B:1208:MET:O   | 2:B:1211:ASN:N    | 2.43                     | 0.51              |
| 4:D:16:LYS:O     | 4:D:18:VAL:N      | 2.42                     | 0.51              |
| 4:D:23:ASN:HA    | 4:D:28:GLN:O      | 2.11                     | 0.51              |
| 7:G:26:LEU:CD1   | 7:G:56:ILE:HD11   | 2.37                     | 0.51              |
| 8:H:138:GLU:C    | 8:H:138:GLU:OE1   | 2.54                     | 0.51              |
| 9:I:105:SER:O    | 9:I:106:CYS:CB    | 2.53                     | 0.51              |
| 11:K:8:GLU:O     | 11:K:37:LYS:HD2   | 2.11                     | 0.51              |
| 1:A:55:ASP:O     | 1:A:55:ASP:OD2    | 2.28                     | 0.51              |
| 1:A:541:ILE:HG21 | 1:A:549:MET:HE3   | 1.91                     | 0.51              |
| 1:A:982:THR:C    | 1:A:984:LYS:N     | 2.69                     | 0.51              |
| 2:B:168:GLY:HA2  | 2:B:450:ALA:O     | 2.10                     | 0.51              |
| 2:B:217:ARG:NE   | 2:B:405:ARG:HB2   | 2.10                     | 0.51              |
| 2:B:766:ARG:NH2  | 2:B:1020:ARG:HD2  | 2.25                     | 0.51              |
| 2:B:850:LEU:HD12 | 2:B:851:PHE:N     | 2.26                     | 0.51              |
| 2:B:955:THR:CG2  | 2:B:956:THR:O     | 2.59                     | 0.51              |
| 5:E:78:LEU:HD23  | 5:E:78:LEU:C      | 2.36                     | 0.51              |
| 5:E:180:ARG:O    | 5:E:186:LEU:HD21  | 2.10                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:H:38:LEU:HD12   | 8:H:124:ARG:O     | 2.10                     | 0.51              |
| 9:I:19:ASP:HB3    | 9:I:24:ARG:HG2    | 1.93                     | 0.51              |
| 11:K:107:THR:O    | 11:K:111:LEU:HG   | 2.09                     | 0.51              |
| 1:A:8:SER:O       | 4:D:3:VAL:HG21    | 2.10                     | 0.51              |
| 1:A:43:GLU:HG2    | 1:A:48:ALA:HB3    | 1.92                     | 0.51              |
| 1:A:164:ARG:HG3   | 1:A:165:GLY:N     | 2.26                     | 0.51              |
| 1:A:898:ARG:HB2   | 1:A:933:TYR:CE1   | 2.46                     | 0.51              |
| 1:A:946:VAL:HG22  | 5:E:201:LYS:HB3   | 1.93                     | 0.51              |
| 2:B:225:VAL:HG11  | 2:B:385:LEU:HA    | 1.92                     | 0.51              |
| 2:B:309:GLN:CG    | 9:I:52:ILE:HD11   | 2.39                     | 0.51              |
| 2:B:604:ARG:HB2   | 2:B:609:ILE:HG13  | 1.92                     | 0.51              |
| 2:B:687:GLU:O     | 2:B:689:LEU:HG    | 2.11                     | 0.51              |
| 3:C:18:VAL:O      | 3:C:20:PHE:HD2    | 1.94                     | 0.51              |
| 3:C:98:VAL:C      | 3:C:99:LEU:HD22   | 2.36                     | 0.51              |
| 4:D:35:LEU:HD11   | 4:D:173:HIS:CD2   | 2.45                     | 0.51              |
| 4:D:118:THR:O     | 4:D:120:GLU:N     | 2.44                     | 0.51              |
| 5:E:26:ARG:HH22   | 5:E:133:GLU:CD    | 2.19                     | 0.51              |
| 6:F:75:PRO:O      | 6:F:77:ASP:O      | 2.29                     | 0.51              |
| 8:H:84:ALA:O      | 8:H:85:GLY:C      | 2.53                     | 0.51              |
| 12:L:55:ILE:O     | 12:L:56:LEU:HB2   | 2.10                     | 0.51              |
| 1:A:71:GLN:C      | 1:A:73:GLY:H      | 2.18                     | 0.51              |
| 1:A:93:VAL:HG21   | 1:A:301:ALA:O     | 2.11                     | 0.51              |
| 1:A:218:ASP:O     | 1:A:219:PHE:C     | 2.53                     | 0.51              |
| 2:B:69:LEU:HB3    | 2:B:429:PHE:HE1   | 1.76                     | 0.51              |
| 2:B:230:ALA:HB3   | 2:B:231:PRO:HD3   | 1.92                     | 0.51              |
| 2:B:408:LEU:HD12  | 2:B:408:LEU:N     | 2.26                     | 0.51              |
| 4:D:134:THR:CG2   | 4:D:135:GLY:H     | 2.24                     | 0.51              |
| 7:G:127:PRO:HG3   | 7:G:139:ILE:HG21  | 1.92                     | 0.51              |
| 11:K:65:HIS:CD2   | 11:K:67:PHE:HB2   | 2.46                     | 0.51              |
| 1:A:98:LYS:HE2    | 1:A:224:PHE:CZ    | 2.46                     | 0.51              |
| 1:A:184:SER:HB2   | 1:A:199:LEU:HD23  | 1.93                     | 0.51              |
| 1:A:670:ILE:HG23  | 1:A:805:LEU:HD21  | 1.93                     | 0.51              |
| 1:A:829:VAL:CG2   | 2:B:508:LEU:HD13  | 2.40                     | 0.51              |
| 1:A:1018:PHE:O    | 1:A:1021:LEU:HB3  | 2.11                     | 0.51              |
| 1:A:1036:ARG:HG2  | 1:A:1036:ARG:HH11 | 1.74                     | 0.51              |
| 1:A:1095:THR:HG21 | 1:A:1112:LYS:HD2  | 1.91                     | 0.51              |
| 2:B:91:SER:OG     | 2:B:133:LYS:HB2   | 2.11                     | 0.51              |
| 2:B:113:TYR:CD2   | 2:B:192:LEU:HD22  | 2.46                     | 0.51              |
| 2:B:508:LEU:N     | 14:N:1:DA:O5'     | 2.38                     | 0.51              |
| 3:C:7:GLN:HE21    | 11:K:104:ASN:HD21 | 1.56                     | 0.51              |
| 5:E:22:MET:HE3    | 5:E:26:ARG:CZ     | 2.40                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:66:ASP:OD2    | 2:B:422:LYS:HG2   | 2.11                     | 0.50              |
| 2:B:118:ARG:HG2   | 2:B:204:ILE:HD13  | 1.93                     | 0.50              |
| 2:B:515:HIS:H     | 2:B:518:HIS:CD2   | 2.29                     | 0.50              |
| 4:D:13:ARG:O      | 4:D:15:LEU:N      | 2.41                     | 0.50              |
| 8:H:38:LEU:HD13   | 8:H:125:LEU:HD13  | 1.93                     | 0.50              |
| 8:H:84:ALA:CA     | 8:H:87:ARG:HB2    | 2.41                     | 0.50              |
| 1:A:306:ASN:ND2   | 1:A:322:VAL:HG12  | 2.26                     | 0.50              |
| 1:A:382:PRO:CB    | 1:A:428:TYR:HE2   | 2.23                     | 0.50              |
| 1:A:556:TRP:CH2   | 1:A:558:GLY:HA2   | 2.46                     | 0.50              |
| 1:A:556:TRP:CZ3   | 1:A:558:GLY:HA2   | 2.46                     | 0.50              |
| 1:A:1130:GLN:HA   | 1:A:1133:LEU:HD12 | 1.92                     | 0.50              |
| 2:B:211:VAL:HG23  | 2:B:483:LEU:HB2   | 1.93                     | 0.50              |
| 2:B:542:MET:HE2   | 2:B:747:MET:HG3   | 1.93                     | 0.50              |
| 2:B:601:ARG:HD3   | 2:B:605:ARG:NH2   | 2.26                     | 0.50              |
| 3:C:80:LEU:HD11   | 3:C:95:CYS:C      | 2.36                     | 0.50              |
| 3:C:120:ILE:HG21  | 3:C:124:LEU:CD1   | 2.40                     | 0.50              |
| 5:E:89:GLY:C      | 5:E:91:LYS:N      | 2.69                     | 0.50              |
| 12:L:26:THR:C     | 12:L:27:LEU:HD23  | 2.36                     | 0.50              |
| 1:A:55:ASP:C      | 1:A:57:ARG:N      | 2.59                     | 0.50              |
| 1:A:306:ASN:HD22  | 1:A:322:VAL:HG12  | 1.77                     | 0.50              |
| 1:A:709:THR:CB    | 1:A:712:GLU:HG3   | 2.41                     | 0.50              |
| 1:A:1316:VAL:O    | 1:A:1316:VAL:HG12 | 2.11                     | 0.50              |
| 2:B:580:VAL:HG22  | 2:B:624:LEU:HB3   | 1.93                     | 0.50              |
| 2:B:827:ILE:HD12  | 2:B:1086:PHE:HD2  | 1.77                     | 0.50              |
| 3:C:183:TRP:O     | 3:C:184:ASN:C     | 2.55                     | 0.50              |
| 4:D:194:LEU:HD22  | 7:G:86:VAL:HG11   | 1.93                     | 0.50              |
| 7:G:1:MET:CE      | 7:G:80:LYS:H      | 2.24                     | 0.50              |
| 1:A:43:GLU:OE2    | 1:A:48:ALA:CB     | 2.58                     | 0.50              |
| 1:A:69:THR:C      | 1:A:71:GLN:N      | 2.68                     | 0.50              |
| 1:A:146:MET:O     | 1:A:147:VAL:HG23  | 2.12                     | 0.50              |
| 1:A:341:MET:CE    | 1:A:843:LYS:HZ3   | 2.24                     | 0.50              |
| 1:A:905:ASP:C     | 1:A:906:HIS:ND1   | 2.70                     | 0.50              |
| 1:A:1197:LEU:HD11 | 1:A:1238:ILE:HD11 | 1.92                     | 0.50              |
| 2:B:31:TRP:CZ3    | 2:B:34:ILE:HD12   | 2.46                     | 0.50              |
| 2:B:650:GLU:OE2   | 2:B:651:LEU:HB2   | 2.10                     | 0.50              |
| 2:B:654:ARG:O     | 2:B:657:HIS:N     | 2.44                     | 0.50              |
| 2:B:705:MET:HA    | 2:B:705:MET:CE    | 2.38                     | 0.50              |
| 8:H:113:ALA:HA    | 8:H:125:LEU:O     | 2.10                     | 0.50              |
| 10:J:52:THR:HG22  | 10:J:52:THR:O     | 2.11                     | 0.50              |
| 1:A:914:GLU:HB2   | 1:A:979:SER:O     | 2.11                     | 0.50              |
| 1:A:1280:GLU:O    | 1:A:1281:ARG:O    | 2.29                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1312:ASN:O    | 1:A:1316:VAL:HG23 | 2.12                     | 0.50              |
| 2:B:227:LYS:HG3   | 2:B:395:GLN:OE1   | 2.11                     | 0.50              |
| 2:B:515:HIS:HD2   | 2:B:517:THR:HG23  | 1.75                     | 0.50              |
| 2:B:1056:SER:HB3  | 2:B:1066:SER:OG   | 2.11                     | 0.50              |
| 3:C:7:GLN:HE21    | 11:K:104:ASN:HD22 | 1.57                     | 0.50              |
| 4:D:56:ARG:HD3    | 4:D:149:THR:HA    | 1.93                     | 0.50              |
| 5:E:48:ASP:OD1    | 5:E:52:ARG:HB2    | 2.11                     | 0.50              |
| 7:G:126:ASN:HD22  | 7:G:126:ASN:C     | 2.15                     | 0.50              |
| 8:H:15:VAL:HG21   | 8:H:49:VAL:O      | 2.11                     | 0.50              |
| 1:A:47:ARG:NH1    | 1:A:254:GLU:HG2   | 2.27                     | 0.50              |
| 1:A:75:ASN:O      | 1:A:76:GLU:CB     | 2.59                     | 0.50              |
| 1:A:105:CYS:SG    | 1:A:139:TRP:HA    | 2.52                     | 0.50              |
| 1:A:655:PHE:O     | 1:A:658:LEU:HB3   | 2.11                     | 0.50              |
| 1:A:1015:VAL:CG1  | 1:A:1019:CYS:SG   | 2.98                     | 0.50              |
| 1:A:1168:GLU:OE2  | 1:A:1172:LEU:HD11 | 2.11                     | 0.50              |
| 1:A:1205:LYS:O    | 1:A:1206:ASP:C    | 2.55                     | 0.50              |
| 2:B:118:ARG:CG    | 2:B:204:ILE:HD13  | 2.41                     | 0.50              |
| 2:B:269:ILE:HD11  | 2:B:386:LEU:HD21  | 1.94                     | 0.50              |
| 2:B:893:LEU:HD22  | 2:B:897:GLY:C     | 2.35                     | 0.50              |
| 2:B:1096:ARG:O    | 2:B:1097:HIS:HB2  | 2.12                     | 0.50              |
| 3:C:67:LEU:HD11   | 3:C:155:LEU:HD13  | 1.93                     | 0.50              |
| 4:D:29:LEU:HB3    | 7:G:82:PHE:CE2    | 2.46                     | 0.50              |
| 4:D:39:ASN:ND2    | 4:D:41:GLN:H      | 2.09                     | 0.50              |
| 5:E:204:THR:HG23  | 5:E:205:SER:H     | 1.73                     | 0.50              |
| 7:G:55:ASP:OD1    | 7:G:57:GLN:HG3    | 2.12                     | 0.50              |
| 7:G:138:THR:CG2   | 7:G:139:ILE:H     | 2.23                     | 0.50              |
| 1:A:180:LYS:HZ2   | 1:A:294:SER:HB3   | 1.77                     | 0.50              |
| 1:A:1395:GLY:HA3  | 1:A:1419:ASP:OD2  | 2.11                     | 0.50              |
| 2:B:599:THR:O     | 2:B:603:LEU:HB2   | 2.11                     | 0.50              |
| 3:C:8:VAL:HG12    | 3:C:9:LYS:H       | 1.76                     | 0.50              |
| 5:E:154:ILE:HG22  | 5:E:155:ARG:O     | 2.11                     | 0.50              |
| 7:G:111:THR:HG23  | 7:G:114:LEU:HB2   | 1.92                     | 0.50              |
| 1:A:54:ASN:HB3    | 1:A:247:ARG:HH12  | 1.77                     | 0.50              |
| 1:A:1207:LEU:HD13 | 1:A:1273:LEU:HD23 | 1.94                     | 0.50              |
| 1:A:1376:THR:O    | 1:A:1377:THR:C    | 2.55                     | 0.50              |
| 2:B:105:SER:O     | 2:B:106:ASP:HB2   | 2.12                     | 0.50              |
| 2:B:172:ILE:CD1   | 2:B:178:ASN:ND2   | 2.73                     | 0.50              |
| 2:B:244:LEU:HD11  | 2:B:250:PHE:HD1   | 1.77                     | 0.50              |
| 2:B:605:ARG:HH12  | 2:B:641:GLU:CG    | 2.25                     | 0.50              |
| 2:B:953:LEU:CB    | 12:L:57:LEU:HD23  | 2.42                     | 0.50              |
| 4:D:50:LEU:HD11   | 7:G:4:ILE:HD11    | 1.93                     | 0.50              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 7:G:126:ASN:HA   | 7:G:127:PRO:C     | 2.35                     | 0.50              |
| 8:H:77:ARG:HG2   | 8:H:78:SER:H      | 1.77                     | 0.50              |
| 8:H:84:ALA:CB    | 8:H:87:ARG:HB2    | 2.41                     | 0.50              |
| 8:H:98:TYR:C     | 8:H:118:PHE:HD2   | 2.20                     | 0.50              |
| 9:I:111:THR:CG2  | 9:I:113:ASP:H     | 2.14                     | 0.50              |
| 13:T:16:DT:H2''  | 13:T:17:DT:C5'    | 2.41                     | 0.50              |
| 1:A:547:LEU:HD21 | 1:A:560:ILE:HD13  | 1.94                     | 0.50              |
| 1:A:1081:LEU:CD1 | 1:A:1098:VAL:HG23 | 2.42                     | 0.50              |
| 1:A:1313:LEU:O   | 1:A:1315:GLU:N    | 2.44                     | 0.50              |
| 2:B:37:PHE:HD2   | 2:B:542:MET:SD    | 2.35                     | 0.50              |
| 2:B:552:MET:C    | 2:B:554:ILE:H     | 2.20                     | 0.50              |
| 2:B:570:VAL:HB   | 2:B:573:GLN:HB3   | 1.94                     | 0.50              |
| 2:B:1106:ARG:HG3 | 2:B:1107:ALA:N    | 2.26                     | 0.50              |
| 6:F:76:LYS:HA    | 6:F:79:ARG:CD     | 2.42                     | 0.50              |
| 9:I:58:VAL:HG13  | 9:I:62:ILE:HD13   | 1.93                     | 0.50              |
| 12:L:47:ARG:CG   | 12:L:48:CYS:N     | 2.74                     | 0.50              |
| 1:A:401:GLY:C    | 1:A:435:HIS:CD2   | 2.90                     | 0.49              |
| 1:A:447:GLN:NE2  | 13:T:20:DG:H4'    | 2.27                     | 0.49              |
| 1:A:831:THR:HG23 | 1:A:832:ALA:N     | 2.27                     | 0.49              |
| 1:A:1171:GLN:OE1 | 1:A:1172:LEU:N    | 2.45                     | 0.49              |
| 1:A:1402:PHE:CD2 | 1:A:1403:GLU:HG2  | 2.47                     | 0.49              |
| 2:B:56:ASP:HB3   | 2:B:57:TYR:CE1    | 2.48                     | 0.49              |
| 2:B:96:TYR:HB2   | 2:B:129:PHE:HB2   | 1.94                     | 0.49              |
| 2:B:115:GLN:HG2  | 2:B:193:LYS:CB    | 2.41                     | 0.49              |
| 2:B:579:ARG:N    | 2:B:589:VAL:HG13  | 2.26                     | 0.49              |
| 2:B:582:VAL:O    | 2:B:582:VAL:HG12  | 2.11                     | 0.49              |
| 2:B:957:ASN:HD22 | 2:B:961:LEU:HB2   | 1.76                     | 0.49              |
| 3:C:101:LEU:HD21 | 3:C:113:VAL:HG11  | 1.94                     | 0.49              |
| 1:A:145:LYS:HE3  | 1:A:145:LYS:CA    | 2.43                     | 0.49              |
| 1:A:266:LEU:HD21 | 1:A:303:TYR:CZ    | 2.47                     | 0.49              |
| 1:A:626:ASN:O    | 1:A:631:HIS:HD2   | 1.94                     | 0.49              |
| 1:A:860:LEU:CD1  | 1:A:1393:ASN:HD22 | 2.24                     | 0.49              |
| 1:A:1050:GLU:O   | 1:A:1054:LEU:HD12 | 2.13                     | 0.49              |
| 1:A:1389:PHE:C   | 1:A:1391:ARG:H    | 2.20                     | 0.49              |
| 1:A:1402:PHE:CE2 | 1:A:1403:GLU:HG2  | 2.47                     | 0.49              |
| 2:B:473:MET:HE3  | 2:B:474:SER:N     | 2.27                     | 0.49              |
| 2:B:707:PRO:CG   | 2:B:708:GLU:H     | 2.24                     | 0.49              |
| 2:B:1095:LEU:H   | 2:B:1095:LEU:CD1  | 2.22                     | 0.49              |
| 4:D:156:ASP:HB2  | 4:D:159:THR:CG2   | 2.41                     | 0.49              |
| 4:D:161:GLY:O    | 4:D:165:GLN:HG3   | 2.11                     | 0.49              |
| 7:G:132:SER:HB3  | 7:G:135:ASP:H     | 1.77                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:21:LEU:HD12   | 1:A:229:SER:HB2   | 1.94                     | 0.49              |
| 1:A:152:VAL:CG1   | 1:A:153:PRO:HD2   | 2.42                     | 0.49              |
| 1:A:378:GLU:OE1   | 1:A:434:ARG:HD3   | 2.12                     | 0.49              |
| 1:A:669:THR:HG22  | 1:A:761:MET:HE3   | 1.94                     | 0.49              |
| 1:A:1076:ALA:HA   | 1:A:1079:MET:HG3  | 1.93                     | 0.49              |
| 1:A:1150:SER:CB   | 1:A:1195:LEU:HD23 | 2.42                     | 0.49              |
| 1:A:1399:ARG:HB3  | 1:A:1408:ILE:HD13 | 1.95                     | 0.49              |
| 2:B:558:LEU:CD2   | 2:B:596:LEU:HD11  | 2.43                     | 0.49              |
| 8:H:7:ASP:O       | 8:H:8:ASP:HB2     | 2.11                     | 0.49              |
| 8:H:106:GLU:O     | 8:H:108:SER:N     | 2.36                     | 0.49              |
| 1:A:47:ARG:CZ     | 1:A:254:GLU:HG2   | 2.43                     | 0.49              |
| 1:A:53:LEU:O      | 1:A:54:ASN:C      | 2.56                     | 0.49              |
| 1:A:54:ASN:HB3    | 1:A:247:ARG:HH22  | 1.77                     | 0.49              |
| 1:A:67:CYS:O      | 1:A:70:CYS:HB3    | 2.12                     | 0.49              |
| 1:A:794:PRO:C     | 1:A:796:SER:H     | 2.20                     | 0.49              |
| 1:A:807:GLY:HA2   | 2:B:760:ASP:O     | 2.12                     | 0.49              |
| 1:A:997:LEU:HD13  | 1:A:1018:PHE:CE2  | 2.47                     | 0.49              |
| 1:A:1081:LEU:HD11 | 1:A:1098:VAL:HG23 | 1.94                     | 0.49              |
| 2:B:508:LEU:O     | 2:B:509:ALA:CB    | 2.60                     | 0.49              |
| 2:B:580:VAL:HG22  | 2:B:624:LEU:HD23  | 1.95                     | 0.49              |
| 2:B:638:PHE:HB3   | 2:B:651:LEU:CD2   | 2.42                     | 0.49              |
| 2:B:796:LEU:CD2   | 2:B:821:GLN:HE21  | 2.23                     | 0.49              |
| 2:B:887:HIS:CD2   | 2:B:887:HIS:N     | 2.81                     | 0.49              |
| 4:D:14:ARG:HH22   | 4:D:16:LYS:NZ     | 2.02                     | 0.49              |
| 5:E:127:ILE:O     | 5:E:127:ILE:HG13  | 2.13                     | 0.49              |
| 9:I:6:PHE:CB      | 9:I:12:ASN:O      | 2.56                     | 0.49              |
| 9:I:101:PHE:N     | 9:I:101:PHE:CD1   | 2.81                     | 0.49              |
| 1:A:125:ALA:C     | 1:A:127:ALA:H     | 2.21                     | 0.49              |
| 1:A:378:GLU:OE2   | 1:A:387:ARG:NH2   | 2.46                     | 0.49              |
| 1:A:982:THR:C     | 1:A:984:LYS:H     | 2.19                     | 0.49              |
| 2:B:785:TYR:CD1   | 2:B:785:TYR:C     | 2.91                     | 0.49              |
| 2:B:953:LEU:CD2   | 2:B:965:LYS:HB2   | 2.42                     | 0.49              |
| 2:B:1095:LEU:HD12 | 2:B:1095:LEU:N    | 2.26                     | 0.49              |
| 4:D:220:LEU:CG    | 4:D:221:TYR:N     | 2.75                     | 0.49              |
| 5:E:145:THR:HG21  | 5:E:187:TYR:CE2   | 2.48                     | 0.49              |
| 8:H:12:VAL:HG11   | 8:H:15:VAL:HG23   | 1.94                     | 0.49              |
| 10:J:64:ASN:CB    | 10:J:65:PRO:CD    | 2.78                     | 0.49              |
| 1:A:75:ASN:O      | 1:A:76:GLU:HB2    | 2.12                     | 0.49              |
| 1:A:1021:LEU:O    | 1:A:1024:SER:HB3  | 2.12                     | 0.49              |
| 1:A:1138:ILE:HG21 | 1:A:1316:VAL:HG13 | 1.95                     | 0.49              |
| 1:A:1142:THR:O    | 1:A:1145:SER:OG   | 2.31                     | 0.49              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:1315:GLU:O   | 1:A:1317:MET:N    | 2.46                     | 0.49              |
| 2:B:102:VAL:CG2  | 2:B:112:LEU:HD13  | 2.42                     | 0.49              |
| 3:C:69:LEU:HD12  | 3:C:69:LEU:H      | 1.77                     | 0.49              |
| 3:C:239:PRO:O    | 3:C:240:VAL:C     | 2.54                     | 0.49              |
| 5:E:169:ARG:HD3  | 6:F:140:ASP:CG    | 2.38                     | 0.49              |
| 10:J:48:ARG:HE   | 10:J:49:MET:HE1   | 1.75                     | 0.49              |
| 1:A:304:MET:O    | 1:A:324:SER:HB2   | 2.12                     | 0.49              |
| 1:A:598:LEU:O    | 1:A:598:LEU:HD23  | 2.12                     | 0.49              |
| 1:A:1207:LEU:CD1 | 1:A:1273:LEU:HD23 | 2.42                     | 0.49              |
| 1:A:1237:ILE:CG2 | 1:A:1238:ILE:N    | 2.75                     | 0.49              |
| 2:B:90:ILE:CD1   | 2:B:432:MET:SD    | 3.00                     | 0.49              |
| 2:B:203:PHE:N    | 2:B:203:PHE:HD1   | 2.11                     | 0.49              |
| 2:B:280:ILE:CG2  | 2:B:285:ILE:HG13  | 2.43                     | 0.49              |
| 2:B:390:LEU:O    | 2:B:392:ARG:N     | 2.45                     | 0.49              |
| 2:B:417:PHE:CE1  | 2:B:453:ILE:HD13  | 2.47                     | 0.49              |
| 2:B:557:PHE:HZ   | 2:B:603:LEU:HD21  | 1.77                     | 0.49              |
| 2:B:604:ARG:C    | 2:B:606:LYS:N     | 2.69                     | 0.49              |
| 2:B:605:ARG:HH12 | 2:B:641:GLU:HG3   | 1.78                     | 0.49              |
| 2:B:642:ASP:N    | 2:B:649:LYS:HG3   | 2.27                     | 0.49              |
| 2:B:866:TYR:HB2  | 2:B:870:ILE:HB    | 1.94                     | 0.49              |
| 4:D:33:PHE:HE1   | 7:G:80:LYS:HD3    | 1.74                     | 0.49              |
| 4:D:51:ASN:C     | 4:D:52:LEU:O      | 2.53                     | 0.49              |
| 4:D:195:ILE:HG22 | 4:D:198:LEU:HG    | 1.95                     | 0.49              |
| 5:E:61:GLN:NE2   | 5:E:105:PHE:CZ    | 2.80                     | 0.49              |
| 9:I:118:ARG:HH22 | 9:I:120:GLN:HB2   | 1.78                     | 0.49              |
| 1:A:265:LYS:HA   | 1:A:265:LYS:CE    | 2.42                     | 0.49              |
| 1:A:855:THR:CG2  | 1:A:857:ARG:HE    | 2.16                     | 0.49              |
| 1:A:857:ARG:HD3  | 1:A:861:GLY:O     | 2.13                     | 0.49              |
| 1:A:883:LEU:HD23 | 1:A:1021:LEU:HD13 | 1.94                     | 0.49              |
| 1:A:1315:GLU:C   | 1:A:1317:MET:N    | 2.69                     | 0.49              |
| 2:B:377:PHE:CE2  | 2:B:381:MET:HE2   | 2.48                     | 0.49              |
| 2:B:468:GLU:HB3  | 2:B:469:GLN:H     | 1.39                     | 0.49              |
| 2:B:827:ILE:HD12 | 2:B:1086:PHE:CD2  | 2.48                     | 0.49              |
| 2:B:910:VAL:CG1  | 2:B:938:SER:HB3   | 2.43                     | 0.49              |
| 3:C:105:GLY:O    | 3:C:149:LYS:O     | 2.31                     | 0.49              |
| 3:C:124:LEU:O    | 3:C:125:MET:C     | 2.55                     | 0.49              |
| 8:H:81:PRO:HB3   | 8:H:82:PRO:HD2    | 1.93                     | 0.49              |
| 8:H:129:TYR:C    | 8:H:131:ASN:H     | 2.21                     | 0.49              |
| 1:A:145:LYS:HA   | 1:A:145:LYS:CE    | 2.43                     | 0.49              |
| 2:B:247:GLY:C    | 2:B:249:ARG:N     | 2.70                     | 0.49              |
| 2:B:797:TYR:HE1  | 2:B:854:LEU:CD2   | 2.25                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:857:ARG:HD2   | 2:B:945:GLU:OE1   | 2.12                     | 0.49              |
| 3:C:44:LEU:HD13   | 3:C:129:ILE:HG23  | 1.95                     | 0.49              |
| 4:D:50:LEU:HD21   | 7:G:4:ILE:HD12    | 1.94                     | 0.49              |
| 7:G:14:HIS:HD2    | 7:G:16:SER:CB     | 2.26                     | 0.49              |
| 12:L:34:CYS:O     | 12:L:35:SER:C     | 2.56                     | 0.49              |
| 1:A:341:MET:CE    | 2:B:1135:ARG:NH1  | 2.75                     | 0.49              |
| 1:A:1325:THR:O    | 5:E:148:GLU:HB2   | 2.12                     | 0.49              |
| 3:C:11:ARG:NH2    | 3:C:206:ASN:OD1   | 2.46                     | 0.49              |
| 5:E:50:MET:HG2    | 5:E:52:ARG:NH2    | 2.28                     | 0.49              |
| 9:I:73:ARG:O      | 9:I:83:ASN:ND2    | 2.44                     | 0.49              |
| 11:K:55:LYS:CB    | 11:K:81:TYR:CD1   | 2.96                     | 0.49              |
| 1:A:162:VAL:HG12  | 1:A:163:SER:N     | 2.28                     | 0.48              |
| 1:A:470:LEU:HD23  | 1:A:470:LEU:H     | 1.78                     | 0.48              |
| 1:A:1155:ASP:OD2  | 1:A:1162:VAL:N    | 2.38                     | 0.48              |
| 2:B:43:LEU:HD13   | 2:B:492:LEU:HD13  | 1.94                     | 0.48              |
| 2:B:326:ASP:OD2   | 2:B:328:GLU:HB3   | 2.12                     | 0.48              |
| 2:B:449:ASN:O     | 2:B:451:LYS:N     | 2.46                     | 0.48              |
| 2:B:467:GLY:N     | 2:B:475:SER:HB3   | 2.28                     | 0.48              |
| 2:B:729:ILE:O     | 2:B:729:ILE:HG22  | 2.11                     | 0.48              |
| 2:B:941:LEU:O     | 2:B:942:ARG:C     | 2.55                     | 0.48              |
| 2:B:1197:PRO:HG2  | 2:B:1200:ALA:CB   | 2.43                     | 0.48              |
| 3:C:104:PHE:HD2   | 3:C:105:GLY:H     | 1.60                     | 0.48              |
| 3:C:242:GLN:C     | 3:C:244:VAL:N     | 2.71                     | 0.48              |
| 4:D:218:GLU:O     | 4:D:219:THR:C     | 2.55                     | 0.48              |
| 5:E:48:ASP:HB3    | 5:E:54:GLN:NE2    | 2.28                     | 0.48              |
| 7:G:145:VAL:HG12  | 7:G:146:LYS:N     | 2.27                     | 0.48              |
| 8:H:38:LEU:HD13   | 8:H:125:LEU:HD12  | 1.94                     | 0.48              |
| 8:H:100:THR:HG22  | 8:H:101:ALA:N     | 2.28                     | 0.48              |
| 1:A:122:MET:CA    | 1:A:141:LEU:HD11  | 2.41                     | 0.48              |
| 1:A:288:ALA:HA    | 1:A:291:GLU:CG    | 2.43                     | 0.48              |
| 1:A:1161:THR:HG22 | 1:A:1163:ILE:HG13 | 1.94                     | 0.48              |
| 2:B:263:GLY:O     | 2:B:264:SER:C     | 2.56                     | 0.48              |
| 2:B:284:ILE:HD13  | 2:B:333:PHE:HD2   | 1.77                     | 0.48              |
| 2:B:750:GLY:O     | 2:B:751:VAL:C     | 2.55                     | 0.48              |
| 2:B:831:SER:CB    | 2:B:994:TYR:OH    | 2.61                     | 0.48              |
| 1:A:35:ILE:HD12   | 1:A:241:VAL:HG21  | 1.95                     | 0.48              |
| 1:A:41:MET:O      | 1:A:50:ILE:HG13   | 2.12                     | 0.48              |
| 1:A:1140:HIS:NE2  | 1:A:1142:THR:HG23 | 2.28                     | 0.48              |
| 2:B:95:ILE:HG13   | 2:B:130:VAL:CG2   | 2.43                     | 0.48              |
| 2:B:812:LEU:O     | 2:B:813:LYS:HB2   | 2.13                     | 0.48              |
| 8:H:15:VAL:HG22   | 8:H:26:ILE:CD1    | 2.43                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:325:ILE:HG22  | 2:B:1210:MET:HE2  | 1.96                     | 0.48              |
| 1:A:475:THR:CG2   | 1:A:476:SER:N     | 2.75                     | 0.48              |
| 2:B:95:ILE:HG13   | 2:B:130:VAL:HG22  | 1.95                     | 0.48              |
| 2:B:237:VAL:HG22  | 2:B:257:LYS:HG3   | 1.94                     | 0.48              |
| 2:B:273:LEU:HD12  | 2:B:280:ILE:HD12  | 1.95                     | 0.48              |
| 2:B:309:GLN:HG3   | 9:I:52:ILE:HD12   | 1.95                     | 0.48              |
| 2:B:516:ASN:N     | 2:B:516:ASN:ND2   | 2.44                     | 0.48              |
| 2:B:597:MET:SD    | 2:B:624:LEU:HD11  | 2.53                     | 0.48              |
| 2:B:654:ARG:N     | 2:B:657:HIS:HD2   | 2.11                     | 0.48              |
| 2:B:773:MET:CE    | 2:B:987:LYS:HD2   | 2.44                     | 0.48              |
| 2:B:839:MET:HE3   | 2:B:1010:LEU:HD21 | 1.95                     | 0.48              |
| 5:E:177:ARG:O     | 5:E:212:ARG:HD3   | 2.13                     | 0.48              |
| 6:F:101:ILE:HD13  | 6:F:120:ILE:CG2   | 2.43                     | 0.48              |
| 7:G:126:ASN:C     | 7:G:126:ASN:ND2   | 2.71                     | 0.48              |
| 7:G:126:ASN:ND2   | 7:G:127:PRO:HA    | 2.24                     | 0.48              |
| 7:G:129:SER:HB3   | 7:G:138:THR:OG1   | 2.13                     | 0.48              |
| 1:A:773:LYS:H     | 1:A:773:LYS:HD2   | 1.79                     | 0.48              |
| 1:A:1035:TYR:O    | 1:A:1036:ARG:HB2  | 2.13                     | 0.48              |
| 2:B:976:ILE:O     | 2:B:990:ILE:HB    | 2.13                     | 0.48              |
| 8:H:51:ALA:O      | 8:H:52:GLN:HB2    | 2.13                     | 0.48              |
| 8:H:82:PRO:HG2    | 8:H:83:GLN:H      | 1.78                     | 0.48              |
| 8:H:128:ASN:ND2   | 8:H:128:ASN:C     | 2.71                     | 0.48              |
| 9:I:82:GLU:HB3    | 9:I:104:LEU:CD1   | 2.43                     | 0.48              |
| 11:K:59:ALA:HA    | 11:K:74:ARG:O     | 2.14                     | 0.48              |
| 1:A:23:SER:HA     | 1:A:233:TRP:CD1   | 2.48                     | 0.48              |
| 1:A:196:GLU:CG    | 1:A:197:PRO:HD2   | 2.44                     | 0.48              |
| 1:A:963:ILE:HD11  | 1:A:1048:ASN:CB   | 2.43                     | 0.48              |
| 2:B:24:PRO:O      | 2:B:25:ILE:HG23   | 2.13                     | 0.48              |
| 2:B:529:GLU:OE1   | 2:B:769:TYR:CE2   | 2.66                     | 0.48              |
| 2:B:638:PHE:HB2   | 2:B:741:CYS:O     | 2.13                     | 0.48              |
| 2:B:1116:ARG:HG3  | 2:B:1198:TYR:CD1  | 2.48                     | 0.48              |
| 5:E:10:SER:O      | 5:E:14:ARG:HG3    | 2.13                     | 0.48              |
| 7:G:34:VAL:CG1    | 7:G:45:ILE:HG21   | 2.43                     | 0.48              |
| 1:A:41:MET:HA     | 1:A:50:ILE:H      | 1.78                     | 0.48              |
| 1:A:88:LYS:HD3    | 1:A:293:GLU:CD    | 2.38                     | 0.48              |
| 1:A:344:ARG:HB2   | 2:B:1118:PRO:HB2  | 1.96                     | 0.48              |
| 1:A:364:VAL:O     | 1:A:364:VAL:HG13  | 2.13                     | 0.48              |
| 1:A:850:VAL:HG12  | 1:A:1060:PRO:HA   | 1.94                     | 0.48              |
| 1:A:1095:THR:HG21 | 1:A:1112:LYS:HB2  | 1.95                     | 0.48              |
| 1:A:1152:ILE:CD1  | 1:A:1260:LEU:HD23 | 2.43                     | 0.48              |
| 1:A:1453:TYR:O    | 1:A:1454:MET:HB3  | 2.13                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:D:119:ARG:HD3   | 4:D:221:TYR:CE2   | 2.49                     | 0.48              |
| 5:E:29:PHE:C      | 5:E:30:ILE:HG13   | 2.38                     | 0.48              |
| 5:E:78:LEU:CA     | 5:E:107:THR:HB    | 2.43                     | 0.48              |
| 6:F:103:MET:O     | 6:F:104:ASN:HB2   | 2.14                     | 0.48              |
| 7:G:21:ARG:HD3    | 7:G:21:ARG:HA     | 1.75                     | 0.48              |
| 7:G:91:VAL:HG12   | 7:G:92:VAL:N      | 2.29                     | 0.48              |
| 9:I:119:THR:O     | 9:I:119:THR:HG22  | 2.12                     | 0.48              |
| 10:J:1:MET:H1     | 10:J:56:LEU:N     | 2.12                     | 0.48              |
| 10:J:3:VAL:HG21   | 10:J:18:TRP:CG    | 2.48                     | 0.48              |
| 12:L:61:THR:HG21  | 12:L:63:ARG:HG3   | 1.96                     | 0.48              |
| 1:A:49:LYS:CD     | 1:A:55:ASP:HB3    | 2.44                     | 0.48              |
| 1:A:66:LYS:NZ     | 1:A:68:GLN:N      | 2.48                     | 0.48              |
| 1:A:629:LEU:CD1   | 1:A:645:LEU:HD21  | 2.44                     | 0.48              |
| 1:A:1107:VAL:CG1  | 1:A:1333:ILE:HD11 | 2.44                     | 0.48              |
| 2:B:710:LEU:HA    | 2:B:733:HIS:CB    | 2.34                     | 0.48              |
| 2:B:840:ILE:HB    | 2:B:1011:ILE:HB   | 1.95                     | 0.48              |
| 2:B:1102:LYS:O    | 2:B:1103:ILE:C    | 2.57                     | 0.48              |
| 2:B:1197:PRO:HG2  | 2:B:1200:ALA:HB2  | 1.95                     | 0.48              |
| 3:C:91:HIS:HD2    | 3:C:91:HIS:O      | 1.97                     | 0.48              |
| 3:C:186:LEU:HD21  | 3:C:225:ALA:HB2   | 1.95                     | 0.48              |
| 3:C:233:GLU:OE1   | 10:J:12:LYS:HE2   | 2.13                     | 0.48              |
| 7:G:137:ILE:CG2   | 7:G:143:ILE:HD11  | 2.44                     | 0.48              |
| 9:I:84:VAL:HG13   | 9:I:84:VAL:O      | 2.12                     | 0.48              |
| 1:A:341:MET:HE2   | 1:A:843:LYS:NZ    | 2.28                     | 0.48              |
| 1:A:690:VAL:CG1   | 1:A:691:LEU:N     | 2.77                     | 0.48              |
| 1:A:986:ILE:HG21  | 1:A:1028:THR:HA   | 1.96                     | 0.48              |
| 1:A:1293:SER:HB3  | 1:A:1297:GLU:OE1  | 2.14                     | 0.48              |
| 2:B:244:LEU:CD2   | 2:B:366:GLN:HE21  | 2.25                     | 0.48              |
| 2:B:324:ILE:HD13  | 2:B:330:ALA:HA    | 1.96                     | 0.48              |
| 5:E:172:GLU:HG2   | 5:E:213:ILE:CD1   | 2.44                     | 0.48              |
| 1:A:106:VAL:CG1   | 1:A:107:CYS:N     | 2.77                     | 0.48              |
| 1:A:305:ASP:OD2   | 1:A:326:ARG:HD3   | 2.12                     | 0.48              |
| 1:A:973:ILE:O     | 1:A:973:ILE:HG22  | 2.14                     | 0.48              |
| 1:A:1168:GLU:O    | 1:A:1171:GLN:OE1  | 2.30                     | 0.48              |
| 1:A:1317:MET:O    | 1:A:1322:ILE:HD11 | 2.14                     | 0.48              |
| 1:A:1430:LEU:O    | 2:B:1196:ILE:HG22 | 2.13                     | 0.48              |
| 1:A:738:LYS:CG    | 1:A:740:LEU:HG    | 2.38                     | 0.47              |
| 1:A:1081:LEU:HD11 | 1:A:1097:GLY:HA3  | 1.96                     | 0.47              |
| 2:B:123:THR:O     | 2:B:125:SER:N     | 2.44                     | 0.47              |
| 2:B:258:LEU:O     | 2:B:258:LEU:CG    | 2.61                     | 0.47              |
| 2:B:839:MET:HE3   | 2:B:1010:LEU:HD23 | 1.95                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:1138:MET:HE2  | 2:B:1146:PHE:CE2  | 2.49                     | 0.47              |
| 3:C:22:LEU:HG     | 3:C:25:VAL:HG21   | 1.96                     | 0.47              |
| 5:E:55:ARG:C      | 5:E:57:MET:N      | 2.71                     | 0.47              |
| 6:F:69:LEU:C      | 6:F:71:GLU:HG3    | 2.39                     | 0.47              |
| 7:G:125:SER:OG    | 7:G:128:PRO:HA    | 2.13                     | 0.47              |
| 8:H:89:LEU:HD13   | 8:H:91:ASP:OD1    | 2.13                     | 0.47              |
| 8:H:145:ARG:O     | 8:H:146:ARG:CB    | 2.61                     | 0.47              |
| 1:A:608:ILE:HG13  | 1:A:613:ILE:HD12  | 1.95                     | 0.47              |
| 1:A:1121:GLU:HB3  | 1:A:1124:HIS:NE2  | 2.29                     | 0.47              |
| 1:A:1239:ARG:HH12 | 1:A:1241:ARG:HH12 | 1.63                     | 0.47              |
| 1:A:1324:PRO:HB2  | 5:E:142:VAL:HG11  | 1.96                     | 0.47              |
| 2:B:23:ALA:HB1    | 2:B:24:PRO:HD2    | 1.95                     | 0.47              |
| 2:B:108:VAL:CG2   | 2:B:109:THR:H     | 2.25                     | 0.47              |
| 2:B:123:THR:HG23  | 2:B:205:ILE:HA    | 1.96                     | 0.47              |
| 2:B:314:LEU:O     | 2:B:318:VAL:HG23  | 2.13                     | 0.47              |
| 2:B:642:ASP:CA    | 2:B:649:LYS:HA    | 2.38                     | 0.47              |
| 2:B:696:GLU:O     | 2:B:699:GLU:HB2   | 2.15                     | 0.47              |
| 2:B:862:GLN:O     | 2:B:914:LYS:HE3   | 2.13                     | 0.47              |
| 3:C:109:SER:O     | 3:C:110:THR:C     | 2.56                     | 0.47              |
| 3:C:191:TYR:HD2   | 3:C:201:TRP:CD1   | 2.32                     | 0.47              |
| 3:C:193:TYR:C     | 3:C:193:TYR:CD1   | 2.92                     | 0.47              |
| 4:D:160:VAL:O     | 4:D:164:ILE:HG13  | 2.15                     | 0.47              |
| 4:D:220:LEU:CD2   | 4:D:221:TYR:H     | 2.27                     | 0.47              |
| 5:E:65:THR:O      | 5:E:69:ILE:CD1    | 2.62                     | 0.47              |
| 5:E:157:SER:C     | 5:E:159:ASP:N     | 2.71                     | 0.47              |
| 7:G:88:ASP:OD2    | 7:G:88:ASP:N      | 2.47                     | 0.47              |
| 1:A:92:HIS:O      | 1:A:94:GLY:N      | 2.47                     | 0.47              |
| 1:A:289:ILE:HG22  | 1:A:290:GLU:N     | 2.29                     | 0.47              |
| 1:A:385:ILE:HG22  | 1:A:386:ASP:N     | 2.26                     | 0.47              |
| 1:A:832:ALA:O     | 13:T:18:DA:H5'    | 2.15                     | 0.47              |
| 1:A:1111:MET:HG3  | 1:A:1114:PRO:HB3  | 1.95                     | 0.47              |
| 1:A:1255:GLU:OE1  | 1:A:1258:HIS:HB2  | 2.15                     | 0.47              |
| 1:A:1294:PRO:HG2  | 1:A:1295:THR:HG22 | 1.97                     | 0.47              |
| 2:B:244:LEU:O     | 2:B:246:LYS:N     | 2.47                     | 0.47              |
| 2:B:287:ARG:NH1   | 2:B:324:ILE:O     | 2.47                     | 0.47              |
| 2:B:591:ARG:O     | 2:B:592:ASN:C     | 2.57                     | 0.47              |
| 2:B:766:ARG:NH2   | 2:B:1020:ARG:CD   | 2.73                     | 0.47              |
| 2:B:955:THR:HG23  | 2:B:956:THR:N     | 2.28                     | 0.47              |
| 2:B:996:ARG:HH22  | 3:C:175:ALA:H     | 1.61                     | 0.47              |
| 3:C:89:GLU:O      | 3:C:90:ASP:CB     | 2.63                     | 0.47              |
| 3:C:221:TYR:CD1   | 3:C:222:LYS:N     | 2.83                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:E:10:SER:O      | 5:E:13:TRP:HB3    | 2.14                     | 0.47              |
| 7:G:21:ARG:CZ     | 7:G:24:GLN:HB2    | 2.45                     | 0.47              |
| 8:H:103:LYS:HG2   | 8:H:104:PHE:N     | 2.29                     | 0.47              |
| 8:H:104:PHE:CE2   | 8:H:136:LYS:HG3   | 2.49                     | 0.47              |
| 13:T:16:DT:H2''   | 13:T:17:DT:O5'    | 2.14                     | 0.47              |
| 1:A:323:LYS:HD2   | 1:A:323:LYS:N     | 2.28                     | 0.47              |
| 1:A:1203:ASN:O    | 1:A:1204:ASP:C    | 2.57                     | 0.47              |
| 1:A:1402:PHE:CE2  | 1:A:1403:GLU:CG   | 2.98                     | 0.47              |
| 2:B:222:ILE:N     | 2:B:240:ILE:HD12  | 2.28                     | 0.47              |
| 2:B:620:ARG:NH2   | 9:I:68:LEU:HD21   | 2.28                     | 0.47              |
| 3:C:3:GLU:CD      | 3:C:4:GLU:HG3     | 2.40                     | 0.47              |
| 5:E:56:LYS:CE     | 5:E:84:ASP:H      | 2.27                     | 0.47              |
| 5:E:155:ARG:HG2   | 5:E:155:ARG:HH11  | 1.80                     | 0.47              |
| 5:E:192:ARG:HH11  | 5:E:192:ARG:HG3   | 1.78                     | 0.47              |
| 8:H:27:GLU:CG     | 8:H:39:THR:HG23   | 2.45                     | 0.47              |
| 12:L:30:ILE:CG2   | 12:L:31:CYS:N     | 2.77                     | 0.47              |
| 1:A:36:ARG:HB2    | 1:A:37:PHE:CE1    | 2.49                     | 0.47              |
| 1:A:61:ILE:O      | 1:A:62:ASP:C      | 2.56                     | 0.47              |
| 1:A:698:GLN:HE22  | 9:I:99:LEU:HD11   | 1.78                     | 0.47              |
| 1:A:845:LEU:O     | 1:A:846:GLU:C     | 2.58                     | 0.47              |
| 1:A:1011:GLN:NE2  | 1:A:1015:VAL:CG2  | 2.78                     | 0.47              |
| 1:A:1029:ARG:HH11 | 1:A:1029:ARG:CG   | 2.26                     | 0.47              |
| 2:B:199:MET:HE2   | 2:B:492:LEU:CD2   | 2.44                     | 0.47              |
| 2:B:605:ARG:CZ    | 2:B:639:ILE:HD13  | 2.45                     | 0.47              |
| 2:B:1001:PHE:CE1  | 2:B:1073:TYR:HB2  | 2.49                     | 0.47              |
| 2:B:1045:SER:O    | 2:B:1048:THR:HG23 | 2.14                     | 0.47              |
| 3:C:22:LEU:CD2    | 3:C:25:VAL:HG21   | 2.45                     | 0.47              |
| 3:C:43:THR:HG22   | 3:C:44:LEU:N      | 2.30                     | 0.47              |
| 5:E:180:ARG:HH21  | 5:E:192:ARG:HB2   | 1.79                     | 0.47              |
| 8:H:44:VAL:O      | 8:H:44:VAL:HG12   | 2.15                     | 0.47              |
| 1:A:336:ILE:HD13  | 1:A:340:LEU:HD12  | 1.97                     | 0.47              |
| 1:A:347:PHE:HE2   | 1:A:375:THR:CG2   | 2.27                     | 0.47              |
| 1:A:565:ILE:HG22  | 1:A:565:ILE:O     | 2.13                     | 0.47              |
| 1:A:1015:VAL:HG12 | 1:A:1015:VAL:O    | 2.14                     | 0.47              |
| 1:A:1141:THR:HG23 | 1:A:1205:LYS:HZ2  | 1.79                     | 0.47              |
| 1:A:1141:THR:HG23 | 1:A:1205:LYS:CD   | 2.42                     | 0.47              |
| 1:A:1141:THR:HA   | 1:A:1205:LYS:NZ   | 2.29                     | 0.47              |
| 2:B:235:SER:C     | 2:B:236:HIS:HD2   | 2.21                     | 0.47              |
| 2:B:466:TRP:HA    | 2:B:466:TRP:CE3   | 2.49                     | 0.47              |
| 2:B:483:LEU:CD1   | 2:B:491:THR:HG23  | 2.42                     | 0.47              |
| 2:B:792:MET:H     | 2:B:857:ARG:HA    | 1.78                     | 0.47              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B:819:ALA:O    | 2:B:1093:GLN:HG2  | 2.14                     | 0.47              |
| 4:D:155:ARG:HB3  | 4:D:155:ARG:HH11  | 1.80                     | 0.47              |
| 7:G:55:ASP:HB3   | 7:G:73:LYS:HB2    | 1.96                     | 0.47              |
| 1:A:71:GLN:O     | 1:A:73:GLY:N      | 2.41                     | 0.47              |
| 1:A:268:ASP:HB3  | 1:A:299:HIS:CE1   | 2.50                     | 0.47              |
| 1:A:281:HIS:O    | 1:A:282:ASN:ND2   | 2.41                     | 0.47              |
| 1:A:305:ASP:C    | 1:A:305:ASP:OD1   | 2.57                     | 0.47              |
| 1:A:316:GLN:HG2  | 1:A:317:LYS:H     | 1.78                     | 0.47              |
| 1:A:322:VAL:O    | 1:A:322:VAL:CG1   | 2.61                     | 0.47              |
| 1:A:598:LEU:HD11 | 8:H:124:ARG:HB2   | 1.97                     | 0.47              |
| 1:A:741:ASN:HD21 | 1:A:743:VAL:HB    | 1.80                     | 0.47              |
| 1:A:953:ASN:C    | 1:A:954:TRP:CD1   | 2.93                     | 0.47              |
| 1:A:1001:ARG:O   | 1:A:1002:GLY:C    | 2.57                     | 0.47              |
| 1:A:1081:LEU:CD1 | 1:A:1097:GLY:HA3  | 2.45                     | 0.47              |
| 1:A:1345:ARG:CG  | 1:A:1372:VAL:HG12 | 2.45                     | 0.47              |
| 2:B:363:HIS:O    | 2:B:364:ILE:CB    | 2.60                     | 0.47              |
| 2:B:448:ILE:O    | 2:B:450:ALA:N     | 2.47                     | 0.47              |
| 2:B:516:ASN:H    | 2:B:516:ASN:ND2   | 2.11                     | 0.47              |
| 2:B:1048:THR:OG1 | 2:B:1050:ILE:HD12 | 2.14                     | 0.47              |
| 2:B:1068:GLY:O   | 2:B:1069:PHE:C    | 2.58                     | 0.47              |
| 2:B:1068:GLY:O   | 2:B:1069:PHE:O    | 2.32                     | 0.47              |
| 4:D:12:ARG:NH1   | 4:D:14:ARG:HG2    | 2.30                     | 0.47              |
| 4:D:15:LEU:O     | 4:D:17:LYS:HG3    | 2.14                     | 0.47              |
| 4:D:69:ALA:C     | 4:D:71:LYS:N      | 2.72                     | 0.47              |
| 5:E:37:LEU:HD11  | 5:E:41:ASP:HB2    | 1.94                     | 0.47              |
| 5:E:56:LYS:NZ    | 5:E:84:ASP:N      | 2.63                     | 0.47              |
| 7:G:59:GLY:HA3   | 7:G:70:PHE:CD2    | 2.50                     | 0.47              |
| 8:H:9:ILE:HA     | 8:H:55:LEU:O      | 2.15                     | 0.47              |
| 11:K:18:LYS:HZ2  | 11:K:38:GLU:HG2   | 1.80                     | 0.47              |
| 11:K:65:HIS:CD2  | 11:K:67:PHE:N     | 2.76                     | 0.47              |
| 1:A:298:PHE:CD2  | 1:A:299:HIS:HD2   | 2.33                     | 0.47              |
| 1:A:590:ARG:HG2  | 1:A:590:ARG:NH1   | 2.27                     | 0.47              |
| 1:A:672:ASP:OD2  | 1:A:674:PRO:HG2   | 2.15                     | 0.47              |
| 1:A:1362:TYR:CD1 | 1:A:1363:VAL:N    | 2.83                     | 0.47              |
| 2:B:129:PHE:CE2  | 2:B:166:PHE:HB2   | 2.50                     | 0.47              |
| 2:B:638:PHE:HB3  | 2:B:651:LEU:HD22  | 1.97                     | 0.47              |
| 3:C:73:GLN:HE21  | 3:C:75:MET:N      | 2.11                     | 0.47              |
| 4:D:13:ARG:C     | 4:D:15:LEU:N      | 2.73                     | 0.47              |
| 5:E:191:LYS:O    | 5:E:192:ARG:C     | 2.57                     | 0.47              |
| 7:G:106:MET:CG   | 7:G:107:LYS:N     | 2.77                     | 0.47              |
| 1:A:55:ASP:N     | 1:A:56:PRO:CD     | 2.73                     | 0.47              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:226:GLU:O    | 1:A:226:GLU:HG2   | 2.13                     | 0.47              |
| 1:A:518:LYS:HB2  | 1:A:519:PRO:HD2   | 1.96                     | 0.47              |
| 1:A:682:THR:HG23 | 1:A:728:LYS:HE3   | 1.96                     | 0.47              |
| 1:A:916:GLY:O    | 1:A:919:ILE:HG22  | 2.14                     | 0.47              |
| 1:A:1027:ALA:O   | 1:A:1031:VAL:HG23 | 2.15                     | 0.47              |
| 1:A:1120:LEU:H   | 1:A:1120:LEU:HG   | 1.48                     | 0.47              |
| 1:A:1366:ARG:HG2 | 1:A:1366:ARG:HH11 | 1.80                     | 0.47              |
| 2:B:37:PHE:HE1   | 2:B:41:LYS:CD     | 2.25                     | 0.47              |
| 2:B:235:SER:OG   | 2:B:236:HIS:CD2   | 2.68                     | 0.47              |
| 2:B:317:CYS:O    | 2:B:320:ASP:HB3   | 2.15                     | 0.47              |
| 2:B:335:GLY:O    | 2:B:336:ARG:HB2   | 2.15                     | 0.47              |
| 2:B:527:THR:OG1  | 2:B:528:PRO:HD2   | 2.15                     | 0.47              |
| 2:B:776:GLN:OE1  | 2:B:1097:HIS:NE2  | 2.47                     | 0.47              |
| 2:B:1190:ASP:C   | 2:B:1191:ILE:HG13 | 2.40                     | 0.47              |
| 2:B:1222:ARG:O   | 2:B:1222:ARG:HG2  | 2.15                     | 0.47              |
| 3:C:10:ILE:HG13  | 11:K:108:GLU:HB3  | 1.95                     | 0.47              |
| 3:C:11:ARG:HE    | 3:C:21:ILE:HD11   | 1.80                     | 0.47              |
| 3:C:47:ASP:CG    | 3:C:47:ASP:O      | 2.58                     | 0.47              |
| 3:C:196:ASP:OD1  | 3:C:198:ALA:HB3   | 2.15                     | 0.47              |
| 3:C:254:LYS:O    | 3:C:258:ILE:CD1   | 2.63                     | 0.47              |
| 5:E:29:PHE:HA    | 5:E:65:THR:HG22   | 1.97                     | 0.47              |
| 6:F:111:LEU:O    | 6:F:113:GLY:N     | 2.39                     | 0.47              |
| 8:H:59:ILE:CG2   | 8:H:60:ALA:N      | 2.66                     | 0.47              |
| 8:H:84:ALA:C     | 8:H:86:ASP:N      | 2.70                     | 0.47              |
| 9:I:4:PHE:CE1    | 9:I:13:MET:HG3    | 2.50                     | 0.47              |
| 9:I:50:THR:HG22  | 9:I:52:ILE:N      | 2.27                     | 0.47              |
| 1:A:416:ARG:HG3  | 1:A:417:TYR:CD1   | 2.49                     | 0.47              |
| 1:A:478:TYR:O    | 1:A:479:ASN:CB    | 2.62                     | 0.47              |
| 1:A:482:PHE:CE1  | 2:B:836:GLU:HB2   | 2.50                     | 0.47              |
| 1:A:589:GLN:HA   | 1:A:605:MET:O     | 2.15                     | 0.47              |
| 1:A:821:ARG:O    | 1:A:821:ARG:HG3   | 2.14                     | 0.47              |
| 1:A:1444:MET:HE3 | 1:A:1444:MET:HB2  | 1.63                     | 0.47              |
| 2:B:806:THR:HA   | 2:B:1045:SER:OG   | 2.15                     | 0.47              |
| 2:B:810:GLU:CB   | 2:B:815:ARG:HH22  | 2.28                     | 0.47              |
| 3:C:44:LEU:CD2   | 3:C:159:ALA:HB1   | 2.44                     | 0.47              |
| 3:C:213:PRO:HG2  | 3:C:214:ASN:H     | 1.80                     | 0.47              |
| 4:D:52:LEU:C     | 4:D:53:SER:HG     | 2.21                     | 0.47              |
| 6:F:106:PRO:HG2  | 7:G:18:PHE:O      | 2.15                     | 0.47              |
| 8:H:129:TYR:HA   | 8:H:131:ASN:HD21  | 1.80                     | 0.47              |
| 1:A:567:LYS:HB3  | 8:H:95:TYR:CA     | 2.44                     | 0.46              |
| 1:A:672:ASP:HB3  | 1:A:736:ASN:CG    | 2.40                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:852:TYR:CD2   | 1:A:1060:PRO:HB2  | 2.49                     | 0.46              |
| 2:B:129:PHE:HE2   | 2:B:166:PHE:HB2   | 1.81                     | 0.46              |
| 2:B:345:LYS:HA    | 2:B:348:ARG:HE    | 1.80                     | 0.46              |
| 2:B:470:LYS:O     | 2:B:472:ALA:N     | 2.46                     | 0.46              |
| 3:C:34:ARG:O      | 3:C:38:ILE:HG13   | 2.15                     | 0.46              |
| 5:E:26:ARG:NH1    | 5:E:133:GLU:OE2   | 2.37                     | 0.46              |
| 8:H:26:ILE:CD1    | 8:H:49:VAL:HG11   | 2.45                     | 0.46              |
| 9:I:80:SER:HB2    | 9:I:103:CYS:SG    | 2.54                     | 0.46              |
| 1:A:252:PHE:HB2   | 1:A:256:GLN:NE2   | 2.30                     | 0.46              |
| 1:A:494:SER:O     | 1:A:498:ARG:HG2   | 2.15                     | 0.46              |
| 1:A:549:MET:SD    | 1:A:577:ILE:CD1   | 3.03                     | 0.46              |
| 1:A:568:PRO:HG3   | 8:H:46:LEU:O      | 2.15                     | 0.46              |
| 1:A:697:ALA:HA    | 1:A:702:LEU:HG    | 1.96                     | 0.46              |
| 1:A:858:ASN:HD21  | 1:A:860:LEU:HB2   | 1.79                     | 0.46              |
| 1:A:1107:VAL:HG13 | 1:A:1333:ILE:HD11 | 1.97                     | 0.46              |
| 2:B:618:ASP:O     | 2:B:622:LYS:N     | 2.48                     | 0.46              |
| 2:B:745:PRO:O     | 2:B:747:MET:N     | 2.47                     | 0.46              |
| 3:C:116:LYS:HD3   | 3:C:140:ASN:HA    | 1.96                     | 0.46              |
| 9:I:88:SER:HB3    | 9:I:95:THR:HG21   | 1.98                     | 0.46              |
| 12:L:61:THR:HG22  | 12:L:62:LYS:N     | 2.30                     | 0.46              |
| 1:A:270:LEU:O     | 1:A:274:ILE:HG13  | 2.15                     | 0.46              |
| 1:A:886:ILE:CG2   | 1:A:887:GLY:N     | 2.79                     | 0.46              |
| 1:A:993:LEU:CD2   | 1:A:1022:LEU:HD21 | 2.46                     | 0.46              |
| 1:A:1241:ARG:O    | 1:A:1242:VAL:CG2  | 2.62                     | 0.46              |
| 2:B:652:LYS:HB3   | 2:B:689:LEU:CD2   | 2.43                     | 0.46              |
| 2:B:885:MET:HA    | 2:B:936:ASP:HB2   | 1.96                     | 0.46              |
| 8:H:94:ASP:O      | 8:H:95:TYR:HB2    | 2.14                     | 0.46              |
| 11:K:67:PHE:C     | 11:K:68:PHE:CD2   | 2.93                     | 0.46              |
| 1:A:65:LEU:HA     | 1:A:73:GLY:HA2    | 1.97                     | 0.46              |
| 1:A:601:LYS:HB2   | 1:A:603:ASN:ND2   | 2.30                     | 0.46              |
| 2:B:293:PRO:C     | 2:B:294:ASP:O     | 2.56                     | 0.46              |
| 2:B:496:ARG:NH1   | 2:B:539:LEU:HB2   | 2.29                     | 0.46              |
| 2:B:801:LYS:O     | 10:J:52:THR:CG2   | 2.64                     | 0.46              |
| 2:B:871:THR:HG22  | 2:B:872:GLU:N     | 2.29                     | 0.46              |
| 3:C:15:LYS:O      | 3:C:240:VAL:HG22  | 2.14                     | 0.46              |
| 3:C:189:THR:CG2   | 3:C:190:ASP:H     | 2.27                     | 0.46              |
| 3:C:212:PRO:HB3   | 3:C:213:PRO:HD2   | 1.97                     | 0.46              |
| 4:D:47:LEU:HD11   | 7:G:3:PHE:CD2     | 2.51                     | 0.46              |
| 5:E:175:LEU:HA    | 5:E:176:PRO:HD3   | 1.81                     | 0.46              |
| 7:G:111:THR:HG23  | 7:G:114:LEU:HD13  | 1.96                     | 0.46              |
| 12:L:47:ARG:CD    | 12:L:52:GLY:HA2   | 2.45                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:T:12:DG:H2''   | 13:T:13:DT:O5'    | 2.16                     | 0.46              |
| 1:A:744:LYS:CD    | 1:A:748:MET:HE2   | 2.46                     | 0.46              |
| 2:B:38:PHE:HD1    | 2:B:811:TYR:CD2   | 2.34                     | 0.46              |
| 2:B:243:ALA:HB2   | 2:B:251:ILE:HG12  | 1.97                     | 0.46              |
| 2:B:600:LEU:O     | 2:B:609:ILE:HD11  | 2.16                     | 0.46              |
| 2:B:999:MET:HE2   | 2:B:1011:ILE:HD12 | 1.98                     | 0.46              |
| 2:B:1001:PHE:CZ   | 2:B:1073:TYR:HB2  | 2.51                     | 0.46              |
| 3:C:67:LEU:HA     | 3:C:70:ILE:HD12   | 1.97                     | 0.46              |
| 5:E:145:THR:HG21  | 5:E:187:TYR:CD2   | 2.51                     | 0.46              |
| 7:G:1:MET:HE2     | 7:G:1:MET:O       | 2.15                     | 0.46              |
| 11:K:31:VAL:CG1   | 11:K:32:VAL:N     | 2.77                     | 0.46              |
| 11:K:65:HIS:NE2   | 11:K:67:PHE:CG    | 2.81                     | 0.46              |
| 1:A:72:GLU:HB3    | 1:A:76:GLU:CG     | 2.44                     | 0.46              |
| 1:A:75:ASN:ND2    | 2:B:1116:ARG:NH1  | 2.59                     | 0.46              |
| 1:A:247:ARG:NH1   | 1:A:263:THR:HG23  | 2.30                     | 0.46              |
| 1:A:464:PRO:HG2   | 1:A:465:TYR:CD1   | 2.51                     | 0.46              |
| 1:A:540:PHE:CE2   | 1:A:565:ILE:HD12  | 2.51                     | 0.46              |
| 1:A:540:PHE:HE2   | 1:A:565:ILE:HD12  | 1.80                     | 0.46              |
| 1:A:1191:TRP:CZ3  | 9:I:43:VAL:HG21   | 2.48                     | 0.46              |
| 1:A:1313:LEU:C    | 1:A:1315:GLU:N    | 2.71                     | 0.46              |
| 2:B:31:TRP:CZ2    | 2:B:807:ARG:HB2   | 2.50                     | 0.46              |
| 2:B:274:PRO:HG2   | 2:B:359:GLU:HB3   | 1.98                     | 0.46              |
| 2:B:449:ASN:C     | 2:B:451:LYS:N     | 2.73                     | 0.46              |
| 4:D:7:THR:HB      | 7:G:42:PHE:CE2    | 2.51                     | 0.46              |
| 4:D:14:ARG:NH2    | 4:D:16:LYS:HZ3    | 2.03                     | 0.46              |
| 4:D:128:VAL:CG1   | 4:D:129:LEU:N     | 2.79                     | 0.46              |
| 8:H:12:VAL:HG13   | 8:H:26:ILE:HD11   | 1.96                     | 0.46              |
| 8:H:133:ASN:O     | 8:H:135:LEU:N     | 2.48                     | 0.46              |
| 9:I:58:VAL:O      | 9:I:58:VAL:HG12   | 2.16                     | 0.46              |
| 1:A:407:ARG:HG2   | 1:A:430:TRP:CH2   | 2.50                     | 0.46              |
| 1:A:709:THR:CG2   | 1:A:710:LEU:H     | 2.21                     | 0.46              |
| 1:A:774:ARG:NH1   | 1:A:797:LYS:HG3   | 2.30                     | 0.46              |
| 1:A:1042:PHE:CE2  | 1:A:1046:LEU:HD11 | 2.51                     | 0.46              |
| 1:A:1450:LEU:HD11 | 6:F:108:PHE:CZ    | 2.51                     | 0.46              |
| 2:B:458:LYS:O     | 2:B:459:TYR:C     | 2.59                     | 0.46              |
| 2:B:733:HIS:O     | 2:B:735:ALA:N     | 2.44                     | 0.46              |
| 2:B:798:TYR:CE2   | 3:C:62:PHE:CZ     | 2.97                     | 0.46              |
| 2:B:1072:MET:HB2  | 2:B:1085:ILE:HD13 | 1.98                     | 0.46              |
| 3:C:11:ARG:HD3    | 3:C:209:TYR:CZ    | 2.49                     | 0.46              |
| 3:C:66:ARG:NH1    | 10:J:2:ILE:CG2    | 2.75                     | 0.46              |
| 3:C:91:HIS:ND1    | 3:C:158:VAL:HG11  | 2.30                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:177:GLU:HG3   | 3:C:231:ASN:ND2   | 2.31                     | 0.46              |
| 5:E:79:TRP:HB2    | 5:E:105:PHE:HE1   | 1.77                     | 0.46              |
| 5:E:124:VAL:HB    | 5:E:125:PRO:CD    | 2.46                     | 0.46              |
| 5:E:135:PHE:HD2   | 5:E:140:LEU:CD2   | 2.27                     | 0.46              |
| 5:E:153:HIS:C     | 5:E:154:ILE:HG13  | 2.39                     | 0.46              |
| 7:G:14:HIS:CD2    | 7:G:16:SER:HB3    | 2.51                     | 0.46              |
| 9:I:82:GLU:OE2    | 9:I:104:LEU:HB2   | 2.15                     | 0.46              |
| 1:A:23:SER:HB3    | 1:A:233:TRP:CE2   | 2.51                     | 0.46              |
| 1:A:133:LYS:O     | 1:A:136:ALA:HB3   | 2.16                     | 0.46              |
| 1:A:137:ALA:O     | 1:A:138:ILE:C     | 2.58                     | 0.46              |
| 1:A:555:ASP:O     | 1:A:556:TRP:O     | 2.33                     | 0.46              |
| 1:A:709:THR:CG2   | 1:A:710:LEU:N     | 2.75                     | 0.46              |
| 2:B:95:ILE:CG1    | 2:B:130:VAL:HG22  | 2.46                     | 0.46              |
| 2:B:249:ARG:O     | 2:B:251:ILE:HG13  | 2.15                     | 0.46              |
| 2:B:277:LYS:HG2   | 2:B:336:ARG:CB    | 2.46                     | 0.46              |
| 2:B:486:TYR:CE1   | 2:B:1096:ARG:NH2  | 2.84                     | 0.46              |
| 2:B:640:VAL:HG23  | 2:B:740:HIS:CA    | 2.46                     | 0.46              |
| 2:B:1165:ILE:CD1  | 2:B:1187:ASN:HD22 | 2.28                     | 0.46              |
| 2:B:1170:THR:O    | 2:B:1171:VAL:C    | 2.59                     | 0.46              |
| 3:C:79:GLN:HE21   | 3:C:127:ARG:HD3   | 1.81                     | 0.46              |
| 5:E:178:ILE:HB    | 5:E:212:ARG:HB3   | 1.97                     | 0.46              |
| 6:F:85:MET:HE2    | 6:F:93:ILE:HD13   | 1.97                     | 0.46              |
| 11:K:49:GLU:HG3   | 11:K:94:ILE:CG1   | 2.45                     | 0.46              |
| 12:L:55:ILE:CG1   | 12:L:56:LEU:H     | 2.10                     | 0.46              |
| 1:A:752:LYS:HD3   | 1:A:752:LYS:HA    | 1.72                     | 0.46              |
| 1:A:1100:ARG:O    | 1:A:1104:ILE:HG13 | 2.16                     | 0.46              |
| 1:A:1100:ARG:NH2  | 1:A:1351:GLU:HG2  | 2.31                     | 0.46              |
| 2:B:100:PRO:HB2   | 2:B:180:TYR:HE1   | 1.79                     | 0.46              |
| 2:B:390:LEU:O     | 2:B:391:ASP:C     | 2.58                     | 0.46              |
| 2:B:889:THR:HG23  | 2:B:891:ASP:N     | 2.31                     | 0.46              |
| 3:C:189:THR:CG2   | 3:C:190:ASP:N     | 2.78                     | 0.46              |
| 7:G:74:TYR:H      | 7:G:74:TYR:HD2    | 1.62                     | 0.46              |
| 10:J:21:TYR:HB2   | 10:J:39:LEU:CD1   | 2.46                     | 0.46              |
| 1:A:116:ASP:C     | 1:A:118:HIS:N     | 2.74                     | 0.46              |
| 1:A:1066:VAL:O    | 1:A:1070:GLN:HG3  | 2.16                     | 0.46              |
| 1:A:1115:SER:OG   | 1:A:1116:LEU:N    | 2.49                     | 0.46              |
| 1:A:1206:ASP:O    | 1:A:1274:ARG:NH1  | 2.48                     | 0.46              |
| 1:A:1268:LEU:HD11 | 9:I:48:LEU:HD11   | 1.98                     | 0.46              |
| 2:B:469:GLN:HB3   | 2:B:470:LYS:H     | 1.50                     | 0.46              |
| 2:B:651:LEU:HD21  | 2:B:741:CYS:HB3   | 1.98                     | 0.46              |
| 2:B:770:GLN:HB2   | 2:B:985:GLY:H     | 1.81                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:790:ASP:OD2  | 2:B:790:ASP:N    | 2.46                     | 0.46              |
| 3:C:118:LEU:HB2  | 3:C:132:PRO:HG2  | 1.98                     | 0.46              |
| 3:C:243:VAL:O    | 3:C:243:VAL:CG1  | 2.64                     | 0.46              |
| 5:E:45:LYS:HD3   | 5:E:46:TYR:CE1   | 2.51                     | 0.46              |
| 5:E:50:MET:HE3   | 5:E:50:MET:O     | 2.16                     | 0.46              |
| 5:E:169:ARG:HD3  | 6:F:140:ASP:OD2  | 2.15                     | 0.46              |
| 8:H:30:SER:HB2   | 8:H:36:CYS:HB3   | 1.98                     | 0.46              |
| 10:J:7:CYS:HA    | 10:J:49:MET:HE3  | 1.97                     | 0.46              |
| 12:L:46:VAL:O    | 12:L:46:VAL:HG12 | 2.16                     | 0.46              |
| 1:A:69:THR:O     | 1:A:70:CYS:C     | 2.59                     | 0.45              |
| 1:A:541:ILE:HG22 | 1:A:546:VAL:CG2  | 2.39                     | 0.45              |
| 1:A:1386:ARG:HB2 | 1:A:1403:GLU:CG  | 2.45                     | 0.45              |
| 2:B:436:VAL:O    | 2:B:436:VAL:HG12 | 2.17                     | 0.45              |
| 2:B:629:ASP:HB3  | 2:B:632:ARG:HE   | 1.81                     | 0.45              |
| 2:B:886:LYS:HB2  | 2:B:890:TYR:OH   | 2.16                     | 0.45              |
| 2:B:916:THR:CB   | 2:B:935:ARG:HD2  | 2.41                     | 0.45              |
| 2:B:999:MET:HA   | 2:B:999:MET:CE   | 2.41                     | 0.45              |
| 2:B:1115:THR:CG2 | 2:B:1117:GLN:HB2 | 2.46                     | 0.45              |
| 3:C:58:LEU:HD11  | 10:J:2:ILE:HG13  | 1.98                     | 0.45              |
| 4:D:119:ARG:HD3  | 4:D:221:TYR:CD2  | 2.51                     | 0.45              |
| 5:E:63:ASN:HB3   | 5:E:64:PRO:HD2   | 1.97                     | 0.45              |
| 6:F:111:LEU:N    | 6:F:111:LEU:CD1  | 2.78                     | 0.45              |
| 7:G:14:HIS:HD2   | 7:G:16:SER:HB3   | 1.80                     | 0.45              |
| 7:G:77:VAL:O     | 7:G:77:VAL:HG12  | 2.15                     | 0.45              |
| 8:H:62:SER:OG    | 8:H:63:LEU:N     | 2.49                     | 0.45              |
| 11:K:113:THR:O   | 11:K:114:LEU:CB  | 2.63                     | 0.45              |
| 1:A:335:ARG:O    | 1:A:339:ASN:HB2  | 2.15                     | 0.45              |
| 1:A:401:GLY:CA   | 1:A:435:HIS:HD2  | 2.29                     | 0.45              |
| 1:A:506:ALA:O    | 1:A:507:VAL:C    | 2.58                     | 0.45              |
| 1:A:567:LYS:CG   | 1:A:568:PRO:CD   | 2.89                     | 0.45              |
| 1:A:705:LYS:O    | 1:A:706:HIS:C    | 2.60                     | 0.45              |
| 1:A:705:LYS:CB   | 1:A:708:MET:HE3  | 2.45                     | 0.45              |
| 1:A:789:LYS:HE3  | 9:I:67:THR:CB    | 2.46                     | 0.45              |
| 1:A:1121:GLU:O   | 1:A:1122:PRO:C   | 2.59                     | 0.45              |
| 1:A:1323:ASP:C   | 1:A:1325:THR:H   | 2.24                     | 0.45              |
| 2:B:769:TYR:HD1  | 2:B:987:LYS:NZ   | 2.14                     | 0.45              |
| 2:B:1079:LYS:HA  | 3:C:27:LEU:HD21  | 1.98                     | 0.45              |
| 2:B:1212:ILE:O   | 2:B:1214:PRO:HD3 | 2.14                     | 0.45              |
| 3:C:34:ARG:NH1   | 3:C:35:ARG:HG2   | 2.32                     | 0.45              |
| 3:C:264:GLN:H    | 3:C:264:GLN:HG3  | 1.60                     | 0.45              |
| 4:D:8:PHE:CD2    | 7:G:6:ASP:HB2    | 2.51                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:E:56:LYS:NZ     | 5:E:85:GLU:HG3    | 2.30                     | 0.45              |
| 5:E:147:HIS:HB3   | 5:E:150:VAL:CG2   | 2.41                     | 0.45              |
| 1:A:100:LYS:O     | 1:A:103:CYS:HB2   | 2.17                     | 0.45              |
| 1:A:173:THR:O     | 1:A:173:THR:CG2   | 2.64                     | 0.45              |
| 1:A:196:GLU:HG2   | 1:A:197:PRO:HD2   | 1.99                     | 0.45              |
| 1:A:590:ARG:O     | 1:A:591:PHE:CB    | 2.60                     | 0.45              |
| 1:A:838:GLN:O     | 1:A:842:VAL:HG23  | 2.17                     | 0.45              |
| 1:A:843:LYS:HD3   | 1:A:843:LYS:HA    | 1.71                     | 0.45              |
| 1:A:1395:GLY:O    | 1:A:1396:ALA:C    | 2.59                     | 0.45              |
| 2:B:230:ALA:N     | 2:B:231:PRO:HD2   | 2.32                     | 0.45              |
| 2:B:308:TRP:HB2   | 9:I:2:THR:HG22    | 1.97                     | 0.45              |
| 2:B:364:ILE:O     | 2:B:365:THR:CB    | 2.60                     | 0.45              |
| 2:B:664:THR:CG2   | 2:B:678:GLU:N     | 2.79                     | 0.45              |
| 2:B:878:GLN:HB2   | 2:B:879:ARG:NH1   | 2.31                     | 0.45              |
| 3:C:97:VAL:HG12   | 3:C:99:LEU:CD2    | 2.46                     | 0.45              |
| 3:C:97:VAL:HG12   | 3:C:99:LEU:HD22   | 1.97                     | 0.45              |
| 3:C:137:LYS:HB3   | 3:C:138:GLU:OE1   | 2.16                     | 0.45              |
| 4:D:8:PHE:CZ      | 4:D:37:GLN:HB2    | 2.51                     | 0.45              |
| 7:G:129:SER:CB    | 7:G:138:THR:OG1   | 2.65                     | 0.45              |
| 9:I:82:GLU:HB3    | 9:I:104:LEU:HG    | 1.97                     | 0.45              |
| 1:A:283:GLY:O     | 1:A:285:PRO:HD2   | 2.16                     | 0.45              |
| 1:A:382:PRO:HD3   | 1:A:428:TYR:CE2   | 2.50                     | 0.45              |
| 1:A:675:THR:HG21  | 1:A:736:ASN:CB    | 2.47                     | 0.45              |
| 1:A:676:MET:O     | 1:A:677:ARG:C     | 2.60                     | 0.45              |
| 1:A:1220:PHE:O    | 1:A:1221:LYS:HB2  | 2.15                     | 0.45              |
| 2:B:461:LEU:N     | 2:B:461:LEU:HD12  | 2.31                     | 0.45              |
| 3:C:22:LEU:HD22   | 3:C:230:MET:CE    | 2.45                     | 0.45              |
| 3:C:117:ASP:N     | 3:C:117:ASP:OD1   | 2.48                     | 0.45              |
| 4:D:217:LEU:O     | 4:D:219:THR:N     | 2.48                     | 0.45              |
| 5:E:124:VAL:C     | 5:E:126:SER:H     | 2.24                     | 0.45              |
| 5:E:177:ARG:C     | 5:E:212:ARG:HD3   | 2.42                     | 0.45              |
| 6:F:85:MET:HB2    | 6:F:151:LEU:HB3   | 1.98                     | 0.45              |
| 9:I:78:CYS:SG     | 9:I:106:CYS:SG    | 3.14                     | 0.45              |
| 12:L:38:LEU:CG    | 12:L:39:SER:N     | 2.79                     | 0.45              |
| 1:A:49:LYS:HD3    | 1:A:55:ASP:HB3    | 1.99                     | 0.45              |
| 1:A:305:ASP:OD1   | 1:A:306:ASN:N     | 2.48                     | 0.45              |
| 1:A:335:ARG:HA    | 1:A:339:ASN:HD22  | 1.82                     | 0.45              |
| 1:A:919:ILE:CD1   | 1:A:983:ILE:HD12  | 2.47                     | 0.45              |
| 1:A:1127:ASP:O    | 1:A:1128:GLN:C    | 2.58                     | 0.45              |
| 1:A:1313:LEU:HD23 | 1:A:1338:VAL:HG21 | 1.99                     | 0.45              |
| 2:B:33:VAL:O      | 2:B:36:ALA:HB3    | 2.16                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:334:ILE:O     | 2:B:334:ILE:CG2   | 2.64                     | 0.45              |
| 2:B:639:ILE:HD11  | 2:B:691:GLU:HB2   | 1.97                     | 0.45              |
| 2:B:825:VAL:HG21  | 2:B:1092:TYR:HE1  | 1.82                     | 0.45              |
| 2:B:842:ASN:HD22  | 2:B:845:SER:H     | 1.61                     | 0.45              |
| 2:B:859:TYR:N     | 2:B:859:TYR:CD1   | 2.85                     | 0.45              |
| 2:B:866:TYR:HD2   | 2:B:870:ILE:HD12  | 1.82                     | 0.45              |
| 4:D:7:THR:HG21    | 4:D:32:GLU:OE1    | 2.17                     | 0.45              |
| 4:D:20:GLU:O      | 4:D:20:GLU:HG2    | 2.16                     | 0.45              |
| 4:D:71:LYS:HA     | 4:D:74:GLN:HG3    | 1.97                     | 0.45              |
| 1:A:443:LEU:O     | 1:A:489:LEU:HD12  | 2.16                     | 0.45              |
| 1:A:1313:LEU:C    | 1:A:1315:GLU:H    | 2.24                     | 0.45              |
| 1:A:1339:LEU:HD23 | 5:E:144:ILE:HG22  | 1.98                     | 0.45              |
| 2:B:230:ALA:N     | 2:B:231:PRO:CD    | 2.79                     | 0.45              |
| 2:B:377:PHE:O     | 2:B:380:TYR:N     | 2.50                     | 0.45              |
| 2:B:662:MET:HA    | 2:B:665:GLU:HG3   | 1.99                     | 0.45              |
| 2:B:999:MET:HE2   | 2:B:1011:ILE:HD11 | 1.97                     | 0.45              |
| 2:B:1007:VAL:HG22 | 2:B:1008:PRO:HD2  | 1.99                     | 0.45              |
| 2:B:1095:LEU:C    | 2:B:1096:ARG:O    | 2.57                     | 0.45              |
| 2:B:1169:MET:HE1  | 2:B:1201:LYS:CA   | 2.47                     | 0.45              |
| 3:C:186:LEU:CD2   | 3:C:225:ALA:HB2   | 2.47                     | 0.45              |
| 8:H:30:SER:CB     | 8:H:36:CYS:HB3    | 2.47                     | 0.45              |
| 8:H:103:LYS:HB3   | 8:H:115:TYR:HD1   | 1.82                     | 0.45              |
| 10:J:1:MET:H3     | 10:J:56:LEU:H     | 1.65                     | 0.45              |
| 1:A:146:MET:C     | 1:A:171:GLN:HB2   | 2.40                     | 0.45              |
| 1:A:265:LYS:CA    | 1:A:265:LYS:CE    | 2.92                     | 0.45              |
| 1:A:381:THR:CG2   | 1:A:383:TYR:H     | 2.18                     | 0.45              |
| 1:A:399:HIS:CG    | 1:A:400:PRO:N     | 2.81                     | 0.45              |
| 1:A:483:ASP:O     | 2:B:979:LYS:HE3   | 2.16                     | 0.45              |
| 1:A:514:PRO:O     | 1:A:515:GLN:C     | 2.59                     | 0.45              |
| 1:A:523:ILE:HG13  | 1:A:622:VAL:HG22  | 1.99                     | 0.45              |
| 1:A:577:ILE:O     | 1:A:580:VAL:HG23  | 2.16                     | 0.45              |
| 1:A:831:THR:O     | 1:A:834:THR:HG22  | 2.16                     | 0.45              |
| 2:B:51:PHE:O      | 2:B:54:PHE:HB3    | 2.17                     | 0.45              |
| 2:B:193:LYS:HZ3   | 12:L:32:ALA:HB1   | 1.81                     | 0.45              |
| 2:B:277:LYS:HG2   | 2:B:336:ARG:HB3   | 1.98                     | 0.45              |
| 2:B:550:ASP:OD1   | 2:B:552:MET:HB2   | 2.17                     | 0.45              |
| 2:B:838:SER:HA    | 2:B:989:THR:O     | 2.16                     | 0.45              |
| 2:B:942:ARG:HB2   | 2:B:945:GLU:HB2   | 1.99                     | 0.45              |
| 2:B:952:VAL:HG12  | 2:B:953:LEU:N     | 2.32                     | 0.45              |
| 3:C:46:ILE:HG23   | 3:C:157:CYS:HB3   | 1.97                     | 0.45              |
| 5:E:61:GLN:NE2    | 5:E:105:PHE:CE2   | 2.84                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:G:155:SER:O    | 7:G:156:SER:HB3  | 2.16                     | 0.45              |
| 8:H:128:ASN:C    | 8:H:128:ASN:HD22 | 2.25                     | 0.45              |
| 1:A:130:ASP:O    | 1:A:131:SER:C    | 2.60                     | 0.45              |
| 1:A:332:LYS:H    | 1:A:337:ARG:CB   | 2.30                     | 0.45              |
| 1:A:543:LEU:O    | 1:A:544:ASP:C    | 2.60                     | 0.45              |
| 1:A:849:MET:HB3  | 1:A:1063:MET:SD  | 2.57                     | 0.45              |
| 1:A:1095:THR:CG2 | 1:A:1112:LYS:HB2 | 2.47                     | 0.45              |
| 1:A:1393:ASN:O   | 1:A:1394:THR:C   | 2.59                     | 0.45              |
| 2:B:205:ILE:N    | 2:B:205:ILE:CD1  | 2.80                     | 0.45              |
| 2:B:1166:CYS:O   | 2:B:1166:CYS:SG  | 2.75                     | 0.45              |
| 4:D:50:LEU:HD21  | 7:G:4:ILE:CD1    | 2.47                     | 0.45              |
| 5:E:116:ILE:CB   | 5:E:121:MET:HE2  | 2.45                     | 0.45              |
| 6:F:82:THR:CG2   | 6:F:84:TYR:O     | 2.64                     | 0.45              |
| 8:H:84:ALA:HA    | 8:H:87:ARG:HB2   | 1.97                     | 0.45              |
| 8:H:100:THR:OG1  | 8:H:138:GLU:HG2  | 2.16                     | 0.45              |
| 9:I:10:CYS:O     | 9:I:11:ASN:C     | 2.59                     | 0.45              |
| 1:A:106:VAL:HG21 | 1:A:214:ILE:HD13 | 1.96                     | 0.45              |
| 1:A:162:VAL:HG12 | 1:A:163:SER:H    | 1.82                     | 0.45              |
| 1:A:298:PHE:CZ   | 1:A:314:ALA:HB2  | 2.52                     | 0.45              |
| 1:A:549:MET:HE1  | 1:A:656:TRP:HD1  | 1.81                     | 0.45              |
| 1:A:593:GLU:C    | 1:A:595:THR:N    | 2.74                     | 0.45              |
| 1:A:715:GLU:OE1  | 1:A:774:ARG:HD3  | 2.16                     | 0.45              |
| 1:A:743:VAL:O    | 1:A:747:VAL:HG23 | 2.17                     | 0.45              |
| 1:A:962:ARG:O    | 1:A:964:ILE:N    | 2.49                     | 0.45              |
| 1:A:963:ILE:HD11 | 1:A:1048:ASN:HB2 | 1.98                     | 0.45              |
| 1:A:1242:VAL:CG1 | 1:A:1243:VAL:H   | 2.29                     | 0.45              |
| 1:A:1451:VAL:C   | 1:A:1453:TYR:N   | 2.73                     | 0.45              |
| 2:B:408:LEU:HD21 | 2:B:545:ILE:HD12 | 1.98                     | 0.45              |
| 2:B:487:THR:O    | 2:B:490:SER:HB3  | 2.17                     | 0.45              |
| 2:B:705:MET:HB3  | 2:B:706:GLN:H    | 1.61                     | 0.45              |
| 2:B:906:SER:O    | 2:B:941:LEU:HD23 | 2.17                     | 0.45              |
| 2:B:1167:GLY:N   | 2:B:1215:ARG:HG2 | 2.32                     | 0.45              |
| 3:C:101:LEU:C    | 3:C:102:GLN:CG   | 2.90                     | 0.45              |
| 5:E:182:ASP:HB3  | 5:E:185:ALA:CB   | 2.47                     | 0.45              |
| 8:H:4:THR:CG2    | 8:H:5:LEU:N      | 2.80                     | 0.45              |
| 1:A:33:ALA:HB1   | 1:A:56:PRO:HB2   | 1.99                     | 0.45              |
| 1:A:671:ALA:H    | 1:A:676:MET:HE2  | 1.81                     | 0.45              |
| 1:A:898:ARG:O    | 1:A:1029:ARG:NH1 | 2.50                     | 0.45              |
| 1:A:1189:SER:HB2 | 1:A:1256:GLU:OE1 | 2.17                     | 0.45              |
| 1:A:1217:LYS:O   | 1:A:1221:LYS:HA  | 2.17                     | 0.45              |
| 1:A:1441:PHE:CZ  | 6:F:89:GLU:HA    | 2.52                     | 0.45              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B:62:ILE:HG23  | 2:B:418:LYS:HG3   | 1.99                     | 0.45              |
| 2:B:227:LYS:H    | 2:B:395:GLN:CD    | 2.25                     | 0.45              |
| 2:B:257:LYS:HB3  | 2:B:258:LEU:H     | 1.53                     | 0.45              |
| 2:B:969:ARG:HH11 | 3:C:61:GLU:CD     | 2.25                     | 0.45              |
| 3:C:101:LEU:O    | 3:C:102:GLN:HG2   | 2.17                     | 0.45              |
| 10:J:31:ASP:O    | 10:J:32:GLU:C     | 2.60                     | 0.45              |
| 1:A:23:SER:HA    | 1:A:233:TRP:NE1   | 2.32                     | 0.44              |
| 1:A:456:MET:HE3  | 1:A:478:TYR:CZ    | 2.52                     | 0.44              |
| 1:A:690:VAL:CG2  | 1:A:718:VAL:HG13  | 2.47                     | 0.44              |
| 1:A:715:GLU:O    | 1:A:716:ASP:C     | 2.60                     | 0.44              |
| 1:A:789:LYS:HE3  | 9:I:67:THR:HB     | 1.99                     | 0.44              |
| 1:A:853:ASP:OD1  | 1:A:853:ASP:C     | 2.59                     | 0.44              |
| 1:A:888:GLY:O    | 1:A:940:ARG:NH2   | 2.51                     | 0.44              |
| 1:A:904:THR:O    | 1:A:904:THR:HG22  | 2.17                     | 0.44              |
| 1:A:929:LEU:CD2  | 1:A:929:LEU:N     | 2.80                     | 0.44              |
| 1:A:1297:GLU:OE1 | 1:A:1297:GLU:N    | 2.50                     | 0.44              |
| 2:B:29:ASP:CB    | 2:B:658:ILE:HD13  | 2.46                     | 0.44              |
| 2:B:286:PHE:CG   | 2:B:297:ILE:HG23  | 2.52                     | 0.44              |
| 2:B:425:THR:HG22 | 2:B:426:LYS:N     | 2.32                     | 0.44              |
| 2:B:996:ARG:NH2  | 3:C:38:ILE:HG23   | 2.32                     | 0.44              |
| 5:E:192:ARG:HG3  | 5:E:192:ARG:NH1   | 2.31                     | 0.44              |
| 1:A:105:CYS:O    | 1:A:114:LEU:HG    | 2.17                     | 0.44              |
| 1:A:146:MET:CA   | 1:A:171:GLN:HB2   | 2.47                     | 0.44              |
| 1:A:220:THR:O    | 1:A:223:GLY:N     | 2.44                     | 0.44              |
| 1:A:1138:ILE:C   | 1:A:1275:GLY:HA2  | 2.41                     | 0.44              |
| 1:A:1148:ILE:O   | 1:A:1149:ALA:HB2  | 2.17                     | 0.44              |
| 1:A:1345:ARG:HG2 | 1:A:1372:VAL:HG12 | 1.98                     | 0.44              |
| 2:B:31:TRP:CE3   | 2:B:31:TRP:HA     | 2.52                     | 0.44              |
| 2:B:110:HIS:CB   | 12:L:54:ARG:HH22  | 2.30                     | 0.44              |
| 2:B:254:LEU:HD22 | 2:B:361:LEU:CD1   | 2.47                     | 0.44              |
| 2:B:434:ARG:O    | 2:B:436:VAL:N     | 2.50                     | 0.44              |
| 2:B:769:TYR:C    | 2:B:771:SER:N     | 2.75                     | 0.44              |
| 3:C:146:LYS:C    | 3:C:147:LEU:HD23  | 2.42                     | 0.44              |
| 3:C:235:VAL:HG21 | 10:J:6:ARG:HH21   | 1.81                     | 0.44              |
| 9:I:15:TYR:N     | 9:I:15:TYR:CD1    | 2.85                     | 0.44              |
| 11:K:46:ILE:O    | 11:K:50:LEU:HB2   | 2.17                     | 0.44              |
| 1:A:289:ILE:CG2  | 1:A:290:GLU:N     | 2.80                     | 0.44              |
| 1:A:676:MET:O    | 1:A:679:ILE:N     | 2.48                     | 0.44              |
| 1:A:1157:ASP:C   | 1:A:1159:ARG:H    | 2.25                     | 0.44              |
| 2:B:274:PRO:O    | 2:B:275:TYR:HB2   | 2.17                     | 0.44              |
| 2:B:293:PRO:O    | 2:B:294:ASP:O     | 2.36                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:401:PHE:HD2   | 2:B:521:LEU:HD12  | 1.83                     | 0.44              |
| 2:B:479:VAL:O     | 2:B:480:SER:HB3   | 2.17                     | 0.44              |
| 2:B:644:GLU:C     | 2:B:646:LEU:N     | 2.75                     | 0.44              |
| 3:C:133:ILE:CD1   | 3:C:236:GLY:C     | 2.90                     | 0.44              |
| 4:D:12:ARG:NH1    | 4:D:14:ARG:CA     | 2.79                     | 0.44              |
| 4:D:29:LEU:HD12   | 7:G:82:PHE:CZ     | 2.52                     | 0.44              |
| 7:G:116:PRO:HG2   | 7:G:119:LEU:CB    | 2.44                     | 0.44              |
| 1:A:34:LYS:HG2    | 1:A:57:ARG:NH2    | 2.31                     | 0.44              |
| 1:A:34:LYS:NZ     | 1:A:57:ARG:NH2    | 2.57                     | 0.44              |
| 1:A:691:LEU:O     | 1:A:694:THR:HB    | 2.17                     | 0.44              |
| 1:A:1050:GLU:HG3  | 1:A:1054:LEU:HD11 | 1.99                     | 0.44              |
| 1:A:1165:GLU:H    | 1:A:1165:GLU:HG2  | 1.44                     | 0.44              |
| 1:A:1385:THR:HG22 | 1:A:1388:GLY:N    | 2.17                     | 0.44              |
| 2:B:204:ILE:O     | 2:B:204:ILE:HG22  | 2.16                     | 0.44              |
| 2:B:431:TYR:CD1   | 2:B:447:ALA:HB2   | 2.52                     | 0.44              |
| 2:B:807:ARG:HH11  | 2:B:807:ARG:CB    | 2.29                     | 0.44              |
| 2:B:1096:ARG:HB2  | 2:B:1096:ARG:HH11 | 1.83                     | 0.44              |
| 3:C:73:GLN:NE2    | 3:C:75:MET:N      | 2.65                     | 0.44              |
| 3:C:181:ASP:N     | 3:C:182:PRO:CD    | 2.80                     | 0.44              |
| 4:D:146:GLN:CA    | 4:D:149:THR:HG22  | 2.47                     | 0.44              |
| 6:F:148:VAL:O     | 6:F:149:GLU:C     | 2.60                     | 0.44              |
| 12:L:47:ARG:HG2   | 12:L:48:CYS:N     | 2.23                     | 0.44              |
| 1:A:260:ASP:O     | 1:A:261:ASP:C     | 2.60                     | 0.44              |
| 1:A:451:HIS:O     | 1:A:452:LYS:C     | 2.60                     | 0.44              |
| 1:A:700:ASN:O     | 9:I:115:LYS:HD2   | 2.18                     | 0.44              |
| 1:A:781:ASP:HB3   | 1:A:790:ASP:H     | 1.82                     | 0.44              |
| 1:A:874:ASP:C     | 1:A:874:ASP:OD1   | 2.60                     | 0.44              |
| 1:A:1385:THR:CG2  | 1:A:1388:GLY:H    | 2.18                     | 0.44              |
| 1:A:1446:ASP:O    | 1:A:1448:GLU:N    | 2.51                     | 0.44              |
| 2:B:302:CYS:C     | 2:B:303:TYR:HD2   | 2.26                     | 0.44              |
| 2:B:370:PHE:HD2   | 2:B:373:ARG:CD    | 2.29                     | 0.44              |
| 2:B:622:LYS:CE    | 9:I:59:VAL:HG13   | 2.47                     | 0.44              |
| 2:B:744:HIS:CD2   | 2:B:745:PRO:CD    | 2.83                     | 0.44              |
| 2:B:860:MET:HG3   | 2:B:965:LYS:HG2   | 1.98                     | 0.44              |
| 3:C:236:GLY:O     | 3:C:238:ILE:N     | 2.51                     | 0.44              |
| 4:D:142:LYS:O     | 4:D:146:GLN:HG3   | 2.18                     | 0.44              |
| 5:E:78:LEU:HD23   | 5:E:78:LEU:O      | 2.18                     | 0.44              |
| 8:H:11:GLN:O      | 8:H:28:ALA:HB1    | 2.17                     | 0.44              |
| 8:H:77:ARG:O      | 8:H:78:SER:C      | 2.60                     | 0.44              |
| 8:H:130:ARG:HH11  | 8:H:130:ARG:H     | 1.64                     | 0.44              |
| 9:I:106:CYS:O     | 9:I:107:SER:HB2   | 2.17                     | 0.44              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 11:K:50:LEU:HD13  | 11:K:75:ILE:HG12 | 2.00                     | 0.44              |
| 12:L:43:THR:HG22  | 12:L:43:THR:O    | 2.17                     | 0.44              |
| 1:A:26:GLU:O      | 1:A:29:ALA:HB3   | 2.17                     | 0.44              |
| 1:A:40:THR:HG21   | 1:A:259:GLU:OE2  | 2.18                     | 0.44              |
| 1:A:69:THR:HG22   | 2:B:1174:LYS:HD3 | 2.00                     | 0.44              |
| 1:A:93:VAL:HG22   | 1:A:301:ALA:CA   | 2.41                     | 0.44              |
| 1:A:590:ARG:NH1   | 1:A:592:ASP:OD2  | 2.44                     | 0.44              |
| 1:A:806:ARG:HH12  | 2:B:729:ILE:HD11 | 1.81                     | 0.44              |
| 1:A:1123:GLY:O    | 1:A:1125:ALA:N   | 2.51                     | 0.44              |
| 1:A:1127:ASP:HB3  | 1:A:1130:GLN:HB3 | 1.99                     | 0.44              |
| 1:A:1209:MET:O    | 1:A:1210:GLY:C   | 2.60                     | 0.44              |
| 1:A:1313:LEU:HD23 | 1:A:1338:VAL:CG2 | 2.48                     | 0.44              |
| 2:B:110:HIS:CB    | 12:L:54:ARG:NH2  | 2.80                     | 0.44              |
| 2:B:244:LEU:O     | 2:B:245:GLU:C    | 2.61                     | 0.44              |
| 2:B:384:ARG:HE    | 2:B:384:ARG:HB3  | 1.59                     | 0.44              |
| 2:B:629:ASP:HB3   | 2:B:632:ARG:HD3  | 2.00                     | 0.44              |
| 2:B:637:LEU:HB2   | 2:B:693:ILE:CD1  | 2.48                     | 0.44              |
| 2:B:886:LYS:HB2   | 2:B:890:TYR:CE1  | 2.53                     | 0.44              |
| 2:B:918:ILE:HG21  | 2:B:935:ARG:NH2  | 2.32                     | 0.44              |
| 2:B:958:GLN:C     | 2:B:960:GLY:H    | 2.26                     | 0.44              |
| 4:D:54:GLU:O      | 4:D:58:VAL:HG23  | 2.18                     | 0.44              |
| 4:D:136:GLY:HA2   | 4:D:142:LYS:NZ   | 2.32                     | 0.44              |
| 5:E:128:PRO:HA    | 5:E:129:PRO:O    | 2.18                     | 0.44              |
| 8:H:81:PRO:CB     | 8:H:82:PRO:CD    | 2.95                     | 0.44              |
| 11:K:53:ASP:OD1   | 11:K:55:LYS:HB2  | 2.18                     | 0.44              |
| 11:K:53:ASP:HB3   | 11:K:56:VAL:HG23 | 2.00                     | 0.44              |
| 1:A:298:PHE:O     | 1:A:302:THR:HB   | 2.17                     | 0.44              |
| 1:A:458:HIS:NE2   | 1:A:478:TYR:OH   | 2.35                     | 0.44              |
| 1:A:492:PRO:O     | 1:A:493:GLN:NE2  | 2.50                     | 0.44              |
| 1:A:934:LYS:HB2   | 1:A:934:LYS:NZ   | 2.33                     | 0.44              |
| 1:A:1350:LYS:O    | 1:A:1354:ASN:ND2 | 2.51                     | 0.44              |
| 2:B:260:GLY:O     | 2:B:267:ARG:HD3  | 2.17                     | 0.44              |
| 3:C:6:PRO:CB      | 3:C:25:VAL:HG22  | 2.45                     | 0.44              |
| 3:C:113:VAL:HG23  | 3:C:147:LEU:CD2  | 2.48                     | 0.44              |
| 4:D:29:LEU:N      | 4:D:29:LEU:CD2   | 2.78                     | 0.44              |
| 5:E:180:ARG:NH2   | 5:E:192:ARG:HB2  | 2.32                     | 0.44              |
| 6:F:97:ARG:HH11   | 6:F:97:ARG:HG3   | 1.82                     | 0.44              |
| 8:H:40:LEU:HD13   | 8:H:123:MET:CE   | 2.36                     | 0.44              |
| 12:L:44:ASP:O     | 12:L:45:ALA:HB3  | 2.17                     | 0.44              |
| 13:T:23:BRU:H2''  | 13:T:24:DG:O5'   | 2.18                     | 0.44              |
| 1:A:115:LEU:CD1   | 1:A:142:CYS:HB3  | 2.48                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:157:ASP:C     | 1:A:159:THR:H     | 2.26                     | 0.44              |
| 1:A:211:PHE:HD1   | 1:A:214:ILE:HD12  | 1.83                     | 0.44              |
| 1:A:666:ILE:O     | 1:A:670:ILE:HD13  | 2.18                     | 0.44              |
| 1:A:1329:THR:H    | 1:A:1335:ILE:HD11 | 1.83                     | 0.44              |
| 2:B:240:ILE:HG23  | 2:B:240:ILE:O     | 2.17                     | 0.44              |
| 2:B:244:LEU:CD1   | 2:B:250:PHE:HD1   | 2.31                     | 0.44              |
| 2:B:280:ILE:HG22  | 2:B:285:ILE:HG13  | 2.00                     | 0.44              |
| 2:B:287:ARG:CG    | 2:B:292:ILE:HA    | 2.46                     | 0.44              |
| 2:B:291:ILE:CD1   | 2:B:300:HIS:NE2   | 2.81                     | 0.44              |
| 2:B:616:ILE:CG2   | 2:B:700:SER:OG    | 2.66                     | 0.44              |
| 2:B:1124:ARG:HH22 | 15:P:2:G:P        | 2.40                     | 0.44              |
| 3:C:52:GLU:OE2    | 3:C:154:LYS:HD2   | 2.17                     | 0.44              |
| 13:T:21:DC:C2     | 13:T:22:DC:C5     | 3.06                     | 0.44              |
| 1:A:883:LEU:CD1   | 1:A:1017:LEU:HD11 | 2.46                     | 0.44              |
| 1:A:899:VAL:CB    | 1:A:929:LEU:HD12  | 2.45                     | 0.44              |
| 1:A:1268:LEU:O    | 1:A:1269:GLU:HG3  | 2.17                     | 0.44              |
| 1:A:1354:ASN:O    | 1:A:1358:SER:HB3  | 2.17                     | 0.44              |
| 2:B:467:GLY:HA3   | 2:B:475:SER:HB3   | 1.99                     | 0.44              |
| 2:B:617:ARG:HH22  | 9:I:61:ASP:CG     | 2.26                     | 0.44              |
| 2:B:707:PRO:O     | 2:B:708:GLU:O     | 2.36                     | 0.44              |
| 2:B:708:GLU:HG3   | 2:B:709:ASP:N     | 2.32                     | 0.44              |
| 2:B:1119:VAL:O    | 2:B:1126:GLY:HA3  | 2.17                     | 0.44              |
| 3:C:69:LEU:N      | 3:C:69:LEU:CD1    | 2.81                     | 0.44              |
| 4:D:39:ASN:HD22   | 4:D:41:GLN:HB2    | 1.83                     | 0.44              |
| 5:E:28:TYR:CE1    | 5:E:78:LEU:HB3    | 2.53                     | 0.44              |
| 6:F:97:ARG:NH2    | 6:F:108:PHE:HE1   | 2.15                     | 0.44              |
| 12:L:48:CYS:HB3   | 12:L:51:CYS:O     | 2.17                     | 0.44              |
| 13:T:22:DC:H2"    | 13:T:23:BRU:OP2   | 2.18                     | 0.44              |
| 1:A:92:HIS:O      | 1:A:93:VAL:C      | 2.61                     | 0.43              |
| 1:A:613:ILE:O     | 1:A:614:PHE:HB3   | 2.18                     | 0.43              |
| 2:B:664:THR:HG23  | 2:B:678:GLU:N     | 2.32                     | 0.43              |
| 2:B:866:TYR:CD2   | 2:B:870:ILE:HB    | 2.53                     | 0.43              |
| 2:B:984:HIS:NE2   | 2:B:1025:HIS:HA   | 2.33                     | 0.43              |
| 2:B:984:HIS:CD2   | 2:B:1025:HIS:HB2  | 2.53                     | 0.43              |
| 3:C:112:ASN:CB    | 3:C:114:TYR:CE1   | 2.91                     | 0.43              |
| 4:D:29:LEU:HD22   | 4:D:29:LEU:H      | 1.81                     | 0.43              |
| 4:D:166:LEU:O     | 4:D:169:SER:OG    | 2.36                     | 0.43              |
| 5:E:79:TRP:NE1    | 5:E:81:GLU:HB2    | 2.30                     | 0.43              |
| 5:E:180:ARG:O     | 5:E:180:ARG:HG2   | 2.18                     | 0.43              |
| 6:F:147:SER:HG    | 6:F:150:GLU:HG3   | 1.80                     | 0.43              |
| 7:G:127:PRO:HG2   | 7:G:138:THR:HG21  | 2.00                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:I:4:PHE:HE1     | 9:I:13:MET:HG3    | 1.83                     | 0.43              |
| 9:I:73:ARG:NH1    | 9:I:112:SER:HB3   | 2.32                     | 0.43              |
| 10:J:16:ASP:OD1   | 10:J:17:LYS:N     | 2.48                     | 0.43              |
| 11:K:91:CYS:O     | 11:K:94:ILE:HB    | 2.18                     | 0.43              |
| 1:A:36:ARG:HB2    | 1:A:37:PHE:CD1    | 2.53                     | 0.43              |
| 1:A:61:ILE:CG2    | 1:A:62:ASP:N      | 2.74                     | 0.43              |
| 1:A:139:TRP:O     | 1:A:140:THR:C     | 2.61                     | 0.43              |
| 1:A:310:GLY:C     | 1:A:312:PRO:HD2   | 2.42                     | 0.43              |
| 1:A:664:THR:HG22  | 2:B:1014:PRO:HB3  | 2.00                     | 0.43              |
| 1:A:744:LYS:HD3   | 1:A:748:MET:HE2   | 2.00                     | 0.43              |
| 1:A:836:TYR:CZ    | 1:A:840:ARG:HD2   | 2.53                     | 0.43              |
| 1:A:987:VAL:HG12  | 1:A:988:LEU:N     | 2.33                     | 0.43              |
| 1:A:1072:ILE:O    | 1:A:1075:PRO:HG2  | 2.18                     | 0.43              |
| 1:A:1155:ASP:OD2  | 1:A:1161:THR:CG2  | 2.64                     | 0.43              |
| 1:A:1444:MET:HG2  | 7:G:60:ARG:CA     | 2.47                     | 0.43              |
| 2:B:427:ASP:HA    | 2:B:430:ARG:CG    | 2.49                     | 0.43              |
| 2:B:593:PRO:HG2   | 2:B:617:ARG:CZ    | 2.48                     | 0.43              |
| 2:B:611:PRO:O     | 2:B:692:TYR:HB2   | 2.18                     | 0.43              |
| 2:B:616:ILE:HD12  | 2:B:616:ILE:H     | 1.79                     | 0.43              |
| 2:B:758:PHE:N     | 2:B:759:PRO:CD    | 2.81                     | 0.43              |
| 2:B:785:TYR:CD2   | 2:B:795:ILE:HG12  | 2.53                     | 0.43              |
| 2:B:1064:TYR:O    | 2:B:1065:GLN:C    | 2.61                     | 0.43              |
| 5:E:48:ASP:CG     | 5:E:49:SER:N      | 2.75                     | 0.43              |
| 11:K:53:ASP:HB3   | 11:K:56:VAL:CG2   | 2.48                     | 0.43              |
| 1:A:63:ARG:HA     | 1:A:74:MET:CE     | 2.39                     | 0.43              |
| 1:A:93:VAL:CG1    | 1:A:301:ALA:HB1   | 2.46                     | 0.43              |
| 1:A:828:ALA:C     | 1:A:831:THR:HG22  | 2.42                     | 0.43              |
| 1:A:1308:THR:HG23 | 1:A:1310:GLY:H    | 1.82                     | 0.43              |
| 2:B:35:SER:HA     | 2:B:811:TYR:CE2   | 2.44                     | 0.43              |
| 2:B:558:LEU:HD23  | 2:B:596:LEU:HD11  | 2.00                     | 0.43              |
| 2:B:619:ILE:O     | 2:B:622:LYS:N     | 2.46                     | 0.43              |
| 2:B:635:ARG:HH22  | 2:B:742:GLU:CD    | 2.23                     | 0.43              |
| 2:B:635:ARG:NH1   | 2:B:742:GLU:OE2   | 2.51                     | 0.43              |
| 2:B:640:VAL:O     | 2:B:640:VAL:HG12  | 2.18                     | 0.43              |
| 2:B:955:THR:HG22  | 2:B:956:THR:N     | 2.33                     | 0.43              |
| 2:B:1181:GLU:HB2  | 2:B:1188:LYS:HG2  | 2.00                     | 0.43              |
| 3:C:6:PRO:HB2     | 11:K:101:LEU:HD12 | 1.99                     | 0.43              |
| 3:C:254:LYS:O     | 3:C:258:ILE:HD13  | 2.18                     | 0.43              |
| 4:D:46:GLU:HG2    | 4:D:47:LEU:N      | 2.33                     | 0.43              |
| 7:G:123:ALA:C     | 7:G:125:SER:H     | 2.25                     | 0.43              |
| 8:H:41:ASP:HB3    | 8:H:121:LEU:HD22  | 1.98                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 9:I:8:ARG:O      | 9:I:10:CYS:N      | 2.52                     | 0.43              |
| 1:A:37:PHE:HD1   | 1:A:37:PHE:H      | 1.66                     | 0.43              |
| 1:A:66:LYS:HD3   | 1:A:67:CYS:H      | 1.81                     | 0.43              |
| 1:A:186:LYS:HZ1  | 1:A:197:PRO:HD3   | 1.81                     | 0.43              |
| 1:A:417:TYR:O    | 1:A:418:SER:C     | 2.61                     | 0.43              |
| 1:A:456:MET:HE1  | 1:A:474:VAL:CG2   | 2.48                     | 0.43              |
| 1:A:722:LEU:HD23 | 1:A:799:PHE:CG    | 2.52                     | 0.43              |
| 1:A:723:ASN:O    | 1:A:724:GLU:C     | 2.62                     | 0.43              |
| 1:A:959:ASN:OD1  | 1:A:959:ASN:C     | 2.62                     | 0.43              |
| 1:A:1097:GLY:C   | 1:A:1099:PRO:HD2  | 2.44                     | 0.43              |
| 1:A:1364:ASN:O   | 1:A:1365:TYR:C    | 2.61                     | 0.43              |
| 2:B:125:SER:O    | 2:B:126:SER:HB3   | 2.17                     | 0.43              |
| 2:B:803:LEU:CD1  | 2:B:1032:SER:HB3  | 2.47                     | 0.43              |
| 2:B:948:ILE:HG22 | 2:B:949:VAL:O     | 2.18                     | 0.43              |
| 5:E:21:GLU:HG2   | 5:E:35:VAL:HG11   | 1.99                     | 0.43              |
| 5:E:117:THR:C    | 5:E:119:SER:H     | 2.26                     | 0.43              |
| 5:E:186:LEU:O    | 5:E:187:TYR:C     | 2.60                     | 0.43              |
| 6:F:101:ILE:HD13 | 6:F:120:ILE:HG22  | 1.99                     | 0.43              |
| 11:K:79:GLU:C    | 11:K:81:TYR:H     | 2.26                     | 0.43              |
| 1:A:90:VAL:HB    | 1:A:297:GLN:HE22  | 1.74                     | 0.43              |
| 1:A:116:ASP:C    | 1:A:118:HIS:H     | 2.26                     | 0.43              |
| 1:A:350:ARG:HB2  | 2:B:1128:LEU:HD13 | 2.00                     | 0.43              |
| 1:A:409:SER:O    | 1:A:410:GLY:C     | 2.62                     | 0.43              |
| 1:A:780:VAL:O    | 1:A:782:ARG:HG2   | 2.18                     | 0.43              |
| 1:A:1063:MET:SD  | 1:A:1436:ILE:CG2  | 3.06                     | 0.43              |
| 1:A:1171:GLN:O   | 1:A:1174:PHE:HB2  | 2.19                     | 0.43              |
| 1:A:1444:MET:HG2 | 7:G:59:GLY:O      | 2.19                     | 0.43              |
| 1:A:1451:VAL:O   | 1:A:1454:MET:HG2  | 2.19                     | 0.43              |
| 2:B:209:GLU:CD   | 2:B:485:ARG:HE    | 2.22                     | 0.43              |
| 2:B:293:PRO:O    | 2:B:296:GLU:HB3   | 2.18                     | 0.43              |
| 2:B:473:MET:C    | 2:B:475:SER:H     | 2.26                     | 0.43              |
| 2:B:552:MET:C    | 2:B:554:ILE:N     | 2.77                     | 0.43              |
| 2:B:908:GLU:O    | 2:B:909:ASP:C     | 2.62                     | 0.43              |
| 2:B:1034:VAL:O   | 2:B:1037:LEU:N    | 2.51                     | 0.43              |
| 6:F:76:LYS:HA    | 6:F:79:ARG:HD2    | 1.99                     | 0.43              |
| 6:F:119:ARG:HH11 | 6:F:119:ARG:CG    | 2.30                     | 0.43              |
| 8:H:40:LEU:HD22  | 8:H:123:MET:HE3   | 1.99                     | 0.43              |
| 9:I:77:LYS:O     | 9:I:79:HIS:N      | 2.51                     | 0.43              |
| 10:J:36:LEU:HD12 | 10:J:47:ARG:NH1   | 2.33                     | 0.43              |
| 12:L:33:GLU:CD   | 12:L:33:GLU:N     | 2.75                     | 0.43              |
| 12:L:34:CYS:CB   | 12:L:51:CYS:SG    | 3.05                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:65:LEU:O      | 1:A:66:LYS:O      | 2.36                     | 0.43              |
| 1:A:134:ARG:HH11  | 1:A:221:SER:HA    | 1.83                     | 0.43              |
| 1:A:137:ALA:O     | 1:A:139:TRP:N     | 2.51                     | 0.43              |
| 1:A:219:PHE:CE2   | 1:A:231:PRO:HD2   | 2.54                     | 0.43              |
| 1:A:224:PHE:CD2   | 1:A:231:PRO:HG3   | 2.54                     | 0.43              |
| 1:A:392:VAL:HG13  | 1:A:415:LEU:CD1   | 2.44                     | 0.43              |
| 1:A:675:THR:OG1   | 1:A:736:ASN:ND2   | 2.52                     | 0.43              |
| 1:A:709:THR:HG23  | 9:I:94:ASP:HA     | 2.01                     | 0.43              |
| 1:A:713:SER:O     | 1:A:717:ASN:ND2   | 2.52                     | 0.43              |
| 1:A:846:GLU:OE1   | 1:A:1425:SER:OG   | 2.36                     | 0.43              |
| 1:A:868:TYR:CE1   | 1:A:1064:VAL:CG1  | 3.01                     | 0.43              |
| 1:A:1001:ARG:O    | 1:A:1002:GLY:O    | 2.36                     | 0.43              |
| 2:B:292:ILE:CG2   | 2:B:325:GLN:O     | 2.66                     | 0.43              |
| 2:B:641:GLU:O     | 2:B:643:ASP:N     | 2.51                     | 0.43              |
| 2:B:810:GLU:HB2   | 2:B:815:ARG:NH2   | 2.33                     | 0.43              |
| 2:B:840:ILE:CG2   | 2:B:994:TYR:HD1   | 2.31                     | 0.43              |
| 2:B:880:THR:HG21  | 2:B:934:LYS:HE3   | 2.00                     | 0.43              |
| 2:B:1060:ARG:C    | 2:B:1062:HIS:H    | 2.26                     | 0.43              |
| 2:B:1065:GLN:HE22 | 2:B:1067:ARG:HG2  | 1.81                     | 0.43              |
| 3:C:213:PRO:O     | 3:C:214:ASN:CB    | 2.66                     | 0.43              |
| 3:C:235:VAL:HG13  | 10:J:13:VAL:HG22  | 2.01                     | 0.43              |
| 3:C:239:PRO:O     | 3:C:242:GLN:N     | 2.51                     | 0.43              |
| 5:E:55:ARG:C      | 5:E:57:MET:H      | 2.26                     | 0.43              |
| 5:E:62:ALA:HB3    | 5:E:78:LEU:CD2    | 2.48                     | 0.43              |
| 7:G:28:THR:HG22   | 7:G:32:GLU:OE1    | 2.18                     | 0.43              |
| 8:H:4:THR:HG22    | 8:H:5:LEU:H       | 1.80                     | 0.43              |
| 10:J:53:HIS:CD2   | 10:J:53:HIS:C     | 2.97                     | 0.43              |
| 11:K:37:LYS:HA    | 11:K:37:LYS:HD3   | 1.92                     | 0.43              |
| 11:K:47:ARG:HD2   | 11:K:47:ARG:C     | 2.44                     | 0.43              |
| 11:K:55:LYS:HB2   | 11:K:81:TYR:CE1   | 2.54                     | 0.43              |
| 11:K:85:ASP:O     | 11:K:88:LYS:HB2   | 2.17                     | 0.43              |
| 1:A:79:GLY:H      | 2:B:1205:GLN:HE22 | 1.66                     | 0.43              |
| 1:A:476:SER:HB2   | 1:A:477:PRO:HD3   | 2.00                     | 0.43              |
| 1:A:767:GLN:HA    | 1:A:799:PHE:HA    | 2.00                     | 0.43              |
| 1:A:814:PHE:CD2   | 1:A:814:PHE:O     | 2.71                     | 0.43              |
| 1:A:962:ARG:C     | 1:A:964:ILE:H     | 2.27                     | 0.43              |
| 1:A:1278:ASN:O    | 1:A:1310:GLY:HA3  | 2.17                     | 0.43              |
| 2:B:365:THR:HG21  | 2:B:370:PHE:CD1   | 2.54                     | 0.43              |
| 2:B:487:THR:H     | 2:B:490:SER:HB3   | 1.84                     | 0.43              |
| 2:B:508:LEU:HD23  | 14:N:2:DC:OP1     | 2.19                     | 0.43              |
| 2:B:957:ASN:O     | 2:B:958:GLN:C     | 2.62                     | 0.43              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:B:1096:ARG:HH11 | 2:B:1096:ARG:CB  | 2.32                     | 0.43              |
| 5:E:17:ARG:CG     | 5:E:18:THR:N     | 2.82                     | 0.43              |
| 6:F:84:TYR:N      | 6:F:84:TYR:CD1   | 2.87                     | 0.43              |
| 6:F:97:ARG:HD2    | 6:F:97:ARG:HA    | 1.75                     | 0.43              |
| 11:K:13:GLY:O     | 11:K:16:GLU:HG3  | 2.18                     | 0.43              |
| 1:A:88:LYS:HG3    | 1:A:276:LEU:HD21 | 2.01                     | 0.43              |
| 1:A:204:THR:C     | 1:A:206:GLU:N    | 2.74                     | 0.43              |
| 1:A:504:LEU:HD13  | 6:F:91:ALA:HB2   | 1.99                     | 0.43              |
| 1:A:688:LYS:C     | 1:A:690:VAL:N    | 2.75                     | 0.43              |
| 1:A:740:LEU:C     | 1:A:740:LEU:HD12 | 2.44                     | 0.43              |
| 1:A:870:GLU:HG2   | 5:E:208:TYR:CD2  | 2.53                     | 0.43              |
| 1:A:1100:ARG:O    | 1:A:1100:ARG:HD2 | 2.19                     | 0.43              |
| 1:A:1147:THR:HB   | 9:I:48:LEU:CD1   | 2.47                     | 0.43              |
| 1:A:1154:TYR:CD2  | 1:A:1156:PRO:HD3 | 2.54                     | 0.43              |
| 1:A:1386:ARG:HB2  | 1:A:1403:GLU:CB  | 2.49                     | 0.43              |
| 2:B:282:ILE:HG21  | 2:B:382:ILE:CD1  | 2.48                     | 0.43              |
| 2:B:569:TYR:CE1   | 2:B:589:VAL:HG21 | 2.54                     | 0.43              |
| 2:B:798:TYR:CE2   | 3:C:62:PHE:CE2   | 3.03                     | 0.43              |
| 2:B:810:GLU:HB2   | 2:B:815:ARG:HH22 | 1.83                     | 0.43              |
| 2:B:842:ASN:HD22  | 2:B:845:SER:CB   | 2.30                     | 0.43              |
| 2:B:1131:GLY:N    | 2:B:1134:GLU:OE1 | 2.51                     | 0.43              |
| 3:C:11:ARG:H      | 3:C:20:PHE:HA    | 1.83                     | 0.43              |
| 3:C:39:ALA:HA     | 3:C:164:ALA:CB   | 2.49                     | 0.43              |
| 3:C:214:ASN:O     | 3:C:217:ASP:OD2  | 2.37                     | 0.43              |
| 3:C:264:GLN:O     | 3:C:267:GLN:HG2  | 2.19                     | 0.43              |
| 4:D:212:LYS:O     | 4:D:215:SER:OG   | 2.35                     | 0.43              |
| 5:E:55:ARG:N      | 5:E:84:ASP:OD1   | 2.51                     | 0.43              |
| 5:E:212:ARG:HG3   | 5:E:212:ARG:NH1  | 2.33                     | 0.43              |
| 8:H:43:ASN:C      | 8:H:45:GLU:H     | 2.27                     | 0.43              |
| 11:K:60:ALA:O     | 11:K:73:LEU:HD12 | 2.18                     | 0.43              |
| 1:A:13:THR:HB     | 1:A:1432:GLN:NE2 | 2.34                     | 0.43              |
| 1:A:125:ALA:C     | 1:A:127:ALA:N    | 2.77                     | 0.43              |
| 1:A:690:VAL:HG21  | 1:A:718:VAL:HG13 | 1.99                     | 0.43              |
| 1:A:897:TYR:N     | 1:A:897:TYR:CD1  | 2.87                     | 0.43              |
| 1:A:962:ARG:C     | 1:A:964:ILE:N    | 2.75                     | 0.43              |
| 1:A:1208:THR:O    | 1:A:1211:GLN:HB2 | 2.18                     | 0.43              |
| 1:A:1450:LEU:HD11 | 6:F:108:PHE:HZ   | 1.83                     | 0.43              |
| 2:B:290:GLY:O     | 2:B:292:ILE:HG13 | 2.19                     | 0.43              |
| 2:B:376:PHE:CB    | 2:B:566:LEU:HD21 | 2.49                     | 0.43              |
| 2:B:377:PHE:C     | 2:B:379:GLY:N    | 2.76                     | 0.43              |
| 2:B:486:TYR:HD1   | 2:B:775:LYS:O    | 2.01                     | 0.43              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:B:552:MET:HA    | 2:B:552:MET:CE   | 2.46                     | 0.43              |
| 3:C:16:ASP:C      | 3:C:240:VAL:HG11 | 2.43                     | 0.43              |
| 4:D:156:ASP:O     | 4:D:157:GLN:C    | 2.61                     | 0.43              |
| 4:D:216:ASN:O     | 4:D:218:GLU:N    | 2.52                     | 0.43              |
| 5:E:102:GLU:C     | 5:E:104:ASN:N    | 2.77                     | 0.43              |
| 5:E:117:THR:HB    | 5:E:120:ALA:H    | 1.84                     | 0.43              |
| 9:I:17:ARG:HG3    | 9:I:28:GLU:OE1   | 2.19                     | 0.43              |
| 12:L:53:HIS:HB3   | 12:L:55:ILE:HD11 | 1.95                     | 0.43              |
| 1:A:153:PRO:CB    | 1:A:161:LEU:HD22 | 2.47                     | 0.43              |
| 1:A:399:HIS:O     | 1:A:400:PRO:C    | 2.60                     | 0.43              |
| 1:A:444:PHE:CZ    | 1:A:487:MET:HE3  | 2.52                     | 0.43              |
| 1:A:471:ASN:O     | 1:A:474:VAL:HG12 | 2.19                     | 0.43              |
| 1:A:751:SER:O     | 1:A:752:LYS:HG2  | 2.19                     | 0.43              |
| 1:A:768:GLN:HG2   | 1:A:816:HIS:CA   | 2.39                     | 0.43              |
| 1:A:1100:ARG:HH21 | 1:A:1351:GLU:CG  | 2.32                     | 0.43              |
| 1:A:1148:ILE:HG12 | 9:I:49:ILE:HD12  | 2.01                     | 0.43              |
| 1:A:1154:TYR:CE2  | 1:A:1156:PRO:HD3 | 2.54                     | 0.43              |
| 1:A:1213:GLY:O    | 1:A:1214:GLU:C   | 2.62                     | 0.43              |
| 1:A:1215:ARG:O    | 1:A:1219:THR:N   | 2.50                     | 0.43              |
| 2:B:186:GLU:HG2   | 10:J:62:ARG:NH2  | 2.34                     | 0.43              |
| 2:B:299:GLU:OE2   | 2:B:571:PRO:CG   | 2.66                     | 0.43              |
| 2:B:432:MET:C     | 2:B:434:ARG:H    | 2.27                     | 0.43              |
| 2:B:555:ILE:HG22  | 2:B:556:THR:N    | 2.34                     | 0.43              |
| 3:C:69:LEU:O      | 10:J:6:ARG:HD2   | 2.19                     | 0.43              |
| 3:C:187:LYS:HG2   | 3:C:219:PHE:CE1  | 2.54                     | 0.43              |
| 3:C:226:ASP:O     | 3:C:227:THR:CB   | 2.66                     | 0.43              |
| 4:D:173:HIS:ND1   | 4:D:174:PRO:HD2  | 2.34                     | 0.43              |
| 8:H:13:SER:HB3    | 8:H:27:GLU:O     | 2.19                     | 0.43              |
| 1:A:414:ASP:OD1   | 1:A:416:ARG:CG   | 2.66                     | 0.42              |
| 1:A:963:ILE:HD13  | 1:A:1049:ILE:CG1 | 2.49                     | 0.42              |
| 1:A:1308:THR:HG23 | 1:A:1309:ASP:H   | 1.81                     | 0.42              |
| 2:B:129:PHE:CE2   | 2:B:166:PHE:CD1  | 3.07                     | 0.42              |
| 3:C:22:LEU:HD22   | 3:C:230:MET:HE1  | 2.01                     | 0.42              |
| 3:C:181:ASP:OD2   | 3:C:185:LYS:N    | 2.49                     | 0.42              |
| 3:C:196:ASP:CB    | 3:C:199:LYS:HD3  | 2.49                     | 0.42              |
| 4:D:35:LEU:HA     | 4:D:47:LEU:HB2   | 2.00                     | 0.42              |
| 7:G:99:PHE:HZ     | 7:G:163:ILE:HD13 | 1.85                     | 0.42              |
| 8:H:47:PHE:CD2    | 8:H:95:TYR:HD1   | 2.37                     | 0.42              |
| 8:H:142:LEU:C     | 8:H:143:LEU:HD12 | 2.43                     | 0.42              |
| 9:I:95:THR:HG22   | 9:I:96:SER:O     | 2.18                     | 0.42              |
| 1:A:2:VAL:CG1     | 2:B:1157:ALA:O   | 2.67                     | 0.42              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:565:ILE:HG23  | 1:A:567:LYS:HG2  | 2.00                     | 0.42              |
| 1:A:834:THR:CG2   | 1:A:835:GLY:N    | 2.81                     | 0.42              |
| 1:A:846:GLU:OE2   | 1:A:1398:MET:HE2 | 2.18                     | 0.42              |
| 1:A:996:ASN:C     | 1:A:998:LEU:HD12 | 2.44                     | 0.42              |
| 1:A:1227:ILE:HG22 | 1:A:1228:TRP:N   | 2.33                     | 0.42              |
| 1:A:1280:GLU:HB3  | 1:A:1281:ARG:H   | 1.64                     | 0.42              |
| 1:A:1342:GLU:HG3  | 5:E:198:ILE:HD13 | 2.00                     | 0.42              |
| 2:B:126:SER:CB    | 2:B:172:ILE:HD11 | 2.49                     | 0.42              |
| 2:B:269:ILE:HG21  | 2:B:282:ILE:HD13 | 2.01                     | 0.42              |
| 2:B:317:CYS:O     | 2:B:320:ASP:N    | 2.52                     | 0.42              |
| 2:B:953:LEU:HB2   | 12:L:57:LEU:HD23 | 2.00                     | 0.42              |
| 2:B:1152:MET:HE1  | 2:B:1157:ALA:HA  | 2.00                     | 0.42              |
| 3:C:177:GLU:CG    | 3:C:231:ASN:HD22 | 2.32                     | 0.42              |
| 5:E:35:VAL:C      | 5:E:37:LEU:H     | 2.26                     | 0.42              |
| 5:E:55:ARG:HG3    | 5:E:55:ARG:NH1   | 2.34                     | 0.42              |
| 5:E:135:PHE:CD2   | 5:E:140:LEU:HD21 | 2.50                     | 0.42              |
| 7:G:29:LYS:O      | 7:G:30:LEU:C     | 2.62                     | 0.42              |
| 9:I:69:PRO:HB2    | 9:I:85:PHE:CZ    | 2.54                     | 0.42              |
| 1:A:117:GLU:CD    | 1:A:117:GLU:N    | 2.77                     | 0.42              |
| 1:A:207:ILE:HG22  | 1:A:211:PHE:CD2  | 2.53                     | 0.42              |
| 1:A:419:LYS:HG3   | 1:A:420:ARG:HG3  | 2.01                     | 0.42              |
| 1:A:537:ARG:NH1   | 8:H:120:GLY:O    | 2.50                     | 0.42              |
| 1:A:648:ASN:O     | 1:A:649:ILE:C    | 2.61                     | 0.42              |
| 1:A:901:LEU:HB2   | 1:A:926:GLN:HG2  | 2.01                     | 0.42              |
| 1:A:1166:ASP:OD2  | 1:A:1239:ARG:HD2 | 2.19                     | 0.42              |
| 1:A:1268:LEU:CD1  | 9:I:48:LEU:HD11  | 2.49                     | 0.42              |
| 1:A:1289:ARG:HH12 | 1:A:1326:ARG:NH1 | 2.18                     | 0.42              |
| 1:A:1325:THR:OG1  | 5:E:146:HIS:O    | 2.37                     | 0.42              |
| 2:B:558:LEU:O     | 2:B:560:GLU:N    | 2.52                     | 0.42              |
| 2:B:570:VAL:HG21  | 2:B:573:GLN:NE2  | 2.34                     | 0.42              |
| 2:B:629:ASP:HB3   | 2:B:632:ARG:CD   | 2.49                     | 0.42              |
| 2:B:745:PRO:C     | 2:B:747:MET:N    | 2.76                     | 0.42              |
| 2:B:766:ARG:HD3   | 2:B:766:ARG:HA   | 1.78                     | 0.42              |
| 2:B:992:ILE:HD11  | 11:K:66:PRO:HB2  | 2.00                     | 0.42              |
| 3:C:7:GLN:NE2     | 11:K:104:ASN:ND2 | 2.55                     | 0.42              |
| 3:C:147:LEU:N     | 3:C:147:LEU:CD2  | 2.79                     | 0.42              |
| 3:C:174:ALA:O     | 3:C:175:ALA:HB3  | 2.18                     | 0.42              |
| 4:D:6:SER:OG      | 4:D:7:THR:N      | 2.52                     | 0.42              |
| 5:E:13:TRP:O      | 5:E:16:PHE:HB3   | 2.19                     | 0.42              |
| 5:E:78:LEU:HB2    | 5:E:107:THR:CG2  | 2.49                     | 0.42              |
| 5:E:99:HIS:C      | 5:E:99:HIS:HD1   | 2.27                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 6:F:97:ARG:NH2   | 6:F:108:PHE:CE1   | 2.87                     | 0.42              |
| 6:F:127:GLU:O    | 6:F:129:LYS:HG3   | 2.18                     | 0.42              |
| 1:A:65:LEU:HB2   | 1:A:71:GLN:NE2    | 2.34                     | 0.42              |
| 1:A:153:PRO:HB3  | 1:A:161:LEU:CD2   | 2.47                     | 0.42              |
| 1:A:279:LEU:C    | 1:A:289:ILE:HD11  | 2.43                     | 0.42              |
| 1:A:322:VAL:HG12 | 1:A:322:VAL:O     | 2.19                     | 0.42              |
| 1:A:567:LYS:HD3  | 8:H:95:TYR:CE2    | 2.54                     | 0.42              |
| 1:A:642:CYS:O    | 1:A:645:LEU:HB3   | 2.19                     | 0.42              |
| 1:A:674:PRO:C    | 1:A:676:MET:N     | 2.75                     | 0.42              |
| 1:A:817:ALA:O    | 1:A:818:MET:C     | 2.63                     | 0.42              |
| 1:A:878:ILE:HG22 | 1:A:879:GLU:N     | 2.34                     | 0.42              |
| 1:A:883:LEU:O    | 1:A:884:ASP:C     | 2.63                     | 0.42              |
| 1:A:1293:SER:HG  | 1:A:1295:THR:HG23 | 1.84                     | 0.42              |
| 2:B:44:VAL:HG21  | 2:B:199:MET:O     | 2.20                     | 0.42              |
| 2:B:174:LEU:HD22 | 2:B:202:TYR:CE1   | 2.54                     | 0.42              |
| 2:B:216:GLU:OE2  | 2:B:401:PHE:HE1   | 2.03                     | 0.42              |
| 2:B:431:TYR:CG   | 2:B:447:ALA:CB    | 3.02                     | 0.42              |
| 2:B:704:ALA:HB2  | 2:B:738:PHE:CE2   | 2.54                     | 0.42              |
| 2:B:863:GLU:OE1  | 2:B:962:LYS:HB2   | 2.19                     | 0.42              |
| 2:B:900:ALA:HB3  | 12:L:61:THR:OG1   | 2.19                     | 0.42              |
| 2:B:1161:HIS:NE2 | 2:B:1175:LEU:HD21 | 2.34                     | 0.42              |
| 4:D:35:LEU:H     | 4:D:35:LEU:CD1    | 2.31                     | 0.42              |
| 4:D:170:THR:HB   | 4:D:172:LEU:HG    | 2.01                     | 0.42              |
| 5:E:62:ALA:HB3   | 5:E:78:LEU:HD22   | 2.01                     | 0.42              |
| 5:E:157:SER:O    | 5:E:159:ASP:N     | 2.52                     | 0.42              |
| 8:H:15:VAL:HG22  | 8:H:26:ILE:HD12   | 2.01                     | 0.42              |
| 8:H:82:PRO:O     | 8:H:83:GLN:HB3    | 2.18                     | 0.42              |
| 11:K:52:ASN:O    | 11:K:54:ARG:N     | 2.53                     | 0.42              |
| 1:A:38:PRO:HA    | 1:A:270:LEU:HD23  | 2.00                     | 0.42              |
| 1:A:350:ARG:HB2  | 2:B:1128:LEU:CD1  | 2.49                     | 0.42              |
| 1:A:865:GLN:OE1  | 1:A:1370:LEU:HD23 | 2.20                     | 0.42              |
| 1:A:1030:ARG:NH1 | 1:A:1035:TYR:OH   | 2.52                     | 0.42              |
| 2:B:110:HIS:HB3  | 12:L:54:ARG:HH22  | 1.84                     | 0.42              |
| 2:B:447:ALA:O    | 2:B:449:ASN:N     | 2.52                     | 0.42              |
| 2:B:545:ILE:HG12 | 2:B:633:VAL:HG22  | 2.01                     | 0.42              |
| 2:B:644:GLU:HG3  | 2:B:646:LEU:C     | 2.44                     | 0.42              |
| 2:B:956:THR:HA   | 2:B:961:LEU:O     | 2.20                     | 0.42              |
| 2:B:986:GLN:NE2  | 2:B:1022:THR:HG21 | 2.34                     | 0.42              |
| 3:C:31:ASN:O     | 3:C:35:ARG:HG3    | 2.19                     | 0.42              |
| 3:C:175:ALA:HB2  | 10:J:10:CYS:HB2   | 2.00                     | 0.42              |
| 5:E:64:PRO:O     | 5:E:69:ILE:HD11   | 2.20                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 9:I:70:ARG:HA    | 9:I:83:ASN:O      | 2.20                     | 0.42              |
| 10:J:43:ARG:HD3  | 10:J:43:ARG:H     | 1.83                     | 0.42              |
| 10:J:56:LEU:O    | 10:J:57:ILE:C     | 2.63                     | 0.42              |
| 11:K:48:ALA:O    | 11:K:51:LEU:N     | 2.45                     | 0.42              |
| 12:L:53:HIS:C    | 12:L:55:ILE:HD13  | 2.44                     | 0.42              |
| 1:A:120:GLU:O    | 1:A:121:LEU:C     | 2.63                     | 0.42              |
| 1:A:614:PHE:HB3  | 8:H:122:LEU:HD21  | 2.01                     | 0.42              |
| 1:A:838:GLN:HG2  | 1:A:1073:GLY:HA3  | 2.01                     | 0.42              |
| 1:A:1029:ARG:CG  | 1:A:1029:ARG:NH1  | 2.81                     | 0.42              |
| 2:B:281:PRO:O    | 2:B:283:VAL:N     | 2.52                     | 0.42              |
| 2:B:601:ARG:HD3  | 2:B:605:ARG:CZ    | 2.49                     | 0.42              |
| 2:B:847:ASP:OD2  | 11:K:6:ARG:NH2    | 2.52                     | 0.42              |
| 2:B:912:ILE:O    | 2:B:938:SER:HA    | 2.20                     | 0.42              |
| 2:B:996:ARG:NH1  | 3:C:175:ALA:H     | 2.18                     | 0.42              |
| 2:B:1110:PRO:C   | 2:B:1119:VAL:HG13 | 2.44                     | 0.42              |
| 3:C:260:LEU:O    | 3:C:264:GLN:HG3   | 2.20                     | 0.42              |
| 4:D:8:PHE:HD2    | 7:G:6:ASP:O       | 2.02                     | 0.42              |
| 4:D:162:ALA:HA   | 4:D:165:GLN:NE2   | 2.26                     | 0.42              |
| 4:D:179:GLN:O    | 4:D:183:LEU:HB2   | 2.20                     | 0.42              |
| 8:H:24:CYS:CB    | 8:H:44:VAL:HG21   | 2.41                     | 0.42              |
| 9:I:76:PRO:HD3   | 9:I:110:PHE:CG    | 2.55                     | 0.42              |
| 9:I:88:SER:C     | 9:I:90:GLN:N      | 2.78                     | 0.42              |
| 11:K:13:GLY:O    | 11:K:14:GLU:C     | 2.62                     | 0.42              |
| 11:K:17:SER:O    | 11:K:18:LYS:C     | 2.63                     | 0.42              |
| 1:A:108:MET:O    | 1:A:109:HIS:CB    | 2.62                     | 0.42              |
| 1:A:125:ALA:O    | 1:A:127:ALA:N     | 2.53                     | 0.42              |
| 1:A:596:THR:C    | 1:A:597:LEU:HD12  | 2.44                     | 0.42              |
| 1:A:820:GLY:O    | 1:A:823:GLY:N     | 2.53                     | 0.42              |
| 1:A:1444:MET:O   | 6:F:133:VAL:N     | 2.50                     | 0.42              |
| 2:B:34:ILE:HG12  | 2:B:542:MET:CE    | 2.48                     | 0.42              |
| 2:B:189:LEU:O    | 2:B:190:TYR:C     | 2.61                     | 0.42              |
| 2:B:376:PHE:HB2  | 2:B:566:LEU:HD21  | 2.02                     | 0.42              |
| 4:D:12:ARG:NH1   | 4:D:14:ARG:N      | 2.68                     | 0.42              |
| 5:E:112:TYR:OH   | 5:E:136:ASN:HB2   | 2.19                     | 0.42              |
| 7:G:81:PRO:HG3   | 7:G:106:MET:SD    | 2.59                     | 0.42              |
| 12:L:47:ARG:NH2  | 12:L:54:ARG:HG2   | 2.34                     | 0.42              |
| 1:A:67:CYS:O     | 1:A:68:GLN:C      | 2.63                     | 0.42              |
| 1:A:441:PRO:HD2  | 1:A:498:ARG:NH2   | 2.35                     | 0.42              |
| 1:A:798:GLY:HA2  | 1:A:815:PHE:CD1   | 2.55                     | 0.42              |
| 1:A:912:LEU:HB2  | 1:A:913:LEU:H     | 1.72                     | 0.42              |
| 1:A:1166:ASP:OD2 | 1:A:1239:ARG:CD   | 2.68                     | 0.42              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:B:129:PHE:CE2   | 2:B:166:PHE:HD1  | 2.38                     | 0.42              |
| 2:B:191:LYS:HB3   | 2:B:191:LYS:HE2  | 1.85                     | 0.42              |
| 2:B:228:LYS:HD3   | 2:B:228:LYS:HA   | 1.87                     | 0.42              |
| 2:B:310:MET:HB2   | 2:B:310:MET:HE3  | 1.95                     | 0.42              |
| 2:B:535:LEU:HD23  | 2:B:535:LEU:HA   | 1.79                     | 0.42              |
| 2:B:558:LEU:O     | 2:B:561:TRP:N    | 2.53                     | 0.42              |
| 2:B:570:VAL:HA    | 2:B:571:PRO:HD2  | 1.86                     | 0.42              |
| 2:B:592:ASN:OD1   | 2:B:595:ARG:HG2  | 2.20                     | 0.42              |
| 2:B:1065:GLN:NE2  | 2:B:1067:ARG:N   | 2.45                     | 0.42              |
| 2:B:1183:LYS:HE3  | 2:B:1183:LYS:N   | 2.35                     | 0.42              |
| 2:B:1221:SER:O    | 2:B:1223:ASP:N   | 2.53                     | 0.42              |
| 3:C:132:PRO:O     | 3:C:134:ILE:HG13 | 2.20                     | 0.42              |
| 3:C:186:LEU:N     | 3:C:186:LEU:CD1  | 2.82                     | 0.42              |
| 5:E:149:LEU:O     | 5:E:151:PRO:HD3  | 2.19                     | 0.42              |
| 5:E:162:ARG:HH11  | 5:E:162:ARG:HG2  | 1.85                     | 0.42              |
| 5:E:164:LEU:CD2   | 5:E:211:TYR:CD2  | 3.02                     | 0.42              |
| 5:E:186:LEU:O     | 5:E:189:GLY:N    | 2.41                     | 0.42              |
| 5:E:204:THR:CG2   | 5:E:205:SER:H    | 2.30                     | 0.42              |
| 7:G:22:MET:O      | 7:G:23:LYS:C     | 2.63                     | 0.42              |
| 7:G:61:ILE:O      | 7:G:62:LEU:C     | 2.61                     | 0.42              |
| 10:J:53:HIS:NE2   | 10:J:55:ASP:HA   | 2.34                     | 0.42              |
| 11:K:82:ASP:OD1   | 11:K:82:ASP:C    | 2.63                     | 0.42              |
| 1:A:160:GLN:OE1   | 1:A:160:GLN:O    | 2.38                     | 0.42              |
| 1:A:298:PHE:HD2   | 1:A:299:HIS:CD2  | 2.38                     | 0.42              |
| 1:A:316:GLN:CG    | 1:A:317:LYS:N    | 2.80                     | 0.42              |
| 1:A:536:LEU:O     | 1:A:537:ARG:C    | 2.63                     | 0.42              |
| 1:A:548:ASN:HD21  | 11:K:47:ARG:NH2  | 2.18                     | 0.42              |
| 1:A:683:ILE:HG21  | 1:A:801:GLU:CD   | 2.44                     | 0.42              |
| 1:A:856:THR:HB    | 1:A:865:GLN:HB2  | 2.01                     | 0.42              |
| 1:A:973:ILE:CD1   | 1:A:1037:LEU:HA  | 2.45                     | 0.42              |
| 1:A:1135:ARG:NH2  | 1:A:1284:MET:HG3 | 2.34                     | 0.42              |
| 1:A:1141:THR:HG21 | 1:A:1205:LYS:HD3 | 1.99                     | 0.42              |
| 1:A:1341:ILE:CG2  | 1:A:1342:GLU:N   | 2.80                     | 0.42              |
| 2:B:448:ILE:H     | 2:B:448:ILE:HG13 | 1.66                     | 0.42              |
| 2:B:544:CYS:C     | 2:B:545:ILE:HG13 | 2.45                     | 0.42              |
| 2:B:864:LYS:HG3   | 2:B:872:GLU:OE1  | 2.19                     | 0.42              |
| 2:B:1004:GLU:OE2  | 2:B:1064:TYR:HE2 | 2.02                     | 0.42              |
| 2:B:1201:LYS:HE2  | 2:B:1205:GLN:NE2 | 2.33                     | 0.42              |
| 3:C:11:ARG:NH2    | 3:C:229:TYR:HB3  | 2.35                     | 0.42              |
| 4:D:51:ASN:O      | 4:D:52:LEU:C     | 2.63                     | 0.42              |
| 4:D:218:GLU:O     | 4:D:219:THR:O    | 2.38                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:E:207:ARG:NH1   | 5:E:207:ARG:CB    | 2.83                     | 0.42              |
| 5:E:213:ILE:HG12  | 5:E:214:CYS:N     | 2.35                     | 0.42              |
| 1:A:1193:LEU:HD12 | 1:A:1194:ARG:N    | 2.34                     | 0.42              |
| 1:A:1217:LYS:HA   | 1:A:1217:LYS:HE3  | 2.02                     | 0.42              |
| 1:A:1365:TYR:O    | 1:A:1366:ARG:C    | 2.62                     | 0.42              |
| 2:B:34:ILE:HD13   | 2:B:542:MET:HE2   | 2.01                     | 0.42              |
| 2:B:104:GLU:HG3   | 2:B:104:GLU:O     | 2.20                     | 0.42              |
| 2:B:231:PRO:O     | 2:B:231:PRO:HG2   | 2.20                     | 0.42              |
| 2:B:558:LEU:O     | 2:B:559:SER:C     | 2.62                     | 0.42              |
| 2:B:707:PRO:CG    | 2:B:708:GLU:N     | 2.82                     | 0.42              |
| 2:B:837:ASP:OD2   | 2:B:1020:ARG:NH2  | 2.53                     | 0.42              |
| 2:B:1079:LYS:CG   | 2:B:1080:LYS:N    | 2.83                     | 0.42              |
| 3:C:133:ILE:CD1   | 3:C:237:SER:N     | 2.82                     | 0.42              |
| 8:H:56:THR:O      | 8:H:144:ILE:HA    | 2.19                     | 0.42              |
| 1:A:254:GLU:HB3   | 1:A:255:SER:H     | 1.45                     | 0.41              |
| 1:A:316:GLN:O     | 1:A:317:LYS:C     | 2.63                     | 0.41              |
| 1:A:387:ARG:NH1   | 1:A:437:MET:HE1   | 2.35                     | 0.41              |
| 1:A:666:ILE:HD11  | 2:B:1086:PHE:CE1  | 2.54                     | 0.41              |
| 1:A:852:TYR:CE2   | 1:A:1060:PRO:HB2  | 2.56                     | 0.41              |
| 1:A:977:LYS:HB3   | 1:A:978:PRO:CD    | 2.48                     | 0.41              |
| 1:A:1109:LYS:O    | 1:A:1109:LYS:HD2  | 2.20                     | 0.41              |
| 1:A:1191:TRP:CD1  | 1:A:1256:GLU:HB2  | 2.55                     | 0.41              |
| 2:B:25:ILE:HG21   | 2:B:658:ILE:CD1   | 2.45                     | 0.41              |
| 2:B:277:LYS:HG2   | 2:B:336:ARG:HG2   | 2.01                     | 0.41              |
| 2:B:498:THR:CG2   | 2:B:537:LYS:HB2   | 2.50                     | 0.41              |
| 2:B:546:SER:OG    | 2:B:631:GLY:N     | 2.51                     | 0.41              |
| 2:B:610:ASN:HA    | 2:B:611:PRO:HD3   | 1.81                     | 0.41              |
| 2:B:899:ILE:HG22  | 2:B:900:ALA:O     | 2.20                     | 0.41              |
| 2:B:986:GLN:HE22  | 2:B:1022:THR:HG21 | 1.84                     | 0.41              |
| 2:B:1017:ILE:HD13 | 2:B:1017:ILE:HA   | 1.86                     | 0.41              |
| 3:C:221:TYR:C     | 3:C:223:ALA:N     | 2.76                     | 0.41              |
| 8:H:10:PHE:CD1    | 8:H:10:PHE:N      | 2.88                     | 0.41              |
| 9:I:8:ARG:O       | 9:I:9:ASP:C       | 2.63                     | 0.41              |
| 9:I:75:CYS:SG     | 9:I:78:CYS:SG     | 3.18                     | 0.41              |
| 1:A:84:ILE:HD13   | 1:A:270:LEU:HD13  | 1.99                     | 0.41              |
| 1:A:427:GLN:HB2   | 1:A:430:TRP:CD1   | 2.55                     | 0.41              |
| 1:A:463:ILE:HB    | 1:A:464:PRO:CD    | 2.48                     | 0.41              |
| 1:A:666:ILE:HD11  | 2:B:1086:PHE:HE1  | 1.85                     | 0.41              |
| 1:A:767:GLN:NE2   | 1:A:774:ARG:CB    | 2.75                     | 0.41              |
| 1:A:1019:CYS:O    | 1:A:1020:CYS:C    | 2.60                     | 0.41              |
| 1:A:1036:ARG:HG2  | 1:A:1036:ARG:NH1  | 2.35                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:37:PHE:C     | 2:B:37:PHE:CD1   | 2.97                     | 0.41              |
| 2:B:225:VAL:HA   | 2:B:237:VAL:O    | 2.20                     | 0.41              |
| 2:B:265:SER:O    | 2:B:266:ALA:HB3  | 2.20                     | 0.41              |
| 2:B:457:LEU:O    | 2:B:461:LEU:HD13 | 2.21                     | 0.41              |
| 2:B:500:THR:O    | 2:B:501:PRO:C    | 2.62                     | 0.41              |
| 3:C:11:ARG:O     | 3:C:12:GLU:C     | 2.63                     | 0.41              |
| 3:C:133:ILE:HD12 | 3:C:237:SER:CA   | 2.49                     | 0.41              |
| 3:C:203:GLN:CG   | 3:C:207:CYS:SG   | 3.06                     | 0.41              |
| 3:C:259:LEU:HD21 | 11:K:91:CYS:HB3  | 2.02                     | 0.41              |
| 4:D:130:LEU:C    | 4:D:132:GLN:N    | 2.78                     | 0.41              |
| 5:E:63:ASN:HB3   | 5:E:64:PRO:CD    | 2.50                     | 0.41              |
| 10:J:42:LYS:HD3  | 10:J:43:ARG:N    | 2.35                     | 0.41              |
| 12:L:32:ALA:HB3  | 12:L:33:GLU:OE2  | 2.20                     | 0.41              |
| 13:T:16:DT:H2''  | 13:T:17:DT:H5'   | 2.01                     | 0.41              |
| 1:A:77:CYS:C     | 1:A:78:PRO:O     | 2.60                     | 0.41              |
| 1:A:452:LYS:HB3  | 2:B:1141:HIS:CE1 | 2.55                     | 0.41              |
| 1:A:1140:HIS:N   | 1:A:1275:GLY:HA3 | 2.36                     | 0.41              |
| 1:A:1215:ARG:O   | 1:A:1216:ILE:C   | 2.62                     | 0.41              |
| 2:B:292:ILE:HG23 | 2:B:325:GLN:O    | 2.20                     | 0.41              |
| 2:B:830:TYR:CE2  | 2:B:1000:PRO:HD3 | 2.56                     | 0.41              |
| 2:B:835:GLN:HE21 | 2:B:835:GLN:HB2  | 1.52                     | 0.41              |
| 2:B:995:ARG:HB3  | 2:B:997:GLU:OE2  | 2.20                     | 0.41              |
| 3:C:133:ILE:CD1  | 3:C:237:SER:CA   | 2.95                     | 0.41              |
| 5:E:33:GLU:OE1   | 5:E:33:GLU:N     | 2.51                     | 0.41              |
| 7:G:9:LEU:HD23   | 7:G:30:LEU:HD12  | 2.02                     | 0.41              |
| 1:A:132:LYS:HZ2  | 1:A:1415:SER:CB  | 2.33                     | 0.41              |
| 1:A:150:THR:O    | 1:A:150:THR:HG22 | 2.21                     | 0.41              |
| 1:A:239:LEU:HD12 | 1:A:239:LEU:HA   | 1.65                     | 0.41              |
| 1:A:347:PHE:CE2  | 1:A:375:THR:HG22 | 2.56                     | 0.41              |
| 1:A:446:ARG:CD   | 1:A:480:ALA:HB2  | 2.50                     | 0.41              |
| 1:A:456:MET:HE1  | 1:A:474:VAL:HG22 | 2.03                     | 0.41              |
| 1:A:789:LYS:HD2  | 2:B:620:ARG:HH12 | 1.84                     | 0.41              |
| 1:A:1141:THR:HA  | 1:A:1205:LYS:HZ3 | 1.86                     | 0.41              |
| 1:A:1421:CYS:HA  | 1:A:1426:GLU:HG3 | 2.02                     | 0.41              |
| 2:B:36:ALA:O     | 2:B:39:ARG:HB2   | 2.21                     | 0.41              |
| 2:B:272:THR:HG23 | 2:B:279:ASP:OD1  | 2.20                     | 0.41              |
| 2:B:757:PRO:HG2  | 2:B:984:HIS:HE1  | 1.86                     | 0.41              |
| 2:B:831:SER:HB3  | 2:B:994:TYR:OH   | 2.20                     | 0.41              |
| 2:B:996:ARG:CZ   | 3:C:175:ALA:H    | 2.34                     | 0.41              |
| 2:B:1060:ARG:HA  | 2:B:1060:ARG:HD2 | 1.80                     | 0.41              |
| 3:C:36:VAL:CG2   | 3:C:251:LEU:HD13 | 2.48                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:D:27:LEU:HA     | 4:D:27:LEU:HD23   | 1.85                     | 0.41              |
| 4:D:204:ASP:O     | 4:D:208:GLU:HB2   | 2.20                     | 0.41              |
| 5:E:186:LEU:HD23  | 5:E:186:LEU:HA    | 1.76                     | 0.41              |
| 11:K:40:HIS:O     | 11:K:41:THR:C     | 2.63                     | 0.41              |
| 1:A:692:ASP:C     | 1:A:694:THR:N     | 2.77                     | 0.41              |
| 1:A:913:LEU:HD13  | 1:A:981:LEU:O     | 2.21                     | 0.41              |
| 1:A:1254:ALA:O    | 1:A:1255:GLU:CB   | 2.68                     | 0.41              |
| 2:B:23:ALA:O      | 2:B:24:PRO:O      | 2.39                     | 0.41              |
| 2:B:56:ASP:CB     | 2:B:57:TYR:HD1    | 2.26                     | 0.41              |
| 2:B:301:ILE:CG2   | 2:B:314:LEU:HD11  | 2.49                     | 0.41              |
| 2:B:515:HIS:CD2   | 2:B:517:THR:H     | 2.39                     | 0.41              |
| 2:B:1050:ILE:HG22 | 2:B:1051:THR:N    | 2.35                     | 0.41              |
| 4:D:126:ILE:HG21  | 4:D:145:MET:HB3   | 2.03                     | 0.41              |
| 5:E:96:PHE:O      | 5:E:99:HIS:HB3    | 2.21                     | 0.41              |
| 8:H:12:VAL:HG13   | 8:H:26:ILE:CG1    | 2.50                     | 0.41              |
| 10:J:27:GLU:O     | 10:J:29:GLU:N     | 2.53                     | 0.41              |
| 11:K:5:ASP:HB3    | 11:K:7:PHE:CE2    | 2.55                     | 0.41              |
| 13:T:25:DG:C2'    | 13:T:26:DT:H72    | 2.50                     | 0.41              |
| 1:A:91:PHE:HB2    | 1:A:297:GLN:OE1   | 2.21                     | 0.41              |
| 1:A:262:LEU:O     | 1:A:266:LEU:HG    | 2.21                     | 0.41              |
| 1:A:357:PRO:HD2   | 2:B:833:TYR:CZ    | 2.56                     | 0.41              |
| 1:A:380:VAL:HG22  | 1:A:426:LEU:HD13  | 2.02                     | 0.41              |
| 1:A:482:PHE:C     | 1:A:484:GLY:N     | 2.77                     | 0.41              |
| 1:A:710:LEU:HD22  | 9:I:96:SER:HA     | 2.03                     | 0.41              |
| 1:A:820:GLY:O     | 1:A:822:GLU:N     | 2.54                     | 0.41              |
| 1:A:868:TYR:CE1   | 1:A:1064:VAL:HG11 | 2.56                     | 0.41              |
| 1:A:886:ILE:CG2   | 1:A:952:ALA:HB2   | 2.50                     | 0.41              |
| 1:A:1341:ILE:HG23 | 1:A:1342:GLU:H    | 1.84                     | 0.41              |
| 1:A:1342:GLU:HG2  | 5:E:198:ILE:HD13  | 2.02                     | 0.41              |
| 2:B:134:LYS:NZ    | 2:B:164:LYS:NZ    | 2.68                     | 0.41              |
| 2:B:240:ILE:HG21  | 2:B:381:MET:HE1   | 2.03                     | 0.41              |
| 2:B:280:ILE:HD11  | 2:B:334:ILE:HG12  | 2.02                     | 0.41              |
| 2:B:621:GLU:HG3   | 2:B:621:GLU:O     | 2.20                     | 0.41              |
| 2:B:1045:SER:HB3  | 2:B:1046:PRO:HD2  | 2.03                     | 0.41              |
| 3:C:66:ARG:NH2    | 10:J:5:VAL:HG23   | 2.34                     | 0.41              |
| 3:C:136:ASP:OD2   | 3:C:137:LYS:N     | 2.53                     | 0.41              |
| 3:C:215:GLU:O     | 3:C:217:ASP:N     | 2.54                     | 0.41              |
| 4:D:135:GLY:C     | 4:D:137:ASN:H     | 2.28                     | 0.41              |
| 4:D:146:GLN:O     | 4:D:147:TYR:C     | 2.64                     | 0.41              |
| 5:E:13:TRP:CE3    | 5:E:39:LEU:HD13   | 2.55                     | 0.41              |
| 6:F:97:ARG:HG3    | 6:F:97:ARG:NH1    | 2.35                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 10:J:1:MET:H3    | 10:J:56:LEU:N    | 2.13                     | 0.41              |
| 12:L:47:ARG:HD3  | 12:L:52:GLY:HA2  | 2.02                     | 0.41              |
| 15:P:5:C:H2'     | 15:P:6:A:C8      | 2.56                     | 0.41              |
| 1:A:34:LYS:HG2   | 1:A:34:LYS:H     | 1.63                     | 0.41              |
| 1:A:51:GLY:HA2   | 1:A:56:PRO:HA    | 2.02                     | 0.41              |
| 1:A:180:LYS:NZ   | 1:A:294:SER:HB3  | 2.35                     | 0.41              |
| 1:A:562:THR:HA   | 1:A:563:PRO:HD3  | 1.85                     | 0.41              |
| 1:A:753:GLY:HA2  | 1:A:757:ASN:ND2  | 2.35                     | 0.41              |
| 1:A:899:VAL:HG22 | 1:A:908:LEU:HD21 | 2.02                     | 0.41              |
| 1:A:1385:THR:C   | 1:A:1387:HIS:N   | 2.79                     | 0.41              |
| 2:B:309:GLN:HG3  | 9:I:52:ILE:HD11  | 2.00                     | 0.41              |
| 2:B:418:LYS:CG   | 2:B:422:LYS:HE3  | 2.50                     | 0.41              |
| 2:B:619:ILE:O    | 2:B:620:ARG:C    | 2.63                     | 0.41              |
| 2:B:629:ASP:HB3  | 2:B:632:ARG:NE   | 2.36                     | 0.41              |
| 2:B:806:THR:N    | 2:B:809:MET:HE3  | 2.36                     | 0.41              |
| 2:B:1168:LEU:C   | 2:B:1170:THR:H   | 2.29                     | 0.41              |
| 3:C:259:LEU:CD2  | 11:K:91:CYS:HB3  | 2.51                     | 0.41              |
| 4:D:166:LEU:HD21 | 4:D:213:GLU:HB3  | 2.02                     | 0.41              |
| 10:J:30:LEU:HD22 | 10:J:34:THR:CG2  | 2.50                     | 0.41              |
| 1:A:120:GLU:C    | 1:A:122:MET:N    | 2.76                     | 0.41              |
| 1:A:344:ARG:HD3  | 2:B:1118:PRO:O   | 2.21                     | 0.41              |
| 1:A:573:SER:O    | 1:A:574:GLY:C    | 2.63                     | 0.41              |
| 1:A:650:GLN:O    | 1:A:654:ASN:HB2  | 2.21                     | 0.41              |
| 1:A:1161:THR:CG2 | 1:A:1162:VAL:N   | 2.84                     | 0.41              |
| 1:A:1171:GLN:H   | 1:A:1171:GLN:HG3 | 1.66                     | 0.41              |
| 1:A:1393:ASN:C   | 1:A:1394:THR:O   | 2.59                     | 0.41              |
| 2:B:27:ALA:O     | 2:B:29:ASP:N     | 2.54                     | 0.41              |
| 2:B:67:SER:HB3   | 2:B:92:PHE:HD1   | 1.84                     | 0.41              |
| 2:B:618:ASP:OD1  | 2:B:621:GLU:HB3  | 2.20                     | 0.41              |
| 2:B:773:MET:C    | 2:B:775:LYS:N    | 2.79                     | 0.41              |
| 3:C:164:ALA:HA   | 3:C:167:HIS:O    | 2.21                     | 0.41              |
| 4:D:32:GLU:HG3   | 7:G:5:LYS:HE2    | 2.03                     | 0.41              |
| 5:E:99:HIS:ND1   | 5:E:103:LYS:HG3  | 2.36                     | 0.41              |
| 7:G:92:VAL:HG21  | 7:G:102:GLN:HB2  | 2.03                     | 0.41              |
| 7:G:122:ASN:HB2  | 7:G:131:GLN:HE21 | 1.85                     | 0.41              |
| 9:I:56:ALA:O     | 9:I:57:GLY:O     | 2.39                     | 0.41              |
| 12:L:30:ILE:HD11 | 12:L:59:ALA:HB2  | 2.01                     | 0.41              |
| 1:A:331:GLY:C    | 1:A:332:LYS:O    | 2.63                     | 0.41              |
| 1:A:443:LEU:HD13 | 1:A:455:MET:HE2  | 2.03                     | 0.41              |
| 1:A:574:GLY:O    | 1:A:575:LYS:C    | 2.63                     | 0.41              |
| 1:A:665:GLY:C    | 1:A:667:GLY:N    | 2.78                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:907:THR:HG23  | 1:A:908:LEU:H     | 1.86                     | 0.41              |
| 1:A:982:THR:N     | 1:A:985:ASP:HB2   | 2.36                     | 0.41              |
| 1:A:1120:LEU:CD2  | 1:A:1125:ALA:HA   | 2.48                     | 0.41              |
| 1:A:1148:ILE:O    | 1:A:1148:ILE:HG22 | 2.21                     | 0.41              |
| 1:A:1381:LEU:HD23 | 1:A:1381:LEU:HA   | 1.92                     | 0.41              |
| 2:B:105:SER:O     | 2:B:106:ASP:CB    | 2.69                     | 0.41              |
| 2:B:129:PHE:CD2   | 2:B:166:PHE:HA    | 2.52                     | 0.41              |
| 2:B:185:THR:O     | 2:B:188:ASP:HB2   | 2.21                     | 0.41              |
| 2:B:220:GLY:O     | 2:B:221:ASN:C     | 2.64                     | 0.41              |
| 2:B:241:ARG:CZ    | 2:B:241:ARG:HB3   | 2.51                     | 0.41              |
| 2:B:408:LEU:N     | 2:B:408:LEU:CD1   | 2.84                     | 0.41              |
| 2:B:496:ARG:HH11  | 2:B:496:ARG:HB3   | 1.86                     | 0.41              |
| 2:B:710:LEU:C     | 2:B:711:GLU:HG2   | 2.45                     | 0.41              |
| 2:B:722:ASP:HB3   | 2:B:723:VAL:H     | 1.62                     | 0.41              |
| 2:B:763:GLN:O     | 2:B:764:SER:C     | 2.64                     | 0.41              |
| 2:B:809:MET:O     | 2:B:812:LEU:N     | 2.47                     | 0.41              |
| 2:B:906:SER:O     | 2:B:907:GLY:O     | 2.39                     | 0.41              |
| 2:B:976:ILE:HD13  | 2:B:992:ILE:HA    | 2.03                     | 0.41              |
| 2:B:1110:PRO:HB2  | 2:B:1119:VAL:HG11 | 2.03                     | 0.41              |
| 2:B:1125:ASP:O    | 2:B:1125:ASP:CG   | 2.64                     | 0.41              |
| 2:B:1159:ARG:HD3  | 2:B:1193:GLN:HB2  | 2.03                     | 0.41              |
| 2:B:1221:SER:C    | 2:B:1223:ASP:H    | 2.29                     | 0.41              |
| 3:C:43:THR:HG23   | 3:C:44:LEU:H      | 1.86                     | 0.41              |
| 3:C:58:LEU:HD12   | 3:C:145:CYS:HB2   | 2.01                     | 0.41              |
| 3:C:107:SER:C     | 3:C:109:SER:N     | 2.78                     | 0.41              |
| 3:C:179:GLU:HG2   | 3:C:180:TYR:H     | 1.86                     | 0.41              |
| 3:C:236:GLY:C     | 3:C:238:ILE:N     | 2.79                     | 0.41              |
| 4:D:24:ALA:HB1    | 4:D:25:ALA:H      | 1.72                     | 0.41              |
| 4:D:33:PHE:HE1    | 7:G:80:LYS:CD     | 2.33                     | 0.41              |
| 4:D:36:LYS:HE2    | 4:D:44:GLU:OE1    | 2.20                     | 0.41              |
| 4:D:126:ILE:CD1   | 4:D:145:MET:HE3   | 2.51                     | 0.41              |
| 4:D:138:ASN:C     | 4:D:140:ASP:N     | 2.78                     | 0.41              |
| 5:E:157:SER:O     | 5:E:158:SER:C     | 2.64                     | 0.41              |
| 5:E:164:LEU:HD22  | 5:E:211:TYR:CD2   | 2.56                     | 0.41              |
| 7:G:56:ILE:O      | 7:G:57:GLN:HB2    | 2.20                     | 0.41              |
| 8:H:35:GLN:HB3    | 8:H:111:LEU:HD21  | 2.03                     | 0.41              |
| 8:H:41:ASP:HB2    | 8:H:121:LEU:HB3   | 2.02                     | 0.41              |
| 8:H:91:ASP:C      | 8:H:93:TYR:H      | 2.29                     | 0.41              |
| 8:H:138:GLU:C     | 8:H:139:ASN:O     | 2.64                     | 0.41              |
| 9:I:65:ASP:HA     | 9:I:66:PRO:HD2    | 1.92                     | 0.41              |
| 10:J:48:ARG:HH21  | 10:J:49:MET:HE1   | 1.86                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:L:28:LYS:HB2   | 12:L:39:SER:HB2   | 2.03                     | 0.41              |
| 12:L:34:CYS:SG    | 12:L:51:CYS:SG    | 3.18                     | 0.41              |
| 1:A:202:LEU:HA    | 1:A:206:GLU:OE1   | 2.21                     | 0.41              |
| 1:A:443:LEU:HD23  | 1:A:443:LEU:HA    | 1.79                     | 0.41              |
| 1:A:688:LYS:CD    | 1:A:691:LEU:HD23  | 2.34                     | 0.41              |
| 1:A:720:ARG:O     | 1:A:724:GLU:CB    | 2.68                     | 0.41              |
| 1:A:1386:ARG:HD3  | 1:A:1403:GLU:HB3  | 2.03                     | 0.41              |
| 2:B:571:PRO:O     | 2:B:574:SER:O     | 2.39                     | 0.41              |
| 2:B:910:VAL:HG13  | 2:B:938:SER:HB3   | 2.01                     | 0.41              |
| 2:B:975:GLN:O     | 2:B:990:ILE:HD12  | 2.20                     | 0.41              |
| 2:B:1117:GLN:HE21 | 2:B:1199:ALA:HB2  | 1.85                     | 0.41              |
| 3:C:44:LEU:HD21   | 3:C:159:ALA:HB3   | 2.03                     | 0.41              |
| 3:C:239:PRO:O     | 3:C:241:ASP:N     | 2.54                     | 0.41              |
| 4:D:155:ARG:NH1   | 4:D:155:ARG:CB    | 2.84                     | 0.41              |
| 5:E:24:LYS:HB3    | 5:E:30:ILE:HB     | 2.03                     | 0.41              |
| 5:E:102:GLU:C     | 5:E:104:ASN:H     | 2.28                     | 0.41              |
| 5:E:161:LYS:HD2   | 5:E:195:VAL:HG23  | 2.02                     | 0.41              |
| 8:H:63:LEU:HD11   | 8:H:141:TYR:CD2   | 2.55                     | 0.41              |
| 13:T:25:DG:H2'    | 13:T:26:DT:H72    | 2.03                     | 0.41              |
| 1:A:132:LYS:HE3   | 1:A:1411:GLU:CG   | 2.51                     | 0.40              |
| 1:A:150:THR:HA    | 1:A:165:GLY:O     | 2.20                     | 0.40              |
| 1:A:295:LEU:O     | 1:A:298:PHE:HB3   | 2.21                     | 0.40              |
| 1:A:369:SER:CB    | 11:K:2:ASN:OD1    | 2.66                     | 0.40              |
| 1:A:531:ILE:HG13  | 1:A:653:VAL:HG21  | 2.03                     | 0.40              |
| 1:A:709:THR:HG22  | 1:A:711:ARG:H     | 1.86                     | 0.40              |
| 1:A:956:LEU:HD21  | 1:A:1017:LEU:HD23 | 2.03                     | 0.40              |
| 1:A:992:ASP:O     | 1:A:995:GLU:HB2   | 2.21                     | 0.40              |
| 1:A:1079:MET:HG2  | 1:A:1359:ASP:CG   | 2.47                     | 0.40              |
| 1:A:1362:TYR:CD1  | 1:A:1362:TYR:C    | 2.98                     | 0.40              |
| 1:A:1412:ALA:HA   | 1:A:1417:GLU:HG3  | 2.03                     | 0.40              |
| 1:A:1438:THR:HB   | 2:B:1144:ALA:CB   | 2.49                     | 0.40              |
| 2:B:69:LEU:HB3    | 2:B:429:PHE:CD1   | 2.56                     | 0.40              |
| 2:B:224:GLN:HA    | 2:B:396:ASP:OD2   | 2.21                     | 0.40              |
| 2:B:282:ILE:HG21  | 2:B:382:ILE:HD11  | 2.03                     | 0.40              |
| 2:B:331:LEU:CD2   | 2:B:353:LYS:HG2   | 2.51                     | 0.40              |
| 2:B:570:VAL:CG2   | 2:B:573:GLN:HB3   | 2.51                     | 0.40              |
| 2:B:660:LYS:HG2   | 2:B:679:TYR:CD2   | 2.56                     | 0.40              |
| 2:B:780:VAL:HG21  | 10:J:56:LEU:HD11  | 2.04                     | 0.40              |
| 2:B:860:MET:CG    | 2:B:861:ASP:N     | 2.84                     | 0.40              |
| 2:B:1177:HIS:HB2  | 2:B:1179:GLN:HE21 | 1.80                     | 0.40              |
| 3:C:260:LEU:O     | 3:C:263:THR:HB    | 2.21                     | 0.40              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 5:E:28:TYR:C      | 5:E:65:THR:CG2   | 2.95                     | 0.40              |
| 6:F:109:VAL:HG21  | 6:F:124:GLU:HA   | 2.02                     | 0.40              |
| 9:I:2:THR:O       | 9:I:2:THR:HG23   | 2.21                     | 0.40              |
| 9:I:77:LYS:C      | 9:I:79:HIS:H     | 2.28                     | 0.40              |
| 1:A:219:PHE:HE1   | 1:A:230:ARG:NE   | 2.18                     | 0.40              |
| 1:A:298:PHE:HD2   | 1:A:299:HIS:HD2  | 1.68                     | 0.40              |
| 1:A:997:LEU:HD13  | 1:A:1018:PHE:HE2 | 1.84                     | 0.40              |
| 1:A:1163:ILE:HG22 | 1:A:1165:GLU:HG2 | 2.04                     | 0.40              |
| 2:B:229:ALA:CB    | 2:B:231:PRO:HD2  | 2.50                     | 0.40              |
| 2:B:269:ILE:CG2   | 2:B:282:ILE:HD13 | 2.52                     | 0.40              |
| 2:B:357:GLN:HA    | 2:B:374:LYS:NZ   | 2.36                     | 0.40              |
| 2:B:642:ASP:C     | 2:B:644:GLU:H    | 2.25                     | 0.40              |
| 2:B:880:THR:HG22  | 2:B:934:LYS:HG3  | 2.03                     | 0.40              |
| 2:B:1081:LEU:C    | 2:B:1083:ALA:N   | 2.79                     | 0.40              |
| 3:C:82:TYR:O      | 3:C:83:SER:C     | 2.63                     | 0.40              |
| 3:C:249:ASP:O     | 3:C:250:THR:C    | 2.63                     | 0.40              |
| 6:F:130:ILE:O     | 6:F:148:VAL:HG22 | 2.21                     | 0.40              |
| 7:G:119:LEU:HD12  | 7:G:131:GLN:C    | 2.46                     | 0.40              |
| 8:H:58:THR:HB     | 8:H:143:LEU:HD13 | 2.03                     | 0.40              |
| 1:A:254:GLU:O     | 1:A:256:GLN:N    | 2.54                     | 0.40              |
| 1:A:347:PHE:HE2   | 1:A:375:THR:HG22 | 1.86                     | 0.40              |
| 1:A:798:GLY:HA2   | 1:A:815:PHE:HD1  | 1.86                     | 0.40              |
| 1:A:963:ILE:HD11  | 1:A:1048:ASN:C   | 2.46                     | 0.40              |
| 1:A:983:ILE:HG23  | 1:A:983:ILE:O    | 2.20                     | 0.40              |
| 1:A:1061:GLY:O    | 1:A:1062:GLU:C   | 2.64                     | 0.40              |
| 1:A:1446:ASP:C    | 1:A:1448:GLU:N   | 2.80                     | 0.40              |
| 2:B:113:TYR:O     | 2:B:114:PRO:C    | 2.65                     | 0.40              |
| 2:B:216:GLU:HA    | 2:B:406:LEU:HD23 | 2.03                     | 0.40              |
| 2:B:778:MET:HB2   | 2:B:1094:ARG:O   | 2.22                     | 0.40              |
| 2:B:861:ASP:OD1   | 2:B:914:LYS:HD2  | 2.22                     | 0.40              |
| 2:B:918:ILE:HD12  | 2:B:935:ARG:CZ   | 2.51                     | 0.40              |
| 2:B:970:THR:HG22  | 2:B:971:THR:N    | 2.36                     | 0.40              |
| 2:B:1159:ARG:HH11 | 2:B:1159:ARG:HB3 | 1.86                     | 0.40              |
| 3:C:77:ILE:HA     | 3:C:77:ILE:HD13  | 1.74                     | 0.40              |
| 4:D:53:SER:HA     | 4:D:56:ARG:HB3   | 2.04                     | 0.40              |
| 4:D:130:LEU:O     | 4:D:132:GLN:N    | 2.53                     | 0.40              |
| 4:D:167:LEU:HB3   | 4:D:177:VAL:HG13 | 2.03                     | 0.40              |
| 7:G:115:MET:HE1   | 7:G:130:TYR:CZ   | 2.56                     | 0.40              |
| 8:H:99:GLY:HA3    | 8:H:118:PHE:CD2  | 2.57                     | 0.40              |
| 11:K:94:ILE:O     | 11:K:98:LEU:HG   | 2.22                     | 0.40              |
| 12:L:38:LEU:O     | 12:L:39:SER:CB   | 2.69                     | 0.40              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:6:TYR:CG     | 1:A:7:SER:N       | 2.88                     | 0.40              |
| 1:A:50:ILE:C     | 1:A:52:GLY:N      | 2.72                     | 0.40              |
| 1:A:262:LEU:HD23 | 1:A:262:LEU:HA    | 1.89                     | 0.40              |
| 1:A:380:VAL:HG12 | 1:A:428:TYR:HA    | 2.03                     | 0.40              |
| 1:A:855:THR:CG2  | 1:A:857:ARG:HG3   | 2.39                     | 0.40              |
| 1:A:1169:ILE:H   | 1:A:1169:ILE:HG13 | 1.66                     | 0.40              |
| 2:B:114:PRO:O    | 2:B:115:GLN:C     | 2.64                     | 0.40              |
| 2:B:300:HIS:O    | 2:B:303:TYR:CE2   | 2.73                     | 0.40              |
| 2:B:304:ASP:OD1  | 2:B:306:ASN:N     | 2.36                     | 0.40              |
| 3:C:7:GLN:NE2    | 11:K:104:ASN:HD21 | 2.18                     | 0.40              |
| 4:D:155:ARG:HH11 | 4:D:155:ARG:CB    | 2.35                     | 0.40              |
| 4:D:156:ASP:C    | 4:D:158:GLU:N     | 2.79                     | 0.40              |
| 5:E:28:TYR:HE1   | 5:E:78:LEU:HD13   | 1.84                     | 0.40              |
| 5:E:55:ARG:HD2   | 5:E:113:GLN:HE21  | 1.86                     | 0.40              |
| 5:E:92:THR:O     | 5:E:95:THR:HB     | 2.21                     | 0.40              |
| 6:F:82:THR:HA    | 6:F:83:PRO:HD3    | 1.84                     | 0.40              |
| 6:F:100:GLN:HA   | 6:F:103:MET:HG3   | 2.03                     | 0.40              |
| 7:G:111:THR:O    | 7:G:112:LYS:C     | 2.65                     | 0.40              |
| 8:H:100:THR:CG2  | 8:H:101:ALA:N     | 2.84                     | 0.40              |
| 14:N:4:DA:N3     | 14:N:5:DC:C5      | 2.89                     | 0.40              |
| 1:A:279:LEU:HB3  | 1:A:289:ILE:HG13  | 2.04                     | 0.40              |
| 1:A:760:GLN:OE1  | 2:B:1021:MET:HE1  | 2.22                     | 0.40              |
| 1:A:1111:MET:HE3 | 1:A:1111:MET:HB2  | 1.81                     | 0.40              |
| 1:A:1148:ILE:CG1 | 1:A:1198:ASP:HB2  | 2.51                     | 0.40              |
| 2:B:311:LEU:O    | 2:B:314:LEU:N     | 2.54                     | 0.40              |
| 2:B:530:GLY:C    | 2:B:531:GLN:OE1   | 2.65                     | 0.40              |
| 2:B:557:PHE:O    | 2:B:557:PHE:HD2   | 2.04                     | 0.40              |
| 2:B:737:THR:HG21 | 9:I:70:ARG:HH21   | 1.86                     | 0.40              |
| 2:B:809:MET:HA   | 2:B:812:LEU:HD12  | 2.02                     | 0.40              |
| 2:B:990:ILE:HG22 | 2:B:991:GLY:N     | 2.36                     | 0.40              |
| 2:B:1074:ASN:HB2 | 2:B:1081:LEU:HD21 | 2.04                     | 0.40              |
| 2:B:1116:ARG:HG3 | 2:B:1198:TYR:CE2  | 2.56                     | 0.40              |
| 5:E:30:ILE:HG22  | 5:E:31:THR:O      | 2.22                     | 0.40              |
| 6:F:106:PRO:HG2  | 7:G:18:PHE:C      | 2.47                     | 0.40              |
| 10:J:31:ASP:OD1  | 10:J:34:THR:HB    | 2.21                     | 0.40              |
| 11:K:102:LYS:O   | 11:K:106:GLU:HG3  | 2.20                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|-----------|----------|-------------|----|
| 1   | A     | 1406/1733 (81%) | 1062 (76%) | 240 (17%) | 104 (7%) | 1           | 9  |
| 2   | B     | 1082/1224 (88%) | 795 (74%)  | 188 (17%) | 99 (9%)  | 0           | 7  |
| 3   | C     | 264/318 (83%)   | 200 (76%)  | 45 (17%)  | 19 (7%)  | 1           | 9  |
| 4   | D     | 174/221 (79%)   | 131 (75%)  | 29 (17%)  | 14 (8%)  | 1           | 8  |
| 5   | E     | 212/215 (99%)   | 159 (75%)  | 40 (19%)  | 13 (6%)  | 1           | 12 |
| 6   | F     | 85/155 (55%)    | 72 (85%)   | 12 (14%)  | 1 (1%)   | 10          | 41 |
| 7   | G     | 169/171 (99%)   | 143 (85%)  | 20 (12%)  | 6 (4%)   | 2           | 22 |
| 8   | H     | 130/146 (89%)   | 86 (66%)   | 23 (18%)  | 21 (16%) | 0           | 2  |
| 9   | I     | 117/122 (96%)   | 76 (65%)   | 31 (26%)  | 10 (8%)  | 0           | 7  |
| 10  | J     | 63/70 (90%)     | 44 (70%)   | 10 (16%)  | 9 (14%)  | 0           | 3  |
| 11  | K     | 112/120 (93%)   | 90 (80%)   | 19 (17%)  | 3 (3%)   | 4           | 27 |
| 12  | L     | 44/70 (63%)     | 18 (41%)   | 16 (36%)  | 10 (23%) | 0           | 1  |
| All | All   | 3858/4565 (84%) | 2876 (74%) | 673 (17%) | 309 (8%) | 1           | 8  |

All (309) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 4   | GLN  |
| 1   | A     | 43  | GLU  |
| 1   | A     | 54  | ASN  |
| 1   | A     | 57  | ARG  |
| 1   | A     | 58  | LEU  |
| 1   | A     | 62  | ASP  |
| 1   | A     | 63  | ARG  |
| 1   | A     | 67  | CYS  |
| 1   | A     | 70  | CYS  |
| 1   | A     | 130 | ASP  |
| 1   | A     | 167 | CYS  |
| 1   | A     | 250 | ILE  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 255  | SER  |
| 1   | A     | 257  | ARG  |
| 1   | A     | 286  | HIS  |
| 1   | A     | 318  | SER  |
| 1   | A     | 332  | LYS  |
| 1   | A     | 399  | HIS  |
| 1   | A     | 410  | GLY  |
| 1   | A     | 567  | LYS  |
| 1   | A     | 597  | LEU  |
| 1   | A     | 1002 | GLY  |
| 1   | A     | 1112 | LYS  |
| 1   | A     | 1114 | PRO  |
| 1   | A     | 1120 | LEU  |
| 1   | A     | 1122 | PRO  |
| 1   | A     | 1124 | HIS  |
| 1   | A     | 1223 | ASP  |
| 1   | A     | 1233 | ASP  |
| 1   | A     | 1242 | VAL  |
| 1   | A     | 1255 | GLU  |
| 1   | A     | 1281 | ARG  |
| 1   | A     | 1403 | GLU  |
| 1   | A     | 1405 | THR  |
| 1   | A     | 1438 | THR  |
| 2   | B     | 21   | GLU  |
| 2   | B     | 58   | THR  |
| 2   | B     | 67   | SER  |
| 2   | B     | 68   | THR  |
| 2   | B     | 108  | VAL  |
| 2   | B     | 186  | GLU  |
| 2   | B     | 258  | LEU  |
| 2   | B     | 259  | TYR  |
| 2   | B     | 294  | ASP  |
| 2   | B     | 295  | GLY  |
| 2   | B     | 334  | ILE  |
| 2   | B     | 365  | THR  |
| 2   | B     | 367  | LEU  |
| 2   | B     | 391  | ASP  |
| 2   | B     | 435  | THR  |
| 2   | B     | 509  | ALA  |
| 2   | B     | 642  | ASP  |
| 2   | B     | 643  | ASP  |
| 2   | B     | 708  | GLU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 709  | ASP  |
| 2   | B     | 728  | ARG  |
| 2   | B     | 731  | VAL  |
| 2   | B     | 879  | ARG  |
| 2   | B     | 907  | GLY  |
| 2   | B     | 958  | GLN  |
| 2   | B     | 1046 | PRO  |
| 2   | B     | 1069 | PHE  |
| 2   | B     | 1155 | SER  |
| 2   | B     | 1156 | ASP  |
| 2   | B     | 1175 | LEU  |
| 3   | C     | 110  | THR  |
| 3   | C     | 141  | GLY  |
| 3   | C     | 149  | LYS  |
| 3   | C     | 184  | ASN  |
| 3   | C     | 209  | TYR  |
| 3   | C     | 215  | GLU  |
| 3   | C     | 216  | GLY  |
| 4   | D     | 5    | THR  |
| 4   | D     | 8    | PHE  |
| 4   | D     | 17   | LYS  |
| 4   | D     | 19   | GLU  |
| 4   | D     | 52   | LEU  |
| 4   | D     | 119  | ARG  |
| 4   | D     | 218  | GLU  |
| 5   | E     | 45   | LYS  |
| 5   | E     | 106  | GLN  |
| 5   | E     | 115  | ASN  |
| 5   | E     | 129  | PRO  |
| 7   | G     | 139  | ILE  |
| 8   | H     | 82   | PRO  |
| 8   | H     | 107  | VAL  |
| 8   | H     | 128  | ASN  |
| 8   | H     | 140  | ALA  |
| 9   | I     | 11   | ASN  |
| 9   | I     | 62   | ILE  |
| 9   | I     | 78   | CYS  |
| 10  | J     | 2    | ILE  |
| 10  | J     | 6    | ARG  |
| 10  | J     | 55   | ASP  |
| 10  | J     | 64   | ASN  |
| 12  | L     | 50   | ASP  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 12  | L     | 53   | HIS  |
| 12  | L     | 59   | ALA  |
| 12  | L     | 60   | ARG  |
| 1   | A     | 41   | MET  |
| 1   | A     | 42   | ASP  |
| 1   | A     | 76   | GLU  |
| 1   | A     | 93   | VAL  |
| 1   | A     | 128  | ILE  |
| 1   | A     | 138  | ILE  |
| 1   | A     | 253  | ASN  |
| 1   | A     | 311  | GLN  |
| 1   | A     | 312  | PRO  |
| 1   | A     | 322  | VAL  |
| 1   | A     | 331  | GLY  |
| 1   | A     | 423  | ASP  |
| 1   | A     | 424  | ILE  |
| 1   | A     | 517  | ASN  |
| 1   | A     | 556  | TRP  |
| 1   | A     | 846  | GLU  |
| 1   | A     | 958  | VAL  |
| 1   | A     | 1123 | GLY  |
| 1   | A     | 1139 | GLU  |
| 1   | A     | 1169 | ILE  |
| 1   | A     | 1221 | LYS  |
| 1   | A     | 1308 | THR  |
| 1   | A     | 1309 | ASP  |
| 1   | A     | 1314 | SER  |
| 1   | A     | 1448 | GLU  |
| 2   | B     | 24   | PRO  |
| 2   | B     | 28   | GLU  |
| 2   | B     | 65   | GLU  |
| 2   | B     | 124  | TYR  |
| 2   | B     | 206  | ASN  |
| 2   | B     | 257  | LYS  |
| 2   | B     | 291  | ILE  |
| 2   | B     | 369  | GLY  |
| 2   | B     | 448  | ILE  |
| 2   | B     | 449  | ASN  |
| 2   | B     | 450  | ALA  |
| 2   | B     | 467  | GLY  |
| 2   | B     | 468  | GLU  |
| 2   | B     | 531  | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 591  | ARG  |
| 2   | B     | 641  | GLU  |
| 2   | B     | 734  | HIS  |
| 2   | B     | 751  | VAL  |
| 2   | B     | 848  | ARG  |
| 2   | B     | 992  | ILE  |
| 2   | B     | 1097 | HIS  |
| 2   | B     | 1103 | ILE  |
| 2   | B     | 1167 | GLY  |
| 2   | B     | 1171 | VAL  |
| 2   | B     | 1176 | ASN  |
| 2   | B     | 1181 | GLU  |
| 2   | B     | 1222 | ARG  |
| 3   | C     | 90   | ASP  |
| 3   | C     | 126  | GLY  |
| 4   | D     | 14   | ARG  |
| 4   | D     | 198  | LEU  |
| 4   | D     | 219  | THR  |
| 5   | E     | 74   | ASP  |
| 5   | E     | 130  | ALA  |
| 8   | H     | 17   | PRO  |
| 8   | H     | 32   | THR  |
| 8   | H     | 59   | ILE  |
| 8   | H     | 62   | SER  |
| 8   | H     | 77   | ARG  |
| 8   | H     | 108  | SER  |
| 8   | H     | 134  | ASN  |
| 9   | I     | 57   | GLY  |
| 9   | I     | 79   | HIS  |
| 9   | I     | 106  | CYS  |
| 10  | J     | 28   | ASP  |
| 11  | K     | 53   | ASP  |
| 12  | L     | 27   | LEU  |
| 12  | L     | 28   | LYS  |
| 12  | L     | 35   | SER  |
| 12  | L     | 54   | ARG  |
| 1   | A     | 48   | ALA  |
| 1   | A     | 65   | LEU  |
| 1   | A     | 69   | THR  |
| 1   | A     | 126  | LEU  |
| 1   | A     | 169  | ASN  |
| 1   | A     | 314  | ALA  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 317  | LYS  |
| 1   | A     | 400  | PRO  |
| 1   | A     | 453  | MET  |
| 1   | A     | 543  | LEU  |
| 1   | A     | 628  | GLY  |
| 1   | A     | 755  | PHE  |
| 1   | A     | 821  | ARG  |
| 1   | A     | 852  | TYR  |
| 1   | A     | 884  | ASP  |
| 1   | A     | 1140 | HIS  |
| 1   | A     | 1206 | ASP  |
| 1   | A     | 1270 | ASN  |
| 1   | A     | 1447 | GLU  |
| 2   | B     | 43   | LEU  |
| 2   | B     | 45   | SER  |
| 2   | B     | 245  | GLU  |
| 2   | B     | 266  | ALA  |
| 2   | B     | 282  | ILE  |
| 2   | B     | 466  | TRP  |
| 2   | B     | 655  | LYS  |
| 2   | B     | 705  | MET  |
| 2   | B     | 711  | GLU  |
| 2   | B     | 746  | SER  |
| 2   | B     | 792  | MET  |
| 2   | B     | 810  | GLU  |
| 2   | B     | 906  | SER  |
| 2   | B     | 1075 | GLY  |
| 2   | B     | 1108 | ARG  |
| 2   | B     | 1157 | ALA  |
| 3   | C     | 132  | PRO  |
| 3   | C     | 213  | PRO  |
| 3   | C     | 237  | SER  |
| 4   | D     | 16   | LYS  |
| 4   | D     | 30   | GLY  |
| 4   | D     | 53   | SER  |
| 5   | E     | 36   | GLU  |
| 5   | E     | 95   | THR  |
| 6   | F     | 128  | LYS  |
| 7   | G     | 112  | LYS  |
| 7   | G     | 154  | VAL  |
| 8   | H     | 90   | ALA  |
| 8   | H     | 92   | ASP  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 8   | H     | 95   | TYR  |
| 8   | H     | 139  | ASN  |
| 9   | I     | 8    | ARG  |
| 9   | I     | 9    | ASP  |
| 10  | J     | 17   | LYS  |
| 10  | J     | 24   | LEU  |
| 10  | J     | 29   | GLU  |
| 1   | A     | 5    | GLN  |
| 1   | A     | 59   | GLY  |
| 1   | A     | 61   | ILE  |
| 1   | A     | 154  | SER  |
| 1   | A     | 256  | GLN  |
| 1   | A     | 415  | LEU  |
| 1   | A     | 591  | PHE  |
| 1   | A     | 604  | GLY  |
| 1   | A     | 1168 | GLU  |
| 1   | A     | 1316 | VAL  |
| 1   | A     | 1390 | ASN  |
| 2   | B     | 27   | ALA  |
| 2   | B     | 249  | ARG  |
| 2   | B     | 264  | SER  |
| 2   | B     | 323  | VAL  |
| 2   | B     | 559  | SER  |
| 2   | B     | 575  | PRO  |
| 2   | B     | 594  | ALA  |
| 2   | B     | 636  | PRO  |
| 2   | B     | 738  | PHE  |
| 2   | B     | 1017 | ILE  |
| 2   | B     | 1035 | ALA  |
| 2   | B     | 1223 | ASP  |
| 3   | C     | 142  | VAL  |
| 3   | C     | 214  | ASN  |
| 5   | E     | 44   | ALA  |
| 5   | E     | 154  | ILE  |
| 5   | E     | 192  | ARG  |
| 7   | G     | 63   | PRO  |
| 9   | I     | 54   | GLU  |
| 11  | K     | 14   | GLU  |
| 12  | L     | 26   | THR  |
| 12  | L     | 55   | ILE  |
| 1   | A     | 35   | ILE  |
| 1   | A     | 66   | LYS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 219  | PHE  |
| 1   | A     | 308  | ILE  |
| 1   | A     | 871  | ASP  |
| 1   | A     | 885  | THR  |
| 2   | B     | 114  | PRO  |
| 2   | B     | 433  | GLN  |
| 2   | B     | 667  | GLN  |
| 2   | B     | 869  | SER  |
| 3   | C     | 208  | GLU  |
| 3   | C     | 240  | VAL  |
| 4   | D     | 131  | GLU  |
| 5   | E     | 51   | GLY  |
| 8   | H     | 12   | VAL  |
| 8   | H     | 47   | PHE  |
| 10  | J     | 14   | VAL  |
| 1   | A     | 598  | LEU  |
| 1   | A     | 780  | VAL  |
| 1   | A     | 1280 | GLU  |
| 1   | A     | 1297 | GLU  |
| 2   | B     | 56   | ASP  |
| 2   | B     | 115  | GLN  |
| 2   | B     | 260  | GLY  |
| 2   | B     | 1214 | PRO  |
| 5   | E     | 73   | PRO  |
| 8   | H     | 21   | ASN  |
| 8   | H     | 44   | VAL  |
| 8   | H     | 81   | PRO  |
| 8   | H     | 83   | GLN  |
| 11  | K     | 107  | THR  |
| 1   | A     | 283  | GLY  |
| 1   | A     | 963  | ILE  |
| 2   | B     | 729  | ILE  |
| 7   | G     | 136  | VAL  |
| 1   | A     | 284  | ALA  |
| 2   | B     | 25   | ILE  |
| 2   | B     | 619  | ILE  |
| 2   | B     | 764  | SER  |
| 3   | C     | 172  | PRO  |
| 9   | I     | 59   | VAL  |
| 2   | B     | 55   | VAL  |
| 3   | C     | 182  | PRO  |
| 1   | A     | 1388 | GLY  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 501 | PRO  |
| 3   | C     | 217 | ASP  |
| 7   | G     | 20  | 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     | 1239/1520 (82%) | 1089 (88%) | 150 (12%) | 5           | 22 |
| 2   | B     | 958/1061 (90%)  | 841 (88%)  | 117 (12%) | 5           | 22 |
| 3   | C     | 234/274 (85%)   | 202 (86%)  | 32 (14%)  | 3           | 19 |
| 4   | D     | 160/200 (80%)   | 133 (83%)  | 27 (17%)  | 2           | 13 |
| 5   | E     | 196/197 (100%)  | 184 (94%)  | 12 (6%)   | 17          | 43 |
| 6   | F     | 77/137 (56%)    | 67 (87%)   | 10 (13%)  | 4           | 21 |
| 7   | G     | 152/152 (100%)  | 135 (89%)  | 17 (11%)  | 6           | 25 |
| 8   | H     | 118/128 (92%)   | 106 (90%)  | 12 (10%)  | 7           | 28 |
| 9   | I     | 113/116 (97%)   | 106 (94%)  | 7 (6%)    | 16          | 43 |
| 10  | J     | 60/65 (92%)     | 54 (90%)   | 6 (10%)   | 7           | 28 |
| 11  | K     | 99/102 (97%)    | 88 (89%)   | 11 (11%)  | 6           | 25 |
| 12  | L     | 40/57 (70%)     | 35 (88%)   | 5 (12%)   | 4           | 22 |
| All | All   | 3446/4009 (86%) | 3040 (88%) | 406 (12%) | 5           | 23 |

All (406) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 11  | LEU  |
| 1   | A     | 18  | GLN  |
| 1   | A     | 32  | VAL  |
| 1   | A     | 34  | LYS  |
| 1   | A     | 36  | ARG  |
| 1   | A     | 37  | PHE  |
| 1   | A     | 41  | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 68  | GLN  |
| 1   | A     | 70  | CYS  |
| 1   | A     | 93  | VAL  |
| 1   | A     | 121 | LEU  |
| 1   | A     | 141 | LEU  |
| 1   | A     | 145 | LYS  |
| 1   | A     | 160 | GLN  |
| 1   | A     | 161 | LEU  |
| 1   | A     | 173 | THR  |
| 1   | A     | 185 | TRP  |
| 1   | A     | 200 | ARG  |
| 1   | A     | 207 | ILE  |
| 1   | A     | 208 | LEU  |
| 1   | A     | 221 | SER  |
| 1   | A     | 244 | PRO  |
| 1   | A     | 245 | PRO  |
| 1   | A     | 249 | SER  |
| 1   | A     | 265 | LYS  |
| 1   | A     | 289 | ILE  |
| 1   | A     | 297 | GLN  |
| 1   | A     | 302 | THR  |
| 1   | A     | 315 | LEU  |
| 1   | A     | 320 | ARG  |
| 1   | A     | 322 | VAL  |
| 1   | A     | 324 | SER  |
| 1   | A     | 329 | LEU  |
| 1   | A     | 337 | ARG  |
| 1   | A     | 344 | ARG  |
| 1   | A     | 353 | ILE  |
| 1   | A     | 369 | SER  |
| 1   | A     | 381 | THR  |
| 1   | A     | 385 | ILE  |
| 1   | A     | 394 | ASN  |
| 1   | A     | 408 | ASP  |
| 1   | A     | 425 | GLN  |
| 1   | A     | 443 | LEU  |
| 1   | A     | 445 | ASN  |
| 1   | A     | 449 | SER  |
| 1   | A     | 451 | HIS  |
| 1   | A     | 461 | LYS  |
| 1   | A     | 469 | ARG  |
| 1   | A     | 470 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 475 | THR  |
| 1   | A     | 479 | ASN  |
| 1   | A     | 481 | ASP  |
| 1   | A     | 493 | GLN  |
| 1   | A     | 504 | LEU  |
| 1   | A     | 505 | CYS  |
| 1   | A     | 512 | VAL  |
| 1   | A     | 524 | VAL  |
| 1   | A     | 562 | THR  |
| 1   | A     | 565 | ILE  |
| 1   | A     | 596 | THR  |
| 1   | A     | 597 | LEU  |
| 1   | A     | 618 | GLU  |
| 1   | A     | 635 | ARG  |
| 1   | A     | 666 | ILE  |
| 1   | A     | 670 | ILE  |
| 1   | A     | 672 | ASP  |
| 1   | A     | 685 | GLU  |
| 1   | A     | 690 | VAL  |
| 1   | A     | 691 | LEU  |
| 1   | A     | 701 | LEU  |
| 1   | A     | 710 | LEU  |
| 1   | A     | 737 | LEU  |
| 1   | A     | 738 | LYS  |
| 1   | A     | 758 | ILE  |
| 1   | A     | 768 | GLN  |
| 1   | A     | 774 | ARG  |
| 1   | A     | 788 | SER  |
| 1   | A     | 805 | LEU  |
| 1   | A     | 810 | PRO  |
| 1   | A     | 821 | ARG  |
| 1   | A     | 827 | THR  |
| 1   | A     | 833 | GLU  |
| 1   | A     | 834 | THR  |
| 1   | A     | 838 | GLN  |
| 1   | A     | 849 | MET  |
| 1   | A     | 855 | THR  |
| 1   | A     | 858 | ASN  |
| 1   | A     | 867 | ILE  |
| 1   | A     | 882 | SER  |
| 1   | A     | 907 | THR  |
| 1   | A     | 920 | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 929  | LEU  |
| 1   | A     | 934  | LYS  |
| 1   | A     | 937  | VAL  |
| 1   | A     | 941  | LYS  |
| 1   | A     | 961  | ARG  |
| 1   | A     | 976  | THR  |
| 1   | A     | 978  | PRO  |
| 1   | A     | 982  | THR  |
| 1   | A     | 983  | ILE  |
| 1   | A     | 987  | VAL  |
| 1   | A     | 993  | LEU  |
| 1   | A     | 1005 | GLU  |
| 1   | A     | 1029 | ARG  |
| 1   | A     | 1033 | GLN  |
| 1   | A     | 1060 | PRO  |
| 1   | A     | 1067 | LEU  |
| 1   | A     | 1095 | THR  |
| 1   | A     | 1110 | ASN  |
| 1   | A     | 1114 | PRO  |
| 1   | A     | 1116 | LEU  |
| 1   | A     | 1120 | LEU  |
| 1   | A     | 1122 | PRO  |
| 1   | A     | 1124 | HIS  |
| 1   | A     | 1129 | GLU  |
| 1   | A     | 1145 | SER  |
| 1   | A     | 1160 | SER  |
| 1   | A     | 1165 | GLU  |
| 1   | A     | 1170 | ILE  |
| 1   | A     | 1171 | GLN  |
| 1   | A     | 1193 | LEU  |
| 1   | A     | 1206 | ASP  |
| 1   | A     | 1217 | LYS  |
| 1   | A     | 1255 | GLU  |
| 1   | A     | 1257 | ASP  |
| 1   | A     | 1264 | GLU  |
| 1   | A     | 1265 | ASN  |
| 1   | A     | 1276 | VAL  |
| 1   | A     | 1280 | GLU  |
| 1   | A     | 1288 | ASP  |
| 1   | A     | 1295 | THR  |
| 1   | A     | 1297 | GLU  |
| 1   | A     | 1299 | VAL  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1325 | THR  |
| 1   | A     | 1349 | TYR  |
| 1   | A     | 1353 | TYR  |
| 1   | A     | 1355 | VAL  |
| 1   | A     | 1365 | TYR  |
| 1   | A     | 1370 | LEU  |
| 1   | A     | 1383 | SER  |
| 1   | A     | 1385 | THR  |
| 1   | A     | 1393 | ASN  |
| 1   | A     | 1394 | THR  |
| 1   | A     | 1410 | PHE  |
| 1   | A     | 1424 | VAL  |
| 1   | A     | 1426 | GLU  |
| 1   | A     | 1442 | ASP  |
| 1   | A     | 1444 | MET  |
| 1   | A     | 1445 | ILE  |
| 1   | A     | 1451 | VAL  |
| 2   | B     | 20   | ASP  |
| 2   | B     | 25   | ILE  |
| 2   | B     | 46   | GLN  |
| 2   | B     | 57   | TYR  |
| 2   | B     | 63   | ILE  |
| 2   | B     | 98   | THR  |
| 2   | B     | 128  | LEU  |
| 2   | B     | 194  | GLU  |
| 2   | B     | 203  | PHE  |
| 2   | B     | 218  | SER  |
| 2   | B     | 225  | VAL  |
| 2   | B     | 241  | ARG  |
| 2   | B     | 249  | ARG  |
| 2   | B     | 261  | ARG  |
| 2   | B     | 267  | ARG  |
| 2   | B     | 272  | THR  |
| 2   | B     | 294  | ASP  |
| 2   | B     | 298  | LEU  |
| 2   | B     | 299  | GLU  |
| 2   | B     | 303  | TYR  |
| 2   | B     | 323  | VAL  |
| 2   | B     | 325  | GLN  |
| 2   | B     | 334  | ILE  |
| 2   | B     | 336  | ARG  |
| 2   | B     | 364  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 368 | GLU  |
| 2   | B     | 371 | GLU  |
| 2   | B     | 393 | LYS  |
| 2   | B     | 396 | ASP  |
| 2   | B     | 401 | PHE  |
| 2   | B     | 425 | THR  |
| 2   | B     | 429 | PHE  |
| 2   | B     | 430 | ARG  |
| 2   | B     | 446 | LEU  |
| 2   | B     | 452 | THR  |
| 2   | B     | 455 | SER  |
| 2   | B     | 465 | ASN  |
| 2   | B     | 466 | TRP  |
| 2   | B     | 475 | SER  |
| 2   | B     | 485 | ARG  |
| 2   | B     | 493 | SER  |
| 2   | B     | 498 | THR  |
| 2   | B     | 502 | ILE  |
| 2   | B     | 516 | ASN  |
| 2   | B     | 552 | MET  |
| 2   | B     | 555 | ILE  |
| 2   | B     | 570 | VAL  |
| 2   | B     | 582 | VAL  |
| 2   | B     | 603 | LEU  |
| 2   | B     | 609 | ILE  |
| 2   | B     | 615 | MET  |
| 2   | B     | 616 | ILE  |
| 2   | B     | 620 | ARG  |
| 2   | B     | 635 | ARG  |
| 2   | B     | 636 | PRO  |
| 2   | B     | 645 | SER  |
| 2   | B     | 648 | HIS  |
| 2   | B     | 682 | SER  |
| 2   | B     | 694 | ASP  |
| 2   | B     | 705 | MET  |
| 2   | B     | 714 | GLU  |
| 2   | B     | 737 | THR  |
| 2   | B     | 743 | ILE  |
| 2   | B     | 748 | ILE  |
| 2   | B     | 780 | VAL  |
| 2   | B     | 786 | ASN  |
| 2   | B     | 790 | ASP  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 805  | THR  |
| 2   | B     | 807  | ARG  |
| 2   | B     | 811  | TYR  |
| 2   | B     | 816  | GLU  |
| 2   | B     | 835  | GLN  |
| 2   | B     | 837  | ASP  |
| 2   | B     | 839  | MET  |
| 2   | B     | 857  | ARG  |
| 2   | B     | 865  | LYS  |
| 2   | B     | 868  | MET  |
| 2   | B     | 878  | GLN  |
| 2   | B     | 887  | HIS  |
| 2   | B     | 889  | THR  |
| 2   | B     | 895  | ASP  |
| 2   | B     | 915  | THR  |
| 2   | B     | 933  | SER  |
| 2   | B     | 944  | THR  |
| 2   | B     | 946  | ASN  |
| 2   | B     | 953  | LEU  |
| 2   | B     | 955  | THR  |
| 2   | B     | 956  | THR  |
| 2   | B     | 957  | ASN  |
| 2   | B     | 959  | ASP  |
| 2   | B     | 969  | ARG  |
| 2   | B     | 997  | GLU  |
| 2   | B     | 1006 | ILE  |
| 2   | B     | 1007 | VAL  |
| 2   | B     | 1017 | ILE  |
| 2   | B     | 1046 | PRO  |
| 2   | B     | 1047 | PHE  |
| 2   | B     | 1049 | ASP  |
| 2   | B     | 1053 | GLU  |
| 2   | B     | 1077 | THR  |
| 2   | B     | 1084 | GLN  |
| 2   | B     | 1095 | LEU  |
| 2   | B     | 1096 | ARG  |
| 2   | B     | 1103 | ILE  |
| 2   | B     | 1112 | GLN  |
| 2   | B     | 1147 | LEU  |
| 2   | B     | 1150 | ARG  |
| 2   | B     | 1151 | LEU  |
| 2   | B     | 1159 | ARG  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 1160 | VAL  |
| 2   | B     | 1169 | MET  |
| 2   | B     | 1172 | ILE  |
| 2   | B     | 1175 | LEU  |
| 2   | B     | 1178 | ASN  |
| 2   | B     | 1183 | LYS  |
| 2   | B     | 1185 | CYS  |
| 2   | B     | 1202 | LEU  |
| 3   | C     | 3    | GLU  |
| 3   | C     | 22   | LEU  |
| 3   | C     | 25   | VAL  |
| 3   | C     | 26   | ASP  |
| 3   | C     | 43   | THR  |
| 3   | C     | 55   | THR  |
| 3   | C     | 56   | THR  |
| 3   | C     | 57   | VAL  |
| 3   | C     | 77   | ILE  |
| 3   | C     | 78   | GLU  |
| 3   | C     | 91   | HIS  |
| 3   | C     | 99   | LEU  |
| 3   | C     | 100  | THR  |
| 3   | C     | 101  | LEU  |
| 3   | C     | 106  | GLU  |
| 3   | C     | 115  | SER  |
| 3   | C     | 124  | LEU  |
| 3   | C     | 129  | ILE  |
| 3   | C     | 138  | GLU  |
| 3   | C     | 145  | CYS  |
| 3   | C     | 147  | LEU  |
| 3   | C     | 151  | GLN  |
| 3   | C     | 156  | THR  |
| 3   | C     | 158  | VAL  |
| 3   | C     | 166  | GLU  |
| 3   | C     | 177  | GLU  |
| 3   | C     | 186  | LEU  |
| 3   | C     | 232  | VAL  |
| 3   | C     | 238  | ILE  |
| 3   | C     | 240  | VAL  |
| 3   | C     | 259  | LEU  |
| 3   | C     | 266  | ASP  |
| 4   | D     | 4    | SER  |
| 4   | D     | 11   | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | D     | 12  | ARG  |
| 4   | D     | 14  | ARG  |
| 4   | D     | 17  | LYS  |
| 4   | D     | 18  | VAL  |
| 4   | D     | 22  | GLU  |
| 4   | D     | 26  | THR  |
| 4   | D     | 29  | LEU  |
| 4   | D     | 34  | GLN  |
| 4   | D     | 38  | ILE  |
| 4   | D     | 40  | HIS  |
| 4   | D     | 47  | LEU  |
| 4   | D     | 65  | GLU  |
| 4   | D     | 120 | GLU  |
| 4   | D     | 124 | GLU  |
| 4   | D     | 125 | SER  |
| 4   | D     | 126 | ILE  |
| 4   | D     | 128 | VAL  |
| 4   | D     | 169 | SER  |
| 4   | D     | 187 | THR  |
| 4   | D     | 200 | ASN  |
| 4   | D     | 206 | GLU  |
| 4   | D     | 207 | LEU  |
| 4   | D     | 213 | GLU  |
| 4   | D     | 219 | THR  |
| 4   | D     | 221 | TYR  |
| 5   | E     | 9   | ILE  |
| 5   | E     | 37  | LEU  |
| 5   | E     | 72  | PHE  |
| 5   | E     | 78  | LEU  |
| 5   | E     | 83  | CYS  |
| 5   | E     | 99  | HIS  |
| 5   | E     | 115 | ASN  |
| 5   | E     | 123 | LEU  |
| 5   | E     | 131 | THR  |
| 5   | E     | 140 | LEU  |
| 5   | E     | 150 | VAL  |
| 5   | E     | 202 | SER  |
| 6   | F     | 79  | ARG  |
| 6   | F     | 82  | THR  |
| 6   | F     | 90  | ARG  |
| 6   | F     | 93  | ILE  |
| 6   | F     | 103 | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | F     | 111 | LEU  |
| 6   | F     | 112 | GLU  |
| 6   | F     | 116 | ASP  |
| 6   | F     | 119 | ARG  |
| 6   | F     | 153 | VAL  |
| 7   | G     | 1   | MET  |
| 7   | G     | 8   | SER  |
| 7   | G     | 12  | THR  |
| 7   | G     | 13  | LEU  |
| 7   | G     | 21  | ARG  |
| 7   | G     | 24  | GLN  |
| 7   | G     | 53  | ASN  |
| 7   | G     | 74  | TYR  |
| 7   | G     | 77  | VAL  |
| 7   | G     | 93  | SER  |
| 7   | G     | 113 | HIS  |
| 7   | G     | 114 | LEU  |
| 7   | G     | 120 | THR  |
| 7   | G     | 134 | GLU  |
| 7   | G     | 151 | ILE  |
| 7   | G     | 165 | GLU  |
| 7   | G     | 171 | ILE  |
| 8   | H     | 2   | SER  |
| 8   | H     | 10  | PHE  |
| 8   | H     | 33  | GLN  |
| 8   | H     | 53  | ASP  |
| 8   | H     | 61  | SER  |
| 8   | H     | 64  | ASN  |
| 8   | H     | 89  | LEU  |
| 8   | H     | 95  | TYR  |
| 8   | H     | 129 | TYR  |
| 8   | H     | 130 | ARG  |
| 8   | H     | 138 | GLU  |
| 8   | H     | 143 | LEU  |
| 9   | I     | 7   | CYS  |
| 9   | I     | 8   | ARG  |
| 9   | I     | 15  | TYR  |
| 9   | I     | 59  | VAL  |
| 9   | I     | 86  | PHE  |
| 9   | I     | 93  | LYS  |
| 9   | I     | 94  | ASP  |
| 10  | J     | 2   | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | J     | 13  | VAL  |
| 10  | J     | 22  | LEU  |
| 10  | J     | 23  | ASN  |
| 10  | J     | 43  | ARG  |
| 10  | J     | 44  | TYR  |
| 11  | K     | 12  | LEU  |
| 11  | K     | 25  | THR  |
| 11  | K     | 42  | LEU  |
| 11  | K     | 47  | ARG  |
| 11  | K     | 70  | ARG  |
| 11  | K     | 76  | GLN  |
| 11  | K     | 78  | THR  |
| 11  | K     | 101 | LEU  |
| 11  | K     | 107 | THR  |
| 11  | K     | 111 | LEU  |
| 11  | K     | 114 | LEU  |
| 12  | L     | 27  | LEU  |
| 12  | L     | 28  | LYS  |
| 12  | L     | 55  | ILE  |
| 12  | L     | 65  | VAL  |
| 12  | L     | 68  | GLU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (131) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 18  | GLN  |
| 1   | A     | 54  | ASN  |
| 1   | A     | 71  | GLN  |
| 1   | A     | 75  | ASN  |
| 1   | A     | 160 | GLN  |
| 1   | A     | 169 | ASN  |
| 1   | A     | 171 | GLN  |
| 1   | A     | 225 | ASN  |
| 1   | A     | 253 | ASN  |
| 1   | A     | 256 | GLN  |
| 1   | A     | 282 | ASN  |
| 1   | A     | 299 | HIS  |
| 1   | A     | 313 | GLN  |
| 1   | A     | 316 | GLN  |
| 1   | A     | 339 | ASN  |
| 1   | A     | 394 | ASN  |
| 1   | A     | 435 | HIS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 447  | GLN  |
| 1   | A     | 451  | HIS  |
| 1   | A     | 479  | ASN  |
| 1   | A     | 490  | HIS  |
| 1   | A     | 493  | GLN  |
| 1   | A     | 503  | GLN  |
| 1   | A     | 515  | GLN  |
| 1   | A     | 517  | ASN  |
| 1   | A     | 545  | GLN  |
| 1   | A     | 548  | ASN  |
| 1   | A     | 603  | ASN  |
| 1   | A     | 611  | GLN  |
| 1   | A     | 640  | GLN  |
| 1   | A     | 650  | GLN  |
| 1   | A     | 698  | GLN  |
| 1   | A     | 741  | ASN  |
| 1   | A     | 745  | GLN  |
| 1   | A     | 757  | ASN  |
| 1   | A     | 786  | HIS  |
| 1   | A     | 802  | ASN  |
| 1   | A     | 854  | ASN  |
| 1   | A     | 858  | ASN  |
| 1   | A     | 877  | HIS  |
| 1   | A     | 903  | ASN  |
| 1   | A     | 926  | GLN  |
| 1   | A     | 969  | GLN  |
| 1   | A     | 975  | HIS  |
| 1   | A     | 1048 | ASN  |
| 1   | A     | 1110 | ASN  |
| 1   | A     | 1187 | GLN  |
| 1   | A     | 1188 | GLN  |
| 1   | A     | 1203 | ASN  |
| 1   | A     | 1312 | ASN  |
| 1   | A     | 1354 | ASN  |
| 1   | A     | 1393 | ASN  |
| 1   | A     | 1432 | GLN  |
| 2   | B     | 178  | ASN  |
| 2   | B     | 236  | HIS  |
| 2   | B     | 366  | GLN  |
| 2   | B     | 433  | GLN  |
| 2   | B     | 465  | ASN  |
| 2   | B     | 484  | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 513  | GLN  |
| 2   | B     | 515  | HIS  |
| 2   | B     | 516  | ASN  |
| 2   | B     | 518  | HIS  |
| 2   | B     | 587  | HIS  |
| 2   | B     | 657  | HIS  |
| 2   | B     | 686  | ASN  |
| 2   | B     | 744  | HIS  |
| 2   | B     | 786  | ASN  |
| 2   | B     | 835  | GLN  |
| 2   | B     | 842  | ASN  |
| 2   | B     | 862  | GLN  |
| 2   | B     | 887  | HIS  |
| 2   | B     | 951  | GLN  |
| 2   | B     | 957  | ASN  |
| 2   | B     | 975  | GLN  |
| 2   | B     | 986  | GLN  |
| 2   | B     | 1062 | HIS  |
| 2   | B     | 1065 | GLN  |
| 2   | B     | 1076 | HIS  |
| 2   | B     | 1084 | GLN  |
| 2   | B     | 1161 | HIS  |
| 2   | B     | 1179 | GLN  |
| 2   | B     | 1193 | GLN  |
| 2   | B     | 1205 | GLN  |
| 2   | B     | 1211 | ASN  |
| 3   | C     | 7    | GLN  |
| 3   | C     | 17   | ASN  |
| 3   | C     | 65   | HIS  |
| 3   | C     | 73   | GLN  |
| 3   | C     | 79   | GLN  |
| 3   | C     | 91   | HIS  |
| 3   | C     | 102  | GLN  |
| 3   | C     | 112  | ASN  |
| 3   | C     | 123  | ASN  |
| 3   | C     | 131  | HIS  |
| 3   | C     | 135  | GLN  |
| 3   | C     | 151  | GLN  |
| 3   | C     | 195  | GLN  |
| 3   | C     | 231  | ASN  |
| 4   | D     | 37   | GLN  |
| 4   | D     | 39   | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | D     | 40  | HIS  |
| 4   | D     | 138 | ASN  |
| 4   | D     | 165 | GLN  |
| 5   | E     | 3   | GLN  |
| 5   | E     | 54  | GLN  |
| 5   | E     | 104 | ASN  |
| 5   | E     | 113 | GLN  |
| 5   | E     | 143 | ASN  |
| 5   | E     | 147 | HIS  |
| 6   | F     | 100 | GLN  |
| 7   | G     | 14  | HIS  |
| 7   | G     | 53  | ASN  |
| 7   | G     | 102 | GLN  |
| 7   | G     | 122 | ASN  |
| 7   | G     | 126 | ASN  |
| 7   | G     | 131 | GLN  |
| 7   | G     | 158 | HIS  |
| 8   | H     | 83  | GLN  |
| 8   | H     | 128 | ASN  |
| 8   | H     | 131 | ASN  |
| 8   | H     | 133 | ASN  |
| 8   | H     | 137 | GLN  |
| 9   | I     | 12  | ASN  |
| 9   | I     | 79  | HIS  |
| 9   | I     | 90  | GLN  |
| 9   | I     | 108 | HIS  |
| 9   | I     | 114 | GLN  |
| 10  | J     | 64  | ASN  |
| 11  | K     | 44  | ASN  |
| 11  | K     | 76  | GLN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed   | Backbone Outliers | Pucker Outliers |
|-----|-------|------------|-------------------|-----------------|
| 15  | P     | 9/17 (52%) | 0                 | 0               |

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

| Mol | Type | Chain | Res | Link  | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|-------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |       | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 13  | BRU  | T     | 23  | 13,15 | 18,21,22     | 3.92 | 1 (5%)      | 25,30,33    | 0.94 | 1 (4%)      |

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

| Mol | Type | Chain | Res | Link  | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|-------|---------|-----------|---------|
| 13  | BRU  | T     | 23  | 13,15 | -       | 1/7/21/22 | 0/2/2/2 |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 13  | T     | 23  | BRU  | BR-C5 | -16.56 | 1.50        | 1.88     |

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 13  | T     | 23  | BRU  | C6-C5-C4 | -2.83 | 117.80      | 120.67   |

There are no chirality outliers.

All (1) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 13  | T     | 23  | BRU  | O4'-C4'-C5'-O5' |

There are no ring outliers.

1 monomer is involved in 3 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 13  | T     | 23  | BRU  | 3       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 9 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 [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 1   | A     | 1416/1733 (81%) | 0.05   | 37 (2%) 57 33  | 28, 72, 115, 145      | 0     |
| 2   | B     | 1104/1224 (90%) | 0.33   | 57 (5%) 33 19  | 28, 85, 126, 140      | 0     |
| 3   | C     | 266/318 (83%)   | -0.03  | 1 (0%) 88 72   | 41, 71, 107, 125      | 0     |
| 4   | D     | 178/221 (80%)   | 0.35   | 8 (4%) 38 20   | 52, 84, 120, 134      | 0     |
| 5   | E     | 214/215 (99%)   | 0.42   | 4 (1%) 66 41   | 52, 103, 130, 138     | 0     |
| 6   | F     | 87/155 (56%)    | -0.32  | 2 (2%) 61 37   | 32, 51, 81, 91        | 0     |
| 7   | G     | 171/171 (100%)  | 0.00   | 2 (1%) 76 52   | 48, 71, 104, 117      | 0     |
| 8   | H     | 134/146 (91%)   | 0.74   | 9 (6%) 24 15   | 79, 109, 127, 138     | 0     |
| 9   | I     | 119/122 (97%)   | 0.68   | 8 (6%) 24 15   | 66, 106, 126, 144     | 0     |
| 10  | J     | 65/70 (92%)     | -0.09  | 0 100 100      | 49, 68, 95, 107       | 0     |
| 11  | K     | 114/120 (95%)   | -0.18  | 1 (0%) 81 58   | 36, 76, 95, 112       | 0     |
| 12  | L     | 46/70 (65%)     | 1.02   | 6 (13%) 7 6    | 48, 111, 129, 130     | 0     |
| 13  | T     | 16/26 (61%)     | 1.66   | 6 (37%) 1 1    | 99, 137, 166, 166     | 0     |
| 14  | N     | 5/13 (38%)      | 2.40   | 3 (60%) 0 0    | 143, 147, 156, 171    | 0     |
| 15  | P     | 10/17 (58%)     | 2.37   | 6 (60%) 0 0    | 122, 129, 147, 153    | 0     |
| All | All   | 3945/4621 (85%) | 0.21   | 150 (3%) 44 24 | 28, 80, 124, 171      | 0     |

All (150) RSRZ outliers are listed below:

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | A     | 1081 | LEU  | 5.4  |
| 15  | P     | 1    | C    | 5.2  |
| 2   | B     | 446  | LEU  | 4.8  |
| 1   | A     | 3    | GLY  | 4.7  |
| 2   | B     | 509  | ALA  | 4.6  |
| 1   | A     | 2    | VAL  | 4.6  |
| 2   | B     | 70   | ILE  | 4.6  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 14  | N     | 1    | DA   | 4.5  |
| 1   | A     | 1254 | ALA  | 4.2  |
| 1   | A     | 69   | THR  | 4.1  |
| 9   | I     | 120  | GLN  | 4.0  |
| 4   | D     | 24   | ALA  | 3.9  |
| 11  | K     | 114  | LEU  | 3.9  |
| 1   | A     | 1455 | PRO  | 3.6  |
| 9   | I     | 117  | LYS  | 3.6  |
| 2   | B     | 250  | PHE  | 3.5  |
| 2   | B     | 733  | HIS  | 3.5  |
| 15  | P     | 9    | C    | 3.4  |
| 15  | P     | 10   | A    | 3.4  |
| 1   | A     | 1080 | THR  | 3.4  |
| 1   | A     | 51   | GLY  | 3.4  |
| 2   | B     | 710  | LEU  | 3.3  |
| 4   | D     | 3    | VAL  | 3.3  |
| 1   | A     | 1187 | GLN  | 3.3  |
| 2   | B     | 715  | ALA  | 3.3  |
| 2   | B     | 249  | ARG  | 3.3  |
| 2   | B     | 467  | GLY  | 3.3  |
| 1   | A     | 56   | PRO  | 3.2  |
| 15  | P     | 2    | G    | 3.2  |
| 9   | I     | 4    | PHE  | 3.2  |
| 9   | I     | 116  | ASN  | 3.2  |
| 12  | L     | 25   | ALA  | 3.2  |
| 2   | B     | 918  | ILE  | 3.1  |
| 2   | B     | 108  | VAL  | 3.1  |
| 4   | D     | 18   | VAL  | 3.1  |
| 13  | T     | 12   | DG   | 3.1  |
| 8   | H     | 132  | LEU  | 3.1  |
| 8   | H     | 84   | ALA  | 3.0  |
| 1   | A     | 265  | LYS  | 3.0  |
| 2   | B     | 734  | HIS  | 3.0  |
| 2   | B     | 508  | LEU  | 3.0  |
| 2   | B     | 880  | THR  | 3.0  |
| 1   | A     | 594  | GLY  | 3.0  |
| 1   | A     | 159  | THR  | 3.0  |
| 8   | H     | 90   | ALA  | 2.9  |
| 9   | I     | 119  | THR  | 2.9  |
| 2   | B     | 266  | ALA  | 2.9  |
| 2   | B     | 709  | ASP  | 2.9  |
| 13  | T     | 13   | DT   | 2.9  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 483 | ASP  | 2.8  |
| 12  | L     | 27  | LEU  | 2.8  |
| 2   | B     | 241 | ARG  | 2.8  |
| 1   | A     | 66  | LYS  | 2.8  |
| 2   | B     | 134 | LYS  | 2.7  |
| 14  | N     | 5   | DC   | 2.7  |
| 2   | B     | 101 | MET  | 2.7  |
| 5   | E     | 90  | VAL  | 2.7  |
| 9   | I     | 56  | ALA  | 2.7  |
| 13  | T     | 28  | DA   | 2.7  |
| 2   | B     | 502 | ILE  | 2.7  |
| 12  | L     | 43  | THR  | 2.7  |
| 5   | E     | 114 | ASN  | 2.7  |
| 2   | B     | 265 | SER  | 2.7  |
| 15  | P     | 7   | G    | 2.7  |
| 15  | P     | 8   | G    | 2.7  |
| 7   | G     | 21  | ARG  | 2.7  |
| 13  | T     | 14  | DA   | 2.7  |
| 8   | H     | 135 | LEU  | 2.7  |
| 2   | B     | 472 | ALA  | 2.6  |
| 2   | B     | 251 | ILE  | 2.6  |
| 12  | L     | 26  | THR  | 2.6  |
| 2   | B     | 712 | PRO  | 2.6  |
| 4   | D     | 4   | SER  | 2.6  |
| 2   | B     | 436 | VAL  | 2.5  |
| 2   | B     | 295 | GLY  | 2.5  |
| 2   | B     | 866 | TYR  | 2.5  |
| 2   | B     | 868 | MET  | 2.5  |
| 2   | B     | 594 | ALA  | 2.5  |
| 2   | B     | 870 | ILE  | 2.5  |
| 2   | B     | 66  | ASP  | 2.5  |
| 2   | B     | 468 | GLU  | 2.4  |
| 12  | L     | 49  | LYS  | 2.4  |
| 1   | A     | 257 | ARG  | 2.4  |
| 4   | D     | 13  | ARG  | 2.4  |
| 2   | B     | 731 | VAL  | 2.4  |
| 2   | B     | 510 | LYS  | 2.4  |
| 6   | F     | 69  | LEU  | 2.4  |
| 1   | A     | 71  | GLN  | 2.4  |
| 1   | A     | 251 | SER  | 2.4  |
| 1   | A     | 252 | PHE  | 2.4  |
| 9   | I     | 118 | ARG  | 2.4  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 2   | B     | 867  | GLY  | 2.4  |
| 8   | H     | 76   | THR  | 2.4  |
| 2   | B     | 335  | GLY  | 2.4  |
| 2   | B     | 1224 | PHE  | 2.4  |
| 8   | H     | 83   | GLN  | 2.4  |
| 1   | A     | 155  | GLU  | 2.4  |
| 2   | B     | 713  | ALA  | 2.3  |
| 4   | D     | 221  | TYR  | 2.3  |
| 3   | C     | 3    | GLU  | 2.3  |
| 2   | B     | 962  | LYS  | 2.3  |
| 1   | A     | 255  | SER  | 2.3  |
| 14  | N     | 2    | DC   | 2.3  |
| 1   | A     | 65   | LEU  | 2.3  |
| 2   | B     | 431  | TYR  | 2.3  |
| 1   | A     | 256  | GLN  | 2.3  |
| 13  | T     | 25   | DG   | 2.3  |
| 1   | A     | 149  | GLU  | 2.3  |
| 9   | I     | 52   | ILE  | 2.2  |
| 5   | E     | 41   | ASP  | 2.2  |
| 6   | F     | 76   | LYS  | 2.2  |
| 1   | A     | 253  | ASN  | 2.2  |
| 2   | B     | 115  | GLN  | 2.2  |
| 2   | B     | 473  | MET  | 2.2  |
| 2   | B     | 885  | MET  | 2.2  |
| 2   | B     | 336  | ARG  | 2.2  |
| 1   | A     | 158  | PRO  | 2.2  |
| 1   | A     | 1158 | PRO  | 2.2  |
| 1   | A     | 567  | LYS  | 2.2  |
| 2   | B     | 933  | SER  | 2.1  |
| 1   | A     | 186  | LYS  | 2.1  |
| 1   | A     | 1321 | GLY  | 2.1  |
| 2   | B     | 24   | PRO  | 2.1  |
| 4   | D     | 17   | LYS  | 2.1  |
| 2   | B     | 736  | THR  | 2.1  |
| 13  | T     | 24   | DG   | 2.1  |
| 12  | L     | 42   | ARG  | 2.1  |
| 2   | B     | 105  | SER  | 2.1  |
| 1   | A     | 587  | HIS  | 2.1  |
| 8   | H     | 82   | PRO  | 2.1  |
| 1   | A     | 1244 | ARG  | 2.1  |
| 1   | A     | 50   | ILE  | 2.1  |
| 2   | B     | 164  | LYS  | 2.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | A     | 1277 | GLU  | 2.1  |
| 5   | E     | 95   | THR  | 2.1  |
| 2   | B     | 267  | ARG  | 2.1  |
| 2   | B     | 887  | HIS  | 2.1  |
| 2   | B     | 263  | GLY  | 2.1  |
| 8   | H     | 85   | GLY  | 2.1  |
| 1   | A     | 150  | THR  | 2.1  |
| 8   | H     | 64   | ASN  | 2.1  |
| 2   | B     | 132  | VAL  | 2.1  |
| 1   | A     | 310  | GLY  | 2.1  |
| 7   | G     | 139  | ILE  | 2.1  |
| 2   | B     | 133  | LYS  | 2.0  |
| 2   | B     | 111  | ALA  | 2.0  |
| 2   | B     | 243  | ALA  | 2.0  |
| 1   | A     | 63   | ARG  | 2.0  |
| 4   | D     | 20   | GLU  | 2.0  |
| 2   | B     | 602  | THR  | 2.0  |

## 6.2 Non-standard residues in protein, DNA, RNA chains [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(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 13  | BRU  | T     | 23  | 20/21 | 0.66 | 0.22 | 127,131,137,139            | 0     |

## 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 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 17  | MG   | A     | 2458 | 1/1   | 0.81 | 0.14 | 123,123,123,123             | 0     |
| 16  | ZN   | I     | 1122 | 1/1   | 0.96 | 0.06 | 122,122,122,122             | 0     |
| 16  | ZN   | L     | 1071 | 1/1   | 0.99 | 0.04 | 111,111,111,111             | 0     |
| 16  | ZN   | A     | 2456 | 1/1   | 0.99 | 0.03 | 86,86,86,86                 | 0     |
| 16  | ZN   | I     | 1121 | 1/1   | 1.00 | 0.04 | 90,90,90,90                 | 0     |
| 16  | ZN   | A     | 2457 | 1/1   | 1.00 | 0.02 | 51,51,51,51                 | 0     |
| 16  | ZN   | J     | 1066 | 1/1   | 1.00 | 0.03 | 61,61,61,61                 | 0     |
| 16  | ZN   | B     | 2225 | 1/1   | 1.00 | 0.03 | 54,54,54,54                 | 0     |
| 16  | ZN   | C     | 1269 | 1/1   | 1.00 | 0.03 | 49,49,49,49                 | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.