



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:09 PM UTC

PDB ID : 4XLS / pdb\_00004xls  
Title : Crystal structure of T. aquaticus transcription initiation complex with CarD containing upstream fork promoter.  
Authors : Bae, B.; Darst, S.A.  
Deposited on : 2015-01-13  
Resolution : 4.01 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

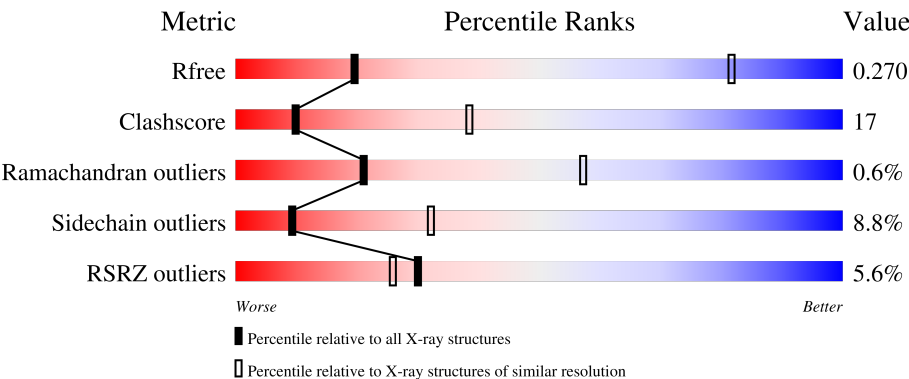
|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                             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

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 4.01 Å.

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



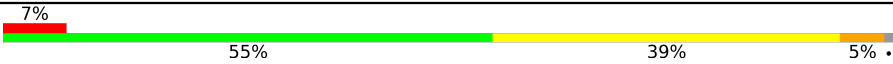
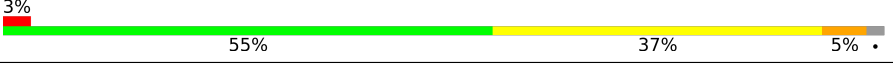
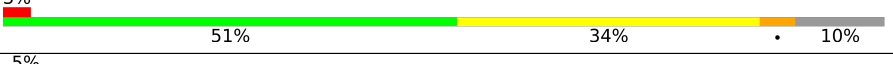
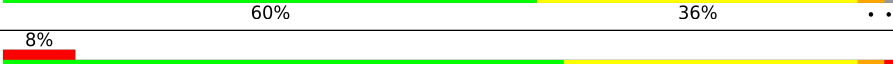
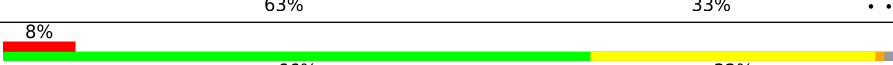
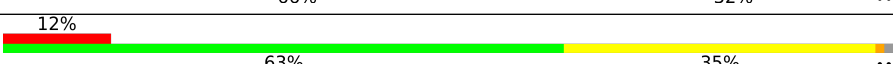
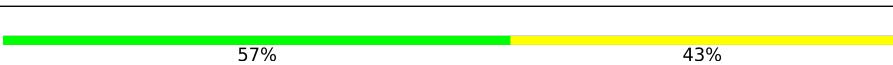
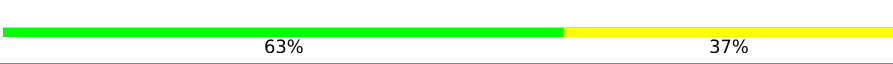
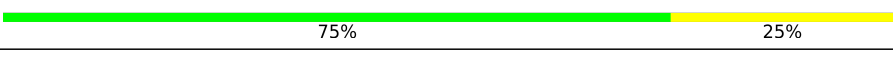
| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| R <sub>free</sub>     | 180053                      | 1095 (4.24-3.80)                                      |
| Clashscore            | 190562                      | 1142 (4.24-3.80)                                      |
| Ramachandran outliers | 187476                      | 1074 (4.24-3.80)                                      |
| Sidechain outliers    | 187428                      | 1065 (4.24-3.80)                                      |
| RSRZ outliers         | 180081                      | 1095 (4.24-3.80)                                      |

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

| Mol | Chain | Length | Quality of chain                                                               |
|-----|-------|--------|--------------------------------------------------------------------------------|
| 1   | A     | 314    | <div><div>4%</div><div>40%</div><div>29%</div><div>•</div><div>28%</div></div> |
| 1   | B     | 314    | <div><div>4%</div><div>43%</div><div>27%</div><div>•</div><div>28%</div></div> |
| 1   | G     | 314    | <div><div>9%</div><div>40%</div><div>29%</div><div>•</div><div>28%</div></div> |
| 1   | H     | 314    | <div><div>4%</div><div>38%</div><div>32%</div><div>•</div><div>28%</div></div> |
| 2   | C     | 1119   | <div><div>6%</div><div>55%</div><div>39%</div><div>5%</div><div>•</div></div>  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 2   | I     | 1119   |    |
| 3   | D     | 1524   |    |
| 3   | J     | 1524   |    |
| 4   | E     | 99     |    |
| 4   | K     | 99     |    |
| 5   | F     | 347    |    |
| 5   | L     | 347    |    |
| 6   | M     | 164    |    |
| 6   | N     | 164    |    |
| 7   | O     | 30     |    |
| 7   | R     | 30     |   |
| 8   | P     | 24     |  |
| 8   | S     | 24     |  |

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 58966 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 subunit alpha.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | A     | 227      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1770  | 1130 | 303 | 334 | 3 |         |         |       |
| 1   | B     | 227      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1770  | 1130 | 303 | 334 | 3 |         |         |       |
| 1   | G     | 227      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1770  | 1130 | 303 | 334 | 3 |         |         |       |
| 1   | H     | 227      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1770  | 1130 | 303 | 334 | 3 |         |         |       |

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

| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 2   | C     | 1112     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 8739  | 5531 | 1553 | 1632 | 23 |         |         |       |
| 2   | I     | 1112     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 8739  | 5531 | 1553 | 1632 | 23 |         |         |       |

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 3   | D     | 1490     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 11761 | 7439 | 2088 | 2196 | 38 |         |         |       |
| 3   | J     | 1367     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 10779 | 6810 | 1923 | 2010 | 36 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 4   | E     | 93       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 768   | 490 | 136 | 138 | 4 |         |         |       |
| 4   | K     | 93       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 768   | 490 | 136 | 138 | 4 |         |         |       |

- Molecule 5 is a protein called RNA polymerase sigma factor SigA.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 5   | F     | 345      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2787  | 1758 | 502 | 523 | 4 |         |         |       |
| 5   | L     | 345      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2787  | 1758 | 502 | 523 | 4 |         |         |       |

- Molecule 6 is a protein called CarD-like transcriptional regulator.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6   | M     | 162      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1274  | 807 | 234 | 231 | 2 |         |         |       |
| 6   | N     | 162      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1274  | 807 | 234 | 231 | 2 |         |         |       |

- Molecule 7 is a DNA chain called DNA (30-MER).

| Mol | Chain | Residues | Atoms |     |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 7   | O     | 30       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 613   | 296 | 109 | 179 | 29 |         |         |       |
| 7   | R     | 30       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 613   | 296 | 109 | 179 | 29 |         |         |       |

- Molecule 8 is a DNA chain called DNA (5'-D(P\*GP\*CP\*AP\*CP\*AP\*AP\*TP\*TP\*TP\*AP\*AP\*CP\*AP\*CP\*TP\*TP\*TP\*TP\*GP\*TP\*CP\*AP\*AP\*G)-3').

| Mol | Chain | Residues | Atoms |     |    |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|---------|-------|
| 8   | P     | 24       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 489   | 235 | 86 | 144 | 24 |         |         |       |
| 8   | S     | 24       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 489   | 235 | 86 | 144 | 24 |         |         |       |

- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 9   | D     | 2        | Total | Zn | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 9   | J     | 2        | Total | Zn | 0       | 0       |
|     |       |          | 2     | 2  |         |         |

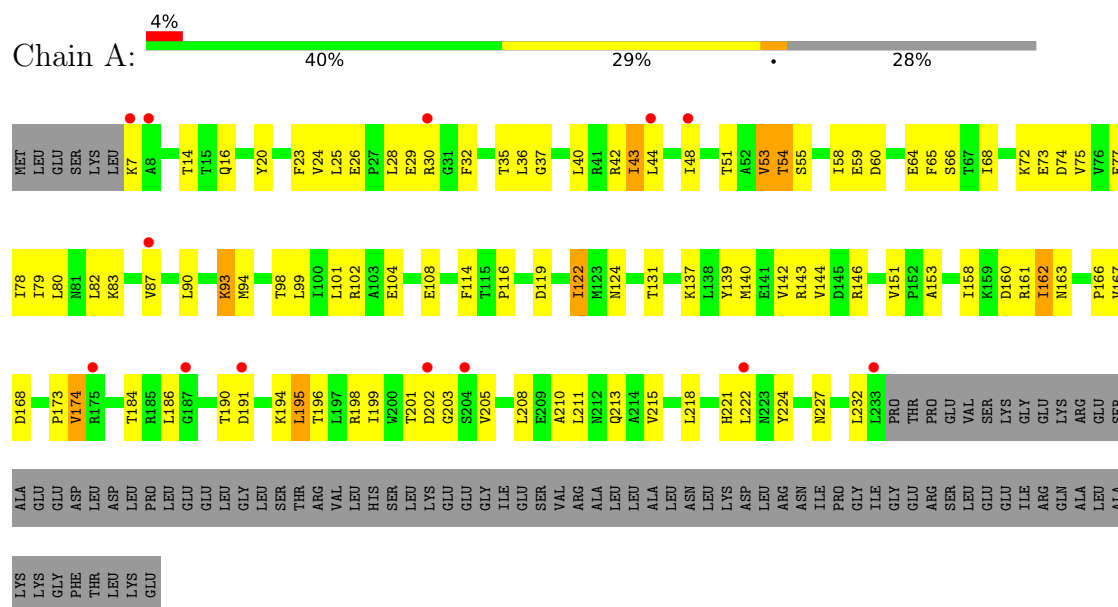
- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 10  | D     | 1        | Total<br>1 | Mg<br>1 | 0       | 0       |
| 10  | J     | 1        | Total<br>1 | Mg<br>1 | 0       | 0       |

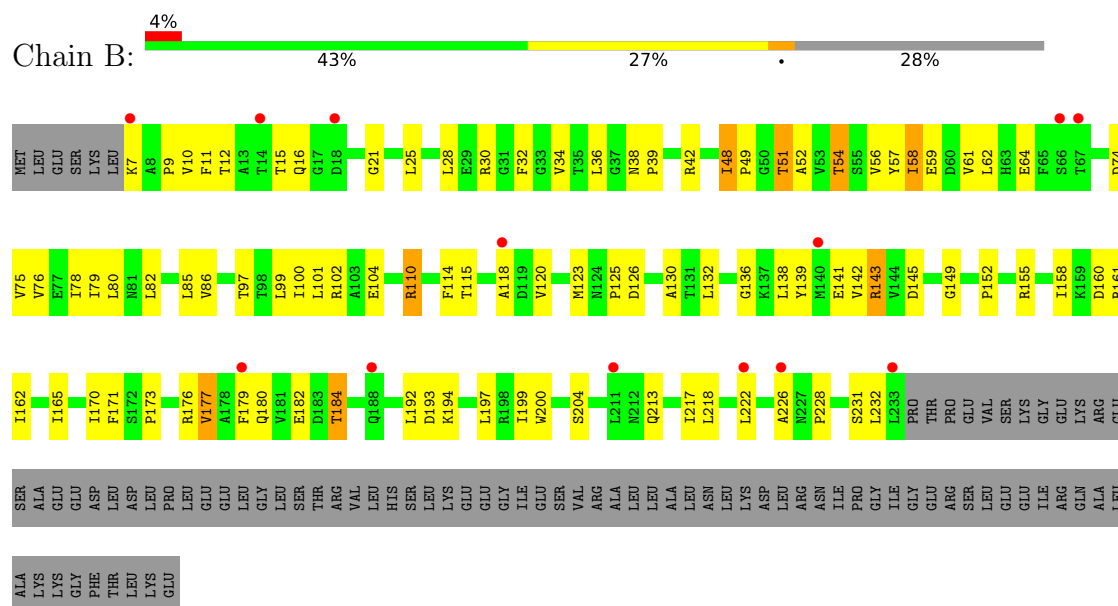
### 3 Residue-property plots [i](#)

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

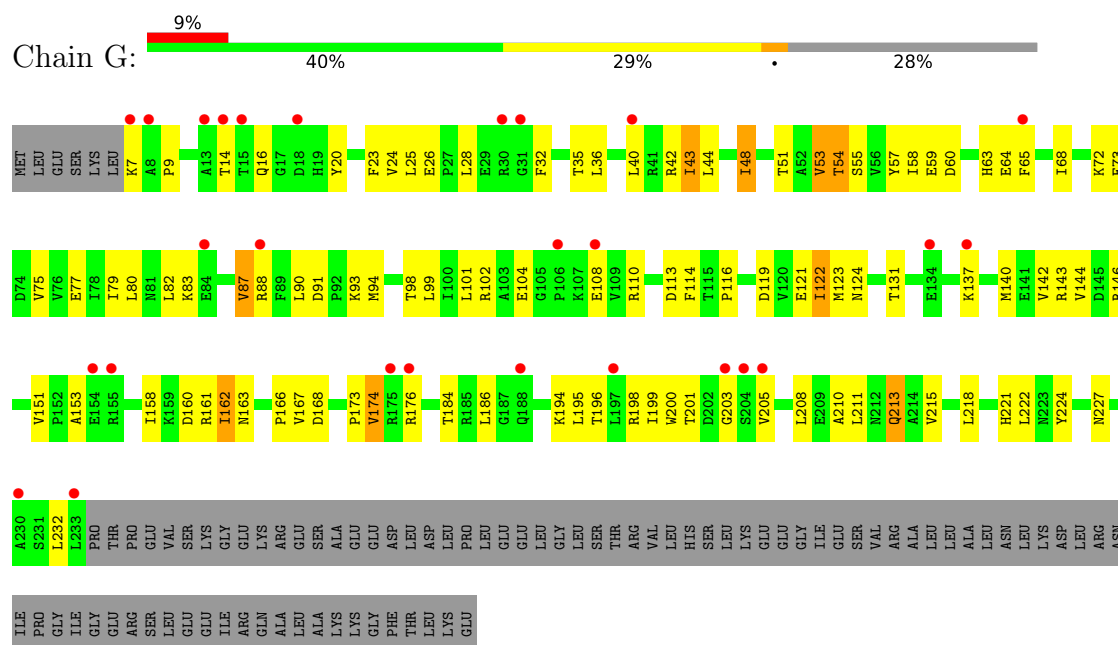
#### • Molecule 1: DNA-directed RNA polymerase subunit alpha



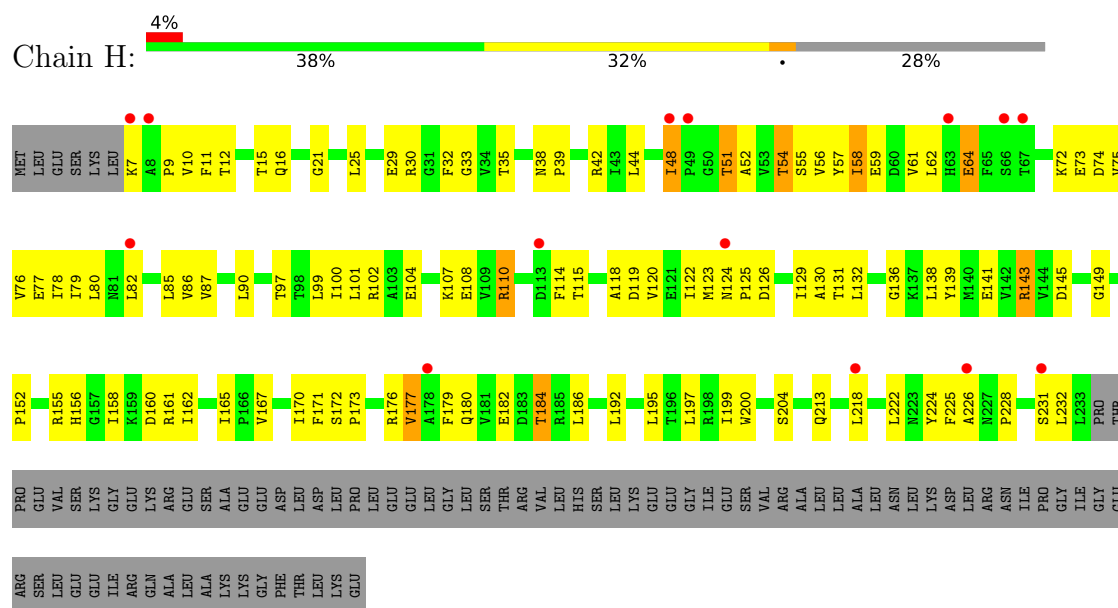
#### • Molecule 1: DNA-directed RNA polymerase subunit alpha



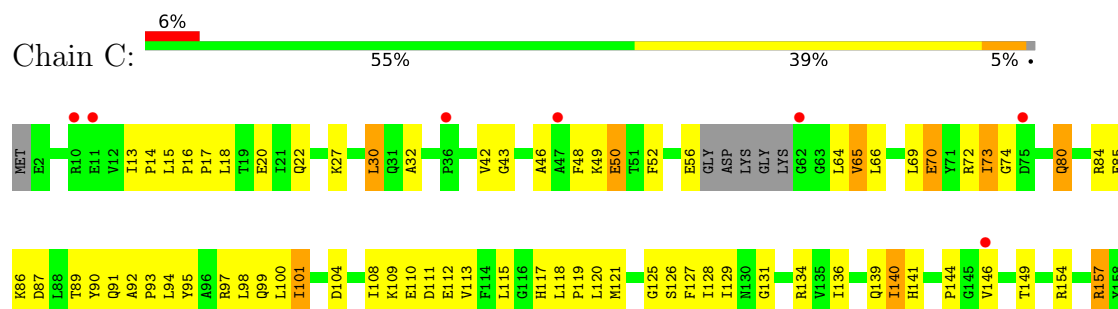
- Molecule 1: DNA-directed RNA polymerase subunit alpha



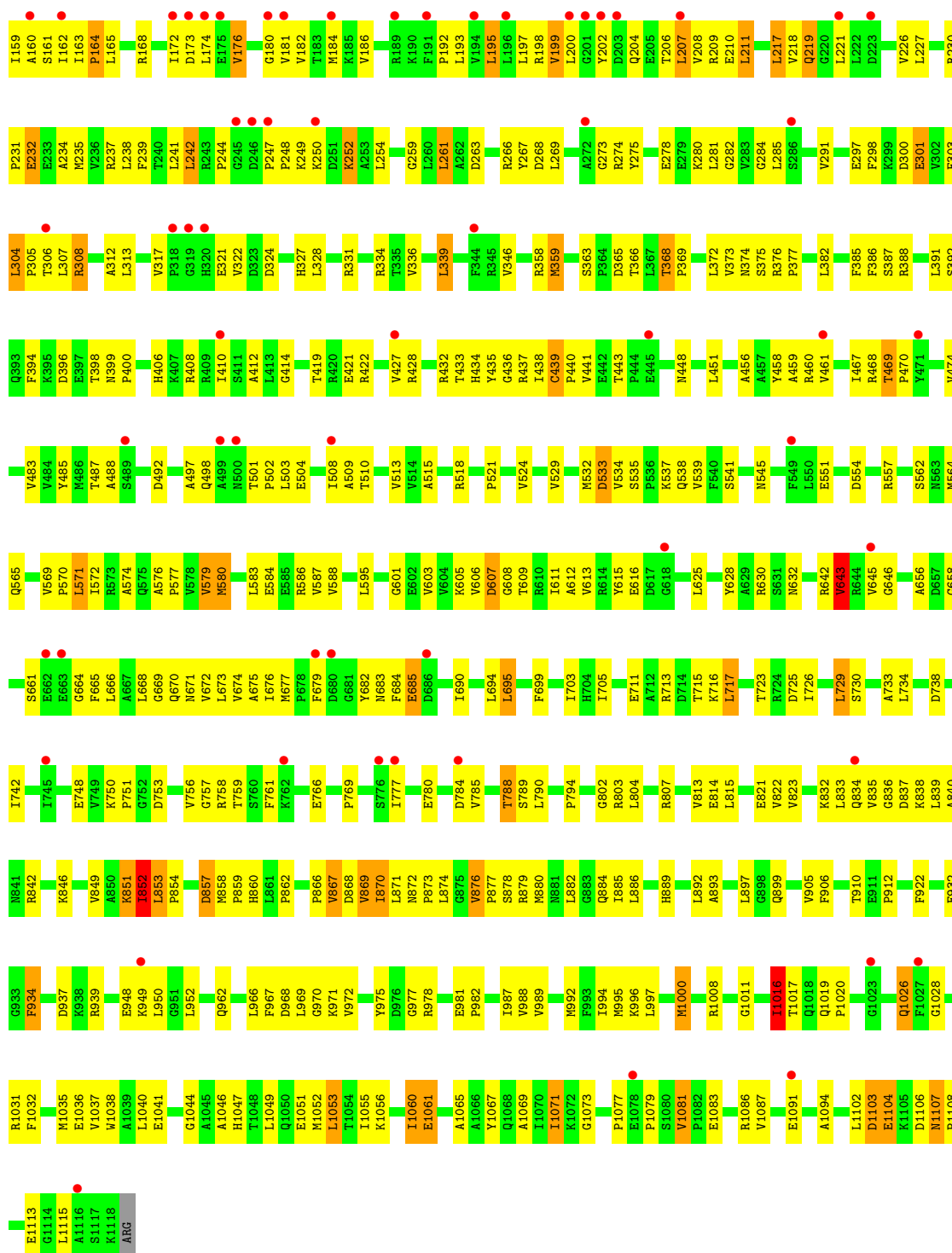
- Molecule 1: DNA-directed RNA polymerase subunit alpha



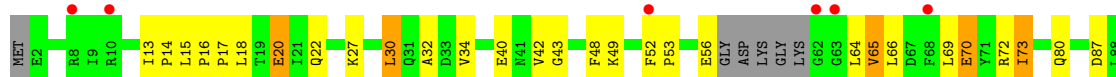
- Molecule 2: DNA-directed RNA polymerase subunit beta

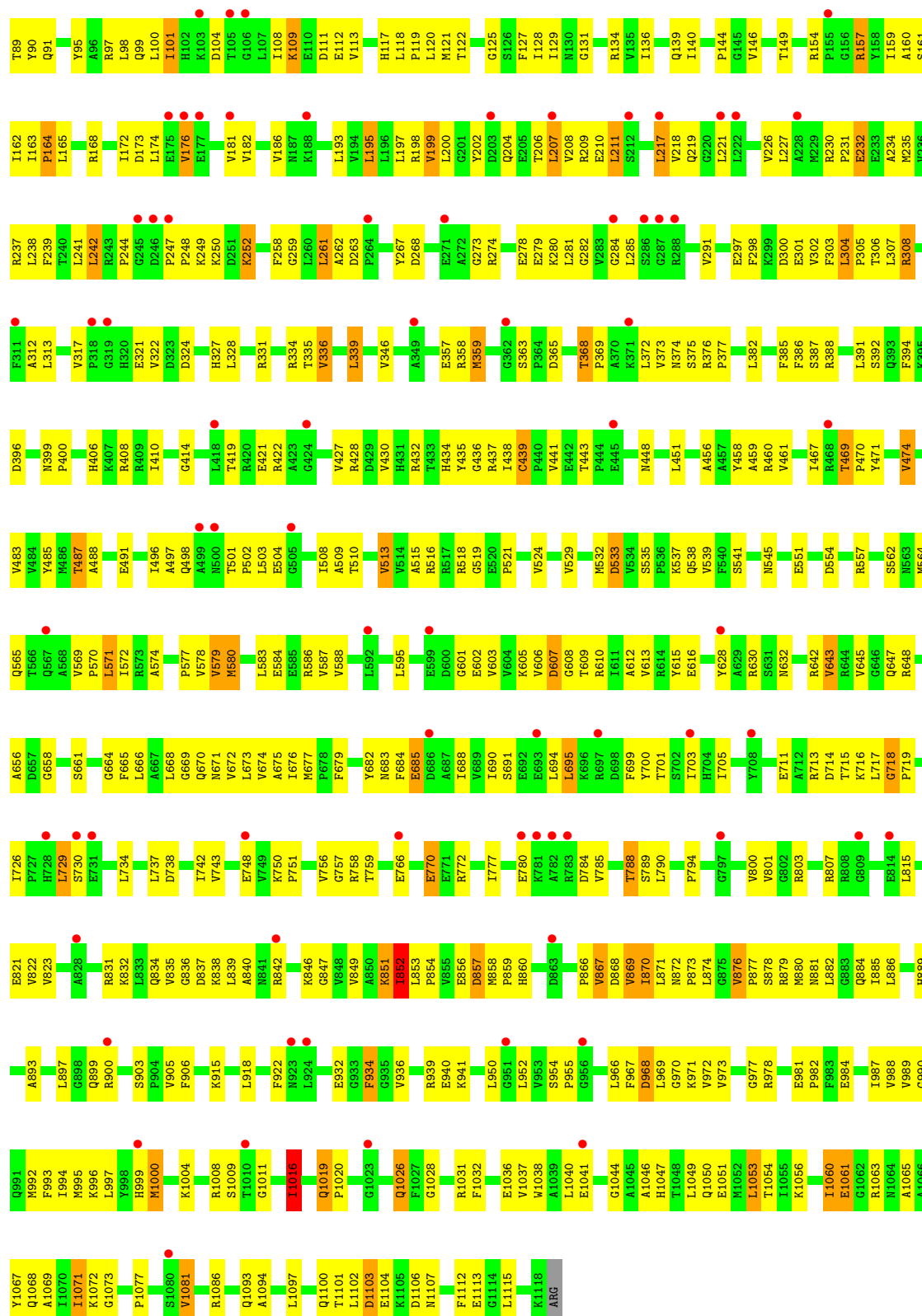






• Molecule 2: DNA-directed RNA polymerase subunit beta

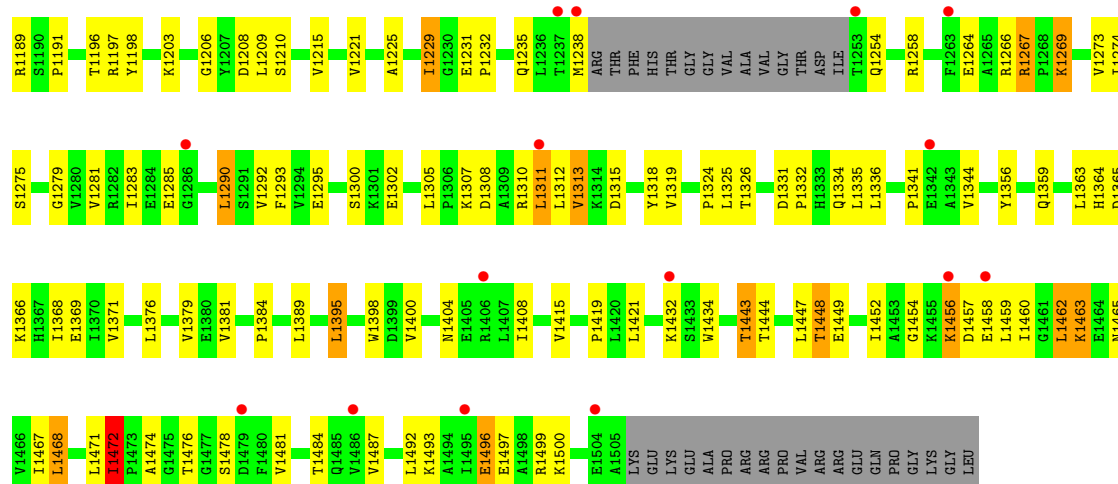




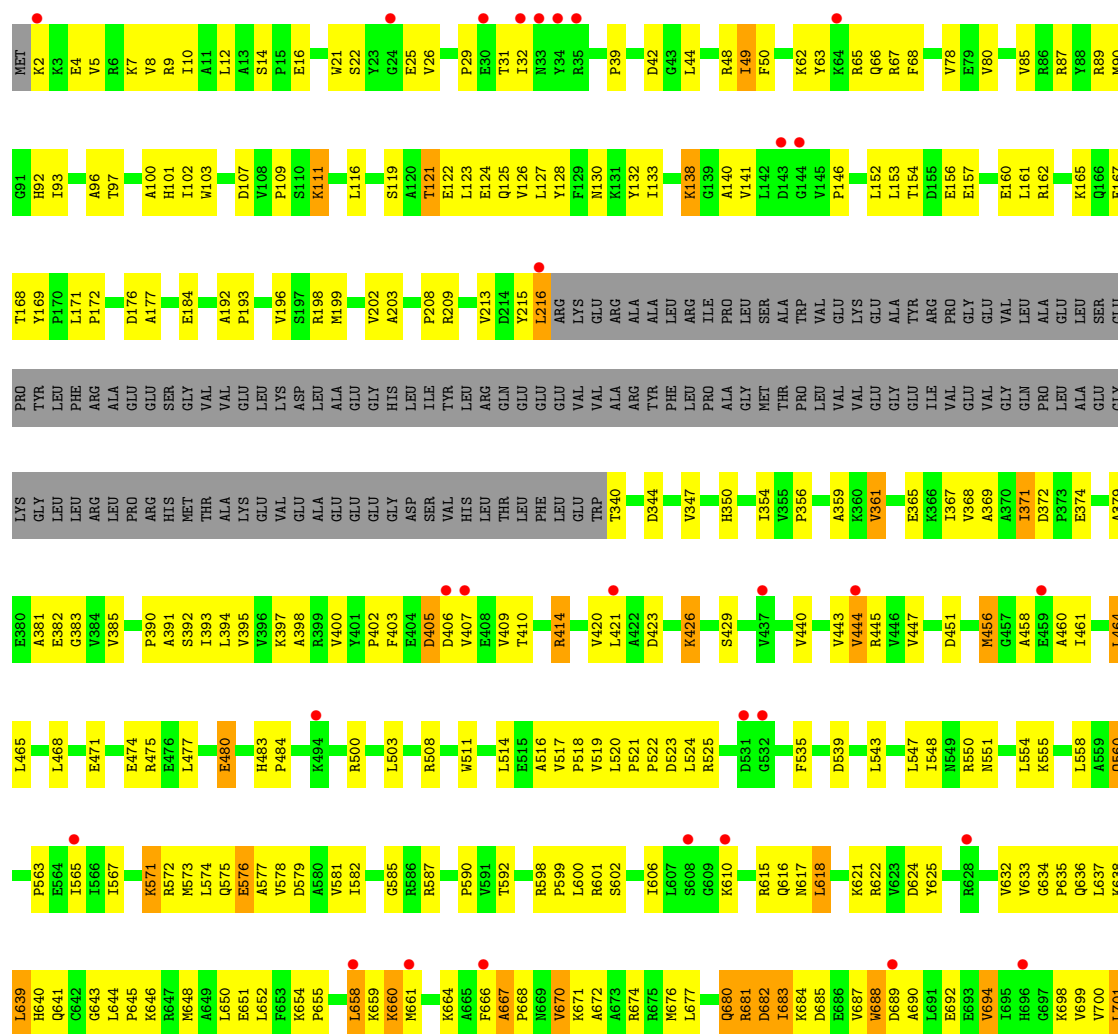
• Molecule 3: DNA-directed RNA polymerase subunit beta'

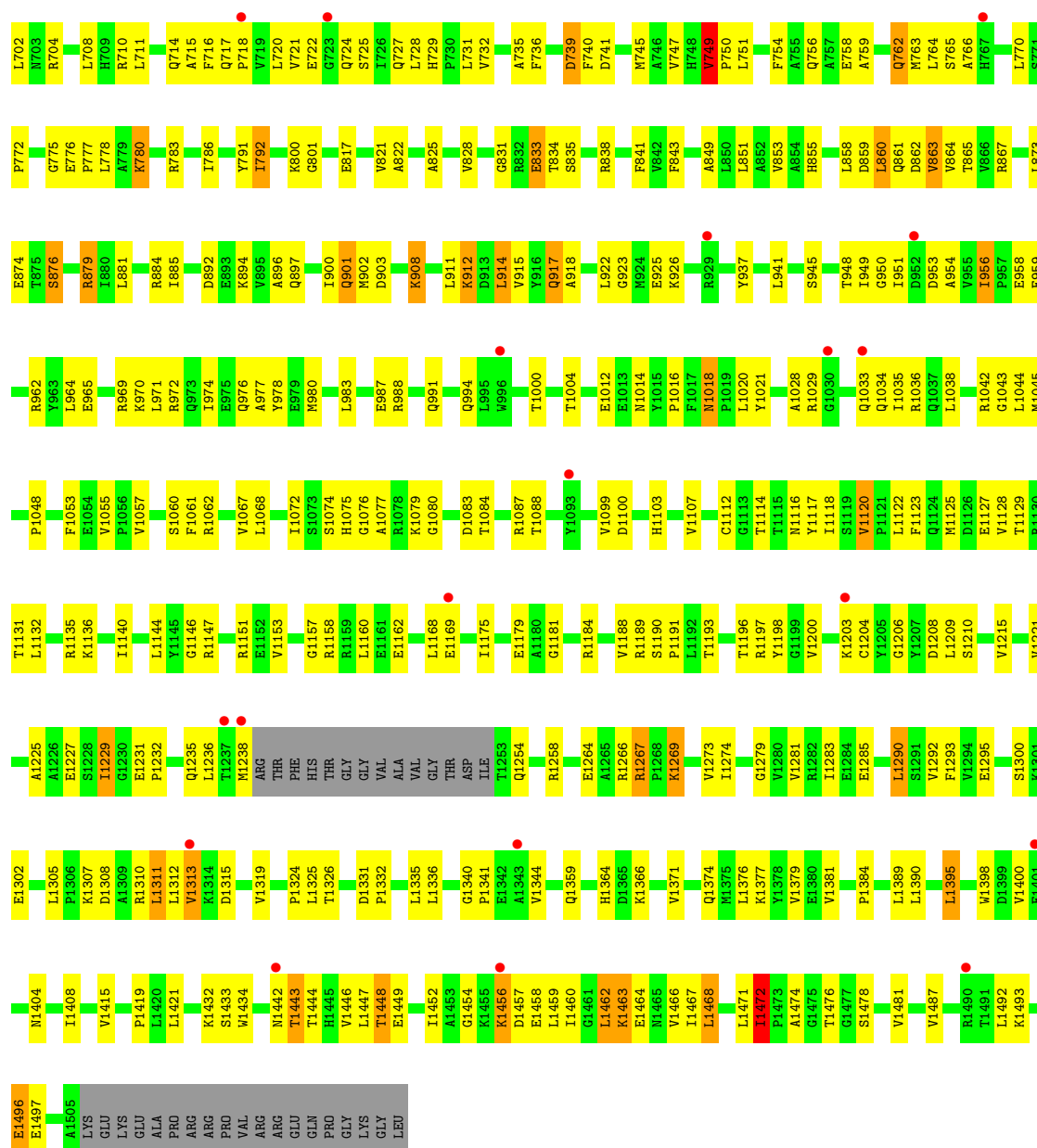




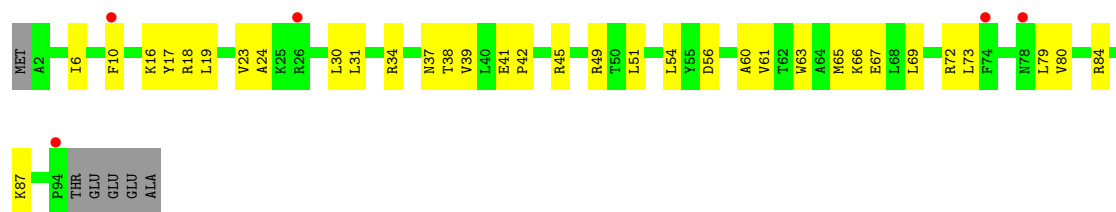


● Molecule 3: DNA-directed RNA polymerase subunit beta'



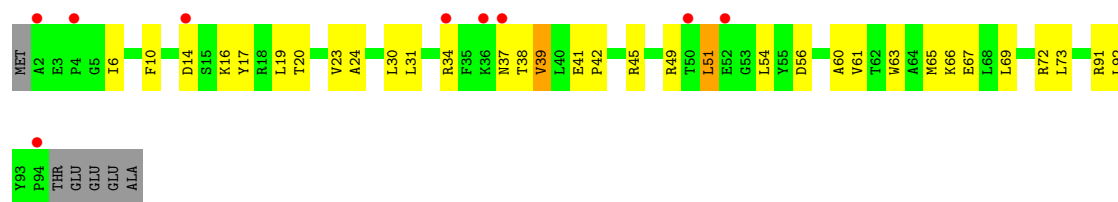


- Molecule 4: DNA-directed RNA polymerase subunit omega

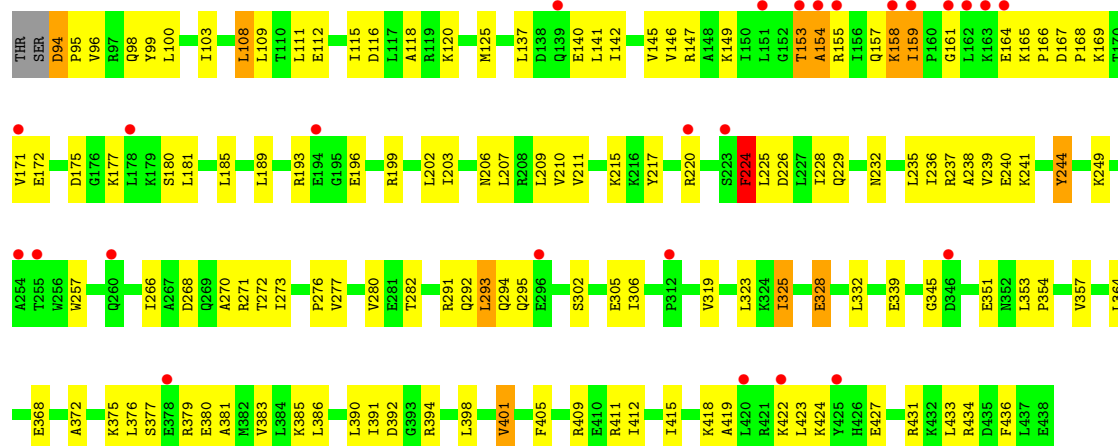


- Molecule 4: DNA-directed RNA polymerase subunit omega

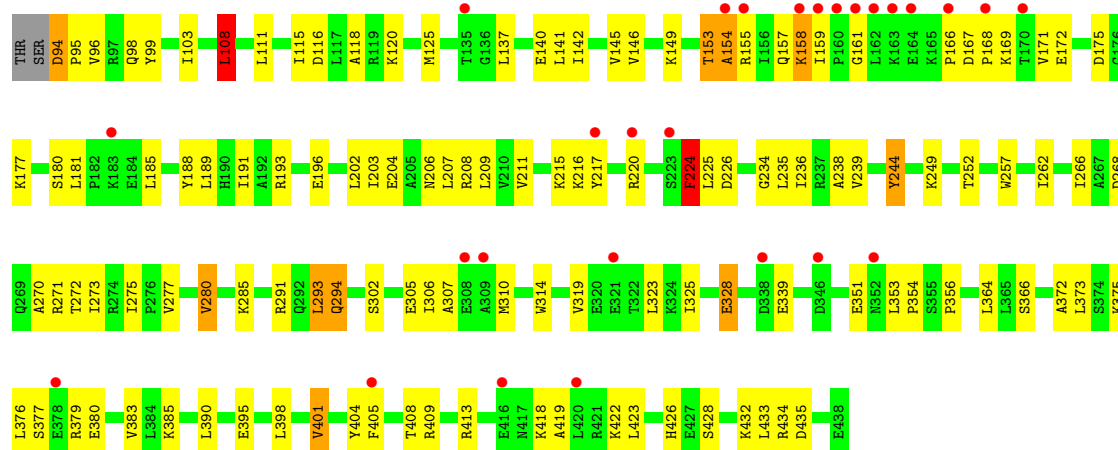




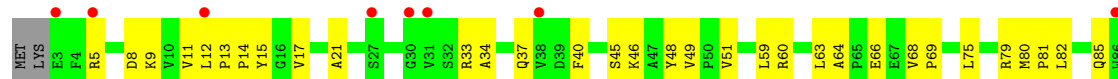
• Molecule 5: RNA polymerase sigma factor SigA



• Molecule 5: RNA polymerase sigma factor SigA

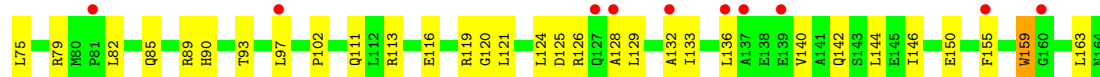
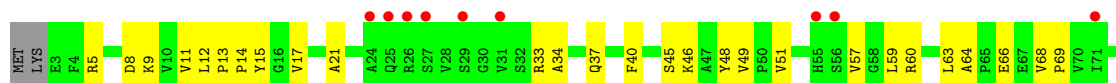


• Molecule 6: CarD-like transcriptional regulator





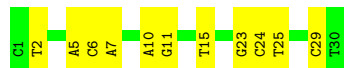
- Molecule 6: CarD-like transcriptional regulator



- Molecule 7: DNA (30-MER)



- Molecule 7: DNA (30-MER)



- Molecule 8: DNA (5'-D(P\*GP\*CP\*AP\*CP\*AP\*AP\*TP\*TP\*TP\*AP\*AP\*CP\*AP\*CP\*TP\*T  
P\*TP\*TP\*GP\*TP\*CP\*AP\*AP\*G)-3')



- Molecule 8: DNA (5'-D(P\*GP\*CP\*AP\*CP\*AP\*AP\*TP\*TP\*TP\*AP\*AP\*CP\*AP\*CP\*TP\*T  
P\*TP\*TP\*GP\*TP\*CP\*AP\*AP\*G)-3')



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 43 21 2                                                   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 293.15Å 293.15Å 539.13Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 49.79 – 4.01<br>49.79 – 4.01                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 75.7 (49.79-4.01)<br>75.7 (49.79-4.01)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 0.79 (at 4.00Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX (PHENIX.REFINE: DEV_1839)                            | Depositor        |
| R, $R_{free}$                                                           | 0.232 , 0.272<br>0.234 , 0.270                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 7463 reflections (3.75%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 146.9                                                       | Xtriage          |
| Anisotropy                                                              | 0.030                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.32 , 243.3                                                | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.36$ , $\langle L^2 \rangle = 0.20$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.88                                                        | EDS              |
| Total number of atoms                                                   | 58966                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 173.0                                                       | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.80% 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: ZN, MG

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     | 0.37         | 0/1804         | 0.88        | 2/2455 (0.1%)   |
| 1   | B     | 0.39         | 0/1804         | 0.87        | 3/2455 (0.1%)   |
| 1   | G     | 0.39         | 0/1804         | 0.87        | 6/2455 (0.2%)   |
| 1   | H     | 0.41         | 0/1804         | 0.87        | 5/2455 (0.2%)   |
| 2   | C     | 0.36         | 0/8905         | 0.88        | 16/12040 (0.1%) |
| 2   | I     | 0.37         | 0/8905         | 0.88        | 16/12040 (0.1%) |
| 3   | D     | 0.36         | 1/11963 (0.0%) | 0.86        | 18/16165 (0.1%) |
| 3   | J     | 0.37         | 1/10959 (0.0%) | 0.86        | 13/14802 (0.1%) |
| 4   | E     | 0.31         | 0/783          | 0.82        | 0/1054          |
| 4   | K     | 0.32         | 0/783          | 0.82        | 0/1054          |
| 5   | F     | 0.34         | 0/2829         | 0.85        | 6/3804 (0.2%)   |
| 5   | L     | 0.36         | 0/2829         | 0.86        | 4/3804 (0.1%)   |
| 6   | M     | 0.34         | 0/1302         | 0.89        | 3/1765 (0.2%)   |
| 6   | N     | 0.35         | 0/1302         | 0.84        | 2/1765 (0.1%)   |
| 7   | O     | 0.12         | 0/687          | 0.56        | 0/1059          |
| 7   | R     | 0.13         | 0/687          | 0.59        | 0/1059          |
| 8   | P     | 0.13         | 0/547          | 0.66        | 0/841           |
| 8   | S     | 0.14         | 0/547          | 0.66        | 1/841 (0.1%)    |
| All | All   | 0.36         | 2/60244 (0.0%) | 0.85        | 95/81913 (0.1%) |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 3   | J     | 670 | VAL  | C-O   | 6.50 | 1.31        | 1.24     |
| 3   | D     | 670 | VAL  | C-O   | 5.96 | 1.30        | 1.24     |

All (95) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 2   | I     | 414 | GLY  | CA-C-N | 7.59 | 129.32      | 119.84   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 2   | I     | 414  | GLY  | C-N-CA    | 7.59  | 129.32      | 119.84   |
| 5   | L     | 277  | VAL  | N-CA-C    | 7.54  | 117.66      | 110.42   |
| 3   | J     | 1472 | ILE  | CA-C-N    | 7.16  | 126.83      | 119.82   |
| 3   | J     | 1472 | ILE  | C-N-CA    | 7.16  | 126.83      | 119.82   |
| 1   | A     | 227  | ASN  | CA-C-N    | 7.08  | 128.69      | 119.84   |
| 1   | A     | 227  | ASN  | C-N-CA    | 7.08  | 128.69      | 119.84   |
| 3   | D     | 1472 | ILE  | CA-C-N    | 6.86  | 126.56      | 119.56   |
| 3   | D     | 1472 | ILE  | C-N-CA    | 6.86  | 126.56      | 119.56   |
| 2   | I     | 718  | GLY  | CA-C-N    | 6.72  | 126.70      | 119.78   |
| 2   | I     | 718  | GLY  | C-N-CA    | 6.72  | 126.70      | 119.78   |
| 2   | C     | 414  | GLY  | CA-C-N    | 6.68  | 128.19      | 119.84   |
| 2   | C     | 414  | GLY  | C-N-CA    | 6.68  | 128.19      | 119.84   |
| 1   | G     | 227  | ASN  | CA-C-N    | 6.54  | 128.01      | 119.84   |
| 1   | G     | 227  | ASN  | C-N-CA    | 6.54  | 128.01      | 119.84   |
| 3   | D     | 406  | ASP  | CB-CA-C   | -6.52 | 108.03      | 115.79   |
| 3   | D     | 245  | LEU  | CB-CA-C   | -6.52 | 107.29      | 115.89   |
| 1   | G     | 48   | ILE  | CA-C-N    | 6.48  | 126.43      | 119.76   |
| 1   | G     | 48   | ILE  | C-N-CA    | 6.48  | 126.43      | 119.76   |
| 3   | J     | 616  | GLN  | CA-C-N    | -6.31 | 114.50      | 123.20   |
| 3   | J     | 616  | GLN  | C-N-CA    | -6.31 | 114.50      | 123.20   |
| 2   | I     | 1081 | VAL  | N-CA-C    | 6.30  | 114.13      | 107.76   |
| 2   | C     | 363  | SER  | CA-C-N    | 6.29  | 125.98      | 119.82   |
| 2   | C     | 363  | SER  | C-N-CA    | 6.29  | 125.98      | 119.82   |
| 5   | F     | 277  | VAL  | N-CA-C    | 6.27  | 116.44      | 110.42   |
| 3   | D     | 341  | GLU  | CA-C-N    | 6.13  | 126.10      | 120.03   |
| 3   | D     | 341  | GLU  | C-N-CA    | 6.13  | 126.10      | 120.03   |
| 3   | J     | 383  | GLY  | N-CA-C    | 6.05  | 118.75      | 110.58   |
| 2   | C     | 439  | CYS  | CA-C-N    | 5.99  | 126.10      | 119.87   |
| 2   | C     | 439  | CYS  | C-N-CA    | 5.99  | 126.10      | 119.87   |
| 3   | J     | 634  | GLY  | N-CA-C    | 5.98  | 124.54      | 112.34   |
| 8   | S     | 25   | DG   | P-O5'-C5' | -5.95 | 111.08      | 120.00   |
| 2   | C     | 853  | LEU  | CA-C-N    | 5.90  | 126.24      | 119.93   |
| 2   | C     | 853  | LEU  | C-N-CA    | 5.90  | 126.24      | 119.93   |
| 2   | I     | 1019 | GLN  | CA-C-N    | 5.87  | 125.81      | 119.76   |
| 2   | I     | 1019 | GLN  | C-N-CA    | 5.87  | 125.81      | 119.76   |
| 3   | D     | 634  | GLY  | N-CA-C    | 5.87  | 124.31      | 112.34   |
| 2   | I     | 363  | SER  | CA-C-N    | 5.84  | 125.55      | 119.82   |
| 2   | I     | 363  | SER  | C-N-CA    | 5.84  | 125.55      | 119.82   |
| 2   | I     | 439  | CYS  | CA-C-N    | 5.75  | 125.85      | 119.87   |
| 2   | I     | 439  | CYS  | C-N-CA    | 5.75  | 125.85      | 119.87   |
| 6   | M     | 119  | ARG  | N-CA-C    | -5.74 | 105.30      | 112.93   |
| 5   | F     | 161  | GLY  | N-CA-C    | -5.74 | 105.39      | 112.33   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 2   | C     | 802  | GLY  | N-CA-C | 5.70  | 120.55      | 110.80   |
| 2   | I     | 1103 | ASP  | N-CA-C | 5.69  | 117.18      | 108.30   |
| 3   | D     | 729  | HIS  | CA-C-N | 5.68  | 125.36      | 119.56   |
| 3   | D     | 729  | HIS  | C-N-CA | 5.68  | 125.36      | 119.56   |
| 2   | C     | 1103 | ASP  | N-CA-C | 5.59  | 117.03      | 108.30   |
| 3   | D     | 1030 | GLY  | N-CA-C | 5.58  | 117.73      | 112.04   |
| 1   | B     | 165  | ILE  | N-CA-C | 5.56  | 113.66      | 108.15   |
| 2   | I     | 469  | THR  | CA-C-N | 5.52  | 125.44      | 119.76   |
| 2   | I     | 469  | THR  | C-N-CA | 5.52  | 125.44      | 119.76   |
| 5   | L     | 94   | ASP  | CA-C-N | 5.52  | 125.13      | 119.56   |
| 5   | L     | 94   | ASP  | C-N-CA | 5.52  | 125.13      | 119.56   |
| 3   | J     | 670  | VAL  | CA-C-N | -5.43 | 113.00      | 120.28   |
| 3   | J     | 670  | VAL  | C-N-CA | -5.43 | 113.00      | 120.28   |
| 3   | D     | 521  | PRO  | CA-C-N | 5.41  | 124.59      | 118.97   |
| 3   | D     | 521  | PRO  | C-N-CA | 5.41  | 124.59      | 118.97   |
| 5   | L     | 161  | GLY  | N-CA-C | -5.36 | 105.84      | 112.33   |
| 3   | J     | 749  | VAL  | CA-C-N | 5.36  | 126.53      | 119.84   |
| 3   | J     | 749  | VAL  | C-N-CA | 5.36  | 126.53      | 119.84   |
| 1   | H     | 172  | SER  | CA-C-N | 5.34  | 125.15      | 119.28   |
| 1   | H     | 172  | SER  | C-N-CA | 5.34  | 125.15      | 119.28   |
| 5   | F     | 94   | ASP  | CA-C-N | 5.33  | 124.94      | 119.56   |
| 5   | F     | 94   | ASP  | C-N-CA | 5.33  | 124.94      | 119.56   |
| 3   | J     | 1018 | ASN  | CA-C-N | 5.30  | 124.48      | 118.97   |
| 3   | J     | 1018 | ASN  | C-N-CA | 5.30  | 124.48      | 118.97   |
| 6   | M     | 5    | ARG  | CA-C-N | 5.29  | 126.45      | 119.84   |
| 6   | M     | 5    | ARG  | C-N-CA | 5.29  | 126.45      | 119.84   |
| 1   | G     | 91   | ASP  | CA-C-N | 5.28  | 125.36      | 119.87   |
| 1   | G     | 91   | ASP  | C-N-CA | 5.28  | 125.36      | 119.87   |
| 2   | I     | 1011 | GLY  | CA-C-N | 5.27  | 125.56      | 119.92   |
| 2   | I     | 1011 | GLY  | C-N-CA | 5.27  | 125.56      | 119.92   |
| 2   | C     | 1011 | GLY  | CA-C-N | 5.26  | 125.55      | 119.92   |
| 2   | C     | 1011 | GLY  | C-N-CA | 5.26  | 125.55      | 119.92   |
| 1   | H     | 48   | ILE  | CA-C-N | 5.25  | 125.25      | 119.89   |
| 1   | H     | 48   | ILE  | C-N-CA | 5.25  | 125.25      | 119.89   |
| 1   | B     | 48   | ILE  | CA-C-N | 5.22  | 125.22      | 119.89   |
| 1   | B     | 48   | ILE  | C-N-CA | 5.22  | 125.22      | 119.89   |
| 3   | D     | 245  | LEU  | N-CA-C | 5.22  | 117.79      | 109.02   |
| 2   | C     | 180  | GLY  | N-CA-C | -5.18 | 107.39      | 114.64   |
| 5   | F     | 159  | ILE  | CA-C-N | -5.13 | 113.43      | 119.84   |
| 5   | F     | 159  | ILE  | C-N-CA | -5.13 | 113.43      | 119.84   |
| 3   | D     | 1059 | SER  | N-CA-C | 5.13  | 117.53      | 110.35   |
| 1   | H     | 129  | ILE  | N-CA-C | -5.12 | 107.15      | 111.56   |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | J     | 406  | ASP  | CB-CA-C | -5.10 | 109.72      | 115.79   |
| 3   | D     | 749  | VAL  | CA-C-N  | 5.09  | 126.20      | 119.84   |
| 3   | D     | 749  | VAL  | C-N-CA  | 5.09  | 126.20      | 119.84   |
| 3   | D     | 401  | TYR  | CA-C-N  | 5.08  | 125.01      | 119.78   |
| 3   | D     | 401  | TYR  | C-N-CA  | 5.08  | 125.01      | 119.78   |
| 2   | C     | 469  | THR  | CA-C-N  | 5.06  | 124.97      | 119.76   |
| 2   | C     | 469  | THR  | C-N-CA  | 5.06  | 124.97      | 119.76   |
| 2   | C     | 1081 | VAL  | N-CA-C  | 5.02  | 112.83      | 107.76   |
| 6   | N     | 5    | ARG  | CA-C-N  | 5.00  | 126.10      | 119.84   |
| 6   | N     | 5    | ARG  | C-N-CA  | 5.00  | 126.10      | 119.84   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 1770  | 0        | 1799     | 76      | 0            |
| 1   | B     | 1770  | 0        | 1799     | 61      | 0            |
| 1   | G     | 1770  | 0        | 1799     | 79      | 0            |
| 1   | H     | 1770  | 0        | 1799     | 75      | 0            |
| 2   | C     | 8739  | 0        | 8841     | 373     | 0            |
| 2   | I     | 8739  | 0        | 8841     | 374     | 0            |
| 3   | D     | 11761 | 0        | 11976    | 464     | 0            |
| 3   | J     | 10779 | 0        | 10993    | 410     | 0            |
| 4   | E     | 768   | 0        | 784      | 27      | 0            |
| 4   | K     | 768   | 0        | 784      | 27      | 0            |
| 5   | F     | 2787  | 0        | 2866     | 87      | 0            |
| 5   | L     | 2787  | 0        | 2866     | 80      | 0            |
| 6   | M     | 1274  | 0        | 1288     | 34      | 0            |
| 6   | N     | 1274  | 0        | 1288     | 39      | 0            |
| 7   | O     | 613   | 0        | 343      | 14      | 0            |
| 7   | R     | 613   | 0        | 343      | 9       | 0            |
| 8   | P     | 489   | 0        | 273      | 7       | 0            |
| 8   | S     | 489   | 0        | 273      | 5       | 0            |
| 9   | D     | 2     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 9   | J     | 2     | 0        | 0        | 0       | 0            |
| 10  | D     | 1     | 0        | 0        | 0       | 0            |
| 10  | J     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 58966 | 0        | 58955    | 2059    | 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 17.

All (2059) 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) |
|------------------|------------------|--------------------------|-------------------|
| 5:F:149:LYS:HB3  | 5:F:193:ARG:HH12 | 1.35                     | 0.91              |
| 2:I:204:GLN:HB2  | 2:I:227:LEU:HD21 | 1.54                     | 0.90              |
| 2:C:502:PRO:HG3  | 2:C:510:THR:HG22 | 1.56                     | 0.88              |
| 5:L:149:LYS:HB3  | 5:L:193:ARG:HH12 | 1.37                     | 0.88              |
| 2:C:199:VAL:HA   | 2:C:231:PRO:HB3  | 1.55                     | 0.88              |
| 4:K:30:LEU:HD12  | 4:K:37:ASN:HD21  | 1.38                     | 0.88              |
| 2:C:204:GLN:HB2  | 2:C:227:LEU:HD21 | 1.57                     | 0.86              |
| 2:I:374:ASN:HD21 | 5:L:291:ARG:HD2  | 1.40                     | 0.86              |
| 2:I:502:PRO:HG3  | 2:I:510:THR:HG22 | 1.56                     | 0.86              |
| 4:E:30:LEU:HD12  | 4:E:37:ASN:HD21  | 1.40                     | 0.85              |
| 2:I:199:VAL:HA   | 2:I:231:PRO:HB3  | 1.58                     | 0.85              |
| 2:C:234:ALA:HA   | 2:C:237:ARG:HB2  | 1.58                     | 0.85              |
| 1:G:42:ARG:HH12  | 2:I:857:ASP:HB3  | 1.43                     | 0.84              |
| 2:I:211:LEU:HD11 | 2:I:221:LEU:HB3  | 1.60                     | 0.84              |
| 2:I:428:ARG:HE   | 2:I:451:LEU:HD21 | 1.43                     | 0.84              |
| 2:I:324:ASP:HB3  | 2:I:327:HIS:HB2  | 1.60                     | 0.83              |
| 2:C:751:PRO:HB3  | 2:C:794:PRO:HA   | 1.60                     | 0.83              |
| 2:C:211:LEU:HD11 | 2:C:221:LEU:HB3  | 1.61                     | 0.83              |
| 2:I:313:LEU:HD13 | 2:I:321:GLU:HA   | 1.62                     | 0.81              |
| 2:C:1102:LEU:HB2 | 3:D:7:LYS:HB2    | 1.63                     | 0.81              |
| 2:C:674:VAL:HA   | 2:C:869:VAL:HG13 | 1.63                     | 0.81              |
| 2:I:683:ASN:HB2  | 2:I:872:ASN:HB2  | 1.62                     | 0.81              |
| 4:K:39:VAL:HB    | 4:K:72:ARG:HD2   | 1.62                     | 0.80              |
| 3:J:800:LYS:HB3  | 3:J:822:ALA:HB2  | 1.63                     | 0.80              |
| 3:D:166:GLN:HB3  | 3:D:396:VAL:HG22 | 1.62                     | 0.80              |
| 4:E:67:GLU:HB3   | 4:E:73:LEU:HD11  | 1.62                     | 0.80              |
| 2:I:328:LEU:HD23 | 2:I:437:ARG:HD2  | 1.63                     | 0.80              |
| 2:I:751:PRO:HB3  | 2:I:794:PRO:HA   | 1.62                     | 0.80              |
| 2:I:1102:LEU:HB2 | 3:J:7:LYS:HB2    | 1.62                     | 0.80              |
| 3:D:700:VAL:HG22 | 3:D:718:PRO:HG3  | 1.63                     | 0.79              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:428:ARG:HE    | 2:C:451:LEU:HD21  | 1.48                     | 0.79              |
| 2:I:32:ALA:HB1    | 2:I:73:ILE:HD13   | 1.63                     | 0.79              |
| 3:D:974:ILE:HG12  | 3:D:991:GLN:HE21  | 1.48                     | 0.79              |
| 2:C:313:LEU:HD13  | 2:C:321:GLU:HA    | 1.63                     | 0.79              |
| 2:I:658:GLY:H     | 2:I:661:SER:HB3   | 1.47                     | 0.78              |
| 4:E:39:VAL:HB     | 4:E:72:ARG:HD2    | 1.66                     | 0.78              |
| 3:D:660:LYS:HD2   | 3:D:694:VAL:HG13  | 1.65                     | 0.78              |
| 3:D:226:PRO:HA    | 3:D:330:SER:HA    | 1.63                     | 0.78              |
| 3:D:1122:LEU:HD23 | 3:D:1140:ILE:HD13 | 1.64                     | 0.78              |
| 3:D:167:GLU:HB2   | 3:D:199:MET:HE3   | 1.65                     | 0.77              |
| 3:J:1147:ARG:HH12 | 3:J:1191:PRO:HD3  | 1.50                     | 0.77              |
| 2:C:328:LEU:HD23  | 2:C:437:ARG:HD2   | 1.65                     | 0.77              |
| 2:I:537:LYS:HZ3   | 2:I:905:VAL:H     | 1.31                     | 0.77              |
| 2:C:683:ASN:HB2   | 2:C:872:ASN:HB2   | 1.67                     | 0.77              |
| 2:C:537:LYS:HZ3   | 2:C:905:VAL:H     | 1.33                     | 0.76              |
| 3:J:1122:LEU:HD23 | 3:J:1140:ILE:HD13 | 1.66                     | 0.76              |
| 1:A:53:VAL:HG22   | 1:A:54:THR:H      | 1.49                     | 0.76              |
| 3:D:977:ALA:HB2   | 3:J:831:GLY:HA3   | 1.66                     | 0.76              |
| 3:J:184:GLU:HG2   | 3:J:202:VAL:HG22  | 1.65                     | 0.76              |
| 5:L:271:ARG:HG2   | 5:L:328:GLU:HB3   | 1.67                     | 0.76              |
| 5:F:431:ARG:HG3   | 5:F:434:ARG:HE    | 1.49                     | 0.76              |
| 2:C:32:ALA:HB1    | 2:C:73:ILE:HD13   | 1.67                     | 0.76              |
| 1:A:42:ARG:HH12   | 2:C:857:ASP:HB3   | 1.51                     | 0.75              |
| 2:C:374:ASN:HD22  | 2:C:375:SER:H     | 1.34                     | 0.75              |
| 2:C:502:PRO:HB2   | 2:C:509:ALA:HB3   | 1.68                     | 0.75              |
| 2:I:584:GLU:HB3   | 2:I:666:LEU:H     | 1.52                     | 0.75              |
| 3:D:349:PRO:HB3   | 5:F:112:GLU:HG2   | 1.70                     | 0.74              |
| 3:D:400:VAL:HG23  | 3:D:443:VAL:HG21  | 1.68                     | 0.74              |
| 4:K:30:LEU:HD23   | 4:K:63:TRP:HB3    | 1.69                     | 0.74              |
| 2:C:373:VAL:HG12  | 2:C:374:ASN:H     | 1.53                     | 0.74              |
| 2:I:432:ARG:HH12  | 2:I:518:ARG:HH21  | 1.35                     | 0.74              |
| 2:I:1060:ILE:HD12 | 2:I:1061:GLU:H    | 1.52                     | 0.74              |
| 2:C:197:LEU:HD23  | 2:C:200:LEU:HD23  | 1.70                     | 0.73              |
| 2:I:515:ALA:HB3   | 2:I:524:VAL:HG21  | 1.68                     | 0.73              |
| 3:D:1267:ARG:HE   | 3:D:1267:ARG:H    | 1.34                     | 0.73              |
| 2:C:684:PHE:HE1   | 3:D:783:ARG:HB2   | 1.52                     | 0.73              |
| 3:J:974:ILE:HG12  | 3:J:991:GLN:HE21  | 1.54                     | 0.73              |
| 2:C:14:PRO:HB3    | 2:C:586:ARG:HH22  | 1.52                     | 0.73              |
| 2:C:324:ASP:HB3   | 2:C:327:HIS:HB2   | 1.69                     | 0.73              |
| 2:C:836:GLY:H     | 2:C:849:VAL:HB    | 1.54                     | 0.73              |
| 2:C:584:GLU:HB3   | 2:C:666:LEU:H     | 1.54                     | 0.73              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:1103:HIS:HB2  | 3:D:1462:LEU:HD11 | 1.69                     | 0.73              |
| 2:I:197:LEU:HD23  | 2:I:200:LEU:HD23  | 1.71                     | 0.73              |
| 2:I:684:PHE:HE1   | 3:J:783:ARG:HB2   | 1.52                     | 0.73              |
| 2:I:373:VAL:HG12  | 2:I:374:ASN:H     | 1.54                     | 0.73              |
| 3:D:1147:ARG:HH12 | 3:D:1191:PRO:HD3  | 1.52                     | 0.72              |
| 4:K:67:GLU:HB3    | 4:K:73:LEU:HD11   | 1.69                     | 0.72              |
| 2:I:278:GLU:HG3   | 2:I:284:GLY:HA2   | 1.70                     | 0.72              |
| 4:K:31:LEU:HG     | 4:K:60:ALA:HB2    | 1.71                     | 0.72              |
| 2:C:146:VAL:HG23  | 2:C:280:LYS:HD2   | 1.71                     | 0.72              |
| 1:G:53:VAL:HG22   | 1:G:54:THR:H      | 1.54                     | 0.72              |
| 2:C:165:LEU:HB2   | 2:C:168:ARG:HB2   | 1.71                     | 0.72              |
| 2:C:1046:ALA:HB1  | 3:D:1471:LEU:HD11 | 1.72                     | 0.72              |
| 2:C:742:ILE:HG22  | 2:C:756:VAL:HG12  | 1.72                     | 0.71              |
| 1:H:52:ALA:HB2    | 1:H:171:PHE:HA    | 1.71                     | 0.71              |
| 2:I:674:VAL:HA    | 2:I:869:VAL:HG13  | 1.70                     | 0.71              |
| 3:D:646:LYS:HE3   | 3:D:688:TRP:HZ2   | 1.56                     | 0.71              |
| 1:A:158:ILE:HG22  | 1:A:160:ASP:H     | 1.56                     | 0.71              |
| 1:B:161:ARG:HG3   | 1:B:162:ILE:H     | 1.55                     | 0.71              |
| 1:H:51:THR:HG21   | 1:H:86:VAL:HG23   | 1.71                     | 0.71              |
| 3:J:1267:ARG:HE   | 3:J:1267:ARG:H    | 1.37                     | 0.71              |
| 2:I:144:PRO:HB3   | 2:I:164:PRO:O     | 1.90                     | 0.71              |
| 2:I:139:GLN:HB3   | 2:I:334:ARG:HB2   | 1.73                     | 0.70              |
| 4:K:49:ARG:HA     | 4:K:54:LEU:HG     | 1.71                     | 0.70              |
| 2:C:261:LEU:HB2   | 2:C:291:VAL:HG22  | 1.71                     | 0.70              |
| 2:C:690:ILE:HG13  | 2:C:852:ILE:HG23  | 1.73                     | 0.70              |
| 2:C:374:ASN:HD21  | 5:F:291:ARG:HD2   | 1.56                     | 0.70              |
| 2:C:995:MET:HE3   | 2:C:996:LYS:H     | 1.57                     | 0.70              |
| 1:G:55:SER:HB3    | 1:G:143:ARG:HB2   | 1.73                     | 0.70              |
| 1:B:52:ALA:HB2    | 1:B:171:PHE:HA    | 1.74                     | 0.70              |
| 2:C:432:ARG:HH12  | 2:C:518:ARG:HH21  | 1.39                     | 0.70              |
| 2:C:278:GLU:HG3   | 2:C:284:GLY:HA2   | 1.73                     | 0.70              |
| 5:L:203:ILE:HG12  | 5:L:239:VAL:HG21  | 1.73                     | 0.70              |
| 1:H:78:ILE:HD12   | 1:H:130:ALA:HB2   | 1.72                     | 0.70              |
| 2:I:261:LEU:HB2   | 2:I:291:VAL:HG22  | 1.72                     | 0.70              |
| 2:I:234:ALA:HA    | 2:I:237:ARG:HB2   | 1.74                     | 0.70              |
| 2:C:1008:ARG:HD3  | 2:C:1028:GLY:HA2  | 1.74                     | 0.69              |
| 1:H:161:ARG:HG3   | 1:H:162:ILE:H     | 1.56                     | 0.69              |
| 2:I:876:VAL:HG11  | 2:I:885:ILE:HD11  | 1.72                     | 0.69              |
| 6:N:85:GLN:HE21   | 7:R:25:DT:H4'     | 1.56                     | 0.69              |
| 2:C:515:ALA:HB3   | 2:C:524:VAL:HG21  | 1.73                     | 0.69              |
| 2:C:1094:ALA:HB2  | 3:D:520:LEU:HD13  | 1.74                     | 0.69              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:C:144:PRO:HB3  | 2:C:164:PRO:O     | 1.92                     | 0.69              |
| 4:E:30:LEU:HD23  | 4:E:63:TRP:HB3    | 1.75                     | 0.69              |
| 3:D:550:ARG:HH21 | 5:F:226:ASP:HB2   | 1.56                     | 0.69              |
| 5:F:411:ARG:HD3  | 7:O:1:DC:H2'      | 1.74                     | 0.69              |
| 3:J:1264:GLU:HB3 | 3:J:1266:ARG:HG3  | 1.75                     | 0.69              |
| 1:G:218:LEU:HG   | 1:H:222:LEU:HD11  | 1.74                     | 0.69              |
| 5:L:428:SER:HA   | 5:L:434:ARG:HH21  | 1.55                     | 0.69              |
| 3:J:543:LEU:HG   | 3:J:600:LEU:HD23  | 1.74                     | 0.69              |
| 1:B:51:THR:HG21  | 1:B:86:VAL:HG23   | 1.74                     | 0.69              |
| 3:D:44:LEU:HB3   | 3:D:525:ARG:HH22  | 1.58                     | 0.69              |
| 3:J:700:VAL:HG22 | 3:J:718:PRO:HG3   | 1.74                     | 0.69              |
| 3:D:213:VAL:HG22 | 3:D:385:VAL:HG12  | 1.75                     | 0.68              |
| 2:I:502:PRO:HB2  | 2:I:509:ALA:HB3   | 1.74                     | 0.68              |
| 1:A:153:ALA:HB1  | 1:A:166:PRO:HB2   | 1.74                     | 0.68              |
| 3:J:44:LEU:HB3   | 3:J:525:ARG:HH22  | 1.57                     | 0.68              |
| 2:I:157:ARG:HH11 | 2:I:157:ARG:HA    | 1.58                     | 0.68              |
| 1:B:78:ILE:HD12  | 1:B:130:ALA:HB2   | 1.74                     | 0.68              |
| 2:C:853:LEU:HD12 | 2:C:854:PRO:HD2   | 1.75                     | 0.68              |
| 5:F:376:LEU:HD21 | 5:F:423:LEU:HG    | 1.74                     | 0.68              |
| 2:I:1094:ALA:HB2 | 3:J:520:LEU:HD13  | 1.75                     | 0.68              |
| 2:C:572:ILE:HD11 | 2:C:703:ILE:HD11  | 1.75                     | 0.68              |
| 2:C:971:LYS:HG2  | 2:C:988:VAL:HG12  | 1.74                     | 0.68              |
| 5:F:157:GLN:HE22 | 5:F:171:VAL:HG21  | 1.59                     | 0.68              |
| 2:I:165:LEU:HB2  | 2:I:168:ARG:HB2   | 1.76                     | 0.68              |
| 2:C:607:ASP:O    | 2:C:609:THR:N     | 2.26                     | 0.68              |
| 3:D:354:ILE:HD11 | 3:D:369:ALA:HB2   | 1.75                     | 0.68              |
| 2:I:154:ARG:HD2  | 2:I:157:ARG:HB2   | 1.75                     | 0.68              |
| 3:J:900:ILE:HG12 | 3:J:914:LEU:HD21  | 1.75                     | 0.68              |
| 5:L:376:LEU:HD21 | 5:L:423:LEU:HG    | 1.74                     | 0.68              |
| 5:L:137:LEU:HD11 | 5:L:177:LYS:HE3   | 1.76                     | 0.68              |
| 3:D:1264:GLU:HB3 | 3:D:1266:ARG:HG3  | 1.75                     | 0.68              |
| 2:I:995:MET:HE3  | 2:I:996:LYS:H     | 1.58                     | 0.68              |
| 2:C:658:GLY:H    | 2:C:661:SER:HB3   | 1.60                     | 0.67              |
| 2:I:571:LEU:HB2  | 2:I:574:ALA:HB2   | 1.76                     | 0.67              |
| 6:N:49:VAL:HG11  | 6:N:59:LEU:HD22   | 1.76                     | 0.67              |
| 2:I:193:LEU:HD22 | 2:I:221:LEU:HD11  | 1.76                     | 0.67              |
| 3:J:96:ALA:HB2   | 3:J:555:LYS:HG2   | 1.76                     | 0.67              |
| 3:J:100:ALA:H    | 3:J:575:GLN:HE22  | 1.42                     | 0.67              |
| 3:J:192:ALA:HB1  | 3:J:193:PRO:HD2   | 1.76                     | 0.67              |
| 1:A:184:THR:HB   | 1:A:194:LYS:HB3   | 1.77                     | 0.67              |
| 3:D:1042:ARG:HB3 | 3:D:1057:VAL:HG21 | 1.77                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:H:184:THR:HG23  | 1:H:192:LEU:HB2   | 1.75                     | 0.67              |
| 3:J:203:ALA:HA    | 3:J:395:VAL:HA    | 1.76                     | 0.67              |
| 6:M:155:PHE:HB2   | 6:M:163:LEU:HD11  | 1.77                     | 0.67              |
| 3:D:520:LEU:HB3   | 3:D:525:ARG:HD3   | 1.77                     | 0.67              |
| 2:C:571:LEU:HB2   | 2:C:574:ALA:HB2   | 1.77                     | 0.67              |
| 3:D:356:PRO:HG2   | 3:D:359:ALA:HB2   | 1.76                     | 0.67              |
| 1:G:174:VAL:HA    | 1:G:201:THR:HG22  | 1.76                     | 0.67              |
| 2:I:603:VAL:HA    | 2:I:613:VAL:HG12  | 1.77                     | 0.67              |
| 2:C:157:ARG:HA    | 2:C:157:ARG:HH11  | 1.59                     | 0.67              |
| 2:I:853:LEU:HD12  | 2:I:854:PRO:HD2   | 1.76                     | 0.67              |
| 1:B:56:VAL:HG21   | 1:B:82:LEU:HD13   | 1.76                     | 0.67              |
| 2:C:376:ARG:HG3   | 2:C:377:PRO:HD3   | 1.77                     | 0.67              |
| 3:D:560:GLN:HE22  | 5:F:236:ILE:HG21  | 1.60                     | 0.67              |
| 4:E:49:ARG:HA     | 4:E:54:LEU:HG     | 1.77                     | 0.67              |
| 2:C:577:PRO:HG2   | 2:C:580:MET:HG2   | 1.77                     | 0.66              |
| 2:I:108:ILE:HB    | 6:N:48:TYR:HB2    | 1.76                     | 0.66              |
| 1:A:222:LEU:HD21  | 1:B:218:LEU:HB3   | 1.77                     | 0.66              |
| 2:C:139:GLN:HB3   | 2:C:334:ARG:HB2   | 1.75                     | 0.66              |
| 3:D:860:LEU:HD12  | 3:D:860:LEU:H     | 1.60                     | 0.66              |
| 1:G:153:ALA:HB1   | 1:G:166:PRO:HB2   | 1.76                     | 0.66              |
| 2:I:874:LEU:HD13  | 3:J:783:ARG:HB3   | 1.76                     | 0.66              |
| 2:I:113:VAL:HG21  | 2:I:373:VAL:HG21  | 1.77                     | 0.66              |
| 2:I:1046:ALA:HB1  | 3:J:1471:LEU:HD11 | 1.78                     | 0.66              |
| 3:J:1254:GLN:HB3  | 3:J:1258:ARG:HB2  | 1.78                     | 0.66              |
| 3:D:166:GLN:HB2   | 3:D:394:LEU:HD21  | 1.77                     | 0.66              |
| 3:D:1493:LYS:HA   | 3:D:1496:GLU:HB2  | 1.78                     | 0.66              |
| 2:I:91:GLN:HA     | 2:I:119:PRO:HA    | 1.76                     | 0.66              |
| 3:J:97:THR:HG21   | 3:J:571:LYS:HG3   | 1.78                     | 0.66              |
| 7:O:24:DC:H42     | 8:P:2:DG:H1       | 1.44                     | 0.66              |
| 3:J:400:VAL:HG12  | 3:J:445:ARG:HG2   | 1.78                     | 0.66              |
| 1:G:184:THR:HB    | 1:G:194:LYS:HB3   | 1.78                     | 0.66              |
| 2:I:282:GLY:HA3   | 2:I:308:ARG:HH21  | 1.59                     | 0.66              |
| 3:D:1462:LEU:HD12 | 3:D:1463:LYS:H    | 1.58                     | 0.65              |
| 2:C:172:ILE:HA    | 2:C:186:VAL:HG22  | 1.79                     | 0.65              |
| 3:D:96:ALA:HB2    | 3:D:555:LYS:HG2   | 1.78                     | 0.65              |
| 3:D:661:MET:HG2   | 3:D:666:PHE:CZ    | 2.31                     | 0.65              |
| 3:D:1379:VAL:HG12 | 3:D:1419:PRO:HA   | 1.77                     | 0.65              |
| 3:D:1131:THR:HG22 | 3:J:1179:GLU:HB3  | 1.78                     | 0.65              |
| 1:A:55:SER:HB3    | 1:A:143:ARG:HB2   | 1.77                     | 0.65              |
| 2:I:304:LEU:HB3   | 2:I:305:PRO:HD3   | 1.78                     | 0.65              |
| 2:I:759:THR:HB    | 2:I:785:VAL:HG21  | 1.77                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:1008:ARG:HD3  | 2:I:1028:GLY:HA2  | 1.77                     | 0.65              |
| 3:J:8:VAL:HG21    | 3:J:1468:LEU:HD21 | 1.77                     | 0.65              |
| 4:E:31:LEU:HG     | 4:E:60:ALA:HB2    | 1.77                     | 0.65              |
| 2:C:101:ILE:HD12  | 2:C:108:ILE:HG23  | 1.79                     | 0.65              |
| 2:C:163:ILE:HD12  | 2:C:164:PRO:HD2   | 1.79                     | 0.65              |
| 3:D:203:ALA:HA    | 3:D:395:VAL:HA    | 1.77                     | 0.65              |
| 3:D:644:LEU:HD12  | 3:D:645:PRO:HD2   | 1.78                     | 0.65              |
| 3:J:1042:ARG:HB3  | 3:J:1057:VAL:HG21 | 1.76                     | 0.65              |
| 6:N:155:PHE:HB2   | 6:N:163:LEU:HD11  | 1.78                     | 0.65              |
| 2:C:304:LEU:HB3   | 2:C:305:PRO:HD3   | 1.78                     | 0.65              |
| 3:J:165:LYS:HE3   | 3:J:199:MET:HE1   | 1.77                     | 0.65              |
| 3:J:560:GLN:HE22  | 5:L:236:ILE:HG21  | 1.62                     | 0.65              |
| 2:C:1037:VAL:HG13 | 2:C:1049:LEU:HD11 | 1.79                     | 0.65              |
| 2:I:577:PRO:HG2   | 2:I:580:MET:HG2   | 1.77                     | 0.65              |
| 1:A:90:LEU:HB2    | 1:A:119:ASP:HA    | 1.77                     | 0.65              |
| 2:C:97:ARG:HE     | 2:C:112:GLU:HB2   | 1.61                     | 0.65              |
| 2:C:168:ARG:HD3   | 2:C:268:ASP:HB3   | 1.79                     | 0.65              |
| 3:D:670:VAL:HB    | 5:F:364:LEU:HD11  | 1.77                     | 0.65              |
| 2:I:607:ASP:O     | 2:I:609:THR:N     | 2.29                     | 0.65              |
| 3:J:698:LYS:HG2   | 3:J:756:GLN:HG2   | 1.79                     | 0.65              |
| 2:I:172:ILE:HA    | 2:I:186:VAL:HG22  | 1.79                     | 0.64              |
| 3:J:367:ILE:HG22  | 3:J:368:VAL:HG23  | 1.79                     | 0.64              |
| 2:C:742:ILE:HD13  | 2:C:803:ARG:HD2   | 1.79                     | 0.64              |
| 3:D:650:LEU:HD12  | 3:D:688:TRP:HZ3   | 1.63                     | 0.64              |
| 2:C:579:VAL:HG13  | 2:C:842:ARG:HH22  | 1.63                     | 0.64              |
| 3:D:241:VAL:HG22  | 3:D:312:ARG:HD3   | 1.80                     | 0.64              |
| 2:I:711:GLU:HG2   | 2:I:822:VAL:HG12  | 1.80                     | 0.64              |
| 3:D:500:ARG:HD3   | 3:D:503:LEU:HD12  | 1.77                     | 0.64              |
| 3:J:670:VAL:HB    | 5:L:364:LEU:HD11  | 1.78                     | 0.64              |
| 3:D:266:GLU:HG3   | 3:D:286:ALA:HB2   | 1.79                     | 0.64              |
| 2:C:282:GLY:HA3   | 2:C:308:ARG:HH21  | 1.61                     | 0.64              |
| 2:C:154:ARG:HD2   | 2:C:157:ARG:HB2   | 1.79                     | 0.64              |
| 2:C:759:THR:HB    | 2:C:785:VAL:HG21  | 1.79                     | 0.64              |
| 3:D:407:VAL:HG22  | 3:D:409:VAL:H     | 1.62                     | 0.64              |
| 4:E:79:LEU:HG     | 4:E:80:VAL:HG13   | 1.80                     | 0.64              |
| 5:F:271:ARG:HG2   | 5:F:328:GLU:HB3   | 1.78                     | 0.64              |
| 2:I:470:PRO:HG3   | 2:I:485:TYR:CZ    | 2.33                     | 0.64              |
| 1:A:108:GLU:HG2   | 1:A:131:THR:HG23  | 1.79                     | 0.64              |
| 3:D:132:TYR:HA    | 3:D:456:MET:HB3   | 1.79                     | 0.64              |
| 3:D:1254:GLN:HB3  | 3:D:1258:ARG:HB2  | 1.79                     | 0.64              |
| 2:I:181:VAL:HG22  | 2:I:182:VAL:H     | 1.63                     | 0.64              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:I:742:ILE:HD13  | 2:I:803:ARG:HD2  | 1.80                     | 0.64              |
| 3:J:1395:LEU:HD11 | 3:J:1400:VAL:HB  | 1.79                     | 0.64              |
| 2:C:886:LEU:HD21  | 3:D:951:ILE:HD13 | 1.80                     | 0.64              |
| 3:J:661:MET:HG2   | 3:J:666:PHE:CZ   | 2.33                     | 0.64              |
| 1:G:158:ILE:HG22  | 1:G:160:ASP:H    | 1.63                     | 0.63              |
| 1:A:174:VAL:HA    | 1:A:201:THR:HG22 | 1.79                     | 0.63              |
| 2:C:91:GLN:HA     | 2:C:119:PRO:HA   | 1.79                     | 0.63              |
| 3:D:543:LEU:HG    | 3:D:600:LEU:HD23 | 1.80                     | 0.63              |
| 3:D:97:THR:HG21   | 3:D:571:LYS:HG3  | 1.80                     | 0.63              |
| 3:J:132:TYR:HA    | 3:J:456:MET:HB3  | 1.80                     | 0.63              |
| 3:J:822:ALA:HB3   | 3:J:825:ALA:HB2  | 1.80                     | 0.63              |
| 3:J:1379:VAL:HG12 | 3:J:1419:PRO:HA  | 1.80                     | 0.63              |
| 5:L:157:GLN:HE22  | 5:L:171:VAL:HG21 | 1.63                     | 0.63              |
| 3:D:831:GLY:HA3   | 3:J:977:ALA:HB2  | 1.80                     | 0.63              |
| 1:A:26:GLU:HG3    | 1:A:186:LEU:HD12 | 1.80                     | 0.63              |
| 3:D:800:LYS:HB3   | 3:D:822:ALA:HB2  | 1.80                     | 0.63              |
| 2:I:101:ILE:HD12  | 2:I:108:ILE:HG23 | 1.80                     | 0.63              |
| 3:J:167:GLU:HB2   | 3:J:199:MET:HE3  | 1.81                     | 0.63              |
| 3:J:520:LEU:HB3   | 3:J:525:ARG:HD3  | 1.79                     | 0.63              |
| 3:J:677:LEU:HD21  | 3:J:687:VAL:HG11 | 1.80                     | 0.63              |
| 3:J:860:LEU:H     | 3:J:860:LEU:HD12 | 1.63                     | 0.63              |
| 3:J:1099:VAL:O    | 3:J:1103:HIS:HB3 | 1.99                     | 0.63              |
| 1:G:90:LEU:HB2    | 1:G:119:ASP:HA   | 1.81                     | 0.63              |
| 1:G:198:ARG:HH22  | 2:I:932:GLU:HB3  | 1.64                     | 0.63              |
| 2:I:742:ILE:HG22  | 2:I:756:VAL:HG12 | 1.81                     | 0.63              |
| 5:L:293:LEU:HD11  | 5:L:306:ILE:HD13 | 1.81                     | 0.63              |
| 2:C:108:ILE:HB    | 6:M:48:TYR:HB2   | 1.81                     | 0.62              |
| 3:J:550:ARG:HH21  | 5:L:226:ASP:HB2  | 1.63                     | 0.62              |
| 2:C:181:VAL:HG22  | 2:C:182:VAL:H    | 1.63                     | 0.62              |
| 1:H:87:VAL:HG12   | 1:H:122:ILE:HG12 | 1.80                     | 0.62              |
| 2:I:682:TYR:HA    | 3:J:633:VAL:HG11 | 1.80                     | 0.62              |
| 2:I:1019:GLN:HE21 | 3:J:617:ASN:HB3  | 1.64                     | 0.62              |
| 3:J:215:TYR:HB3   | 3:J:381:ALA:HB3  | 1.80                     | 0.62              |
| 3:J:1462:LEU:HD12 | 3:J:1463:LYS:H   | 1.64                     | 0.62              |
| 1:B:184:THR:HG23  | 1:B:192:LEU:HB2  | 1.81                     | 0.62              |
| 2:C:470:PRO:HG3   | 2:C:485:TYR:CZ   | 2.34                     | 0.62              |
| 3:D:211:VAL:HG13  | 3:D:345:TYR:HB2  | 1.81                     | 0.62              |
| 1:G:23:PHE:HE2    | 1:G:199:ILE:HD12 | 1.64                     | 0.62              |
| 1:H:58:ILE:HD13   | 1:H:61:VAL:HB    | 1.81                     | 0.62              |
| 3:J:680:GLN:C     | 3:J:682:ASP:H    | 2.06                     | 0.62              |
| 2:C:239:PHE:HA    | 2:C:242:LEU:HD12 | 1.81                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:313:LEU:HG    | 3:D:314:PRO:HD2   | 1.81                     | 0.62              |
| 3:D:353:VAL:HG21  | 3:D:387:LEU:HD21  | 1.81                     | 0.62              |
| 3:D:900:ILE:HG12  | 3:D:914:LEU:HD21  | 1.82                     | 0.62              |
| 1:G:25:LEU:HD23   | 1:G:28:LEU:HD11   | 1.81                     | 0.62              |
| 1:G:26:GLU:HG3    | 1:G:186:LEU:HD12  | 1.80                     | 0.62              |
| 2:I:97:ARG:HE     | 2:I:112:GLU:HB2   | 1.64                     | 0.62              |
| 2:I:14:PRO:HB3    | 2:I:586:ARG:HH22  | 1.64                     | 0.62              |
| 2:I:163:ILE:HD12  | 2:I:164:PRO:HD2   | 1.82                     | 0.62              |
| 1:B:152:PRO:HD2   | 1:B:155:ARG:HG3   | 1.82                     | 0.62              |
| 2:C:498:GLN:HG3   | 3:D:1068:LEU:HD11 | 1.80                     | 0.62              |
| 3:J:1197:ARG:HE   | 3:J:1398:TRP:HB3  | 1.65                     | 0.62              |
| 1:G:222:LEU:HD21  | 1:H:218:LEU:HB3   | 1.81                     | 0.61              |
| 2:I:249:LYS:HB2   | 2:I:252:LYS:HE3   | 1.82                     | 0.61              |
| 1:B:101:LEU:HD22  | 1:B:102:ARG:H     | 1.65                     | 0.61              |
| 2:C:129:ILE:HG12  | 2:C:386:PHE:HB3   | 1.82                     | 0.61              |
| 3:J:792:ILE:HG21  | 3:J:941:LEU:HD13  | 1.82                     | 0.61              |
| 2:I:339:LEU:HD13  | 2:I:385:PHE:CZ    | 2.35                     | 0.61              |
| 3:J:176:ASP:OD1   | 3:J:177:ALA:N     | 2.33                     | 0.61              |
| 3:J:1103:HIS:HB2  | 3:J:1462:LEU:HD11 | 1.82                     | 0.61              |
| 1:B:177:VAL:HG12  | 1:B:199:ILE:HG12  | 1.82                     | 0.61              |
| 2:C:676:ILE:HG22  | 2:C:873:PRO:HB3   | 1.83                     | 0.61              |
| 3:J:1197:ARG:NE   | 3:J:1398:TRP:HB3  | 2.15                     | 0.61              |
| 1:A:218:LEU:HG    | 1:B:222:LEU:HD11  | 1.81                     | 0.61              |
| 3:D:636:GLN:HG2   | 3:D:637:LEU:HD12  | 1.83                     | 0.61              |
| 3:D:1099:VAL:O    | 3:D:1103:HIS:HB3  | 2.01                     | 0.61              |
| 2:I:64:LEU:HD21   | 2:I:66:LEU:HG     | 1.82                     | 0.61              |
| 3:J:365:GLU:H     | 3:J:379:ALA:HB3   | 1.65                     | 0.61              |
| 3:D:314:PRO:HG2   | 3:D:317:MET:HB3   | 1.83                     | 0.61              |
| 1:A:23:PHE:HE2    | 1:A:199:ILE:HD12  | 1.65                     | 0.61              |
| 3:D:698:LYS:HG2   | 3:D:756:GLN:HG2   | 1.83                     | 0.61              |
| 3:D:1197:ARG:NE   | 3:D:1398:TRP:HB3  | 2.15                     | 0.61              |
| 2:I:376:ARG:HG3   | 2:I:377:PRO:HD3   | 1.83                     | 0.61              |
| 2:I:1037:VAL:HG13 | 2:I:1049:LEU:HD11 | 1.82                     | 0.61              |
| 6:N:119:ARG:HG3   | 6:N:120:GLY:H     | 1.65                     | 0.61              |
| 3:J:650:LEU:HD12  | 3:J:688:TRP:HZ3   | 1.66                     | 0.61              |
| 1:A:53:VAL:HG23   | 1:A:144:VAL:HG22  | 1.82                     | 0.61              |
| 3:D:1132:LEU:HD12 | 3:J:1181:GLY:HA3  | 1.83                     | 0.61              |
| 2:I:1019:GLN:HG3  | 3:J:617:ASN:HD22  | 1.65                     | 0.61              |
| 3:J:644:LEU:HD12  | 3:J:645:PRO:HD2   | 1.83                     | 0.61              |
| 2:C:569:VAL:H     | 2:C:995:MET:HE2   | 1.66                     | 0.60              |
| 2:I:694:LEU:HD11  | 2:I:868:ASP:HB3   | 1.82                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:371:ILE:HG23  | 3:D:372:ASP:H     | 1.66                     | 0.60              |
| 4:E:38:THR:OG1    | 4:E:39:VAL:N      | 2.34                     | 0.60              |
| 1:H:101:LEU:HD22  | 1:H:102:ARG:H     | 1.65                     | 0.60              |
| 2:I:886:LEU:HD21  | 3:J:951:ILE:HD13  | 1.83                     | 0.60              |
| 3:D:224:ARG:NH2   | 3:D:254:GLU:OE2   | 2.34                     | 0.60              |
| 3:J:354:ILE:HD11  | 3:J:369:ALA:HB2   | 1.83                     | 0.60              |
| 2:I:369:PRO:O     | 2:I:373:VAL:HG23  | 2.01                     | 0.60              |
| 2:I:756:VAL:HG11  | 2:I:823:VAL:HG11  | 1.84                     | 0.60              |
| 3:J:169:TYR:O     | 3:J:392:SER:HB2   | 2.01                     | 0.60              |
| 1:B:58:ILE:HD13   | 1:B:61:VAL:HB     | 1.84                     | 0.60              |
| 2:I:971:LYS:HG2   | 2:I:988:VAL:HG12  | 1.82                     | 0.60              |
| 2:C:711:GLU:HG2   | 2:C:822:VAL:HG12  | 1.84                     | 0.60              |
| 5:F:293:LEU:HD11  | 5:F:306:ILE:HD13  | 1.83                     | 0.60              |
| 1:G:72:LYS:HG3    | 2:I:606:VAL:HG11  | 1.83                     | 0.60              |
| 2:I:146:VAL:HG23  | 2:I:280:LYS:HD2   | 1.83                     | 0.60              |
| 3:J:1125:MET:HG3  | 3:J:1132:LEU:HG   | 1.84                     | 0.60              |
| 1:B:28:LEU:HB3    | 1:B:193:ASP:HB2   | 1.83                     | 0.59              |
| 2:C:87:ASP:HA     | 2:C:131:GLY:HA3   | 1.84                     | 0.59              |
| 3:D:521:PRO:HD2   | 3:D:524:LEU:HD12  | 1.84                     | 0.59              |
| 5:L:181:LEU:HD23  | 5:L:185:LEU:HB2   | 1.83                     | 0.59              |
| 2:C:603:VAL:HA    | 2:C:613:VAL:HG12  | 1.84                     | 0.59              |
| 3:J:660:LYS:HD2   | 3:J:694:VAL:HG13  | 1.83                     | 0.59              |
| 3:D:192:ALA:HB1   | 3:D:193:PRO:HD2   | 1.83                     | 0.59              |
| 5:F:180:SER:O     | 5:F:181:LEU:HD12  | 2.01                     | 0.59              |
| 2:I:239:PHE:HA    | 2:I:242:LEU:HD12  | 1.84                     | 0.59              |
| 2:C:369:PRO:O     | 2:C:373:VAL:HG23  | 2.01                     | 0.59              |
| 2:C:905:VAL:HG12  | 2:C:906:PHE:HD2   | 1.66                     | 0.59              |
| 1:G:104:GLU:HG3   | 1:G:137:LYS:HG2   | 1.85                     | 0.59              |
| 6:N:82:LEU:HB3    | 6:N:89:ARG:HG3    | 1.84                     | 0.59              |
| 3:D:792:ILE:HG21  | 3:D:941:LEU:HD13  | 1.85                     | 0.59              |
| 3:D:1197:ARG:HE   | 3:D:1398:TRP:HB3  | 1.67                     | 0.59              |
| 2:I:939:ARG:HB3   | 2:I:982:PRO:HG3   | 1.83                     | 0.59              |
| 2:C:1060:ILE:HD12 | 2:C:1061:GLU:H    | 1.67                     | 0.59              |
| 5:F:412:ILE:HD13  | 5:F:415:ILE:HD12  | 1.84                     | 0.59              |
| 2:I:439:CYS:HB2   | 2:I:541:SER:HB3   | 1.84                     | 0.59              |
| 3:J:681:ARG:O     | 3:J:683:ILE:HG12  | 2.02                     | 0.59              |
| 3:J:917:GLN:HE22  | 3:J:1168:LEU:HD11 | 1.67                     | 0.59              |
| 3:J:1123:PHE:HB3  | 3:J:1132:LEU:HD22 | 1.84                     | 0.59              |
| 3:D:310:LEU:H     | 3:D:310:LEU:HD12  | 1.67                     | 0.59              |
| 1:B:179:PHE:HB3   | 1:B:197:LEU:HD13  | 1.85                     | 0.59              |
| 3:D:286:ALA:O     | 3:D:311:LEU:HA    | 2.03                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:160:ALA:HB3   | 2:I:174:LEU:HD13  | 1.85                     | 0.59              |
| 1:A:14:THR:OG1    | 1:B:231:SER:OG    | 2.20                     | 0.59              |
| 3:D:1198:TYR:HE2  | 3:D:1432:LYS:HE2  | 1.68                     | 0.59              |
| 5:F:137:LEU:HD11  | 5:F:177:LYS:HE3   | 1.85                     | 0.59              |
| 2:C:458:TYR:HB3   | 2:C:470:PRO:HG2   | 1.84                     | 0.58              |
| 3:D:367:ILE:HG22  | 3:D:368:VAL:HG23  | 1.85                     | 0.58              |
| 1:G:35:THR:HG23   | 1:H:39:PRO:HA     | 1.85                     | 0.58              |
| 2:I:357:GLU:HG2   | 5:L:216:LYS:HE2   | 1.85                     | 0.58              |
| 1:A:25:LEU:HD23   | 1:A:28:LEU:HD11   | 1.84                     | 0.58              |
| 3:D:48:ARG:HA     | 3:D:78:VAL:HG22   | 1.83                     | 0.58              |
| 2:I:557:ARG:HD3   | 2:I:879:ARG:HB3   | 1.84                     | 0.58              |
| 3:J:48:ARG:HA     | 3:J:78:VAL:HG22   | 1.85                     | 0.58              |
| 3:J:636:GLN:HG2   | 3:J:637:LEU:HD12  | 1.85                     | 0.58              |
| 2:C:64:LEU:HD21   | 2:C:66:LEU:HG     | 1.85                     | 0.58              |
| 2:C:160:ALA:HB3   | 2:C:174:LEU:HD13  | 1.84                     | 0.58              |
| 3:D:8:VAL:HG21    | 3:D:1468:LEU:HD21 | 1.84                     | 0.58              |
| 3:J:141:VAL:HA    | 3:J:146:PRO:HA    | 1.85                     | 0.58              |
| 3:J:402:PRO:HA    | 3:J:443:VAL:HA    | 1.85                     | 0.58              |
| 4:K:38:THR:OG1    | 4:K:39:VAL:N      | 2.36                     | 0.58              |
| 1:B:97:THR:HG21   | 1:B:120:VAL:HG21  | 1.84                     | 0.58              |
| 2:I:690:ILE:HG13  | 2:I:852:ILE:HG23  | 1.86                     | 0.58              |
| 2:C:729:LEU:HD12  | 2:C:734:LEU:HD13  | 1.84                     | 0.58              |
| 5:F:96:VAL:HA     | 5:F:225:LEU:HD11  | 1.86                     | 0.58              |
| 2:I:285:LEU:HD11  | 2:I:301:GLU:HB3   | 1.85                     | 0.58              |
| 2:I:836:GLY:H     | 2:I:849:VAL:HB    | 1.68                     | 0.58              |
| 3:J:715:ALA:HB3   | 3:J:764:LEU:HA    | 1.86                     | 0.58              |
| 6:N:124:LEU:HD21  | 8:S:2:DG:H5"      | 1.85                     | 0.58              |
| 2:C:756:VAL:HG11  | 2:C:823:VAL:HG11  | 1.85                     | 0.58              |
| 2:C:876:VAL:HG11  | 2:C:885:ILE:HD11  | 1.85                     | 0.58              |
| 2:C:682:TYR:HA    | 3:D:633:VAL:HG11  | 1.84                     | 0.58              |
| 1:G:44:LEU:O      | 1:G:174:VAL:HG11  | 2.03                     | 0.58              |
| 3:J:1198:TYR:HE2  | 3:J:1432:LYS:HE2  | 1.69                     | 0.58              |
| 1:H:177:VAL:HG12  | 1:H:199:ILE:HG12  | 1.85                     | 0.58              |
| 2:I:65:VAL:HG13   | 2:I:101:ILE:HB    | 1.86                     | 0.58              |
| 3:D:44:LEU:HD23   | 3:D:525:ARG:HH12  | 1.69                     | 0.58              |
| 5:F:203:ILE:HG12  | 5:F:239:VAL:HG21  | 1.86                     | 0.58              |
| 5:F:319:VAL:O     | 5:F:323:LEU:HB2   | 2.04                     | 0.58              |
| 3:J:853:VAL:HG22  | 3:J:858:LEU:HD23  | 1.85                     | 0.58              |
| 1:A:94:MET:O      | 1:A:146:ARG:HD3   | 2.03                     | 0.58              |
| 3:D:1395:LEU:HD11 | 3:D:1400:VAL:HB   | 1.86                     | 0.58              |
| 2:I:729:LEU:HD12  | 2:I:734:LEU:HD13  | 1.86                     | 0.58              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:C:605:LYS:HG2  | 2:C:612:ALA:HB3   | 1.85                     | 0.57              |
| 3:D:793:THR:O    | 3:D:879:ARG:NH1   | 2.34                     | 0.57              |
| 5:F:372:ALA:HA   | 5:F:375:LYS:HE3   | 1.86                     | 0.57              |
| 2:I:905:VAL:HG12 | 2:I:906:PHE:HD2   | 1.69                     | 0.57              |
| 3:J:216:LEU:N    | 3:J:382:GLU:O     | 2.37                     | 0.57              |
| 1:G:14:THR:OG1   | 1:H:231:SER:OG    | 2.20                     | 0.57              |
| 2:I:339:LEU:HD13 | 2:I:385:PHE:HZ    | 1.68                     | 0.57              |
| 3:J:521:PRO:HD2  | 3:J:524:LEU:HD12  | 1.86                     | 0.57              |
| 1:A:53:VAL:HA    | 1:A:144:VAL:HG13  | 1.86                     | 0.57              |
| 3:D:692:GLU:HG2  | 3:D:720:LEU:HD12  | 1.85                     | 0.57              |
| 3:D:715:ALA:HB3  | 3:D:764:LEU:HA    | 1.86                     | 0.57              |
| 2:I:195:LEU:O    | 2:I:198:ARG:HG3   | 2.04                     | 0.57              |
| 3:J:471:GLU:O    | 3:J:475:ARG:HG2   | 2.04                     | 0.57              |
| 2:C:321:GLU:HG2  | 2:C:322:VAL:N     | 2.20                     | 0.57              |
| 2:C:675:ALA:HB3  | 2:C:870:ILE:HA    | 1.86                     | 0.57              |
| 2:I:498:GLN:HG3  | 3:J:1068:LEU:HD11 | 1.86                     | 0.57              |
| 3:J:1208:ASP:HB2 | 3:J:1215:VAL:HA   | 1.86                     | 0.57              |
| 5:L:428:SER:HA   | 5:L:434:ARG:NH2   | 2.19                     | 0.57              |
| 3:J:125:GLN:HB2  | 3:J:130:ASN:HB3   | 1.87                     | 0.57              |
| 3:J:772:PRO:HG3  | 3:J:1210:SER:HB3  | 1.85                     | 0.57              |
| 3:J:801:GLY:HA2  | 3:J:821:VAL:HA    | 1.86                     | 0.57              |
| 2:C:461:VAL:HG22 | 2:C:467:ILE:HG12  | 1.86                     | 0.57              |
| 3:D:770:LEU:HB2  | 3:D:1210:SER:O    | 2.05                     | 0.57              |
| 5:F:167:ASP:HB3  | 5:F:168:PRO:HD3   | 1.87                     | 0.57              |
| 3:J:896:ALA:O    | 3:J:900:ILE:HG13  | 2.05                     | 0.57              |
| 3:J:1048:PRO:HD3 | 3:J:1075:HIS:HB3  | 1.85                     | 0.57              |
| 1:A:44:LEU:O     | 1:A:174:VAL:HG11  | 2.04                     | 0.57              |
| 1:A:54:THR:O     | 1:A:167:VAL:HG22  | 2.04                     | 0.57              |
| 2:C:113:VAL:HG21 | 2:C:373:VAL:HG21  | 1.85                     | 0.57              |
| 2:C:607:ASP:C    | 2:C:609:THR:H     | 2.11                     | 0.57              |
| 3:D:772:PRO:HG3  | 3:D:1210:SER:HB3  | 1.87                     | 0.57              |
| 1:G:53:VAL:HG23  | 1:G:144:VAL:HG22  | 1.86                     | 0.57              |
| 2:I:207:LEU:O    | 2:I:211:LEU:HD12  | 2.05                     | 0.57              |
| 2:I:607:ASP:C    | 2:I:609:THR:H     | 2.13                     | 0.57              |
| 2:C:874:LEU:HD13 | 3:D:783:ARG:HB3   | 1.86                     | 0.57              |
| 3:D:65:ARG:HD3   | 3:D:66:GLN:H      | 1.68                     | 0.57              |
| 3:D:165:LYS:HG3  | 3:D:199:MET:HE1   | 1.85                     | 0.57              |
| 3:J:881:LEU:O    | 3:J:885:ILE:HG13  | 2.05                     | 0.57              |
| 6:N:124:LEU:HD11 | 8:S:2:DG:H4'      | 1.85                     | 0.57              |
| 2:C:234:ALA:CA   | 2:C:237:ARG:HB2   | 2.34                     | 0.57              |
| 3:D:896:ALA:O    | 3:D:900:ILE:HG13  | 2.05                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:193:LEU:HD22  | 2:C:221:LEU:HD11  | 1.86                     | 0.57              |
| 3:D:261:LEU:HD21  | 3:D:268:HIS:HD2   | 1.70                     | 0.57              |
| 2:I:676:ILE:HG22  | 2:I:873:PRO:HB3   | 1.86                     | 0.57              |
| 2:I:995:MET:HE3   | 2:I:996:LYS:N     | 2.20                     | 0.57              |
| 3:D:323:GLU:HB3   | 3:D:334:THR:H     | 1.69                     | 0.56              |
| 5:L:408:THR:HG21  | 7:R:2:DT:H2'      | 1.87                     | 0.56              |
| 2:C:209:ARG:HG3   | 2:C:210:GLU:HG2   | 1.86                     | 0.56              |
| 3:J:660:LYS:HA    | 3:J:660:LYS:HE3   | 1.87                     | 0.56              |
| 3:J:661:MET:SD    | 3:J:677:LEU:HD11  | 2.45                     | 0.56              |
| 2:C:580:MET:HE1   | 2:C:665:PHE:HB3   | 1.87                     | 0.56              |
| 2:C:1065:ALA:HB1  | 2:C:1077:PRO:HG2  | 1.86                     | 0.56              |
| 2:I:1040:LEU:HG   | 3:J:763:MET:HE1   | 1.87                     | 0.56              |
| 2:C:437:ARG:HB2   | 2:C:438:ILE:HD12  | 1.87                     | 0.56              |
| 3:D:881:LEU:O     | 3:D:885:ILE:HG13  | 2.06                     | 0.56              |
| 1:G:232:LEU:HD23  | 1:H:16:GLN:HA     | 1.87                     | 0.56              |
| 3:J:643:GLY:H     | 3:J:727:GLN:HB2   | 1.70                     | 0.56              |
| 1:A:122:ILE:HG23  | 1:A:124:ASN:H     | 1.70                     | 0.56              |
| 2:C:281:LEU:O     | 2:C:308:ARG:NH2   | 2.38                     | 0.56              |
| 2:C:321:GLU:HG2   | 2:C:322:VAL:H     | 1.70                     | 0.56              |
| 2:I:757:GLY:HA2   | 2:I:789:SER:HB3   | 1.87                     | 0.56              |
| 3:J:87:ARG:HG2    | 3:J:523:ASP:HB2   | 1.86                     | 0.56              |
| 5:L:353:LEU:HD12  | 5:L:354:PRO:HD2   | 1.88                     | 0.56              |
| 2:C:995:MET:HE3   | 2:C:996:LYS:N     | 2.19                     | 0.56              |
| 3:D:775:GLY:HA2   | 3:D:1209:LEU:HB3  | 1.88                     | 0.56              |
| 3:D:1269:LYS:HD3  | 3:D:1269:LYS:H    | 1.71                     | 0.56              |
| 2:I:458:TYR:HB3   | 2:I:470:PRO:HG2   | 1.87                     | 0.56              |
| 2:I:857:ASP:HB2   | 2:I:978:ARG:HG2   | 1.88                     | 0.56              |
| 3:J:664:LYS:NZ    | 3:J:690:ALA:HB2   | 2.21                     | 0.56              |
| 3:J:759:ALA:HA    | 3:J:763:MET:HB3   | 1.88                     | 0.56              |
| 3:J:1487:VAL:HG21 | 3:J:1492:LEU:HD23 | 1.87                     | 0.56              |
| 6:N:90:HIS:CD2    | 6:N:124:LEU:HB3   | 2.40                     | 0.56              |
| 1:A:35:THR:HG23   | 1:B:39:PRO:HA     | 1.88                     | 0.56              |
| 1:A:232:LEU:HD23  | 1:B:16:GLN:HA     | 1.88                     | 0.56              |
| 2:C:588:VAL:HG21  | 2:C:664:GLY:HA2   | 1.88                     | 0.56              |
| 3:D:822:ALA:HB3   | 3:D:825:ALA:HB2   | 1.88                     | 0.56              |
| 2:I:605:LYS:HG2   | 2:I:612:ALA:HB3   | 1.86                     | 0.56              |
| 2:I:672:VAL:HG22  | 2:I:994:ILE:HD13  | 1.88                     | 0.56              |
| 3:J:1458:GLU:HB2  | 3:J:1460:ILE:HG23 | 1.87                     | 0.56              |
| 3:J:1472:ILE:HD11 | 3:J:1474:ALA:HB3  | 1.88                     | 0.56              |
| 3:J:1493:LYS:HA   | 3:J:1496:GLU:HB2  | 1.86                     | 0.56              |
| 5:L:385:LYS:HB3   | 5:L:390:LEU:HD12  | 1.87                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:694:LEU:HD11  | 2:C:868:ASP:HB3   | 1.86                     | 0.56              |
| 1:G:94:MET:O      | 1:G:146:ARG:HD3   | 2.05                     | 0.56              |
| 2:C:285:LEU:HD11  | 2:C:301:GLU:HB3   | 1.87                     | 0.56              |
| 3:D:514:LEU:HD21  | 3:D:518:PRO:HD3   | 1.88                     | 0.56              |
| 3:D:762:GLN:HB3   | 4:E:16:LYS:HE2    | 1.87                     | 0.56              |
| 3:J:640:HIS:CD2   | 3:J:641:GLN:HG3   | 2.41                     | 0.56              |
| 2:C:195:LEU:O     | 2:C:198:ARG:HG3   | 2.05                     | 0.56              |
| 3:D:477:LEU:HA    | 3:D:480:GLU:HB2   | 1.87                     | 0.56              |
| 5:L:376:LEU:HD11  | 5:L:423:LEU:HD11  | 1.88                     | 0.56              |
| 2:C:835:VAL:HG13  | 2:C:851:LYS:H     | 1.71                     | 0.55              |
| 3:D:573:MET:HA    | 3:D:576:GLU:HG2   | 1.88                     | 0.55              |
| 3:D:1487:VAL:HG21 | 3:D:1492:LEU:HD23 | 1.87                     | 0.55              |
| 3:J:1434:TRP:CD1  | 3:J:1434:TRP:H    | 2.23                     | 0.55              |
| 5:L:180:SER:O     | 5:L:181:LEU:HD12  | 2.06                     | 0.55              |
| 5:L:285:LYS:HG2   | 5:L:310:MET:HE1   | 1.88                     | 0.55              |
| 3:D:233:LYS:HG3   | 3:D:235:ALA:H     | 1.70                     | 0.55              |
| 3:D:853:VAL:HG22  | 3:D:858:LEU:HB3   | 1.89                     | 0.55              |
| 3:D:1123:PHE:HB3  | 3:D:1132:LEU:HD22 | 1.88                     | 0.55              |
| 5:F:99:TYR:OH     | 5:F:207:LEU:HD21  | 2.06                     | 0.55              |
| 5:F:203:ILE:HG23  | 5:F:235:LEU:HD23  | 1.87                     | 0.55              |
| 3:J:721:VAL:HG21  | 3:J:727:GLN:NE2   | 2.22                     | 0.55              |
| 5:L:203:ILE:HG23  | 5:L:235:LEU:HD23  | 1.87                     | 0.55              |
| 3:D:12:LEU:HD21   | 3:D:1452:ILE:HD13 | 1.88                     | 0.55              |
| 3:D:288:MET:HA    | 3:D:307:GLY:HA2   | 1.89                     | 0.55              |
| 3:D:413:ASP:O     | 3:D:435:VAL:HG12  | 2.06                     | 0.55              |
| 3:D:680:GLN:C     | 3:D:682:ASP:H     | 2.13                     | 0.55              |
| 3:D:1042:ARG:HH11 | 3:D:1045:MET:HE1  | 1.71                     | 0.55              |
| 2:C:584:GLU:H     | 2:C:584:GLU:CD    | 2.14                     | 0.55              |
| 3:D:660:LYS:HA    | 3:D:660:LYS:HE3   | 1.88                     | 0.55              |
| 3:D:1125:MET:HG3  | 3:D:1132:LEU:HG   | 1.87                     | 0.55              |
| 5:F:376:LEU:HD11  | 5:F:423:LEU:HD11  | 1.89                     | 0.55              |
| 2:I:374:ASN:HD22  | 2:I:375:SER:H     | 1.53                     | 0.55              |
| 2:I:584:GLU:H     | 2:I:584:GLU:CD    | 2.14                     | 0.55              |
| 5:F:385:LYS:HB3   | 5:F:390:LEU:HD12  | 1.88                     | 0.55              |
| 2:I:259:GLY:HA2   | 2:I:263:ASP:HB2   | 1.89                     | 0.55              |
| 6:M:64:ALA:HB3    | 6:M:66:GLU:HG2    | 1.89                     | 0.55              |
| 2:C:328:LEU:HD21  | 2:C:434:HIS:HA    | 1.88                     | 0.55              |
| 2:C:554:ASP:HB2   | 3:D:1061:PHE:HE1  | 1.70                     | 0.55              |
| 3:D:1208:ASP:HB2  | 3:D:1215:VAL:HA   | 1.89                     | 0.55              |
| 3:J:168:THR:HA    | 3:J:394:LEU:HD13  | 1.88                     | 0.55              |
| 3:J:1472:ILE:HG13 | 3:J:1474:ALA:H    | 1.70                     | 0.55              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:D:133:ILE:HG22  | 3:D:152:LEU:HG   | 1.89                     | 0.55              |
| 2:I:15:LEU:H      | 2:I:586:ARG:HH12 | 1.54                     | 0.55              |
| 2:I:456:ALA:HB3   | 2:I:459:ALA:HB2  | 1.89                     | 0.55              |
| 2:I:675:ALA:HB3   | 2:I:870:ILE:HA   | 1.88                     | 0.55              |
| 6:M:49:VAL:HG11   | 6:M:59:LEU:HD22  | 1.89                     | 0.55              |
| 3:D:759:ALA:HA    | 3:D:763:MET:HB3  | 1.88                     | 0.55              |
| 5:F:237:ARG:NH2   | 7:O:24:DC:OP2    | 2.40                     | 0.55              |
| 2:I:15:LEU:N      | 2:I:586:ARG:HH12 | 2.05                     | 0.55              |
| 2:C:230:ARG:HB3   | 2:C:231:PRO:HD2  | 1.88                     | 0.55              |
| 2:C:339:LEU:HD13  | 2:C:385:PHE:CZ   | 2.42                     | 0.55              |
| 2:C:897:LEU:HB2   | 2:C:899:GLN:HG2  | 1.88                     | 0.55              |
| 3:D:471:GLU:O     | 3:D:475:ARG:HG2  | 2.07                     | 0.55              |
| 5:F:418:LYS:O     | 5:F:422:LYS:HB2  | 2.06                     | 0.55              |
| 1:H:179:PHE:HB3   | 1:H:197:LEU:HD13 | 1.89                     | 0.55              |
| 3:J:775:GLY:HA2   | 3:J:1209:LEU:HB3 | 1.87                     | 0.55              |
| 3:D:1130:ARG:HH21 | 3:J:1179:GLU:HB2 | 1.71                     | 0.55              |
| 5:F:249:LYS:HG2   | 7:O:29:DC:OP2    | 2.07                     | 0.55              |
| 1:H:56:VAL:HG21   | 1:H:82:LEU:HD13  | 1.89                     | 0.55              |
| 2:I:595:LEU:HD23  | 2:I:656:ALA:HB3  | 1.89                     | 0.55              |
| 3:J:786:ILE:HD13  | 3:J:908:LYS:HG2  | 1.89                     | 0.55              |
| 2:C:1044:GLY:HA3  | 4:E:17:TYR:CE1   | 2.41                     | 0.54              |
| 3:D:141:VAL:HA    | 3:D:146:PRO:HA   | 1.89                     | 0.54              |
| 3:D:680:GLN:HG3   | 3:D:682:ASP:HB3  | 1.89                     | 0.54              |
| 3:J:668:PRO:HB2   | 5:L:432:LYS:HD3  | 1.89                     | 0.54              |
| 6:N:64:ALA:HB3    | 6:N:66:GLU:HG2   | 1.89                     | 0.54              |
| 2:C:18:LEU:HB3    | 2:C:408:ARG:HD2  | 1.90                     | 0.54              |
| 3:D:1472:ILE:HD11 | 3:D:1474:ALA:HB3 | 1.89                     | 0.54              |
| 3:D:1499:ARG:HE   | 3:D:1500:LYS:HG3 | 1.71                     | 0.54              |
| 2:I:87:ASP:HA     | 2:I:131:GLY:HA3  | 1.89                     | 0.54              |
| 2:I:328:LEU:HD21  | 2:I:434:HIS:HA   | 1.89                     | 0.54              |
| 3:J:1080:GLY:HA2  | 3:J:1083:ASP:HB2 | 1.90                     | 0.54              |
| 2:C:1052:MET:HE1  | 3:D:748:HIS:HD2  | 1.73                     | 0.54              |
| 3:D:702:LEU:HB3   | 3:D:745:MET:HE2  | 1.89                     | 0.54              |
| 3:D:721:VAL:HG21  | 3:D:727:GLN:NE2  | 2.23                     | 0.54              |
| 3:D:1273:VAL:HG23 | 3:D:1325:LEU:HB2 | 1.89                     | 0.54              |
| 3:D:1434:TRP:CD1  | 3:D:1434:TRP:H   | 2.25                     | 0.54              |
| 2:I:17:PRO:O      | 2:I:20:GLU:HG3   | 2.07                     | 0.54              |
| 2:I:437:ARG:HB2   | 2:I:438:ILE:HD12 | 1.89                     | 0.54              |
| 2:I:572:ILE:HD11  | 2:I:703:ILE:HD11 | 1.88                     | 0.54              |
| 3:D:978:TYR:HB2   | 3:D:988:ARG:HD3  | 1.89                     | 0.54              |
| 1:G:14:THR:HG1    | 1:H:231:SER:HG   | 1.56                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:230:ARG:HB3   | 2:I:231:PRO:HD2   | 1.88                     | 0.54              |
| 3:J:209:ARG:HH21  | 3:J:391:ALA:HB1   | 1.71                     | 0.54              |
| 1:A:79:ILE:HD13   | 1:A:167:VAL:HG12  | 1.90                     | 0.54              |
| 3:J:103:TRP:HE3   | 3:J:1448:THR:HG23 | 1.71                     | 0.54              |
| 3:J:216:LEU:HD22  | 3:J:382:GLU:HB3   | 1.90                     | 0.54              |
| 3:J:911:LEU:O     | 3:J:915:VAL:HG23  | 2.08                     | 0.54              |
| 3:J:1123:PHE:HE2  | 3:J:1184:ARG:HA   | 1.73                     | 0.54              |
| 5:L:372:ALA:HA    | 5:L:375:LYS:HE3   | 1.88                     | 0.54              |
| 6:N:17:VAL:HB     | 6:N:142:GLN:HG3   | 1.90                     | 0.54              |
| 2:C:193:LEU:HD21  | 2:C:307:LEU:HD21  | 1.89                     | 0.54              |
| 2:C:439:CYS:HB2   | 2:C:541:SER:HB3   | 1.90                     | 0.54              |
| 3:D:950:GLY:H     | 3:D:953:ASP:CG    | 2.14                     | 0.54              |
| 3:D:1080:GLY:HA2  | 3:D:1083:ASP:HB2  | 1.89                     | 0.54              |
| 2:I:668:LEU:HB3   | 2:I:995:MET:SD    | 2.47                     | 0.54              |
| 2:I:1101:THR:HG22 | 3:J:8:VAL:HG22    | 1.90                     | 0.54              |
| 3:J:477:LEU:HA    | 3:J:480:GLU:HB2   | 1.89                     | 0.54              |
| 3:J:1042:ARG:HH11 | 3:J:1045:MET:HE1  | 1.73                     | 0.54              |
| 1:A:198:ARG:HD2   | 2:C:934:PHE:HE1   | 1.73                     | 0.54              |
| 3:D:223:LEU:HB3   | 3:D:333:LEU:HG    | 1.90                     | 0.54              |
| 3:D:592:THR:HG22  | 3:D:599:PRO:HA    | 1.90                     | 0.54              |
| 3:D:917:GLN:HE22  | 3:D:1168:LEU:HD11 | 1.72                     | 0.54              |
| 3:D:1472:ILE:HG13 | 3:D:1474:ALA:H    | 1.72                     | 0.54              |
| 4:E:42:PRO:HA     | 4:E:45:ARG:HG3    | 1.88                     | 0.54              |
| 1:H:97:THR:HG21   | 1:H:120:VAL:HG21  | 1.88                     | 0.54              |
| 2:I:154:ARG:HH12  | 2:I:176:VAL:HG23  | 1.72                     | 0.54              |
| 2:I:461:VAL:HG22  | 2:I:467:ILE:HG12  | 1.90                     | 0.54              |
| 3:J:735:ALA:HB2   | 3:J:778:LEU:HD11  | 1.89                     | 0.54              |
| 5:L:167:ASP:HB3   | 5:L:168:PRO:HD3   | 1.89                     | 0.54              |
| 2:C:857:ASP:HB2   | 2:C:978:ARG:HG2   | 1.90                     | 0.54              |
| 3:J:140:ALA:HB1   | 3:J:161:LEU:HD23  | 1.89                     | 0.54              |
| 3:J:680:GLN:HG3   | 3:J:682:ASP:HB3   | 1.89                     | 0.54              |
| 3:D:645:PRO:HB2   | 3:D:648:MET:HB3   | 1.89                     | 0.54              |
| 3:D:1484:THR:OG1  | 4:E:18:ARG:NH1    | 2.41                     | 0.54              |
| 1:A:161:ARG:HD2   | 1:A:162:ILE:HG22  | 1.89                     | 0.53              |
| 3:D:671:LYS:HG3   | 5:F:436:PHE:CE2   | 2.42                     | 0.53              |
| 2:I:669:GLY:HA3   | 2:I:994:ILE:O     | 2.08                     | 0.53              |
| 2:I:1103:ASP:OD1  | 2:I:1103:ASP:N    | 2.41                     | 0.53              |
| 3:J:565:ILE:HD12  | 3:J:565:ILE:H     | 1.72                     | 0.53              |
| 3:J:646:LYS:HE3   | 3:J:688:TRP:HZ2   | 1.73                     | 0.53              |
| 3:J:1336:LEU:HD22 | 3:J:1421:LEU:HB3  | 1.90                     | 0.53              |
| 6:N:63:LEU:HD21   | 6:N:102:PRO:HG3   | 1.89                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:P:10:DT:H2"     | 8:P:11:DA:C8      | 2.42                     | 0.53              |
| 2:C:207:LEU:O     | 2:C:211:LEU:HD12  | 2.08                     | 0.53              |
| 2:C:249:LYS:HD3   | 2:C:250:LYS:H     | 1.74                     | 0.53              |
| 3:D:434:ARG:HH11  | 3:D:447:VAL:HG21  | 1.73                     | 0.53              |
| 5:F:368:GLU:HB3   | 5:F:433:LEU:HD21  | 1.90                     | 0.53              |
| 2:I:168:ARG:HD3   | 2:I:268:ASP:HB3   | 1.90                     | 0.53              |
| 2:I:321:GLU:HG2   | 2:I:322:VAL:N     | 2.23                     | 0.53              |
| 2:I:321:GLU:HG2   | 2:I:322:VAL:H     | 1.73                     | 0.53              |
| 6:M:9:LYS:HD3     | 6:M:142:GLN:HE22  | 1.73                     | 0.53              |
| 3:D:859:ASP:HB2   | 3:D:862:ASP:OD2   | 2.09                     | 0.53              |
| 3:D:911:LEU:O     | 3:D:915:VAL:HG23  | 2.08                     | 0.53              |
| 2:I:1019:GLN:HG3  | 3:J:617:ASN:ND2   | 2.24                     | 0.53              |
| 3:J:714:GLN:HB3   | 3:J:765:SER:HB3   | 1.89                     | 0.53              |
| 3:J:1364:HIS:CD2  | 3:J:1366:LYS:HE2  | 2.44                     | 0.53              |
| 3:D:214:ASP:HA    | 3:D:342:PRO:HA    | 1.91                     | 0.53              |
| 3:D:218:LYS:HD3   | 3:D:338:GLU:HB3   | 1.89                     | 0.53              |
| 3:D:658:LEU:HD11  | 3:D:674:ARG:HG2   | 1.91                     | 0.53              |
| 1:G:79:ILE:HD13   | 1:G:167:VAL:HG12  | 1.90                     | 0.53              |
| 1:H:44:LEU:HD13   | 1:H:177:VAL:HG11  | 1.89                     | 0.53              |
| 3:J:514:LEU:HD21  | 3:J:517:VAL:HA    | 1.90                     | 0.53              |
| 5:L:103:ILE:HD13  | 5:L:211:VAL:HG21  | 1.90                     | 0.53              |
| 7:O:24:DC:N4      | 8:P:2:DG:H1       | 2.06                     | 0.53              |
| 2:C:468:ARG:HG2   | 2:C:487:THR:HA    | 1.91                     | 0.53              |
| 2:C:65:VAL:HG13   | 2:C:101:ILE:HB    | 1.90                     | 0.53              |
| 2:C:448:ASN:C     | 2:C:451:LEU:HD23  | 2.34                     | 0.53              |
| 2:I:42:VAL:HG12   | 2:I:43:GLY:H      | 1.73                     | 0.53              |
| 2:I:129:ILE:HG12  | 2:I:386:PHE:HB3   | 1.90                     | 0.53              |
| 8:S:10:DT:H2"     | 8:S:11:DA:C8      | 2.44                     | 0.53              |
| 2:C:675:ALA:HA    | 2:C:989:VAL:HG12  | 1.90                     | 0.53              |
| 3:D:103:TRP:HE3   | 3:D:1448:THR:HG23 | 1.73                     | 0.53              |
| 3:D:248:PRO:HG3   | 3:D:308:LYS:HG3   | 1.90                     | 0.53              |
| 3:D:702:LEU:HG    | 3:D:747:VAL:HG22  | 1.91                     | 0.53              |
| 1:B:101:LEU:HD22  | 1:B:102:ARG:N     | 2.23                     | 0.53              |
| 3:D:125:GLN:HB2   | 3:D:130:ASN:HB3   | 1.91                     | 0.53              |
| 3:D:367:ILE:HB    | 3:D:377:VAL:HB    | 1.90                     | 0.53              |
| 3:D:1274:ILE:HG22 | 3:D:1324:PRO:HA   | 1.89                     | 0.53              |
| 5:F:149:LYS:HD3   | 5:F:193:ARG:HH22  | 1.73                     | 0.53              |
| 3:J:93:ILE:HD13   | 3:J:548:ILE:HG12  | 1.89                     | 0.53              |
| 3:J:702:LEU:HB3   | 3:J:745:MET:HE2   | 1.91                     | 0.53              |
| 5:L:319:VAL:O     | 5:L:323:LEU:HB2   | 2.08                     | 0.53              |
| 1:B:180:GLN:NE2   | 1:B:182:GLU:OE1   | 2.39                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:358:ARG:HB2   | 2:C:372:LEU:HD12  | 1.89                     | 0.53              |
| 2:C:874:LEU:HD22  | 3:D:1029:ARG:HB2  | 1.91                     | 0.53              |
| 3:D:675:ARG:HH21  | 3:D:679:ARG:HH12  | 1.55                     | 0.53              |
| 2:I:1019:GLN:HE22 | 3:J:621:LYS:HD3   | 1.73                     | 0.53              |
| 5:L:379:ARG:HG3   | 5:L:405:PHE:CE2   | 2.44                     | 0.53              |
| 2:C:42:VAL:HG12   | 2:C:43:GLY:H      | 1.73                     | 0.53              |
| 2:C:1103:ASP:OD1  | 2:C:1103:ASP:N    | 2.41                     | 0.53              |
| 3:D:1127:GLU:C    | 3:D:1129:THR:H    | 2.17                     | 0.53              |
| 1:G:53:VAL:HA     | 1:G:144:VAL:HG13  | 1.91                     | 0.53              |
| 2:I:685:GLU:HG2   | 3:J:739:ASP:HB3   | 1.90                     | 0.53              |
| 3:J:1127:GLU:C    | 3:J:1129:THR:H    | 2.16                     | 0.53              |
| 1:B:110:ARG:HH12  | 1:B:126:ASP:HA    | 1.75                     | 0.52              |
| 3:D:87:ARG:HG2    | 3:D:523:ASP:HB2   | 1.91                     | 0.52              |
| 3:D:974:ILE:HG22  | 3:D:988:ARG:HG3   | 1.90                     | 0.52              |
| 5:F:189:LEU:HD21  | 5:F:193:ARG:HE    | 1.74                     | 0.52              |
| 3:D:592:THR:HA    | 3:D:600:LEU:HD13  | 1.91                     | 0.52              |
| 3:D:618:LEU:HG    | 3:D:1467:ILE:HA   | 1.91                     | 0.52              |
| 3:D:1179:GLU:HB3  | 3:J:1131:THR:HG22 | 1.91                     | 0.52              |
| 2:I:874:LEU:HD22  | 3:J:1029:ARG:HB2  | 1.92                     | 0.52              |
| 2:I:1031:ARG:HA   | 3:J:622:ARG:HA    | 1.91                     | 0.52              |
| 3:J:122:GLU:O     | 3:J:126:VAL:HG23  | 2.09                     | 0.52              |
| 3:J:421:LEU:HB3   | 3:J:444:VAL:HG21  | 1.91                     | 0.52              |
| 6:M:85:GLN:NE2    | 7:O:25:DT:O2      | 2.43                     | 0.52              |
| 2:C:683:ASN:OD1   | 2:C:872:ASN:ND2   | 2.42                     | 0.52              |
| 3:D:154:THR:HG22  | 3:D:157:GLU:HG2   | 1.90                     | 0.52              |
| 3:D:714:GLN:HB3   | 3:D:765:SER:HB3   | 1.90                     | 0.52              |
| 5:F:217:TYR:O     | 5:F:220:ARG:HG2   | 2.09                     | 0.52              |
| 2:I:1016:ILE:O    | 3:J:87:ARG:NH2    | 2.42                     | 0.52              |
| 3:J:405:ASP:OD1   | 3:J:405:ASP:N     | 2.42                     | 0.52              |
| 3:J:689:ASP:O     | 3:J:692:GLU:HB2   | 2.09                     | 0.52              |
| 3:J:770:LEU:HD23  | 3:J:777:PRO:HA    | 1.91                     | 0.52              |
| 2:C:1017:THR:HG21 | 3:D:617:ASN:ND2   | 2.25                     | 0.52              |
| 3:D:638:LYS:HG2   | 3:D:639:LEU:N     | 2.25                     | 0.52              |
| 3:D:735:ALA:HB2   | 3:D:778:LEU:HD11  | 1.92                     | 0.52              |
| 2:I:198:ARG:NE    | 2:I:234:ALA:O     | 2.41                     | 0.52              |
| 3:J:729:HIS:HE1   | 3:J:731:LEU:HG    | 1.75                     | 0.52              |
| 5:L:249:LYS:HG2   | 7:R:29:DC:OP2     | 2.09                     | 0.52              |
| 1:B:123:MET:C     | 1:B:125:PRO:HD3   | 2.34                     | 0.52              |
| 2:C:339:LEU:HD13  | 2:C:385:PHE:HZ    | 1.73                     | 0.52              |
| 2:C:1115:LEU:HD23 | 3:D:85:VAL:HG12   | 1.91                     | 0.52              |
| 3:D:208:PRO:HA    | 3:D:390:PRO:HA    | 1.91                     | 0.52              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:D:640:HIS:CD2   | 3:D:641:GLN:HG3  | 2.45                     | 0.52              |
| 1:G:205:VAL:HG11  | 1:G:213:GLN:HE22 | 1.74                     | 0.52              |
| 2:I:118:LEU:HD13  | 2:I:382:LEU:HD23 | 1.92                     | 0.52              |
| 2:I:922:PHE:HB2   | 2:I:967:PHE:CD2  | 2.44                     | 0.52              |
| 2:C:154:ARG:HH12  | 2:C:176:VAL:HG23 | 1.74                     | 0.52              |
| 2:C:241:LEU:O     | 2:C:244:PRO:HD3  | 2.10                     | 0.52              |
| 3:D:127:LEU:HG    | 3:D:461:ILE:HG13 | 1.91                     | 0.52              |
| 3:D:1130:ARG:NH2  | 3:J:1179:GLU:HB2 | 2.24                     | 0.52              |
| 4:K:42:PRO:HA     | 4:K:45:ARG:HG3   | 1.92                     | 0.52              |
| 6:N:60:ARG:CZ     | 6:N:102:PRO:HD3  | 2.40                     | 0.52              |
| 1:A:224:TYR:CD1   | 1:B:9:PRO:HG2    | 2.44                     | 0.52              |
| 2:C:149:THR:HA    | 2:C:322:VAL:HG13 | 1.90                     | 0.52              |
| 2:C:195:LEU:HB3   | 2:C:238:LEU:HD11 | 1.90                     | 0.52              |
| 2:C:580:MET:HE2   | 2:C:584:GLU:HG2  | 1.91                     | 0.52              |
| 2:C:601:GLY:HA2   | 2:C:615:TYR:HA   | 1.91                     | 0.52              |
| 2:C:939:ARG:HB3   | 2:C:982:PRO:HG3  | 1.90                     | 0.52              |
| 2:C:1019:GLN:HE22 | 3:D:621:LYS:HD3  | 1.74                     | 0.52              |
| 3:D:299:GLU:N     | 3:D:302:GLN:OE1  | 2.43                     | 0.52              |
| 3:D:585:GLY:HA2   | 3:D:590:PRO:HG3  | 1.91                     | 0.52              |
| 3:J:1274:ILE:HG22 | 3:J:1324:PRO:HA  | 1.92                     | 0.52              |
| 2:C:630:ARG:HA    | 2:C:705:ILE:HD13 | 1.91                     | 0.52              |
| 2:C:1069:ALA:O    | 2:C:1073:GLY:N   | 2.42                     | 0.52              |
| 5:F:103:ILE:HD13  | 5:F:211:VAL:HG21 | 1.91                     | 0.52              |
| 5:F:353:LEU:HD12  | 5:F:354:PRO:HD2  | 1.91                     | 0.52              |
| 1:H:161:ARG:HG3   | 1:H:162:ILE:N    | 2.25                     | 0.52              |
| 3:J:407:VAL:HG22  | 3:J:409:VAL:H    | 1.74                     | 0.52              |
| 3:J:500:ARG:HD3   | 3:J:503:LEU:HD12 | 1.91                     | 0.52              |
| 2:C:672:VAL:HG22  | 2:C:994:ILE:HD13 | 1.91                     | 0.52              |
| 2:C:695:LEU:HD21  | 2:C:832:LYS:HD3  | 1.92                     | 0.52              |
| 2:C:837:ASP:HB3   | 2:C:1000:MET:HE2 | 1.91                     | 0.52              |
| 2:C:1040:LEU:HG   | 3:D:763:MET:HE1  | 1.92                     | 0.52              |
| 3:D:229:ALA:HB2   | 3:D:245:LEU:HA   | 1.92                     | 0.52              |
| 2:I:852:ILE:HG22  | 2:I:853:LEU:H    | 1.75                     | 0.52              |
| 3:J:508:ARG:HB2   | 3:J:511:TRP:CE2  | 2.45                     | 0.52              |
| 5:L:377:SER:HB3   | 5:L:380:GLU:HG2  | 1.92                     | 0.52              |
| 2:C:146:VAL:HG21  | 2:C:281:LEU:HG   | 1.92                     | 0.52              |
| 2:C:757:GLY:HA2   | 2:C:789:SER:HB3  | 1.92                     | 0.52              |
| 3:J:65:ARG:HD3    | 3:J:66:GLN:H     | 1.74                     | 0.52              |
| 3:J:127:LEU:HG    | 3:J:461:ILE:HG13 | 1.92                     | 0.52              |
| 3:J:974:ILE:HG22  | 3:J:988:ARG:HG3  | 1.92                     | 0.52              |
| 3:J:1273:VAL:HG23 | 3:J:1325:LEU:HB2 | 1.92                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:N:9:LYS:HD3     | 6:N:142:GLN:HE22  | 1.75                     | 0.52              |
| 3:D:521:PRO:HB2   | 3:D:524:LEU:HG    | 1.92                     | 0.51              |
| 3:D:682:ASP:C     | 3:D:684:LYS:H     | 2.18                     | 0.51              |
| 3:D:770:LEU:HD23  | 3:D:777:PRO:HA    | 1.92                     | 0.51              |
| 1:G:153:ALA:HB2   | 1:G:167:VAL:C     | 2.35                     | 0.51              |
| 2:I:897:LEU:HB2   | 2:I:899:GLN:HG2   | 1.93                     | 0.51              |
| 3:J:770:LEU:HB2   | 3:J:1210:SER:O    | 2.09                     | 0.51              |
| 3:J:978:TYR:HB2   | 3:J:988:ARG:HD3   | 1.91                     | 0.51              |
| 3:J:1281:VAL:HG21 | 3:J:1313:VAL:HG11 | 1.91                     | 0.51              |
| 4:K:45:ARG:HD2    | 4:K:63:TRP:HH2    | 1.76                     | 0.51              |
| 1:B:102:ARG:HB2   | 1:B:139:TYR:HD1   | 1.75                     | 0.51              |
| 2:C:374:ASN:HD22  | 2:C:375:SER:N     | 2.05                     | 0.51              |
| 3:D:407:VAL:HG23  | 3:D:422:ALA:HB2   | 1.92                     | 0.51              |
| 3:D:1048:PRO:HD3  | 3:D:1075:HIS:HB3  | 1.92                     | 0.51              |
| 6:N:144:LEU:HB2   | 6:N:146:ILE:HG12  | 1.91                     | 0.51              |
| 2:C:669:GLY:HA3   | 2:C:994:ILE:O     | 2.10                     | 0.51              |
| 3:D:119:SER:HB3   | 3:D:122:GLU:HG2   | 1.91                     | 0.51              |
| 3:D:187:LYS:HG2   | 3:D:198:ARG:C     | 2.36                     | 0.51              |
| 3:D:801:GLY:HA2   | 3:D:821:VAL:HA    | 1.92                     | 0.51              |
| 3:D:1292:VAL:HG21 | 3:D:1311:LEU:HD13 | 1.92                     | 0.51              |
| 5:F:431:ARG:HG3   | 5:F:434:ARG:NE    | 2.22                     | 0.51              |
| 2:I:584:GLU:HB3   | 2:I:666:LEU:N     | 2.24                     | 0.51              |
| 3:J:1269:LYS:HD3  | 3:J:1269:LYS:H    | 1.75                     | 0.51              |
| 5:L:373:LEU:HD12  | 5:L:376:LEU:HD12  | 1.91                     | 0.51              |
| 3:D:1476:THR:HG22 | 4:E:17:TYR:HB3    | 1.91                     | 0.51              |
| 2:I:554:ASP:HB2   | 3:J:1061:PHE:HE1  | 1.75                     | 0.51              |
| 2:I:714:ASP:HA    | 2:I:719:PRO:HA    | 1.91                     | 0.51              |
| 3:J:356:PRO:HG2   | 3:J:359:ALA:HB2   | 1.93                     | 0.51              |
| 6:M:133:ILE:HA    | 6:M:136:LEU:HD12  | 1.92                     | 0.51              |
| 6:N:133:ILE:HA    | 6:N:136:LEU:HD12  | 1.91                     | 0.51              |
| 2:C:606:VAL:HG23  | 2:C:645:VAL:HA    | 1.93                     | 0.51              |
| 2:C:668:LEU:HB3   | 2:C:995:MET:SD    | 2.51                     | 0.51              |
| 3:D:100:ALA:H     | 3:D:575:GLN:HE22  | 1.57                     | 0.51              |
| 2:I:606:VAL:HG23  | 2:I:645:VAL:HA    | 1.92                     | 0.51              |
| 3:J:465:LEU:HA    | 3:J:468:LEU:HD12  | 1.92                     | 0.51              |
| 3:J:1060:SER:OG   | 3:J:1061:PHE:N    | 2.43                     | 0.51              |
| 1:A:58:ILE:HD11   | 1:A:140:MET:HE2   | 1.92                     | 0.51              |
| 3:D:9:ARG:HA      | 3:D:1456:LYS:HA   | 1.93                     | 0.51              |
| 3:D:1181:GLY:HA3  | 3:J:1132:LEU:HD12 | 1.92                     | 0.51              |
| 3:J:154:THR:HG22  | 3:J:157:GLU:HG2   | 1.92                     | 0.51              |
| 5:L:108:LEU:HD23  | 5:L:208:ARG:HD3   | 1.92                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:611:ILE:HG13 | 2:C:625:LEU:HD11 | 1.93                     | 0.51              |
| 1:G:54:THR:O     | 1:G:167:VAL:HG22 | 2.11                     | 0.51              |
| 2:I:1044:GLY:HA3 | 4:K:17:TYR:CE1   | 2.46                     | 0.51              |
| 3:J:950:GLY:H    | 3:J:953:ASP:CG   | 2.18                     | 0.51              |
| 3:J:1476:THR:HA  | 4:K:17:TYR:HB3   | 1.93                     | 0.51              |
| 5:L:189:LEU:HD21 | 5:L:193:ARG:HE   | 1.76                     | 0.51              |
| 5:L:383:VAL:HG13 | 5:L:401:VAL:HG11 | 1.93                     | 0.51              |
| 6:M:34:ALA:HB3   | 6:M:51:VAL:HG21  | 1.92                     | 0.51              |
| 3:D:701:LEU:HD23 | 3:D:763:MET:HG2  | 1.93                     | 0.51              |
| 2:I:587:VAL:HG11 | 2:I:666:LEU:HD22 | 1.92                     | 0.51              |
| 3:J:680:GLN:O    | 3:J:682:ASP:N    | 2.34                     | 0.51              |
| 1:A:53:VAL:HG13  | 1:A:167:VAL:HG21 | 1.93                     | 0.51              |
| 2:C:101:ILE:HG23 | 2:C:108:ILE:HA   | 1.91                     | 0.51              |
| 2:C:857:ASP:OD1  | 2:C:857:ASP:N    | 2.41                     | 0.51              |
| 3:D:508:ARG:HB2  | 3:D:511:TRP:CE2  | 2.45                     | 0.51              |
| 3:D:639:LEU:HD22 | 3:D:766:ALA:HA   | 1.92                     | 0.51              |
| 3:D:783:ARG:NH1  | 3:D:1029:ARG:HD2 | 2.26                     | 0.51              |
| 5:F:199:ARG:HD2  | 5:F:240:GLU:HG2  | 1.93                     | 0.51              |
| 5:F:383:VAL:HG13 | 5:F:401:VAL:HG11 | 1.91                     | 0.51              |
| 1:H:48:ILE:HG13  | 1:H:213:GLN:HE21 | 1.76                     | 0.51              |
| 1:H:186:LEU:HD12 | 4:K:51:LEU:HD13  | 1.92                     | 0.51              |
| 3:J:12:LEU:HD11  | 3:J:1452:ILE:HA  | 1.93                     | 0.51              |
| 3:J:423:ASP:HB3  | 3:J:426:LYS:HE3  | 1.93                     | 0.51              |
| 3:J:754:PHE:HA   | 4:K:24:ALA:HB1   | 1.93                     | 0.51              |
| 5:L:99:TYR:OH    | 5:L:207:LEU:HD21 | 2.10                     | 0.51              |
| 3:D:539:ASP:HB3  | 3:D:600:LEU:HG   | 1.92                     | 0.51              |
| 1:H:15:THR:HA    | 1:H:21:GLY:HA2   | 1.94                     | 0.51              |
| 1:H:123:MET:C    | 1:H:125:PRO:HD3  | 2.36                     | 0.51              |
| 2:I:545:ASN:HB3  | 2:I:583:LEU:HD22 | 1.93                     | 0.51              |
| 3:J:101:HIS:ND1  | 3:J:103:TRP:HB2  | 2.26                     | 0.51              |
| 3:D:10:ILE:O     | 3:D:1454:GLY:HA2 | 2.11                     | 0.50              |
| 3:D:681:ARG:O    | 3:D:683:ILE:HG12 | 2.10                     | 0.50              |
| 3:J:119:SER:HB3  | 3:J:122:GLU:HG2  | 1.92                     | 0.50              |
| 2:C:723:THR:HG23 | 2:C:725:ASP:H    | 1.75                     | 0.50              |
| 3:D:49:ILE:HG13  | 3:D:50:PHE:N     | 2.25                     | 0.50              |
| 3:D:643:GLY:H    | 3:D:727:GLN:HB2  | 1.76                     | 0.50              |
| 2:I:1069:ALA:O   | 2:I:1073:GLY:N   | 2.43                     | 0.50              |
| 3:J:962:ARG:O    | 3:J:965:GLU:HG2  | 2.11                     | 0.50              |
| 1:A:48:ILE:HG22  | 1:A:173:PRO:HD2  | 1.93                     | 0.50              |
| 3:D:786:ILE:HD13 | 3:D:908:LYS:HG2  | 1.92                     | 0.50              |
| 3:D:923:GLY:O    | 3:D:926:LYS:HB2  | 2.12                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:1331:ASP:HB3  | 3:D:1334:GLN:HB2  | 1.94                     | 0.50              |
| 5:F:377:SER:HB3   | 5:F:380:GLU:HG2   | 1.92                     | 0.50              |
| 2:I:580:MET:HE2   | 2:I:584:GLU:HG2   | 1.93                     | 0.50              |
| 2:I:675:ALA:HB2   | 2:I:867:VAL:HG21  | 1.93                     | 0.50              |
| 3:J:654:LYS:HB3   | 3:J:655:PRO:HD3   | 1.94                     | 0.50              |
| 3:J:783:ARG:HD3   | 3:J:1028:ALA:O    | 2.11                     | 0.50              |
| 2:C:164:PRO:HG2   | 2:C:165:LEU:H     | 1.77                     | 0.50              |
| 2:C:584:GLU:HB3   | 2:C:666:LEU:N     | 2.24                     | 0.50              |
| 2:C:1067:TYR:O    | 2:C:1071:ILE:HB   | 2.12                     | 0.50              |
| 3:D:191:LEU:CD1   | 3:D:197:SER:HB2   | 2.42                     | 0.50              |
| 3:D:729:HIS:HE1   | 3:D:731:LEU:HG    | 1.76                     | 0.50              |
| 3:D:918:ALA:HA    | 3:D:922:LEU:HD23  | 1.94                     | 0.50              |
| 4:E:45:ARG:HD2    | 4:E:63:TRP:HH2    | 1.76                     | 0.50              |
| 1:G:53:VAL:HA     | 1:G:144:VAL:HA    | 1.94                     | 0.50              |
| 2:I:673:LEU:HB3   | 2:I:867:VAL:HG12  | 1.92                     | 0.50              |
| 3:J:122:GLU:HB2   | 3:J:152:LEU:HD21  | 1.94                     | 0.50              |
| 6:M:82:LEU:HB3    | 6:M:89:ARG:HG3    | 1.92                     | 0.50              |
| 1:A:72:LYS:HG3    | 2:C:606:VAL:HG11  | 1.93                     | 0.50              |
| 3:D:132:TYR:CE1   | 3:D:456:MET:HG2   | 2.47                     | 0.50              |
| 3:D:977:ALA:HB2   | 3:J:831:GLY:CA    | 2.40                     | 0.50              |
| 2:I:164:PRO:HG2   | 2:I:165:LEU:H     | 1.77                     | 0.50              |
| 3:J:585:GLY:HA2   | 3:J:590:PRO:HG3   | 1.94                     | 0.50              |
| 3:J:1120:VAL:HG12 | 3:J:1135:ARG:HH12 | 1.76                     | 0.50              |
| 5:L:206:ASN:O     | 5:L:209:LEU:HB3   | 2.11                     | 0.50              |
| 1:G:64:GLU:HG3    | 1:G:79:ILE:HD12   | 1.93                     | 0.50              |
| 2:I:18:LEU:HB3    | 2:I:408:ARG:HD2   | 1.93                     | 0.50              |
| 3:D:365:GLU:H     | 3:D:379:ALA:HB3   | 1.77                     | 0.50              |
| 1:G:43:ILE:HD11   | 1:H:35:THR:HG21   | 1.94                     | 0.50              |
| 5:L:238:ALA:HB2   | 5:L:257:TRP:HB2   | 1.94                     | 0.50              |
| 3:D:32:ILE:HG22   | 3:D:39:PRO:HA     | 1.93                     | 0.50              |
| 3:D:1448:THR:O    | 3:D:1452:ILE:HG12 | 2.11                     | 0.50              |
| 1:G:198:ARG:HD2   | 2:I:934:PHE:HE1   | 1.77                     | 0.50              |
| 2:I:1065:ALA:HB1  | 2:I:1077:PRO:HG2  | 1.94                     | 0.50              |
| 2:I:1081:VAL:HG21 | 2:I:1086:ARG:CZ   | 2.42                     | 0.50              |
| 3:J:859:ASP:HB2   | 3:J:862:ASP:OD2   | 2.12                     | 0.50              |
| 3:J:1290:LEU:HB2  | 3:J:1307:LYS:HD2  | 1.93                     | 0.50              |
| 6:N:33:ARG:H      | 6:N:33:ARG:HD2    | 1.77                     | 0.50              |
| 7:O:3:DT:H6       | 7:O:3:DT:H5'      | 1.76                     | 0.50              |
| 3:D:1117:TYR:HB2  | 3:D:1188:VAL:O    | 2.12                     | 0.50              |
| 2:I:249:LYS:HD3   | 2:I:250:LYS:H     | 1.77                     | 0.50              |
| 2:I:881:ASN:OD1   | 2:I:884:GLN:NE2   | 2.45                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:1115:LEU:HD23 | 3:J:85:VAL:HG12   | 1.93                     | 0.50              |
| 1:A:43:ILE:HD11   | 1:A:218:LEU:HD13  | 1.94                     | 0.49              |
| 1:B:149:GLY:O     | 1:B:171:PHE:HB2   | 2.12                     | 0.49              |
| 2:C:72:ARG:HG3    | 2:C:95:TYR:HB2    | 1.94                     | 0.49              |
| 2:C:577:PRO:HA    | 2:C:671:ASN:HD21  | 1.77                     | 0.49              |
| 3:D:14:SER:HB3    | 3:D:511:TRP:CD2   | 2.47                     | 0.49              |
| 3:D:253:ALA:HB2   | 3:D:304:LEU:HG    | 1.93                     | 0.49              |
| 3:D:402:PRO:HA    | 3:D:443:VAL:HA    | 1.93                     | 0.49              |
| 3:D:578:VAL:O     | 3:D:582:ILE:HG12  | 2.12                     | 0.49              |
| 3:D:658:LEU:HD22  | 3:D:670:VAL:HG13  | 1.94                     | 0.49              |
| 1:H:143:ARG:HG3   | 1:H:160:ASP:OD2   | 2.11                     | 0.49              |
| 2:I:999:HIS:CD2   | 2:I:1004:LYS:HE3  | 2.47                     | 0.49              |
| 2:I:1008:ARG:NH2  | 2:I:1020:PRO:HB3  | 2.27                     | 0.49              |
| 3:J:638:LYS:HG2   | 3:J:639:LEU:N     | 2.27                     | 0.49              |
| 1:A:16:GLN:HB3    | 1:A:20:TYR:HB3    | 1.94                     | 0.49              |
| 1:A:114:PHE:O     | 1:A:116:PRO:HD3   | 2.12                     | 0.49              |
| 2:C:327:HIS:CE1   | 2:C:433:THR:HG21  | 2.47                     | 0.49              |
| 2:C:1047:HIS:O    | 2:C:1051:GLU:HG2  | 2.12                     | 0.49              |
| 3:D:1458:GLU:HB2  | 3:D:1460:ILE:HG23 | 1.93                     | 0.49              |
| 5:F:211:VAL:HG13  | 5:F:228:ILE:HD13  | 1.95                     | 0.49              |
| 2:I:146:VAL:HG21  | 2:I:281:LEU:HG    | 1.93                     | 0.49              |
| 3:J:645:PRO:HB2   | 3:J:648:MET:HB3   | 1.94                     | 0.49              |
| 3:J:1107:VAL:HG22 | 3:J:1200:VAL:HG23 | 1.94                     | 0.49              |
| 4:K:38:THR:HG21   | 4:K:63:TRP:CZ3    | 2.47                     | 0.49              |
| 3:D:1048:PRO:HD3  | 3:D:1075:HIS:CG   | 2.47                     | 0.49              |
| 2:I:211:LEU:HB3   | 2:I:218:VAL:HG13  | 1.95                     | 0.49              |
| 2:I:399:ASN:HB2   | 2:I:400:PRO:HD2   | 1.93                     | 0.49              |
| 3:J:851:LEU:O     | 3:J:855:HIS:HB2   | 2.12                     | 0.49              |
| 1:B:99:LEU:HB2    | 1:B:142:VAL:HG22  | 1.94                     | 0.49              |
| 3:D:681:ARG:C     | 3:D:683:ILE:H     | 2.20                     | 0.49              |
| 3:D:754:PHE:HA    | 4:E:24:ALA:HB1    | 1.94                     | 0.49              |
| 5:F:181:LEU:HD23  | 5:F:185:LEU:HB2   | 1.94                     | 0.49              |
| 2:I:209:ARG:HG3   | 2:I:210:GLU:HG2   | 1.95                     | 0.49              |
| 3:J:398:ALA:HB2   | 3:J:447:VAL:HG12  | 1.94                     | 0.49              |
| 3:J:838:ARG:HE    | 3:J:863:VAL:HG11  | 1.78                     | 0.49              |
| 5:L:149:LYS:HD3   | 5:L:193:ARG:HH22  | 1.77                     | 0.49              |
| 5:L:217:TYR:O     | 5:L:220:ARG:HG2   | 2.13                     | 0.49              |
| 1:A:198:ARG:HH22  | 2:C:932:GLU:HB3   | 1.77                     | 0.49              |
| 2:C:209:ARG:HG3   | 2:C:210:GLU:N     | 2.27                     | 0.49              |
| 2:C:858:MET:SD    | 2:C:859:PRO:HD2   | 2.52                     | 0.49              |
| 3:D:12:LEU:HD11   | 3:D:1452:ILE:HA   | 1.93                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:F:103:ILE:HG22  | 5:F:207:LEU:HD13  | 1.92                     | 0.49              |
| 1:G:122:ILE:HG23  | 1:G:124:ASN:H     | 1.77                     | 0.49              |
| 2:I:858:MET:H     | 2:I:977:GLY:HA3   | 1.77                     | 0.49              |
| 3:J:664:LYS:HZ1   | 3:J:690:ALA:HB2   | 1.77                     | 0.49              |
| 2:C:537:LYS:HZ3   | 2:C:905:VAL:N     | 2.07                     | 0.49              |
| 2:C:838:LYS:HG2   | 2:C:997:LEU:HD22  | 1.94                     | 0.49              |
| 3:D:853:VAL:HG22  | 3:D:858:LEU:HD23  | 1.95                     | 0.49              |
| 1:A:210:ALA:HA    | 1:A:213:GLN:HE21  | 1.77                     | 0.49              |
| 3:D:264:LEU:HD21  | 3:D:339:TRP:CE2   | 2.47                     | 0.49              |
| 3:D:664:LYS:NZ    | 3:D:690:ALA:HB2   | 2.27                     | 0.49              |
| 3:D:851:LEU:O     | 3:D:855:HIS:HB2   | 2.13                     | 0.49              |
| 5:F:103:ILE:HG21  | 5:F:207:LEU:HD22  | 1.94                     | 0.49              |
| 1:G:16:GLN:HB3    | 1:G:20:TYR:HB3    | 1.94                     | 0.49              |
| 1:H:226:ALA:O     | 1:H:228:PRO:HD3   | 2.13                     | 0.49              |
| 3:J:44:LEU:HD23   | 3:J:525:ARG:HH12  | 1.77                     | 0.49              |
| 5:L:419:ALA:O     | 5:L:423:LEU:HD12  | 2.13                     | 0.49              |
| 7:R:23:DG:H1'     | 7:R:24:DC:H5'     | 1.94                     | 0.49              |
| 2:C:306:THR:HG23  | 2:C:307:LEU:HD12  | 1.94                     | 0.49              |
| 2:C:456:ALA:HB3   | 2:C:459:ALA:HB2   | 1.95                     | 0.49              |
| 2:C:535:SER:O     | 2:C:538:GLN:HG2   | 2.13                     | 0.49              |
| 2:C:750:LYS:N     | 2:C:753:ASP:OD2   | 2.34                     | 0.49              |
| 2:C:833:LEU:HD21  | 2:C:839:LEU:HD11  | 1.94                     | 0.49              |
| 3:D:273:ARG:HA    | 3:D:279:VAL:HG23  | 1.94                     | 0.49              |
| 3:D:335:LEU:HD13  | 3:D:337:LEU:HD11  | 1.94                     | 0.49              |
| 3:D:710:ARG:HG3   | 3:D:711:LEU:HD22  | 1.95                     | 0.49              |
| 3:D:1336:LEU:HD22 | 3:D:1421:LEU:HB3  | 1.94                     | 0.49              |
| 5:F:157:GLN:NE2   | 5:F:171:VAL:HG21  | 2.26                     | 0.49              |
| 5:F:427:GLU:OE1   | 5:F:433:LEU:HB2   | 2.13                     | 0.49              |
| 1:G:40:LEU:O      | 1:G:44:LEU:HB2    | 2.13                     | 0.49              |
| 1:H:173:PRO:HB3   | 1:H:204:SER:HB2   | 1.94                     | 0.49              |
| 3:J:633:VAL:HG22  | 3:J:635:PRO:HD3   | 1.93                     | 0.49              |
| 3:J:667:ALA:HB1   | 3:J:672:ALA:HB3   | 1.95                     | 0.49              |
| 3:J:1147:ARG:HB3  | 3:J:1188:VAL:HG11 | 1.95                     | 0.49              |
| 1:B:11:PHE:HB2    | 1:B:25:LEU:HD13   | 1.95                     | 0.49              |
| 1:B:226:ALA:O     | 1:B:228:PRO:HD3   | 2.13                     | 0.49              |
| 2:C:874:LEU:O     | 2:C:877:PRO:HD2   | 2.12                     | 0.49              |
| 1:G:210:ALA:HA    | 1:G:213:GLN:HE21  | 1.77                     | 0.49              |
| 3:J:213:VAL:HG13  | 3:J:385:VAL:HG22  | 1.95                     | 0.49              |
| 3:J:601:ARG:HH21  | 3:J:606:ILE:HA    | 1.78                     | 0.49              |
| 5:L:215:LYS:HA    | 5:L:224:PHE:HE2   | 1.77                     | 0.49              |
| 2:C:198:ARG:HG2   | 2:C:234:ALA:CB    | 2.42                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:237:ARG:NH2  | 2:C:241:LEU:HD11 | 2.28                     | 0.49              |
| 3:D:783:ARG:HD3  | 3:D:1028:ALA:O   | 2.13                     | 0.49              |
| 5:F:386:LEU:HD22 | 5:F:391:ILE:HG13 | 1.95                     | 0.49              |
| 1:G:53:VAL:HG13  | 1:G:167:VAL:HG21 | 1.95                     | 0.49              |
| 1:G:58:ILE:HG21  | 1:G:68:ILE:HD13  | 1.94                     | 0.49              |
| 1:H:10:VAL:O     | 1:H:12:THR:HG23  | 2.13                     | 0.49              |
| 1:H:152:PRO:HD2  | 1:H:155:ARG:HG3  | 1.94                     | 0.49              |
| 2:I:1067:TYR:O   | 2:I:1071:ILE:HB  | 2.13                     | 0.49              |
| 8:P:22:DC:H2"    | 8:P:23:DA:C8     | 2.48                     | 0.49              |
| 2:C:168:ARG:HH21 | 2:C:346:VAL:HG22 | 1.78                     | 0.48              |
| 3:D:316:HIS:H    | 3:D:316:HIS:HD1  | 1.59                     | 0.48              |
| 3:D:667:ALA:HB1  | 3:D:672:ALA:HB3  | 1.95                     | 0.48              |
| 3:J:132:TYR:CE1  | 3:J:456:MET:HG2  | 2.48                     | 0.48              |
| 3:J:682:ASP:C    | 3:J:684:LYS:H    | 2.21                     | 0.48              |
| 3:J:758:GLU:O    | 3:J:762:GLN:HG2  | 2.13                     | 0.48              |
| 6:M:63:LEU:HD21  | 6:M:102:PRO:HG3  | 1.95                     | 0.48              |
| 2:C:48:PHE:O     | 2:C:52:PHE:HB2   | 2.12                     | 0.48              |
| 2:C:419:THR:HG22 | 2:C:422:ARG:HG2  | 1.95                     | 0.48              |
| 3:D:288:MET:HE3  | 3:D:311:LEU:HD13 | 1.94                     | 0.48              |
| 1:G:161:ARG:HD2  | 1:G:162:ILE:HG22 | 1.94                     | 0.48              |
| 2:I:432:ARG:NH1  | 2:I:518:ARG:HH21 | 2.06                     | 0.48              |
| 3:J:169:TYR:OH   | 3:J:198:ARG:N    | 2.45                     | 0.48              |
| 3:J:421:LEU:HD11 | 3:J:429:SER:HB2  | 1.94                     | 0.48              |
| 3:J:699:VAL:HA   | 3:J:718:PRO:HD3  | 1.94                     | 0.48              |
| 6:N:34:ALA:HB3   | 6:N:51:VAL:HG21  | 1.95                     | 0.48              |
| 6:N:68:VAL:HB    | 6:N:69:PRO:HD3   | 1.95                     | 0.48              |
| 1:A:24:VAL:HG22  | 1:A:196:THR:HG23 | 1.95                     | 0.48              |
| 2:C:13:ILE:HD13  | 2:C:483:VAL:HG11 | 1.95                     | 0.48              |
| 2:C:259:GLY:HA2  | 2:C:263:ASP:HB2  | 1.95                     | 0.48              |
| 2:C:366:THR:HG23 | 6:M:14:PRO:HD3   | 1.96                     | 0.48              |
| 2:C:1008:ARG:NH2 | 2:C:1020:PRO:HB3 | 2.28                     | 0.48              |
| 3:D:140:ALA:HB1  | 3:D:161:LEU:HD23 | 1.95                     | 0.48              |
| 3:D:238:PRO:HB3  | 3:D:315:ARG:O    | 2.13                     | 0.48              |
| 1:G:43:ILE:HD11  | 1:G:218:LEU:HD13 | 1.95                     | 0.48              |
| 1:G:58:ILE:HD11  | 1:G:140:MET:HE2  | 1.95                     | 0.48              |
| 1:G:108:GLU:HB2  | 1:G:110:ARG:HH11 | 1.78                     | 0.48              |
| 1:G:114:PHE:O    | 1:G:116:PRO:HD3  | 2.14                     | 0.48              |
| 2:I:195:LEU:HB3  | 2:I:238:LEU:HD11 | 1.94                     | 0.48              |
| 2:I:893:ALA:O    | 2:I:897:LEU:HG   | 2.14                     | 0.48              |
| 6:M:17:VAL:HB    | 6:M:142:GLN:HG3  | 1.95                     | 0.48              |
| 2:C:557:ARG:HD3  | 2:C:879:ARG:HB3  | 1.95                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:G:53:VAL:H      | 1:G:144:VAL:HG13  | 1.78                     | 0.48              |
| 2:I:209:ARG:HG3   | 2:I:210:GLU:N     | 2.29                     | 0.48              |
| 2:I:241:LEU:O     | 2:I:244:PRO:HD3   | 2.12                     | 0.48              |
| 2:I:858:MET:SD    | 2:I:859:PRO:HD2   | 2.53                     | 0.48              |
| 3:J:50:PHE:CD2    | 3:J:522:PRO:HD3   | 2.49                     | 0.48              |
| 3:J:65:ARG:HG3    | 3:J:67:ARG:H      | 1.79                     | 0.48              |
| 3:J:162:ARG:HG2   | 3:J:414:ARG:HH21  | 1.77                     | 0.48              |
| 3:J:483:HIS:ND1   | 3:J:484:PRO:HD2   | 2.29                     | 0.48              |
| 3:J:918:ALA:HA    | 3:J:922:LEU:HD23  | 1.94                     | 0.48              |
| 3:J:969:ARG:HG3   | 3:J:972:ARG:HH21  | 1.78                     | 0.48              |
| 3:J:1112:CYS:HB3  | 3:J:1196:THR:OG1  | 2.14                     | 0.48              |
| 3:J:1116:ASN:HB2  | 3:J:1193:THR:HB   | 1.95                     | 0.48              |
| 3:D:1060:SER:OG   | 3:D:1061:PHE:N    | 2.46                     | 0.48              |
| 2:I:674:VAL:HG11  | 2:I:992:MET:HE3   | 1.96                     | 0.48              |
| 2:I:880:MET:HG2   | 3:J:1038:LEU:HD11 | 1.96                     | 0.48              |
| 2:I:882:LEU:HD21  | 3:J:1038:LEU:HD22 | 1.94                     | 0.48              |
| 3:J:103:TRP:CE2   | 3:J:1444:THR:HG23 | 2.48                     | 0.48              |
| 1:B:15:THR:HA     | 1:B:21:GLY:HA2    | 1.96                     | 0.48              |
| 2:C:94:LEU:O      | 2:C:115:LEU:HB2   | 2.14                     | 0.48              |
| 3:D:423:ASP:HB3   | 3:D:426:LYS:HB3   | 1.95                     | 0.48              |
| 5:F:202:LEU:HD22  | 5:F:239:VAL:HG22  | 1.95                     | 0.48              |
| 2:I:750:LYS:HD3   | 3:J:681:ARG:HG3   | 1.95                     | 0.48              |
| 2:I:1047:HIS:O    | 2:I:1051:GLU:HG2  | 2.14                     | 0.48              |
| 3:J:658:LEU:HD11  | 3:J:674:ARG:HG2   | 1.96                     | 0.48              |
| 2:C:508:ILE:HD11  | 2:C:529:VAL:HG11  | 1.96                     | 0.48              |
| 2:C:1081:VAL:HG21 | 2:C:1086:ARG:CZ   | 2.44                     | 0.48              |
| 3:D:122:GLU:O     | 3:D:126:VAL:HG23  | 2.13                     | 0.48              |
| 3:D:1273:VAL:HG22 | 3:D:1326:THR:HG23 | 1.95                     | 0.48              |
| 5:F:266:ILE:O     | 5:F:270:ALA:HB2   | 2.13                     | 0.48              |
| 1:G:48:ILE:HG22   | 1:G:173:PRO:HD2   | 1.94                     | 0.48              |
| 1:H:59:GLU:HG3    | 1:H:139:TYR:HD2   | 1.79                     | 0.48              |
| 1:H:101:LEU:HD22  | 1:H:102:ARG:N     | 2.27                     | 0.48              |
| 2:I:72:ARG:HG3    | 2:I:95:TYR:HB2    | 1.96                     | 0.48              |
| 2:I:99:GLN:HB2    | 2:I:101:ILE:HD11  | 1.96                     | 0.48              |
| 2:I:111:ASP:OD1   | 2:I:368:THR:OG1   | 2.32                     | 0.48              |
| 3:J:49:ILE:HG13   | 3:J:50:PHE:N      | 2.29                     | 0.48              |
| 3:J:567:ILE:HG22  | 3:J:571:LYS:NZ    | 2.29                     | 0.48              |
| 3:J:658:LEU:HD22  | 3:J:670:VAL:HG13  | 1.95                     | 0.48              |
| 5:L:202:LEU:HD22  | 5:L:239:VAL:HG22  | 1.95                     | 0.48              |
| 2:C:46:ALA:O      | 2:C:50:GLU:HB2    | 2.13                     | 0.48              |
| 3:D:1283:ILE:HD12 | 3:D:1315:ASP:HB2  | 1.96                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:734:LEU:HA    | 2:I:737:LEU:HD13  | 1.96                     | 0.48              |
| 2:I:860:HIS:HA    | 2:I:866:PRO:HA    | 1.94                     | 0.48              |
| 3:J:1292:VAL:HG21 | 3:J:1311:LEU:HD13 | 1.96                     | 0.48              |
| 6:M:146:ILE:HB    | 6:M:150:GLU:HB2   | 1.94                     | 0.48              |
| 2:C:206:THR:HG23  | 2:C:209:ARG:CZ    | 2.43                     | 0.48              |
| 3:D:128:TYR:O     | 3:D:572:ARG:NH1   | 2.46                     | 0.48              |
| 4:E:30:LEU:CD2    | 4:E:63:TRP:HB3    | 2.44                     | 0.48              |
| 2:I:193:LEU:HD21  | 2:I:307:LEU:HD21  | 1.94                     | 0.48              |
| 2:I:206:THR:HG23  | 2:I:209:ARG:CZ    | 2.43                     | 0.48              |
| 2:I:874:LEU:O     | 2:I:877:PRO:HD2   | 2.14                     | 0.48              |
| 3:J:1283:ILE:HD12 | 3:J:1315:ASP:HB2  | 1.96                     | 0.48              |
| 3:J:1313:VAL:HG21 | 3:J:1325:LEU:HD13 | 1.96                     | 0.48              |
| 1:A:79:ILE:HA     | 1:A:82:LEU:HB2    | 1.95                     | 0.48              |
| 2:C:399:ASN:HB2   | 2:C:400:PRO:HD2   | 1.95                     | 0.48              |
| 3:D:483:HIS:ND1   | 3:D:484:PRO:HD2   | 2.29                     | 0.48              |
| 3:D:675:ARG:HH21  | 3:D:679:ARG:NH1   | 2.12                     | 0.48              |
| 5:F:379:ARG:HG3   | 5:F:405:PHE:CE2   | 2.48                     | 0.48              |
| 1:G:79:ILE:HA     | 1:G:82:LEU:HB2    | 1.96                     | 0.48              |
| 1:H:72:LYS:HG3    | 1:H:131:THR:HB    | 1.94                     | 0.48              |
| 3:J:701:LEU:HD23  | 3:J:763:MET:HG2   | 1.96                     | 0.48              |
| 3:J:702:LEU:HG    | 3:J:747:VAL:HG22  | 1.95                     | 0.48              |
| 3:J:1434:TRP:CD1  | 3:J:1457:ASP:HB2  | 2.48                     | 0.48              |
| 5:L:157:GLN:NE2   | 5:L:171:VAL:HG21  | 2.28                     | 0.48              |
| 1:B:42:ARG:NH1    | 2:C:981:GLU:OE2   | 2.46                     | 0.47              |
| 1:B:132:LEU:HD12  | 1:B:136:GLY:HA3   | 1.96                     | 0.47              |
| 3:D:1313:VAL:HG21 | 3:D:1325:LEU:HD13 | 1.95                     | 0.47              |
| 1:G:215:VAL:HG13  | 1:H:222:LEU:HD22  | 1.95                     | 0.47              |
| 2:I:198:ARG:HG2   | 2:I:234:ALA:HB1   | 1.96                     | 0.47              |
| 2:I:570:PRO:O     | 2:I:571:LEU:HD13  | 2.14                     | 0.47              |
| 2:I:984:GLU:HG3   | 3:J:945:SER:HA    | 1.94                     | 0.47              |
| 2:I:1053:LEU:HA   | 3:J:621:LYS:HE3   | 1.95                     | 0.47              |
| 3:J:90:MET:HB3    | 3:J:519:VAL:O     | 2.14                     | 0.47              |
| 3:J:592:THR:HG22  | 3:J:599:PRO:HA    | 1.95                     | 0.47              |
| 3:J:858:LEU:HD21  | 3:J:864:VAL:HG11  | 1.96                     | 0.47              |
| 6:M:21:ALA:HB3    | 6:M:37:GLN:HG2    | 1.96                     | 0.47              |
| 2:C:769:PRO:HD3   | 3:D:65:ARG:HH22   | 1.79                     | 0.47              |
| 2:C:1031:ARG:HA   | 3:D:622:ARG:HA    | 1.96                     | 0.47              |
| 3:D:179:VAL:HG11  | 3:D:191:LEU:HG    | 1.95                     | 0.47              |
| 3:D:310:LEU:H     | 3:D:310:LEU:CD1   | 2.27                     | 0.47              |
| 3:D:699:VAL:HA    | 3:D:718:PRO:HD3   | 1.96                     | 0.47              |
| 3:D:954:ALA:HB2   | 3:D:1020:LEU:HD22 | 1.97                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:F:108:LEU:HB2   | 5:F:109:LEU:H     | 1.48                     | 0.47              |
| 1:G:99:LEU:HB2    | 1:G:142:VAL:HG23  | 1.97                     | 0.47              |
| 2:I:13:ILE:HD13   | 2:I:483:VAL:HG11  | 1.95                     | 0.47              |
| 2:I:27:LYS:HA     | 2:I:30:LEU:HD22   | 1.96                     | 0.47              |
| 3:J:731:LEU:HD22  | 3:J:780:LYS:O     | 2.14                     | 0.47              |
| 3:J:1118:ILE:HG12 | 3:J:1190:SER:HB3  | 1.95                     | 0.47              |
| 5:L:418:LYS:O     | 5:L:422:LYS:HB2   | 2.14                     | 0.47              |
| 6:M:68:VAL:HB     | 6:M:69:PRO:HD3    | 1.95                     | 0.47              |
| 2:C:726:ILE:HB    | 2:C:729:LEU:HB2   | 1.96                     | 0.47              |
| 3:D:916:TYR:CE2   | 3:D:1168:LEU:HD13 | 2.49                     | 0.47              |
| 4:E:66:LYS:HA     | 4:E:69:LEU:HD12   | 1.96                     | 0.47              |
| 5:F:95:PRO:O      | 5:F:98:GLN:HB3    | 2.13                     | 0.47              |
| 2:I:146:VAL:HG12  | 2:I:162:ILE:HG13  | 1.94                     | 0.47              |
| 2:I:306:THR:HG23  | 2:I:307:LEU:HD12  | 1.96                     | 0.47              |
| 2:I:1056:LYS:O    | 3:J:624:ASP:N     | 2.48                     | 0.47              |
| 3:J:702:LEU:HD22  | 3:J:728:LEU:HD13  | 1.96                     | 0.47              |
| 1:B:85:LEU:HD12   | 1:B:86:VAL:H      | 1.78                     | 0.47              |
| 3:D:654:LYS:HB3   | 3:D:655:PRO:HD3   | 1.96                     | 0.47              |
| 2:I:274:ARG:O     | 2:I:278:GLU:HB2   | 2.15                     | 0.47              |
| 2:I:713:ARG:HH12  | 2:I:716:LYS:HZ1   | 1.61                     | 0.47              |
| 1:A:59:GLU:HG3    | 1:A:60:ASP:H      | 1.79                     | 0.47              |
| 3:D:400:VAL:HG22  | 3:D:402:PRO:HD3   | 1.96                     | 0.47              |
| 3:D:1364:HIS:CD2  | 3:D:1366:LYS:HE2  | 2.50                     | 0.47              |
| 3:D:1478:SER:HB3  | 3:D:1481:VAL:HG22 | 1.96                     | 0.47              |
| 1:G:32:PHE:O      | 1:G:36:LEU:HG     | 2.15                     | 0.47              |
| 2:I:159:ILE:HG13  | 2:I:174:LEU:O     | 2.14                     | 0.47              |
| 6:M:45:SER:OG     | 6:M:46:LYS:N      | 2.47                     | 0.47              |
| 1:A:53:VAL:HG22   | 1:A:54:THR:N      | 2.25                     | 0.47              |
| 1:A:153:ALA:HB2   | 1:A:167:VAL:C     | 2.39                     | 0.47              |
| 1:B:10:VAL:O      | 1:B:12:THR:HG23   | 2.15                     | 0.47              |
| 2:C:726:ILE:HD12  | 2:C:729:LEU:HG    | 1.96                     | 0.47              |
| 2:C:922:PHE:HB2   | 2:C:967:PHE:CD2   | 2.48                     | 0.47              |
| 3:D:241:VAL:HG13  | 3:D:312:ARG:HG2   | 1.95                     | 0.47              |
| 3:D:272:LEU:O     | 3:D:279:VAL:N     | 2.45                     | 0.47              |
| 5:F:302:SER:H     | 5:F:305:GLU:CG    | 2.28                     | 0.47              |
| 7:R:15:DT:H6      | 7:R:15:DT:H5'     | 1.80                     | 0.47              |
| 1:A:162:ILE:HG23  | 1:A:163:ASN:H     | 1.79                     | 0.47              |
| 1:B:59:GLU:C      | 1:B:61:VAL:H      | 2.23                     | 0.47              |
| 1:B:161:ARG:HG3   | 1:B:162:ILE:N     | 2.24                     | 0.47              |
| 2:C:126:SER:HB3   | 2:C:134:ARG:O     | 2.14                     | 0.47              |
| 2:C:521:PRO:HG2   | 3:D:1072:ILE:HD11 | 1.95                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:685:GLU:HG2   | 3:D:739:ASP:HB3   | 1.96                     | 0.47              |
| 2:C:858:MET:H     | 2:C:977:GLY:HA3   | 1.80                     | 0.47              |
| 3:D:22:SER:HB2    | 3:D:92:HIS:HB3    | 1.95                     | 0.47              |
| 3:D:49:ILE:HD11   | 3:D:50:PHE:CZ     | 2.49                     | 0.47              |
| 3:D:109:PRO:HG2   | 3:D:111:LYS:NZ    | 2.29                     | 0.47              |
| 3:D:858:LEU:HD21  | 3:D:864:VAL:HG11  | 1.97                     | 0.47              |
| 1:H:29:GLU:HB3    | 1:H:32:PHE:CD1    | 2.49                     | 0.47              |
| 2:I:168:ARG:HH21  | 2:I:346:VAL:HG22  | 1.79                     | 0.47              |
| 2:I:579:VAL:HG13  | 2:I:842:ARG:HH22  | 1.80                     | 0.47              |
| 2:I:601:GLY:HA2   | 2:I:615:TYR:HA    | 1.97                     | 0.47              |
| 2:I:726:ILE:HB    | 2:I:729:LEU:HB2   | 1.97                     | 0.47              |
| 2:I:726:ILE:HD12  | 2:I:729:LEU:HG    | 1.96                     | 0.47              |
| 3:J:639:LEU:HD22  | 3:J:766:ALA:HA    | 1.95                     | 0.47              |
| 3:J:648:MET:O     | 3:J:652:LEU:HB2   | 2.14                     | 0.47              |
| 3:J:710:ARG:HG3   | 3:J:711:LEU:HD22  | 1.97                     | 0.47              |
| 3:J:841:PHE:HB3   | 3:J:843:PHE:CE1   | 2.50                     | 0.47              |
| 3:J:853:VAL:HG22  | 3:J:858:LEU:HB3   | 1.97                     | 0.47              |
| 2:C:118:LEU:HD13  | 2:C:382:LEU:HD23  | 1.96                     | 0.47              |
| 2:C:576:ALA:HB1   | 2:C:580:MET:HE3   | 1.96                     | 0.47              |
| 1:G:162:ILE:HG23  | 1:G:163:ASN:H     | 1.77                     | 0.47              |
| 1:G:218:LEU:HD23  | 1:H:222:LEU:HD21  | 1.96                     | 0.47              |
| 2:I:1032:PHE:CZ   | 2:I:1036:GLU:HB3  | 2.50                     | 0.47              |
| 3:J:521:PRO:HB2   | 3:J:524:LEU:HG    | 1.97                     | 0.47              |
| 3:J:977:ALA:HB3   | 3:J:983:LEU:HD12  | 1.96                     | 0.47              |
| 3:J:1168:LEU:HD23 | 3:J:1169:GLU:H    | 1.79                     | 0.47              |
| 1:A:221:HIS:HA    | 1:A:224:TYR:CD1   | 2.50                     | 0.47              |
| 2:C:274:ARG:O     | 2:C:278:GLU:HB2   | 2.15                     | 0.47              |
| 2:C:807:ARG:HB3   | 2:C:821:GLU:HB3   | 1.96                     | 0.47              |
| 3:D:217:ARG:HB2   | 3:D:339:TRP:CE2   | 2.50                     | 0.47              |
| 3:D:717:GLN:HA    | 3:D:718:PRO:HD3   | 1.76                     | 0.47              |
| 3:D:1225:ALA:O    | 3:D:1229:ILE:HG12 | 2.15                     | 0.47              |
| 3:D:1443:THR:HG22 | 3:D:1447:LEU:HD13 | 1.97                     | 0.47              |
| 3:D:1476:THR:HA   | 4:E:17:TYR:HB3    | 1.97                     | 0.47              |
| 5:F:206:ASN:O     | 5:F:209:LEU:HB3   | 2.14                     | 0.47              |
| 1:G:123:MET:HG3   | 1:G:203:GLY:HA3   | 1.95                     | 0.47              |
| 2:I:149:THR:HA    | 2:I:322:VAL:HG13  | 1.96                     | 0.47              |
| 2:I:154:ARG:NH1   | 2:I:176:VAL:HG23  | 2.29                     | 0.47              |
| 2:I:448:ASN:C     | 2:I:451:LEU:HD23  | 2.39                     | 0.47              |
| 2:I:497:ALA:HB1   | 2:I:501:THR:HG21  | 1.97                     | 0.47              |
| 2:I:1038:TRP:CE2  | 3:J:1099:VAL:HG11 | 2.50                     | 0.47              |
| 2:I:1063:ARG:HG3  | 5:L:356:PRO:HG3   | 1.96                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:1086:ARG:HD2  | 2:I:1112:PHE:CE2  | 2.49                     | 0.47              |
| 2:I:1097:LEU:HD22 | 3:J:10:ILE:HD11   | 1.96                     | 0.47              |
| 3:J:828:VAL:HG22  | 3:J:833:GLU:HB2   | 1.96                     | 0.47              |
| 3:J:1381:VAL:HG21 | 3:J:1389:LEU:HD23 | 1.96                     | 0.47              |
| 4:K:41:GLU:HB3    | 4:K:42:PRO:HD2    | 1.96                     | 0.47              |
| 6:M:12:LEU:HD13   | 6:M:59:LEU:HD13   | 1.97                     | 0.47              |
| 2:C:1067:TYR:CZ   | 5:F:357:VAL:HG12  | 2.49                     | 0.47              |
| 3:D:401:TYR:HB3   | 3:D:427:VAL:HG21  | 1.97                     | 0.47              |
| 1:H:149:GLY:O     | 1:H:171:PHE:HB2   | 2.15                     | 0.47              |
| 2:I:146:VAL:HG11  | 2:I:281:LEU:HD11  | 1.96                     | 0.47              |
| 2:I:198:ARG:HG2   | 2:I:234:ALA:CB    | 2.45                     | 0.47              |
| 2:I:893:ALA:HB2   | 2:I:918:LEU:HD22  | 1.96                     | 0.47              |
| 1:B:48:ILE:HG13   | 1:B:213:GLN:HE21  | 1.78                     | 0.46              |
| 2:C:86:LYS:HE2    | 2:C:814:GLU:H     | 1.79                     | 0.46              |
| 2:C:1032:PHE:CZ   | 2:C:1036:GLU:HB3  | 2.50                     | 0.46              |
| 3:D:610:LYS:HD3   | 3:D:615:ARG:NH1   | 2.31                     | 0.46              |
| 3:D:731:LEU:HB3   | 3:D:779:ALA:HB1   | 1.98                     | 0.46              |
| 2:I:336:VAL:HA    | 2:I:339:LEU:HD11  | 1.97                     | 0.46              |
| 3:J:500:ARG:NH1   | 3:J:1390:LEU:HD21 | 2.30                     | 0.46              |
| 5:L:96:VAL:HA     | 5:L:225:LEU:HD11  | 1.96                     | 0.46              |
| 1:A:53:VAL:HA     | 1:A:144:VAL:HA    | 1.96                     | 0.46              |
| 2:C:300:ASP:OD1   | 2:C:301:GLU:N     | 2.48                     | 0.46              |
| 3:D:49:ILE:HG13   | 3:D:50:PHE:H      | 1.81                     | 0.46              |
| 3:D:460:ALA:O     | 3:D:464:LEU:HG    | 2.15                     | 0.46              |
| 3:D:1142:SER:O    | 3:D:1364:HIS:ND1  | 2.48                     | 0.46              |
| 5:F:229:GLN:HA    | 5:F:232:ASN:HD22  | 1.80                     | 0.46              |
| 2:I:300:ASP:OD1   | 2:I:301:GLU:N     | 2.49                     | 0.46              |
| 2:I:537:LYS:HZ3   | 2:I:905:VAL:N     | 2.07                     | 0.46              |
| 3:J:12:LEU:HD21   | 3:J:1452:ILE:HD13 | 1.97                     | 0.46              |
| 3:J:577:ALA:O     | 3:J:581:VAL:HG23  | 2.15                     | 0.46              |
| 3:J:638:LYS:HD3   | 3:J:640:HIS:CD2   | 2.49                     | 0.46              |
| 3:J:681:ARG:C     | 3:J:683:ILE:H     | 2.22                     | 0.46              |
| 3:J:710:ARG:HB3   | 3:J:1227:GLU:OE1  | 2.15                     | 0.46              |
| 6:M:144:LEU:HB2   | 6:M:146:ILE:HG12  | 1.97                     | 0.46              |
| 1:A:215:VAL:HG13  | 1:B:222:LEU:HD22  | 1.97                     | 0.46              |
| 2:C:742:ILE:CD1   | 2:C:803:ARG:HD2   | 2.45                     | 0.46              |
| 2:C:838:LYS:HB3   | 2:C:997:LEU:HB2   | 1.98                     | 0.46              |
| 3:D:26:VAL:HG13   | 3:D:42:ASP:O      | 2.15                     | 0.46              |
| 1:H:76:VAL:HA     | 1:H:79:ILE:HD12   | 1.98                     | 0.46              |
| 2:I:688:ILE:HG12  | 2:I:871:LEU:HD21  | 1.98                     | 0.46              |
| 5:L:302:SER:H     | 5:L:305:GLU:CG    | 2.29                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:58:ILE:HG21   | 1:A:68:ILE:HD13   | 1.97                     | 0.46              |
| 2:C:89:THR:HG23   | 2:C:129:ILE:HA    | 1.96                     | 0.46              |
| 2:C:305:PRO:O     | 2:C:308:ARG:HG2   | 2.16                     | 0.46              |
| 2:C:889:HIS:CE1   | 2:C:970:GLY:HA3   | 2.50                     | 0.46              |
| 3:D:216:LEU:HB3   | 3:D:218:LYS:HZ3   | 1.81                     | 0.46              |
| 3:D:351:MET:HG2   | 3:D:370:ALA:HB2   | 1.97                     | 0.46              |
| 3:D:441:ARG:HH11  | 3:D:445:ARG:HH12  | 1.64                     | 0.46              |
| 3:D:633:VAL:HG22  | 3:D:635:PRO:HD3   | 1.96                     | 0.46              |
| 2:I:98:LEU:HD23   | 2:I:98:LEU:H      | 1.80                     | 0.46              |
| 2:I:508:ILE:HD11  | 2:I:529:VAL:HG11  | 1.97                     | 0.46              |
| 3:J:102:ILE:HB    | 3:J:579:ASP:CG    | 2.40                     | 0.46              |
| 3:J:539:ASP:HB3   | 3:J:600:LEU:HG    | 1.95                     | 0.46              |
| 6:N:75:LEU:HG     | 6:N:159:TRP:CZ3   | 2.51                     | 0.46              |
| 2:C:161:SER:C     | 2:C:162:ILE:HD12  | 2.40                     | 0.46              |
| 2:C:1107:ASN:HD22 | 2:C:1107:ASN:HA   | 1.59                     | 0.46              |
| 3:D:1020:LEU:HG   | 3:D:1035:ILE:HD12 | 1.97                     | 0.46              |
| 5:F:181:LEU:HD23  | 5:F:185:LEU:CB    | 2.46                     | 0.46              |
| 5:F:419:ALA:O     | 5:F:423:LEU:HD12  | 2.16                     | 0.46              |
| 1:G:73:GLU:HB3    | 1:G:77:GLU:HB3    | 1.97                     | 0.46              |
| 1:H:74:ASP:O      | 1:H:78:ILE:HG12   | 2.15                     | 0.46              |
| 2:I:580:MET:HE1   | 2:I:665:PHE:HB3   | 1.98                     | 0.46              |
| 2:I:671:ASN:HA    | 2:I:992:MET:O     | 2.14                     | 0.46              |
| 3:J:100:ALA:N     | 3:J:575:GLN:HE22  | 2.11                     | 0.46              |
| 3:J:1151:ARG:HA   | 3:J:1162:GLU:HG3  | 1.97                     | 0.46              |
| 6:M:11:VAL:O      | 6:M:59:LEU:HD12   | 2.16                     | 0.46              |
| 7:O:23:DG:H1'     | 7:O:24:DC:H5'     | 1.97                     | 0.46              |
| 1:B:32:PHE:O      | 1:B:36:LEU:HG     | 2.16                     | 0.46              |
| 2:C:98:LEU:HD23   | 2:C:98:LEU:H      | 1.81                     | 0.46              |
| 2:C:860:HIS:HA    | 2:C:866:PRO:HA    | 1.97                     | 0.46              |
| 2:C:950:LEU:HD11  | 2:C:952:LEU:HB2   | 1.98                     | 0.46              |
| 2:C:988:VAL:HG22  | 3:D:948:THR:OG1   | 2.15                     | 0.46              |
| 5:F:238:ALA:HB2   | 5:F:257:TRP:HB2   | 1.97                     | 0.46              |
| 1:H:54:THR:HG23   | 1:H:55:SER:H      | 1.80                     | 0.46              |
| 1:H:76:VAL:O      | 1:H:80:LEU:HD13   | 2.15                     | 0.46              |
| 2:I:940:GLU:HG2   | 2:I:973:VAL:HG21  | 1.98                     | 0.46              |
| 5:L:275:ILE:HG22  | 5:L:280:VAL:HG12  | 1.98                     | 0.46              |
| 1:A:32:PHE:O      | 1:A:36:LEU:HG     | 2.16                     | 0.46              |
| 2:C:85:GLU:HB2    | 2:C:804:LEU:HD21  | 1.98                     | 0.46              |
| 2:C:713:ARG:HH12  | 2:C:716:LYS:HZ1   | 1.64                     | 0.46              |
| 3:D:834:THR:OG1   | 3:D:838:ARG:HB2   | 2.16                     | 0.46              |
| 3:D:999:THR:HG22  | 3:D:1041:MET:HE1  | 1.98                     | 0.46              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:J:160:GLU:HG3  | 3:J:165:LYS:HD3   | 1.98                     | 0.46              |
| 5:L:166:PRO:HG2  | 5:L:169:LYS:HE3   | 1.98                     | 0.46              |
| 2:C:672:VAL:HB   | 2:C:868:ASP:HB2   | 1.97                     | 0.46              |
| 3:D:677:LEU:HD21 | 3:D:687:VAL:HG11  | 1.98                     | 0.46              |
| 3:D:1112:CYS:HB3 | 3:D:1196:THR:OG1  | 2.15                     | 0.46              |
| 5:F:154:ALA:HB1  | 5:F:158:LYS:NZ    | 2.31                     | 0.46              |
| 5:F:206:ASN:HA   | 7:O:30:DT:O2      | 2.15                     | 0.46              |
| 1:G:83:LYS:HE3   | 1:G:168:ASP:HB2   | 1.97                     | 0.46              |
| 1:H:176:ARG:HB3  | 1:H:200:TRP:CE3   | 2.51                     | 0.46              |
| 3:J:10:ILE:O     | 3:J:1454:GLY:HA2  | 2.16                     | 0.46              |
| 3:J:1384:PRO:HA  | 3:J:1415:VAL:HG13 | 1.98                     | 0.46              |
| 5:L:294:GLN:HE21 | 5:L:294:GLN:HB3   | 1.57                     | 0.46              |
| 6:N:12:LEU:HD13  | 6:N:59:LEU:HD13   | 1.98                     | 0.46              |
| 3:D:209:ARG:HA   | 3:D:347:VAL:HG12  | 1.96                     | 0.46              |
| 3:D:229:ALA:CB   | 3:D:245:LEU:H     | 2.29                     | 0.46              |
| 3:D:841:PHE:CZ   | 3:D:858:LEU:HD13  | 2.50                     | 0.46              |
| 3:D:954:ALA:O    | 3:D:1062:ARG:NE   | 2.49                     | 0.46              |
| 1:G:108:GLU:HG2  | 1:G:131:THR:HG23  | 1.97                     | 0.46              |
| 3:J:901:GLN:H    | 3:J:901:GLN:HG2   | 1.53                     | 0.46              |
| 5:L:154:ALA:HB1  | 5:L:158:LYS:NZ    | 2.31                     | 0.46              |
| 5:L:234:GLY:O    | 5:L:257:TRP:HB3   | 2.16                     | 0.46              |
| 2:C:232:GLU:CD   | 2:C:232:GLU:H     | 2.24                     | 0.46              |
| 3:D:661:MET:SD   | 3:D:677:LEU:HD11  | 2.56                     | 0.46              |
| 2:I:66:LEU:HA    | 2:I:99:GLN:O      | 2.15                     | 0.46              |
| 2:I:521:PRO:HG2  | 3:J:1072:ILE:HD11 | 1.97                     | 0.46              |
| 2:I:679:PHE:H    | 2:I:683:ASN:HD21  | 1.64                     | 0.46              |
| 2:I:758:ARG:HE   | 2:I:788:THR:HB    | 1.80                     | 0.46              |
| 3:J:834:THR:OG1  | 3:J:838:ARG:HB2   | 2.16                     | 0.46              |
| 4:K:66:LYS:HA    | 4:K:69:LEU:HD12   | 1.98                     | 0.46              |
| 6:M:124:LEU:HD11 | 8:P:2:DG:H4'      | 1.98                     | 0.46              |
| 1:B:57:TYR:HB3   | 1:B:141:GLU:HG3   | 1.97                     | 0.45              |
| 1:B:76:VAL:O     | 1:B:80:LEU:HD13   | 2.16                     | 0.45              |
| 2:C:247:PRO:HA   | 2:C:248:PRO:HD3   | 1.72                     | 0.45              |
| 2:C:435:TYR:HB3  | 2:C:436:GLY:H     | 1.56                     | 0.45              |
| 2:C:675:ALA:HB2  | 2:C:867:VAL:HG21  | 1.98                     | 0.45              |
| 2:C:729:LEU:HD11 | 2:C:733:ALA:HB3   | 1.98                     | 0.45              |
| 3:D:682:ASP:O    | 3:D:684:LYS:N     | 2.45                     | 0.45              |
| 3:D:758:GLU:HA   | 3:D:762:GLN:NE2   | 2.32                     | 0.45              |
| 3:D:1293:PHE:HA  | 3:D:1302:GLU:HA   | 1.98                     | 0.45              |
| 1:G:54:THR:HG23  | 1:G:143:ARG:O     | 2.15                     | 0.45              |
| 1:G:205:VAL:HG11 | 1:G:213:GLN:NE2   | 2.31                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:101:ILE:HG23  | 2:I:108:ILE:HA    | 1.97                     | 0.45              |
| 2:I:835:VAL:HG13  | 2:I:851:LYS:H     | 1.80                     | 0.45              |
| 3:J:1074:SER:HA   | 3:J:1077:ALA:HB3  | 1.98                     | 0.45              |
| 1:B:48:ILE:HA     | 1:B:49:PRO:HD2    | 1.80                     | 0.45              |
| 2:C:154:ARG:NH1   | 2:C:176:VAL:HG23  | 2.30                     | 0.45              |
| 2:C:534:VAL:H     | 2:C:538:GLN:HE22  | 1.64                     | 0.45              |
| 3:D:34:TYR:HD1    | 5:F:325:ILE:HG21  | 1.80                     | 0.45              |
| 3:D:90:MET:HB3    | 3:D:519:VAL:O     | 2.16                     | 0.45              |
| 3:D:441:ARG:NH1   | 3:D:445:ARG:HH12  | 2.14                     | 0.45              |
| 3:D:646:LYS:HE3   | 3:D:688:TRP:CZ2   | 2.44                     | 0.45              |
| 3:D:1381:VAL:HG21 | 3:D:1389:LEU:HD23 | 1.98                     | 0.45              |
| 2:I:232:GLU:CD    | 2:I:232:GLU:H     | 2.24                     | 0.45              |
| 2:I:305:PRO:O     | 2:I:308:ARG:HG2   | 2.16                     | 0.45              |
| 2:I:358:ARG:HB2   | 2:I:372:LEU:HD12  | 1.97                     | 0.45              |
| 2:I:838:LYS:HB3   | 2:I:997:LEU:HB2   | 1.98                     | 0.45              |
| 3:J:838:ARG:HB3   | 3:J:865:THR:HG23  | 1.99                     | 0.45              |
| 5:L:307:ALA:HB1   | 5:L:314:TRP:HB3   | 1.98                     | 0.45              |
| 2:C:671:ASN:HA    | 2:C:992:MET:O     | 2.16                     | 0.45              |
| 2:C:840:ALA:HB3   | 2:C:997:LEU:HD11  | 1.98                     | 0.45              |
| 2:C:882:LEU:HD21  | 3:D:1038:LEU:HD22 | 1.98                     | 0.45              |
| 2:C:1083:GLU:OE2  | 3:D:87:ARG:NH1    | 2.49                     | 0.45              |
| 3:D:689:ASP:O     | 3:D:692:GLU:HB2   | 2.16                     | 0.45              |
| 1:G:63:HIS:NE2    | 2:I:801:VAL:HG13  | 2.31                     | 0.45              |
| 1:G:64:GLU:O      | 1:G:75:VAL:HB     | 2.16                     | 0.45              |
| 2:I:835:VAL:O     | 3:J:725:SER:OG    | 2.34                     | 0.45              |
| 2:I:1086:ARG:HD2  | 2:I:1112:PHE:CD2  | 2.51                     | 0.45              |
| 3:J:717:GLN:HA    | 3:J:718:PRO:HD3   | 1.75                     | 0.45              |
| 3:J:750:PRO:HG2   | 3:J:756:GLN:NE2   | 2.31                     | 0.45              |
| 3:J:1014:ASN:C    | 3:J:1016:PRO:HD3  | 2.41                     | 0.45              |
| 3:J:1043:GLY:O    | 3:J:1045:MET:HE2  | 2.17                     | 0.45              |
| 6:M:33:ARG:H      | 6:M:33:ARG:HD2    | 1.81                     | 0.45              |
| 1:A:83:LYS:HE3    | 1:A:168:ASP:HB2   | 1.98                     | 0.45              |
| 2:C:16:PRO:HB2    | 2:C:460:ARG:NH2   | 2.30                     | 0.45              |
| 2:C:66:LEU:HD23   | 2:C:100:LEU:HA    | 1.98                     | 0.45              |
| 3:D:103:TRP:CE2   | 3:D:1444:THR:HG23 | 2.51                     | 0.45              |
| 3:D:147:VAL:HG23  | 3:D:151:GLN:CD    | 2.42                     | 0.45              |
| 3:D:165:LYS:H     | 3:D:397:LYS:HE3   | 1.81                     | 0.45              |
| 3:D:266:GLU:CD    | 3:D:315:ARG:H     | 2.25                     | 0.45              |
| 3:D:1341:PRO:O    | 3:D:1344:VAL:HB   | 2.17                     | 0.45              |
| 1:H:156:HIS:NE2   | 1:H:167:VAL:O     | 2.49                     | 0.45              |
| 2:I:676:ILE:CG2   | 2:I:873:PRO:HB3   | 2.47                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:691:SER:HB3   | 2:I:868:ASP:HA    | 1.97                     | 0.45              |
| 2:I:729:LEU:HD13  | 2:I:730:SER:O     | 2.17                     | 0.45              |
| 3:J:1448:THR:O    | 3:J:1452:ILE:HG12 | 2.16                     | 0.45              |
| 7:R:5:DA:H1'      | 7:R:6:DC:H5''     | 1.98                     | 0.45              |
| 1:B:180:GLN:NE2   | 1:B:182:GLU:HB3   | 2.31                     | 0.45              |
| 2:C:583:LEU:O     | 2:C:587:VAL:HG23  | 2.16                     | 0.45              |
| 3:D:62:LYS:HE2    | 3:D:62:LYS:HB2    | 1.78                     | 0.45              |
| 3:D:791:TYR:CE2   | 3:D:945:SER:HB3   | 2.51                     | 0.45              |
| 5:F:141:LEU:O     | 5:F:145:VAL:HG23  | 2.17                     | 0.45              |
| 1:G:59:GLU:HG3    | 1:G:60:ASP:H      | 1.81                     | 0.45              |
| 2:I:66:LEU:HD23   | 2:I:100:LEU:HA    | 1.98                     | 0.45              |
| 2:I:200:LEU:HD21  | 2:I:303:PHE:HB2   | 1.98                     | 0.45              |
| 3:J:560:GLN:HE21  | 3:J:560:GLN:HB2   | 1.58                     | 0.45              |
| 3:J:923:GLY:O     | 3:J:926:LYS:HB2   | 2.17                     | 0.45              |
| 3:J:1044:LEU:HD23 | 3:J:1053:PHE:O    | 2.17                     | 0.45              |
| 4:K:19:LEU:O      | 4:K:23:VAL:HG23   | 2.16                     | 0.45              |
| 4:K:30:LEU:CD2    | 4:K:63:TRP:HB3    | 2.44                     | 0.45              |
| 1:A:53:VAL:H      | 1:A:144:VAL:HG13  | 1.82                     | 0.45              |
| 2:C:200:LEU:HD21  | 2:C:303:PHE:HB2   | 1.99                     | 0.45              |
| 2:C:1056:LYS:O    | 3:D:624:ASP:N     | 2.49                     | 0.45              |
| 3:J:618:LEU:HG    | 3:J:1467:ILE:HG23 | 1.97                     | 0.45              |
| 3:J:1012:GLU:HG2  | 3:J:1021:TYR:OH   | 2.17                     | 0.45              |
| 5:L:217:TYR:CD2   | 5:L:262:ILE:HG21  | 2.51                     | 0.45              |
| 7:O:10:DA:H1'     | 7:O:11:DG:H5''    | 1.99                     | 0.45              |
| 7:O:22:DT:H2''    | 7:O:23:DG:C8      | 2.52                     | 0.45              |
| 2:C:118:LEU:HD12  | 2:C:119:PRO:HD2   | 1.99                     | 0.45              |
| 2:C:235:MET:HE1   | 2:C:298:PHE:CE1   | 2.52                     | 0.45              |
| 3:D:699:VAL:HB    | 3:D:716:PHE:O     | 2.17                     | 0.45              |
| 5:F:111:LEU:O     | 5:F:115:ILE:HG12  | 2.16                     | 0.45              |
| 2:I:677:MET:SD    | 2:I:987:ILE:HD13  | 2.56                     | 0.45              |
| 3:J:592:THR:HA    | 3:J:600:LEU:HD13  | 1.99                     | 0.45              |
| 3:J:849:ALA:O     | 3:J:853:VAL:HG23  | 2.17                     | 0.45              |
| 2:C:121:MET:HE2   | 2:C:125:GLY:O     | 2.17                     | 0.45              |
| 2:C:312:ALA:O     | 2:C:317:VAL:HG12  | 2.17                     | 0.45              |
| 2:C:869:VAL:HG21  | 2:C:871:LEU:HG    | 1.99                     | 0.45              |
| 3:D:31:THR:HG21   | 5:F:272:THR:HG22  | 1.98                     | 0.45              |
| 2:I:1086:ARG:HB3  | 2:I:1112:PHE:HE2  | 1.82                     | 0.45              |
| 3:J:1293:PHE:HA   | 3:J:1302:GLU:HA   | 1.99                     | 0.45              |
| 3:J:1295:GLU:HG2  | 3:J:1300:SER:OG   | 2.16                     | 0.45              |
| 3:J:1443:THR:HG22 | 3:J:1447:LEU:HD13 | 1.98                     | 0.45              |
| 6:N:13:PRO:HA     | 6:N:14:PRO:HA     | 1.70                     | 0.45              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 6:N:79:ARG:HB3   | 6:N:111:GLN:HB2   | 1.98                     | 0.45              |
| 2:C:249:LYS:HB2  | 2:C:252:LYS:HE3   | 1.99                     | 0.45              |
| 2:C:971:LYS:HA   | 2:C:988:VAL:HA    | 1.97                     | 0.45              |
| 3:D:65:ARG:HG3   | 3:D:67:ARG:H      | 1.82                     | 0.45              |
| 3:D:421:LEU:HD11 | 3:D:429:SER:HB2   | 1.98                     | 0.45              |
| 3:D:565:ILE:H    | 3:D:565:ILE:HD12  | 1.81                     | 0.45              |
| 1:G:176:ARG:HG3  | 1:G:200:TRP:CE3   | 2.51                     | 0.45              |
| 2:I:134:ARG:HH12 | 2:I:392:SER:C     | 2.25                     | 0.45              |
| 3:J:573:MET:HA   | 3:J:576:GLU:HG2   | 1.97                     | 0.45              |
| 4:K:65:MET:O     | 4:K:69:LEU:HG     | 2.17                     | 0.45              |
| 5:L:95:PRO:O     | 5:L:98:GLN:HB3    | 2.17                     | 0.45              |
| 7:O:14:DT:H3     | 8:P:12:DA:H61     | 1.65                     | 0.45              |
| 1:A:73:GLU:HB3   | 1:A:77:GLU:HB3    | 1.99                     | 0.45              |
| 1:B:11:PHE:HB2   | 1:B:25:LEU:CD1    | 2.47                     | 0.45              |
| 2:C:17:PRO:O     | 2:C:20:GLU:HG3    | 2.16                     | 0.45              |
| 2:C:532:MET:HG2  | 2:C:533:ASP:N     | 2.32                     | 0.45              |
| 2:C:545:ASN:HA   | 2:C:905:VAL:HG21  | 1.99                     | 0.45              |
| 2:C:1053:LEU:HA  | 3:D:621:LYS:HE3   | 1.99                     | 0.45              |
| 5:F:166:PRO:HG2  | 5:F:169:LYS:HE3   | 1.98                     | 0.45              |
| 2:I:144:PRO:HG2  | 2:I:273:GLY:N     | 2.32                     | 0.45              |
| 2:I:235:MET:HE1  | 2:I:298:PHE:CE1   | 2.51                     | 0.45              |
| 2:I:578:VAL:HG12 | 2:I:900:ARG:HA    | 1.98                     | 0.45              |
| 2:I:834:GLN:HG2  | 2:I:835:VAL:H     | 1.82                     | 0.45              |
| 3:J:1374:GLN:HA  | 3:J:1377:LYS:HD2  | 1.99                     | 0.45              |
| 2:C:878:SER:HA   | 3:D:1034:GLN:OE1  | 2.17                     | 0.44              |
| 3:D:1384:PRO:HA  | 3:D:1415:VAL:HG13 | 1.99                     | 0.44              |
| 5:F:332:LEU:HD22 | 5:F:345:GLY:HA2   | 1.98                     | 0.44              |
| 1:H:156:HIS:ND1  | 1:H:158:ILE:HG22  | 2.31                     | 0.44              |
| 2:I:16:PRO:HB2   | 2:I:460:ARG:NH2   | 2.32                     | 0.44              |
| 2:I:22:GLN:O     | 2:I:336:VAL:HG21  | 2.17                     | 0.44              |
| 2:I:535:SER:O    | 2:I:538:GLN:HG2   | 2.16                     | 0.44              |
| 2:I:642:ARG:O    | 2:I:643:VAL:HG13  | 2.17                     | 0.44              |
| 2:I:837:ASP:HB3  | 2:I:1000:MET:HE2  | 1.99                     | 0.44              |
| 3:J:109:PRO:HG2  | 3:J:111:LYS:NZ    | 2.33                     | 0.44              |
| 3:J:565:ILE:HD13 | 5:L:204:GLU:HG2   | 2.00                     | 0.44              |
| 3:J:692:GLU:HG2  | 3:J:720:LEU:HD12  | 1.99                     | 0.44              |
| 6:N:97:LEU:HD21  | 6:N:132:ALA:HB2   | 1.98                     | 0.44              |
| 1:B:74:ASP:O     | 1:B:78:ILE:HG12   | 2.17                     | 0.44              |
| 2:C:192:PRO:HB2  | 2:C:195:LEU:HB2   | 1.99                     | 0.44              |
| 3:D:849:ALA:O    | 3:D:853:VAL:HG23  | 2.18                     | 0.44              |
| 2:I:394:PHE:CE2  | 2:I:632:ASN:HB3   | 2.52                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:428:ARG:NE    | 2:I:451:LEU:HD21  | 2.22                     | 0.44              |
| 2:I:683:ASN:OD1   | 2:I:872:ASN:ND2   | 2.50                     | 0.44              |
| 3:J:371:ILE:HG23  | 3:J:372:ASP:H     | 1.81                     | 0.44              |
| 3:J:1442:ASN:O    | 3:J:1446:VAL:HG23 | 2.18                     | 0.44              |
| 5:L:181:LEU:HD23  | 5:L:185:LEU:CB    | 2.47                     | 0.44              |
| 1:B:38:ASN:HB2    | 1:B:39:PRO:HD3    | 1.99                     | 0.44              |
| 1:B:143:ARG:HG3   | 1:B:160:ASP:OD2   | 2.16                     | 0.44              |
| 2:C:217:LEU:H     | 2:C:217:LEU:HD23  | 1.82                     | 0.44              |
| 2:C:595:LEU:HD23  | 2:C:656:ALA:HB3   | 2.00                     | 0.44              |
| 3:D:264:LEU:HD21  | 3:D:339:TRP:CD1   | 2.52                     | 0.44              |
| 3:D:302:GLN:HG2   | 3:D:303:PRO:HD2   | 1.99                     | 0.44              |
| 3:D:554:LEU:O     | 3:D:558:LEU:HG    | 2.17                     | 0.44              |
| 2:I:335:THR:O     | 2:I:339:LEU:HG    | 2.18                     | 0.44              |
| 2:I:448:ASN:HA    | 2:I:451:LEU:HD23  | 2.00                     | 0.44              |
| 3:J:133:ILE:HG22  | 3:J:152:LEU:HG    | 1.99                     | 0.44              |
| 3:J:762:GLN:HB3   | 4:K:16:LYS:HE2    | 1.99                     | 0.44              |
| 6:N:11:VAL:O      | 6:N:59:LEU:HD12   | 2.17                     | 0.44              |
| 1:A:40:LEU:HD21   | 1:A:215:VAL:HG22  | 2.00                     | 0.44              |
| 1:B:54:THR:OG1    | 1:B:158:ILE:HG21  | 2.17                     | 0.44              |
| 1:B:176:ARG:HD2   | 3:D:884:ARG:HH22  | 1.82                     | 0.44              |
| 2:C:539:VAL:HG21  | 3:D:1067:VAL:HG11 | 1.99                     | 0.44              |
| 2:C:713:ARG:HH22  | 2:C:716:LYS:NZ    | 2.16                     | 0.44              |
| 2:C:834:GLN:HG2   | 2:C:835:VAL:H     | 1.82                     | 0.44              |
| 2:C:1087:VAL:HG12 | 2:C:1091:GLU:OE1  | 2.18                     | 0.44              |
| 3:D:977:ALA:HB3   | 3:D:983:LEU:HD12  | 2.00                     | 0.44              |
| 3:D:1232:PRO:HB2  | 3:D:1356:TYR:HE2  | 1.82                     | 0.44              |
| 1:H:57:TYR:HB3    | 1:H:141:GLU:HG3   | 1.98                     | 0.44              |
| 2:I:950:LEU:HD11  | 2:I:952:LEU:HB2   | 1.99                     | 0.44              |
| 3:J:92:HIS:HD2    | 3:J:516:ALA:HB1   | 1.82                     | 0.44              |
| 2:C:99:GLN:HB3    | 2:C:110:GLU:HG3   | 1.98                     | 0.44              |
| 2:C:428:ARG:NE    | 2:C:451:LEU:HD21  | 2.24                     | 0.44              |
| 2:C:673:LEU:HB3   | 2:C:867:VAL:HG12  | 1.99                     | 0.44              |
| 2:C:690:ILE:CG1   | 2:C:852:ILE:HG23  | 2.45                     | 0.44              |
| 3:D:264:LEU:HD21  | 3:D:339:TRP:CD2   | 2.52                     | 0.44              |
| 3:D:317:MET:HG3   | 3:D:339:TRP:HB3   | 1.99                     | 0.44              |
| 4:E:65:MET:O      | 4:E:69:LEU:HG     | 2.17                     | 0.44              |
| 1:G:53:VAL:HG22   | 1:G:54:THR:N      | 2.28                     | 0.44              |
| 1:H:48:ILE:HG22   | 1:H:173:PRO:HD2   | 1.98                     | 0.44              |
| 2:I:327:HIS:O     | 2:I:331:ARG:HG3   | 2.17                     | 0.44              |
| 2:I:441:VAL:O     | 2:I:443:THR:HG22  | 2.17                     | 0.44              |
| 2:I:630:ARG:HA    | 2:I:705:ILE:HD13  | 2.00                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:J:49:ILE:HD11   | 3:J:50:PHE:CZ     | 2.52                     | 0.44              |
| 3:J:153:LEU:HB3   | 3:J:157:GLU:HG3   | 2.00                     | 0.44              |
| 5:L:266:ILE:O     | 5:L:270:ALA:HB2   | 2.18                     | 0.44              |
| 2:C:839:LEU:HD23  | 2:C:995:MET:O     | 2.18                     | 0.44              |
| 2:C:853:LEU:HA    | 2:C:854:PRO:HD3   | 1.83                     | 0.44              |
| 3:D:206:ARG:HH11  | 3:D:206:ARG:HG3   | 1.83                     | 0.44              |
| 3:D:261:LEU:HD21  | 3:D:268:HIS:CD2   | 2.50                     | 0.44              |
| 3:D:417:PRO:HA    | 3:D:430:GLU:HA    | 1.99                     | 0.44              |
| 5:F:237:ARG:NH2   | 5:F:241:LYS:HD2   | 2.33                     | 0.44              |
| 5:F:302:SER:O     | 5:F:306:ILE:HG22  | 2.17                     | 0.44              |
| 1:G:224:TYR:CD1   | 1:H:9:PRO:HG2     | 2.53                     | 0.44              |
| 2:I:564:MET:SD    | 2:I:846:LYS:HG2   | 2.58                     | 0.44              |
| 2:I:936:VAL:HB    | 2:I:941:LYS:HE2   | 1.99                     | 0.44              |
| 3:J:123:LEU:HG    | 3:J:127:LEU:HD12  | 1.99                     | 0.44              |
| 6:N:49:VAL:HG13   | 6:N:57:VAL:HG21   | 1.99                     | 0.44              |
| 8:P:3:DC:H2"      | 8:P:4:DA:C8       | 2.52                     | 0.44              |
| 2:C:91:GLN:HG3    | 2:C:117:HIS:HB3   | 1.98                     | 0.44              |
| 2:C:198:ARG:CZ    | 2:C:238:LEU:HB2   | 2.47                     | 0.44              |
| 2:C:394:PHE:CE2   | 2:C:632:ASN:HB3   | 2.52                     | 0.44              |
| 2:C:937:ASP:OD2   | 2:C:939:ARG:NE    | 2.51                     | 0.44              |
| 2:C:1035:MET:HB2  | 3:D:707:THR:HB    | 1.99                     | 0.44              |
| 3:D:1281:VAL:HG21 | 3:D:1313:VAL:HG11 | 1.99                     | 0.44              |
| 4:E:41:GLU:HB3    | 4:E:42:PRO:HD2    | 1.99                     | 0.44              |
| 1:H:54:THR:OG1    | 1:H:158:ILE:HG21  | 2.18                     | 0.44              |
| 1:H:176:ARG:HD3   | 1:H:200:TRP:HZ3   | 1.83                     | 0.44              |
| 2:I:164:PRO:HG3   | 2:I:267:TYR:CE1   | 2.53                     | 0.44              |
| 2:I:588:VAL:HG21  | 2:I:664:GLY:HA2   | 2.00                     | 0.44              |
| 3:J:683:ILE:HD12  | 3:J:688:TRP:CZ2   | 2.53                     | 0.44              |
| 3:J:1476:THR:HG22 | 4:K:17:TYR:HB3    | 2.00                     | 0.44              |
| 5:L:103:ILE:HG21  | 5:L:207:LEU:HD22  | 1.99                     | 0.44              |
| 6:N:136:LEU:O     | 6:N:140:VAL:HG23  | 2.17                     | 0.44              |
| 1:A:99:LEU:HB2    | 1:A:142:VAL:HG23  | 2.00                     | 0.44              |
| 1:B:48:ILE:HG22   | 1:B:173:PRO:HD2   | 1.99                     | 0.44              |
| 3:D:268:HIS:HB2   | 3:D:284:LEU:HD22  | 2.00                     | 0.44              |
| 3:D:573:MET:HA    | 3:D:576:GLU:CG    | 2.48                     | 0.44              |
| 4:E:19:LEU:O      | 4:E:23:VAL:HG23   | 2.18                     | 0.44              |
| 1:G:9:PRO:HG3     | 1:H:224:TYR:CG    | 2.53                     | 0.44              |
| 2:I:121:MET:HE2   | 2:I:125:GLY:O     | 2.18                     | 0.44              |
| 2:I:743:VAL:HG21  | 2:I:800:VAL:HG21  | 1.99                     | 0.44              |
| 2:I:839:LEU:HD23  | 2:I:995:MET:O     | 2.18                     | 0.44              |
| 5:L:153:THR:C     | 5:L:155:ARG:H     | 2.25                     | 0.44              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:C:111:ASP:OD1  | 2:C:368:THR:OG1   | 2.35                     | 0.44              |
| 2:C:134:ARG:HH12 | 2:C:392:SER:C     | 2.26                     | 0.44              |
| 3:D:171:LEU:HA   | 3:D:171:LEU:HD23  | 1.75                     | 0.44              |
| 3:D:646:LYS:HA   | 3:D:720:LEU:HD22  | 1.99                     | 0.44              |
| 4:E:6:ILE:HD11   | 4:E:10:PHE:CZ     | 2.53                     | 0.44              |
| 1:H:51:THR:HG23  | 1:H:52:ALA:H      | 1.83                     | 0.44              |
| 2:I:121:MET:HE3  | 2:I:127:PHE:CE1   | 2.52                     | 0.44              |
| 2:I:396:ASP:HB2  | 2:I:406:HIS:ND1   | 2.32                     | 0.44              |
| 2:I:934:PHE:HD2  | 2:I:934:PHE:HA    | 1.74                     | 0.44              |
| 3:J:758:GLU:HG2  | 3:J:1476:THR:HG21 | 1.99                     | 0.44              |
| 3:J:1020:LEU:HG  | 3:J:1035:ILE:HD12 | 2.00                     | 0.44              |
| 5:L:188:TYR:HA   | 5:L:191:ILE:HD12  | 2.00                     | 0.44              |
| 6:N:129:LEU:O    | 6:N:133:ILE:HG12  | 2.18                     | 0.44              |
| 1:A:101:LEU:HD12 | 1:A:102:ARG:H     | 1.82                     | 0.43              |
| 2:C:852:ILE:HG22 | 2:C:853:LEU:H     | 1.83                     | 0.43              |
| 3:D:15:PRO:HG3   | 3:D:514:LEU:HD12  | 2.00                     | 0.43              |
| 3:D:102:ILE:HB   | 3:D:579:ASP:CG    | 2.43                     | 0.43              |
| 3:D:231:VAL:H    | 3:D:243:ALA:H     | 1.66                     | 0.43              |
| 3:D:1074:SER:HA  | 3:D:1077:ALA:HB3  | 2.00                     | 0.43              |
| 2:I:312:ALA:O    | 2:I:317:VAL:HG12  | 2.18                     | 0.43              |
| 2:I:677:MET:HE2  | 2:I:679:PHE:HD1   | 1.83                     | 0.43              |
| 3:J:160:GLU:HG2  | 3:J:165:LYS:HB2   | 2.00                     | 0.43              |
| 3:J:970:LYS:O    | 3:J:974:ILE:HG13  | 2.18                     | 0.43              |
| 2:C:42:VAL:HA    | 2:C:46:ALA:HB2    | 2.00                     | 0.43              |
| 2:C:1038:TRP:CE2 | 3:D:1099:VAL:HG11 | 2.53                     | 0.43              |
| 3:D:124:GLU:OE1  | 3:D:587:ARG:NH2   | 2.52                     | 0.43              |
| 1:H:11:PHE:HB2   | 1:H:25:LEU:CD1    | 2.48                     | 0.43              |
| 1:H:59:GLU:C     | 1:H:61:VAL:H      | 2.25                     | 0.43              |
| 2:I:435:TYR:HB3  | 2:I:436:GLY:H     | 1.54                     | 0.43              |
| 2:I:557:ARG:HG3  | 2:I:881:ASN:HD22  | 1.83                     | 0.43              |
| 2:I:1031:ARG:HG2 | 2:I:1032:PHE:N    | 2.32                     | 0.43              |
| 3:J:876:SER:O    | 3:J:879:ARG:HB3   | 2.17                     | 0.43              |
| 3:J:956:ILE:HD11 | 3:J:1062:ARG:HH11 | 1.83                     | 0.43              |
| 6:M:90:HIS:CD2   | 6:M:124:LEU:HB3   | 2.53                     | 0.43              |
| 2:C:677:MET:SD   | 2:C:987:ILE:HD13  | 2.58                     | 0.43              |
| 2:C:717:LEU:HD23 | 2:C:761:PHE:HB2   | 2.01                     | 0.43              |
| 3:D:156:GLU:O    | 3:D:160:GLU:HB2   | 2.18                     | 0.43              |
| 3:D:648:MET:O    | 3:D:652:LEU:HB2   | 2.17                     | 0.43              |
| 2:I:545:ASN:HA   | 2:I:905:VAL:HG21  | 2.00                     | 0.43              |
| 2:I:583:LEU:O    | 2:I:587:VAL:HG23  | 2.17                     | 0.43              |
| 2:I:874:LEU:O    | 3:J:1029:ARG:HG2  | 2.18                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:915:LYS:HG2   | 2:I:968:ASP:OD2   | 2.18                     | 0.43              |
| 3:J:116:LEU:HD21  | 3:J:465:LEU:HG    | 2.00                     | 0.43              |
| 3:J:554:LEU:O     | 3:J:558:LEU:HG    | 2.17                     | 0.43              |
| 3:J:900:ILE:HB    | 3:J:902:MET:HE3   | 2.00                     | 0.43              |
| 5:L:111:LEU:O     | 5:L:115:ILE:HG12  | 2.18                     | 0.43              |
| 1:A:211:LEU:O     | 1:A:215:VAL:HG23  | 2.17                     | 0.43              |
| 2:C:22:GLN:O      | 2:C:336:VAL:HG21  | 2.18                     | 0.43              |
| 2:C:69:LEU:C      | 2:C:70:GLU:HG3    | 2.43                     | 0.43              |
| 2:C:90:TYR:HB3    | 2:C:128:ILE:HB    | 2.00                     | 0.43              |
| 2:C:159:ILE:HG13  | 2:C:174:LEU:O     | 2.18                     | 0.43              |
| 2:C:569:VAL:HG22  | 2:C:996:LYS:O     | 2.18                     | 0.43              |
| 2:C:880:MET:SD    | 3:D:1034:GLN:HG2  | 2.58                     | 0.43              |
| 3:D:1033:GLN:O    | 3:D:1036:ARG:HB3  | 2.17                     | 0.43              |
| 3:D:1123:PHE:HE2  | 3:D:1184:ARG:HA   | 1.84                     | 0.43              |
| 5:F:94:ASP:HA     | 5:F:95:PRO:HD2    | 1.89                     | 0.43              |
| 1:B:184:THR:HB    | 1:B:194:LYS:HB2   | 2.01                     | 0.43              |
| 2:C:136:ILE:HA    | 2:C:391:LEU:O     | 2.18                     | 0.43              |
| 2:C:164:PRO:HG3   | 2:C:267:TYR:CE1   | 2.53                     | 0.43              |
| 2:C:469:THR:HA    | 2:C:470:PRO:HD3   | 1.85                     | 0.43              |
| 2:C:934:PHE:HD2   | 2:C:934:PHE:HA    | 1.70                     | 0.43              |
| 3:D:632:VAL:O     | 3:D:727:GLN:HA    | 2.19                     | 0.43              |
| 3:D:1048:PRO:HD3  | 3:D:1075:HIS:CB   | 2.49                     | 0.43              |
| 4:E:41:GLU:O      | 4:E:45:ARG:HG2    | 2.19                     | 0.43              |
| 1:G:57:TYR:HD1    | 1:G:163:ASN:O     | 2.02                     | 0.43              |
| 3:J:14:SER:HB3    | 3:J:511:TRP:CD2   | 2.54                     | 0.43              |
| 3:J:585:GLY:CA    | 3:J:590:PRO:HG3   | 2.48                     | 0.43              |
| 3:J:610:LYS:HD3   | 3:J:615:ARG:NH1   | 2.33                     | 0.43              |
| 3:J:1279:GLY:H    | 3:J:1319:VAL:HG23 | 1.83                     | 0.43              |
| 1:A:64:GLU:HG3    | 1:A:79:ILE:HD12   | 2.00                     | 0.43              |
| 2:C:92:ALA:HA     | 2:C:93:PRO:HD3    | 1.89                     | 0.43              |
| 2:C:140:ILE:HG12  | 2:C:141:HIS:N     | 2.33                     | 0.43              |
| 2:C:198:ARG:HG2   | 2:C:234:ALA:HB3   | 2.01                     | 0.43              |
| 2:C:261:LEU:HD13  | 2:C:291:VAL:HG21  | 2.00                     | 0.43              |
| 2:C:336:VAL:HA    | 2:C:339:LEU:HD11  | 2.01                     | 0.43              |
| 2:C:713:ARG:HH22  | 2:C:716:LYS:HZ1   | 1.66                     | 0.43              |
| 2:C:869:VAL:HG22  | 2:C:870:ILE:N     | 2.33                     | 0.43              |
| 3:D:50:PHE:CD2    | 3:D:522:PRO:HD3   | 2.53                     | 0.43              |
| 3:D:147:VAL:HG21  | 3:D:153:LEU:HD21  | 2.00                     | 0.43              |
| 3:D:1168:LEU:HD23 | 3:D:1169:GLU:H    | 1.82                     | 0.43              |
| 1:H:57:TYR:CE1    | 1:H:161:ARG:HG2   | 2.52                     | 0.43              |
| 1:H:87:VAL:HG11   | 1:H:99:LEU:HD21   | 2.01                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:217:LEU:HD23  | 2:I:217:LEU:H     | 1.83                     | 0.43              |
| 2:I:562:SER:O     | 2:I:565:GLN:HB2   | 2.18                     | 0.43              |
| 3:J:103:TRP:CE3   | 3:J:1448:THR:HG23 | 2.52                     | 0.43              |
| 3:J:138:LYS:HD2   | 3:J:451:ASP:O     | 2.18                     | 0.43              |
| 3:J:460:ALA:O     | 3:J:464:LEU:HG    | 2.18                     | 0.43              |
| 3:J:563:PRO:O     | 3:J:567:ILE:HG12  | 2.19                     | 0.43              |
| 5:L:141:LEU:O     | 5:L:145:VAL:HG23  | 2.18                     | 0.43              |
| 1:A:104:GLU:HG3   | 1:A:137:LYS:HG2   | 1.99                     | 0.43              |
| 1:A:158:ILE:HD11  | 1:A:166:PRO:HA    | 2.00                     | 0.43              |
| 2:C:570:PRO:O     | 2:C:571:LEU:HD13  | 2.19                     | 0.43              |
| 2:C:1067:TYR:CE2  | 5:F:357:VAL:HA    | 2.54                     | 0.43              |
| 3:D:236:TYR:CZ    | 3:D:242:LEU:HD13  | 2.53                     | 0.43              |
| 1:H:180:GLN:NE2   | 1:H:182:GLU:HB3   | 2.33                     | 0.43              |
| 2:I:262:ALA:HB2   | 2:I:291:VAL:HG23  | 2.01                     | 0.43              |
| 2:I:532:MET:HG2   | 2:I:533:ASP:N     | 2.33                     | 0.43              |
| 2:I:673:LEU:HA    | 2:I:990:GLY:O     | 2.19                     | 0.43              |
| 3:J:865:THR:HG22  | 3:J:874:GLU:HG2   | 2.00                     | 0.43              |
| 3:J:1000:THR:O    | 3:J:1004:THR:OG1  | 2.30                     | 0.43              |
| 6:N:21:ALA:HB3    | 6:N:37:GLN:HG2    | 2.01                     | 0.43              |
| 2:C:327:HIS:O     | 2:C:331:ARG:HG3   | 2.18                     | 0.43              |
| 2:C:880:MET:HG2   | 3:D:1038:LEU:HD11 | 2.00                     | 0.43              |
| 3:D:103:TRP:HZ3   | 3:D:1447:LEU:HB2  | 1.84                     | 0.43              |
| 3:D:322:VAL:HG22  | 3:D:323:GLU:H     | 1.83                     | 0.43              |
| 3:D:638:LYS:HG2   | 3:D:639:LEU:H     | 1.84                     | 0.43              |
| 3:D:970:LYS:O     | 3:D:974:ILE:HG13  | 2.18                     | 0.43              |
| 1:H:110:ARG:HH12  | 1:H:126:ASP:HA    | 1.84                     | 0.43              |
| 1:H:176:ARG:HD2   | 3:J:884:ARG:HH22  | 1.84                     | 0.43              |
| 2:I:838:LYS:HG2   | 2:I:997:LEU:HD22  | 2.01                     | 0.43              |
| 3:J:1146:GLY:O    | 3:J:1206:GLY:HA3  | 2.18                     | 0.43              |
| 3:J:1225:ALA:O    | 3:J:1229:ILE:HG12 | 2.18                     | 0.43              |
| 3:J:1229:ILE:HG12 | 3:J:1229:ILE:H    | 1.65                     | 0.43              |
| 3:J:1457:ASP:CG   | 3:J:1459:LEU:H    | 2.27                     | 0.43              |
| 5:L:116:ASP:O     | 5:L:120:LYS:HG2   | 2.18                     | 0.43              |
| 1:B:99:LEU:HB2    | 1:B:142:VAL:CG2   | 2.49                     | 0.43              |
| 2:C:893:ALA:O     | 2:C:897:LEU:HG    | 2.19                     | 0.43              |
| 2:C:897:LEU:HB3   | 2:C:899:GLN:HE21  | 1.82                     | 0.43              |
| 3:D:46:ASP:OD2    | 3:D:48:ARG:HB2    | 2.19                     | 0.43              |
| 3:D:56:TYR:CD1    | 3:D:66:GLN:HG2    | 2.54                     | 0.43              |
| 3:D:245:LEU:HD12  | 3:D:311:LEU:HD21  | 2.01                     | 0.43              |
| 3:D:260:GLU:O     | 3:D:270:ILE:HA    | 2.18                     | 0.43              |
| 3:D:277:GLU:H     | 3:D:277:GLU:CD    | 2.27                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:714:GLN:HE22  | 3:D:732:VAL:HB    | 1.83                     | 0.43              |
| 3:D:876:SER:O     | 3:D:879:ARG:HB3   | 2.19                     | 0.43              |
| 3:D:971:LEU:HD21  | 3:D:992:VAL:HG13  | 2.01                     | 0.43              |
| 5:F:142:ILE:O     | 5:F:146:VAL:HG23  | 2.19                     | 0.43              |
| 1:H:90:LEU:HB2    | 1:H:119:ASP:HB3   | 2.01                     | 0.43              |
| 2:I:136:ILE:HA    | 2:I:391:LEU:O     | 2.18                     | 0.43              |
| 2:I:807:ARG:HB3   | 2:I:821:GLU:HB3   | 2.01                     | 0.43              |
| 3:J:32:ILE:HG22   | 3:J:39:PRO:HA     | 2.01                     | 0.43              |
| 5:L:142:ILE:O     | 5:L:146:VAL:HG23  | 2.19                     | 0.43              |
| 5:L:398:LEU:HD23  | 5:L:409:ARG:O     | 2.19                     | 0.43              |
| 2:C:219:GLN:H     | 2:C:219:GLN:HG3   | 1.56                     | 0.43              |
| 2:C:1102:LEU:HD12 | 2:C:1107:ASN:N    | 2.34                     | 0.43              |
| 3:D:251:PHE:HB3   | 3:D:305:ALA:H     | 1.84                     | 0.43              |
| 3:D:1118:ILE:O    | 3:D:1118:ILE:HG13 | 2.19                     | 0.43              |
| 2:I:437:ARG:NH2   | 2:I:491:GLU:OE1   | 2.52                     | 0.43              |
| 2:I:701:THR:HG23  | 2:I:831:ARG:O     | 2.18                     | 0.43              |
| 2:I:880:MET:SD    | 3:J:1034:GLN:HG2  | 2.59                     | 0.43              |
| 3:J:29:PRO:HB3    | 3:J:548:ILE:HB    | 2.00                     | 0.43              |
| 3:J:645:PRO:HG3   | 3:J:725:SER:O     | 2.18                     | 0.43              |
| 3:J:1340:GLY:O    | 3:J:1344:VAL:HG23 | 2.19                     | 0.43              |
| 4:K:91:ARG:HH21   | 4:K:92:LEU:HG     | 1.83                     | 0.43              |
| 6:N:146:ILE:HB    | 6:N:150:GLU:HB2   | 2.00                     | 0.43              |
| 2:C:642:ARG:O     | 2:C:643:VAL:HG13  | 2.18                     | 0.42              |
| 3:D:1238:MET:C    | 3:D:1359:GLN:HE22 | 2.26                     | 0.42              |
| 3:D:1295:GLU:HG2  | 3:D:1300:SER:OG   | 2.19                     | 0.42              |
| 3:D:1465:ASN:O    | 3:D:1468:LEU:N    | 2.52                     | 0.42              |
| 1:G:65:PHE:HB3    | 2:I:628:TYR:CD2   | 2.54                     | 0.42              |
| 1:G:101:LEU:HD12  | 1:G:102:ARG:H     | 1.83                     | 0.42              |
| 2:I:14:PRO:HB3    | 2:I:586:ARG:NH2   | 2.32                     | 0.42              |
| 2:I:89:THR:HG23   | 2:I:129:ILE:HA    | 2.00                     | 0.42              |
| 2:I:146:VAL:HA    | 2:I:161:SER:O     | 2.19                     | 0.42              |
| 2:I:164:PRO:HD3   | 2:I:267:TYR:OH    | 2.19                     | 0.42              |
| 2:I:195:LEU:HD21  | 2:I:226:VAL:HG21  | 2.01                     | 0.42              |
| 2:I:430:VAL:HB    | 3:J:1075:HIS:ND1  | 2.34                     | 0.42              |
| 2:I:674:VAL:HA    | 2:I:869:VAL:CG1   | 2.44                     | 0.42              |
| 2:I:713:ARG:CZ    | 2:I:715:THR:HG22  | 2.49                     | 0.42              |
| 3:J:31:THR:OG1    | 3:J:32:ILE:N      | 2.52                     | 0.42              |
| 3:J:680:GLN:C     | 3:J:682:ASP:N     | 2.76                     | 0.42              |
| 7:R:6:DC:H2"      | 7:R:7:DA:C8       | 2.54                     | 0.42              |
| 1:A:158:ILE:HG13  | 1:A:166:PRO:HG3   | 2.01                     | 0.42              |
| 2:C:884:GLN:HB2   | 2:C:992:MET:HE2   | 2.00                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:1055:ILE:HD11 | 2:C:1079:PRO:HD3  | 2.01                     | 0.42              |
| 3:D:104:PHE:CG    | 3:D:512:MET:HE2   | 2.54                     | 0.42              |
| 3:D:680:GLN:O     | 3:D:682:ASP:N     | 2.44                     | 0.42              |
| 5:F:153:THR:C     | 5:F:155:ARG:H     | 2.28                     | 0.42              |
| 1:G:73:GLU:HG2    | 1:G:77:GLU:HG2    | 2.00                     | 0.42              |
| 2:I:387:SER:HB2   | 2:I:388:ARG:HD2   | 2.00                     | 0.42              |
| 2:I:419:THR:HG22  | 2:I:422:ARG:HG2   | 2.01                     | 0.42              |
| 2:I:658:GLY:N     | 2:I:661:SER:HB3   | 2.26                     | 0.42              |
| 2:I:869:VAL:HG21  | 2:I:871:LEU:HG    | 2.01                     | 0.42              |
| 3:J:62:LYS:HG3    | 3:J:63:TYR:N      | 2.34                     | 0.42              |
| 3:J:640:HIS:O     | 3:J:717:GLN:HB2   | 2.19                     | 0.42              |
| 3:J:721:VAL:HG21  | 3:J:727:GLN:HE22  | 1.82                     | 0.42              |
| 5:L:154:ALA:HB1   | 5:L:158:LYS:HZ3   | 1.84                     | 0.42              |
| 6:M:13:PRO:HA     | 6:M:14:PRO:HA     | 1.73                     | 0.42              |
| 6:M:136:LEU:O     | 6:M:140:VAL:HG23  | 2.19                     | 0.42              |
| 2:C:15:LEU:N      | 2:C:586:ARG:HH12  | 2.16                     | 0.42              |
| 2:C:195:LEU:HD21  | 2:C:226:VAL:HG21  | 2.01                     | 0.42              |
| 2:C:562:SER:O     | 2:C:565:GLN:HB2   | 2.18                     | 0.42              |
| 2:C:676:ILE:CG2   | 2:C:873:PRO:HB3   | 2.48                     | 0.42              |
| 3:D:96:ALA:HB3    | 3:D:554:LEU:HD23  | 2.01                     | 0.42              |
| 3:D:284:LEU:HA    | 3:D:285:PRO:HD2   | 1.91                     | 0.42              |
| 3:D:841:PHE:HB3   | 3:D:843:PHE:CE1   | 2.54                     | 0.42              |
| 3:D:879:ARG:HA    | 3:D:879:ARG:HD3   | 1.93                     | 0.42              |
| 3:D:949:ILE:HD11  | 3:D:1023:MET:HE1  | 2.00                     | 0.42              |
| 3:D:956:ILE:HD11  | 3:D:1062:ARG:HH11 | 1.83                     | 0.42              |
| 3:D:1146:GLY:O    | 3:D:1206:GLY:HA3  | 2.19                     | 0.42              |
| 1:G:9:PRO:HG3     | 1:H:224:TYR:CD2   | 2.53                     | 0.42              |
| 1:H:11:PHE:HB2    | 1:H:25:LEU:HD13   | 2.01                     | 0.42              |
| 1:H:85:LEU:HD12   | 1:H:86:VAL:H      | 1.83                     | 0.42              |
| 2:I:772:ARG:HD3   | 5:L:395:GLU:OE1   | 2.19                     | 0.42              |
| 2:I:889:HIS:CE1   | 2:I:970:GLY:HA3   | 2.54                     | 0.42              |
| 2:I:1044:GLY:HA3  | 4:K:17:TYR:HE1    | 1.83                     | 0.42              |
| 3:J:22:SER:HB2    | 3:J:92:HIS:HB3    | 2.00                     | 0.42              |
| 3:J:87:ARG:HG2    | 3:J:523:ASP:CB    | 2.49                     | 0.42              |
| 3:J:124:GLU:OE1   | 3:J:587:ARG:NH2   | 2.52                     | 0.42              |
| 3:J:171:LEU:HB3   | 3:J:391:ALA:O     | 2.19                     | 0.42              |
| 3:J:1341:PRO:O    | 3:J:1344:VAL:HB   | 2.19                     | 0.42              |
| 5:L:157:GLN:HE22  | 5:L:171:VAL:HG11  | 1.83                     | 0.42              |
| 6:N:113:ARG:HB2   | 6:N:159:TRP:CZ2   | 2.54                     | 0.42              |
| 1:A:58:ILE:HG12   | 1:A:140:MET:HG3   | 2.01                     | 0.42              |
| 1:A:59:GLU:HG2    | 1:A:139:TYR:HB3   | 2.02                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:172:ILE:HG23  | 2:C:184:MET:HE3   | 2.01                     | 0.42              |
| 2:C:497:ALA:HB1   | 2:C:501:THR:HG21  | 2.02                     | 0.42              |
| 3:D:138:LYS:HD2   | 3:D:451:ASP:O     | 2.18                     | 0.42              |
| 3:D:567:ILE:HG22  | 3:D:571:LYS:NZ    | 2.35                     | 0.42              |
| 3:D:1434:TRP:CD1  | 3:D:1457:ASP:HB2  | 2.54                     | 0.42              |
| 1:H:73:GLU:HB3    | 1:H:77:GLU:HB3    | 2.01                     | 0.42              |
| 2:I:258:PHE:HA    | 2:I:298:PHE:HE2   | 1.83                     | 0.42              |
| 2:I:672:VAL:HB    | 2:I:868:ASP:HB2   | 2.01                     | 0.42              |
| 2:I:1026:GLN:HE21 | 2:I:1026:GLN:HB2  | 1.55                     | 0.42              |
| 3:J:403:PHE:HD2   | 3:J:444:VAL:HG22  | 1.84                     | 0.42              |
| 6:M:125:ASP:HA    | 6:M:128:ALA:HB3   | 2.01                     | 0.42              |
| 2:C:80:GLN:O      | 2:C:84:ARG:HG3    | 2.20                     | 0.42              |
| 2:C:121:MET:HE3   | 2:C:127:PHE:CE1   | 2.55                     | 0.42              |
| 2:C:439:CYS:HA    | 2:C:440:PRO:HD2   | 1.92                     | 0.42              |
| 2:C:603:VAL:HB    | 2:C:646:GLY:HA2   | 2.01                     | 0.42              |
| 3:D:658:LEU:CD2   | 3:D:670:VAL:HG13  | 2.50                     | 0.42              |
| 3:D:701:LEU:HD11  | 3:D:750:PRO:HD3   | 2.01                     | 0.42              |
| 3:D:1267:ARG:H    | 3:D:1267:ARG:NE   | 2.09                     | 0.42              |
| 2:I:100:LEU:N     | 2:I:109:LYS:O     | 2.52                     | 0.42              |
| 2:I:516:ARG:HD2   | 2:I:519:GLY:HA2   | 2.01                     | 0.42              |
| 3:J:1117:TYR:HB2  | 3:J:1188:VAL:O    | 2.19                     | 0.42              |
| 3:J:1478:SER:HB3  | 3:J:1481:VAL:HG22 | 2.01                     | 0.42              |
| 5:L:244:TYR:H     | 5:L:244:TYR:HD2   | 1.68                     | 0.42              |
| 1:A:65:PHE:HB3    | 2:C:628:TYR:CD2   | 2.55                     | 0.42              |
| 2:C:670:GLN:HE22  | 2:C:699:PHE:HA    | 1.83                     | 0.42              |
| 2:C:910:THR:OG1   | 2:C:912:PRO:HD2   | 2.20                     | 0.42              |
| 2:C:1041:GLU:OE1  | 3:D:1462:LEU:HD13 | 2.19                     | 0.42              |
| 3:D:1014:ASN:C    | 3:D:1016:PRO:HD3  | 2.44                     | 0.42              |
| 2:I:302:VAL:O     | 2:I:305:PRO:HD2   | 2.20                     | 0.42              |
| 2:I:1071:ILE:HD12 | 3:J:655:PRO:O     | 2.19                     | 0.42              |
| 3:J:49:ILE:HG13   | 3:J:50:PHE:H      | 1.83                     | 0.42              |
| 3:J:791:TYR:CE2   | 3:J:945:SER:HB3   | 2.54                     | 0.42              |
| 5:L:409:ARG:NH2   | 8:S:20:DG:O6      | 2.52                     | 0.42              |
| 1:A:202:ASP:OD1   | 1:A:203:GLY:N     | 2.53                     | 0.42              |
| 2:C:80:GLN:H      | 2:C:80:GLN:HG2    | 1.60                     | 0.42              |
| 2:C:674:VAL:O     | 2:C:989:VAL:HA    | 2.20                     | 0.42              |
| 2:C:994:ILE:HG22  | 2:C:995:MET:N     | 2.35                     | 0.42              |
| 2:C:1083:GLU:O    | 2:C:1087:VAL:HG23 | 2.19                     | 0.42              |
| 3:D:93:ILE:HD13   | 3:D:548:ILE:HG12  | 2.00                     | 0.42              |
| 3:D:268:HIS:HB2   | 3:D:284:LEU:HB2   | 2.02                     | 0.42              |
| 3:D:780:LYS:HE3   | 3:D:908:LYS:HE2   | 2.01                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:F:147:ARG:HH21  | 5:F:199:ARG:HH12  | 1.68                     | 0.42              |
| 1:H:57:TYR:CD1    | 1:H:161:ARG:HG2   | 2.55                     | 0.42              |
| 2:I:48:PHE:O      | 2:I:52:PHE:HB2    | 2.19                     | 0.42              |
| 2:I:376:ARG:H     | 2:I:376:ARG:HG2   | 1.65                     | 0.42              |
| 2:I:840:ALA:HB3   | 2:I:997:LEU:HD11  | 2.02                     | 0.42              |
| 2:I:988:VAL:HG22  | 3:J:948:THR:OG1   | 2.20                     | 0.42              |
| 3:J:704:ARG:HB3   | 3:J:736:PHE:HB3   | 2.01                     | 0.42              |
| 3:J:937:TYR:O     | 3:J:941:LEU:HG    | 2.19                     | 0.42              |
| 6:M:11:VAL:HB     | 6:M:60:ARG:HG3    | 2.01                     | 0.42              |
| 2:C:211:LEU:HD13  | 2:C:218:VAL:HA    | 2.01                     | 0.42              |
| 2:C:230:ARG:CB    | 2:C:231:PRO:HD2   | 2.50                     | 0.42              |
| 2:C:1031:ARG:HG2  | 2:C:1032:PHE:N    | 2.34                     | 0.42              |
| 3:D:521:PRO:HA    | 3:D:522:PRO:HD3   | 1.87                     | 0.42              |
| 3:D:916:TYR:HE2   | 3:D:1168:LEU:HD13 | 1.85                     | 0.42              |
| 3:D:1040:GLY:O    | 3:D:1060:SER:HB2  | 2.19                     | 0.42              |
| 3:D:1044:LEU:HD23 | 3:D:1053:PHE:O    | 2.19                     | 0.42              |
| 3:D:1153:VAL:HB   | 3:D:1160:LEU:HB2  | 2.01                     | 0.42              |
| 1:G:24:VAL:HG22   | 1:G:196:THR:HG23  | 2.01                     | 0.42              |
| 2:I:471:TYR:CZ    | 2:I:496:ILE:HD13  | 2.55                     | 0.42              |
| 3:J:208:PRO:HA    | 3:J:390:PRO:HA    | 2.02                     | 0.42              |
| 3:J:397:LYS:HE3   | 3:J:397:LYS:HB3   | 1.90                     | 0.42              |
| 3:J:551:ASN:O     | 3:J:555:LYS:HG3   | 2.20                     | 0.42              |
| 3:J:670:VAL:O     | 3:J:671:LYS:C     | 2.63                     | 0.42              |
| 3:J:699:VAL:HB    | 3:J:716:PHE:O     | 2.20                     | 0.42              |
| 3:J:892:ASP:HB2   | 3:J:894:LYS:HG2   | 2.02                     | 0.42              |
| 3:J:1404:ASN:O    | 3:J:1408:ILE:HG12 | 2.18                     | 0.42              |
| 2:C:74:GLY:O      | 2:C:92:ALA:HB1    | 2.20                     | 0.42              |
| 2:C:198:ARG:NH2   | 2:C:238:LEU:HB2   | 2.34                     | 0.42              |
| 2:C:202:TYR:HD1   | 2:C:206:THR:HG21  | 1.85                     | 0.42              |
| 3:D:465:LEU:HA    | 3:D:468:LEU:HD12  | 2.01                     | 0.42              |
| 3:D:645:PRO:HG3   | 3:D:725:SER:O     | 2.19                     | 0.42              |
| 3:D:1232:PRO:O    | 3:D:1235:GLN:HG2  | 2.20                     | 0.42              |
| 5:F:398:LEU:HD23  | 5:F:409:ARG:O     | 2.20                     | 0.42              |
| 1:H:38:ASN:HB2    | 1:H:39:PRO:HD3    | 2.01                     | 0.42              |
| 1:H:42:ARG:NH1    | 2:I:981:GLU:OE2   | 2.53                     | 0.42              |
| 2:I:40:GLU:C      | 2:I:42:VAL:H      | 2.28                     | 0.42              |
| 2:I:237:ARG:NH2   | 2:I:241:LEU:HD11  | 2.35                     | 0.42              |
| 2:I:602:GLU:HA    | 2:I:648:ARG:HA    | 2.02                     | 0.42              |
| 2:I:674:VAL:O     | 2:I:989:VAL:HA    | 2.20                     | 0.42              |
| 2:I:897:LEU:HB3   | 2:I:899:GLN:HE21  | 1.85                     | 0.42              |
| 3:J:514:LEU:HD21  | 3:J:518:PRO:HD3   | 2.00                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:J:750:PRO:HG2   | 3:J:756:GLN:HE22  | 1.84                     | 0.42              |
| 3:J:777:PRO:HB2   | 3:J:912:LYS:HE2   | 2.02                     | 0.42              |
| 3:J:1232:PRO:O    | 3:J:1235:GLN:HG2  | 2.19                     | 0.42              |
| 3:J:1238:MET:C    | 3:J:1359:GLN:HE22 | 2.27                     | 0.42              |
| 2:C:100:LEU:HD12  | 2:C:372:LEU:HD22  | 2.01                     | 0.42              |
| 2:C:994:ILE:HG22  | 2:C:995:MET:H     | 1.84                     | 0.42              |
| 3:D:31:THR:OG1    | 3:D:32:ILE:N      | 2.52                     | 0.42              |
| 3:D:401:TYR:HB3   | 3:D:427:VAL:CG2   | 2.50                     | 0.42              |
| 3:D:731:LEU:HD22  | 3:D:780:LYS:O     | 2.19                     | 0.42              |
| 3:D:758:GLU:OE1   | 3:D:1476:THR:OG1  | 2.36                     | 0.42              |
| 3:D:1003:VAL:HG21 | 3:D:1041:MET:HB3  | 2.01                     | 0.42              |
| 3:D:1120:VAL:HG12 | 3:D:1135:ARG:HH12 | 1.84                     | 0.42              |
| 3:D:1331:ASP:HA   | 3:D:1332:PRO:HD3  | 1.90                     | 0.42              |
| 4:E:61:VAL:O      | 4:E:65:MET:HG2    | 2.20                     | 0.42              |
| 1:H:64:GLU:HG3    | 1:H:165:ILE:HG21  | 2.02                     | 0.42              |
| 1:H:132:LEU:HD12  | 1:H:136:GLY:HA3   | 2.02                     | 0.42              |
| 2:I:53:PRO:HB3    | 2:I:66:LEU:O      | 2.19                     | 0.42              |
| 2:I:580:MET:O     | 2:I:903:SER:N     | 2.50                     | 0.42              |
| 2:I:1068:GLN:NE2  | 2:I:1072:LYS:HD2  | 2.35                     | 0.42              |
| 3:J:26:VAL:HG13   | 3:J:42:ASP:O      | 2.19                     | 0.42              |
| 3:J:89:ARG:C      | 3:J:521:PRO:HG3   | 2.44                     | 0.42              |
| 3:J:783:ARG:NH1   | 3:J:1029:ARG:HD2  | 2.35                     | 0.42              |
| 3:J:1048:PRO:HD3  | 3:J:1075:HIS:CG   | 2.55                     | 0.42              |
| 3:J:1114:THR:HG22 | 3:J:1189:ARG:HH22 | 1.85                     | 0.42              |
| 5:L:154:ALA:O     | 5:L:158:LYS:HB2   | 2.20                     | 0.42              |
| 6:N:45:SER:OG     | 6:N:46:LYS:N      | 2.48                     | 0.42              |
| 1:A:30:ARG:HD3    | 1:A:191:ASP:OD2   | 2.20                     | 0.41              |
| 1:A:42:ARG:NH1    | 2:C:978:ARG:HA    | 2.34                     | 0.41              |
| 1:A:205:VAL:HG11  | 1:A:213:GLN:HE22  | 1.84                     | 0.41              |
| 2:C:56:GLU:HB3    | 2:C:359:MET:HE2   | 2.01                     | 0.41              |
| 3:D:102:ILE:HD11  | 3:D:587:ARG:HG3   | 2.02                     | 0.41              |
| 3:D:237:ARG:HG2   | 3:D:240:GLU:HB2   | 2.02                     | 0.41              |
| 3:D:431:ILE:HG13  | 3:D:432:TYR:N     | 2.35                     | 0.41              |
| 3:D:551:ASN:O     | 3:D:555:LYS:HG3   | 2.20                     | 0.41              |
| 3:D:585:GLY:CA    | 3:D:590:PRO:HG3   | 2.50                     | 0.41              |
| 3:D:654:LYS:NZ    | 3:D:674:ARG:HH21  | 2.16                     | 0.41              |
| 5:F:276:PRO:O     | 5:F:280:VAL:HG23  | 2.19                     | 0.41              |
| 5:F:292:GLN:O     | 5:F:295:GLN:HB3   | 2.20                     | 0.41              |
| 2:I:56:GLU:HB3    | 2:I:359:MET:HE2   | 2.01                     | 0.41              |
| 2:I:770:GLU:HG2   | 5:L:366:SER:HA    | 2.00                     | 0.41              |
| 3:J:121:THR:O     | 3:J:124:GLU:HB3   | 2.21                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:J:177:ALA:HB2   | 3:J:393:ILE:HD11  | 2.01                     | 0.41              |
| 3:J:758:GLU:HG3   | 4:K:20:THR:HG21   | 2.02                     | 0.41              |
| 3:J:1087:ARG:HH22 | 3:J:1236:LEU:H    | 1.67                     | 0.41              |
| 6:M:79:ARG:NH1    | 6:M:114:ALA:HB2   | 2.34                     | 0.41              |
| 6:N:12:LEU:O      | 6:N:15:TYR:HB2    | 2.19                     | 0.41              |
| 1:A:37:GLY:N      | 1:A:195:LEU:HD11  | 2.35                     | 0.41              |
| 1:B:176:ARG:HB3   | 1:B:200:TRP:CE3   | 2.55                     | 0.41              |
| 2:C:263:ASP:HB3   | 2:C:266:ARG:HB2   | 2.02                     | 0.41              |
| 2:C:1103:ASP:CG   | 2:C:1104:GLU:H    | 2.28                     | 0.41              |
| 2:C:1107:ASN:HA   | 2:C:1108:PRO:HD3  | 1.86                     | 0.41              |
| 3:D:29:PRO:HB3    | 3:D:548:ILE:HB    | 2.02                     | 0.41              |
| 3:D:750:PRO:HG2   | 3:D:756:GLN:NE2   | 2.35                     | 0.41              |
| 3:D:947:ILE:HG22  | 3:D:1019:PRO:HB3  | 2.02                     | 0.41              |
| 1:G:88:ARG:HD3    | 1:G:121:GLU:OE1   | 2.20                     | 0.41              |
| 1:H:33:GLY:O      | 1:H:195:LEU:HD22  | 2.19                     | 0.41              |
| 1:H:51:THR:O      | 1:H:145:ASP:O     | 2.39                     | 0.41              |
| 2:I:90:TYR:HB3    | 2:I:128:ILE:HB    | 2.02                     | 0.41              |
| 2:I:258:PHE:HA    | 2:I:298:PHE:CE2   | 2.55                     | 0.41              |
| 2:I:279:GLU:H     | 2:I:279:GLU:HG2   | 1.69                     | 0.41              |
| 2:I:695:LEU:HD21  | 2:I:832:LYS:HD3   | 2.01                     | 0.41              |
| 2:I:954:SER:HA    | 2:I:955:PRO:HD3   | 1.88                     | 0.41              |
| 3:J:625:TYR:CE1   | 3:J:751:LEU:HD11  | 2.56                     | 0.41              |
| 3:J:1084:THR:O    | 3:J:1088:THR:HG23 | 2.20                     | 0.41              |
| 7:O:5:DA:H1'      | 7:O:6:DC:H5''     | 2.02                     | 0.41              |
| 1:B:222:LEU:HD23  | 1:B:222:LEU:HA    | 1.92                     | 0.41              |
| 2:C:396:ASP:HB2   | 2:C:406:HIS:ND1   | 2.35                     | 0.41              |
| 2:C:729:LEU:HD13  | 2:C:730:SER:O     | 2.20                     | 0.41              |
| 3:D:39:PRO:HB3    | 3:D:46:ASP:HA     | 2.02                     | 0.41              |
| 3:D:101:HIS:ND1   | 3:D:103:TRP:HB2   | 2.35                     | 0.41              |
| 3:D:704:ARG:HB3   | 3:D:736:PHE:HB3   | 2.01                     | 0.41              |
| 3:D:1188:VAL:HG12 | 3:D:1189:ARG:N    | 2.35                     | 0.41              |
| 1:G:43:ILE:H      | 1:G:43:ILE:HG13   | 1.58                     | 0.41              |
| 1:H:85:LEU:HD12   | 1:H:124:ASN:HB3   | 2.01                     | 0.41              |
| 2:I:69:LEU:C      | 2:I:70:GLU:HG3    | 2.45                     | 0.41              |
| 2:I:247:PRO:HA    | 2:I:248:PRO:HD3   | 1.74                     | 0.41              |
| 2:I:458:TYR:HB2   | 2:I:538:GLN:HB3   | 2.03                     | 0.41              |
| 2:I:1050:GLN:O    | 2:I:1054:THR:N    | 2.53                     | 0.41              |
| 3:J:9:ARG:HA      | 3:J:1456:LYS:HA   | 2.02                     | 0.41              |
| 3:J:500:ARG:HA    | 3:J:503:LEU:HD12  | 2.02                     | 0.41              |
| 5:L:401:VAL:O     | 5:L:404:TYR:HB3   | 2.20                     | 0.41              |
| 6:M:121:LEU:HA    | 6:M:122:PRO:HD3   | 1.88                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 6:M:155:PHE:O    | 6:M:159:TRP:HB2   | 2.20                     | 0.41              |
| 7:O:3:DT:H5'     | 7:O:3:DT:C6       | 2.53                     | 0.41              |
| 2:C:27:LYS:HA    | 2:C:30:LEU:HD22   | 2.01                     | 0.41              |
| 2:C:1044:GLY:HA3 | 4:E:17:TYR:HE1    | 1.82                     | 0.41              |
| 3:D:103:TRP:HH2  | 3:D:1447:LEU:HD22 | 1.86                     | 0.41              |
| 3:D:272:LEU:HD12 | 3:D:272:LEU:HA    | 1.91                     | 0.41              |
| 3:D:758:GLU:O    | 3:D:762:GLN:HG2   | 2.20                     | 0.41              |
| 3:D:907:GLU:O    | 3:D:911:LEU:HG    | 2.21                     | 0.41              |
| 3:D:1290:LEU:O   | 3:D:1305:LEU:HB2  | 2.20                     | 0.41              |
| 5:F:412:ILE:HA   | 5:F:415:ILE:HD12  | 2.02                     | 0.41              |
| 2:I:847:GLY:HA2  | 3:J:741:ASP:HA    | 2.02                     | 0.41              |
| 3:J:925:GLU:H    | 3:J:925:GLU:HG3   | 1.60                     | 0.41              |
| 3:J:1033:GLN:O   | 3:J:1036:ARG:HB3  | 2.20                     | 0.41              |
| 4:K:61:VAL:O     | 4:K:65:MET:HG2    | 2.20                     | 0.41              |
| 1:A:66:SER:O     | 1:A:75:VAL:HG23   | 2.20                     | 0.41              |
| 1:B:76:VAL:HA    | 1:B:79:ILE:HD12   | 2.03                     | 0.41              |
| 2:C:66:LEU:HD11  | 2:C:372:LEU:HD23  | 2.02                     | 0.41              |
| 2:C:441:VAL:O    | 2:C:443:THR:HG22  | 2.19                     | 0.41              |
| 3:D:623:VAL:HG21 | 3:D:748:HIS:CD2   | 2.56                     | 0.41              |
| 3:D:758:GLU:HG2  | 3:D:1476:THR:HG21 | 2.02                     | 0.41              |
| 3:D:835:SER:OG   | 3:D:838:ARG:HG3   | 2.19                     | 0.41              |
| 3:D:892:ASP:HB2  | 3:D:894:LYS:HG2   | 2.03                     | 0.41              |
| 3:D:1231:GLU:HB3 | 3:D:1232:PRO:HD3  | 2.01                     | 0.41              |
| 3:D:1290:LEU:HB2 | 3:D:1307:LYS:HD2  | 2.03                     | 0.41              |
| 5:F:235:LEU:O    | 5:F:239:VAL:HG23  | 2.21                     | 0.41              |
| 1:G:99:LEU:N     | 1:G:142:VAL:O     | 2.51                     | 0.41              |
| 1:G:211:LEU:O    | 1:G:215:VAL:HG23  | 2.20                     | 0.41              |
| 1:H:54:THR:O     | 1:H:167:VAL:HB    | 2.20                     | 0.41              |
| 1:H:107:LYS:HG3  | 1:H:108:GLU:N     | 2.34                     | 0.41              |
| 3:J:128:TYR:O    | 3:J:572:ARG:NH1   | 2.53                     | 0.41              |
| 5:L:118:ALA:HB3  | 5:L:244:TYR:HB3   | 2.03                     | 0.41              |
| 1:A:74:ASP:O     | 1:A:78:ILE:HG13   | 2.21                     | 0.41              |
| 1:B:57:TYR:CD1   | 1:B:161:ARG:HG2   | 2.55                     | 0.41              |
| 2:C:86:LYS:HE2   | 2:C:814:GLU:N     | 2.36                     | 0.41              |
| 2:C:146:VAL:HG12 | 2:C:162:ILE:HG13  | 2.02                     | 0.41              |
| 2:C:285:LEU:CD1  | 2:C:301:GLU:HB3   | 2.49                     | 0.41              |
| 3:D:224:ARG:HB3  | 3:D:251:PHE:CE1   | 2.55                     | 0.41              |
| 3:D:274:GLN:HG3  | 3:D:279:VAL:HG21  | 2.01                     | 0.41              |
| 3:D:409:VAL:HG22 | 3:D:421:LEU:O     | 2.21                     | 0.41              |
| 3:D:606:ILE:HG22 | 3:D:613:ARG:HB2   | 2.01                     | 0.41              |
| 3:D:711:LEU:HG   | 3:D:778:LEU:HD22  | 2.02                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:1459:LEU:HD21 | 3:D:1468:LEU:HG   | 2.03                     | 0.41              |
| 1:G:221:HIS:HA    | 1:G:224:TYR:CD1   | 2.56                     | 0.41              |
| 2:I:161:SER:C     | 2:I:162:ILE:HD12  | 2.45                     | 0.41              |
| 2:I:469:THR:HA    | 2:I:470:PRO:HD3   | 1.83                     | 0.41              |
| 2:I:487:THR:HG22  | 2:I:488:ALA:H     | 1.86                     | 0.41              |
| 2:I:1065:ALA:HA   | 2:I:1068:GLN:HB3  | 2.01                     | 0.41              |
| 3:J:127:LEU:HD23  | 3:J:458:ALA:HA    | 2.02                     | 0.41              |
| 3:J:471:GLU:O     | 3:J:474:GLU:HB3   | 2.19                     | 0.41              |
| 3:J:749:VAL:HA    | 3:J:750:PRO:HD2   | 1.93                     | 0.41              |
| 3:J:1118:ILE:O    | 3:J:1118:ILE:HG13 | 2.20                     | 0.41              |
| 5:L:413:ARG:HE    | 8:S:21:DT:H2'     | 1.86                     | 0.41              |
| 6:N:116:GLU:HG3   | 6:N:121:LEU:HD22  | 2.01                     | 0.41              |
| 6:N:125:ASP:HA    | 6:N:128:ALA:HB3   | 2.02                     | 0.41              |
| 6:N:126:ARG:HH11  | 6:N:126:ARG:HB2   | 1.85                     | 0.41              |
| 1:B:34:VAL:HG11   | 2:C:978:ARG:HB3   | 2.03                     | 0.41              |
| 1:B:213:GLN:O     | 1:B:217:ILE:HG13  | 2.21                     | 0.41              |
| 2:C:14:PRO:HB3    | 2:C:586:ARG:NH2   | 2.30                     | 0.41              |
| 2:C:267:TYR:HE2   | 2:C:269:LEU:HD12  | 1.86                     | 0.41              |
| 2:C:275:TYR:O     | 2:C:278:GLU:HB3   | 2.21                     | 0.41              |
| 2:C:862:PRO:HG3   | 2:C:975:TYR:HE2   | 1.85                     | 0.41              |
| 2:C:892:LEU:HD13  | 2:C:989:VAL:O     | 2.21                     | 0.41              |
| 3:D:632:VAL:N     | 3:D:726:ILE:O     | 2.51                     | 0.41              |
| 3:D:860:LEU:H     | 3:D:860:LEU:CD1   | 2.31                     | 0.41              |
| 3:D:1462:LEU:H    | 3:D:1462:LEU:HG   | 1.66                     | 0.41              |
| 1:G:215:VAL:HG21  | 1:H:225:PHE:HD1   | 1.86                     | 0.41              |
| 2:I:118:LEU:HD12  | 2:I:119:PRO:HD2   | 2.02                     | 0.41              |
| 2:I:202:TYR:HD1   | 2:I:206:THR:HG21  | 1.84                     | 0.41              |
| 2:I:539:VAL:HG21  | 3:J:1067:VAL:HG11 | 2.01                     | 0.41              |
| 2:I:610:ARG:O     | 2:I:610:ARG:HG2   | 2.20                     | 0.41              |
| 2:I:679:PHE:N     | 2:I:683:ASN:HD21  | 2.18                     | 0.41              |
| 2:I:994:ILE:HG22  | 2:I:995:MET:H     | 1.86                     | 0.41              |
| 3:J:602:SER:O     | 3:J:606:ILE:HG13  | 2.20                     | 0.41              |
| 3:J:1331:ASP:HA   | 3:J:1332:PRO:HD3  | 1.87                     | 0.41              |
| 4:K:6:ILE:HD11    | 4:K:10:PHE:CZ     | 2.56                     | 0.41              |
| 1:A:40:LEU:O      | 1:A:44:LEU:HB2    | 2.20                     | 0.41              |
| 2:C:99:GLN:HB2    | 2:C:101:ILE:HD11  | 2.01                     | 0.41              |
| 2:C:432:ARG:NH1   | 2:C:518:ARG:HH21  | 2.13                     | 0.41              |
| 2:C:492:ASP:OD2   | 2:C:518:ARG:HG2   | 2.20                     | 0.41              |
| 2:C:949:LYS:NZ    | 3:D:859:ASP:OD2   | 2.54                     | 0.41              |
| 2:C:1026:GLN:HE21 | 2:C:1026:GLN:HB2  | 1.64                     | 0.41              |
| 3:D:233:LYS:HE3   | 3:D:235:ALA:H     | 1.84                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:D:1365:ASP:O   | 3:D:1369:GLU:HG3  | 2.20                     | 0.41              |
| 1:H:80:LEU:HB3   | 3:J:867:ARG:HH11  | 1.86                     | 0.41              |
| 2:I:80:GLN:HE22  | 2:I:122:THR:HG22  | 1.85                     | 0.41              |
| 2:I:100:LEU:HD12 | 2:I:372:LEU:HD22  | 2.03                     | 0.41              |
| 2:I:100:LEU:CB   | 2:I:369:PRO:HD3   | 2.50                     | 0.41              |
| 2:I:100:LEU:HB3  | 2:I:369:PRO:HD3   | 2.03                     | 0.41              |
| 2:I:285:LEU:CD1  | 2:I:301:GLU:HB3   | 2.48                     | 0.41              |
| 2:I:670:GLN:HE22 | 2:I:699:PHE:HA    | 1.85                     | 0.41              |
| 2:I:1009:SER:HB3 | 3:J:651:GLU:O     | 2.19                     | 0.41              |
| 3:J:103:TRP:O    | 3:J:107:ASP:HB2   | 2.21                     | 0.41              |
| 3:J:156:GLU:O    | 3:J:160:GLU:HB2   | 2.21                     | 0.41              |
| 3:J:783:ARG:NH1  | 3:J:1029:ARG:HA   | 2.36                     | 0.41              |
| 3:J:954:ALA:HB2  | 3:J:1020:LEU:HD22 | 2.02                     | 0.41              |
| 3:J:1122:LEU:HA  | 3:J:1135:ARG:HD3  | 2.03                     | 0.41              |
| 3:J:1231:GLU:HB3 | 3:J:1232:PRO:HD3  | 2.03                     | 0.41              |
| 6:M:75:LEU:HG    | 6:M:159:TRP:CZ3   | 2.55                     | 0.41              |
| 6:M:140:VAL:HG11 | 6:M:154:LEU:HD22  | 2.03                     | 0.41              |
| 1:A:29:GLU:HB3   | 1:A:32:PHE:CD1    | 2.56                     | 0.41              |
| 1:A:93:LYS:HB3   | 1:A:93:LYS:NZ     | 2.35                     | 0.41              |
| 1:B:51:THR:O     | 1:B:145:ASP:O     | 2.38                     | 0.41              |
| 1:B:173:PRO:HB3  | 1:B:204:SER:HB2   | 2.01                     | 0.41              |
| 2:C:144:PRO:HG2  | 2:C:273:GLY:N     | 2.35                     | 0.41              |
| 2:C:254:LEU:HD12 | 2:C:298:PHE:HE1   | 1.86                     | 0.41              |
| 2:C:387:SER:HB2  | 2:C:388:ARG:HD2   | 2.02                     | 0.41              |
| 2:C:437:ARG:NH2  | 2:C:488:ALA:HA    | 2.36                     | 0.41              |
| 2:C:877:PRO:HD3  | 3:D:949:ILE:CD1   | 2.50                     | 0.41              |
| 2:C:948:GLU:OE2  | 2:C:962:GLN:NE2   | 2.50                     | 0.41              |
| 3:D:317:MET:HG2  | 3:D:318:THR:N     | 2.35                     | 0.41              |
| 3:D:348:ALA:HB1  | 3:D:349:PRO:HD2   | 2.02                     | 0.41              |
| 3:D:659:LYS:O    | 3:D:662:GLU:HB3   | 2.20                     | 0.41              |
| 3:D:701:LEU:O    | 3:D:747:VAL:HA    | 2.21                     | 0.41              |
| 3:D:1275:SER:HB2 | 3:D:1325:LEU:HD21 | 2.03                     | 0.41              |
| 3:D:1279:GLY:H   | 3:D:1319:VAL:HG23 | 1.86                     | 0.41              |
| 5:F:116:ASP:O    | 5:F:120:LYS:HG2   | 2.21                     | 0.41              |
| 5:F:381:ALA:O    | 5:F:385:LYS:HG2   | 2.21                     | 0.41              |
| 2:I:238:LEU:HD23 | 2:I:241:LEU:HD12  | 2.02                     | 0.41              |
| 2:I:675:ALA:HA   | 2:I:989:VAL:HG12  | 2.02                     | 0.41              |
| 2:I:992:MET:HG2  | 2:I:993:PHE:N     | 2.35                     | 0.41              |
| 2:I:1041:GLU:OE1 | 3:J:1462:LEU:HD13 | 2.21                     | 0.41              |
| 3:J:632:VAL:O    | 3:J:727:GLN:HA    | 2.21                     | 0.41              |
| 3:J:672:ALA:O    | 3:J:676:MET:HB2   | 2.21                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:J:1103:HIS:HB2  | 3:J:1462:LEU:CD1  | 2.48                     | 0.41              |
| 3:J:1153:VAL:HB   | 3:J:1160:LEU:HB2  | 2.03                     | 0.41              |
| 3:J:1188:VAL:HG12 | 3:J:1189:ARG:N    | 2.36                     | 0.41              |
| 3:J:1462:LEU:O    | 3:J:1466:VAL:HG23 | 2.20                     | 0.41              |
| 4:K:41:GLU:O      | 4:K:45:ARG:HG2    | 2.20                     | 0.41              |
| 6:M:97:LEU:HD23   | 6:M:97:LEU:HA     | 1.87                     | 0.41              |
| 1:A:53:VAL:CG2    | 1:A:54:THR:H      | 2.27                     | 0.41              |
| 1:A:54:THR:HG23   | 1:A:143:ARG:O     | 2.19                     | 0.41              |
| 1:A:158:ILE:HG22  | 1:A:160:ASP:N     | 2.31                     | 0.41              |
| 2:C:758:ARG:HE    | 2:C:788:THR:HB    | 1.86                     | 0.41              |
| 2:C:874:LEU:HD23  | 2:C:874:LEU:HA    | 1.92                     | 0.41              |
| 2:C:1091:GLU:OE2  | 3:D:606:ILE:HG21  | 2.21                     | 0.41              |
| 3:D:410:THR:HB    | 3:D:413:ASP:OD2   | 2.21                     | 0.41              |
| 3:D:841:PHE:CD1   | 3:D:858:LEU:HD22  | 2.55                     | 0.41              |
| 3:D:841:PHE:CE2   | 3:D:858:LEU:HD13  | 2.55                     | 0.41              |
| 3:D:1290:LEU:HD12 | 3:D:1307:LYS:HG3  | 2.02                     | 0.41              |
| 4:E:84:ARG:HA     | 4:E:87:LYS:HB3    | 2.03                     | 0.41              |
| 5:F:118:ALA:HB3   | 5:F:244:TYR:HB3   | 2.03                     | 0.41              |
| 5:F:353:LEU:HA    | 5:F:354:PRO:HD3   | 1.94                     | 0.41              |
| 2:I:699:PHE:HB3   | 2:I:700:TYR:HD1   | 1.85                     | 0.41              |
| 2:I:1093:GLN:O    | 3:J:21:TRP:HZ3    | 2.04                     | 0.41              |
| 3:J:835:SER:OG    | 3:J:838:ARG:HG3   | 2.21                     | 0.41              |
| 3:J:1175:ILE:O    | 3:J:1179:GLU:HG3  | 2.21                     | 0.41              |
| 1:A:190:THR:OG1   | 1:A:191:ASP:N     | 2.52                     | 0.40              |
| 2:C:86:LYS:HE2    | 2:C:813:VAL:HG23  | 2.02                     | 0.40              |
| 2:C:140:ILE:HG23  | 2:C:412:ALA:HA    | 2.03                     | 0.40              |
| 2:C:456:ALA:HB1   | 2:C:538:GLN:O     | 2.21                     | 0.40              |
| 2:C:535:SER:H     | 2:C:538:GLN:HE21  | 1.69                     | 0.40              |
| 3:D:181:ASP:HB3   | 3:D:357:GLU:HG2   | 2.03                     | 0.40              |
| 3:D:264:LEU:HD21  | 3:D:339:TRP:CG    | 2.56                     | 0.40              |
| 3:D:631:ILE:HG13  | 3:D:740:PHE:HD2   | 1.86                     | 0.40              |
| 3:D:684:LYS:HG2   | 3:D:685:ASP:N     | 2.36                     | 0.40              |
| 3:D:722:GLU:H     | 3:D:722:GLU:HG2   | 1.52                     | 0.40              |
| 3:D:760:ARG:HH21  | 4:E:61:VAL:HG12   | 1.87                     | 0.40              |
| 3:D:1151:ARG:HA   | 3:D:1162:GLU:HG3  | 2.03                     | 0.40              |
| 3:D:1404:ASN:O    | 3:D:1408:ILE:HG12 | 2.21                     | 0.40              |
| 5:F:153:THR:HG22  | 5:F:154:ALA:H     | 1.86                     | 0.40              |
| 5:F:210:VAL:HG11  | 5:F:232:ASN:HA    | 2.03                     | 0.40              |
| 5:F:392:ASP:OD2   | 5:F:394:ARG:HB2   | 2.21                     | 0.40              |
| 2:I:91:GLN:HG3    | 2:I:117:HIS:HB3   | 2.02                     | 0.40              |
| 2:I:569:VAL:H     | 2:I:995:MET:HE2   | 1.86                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:J:171:LEU:HD23 | 3:J:172:PRO:O    | 2.21                     | 0.40              |
| 3:J:650:LEU:HD12 | 3:J:688:TRP:CZ3  | 2.52                     | 0.40              |
| 3:J:659:LYS:O    | 3:J:659:LYS:HD3  | 2.20                     | 0.40              |
| 3:J:1076:GLY:HA2 | 3:J:1079:LYS:HB3 | 2.03                     | 0.40              |
| 3:J:1311:LEU:HA  | 3:J:1326:THR:HA  | 2.02                     | 0.40              |
| 6:M:12:LEU:O     | 6:M:15:TYR:HB2   | 2.21                     | 0.40              |
| 6:N:93:THR:O     | 6:N:97:LEU:HG    | 2.21                     | 0.40              |
| 6:N:155:PHE:O    | 6:N:159:TRP:HB2  | 2.21                     | 0.40              |
| 2:C:677:MET:HE2  | 2:C:679:PHE:HD1  | 1.87                     | 0.40              |
| 2:C:1016:ILE:O   | 3:D:87:ARG:NH2   | 2.54                     | 0.40              |
| 3:D:352:ASN:C    | 3:D:368:VAL:HG13 | 2.46                     | 0.40              |
| 3:D:633:VAL:HG13 | 3:D:635:PRO:HD3  | 2.03                     | 0.40              |
| 3:D:1175:ILE:O   | 3:D:1179:GLU:HG3 | 2.21                     | 0.40              |
| 3:D:1318:TYR:HB2 | 3:J:1157:GLY:O   | 2.22                     | 0.40              |
| 5:F:302:SER:H    | 5:F:305:GLU:HG2  | 1.85                     | 0.40              |
| 1:G:161:ARG:HG2  | 1:G:162:ILE:H    | 1.86                     | 0.40              |
| 2:I:474:VAL:HG11 | 2:I:529:VAL:HG22 | 2.03                     | 0.40              |
| 5:L:167:ASP:O    | 5:L:171:VAL:HB   | 2.21                     | 0.40              |
| 6:M:80:MET:HA    | 6:M:81:PRO:HD3   | 1.88                     | 0.40              |
| 1:B:49:PRO:HD2   | 1:B:213:GLN:NE2  | 2.37                     | 0.40              |
| 2:C:564:MET:SD   | 2:C:846:LYS:HG2  | 2.61                     | 0.40              |
| 2:C:1019:GLN:HA  | 2:C:1020:PRO:HD3 | 1.95                     | 0.40              |
| 3:D:918:ALA:O    | 3:D:922:LEU:HB2  | 2.20                     | 0.40              |
| 3:D:1076:GLY:HA2 | 3:D:1079:LYS:HB3 | 2.03                     | 0.40              |
| 2:I:690:ILE:HA   | 2:I:869:VAL:HA   | 2.03                     | 0.40              |
| 2:I:718:GLY:HA2  | 2:I:719:PRO:HD3  | 1.84                     | 0.40              |
| 2:I:877:PRO:HD3  | 3:J:949:ILE:CD1  | 2.52                     | 0.40              |
| 3:J:8:VAL:HG12   | 3:J:1434:TRP:HZ2 | 1.84                     | 0.40              |
| 3:J:1290:LEU:O   | 3:J:1305:LEU:HB2 | 2.21                     | 0.40              |
| 5:L:94:ASP:HA    | 5:L:95:PRO:HD2   | 1.87                     | 0.40              |
| 5:L:252:THR:HA   | 7:R:29:DC:H5     | 1.86                     | 0.40              |
| 1:B:57:TYR:CG    | 1:B:58:ILE:N     | 2.89                     | 0.40              |
| 2:C:86:LYS:CE    | 2:C:814:GLU:H    | 2.35                     | 0.40              |
| 3:D:171:LEU:HA   | 3:D:172:PRO:HD2  | 1.95                     | 0.40              |
| 5:F:215:LYS:HA   | 5:F:224:PHE:HE2  | 1.85                     | 0.40              |
| 1:G:87:VAL:CG1   | 1:G:144:VAL:HG11 | 2.51                     | 0.40              |
| 1:G:161:ARG:NH1  | 1:G:161:ARG:HB3  | 2.36                     | 0.40              |
| 2:I:502:PRO:HD2  | 2:I:513:VAL:HG13 | 2.04                     | 0.40              |
| 2:I:856:GLU:H    | 2:I:856:GLU:HG3  | 1.69                     | 0.40              |
| 3:J:361:VAL:CG2  | 3:J:367:ILE:HD11 | 2.51                     | 0.40              |
| 3:J:578:VAL:O    | 3:J:582:ILE:HG12 | 2.21                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:J:953:ASP:O     | 3:J:1018:ASN:ND2  | 2.37                     | 0.40              |
| 3:J:1048:PRO:HD3  | 3:J:1075:HIS:CB   | 2.48                     | 0.40              |
| 3:J:1189:ARG:NH2  | 3:J:1204:CYS:SG   | 2.94                     | 0.40              |
| 3:J:1433:SER:HB3  | 3:J:1464:GLU:CD   | 2.47                     | 0.40              |
| 6:N:11:VAL:HG12   | 6:N:13:PRO:HD3    | 2.03                     | 0.40              |
| 1:A:161:ARG:HG2   | 1:A:162:ILE:H     | 1.86                     | 0.40              |
| 2:C:713:ARG:CZ    | 2:C:715:THR:HG22  | 2.52                     | 0.40              |
| 3:D:39:PRO:CB     | 3:D:46:ASP:HA     | 2.52                     | 0.40              |
| 3:D:514:LEU:HD21  | 3:D:517:VAL:HA    | 2.03                     | 0.40              |
| 3:D:625:TYR:CE1   | 3:D:751:LEU:HD11  | 2.56                     | 0.40              |
| 3:D:1043:GLY:O    | 3:D:1045:MET:HE2  | 2.22                     | 0.40              |
| 3:D:1363:LEU:HD11 | 3:D:1368:ILE:HD11 | 2.04                     | 0.40              |
| 5:F:164:GLU:OE1   | 5:F:165:LYS:HG2   | 2.21                     | 0.40              |
| 2:I:408:ARG:NH1   | 2:I:408:ARG:HB3   | 2.36                     | 0.40              |
| 2:I:643:VAL:HG12  | 2:I:647:GLN:OE1   | 2.22                     | 0.40              |
| 2:I:878:SER:HA    | 3:J:1034:GLN:OE1  | 2.20                     | 0.40              |
| 3:J:31:THR:HG21   | 5:L:272:THR:HG22  | 2.04                     | 0.40              |
| 3:J:654:LYS:NZ    | 3:J:674:ARG:HH21  | 2.20                     | 0.40              |
| 3:J:991:GLN:HA    | 3:J:994:GLN:HG2   | 2.04                     | 0.40              |
| 7:R:10:DA:H1'     | 7:R:11:DG:H5''    | 2.02                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 1   | A     | 225/314 (72%) | 198 (88%) | 26 (12%) | 1 (0%)   | 30          | 65 |
| 1   | B     | 225/314 (72%) | 199 (88%) | 25 (11%) | 1 (0%)   | 30          | 65 |
| 1   | G     | 225/314 (72%) | 200 (89%) | 24 (11%) | 1 (0%)   | 30          | 65 |
| 1   | H     | 225/314 (72%) | 199 (88%) | 25 (11%) | 1 (0%)   | 30          | 65 |

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| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|-----------|----------|-------------|-----|
| 2   | C     | 1108/1119 (99%) | 980 (88%)  | 119 (11%) | 9 (1%)   | 16          | 51  |
| 2   | I     | 1108/1119 (99%) | 977 (88%)  | 123 (11%) | 8 (1%)   | 18          | 54  |
| 3   | D     | 1486/1524 (98%) | 1333 (90%) | 143 (10%) | 10 (1%)  | 18          | 54  |
| 3   | J     | 1361/1524 (89%) | 1227 (90%) | 126 (9%)  | 8 (1%)   | 21          | 57  |
| 4   | E     | 91/99 (92%)     | 79 (87%)   | 12 (13%)  | 0        | 100         | 100 |
| 4   | K     | 91/99 (92%)     | 80 (88%)   | 11 (12%)  | 0        | 100         | 100 |
| 5   | F     | 343/347 (99%)   | 309 (90%)  | 32 (9%)   | 2 (1%)   | 21          | 57  |
| 5   | L     | 343/347 (99%)   | 309 (90%)  | 31 (9%)   | 3 (1%)   | 14          | 48  |
| 6   | M     | 160/164 (98%)   | 142 (89%)  | 18 (11%)  | 0        | 100         | 100 |
| 6   | N     | 160/164 (98%)   | 141 (88%)  | 19 (12%)  | 0        | 100         | 100 |
| All | All   | 7151/7762 (92%) | 6373 (89%) | 734 (10%) | 44 (1%)  | 21          | 57  |

All (44) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 53   | VAL  |
| 3   | D     | 683  | ILE  |
| 3   | D     | 1128 | VAL  |
| 1   | G     | 53   | VAL  |
| 3   | J     | 681  | ARG  |
| 3   | J     | 683  | ILE  |
| 3   | J     | 1128 | VAL  |
| 2   | C     | 164  | PRO  |
| 2   | C     | 608  | GLY  |
| 2   | C     | 852  | ILE  |
| 3   | D     | 666  | PHE  |
| 3   | D     | 681  | ARG  |
| 2   | I     | 164  | PRO  |
| 2   | I     | 608  | GLY  |
| 2   | I     | 851  | LYS  |
| 2   | I     | 852  | ILE  |
| 3   | J     | 682  | ASP  |
| 1   | B     | 118  | ALA  |
| 2   | C     | 607  | ASP  |
| 2   | C     | 851  | LYS  |
| 3   | D     | 230  | TRP  |
| 3   | D     | 682  | ASP  |
| 1   | H     | 118  | ALA  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | I     | 607  | ASP  |
| 2   | C     | 1106 | ASP  |
| 3   | D     | 680  | GLN  |
| 5   | F     | 224  | PHE  |
| 2   | I     | 1106 | ASP  |
| 5   | F     | 154  | ALA  |
| 3   | J     | 680  | GLN  |
| 3   | J     | 685  | ASP  |
| 5   | L     | 224  | PHE  |
| 3   | D     | 1130 | ARG  |
| 3   | D     | 1221 | VAL  |
| 3   | J     | 1221 | VAL  |
| 5   | L     | 108  | LEU  |
| 5   | L     | 154  | ALA  |
| 3   | D     | 667  | ALA  |
| 2   | C     | 870  | ILE  |
| 2   | C     | 1016 | ILE  |
| 2   | I     | 870  | ILE  |
| 2   | I     | 1016 | ILE  |
| 2   | C     | 643  | VAL  |
| 3   | J     | 667  | ALA  |

### 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     | 194/270 (72%)   | 180 (93%)  | 14 (7%)   | 13          | 37 |
| 1   | B     | 194/270 (72%)   | 175 (90%)  | 19 (10%)  | 7           | 27 |
| 1   | G     | 194/270 (72%)   | 178 (92%)  | 16 (8%)   | 10          | 34 |
| 1   | H     | 194/270 (72%)   | 175 (90%)  | 19 (10%)  | 7           | 27 |
| 2   | C     | 931/936 (100%)  | 849 (91%)  | 82 (9%)   | 9           | 32 |
| 2   | I     | 931/936 (100%)  | 847 (91%)  | 84 (9%)   | 9           | 31 |
| 3   | D     | 1252/1281 (98%) | 1124 (90%) | 128 (10%) | 7           | 25 |
| 3   | J     | 1150/1281 (90%) | 1041 (90%) | 109 (10%) | 8           | 28 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 4   | E     | 83/88 (94%)     | 80 (96%)   | 3 (4%)   | 31          | 53 |
| 4   | K     | 83/88 (94%)     | 78 (94%)   | 5 (6%)   | 17          | 42 |
| 5   | F     | 296/299 (99%)   | 273 (92%)  | 23 (8%)  | 11          | 35 |
| 5   | L     | 296/299 (99%)   | 272 (92%)  | 24 (8%)  | 11          | 34 |
| 6   | M     | 131/133 (98%)   | 128 (98%)  | 3 (2%)   | 44          | 64 |
| 6   | N     | 131/133 (98%)   | 128 (98%)  | 3 (2%)   | 44          | 64 |
| All | All   | 6060/6554 (92%) | 5528 (91%) | 532 (9%) | 9           | 32 |

All (532) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 7   | LYS  |
| 1   | A     | 43  | ILE  |
| 1   | A     | 51  | THR  |
| 1   | A     | 54  | THR  |
| 1   | A     | 80  | LEU  |
| 1   | A     | 87  | VAL  |
| 1   | A     | 93  | LYS  |
| 1   | A     | 98  | THR  |
| 1   | A     | 122 | ILE  |
| 1   | A     | 151 | VAL  |
| 1   | A     | 162 | ILE  |
| 1   | A     | 174 | VAL  |
| 1   | A     | 195 | LEU  |
| 1   | A     | 208 | LEU  |
| 1   | B     | 7   | LYS  |
| 1   | B     | 30  | ARG  |
| 1   | B     | 51  | THR  |
| 1   | B     | 54  | THR  |
| 1   | B     | 58  | ILE  |
| 1   | B     | 62  | LEU  |
| 1   | B     | 64  | GLU  |
| 1   | B     | 75  | VAL  |
| 1   | B     | 100 | ILE  |
| 1   | B     | 104 | GLU  |
| 1   | B     | 110 | ARG  |
| 1   | B     | 114 | PHE  |
| 1   | B     | 115 | THR  |
| 1   | B     | 138 | LEU  |
| 1   | B     | 143 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 170 | ILE  |
| 1   | B     | 177 | VAL  |
| 1   | B     | 184 | THR  |
| 1   | B     | 232 | LEU  |
| 2   | C     | 30  | LEU  |
| 2   | C     | 49  | LYS  |
| 2   | C     | 50  | GLU  |
| 2   | C     | 65  | VAL  |
| 2   | C     | 70  | GLU  |
| 2   | C     | 73  | ILE  |
| 2   | C     | 80  | GLN  |
| 2   | C     | 101 | ILE  |
| 2   | C     | 104 | ASP  |
| 2   | C     | 109 | LYS  |
| 2   | C     | 120 | LEU  |
| 2   | C     | 140 | ILE  |
| 2   | C     | 157 | ARG  |
| 2   | C     | 173 | ASP  |
| 2   | C     | 176 | VAL  |
| 2   | C     | 195 | LEU  |
| 2   | C     | 199 | VAL  |
| 2   | C     | 207 | LEU  |
| 2   | C     | 208 | VAL  |
| 2   | C     | 211 | LEU  |
| 2   | C     | 217 | LEU  |
| 2   | C     | 219 | GLN  |
| 2   | C     | 232 | GLU  |
| 2   | C     | 242 | LEU  |
| 2   | C     | 252 | LYS  |
| 2   | C     | 261 | LEU  |
| 2   | C     | 297 | GLU  |
| 2   | C     | 301 | GLU  |
| 2   | C     | 304 | LEU  |
| 2   | C     | 308 | ARG  |
| 2   | C     | 339 | LEU  |
| 2   | C     | 359 | MET  |
| 2   | C     | 365 | ASP  |
| 2   | C     | 368 | THR  |
| 2   | C     | 398 | THR  |
| 2   | C     | 410 | ILE  |
| 2   | C     | 421 | GLU  |
| 2   | C     | 427 | VAL  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | C     | 474  | VAL  |
| 2   | C     | 503  | LEU  |
| 2   | C     | 504  | GLU  |
| 2   | C     | 513  | VAL  |
| 2   | C     | 533  | ASP  |
| 2   | C     | 551  | GLU  |
| 2   | C     | 571  | LEU  |
| 2   | C     | 579  | VAL  |
| 2   | C     | 580  | MET  |
| 2   | C     | 616  | GLU  |
| 2   | C     | 643  | VAL  |
| 2   | C     | 685  | GLU  |
| 2   | C     | 695  | LEU  |
| 2   | C     | 717  | LEU  |
| 2   | C     | 729  | LEU  |
| 2   | C     | 738  | ASP  |
| 2   | C     | 748  | GLU  |
| 2   | C     | 766  | GLU  |
| 2   | C     | 777  | ILE  |
| 2   | C     | 780  | GLU  |
| 2   | C     | 784  | ASP  |
| 2   | C     | 788  | THR  |
| 2   | C     | 790  | LEU  |
| 2   | C     | 815  | LEU  |
| 2   | C     | 852  | ILE  |
| 2   | C     | 857  | ASP  |
| 2   | C     | 867  | VAL  |
| 2   | C     | 869  | VAL  |
| 2   | C     | 876  | VAL  |
| 2   | C     | 934  | PHE  |
| 2   | C     | 966  | LEU  |
| 2   | C     | 968  | ASP  |
| 2   | C     | 969  | LEU  |
| 2   | C     | 972  | VAL  |
| 2   | C     | 1000 | MET  |
| 2   | C     | 1016 | ILE  |
| 2   | C     | 1026 | GLN  |
| 2   | C     | 1053 | LEU  |
| 2   | C     | 1060 | ILE  |
| 2   | C     | 1061 | GLU  |
| 2   | C     | 1071 | ILE  |
| 2   | C     | 1104 | GLU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | C     | 1107 | ASN  |
| 2   | C     | 1113 | GLU  |
| 3   | D     | 2    | LYS  |
| 3   | D     | 4    | GLU  |
| 3   | D     | 5    | VAL  |
| 3   | D     | 16   | GLU  |
| 3   | D     | 25   | GLU  |
| 3   | D     | 49   | ILE  |
| 3   | D     | 68   | PHE  |
| 3   | D     | 80   | VAL  |
| 3   | D     | 111  | LYS  |
| 3   | D     | 121  | THR  |
| 3   | D     | 138  | LYS  |
| 3   | D     | 155  | ASP  |
| 3   | D     | 166  | GLN  |
| 3   | D     | 168  | THR  |
| 3   | D     | 184  | GLU  |
| 3   | D     | 196  | VAL  |
| 3   | D     | 237  | ARG  |
| 3   | D     | 264  | LEU  |
| 3   | D     | 266  | GLU  |
| 3   | D     | 273  | ARG  |
| 3   | D     | 276  | GLU  |
| 3   | D     | 279  | VAL  |
| 3   | D     | 281  | ARG  |
| 3   | D     | 293  | VAL  |
| 3   | D     | 310  | LEU  |
| 3   | D     | 311  | LEU  |
| 3   | D     | 313  | LEU  |
| 3   | D     | 316  | HIS  |
| 3   | D     | 318  | THR  |
| 3   | D     | 327  | GLU  |
| 3   | D     | 334  | THR  |
| 3   | D     | 335  | LEU  |
| 3   | D     | 347  | VAL  |
| 3   | D     | 371  | ILE  |
| 3   | D     | 385  | VAL  |
| 3   | D     | 394  | LEU  |
| 3   | D     | 397  | LYS  |
| 3   | D     | 400  | VAL  |
| 3   | D     | 405  | ASP  |
| 3   | D     | 406  | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | D     | 409 | VAL  |
| 3   | D     | 411 | THR  |
| 3   | D     | 413 | ASP  |
| 3   | D     | 419 | ASP  |
| 3   | D     | 420 | VAL  |
| 3   | D     | 430 | GLU  |
| 3   | D     | 434 | ARG  |
| 3   | D     | 437 | VAL  |
| 3   | D     | 456 | MET  |
| 3   | D     | 464 | LEU  |
| 3   | D     | 480 | GLU  |
| 3   | D     | 547 | LEU  |
| 3   | D     | 560 | GLN  |
| 3   | D     | 571 | LYS  |
| 3   | D     | 574 | LEU  |
| 3   | D     | 576 | GLU  |
| 3   | D     | 598 | ARG  |
| 3   | D     | 618 | LEU  |
| 3   | D     | 639 | LEU  |
| 3   | D     | 658 | LEU  |
| 3   | D     | 660 | LYS  |
| 3   | D     | 688 | TRP  |
| 3   | D     | 694 | VAL  |
| 3   | D     | 701 | LEU  |
| 3   | D     | 708 | LEU  |
| 3   | D     | 722 | GLU  |
| 3   | D     | 724 | GLN  |
| 3   | D     | 732 | VAL  |
| 3   | D     | 739 | ASP  |
| 3   | D     | 740 | PHE  |
| 3   | D     | 749 | VAL  |
| 3   | D     | 762 | GLN  |
| 3   | D     | 776 | GLU  |
| 3   | D     | 780 | LYS  |
| 3   | D     | 792 | ILE  |
| 3   | D     | 817 | GLU  |
| 3   | D     | 833 | GLU  |
| 3   | D     | 834 | THR  |
| 3   | D     | 861 | GLN  |
| 3   | D     | 863 | VAL  |
| 3   | D     | 873 | LEU  |
| 3   | D     | 879 | ARG  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | D     | 897  | GLN  |
| 3   | D     | 901  | GLN  |
| 3   | D     | 903  | ASP  |
| 3   | D     | 908  | LYS  |
| 3   | D     | 912  | LYS  |
| 3   | D     | 914  | LEU  |
| 3   | D     | 917  | GLN  |
| 3   | D     | 956  | ILE  |
| 3   | D     | 958  | GLU  |
| 3   | D     | 959  | GLU  |
| 3   | D     | 964  | LEU  |
| 3   | D     | 971  | LEU  |
| 3   | D     | 976  | GLN  |
| 3   | D     | 980  | MET  |
| 3   | D     | 987  | GLU  |
| 3   | D     | 1055 | VAL  |
| 3   | D     | 1118 | ILE  |
| 3   | D     | 1120 | VAL  |
| 3   | D     | 1136 | LYS  |
| 3   | D     | 1144 | LEU  |
| 3   | D     | 1158 | ARG  |
| 3   | D     | 1203 | LYS  |
| 3   | D     | 1229 | ILE  |
| 3   | D     | 1267 | ARG  |
| 3   | D     | 1269 | LYS  |
| 3   | D     | 1285 | GLU  |
| 3   | D     | 1290 | LEU  |
| 3   | D     | 1308 | ASP  |
| 3   | D     | 1310 | ARG  |
| 3   | D     | 1311 | LEU  |
| 3   | D     | 1312 | LEU  |
| 3   | D     | 1313 | VAL  |
| 3   | D     | 1335 | LEU  |
| 3   | D     | 1371 | VAL  |
| 3   | D     | 1376 | LEU  |
| 3   | D     | 1395 | LEU  |
| 3   | D     | 1443 | THR  |
| 3   | D     | 1448 | THR  |
| 3   | D     | 1449 | GLU  |
| 3   | D     | 1456 | LYS  |
| 3   | D     | 1462 | LEU  |
| 3   | D     | 1463 | LYS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | D     | 1468 | LEU  |
| 3   | D     | 1472 | ILE  |
| 3   | D     | 1496 | GLU  |
| 3   | D     | 1497 | GLU  |
| 4   | E     | 34   | ARG  |
| 4   | E     | 51   | LEU  |
| 4   | E     | 56   | ASP  |
| 5   | F     | 100  | LEU  |
| 5   | F     | 108  | LEU  |
| 5   | F     | 125  | MET  |
| 5   | F     | 140  | GLU  |
| 5   | F     | 153  | THR  |
| 5   | F     | 158  | LYS  |
| 5   | F     | 159  | ILE  |
| 5   | F     | 172  | GLU  |
| 5   | F     | 175  | ASP  |
| 5   | F     | 196  | GLU  |
| 5   | F     | 224  | PHE  |
| 5   | F     | 244  | TYR  |
| 5   | F     | 268  | ASP  |
| 5   | F     | 273  | ILE  |
| 5   | F     | 282  | THR  |
| 5   | F     | 293  | LEU  |
| 5   | F     | 294  | GLN  |
| 5   | F     | 325  | ILE  |
| 5   | F     | 328  | GLU  |
| 5   | F     | 339  | GLU  |
| 5   | F     | 351  | GLU  |
| 5   | F     | 401  | VAL  |
| 5   | F     | 424  | LYS  |
| 1   | G     | 7    | LYS  |
| 1   | G     | 43   | ILE  |
| 1   | G     | 51   | THR  |
| 1   | G     | 54   | THR  |
| 1   | G     | 80   | LEU  |
| 1   | G     | 87   | VAL  |
| 1   | G     | 93   | LYS  |
| 1   | G     | 98   | THR  |
| 1   | G     | 113  | ASP  |
| 1   | G     | 122  | ILE  |
| 1   | G     | 151  | VAL  |
| 1   | G     | 162  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 174 | VAL  |
| 1   | G     | 195 | LEU  |
| 1   | G     | 208 | LEU  |
| 1   | G     | 213 | GLN  |
| 1   | H     | 7   | LYS  |
| 1   | H     | 30  | ARG  |
| 1   | H     | 51  | THR  |
| 1   | H     | 54  | THR  |
| 1   | H     | 58  | ILE  |
| 1   | H     | 62  | LEU  |
| 1   | H     | 64  | GLU  |
| 1   | H     | 75  | VAL  |
| 1   | H     | 100 | ILE  |
| 1   | H     | 104 | GLU  |
| 1   | H     | 110 | ARG  |
| 1   | H     | 114 | PHE  |
| 1   | H     | 115 | THR  |
| 1   | H     | 138 | LEU  |
| 1   | H     | 143 | ARG  |
| 1   | H     | 170 | ILE  |
| 1   | H     | 177 | VAL  |
| 1   | H     | 184 | THR  |
| 1   | H     | 232 | LEU  |
| 2   | I     | 20  | GLU  |
| 2   | I     | 30  | LEU  |
| 2   | I     | 34  | VAL  |
| 2   | I     | 49  | LYS  |
| 2   | I     | 65  | VAL  |
| 2   | I     | 70  | GLU  |
| 2   | I     | 73  | ILE  |
| 2   | I     | 101 | ILE  |
| 2   | I     | 104 | ASP  |
| 2   | I     | 109 | LYS  |
| 2   | I     | 120 | LEU  |
| 2   | I     | 140 | ILE  |
| 2   | I     | 157 | ARG  |
| 2   | I     | 173 | ASP  |
| 2   | I     | 176 | VAL  |
| 2   | I     | 195 | LEU  |
| 2   | I     | 199 | VAL  |
| 2   | I     | 207 | LEU  |
| 2   | I     | 208 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | I     | 211 | LEU  |
| 2   | I     | 217 | LEU  |
| 2   | I     | 219 | GLN  |
| 2   | I     | 232 | GLU  |
| 2   | I     | 242 | LEU  |
| 2   | I     | 252 | LYS  |
| 2   | I     | 261 | LEU  |
| 2   | I     | 297 | GLU  |
| 2   | I     | 304 | LEU  |
| 2   | I     | 308 | ARG  |
| 2   | I     | 336 | VAL  |
| 2   | I     | 339 | LEU  |
| 2   | I     | 359 | MET  |
| 2   | I     | 365 | ASP  |
| 2   | I     | 368 | THR  |
| 2   | I     | 410 | ILE  |
| 2   | I     | 421 | GLU  |
| 2   | I     | 427 | VAL  |
| 2   | I     | 474 | VAL  |
| 2   | I     | 487 | THR  |
| 2   | I     | 503 | LEU  |
| 2   | I     | 504 | GLU  |
| 2   | I     | 513 | VAL  |
| 2   | I     | 533 | ASP  |
| 2   | I     | 551 | GLU  |
| 2   | I     | 571 | LEU  |
| 2   | I     | 579 | VAL  |
| 2   | I     | 580 | MET  |
| 2   | I     | 616 | GLU  |
| 2   | I     | 643 | VAL  |
| 2   | I     | 685 | GLU  |
| 2   | I     | 695 | LEU  |
| 2   | I     | 717 | LEU  |
| 2   | I     | 729 | LEU  |
| 2   | I     | 738 | ASP  |
| 2   | I     | 748 | GLU  |
| 2   | I     | 766 | GLU  |
| 2   | I     | 770 | GLU  |
| 2   | I     | 777 | ILE  |
| 2   | I     | 780 | GLU  |
| 2   | I     | 784 | ASP  |
| 2   | I     | 788 | THR  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | I     | 790  | LEU  |
| 2   | I     | 815  | LEU  |
| 2   | I     | 852  | ILE  |
| 2   | I     | 857  | ASP  |
| 2   | I     | 867  | VAL  |
| 2   | I     | 869  | VAL  |
| 2   | I     | 876  | VAL  |
| 2   | I     | 934  | PHE  |
| 2   | I     | 966  | LEU  |
| 2   | I     | 968  | ASP  |
| 2   | I     | 969  | LEU  |
| 2   | I     | 972  | VAL  |
| 2   | I     | 1000 | MET  |
| 2   | I     | 1016 | ILE  |
| 2   | I     | 1026 | GLN  |
| 2   | I     | 1053 | LEU  |
| 2   | I     | 1060 | ILE  |
| 2   | I     | 1061 | GLU  |
| 2   | I     | 1071 | ILE  |
| 2   | I     | 1100 | GLN  |
| 2   | I     | 1104 | GLU  |
| 2   | I     | 1107 | ASN  |
| 2   | I     | 1113 | GLU  |
| 3   | J     | 2    | LYS  |
| 3   | J     | 4    | GLU  |
| 3   | J     | 5    | VAL  |
| 3   | J     | 16   | GLU  |
| 3   | J     | 25   | GLU  |
| 3   | J     | 49   | ILE  |
| 3   | J     | 68   | PHE  |
| 3   | J     | 80   | VAL  |
| 3   | J     | 111  | LYS  |
| 3   | J     | 121  | THR  |
| 3   | J     | 138  | LYS  |
| 3   | J     | 196  | VAL  |
| 3   | J     | 216  | LEU  |
| 3   | J     | 340  | THR  |
| 3   | J     | 344  | ASP  |
| 3   | J     | 347  | VAL  |
| 3   | J     | 350  | HIS  |
| 3   | J     | 361  | VAL  |
| 3   | J     | 371  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | J     | 374 | GLU  |
| 3   | J     | 405 | ASP  |
| 3   | J     | 410 | THR  |
| 3   | J     | 414 | ARG  |
| 3   | J     | 420 | VAL  |
| 3   | J     | 426 | LYS  |
| 3   | J     | 440 | VAL  |
| 3   | J     | 444 | VAL  |
| 3   | J     | 456 | MET  |
| 3   | J     | 464 | LEU  |
| 3   | J     | 480 | GLU  |
| 3   | J     | 535 | PHE  |
| 3   | J     | 547 | LEU  |
| 3   | J     | 560 | GLN  |
| 3   | J     | 571 | LYS  |
| 3   | J     | 574 | LEU  |
| 3   | J     | 576 | GLU  |
| 3   | J     | 598 | ARG  |
| 3   | J     | 618 | LEU  |
| 3   | J     | 639 | LEU  |
| 3   | J     | 658 | LEU  |
| 3   | J     | 660 | LYS  |
| 3   | J     | 688 | TRP  |
| 3   | J     | 694 | VAL  |
| 3   | J     | 701 | LEU  |
| 3   | J     | 708 | LEU  |
| 3   | J     | 722 | GLU  |
| 3   | J     | 724 | GLN  |
| 3   | J     | 732 | VAL  |
| 3   | J     | 739 | ASP  |
| 3   | J     | 740 | PHE  |
| 3   | J     | 749 | VAL  |
| 3   | J     | 762 | GLN  |
| 3   | J     | 776 | GLU  |
| 3   | J     | 780 | LYS  |
| 3   | J     | 792 | ILE  |
| 3   | J     | 817 | GLU  |
| 3   | J     | 833 | GLU  |
| 3   | J     | 860 | LEU  |
| 3   | J     | 861 | GLN  |
| 3   | J     | 863 | VAL  |
| 3   | J     | 873 | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | J     | 876  | SER  |
| 3   | J     | 879  | ARG  |
| 3   | J     | 897  | GLN  |
| 3   | J     | 901  | GLN  |
| 3   | J     | 903  | ASP  |
| 3   | J     | 908  | LYS  |
| 3   | J     | 912  | LYS  |
| 3   | J     | 914  | LEU  |
| 3   | J     | 917  | GLN  |
| 3   | J     | 956  | ILE  |
| 3   | J     | 958  | GLU  |
| 3   | J     | 959  | GLU  |
| 3   | J     | 964  | LEU  |
| 3   | J     | 971  | LEU  |
| 3   | J     | 976  | GLN  |
| 3   | J     | 980  | MET  |
| 3   | J     | 987  | GLU  |
| 3   | J     | 1055 | VAL  |
| 3   | J     | 1100 | ASP  |
| 3   | J     | 1120 | VAL  |
| 3   | J     | 1136 | LYS  |
| 3   | J     | 1144 | LEU  |
| 3   | J     | 1158 | ARG  |
| 3   | J     | 1203 | LYS  |
| 3   | J     | 1229 | ILE  |
| 3   | J     | 1267 | ARG  |
| 3   | J     | 1269 | LYS  |
| 3   | J     | 1285 | GLU  |
| 3   | J     | 1290 | LEU  |
| 3   | J     | 1308 | ASP  |
| 3   | J     | 1310 | ARG  |
| 3   | J     | 1311 | LEU  |
| 3   | J     | 1312 | LEU  |
| 3   | J     | 1313 | VAL  |
| 3   | J     | 1335 | LEU  |
| 3   | J     | 1371 | VAL  |
| 3   | J     | 1376 | LEU  |
| 3   | J     | 1395 | LEU  |
| 3   | J     | 1443 | THR  |
| 3   | J     | 1448 | THR  |
| 3   | J     | 1449 | GLU  |
| 3   | J     | 1456 | LYS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | J     | 1462 | LEU  |
| 3   | J     | 1463 | LYS  |
| 3   | J     | 1468 | LEU  |
| 3   | J     | 1472 | ILE  |
| 3   | J     | 1496 | GLU  |
| 3   | J     | 1497 | GLU  |
| 4   | K     | 14   | ASP  |
| 4   | K     | 34   | ARG  |
| 4   | K     | 39   | VAL  |
| 4   | K     | 51   | LEU  |
| 4   | K     | 56   | ASP  |
| 5   | L     | 108  | LEU  |
| 5   | L     | 125  | MET  |
| 5   | L     | 140  | GLU  |
| 5   | L     | 153  | THR  |
| 5   | L     | 158  | LYS  |
| 5   | L     | 159  | ILE  |
| 5   | L     | 172  | GLU  |
| 5   | L     | 175  | ASP  |
| 5   | L     | 196  | GLU  |
| 5   | L     | 224  | PHE  |
| 5   | L     | 244  | TYR  |
| 5   | L     | 268  | ASP  |
| 5   | L     | 273  | ILE  |
| 5   | L     | 280  | VAL  |
| 5   | L     | 293  | LEU  |
| 5   | L     | 294  | GLN  |
| 5   | L     | 325  | ILE  |
| 5   | L     | 328  | GLU  |
| 5   | L     | 339  | GLU  |
| 5   | L     | 351  | GLU  |
| 5   | L     | 401  | VAL  |
| 5   | L     | 426  | HIS  |
| 5   | L     | 433  | LEU  |
| 5   | L     | 435  | ASP  |
| 6   | M     | 8    | ASP  |
| 6   | M     | 40   | PHE  |
| 6   | M     | 159  | TRP  |
| 6   | N     | 8    | ASP  |
| 6   | N     | 40   | PHE  |
| 6   | N     | 159  | TRP  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (130)

such sidechains are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 38   | ASN  |
| 1   | A     | 163  | ASN  |
| 1   | A     | 213  | GLN  |
| 1   | B     | 19   | HIS  |
| 1   | B     | 38   | ASN  |
| 1   | B     | 63   | HIS  |
| 1   | B     | 213  | GLN  |
| 1   | B     | 221  | HIS  |
| 2   | C     | 22   | GLN  |
| 2   | C     | 80   | GLN  |
| 2   | C     | 91   | GLN  |
| 2   | C     | 187  | ASN  |
| 2   | C     | 374  | ASN  |
| 2   | C     | 448  | ASN  |
| 2   | C     | 538  | GLN  |
| 2   | C     | 671  | ASN  |
| 2   | C     | 765  | GLN  |
| 2   | C     | 829  | GLN  |
| 2   | C     | 843  | HIS  |
| 2   | C     | 899  | GLN  |
| 2   | C     | 930  | GLN  |
| 2   | C     | 999  | HIS  |
| 2   | C     | 1026 | GLN  |
| 2   | C     | 1050 | GLN  |
| 2   | C     | 1068 | GLN  |
| 2   | C     | 1107 | ASN  |
| 3   | D     | 151  | GLN  |
| 3   | D     | 268  | HIS  |
| 3   | D     | 274  | GLN  |
| 3   | D     | 388  | HIS  |
| 3   | D     | 462  | GLN  |
| 3   | D     | 507  | ASN  |
| 3   | D     | 549  | ASN  |
| 3   | D     | 552  | ASN  |
| 3   | D     | 560  | GLN  |
| 3   | D     | 575  | GLN  |
| 3   | D     | 617  | ASN  |
| 3   | D     | 640  | HIS  |
| 3   | D     | 680  | GLN  |
| 3   | D     | 756  | GLN  |
| 3   | D     | 762  | GLN  |
| 3   | D     | 897  | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | D     | 917  | GLN  |
| 3   | D     | 991  | GLN  |
| 3   | D     | 1005 | GLN  |
| 3   | D     | 1014 | ASN  |
| 3   | D     | 1202 | GLN  |
| 3   | D     | 1334 | GLN  |
| 4   | E     | 28   | GLN  |
| 4   | E     | 29   | GLN  |
| 4   | E     | 37   | ASN  |
| 5   | F     | 105  | GLN  |
| 5   | F     | 157  | GLN  |
| 5   | F     | 190  | HIS  |
| 5   | F     | 232  | ASN  |
| 5   | F     | 233  | GLN  |
| 5   | F     | 263  | ASN  |
| 5   | F     | 269  | GLN  |
| 5   | F     | 294  | GLN  |
| 5   | F     | 352  | ASN  |
| 5   | F     | 414  | GLN  |
| 5   | F     | 426  | HIS  |
| 1   | G     | 38   | ASN  |
| 1   | G     | 163  | ASN  |
| 1   | G     | 213  | GLN  |
| 1   | H     | 38   | ASN  |
| 1   | H     | 63   | HIS  |
| 1   | H     | 213  | GLN  |
| 2   | I     | 80   | GLN  |
| 2   | I     | 187  | ASN  |
| 2   | I     | 374  | ASN  |
| 2   | I     | 448  | ASN  |
| 2   | I     | 538  | GLN  |
| 2   | I     | 671  | ASN  |
| 2   | I     | 765  | GLN  |
| 2   | I     | 829  | GLN  |
| 2   | I     | 843  | HIS  |
| 2   | I     | 845  | ASN  |
| 2   | I     | 899  | GLN  |
| 2   | I     | 930  | GLN  |
| 2   | I     | 999  | HIS  |
| 2   | I     | 1019 | GLN  |
| 2   | I     | 1026 | GLN  |
| 2   | I     | 1050 | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | I     | 1068 | GLN  |
| 2   | I     | 1107 | ASN  |
| 3   | J     | 130  | ASN  |
| 3   | J     | 151  | GLN  |
| 3   | J     | 350  | HIS  |
| 3   | J     | 442  | ASN  |
| 3   | J     | 462  | GLN  |
| 3   | J     | 549  | ASN  |
| 3   | J     | 552  | ASN  |
| 3   | J     | 560  | GLN  |
| 3   | J     | 575  | GLN  |
| 3   | J     | 617  | ASN  |
| 3   | J     | 640  | HIS  |
| 3   | J     | 680  | GLN  |
| 3   | J     | 724  | GLN  |
| 3   | J     | 727  | GLN  |
| 3   | J     | 756  | GLN  |
| 3   | J     | 762  | GLN  |
| 3   | J     | 897  | GLN  |
| 3   | J     | 917  | GLN  |
| 3   | J     | 976  | GLN  |
| 3   | J     | 991  | GLN  |
| 3   | J     | 994  | GLN  |
| 3   | J     | 1014 | ASN  |
| 3   | J     | 1116 | ASN  |
| 3   | J     | 1334 | GLN  |
| 3   | J     | 1374 | GLN  |
| 3   | J     | 1393 | GLN  |
| 3   | J     | 1441 | GLN  |
| 4   | K     | 28   | GLN  |
| 4   | K     | 29   | GLN  |
| 4   | K     | 37   | ASN  |
| 5   | L     | 105  | GLN  |
| 5   | L     | 157  | GLN  |
| 5   | L     | 232  | ASN  |
| 5   | L     | 263  | ASN  |
| 5   | L     | 269  | GLN  |
| 5   | L     | 294  | GLN  |
| 5   | L     | 352  | ASN  |
| 6   | M     | 85   | GLN  |
| 6   | M     | 90   | HIS  |
| 6   | M     | 107  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | M     | 134 | HIS  |
| 6   | N     | 37  | GLN  |
| 6   | N     | 85  | GLN  |
| 6   | N     | 134 | HIS  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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

Of 6 ligands modelled in this entry, 6 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     | 227/314 (72%)   | 0.48   | 13 (5%) 29 26  | 120, 182, 228, 247    | 0       |
| 1   | B     | 227/314 (72%)   | 0.44   | 13 (5%) 29 26  | 83, 155, 210, 239     | 0       |
| 1   | G     | 227/314 (72%)   | 0.70   | 27 (11%) 9 12  | 127, 193, 236, 261    | 0       |
| 1   | H     | 227/314 (72%)   | 0.47   | 14 (6%) 26 24  | 93, 165, 210, 245     | 0       |
| 2   | C     | 1112/1119 (99%) | 0.47   | 67 (6%) 27 25  | 70, 174, 245, 303     | 0       |
| 2   | I     | 1112/1119 (99%) | 0.49   | 78 (7%) 22 21  | 82, 182, 250, 314     | 0       |
| 3   | D     | 1490/1524 (97%) | 0.34   | 50 (3%) 48 35  | 66, 147, 206, 277     | 0       |
| 3   | J     | 1367/1524 (89%) | 0.35   | 48 (3%) 47 35  | 70, 153, 211, 274     | 0       |
| 4   | E     | 93/99 (93%)     | 0.60   | 5 (5%) 31 27   | 93, 158, 217, 254     | 0       |
| 4   | K     | 93/99 (93%)     | 0.67   | 9 (9%) 13 15   | 106, 166, 222, 247    | 0       |
| 5   | F     | 345/347 (99%)   | 0.58   | 26 (7%) 20 20  | 108, 178, 259, 323    | 0       |
| 5   | L     | 345/347 (99%)   | 0.60   | 27 (7%) 19 19  | 119, 184, 260, 323    | 0       |
| 6   | M     | 162/164 (98%)   | 0.68   | 13 (8%) 18 19  | 154, 223, 269, 295    | 0       |
| 6   | N     | 162/164 (98%)   | 0.77   | 19 (11%) 9 12  | 161, 228, 271, 302    | 0       |
| 7   | O     | 30/30 (100%)    | 0.14   | 0 100 100      | 139, 200, 269, 277    | 0       |
| 7   | R     | 30/30 (100%)    | 0.15   | 0 100 100      | 156, 209, 257, 267    | 0       |
| 8   | P     | 24/24 (100%)    | 0.23   | 0 100 100      | 162, 229, 257, 280    | 0       |
| 8   | S     | 24/24 (100%)    | 0.28   | 0 100 100      | 173, 222, 252, 265    | 0       |
| All | All   | 7297/7870 (92%) | 0.45   | 409 (5%) 30 26 | 66, 168, 242, 323     | 0       |

All (409) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 5   | L     | 161 | GLY  | 6.4  |
| 2   | C     | 207 | LEU  | 6.0  |
| 5   | F     | 159 | ILE  | 5.6  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 5   | L     | 159  | ILE  | 5.5  |
| 2   | I     | 221  | LEU  | 5.5  |
| 5   | F     | 161  | GLY  | 5.4  |
| 4   | E     | 94   | PRO  | 5.2  |
| 2   | I     | 1023 | GLY  | 4.7  |
| 5   | L     | 162  | LEU  | 4.7  |
| 2   | I     | 207  | LEU  | 4.6  |
| 2   | C     | 247  | PRO  | 4.5  |
| 2   | I     | 500  | ASN  | 4.5  |
| 5   | F     | 162  | LEU  | 4.4  |
| 5   | F     | 155  | ARG  | 4.4  |
| 2   | I     | 445  | GLU  | 4.4  |
| 1   | G     | 204  | SER  | 4.3  |
| 4   | K     | 94   | PRO  | 4.3  |
| 2   | I     | 319  | GLY  | 4.3  |
| 5   | L     | 220  | ARG  | 4.2  |
| 1   | G     | 7    | LYS  | 4.2  |
| 2   | C     | 62   | GLY  | 4.2  |
| 2   | C     | 745  | ILE  | 4.1  |
| 2   | I     | 1080 | SER  | 4.1  |
| 2   | I     | 247  | PRO  | 4.0  |
| 3   | J     | 35   | ARG  | 4.0  |
| 2   | I     | 245  | GLY  | 3.9  |
| 2   | I     | 8    | ARG  | 3.9  |
| 2   | I     | 62   | GLY  | 3.9  |
| 3   | J     | 444  | VAL  | 3.8  |
| 5   | L     | 154  | ALA  | 3.8  |
| 1   | G     | 13   | ALA  | 3.8  |
| 1   | H     | 67   | THR  | 3.8  |
| 3   | D     | 666  | PHE  | 3.7  |
| 2   | C     | 162  | ILE  | 3.7  |
| 3   | J     | 34   | TYR  | 3.7  |
| 4   | K     | 2    | ALA  | 3.7  |
| 3   | J     | 1237 | THR  | 3.6  |
| 2   | C     | 663  | GLU  | 3.6  |
| 1   | G     | 188  | GLN  | 3.6  |
| 3   | J     | 2    | LYS  | 3.6  |
| 2   | C     | 306  | THR  | 3.6  |
| 1   | G     | 203  | GLY  | 3.6  |
| 1   | G     | 84   | GLU  | 3.5  |
| 5   | F     | 158  | LYS  | 3.5  |
| 2   | C     | 1023 | GLY  | 3.5  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | B     | 14   | THR  | 3.4  |
| 4   | E     | 26   | ARG  | 3.4  |
| 5   | F     | 420  | LEU  | 3.4  |
| 2   | I     | 286  | SER  | 3.3  |
| 3   | J     | 767  | HIS  | 3.3  |
| 5   | L     | 346  | ASP  | 3.3  |
| 2   | I     | 106  | GLY  | 3.3  |
| 2   | I     | 181  | VAL  | 3.3  |
| 2   | C     | 686  | ASP  | 3.3  |
| 6   | M     | 160  | GLY  | 3.3  |
| 2   | C     | 445  | GLU  | 3.3  |
| 5   | L     | 420  | LEU  | 3.3  |
| 5   | L     | 160  | PRO  | 3.3  |
| 5   | L     | 158  | LYS  | 3.2  |
| 6   | M     | 31   | VAL  | 3.2  |
| 3   | J     | 1030 | GLY  | 3.2  |
| 2   | C     | 662  | GLU  | 3.2  |
| 2   | C     | 196  | LEU  | 3.2  |
| 1   | B     | 233  | LEU  | 3.2  |
| 5   | L     | 416  | GLU  | 3.2  |
| 2   | I     | 686  | ASP  | 3.2  |
| 3   | D     | 1486 | VAL  | 3.1  |
| 3   | J     | 666  | PHE  | 3.1  |
| 2   | C     | 318  | PRO  | 3.1  |
| 2   | I     | 318  | PRO  | 3.1  |
| 3   | J     | 33   | ASN  | 3.1  |
| 3   | J     | 1238 | MET  | 3.1  |
| 5   | L     | 338  | ASP  | 3.1  |
| 5   | F     | 255  | THR  | 3.1  |
| 3   | D     | 1263 | PHE  | 3.1  |
| 3   | J     | 459  | GLU  | 3.1  |
| 5   | F     | 153  | THR  | 3.1  |
| 2   | I     | 780  | GLU  | 3.1  |
| 2   | C     | 202  | TYR  | 3.0  |
| 1   | G     | 14   | THR  | 3.0  |
| 1   | G     | 197  | LEU  | 3.0  |
| 3   | J     | 531  | ASP  | 3.0  |
| 6   | N     | 24   | ALA  | 3.0  |
| 6   | N     | 139  | GLU  | 3.0  |
| 2   | C     | 221  | LEU  | 3.0  |
| 2   | I     | 693  | GLU  | 3.0  |
| 5   | L     | 223  | SER  | 3.0  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 6   | N     | 27   | SER  | 3.0  |
| 5   | L     | 352  | ASN  | 3.0  |
| 3   | D     | 82   | ARG  | 3.0  |
| 3   | D     | 1479 | ASP  | 3.0  |
| 2   | I     | 999  | HIS  | 2.9  |
| 3   | J     | 661  | MET  | 2.9  |
| 6   | M     | 12   | LEU  | 2.9  |
| 6   | N     | 160  | GLY  | 2.9  |
| 2   | C     | 203  | ASP  | 2.9  |
| 2   | C     | 11   | GLU  | 2.9  |
| 3   | D     | 459  | GLU  | 2.9  |
| 5   | F     | 296  | GLU  | 2.9  |
| 5   | F     | 139  | GLN  | 2.9  |
| 2   | I     | 63   | GLY  | 2.9  |
| 2   | I     | 203  | ASP  | 2.9  |
| 2   | C     | 194  | VAL  | 2.9  |
| 2   | I     | 228  | ALA  | 2.9  |
| 3   | D     | 486  | ARG  | 2.9  |
| 6   | N     | 55   | HIS  | 2.9  |
| 1   | G     | 18   | ASP  | 2.9  |
| 3   | J     | 406  | ASP  | 2.8  |
| 2   | I     | 782  | ALA  | 2.8  |
| 2   | I     | 708  | TYR  | 2.8  |
| 2   | I     | 781  | LYS  | 2.8  |
| 2   | C     | 174  | LEU  | 2.8  |
| 1   | H     | 66   | SER  | 2.8  |
| 2   | C     | 173  | ASP  | 2.8  |
| 2   | I     | 288  | ARG  | 2.8  |
| 1   | A     | 7    | LYS  | 2.8  |
| 1   | G     | 8    | ALA  | 2.8  |
| 2   | C     | 10   | ARG  | 2.8  |
| 3   | D     | 444  | VAL  | 2.8  |
| 3   | J     | 1313 | VAL  | 2.8  |
| 6   | N     | 31   | VAL  | 2.8  |
| 6   | M     | 3    | GLU  | 2.8  |
| 1   | H     | 8    | ALA  | 2.8  |
| 1   | G     | 30   | ARG  | 2.8  |
| 3   | D     | 150  | ARG  | 2.8  |
| 3   | J     | 565  | ILE  | 2.8  |
| 5   | L     | 170  | THR  | 2.7  |
| 5   | F     | 346  | ASP  | 2.7  |
| 3   | D     | 1009 | LYS  | 2.7  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 6   | N     | 136  | LEU  | 2.7  |
| 5   | F     | 154  | ALA  | 2.7  |
| 3   | J     | 718  | PRO  | 2.7  |
| 1   | A     | 204  | SER  | 2.7  |
| 3   | J     | 1442 | ASN  | 2.7  |
| 1   | A     | 8    | ALA  | 2.7  |
| 2   | I     | 592  | LEU  | 2.7  |
| 2   | C     | 1027 | PHE  | 2.7  |
| 5   | F     | 312  | PRO  | 2.7  |
| 1   | G     | 134  | GLU  | 2.7  |
| 3   | D     | 722  | GLU  | 2.7  |
| 2   | I     | 924  | LEU  | 2.7  |
| 6   | N     | 127  | GLN  | 2.7  |
| 1   | B     | 67   | THR  | 2.7  |
| 3   | J     | 608  | SER  | 2.7  |
| 5   | F     | 254  | ALA  | 2.6  |
| 1   | G     | 176  | ARG  | 2.6  |
| 2   | C     | 146  | VAL  | 2.6  |
| 2   | I     | 797  | GLY  | 2.6  |
| 3   | J     | 532  | GLY  | 2.6  |
| 2   | C     | 246  | ASP  | 2.6  |
| 6   | M     | 123  | ASP  | 2.6  |
| 3   | D     | 1458 | GLU  | 2.6  |
| 1   | G     | 40   | LEU  | 2.6  |
| 5   | L     | 168  | PRO  | 2.6  |
| 3   | J     | 24   | GLY  | 2.6  |
| 1   | A     | 48   | ILE  | 2.6  |
| 1   | G     | 137  | LYS  | 2.6  |
| 3   | D     | 2    | LYS  | 2.6  |
| 3   | J     | 421  | LEU  | 2.6  |
| 1   | B     | 18   | ASP  | 2.6  |
| 1   | G     | 65   | PHE  | 2.6  |
| 3   | J     | 64   | LYS  | 2.6  |
| 5   | F     | 163  | LYS  | 2.6  |
| 1   | G     | 155  | ARG  | 2.6  |
| 5   | L     | 166  | PRO  | 2.6  |
| 1   | H     | 7    | LYS  | 2.6  |
| 4   | K     | 37   | ASN  | 2.5  |
| 2   | C     | 36   | PRO  | 2.5  |
| 3   | D     | 655  | PRO  | 2.5  |
| 3   | D     | 64   | LYS  | 2.5  |
| 1   | H     | 48   | ILE  | 2.5  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | H     | 231  | SER  | 2.5  |
| 2   | C     | 172  | ILE  | 2.5  |
| 2   | I     | 217  | LEU  | 2.5  |
| 1   | H     | 226  | ALA  | 2.5  |
| 2   | C     | 189  | ARG  | 2.5  |
| 3   | D     | 385  | VAL  | 2.5  |
| 2   | I     | 923  | ASN  | 2.5  |
| 2   | I     | 371  | LYS  | 2.5  |
| 1   | A     | 175  | ARG  | 2.5  |
| 6   | M     | 27   | SER  | 2.5  |
| 2   | C     | 75   | ASP  | 2.5  |
| 1   | G     | 106  | PRO  | 2.5  |
| 1   | H     | 178  | ALA  | 2.5  |
| 5   | F     | 378  | GLU  | 2.5  |
| 4   | K     | 14   | ASP  | 2.5  |
| 4   | K     | 36   | LYS  | 2.5  |
| 2   | C     | 834  | GLN  | 2.5  |
| 3   | D     | 220  | ARG  | 2.5  |
| 3   | D     | 247  | GLU  | 2.5  |
| 5   | F     | 171  | VAL  | 2.5  |
| 2   | I     | 424  | GLY  | 2.5  |
| 1   | B     | 222  | LEU  | 2.4  |
| 3   | D     | 1237 | THR  | 2.4  |
| 1   | A     | 191  | ASP  | 2.4  |
| 1   | A     | 202  | ASP  | 2.4  |
| 1   | B     | 226  | ALA  | 2.4  |
| 2   | I     | 271  | GLU  | 2.4  |
| 6   | N     | 56   | SER  | 2.4  |
| 3   | D     | 1238 | MET  | 2.4  |
| 3   | J     | 952  | ASP  | 2.4  |
| 3   | J     | 144  | GLY  | 2.4  |
| 3   | J     | 494  | LYS  | 2.4  |
| 3   | J     | 407  | VAL  | 2.4  |
| 1   | G     | 31   | GLY  | 2.4  |
| 2   | C     | 319  | GLY  | 2.4  |
| 6   | M     | 86   | TRP  | 2.4  |
| 5   | L     | 405  | PHE  | 2.4  |
| 2   | C     | 181  | VAL  | 2.4  |
| 3   | J     | 610  | LYS  | 2.4  |
| 1   | H     | 113  | ASP  | 2.4  |
| 3   | J     | 143  | ASP  | 2.4  |
| 3   | D     | 75   | ARG  | 2.4  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 2   | I     | 1010 | THR  | 2.4  |
| 5   | F     | 194  | GLU  | 2.4  |
| 2   | I     | 505  | GLY  | 2.4  |
| 3   | D     | 184  | GLU  | 2.4  |
| 3   | D     | 1495 | ILE  | 2.4  |
| 2   | I     | 863  | ASP  | 2.4  |
| 2   | C     | 762  | LYS  | 2.4  |
| 6   | N     | 81   | PRO  | 2.3  |
| 5   | L     | 135  | THR  | 2.3  |
| 3   | J     | 1490 | ARG  | 2.3  |
| 3   | D     | 191  | LEU  | 2.3  |
| 6   | N     | 97   | LEU  | 2.3  |
| 2   | C     | 344  | PHE  | 2.3  |
| 2   | I     | 175  | GLU  | 2.3  |
| 2   | I     | 567  | GLN  | 2.3  |
| 3   | D     | 1504 | GLU  | 2.3  |
| 5   | L     | 321  | GLU  | 2.3  |
| 2   | I     | 105  | THR  | 2.3  |
| 2   | C     | 201  | GLY  | 2.3  |
| 2   | C     | 489  | SER  | 2.3  |
| 5   | F     | 151  | LEU  | 2.3  |
| 5   | F     | 178  | LEU  | 2.3  |
| 4   | K     | 4    | PRO  | 2.3  |
| 2   | C     | 272  | ALA  | 2.3  |
| 2   | I     | 766  | GLU  | 2.3  |
| 5   | L     | 378  | GLU  | 2.3  |
| 6   | M     | 157  | GLU  | 2.3  |
| 2   | I     | 900  | ARG  | 2.3  |
| 3   | D     | 664  | LYS  | 2.3  |
| 2   | C     | 286  | SER  | 2.3  |
| 4   | E     | 74   | PHE  | 2.3  |
| 2   | I     | 246  | ASP  | 2.3  |
| 1   | G     | 108  | GLU  | 2.3  |
| 2   | C     | 1091 | GLU  | 2.3  |
| 6   | N     | 71   | ILE  | 2.3  |
| 2   | C     | 47   | ALA  | 2.3  |
| 2   | I     | 783  | ARG  | 2.3  |
| 5   | L     | 155  | ARG  | 2.3  |
| 2   | I     | 748  | GLU  | 2.3  |
| 2   | I     | 814  | GLU  | 2.3  |
| 2   | C     | 245  | GLY  | 2.3  |
| 2   | I     | 956  | GLY  | 2.3  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 3   | D     | 1432 | LYS  | 2.3  |
| 1   | H     | 82   | LEU  | 2.3  |
| 3   | D     | 1171 | VAL  | 2.3  |
| 3   | D     | 1311 | LEU  | 2.3  |
| 3   | D     | 4    | GLU  | 2.2  |
| 2   | C     | 500  | ASN  | 2.2  |
| 3   | J     | 1093 | TYR  | 2.2  |
| 4   | K     | 50   | THR  | 2.2  |
| 2   | I     | 264  | PRO  | 2.2  |
| 3   | D     | 981  | GLY  | 2.2  |
| 2   | C     | 499  | ALA  | 2.2  |
| 5   | L     | 308  | GLU  | 2.2  |
| 2   | I     | 284  | GLY  | 2.2  |
| 4   | E     | 10   | PHE  | 2.2  |
| 2   | I     | 628  | TYR  | 2.2  |
| 5   | L     | 217  | TYR  | 2.2  |
| 3   | D     | 660  | LYS  | 2.2  |
| 2   | C     | 618  | GLY  | 2.2  |
| 3   | D     | 1253 | THR  | 2.2  |
| 3   | D     | 1286 | GLY  | 2.2  |
| 1   | B     | 179  | PHE  | 2.2  |
| 1   | B     | 188  | GLN  | 2.2  |
| 2   | C     | 679  | PHE  | 2.2  |
| 2   | C     | 223  | ASP  | 2.2  |
| 2   | I     | 177  | GLU  | 2.2  |
| 2   | C     | 250  | LYS  | 2.2  |
| 3   | D     | 88   | TYR  | 2.2  |
| 3   | J     | 1456 | LYS  | 2.2  |
| 5   | F     | 422  | LYS  | 2.2  |
| 5   | F     | 425  | TYR  | 2.2  |
| 1   | H     | 124  | ASN  | 2.2  |
| 6   | N     | 137  | ALA  | 2.2  |
| 1   | G     | 15   | THR  | 2.2  |
| 1   | B     | 7    | LYS  | 2.2  |
| 1   | G     | 233  | LEU  | 2.2  |
| 2   | I     | 418  | LEU  | 2.2  |
| 3   | J     | 216  | LEU  | 2.2  |
| 3   | J     | 658  | LEU  | 2.2  |
| 1   | A     | 87   | VAL  | 2.2  |
| 2   | C     | 184  | MET  | 2.2  |
| 6   | M     | 126  | ARG  | 2.2  |
| 2   | C     | 410  | ILE  | 2.2  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 2   | C     | 777  | ILE  | 2.2  |
| 2   | I     | 311  | PHE  | 2.2  |
| 3   | J     | 1401 | GLU  | 2.2  |
| 4   | K     | 52   | GLU  | 2.2  |
| 2   | C     | 427  | VAL  | 2.2  |
| 3   | J     | 437  | VAL  | 2.2  |
| 3   | J     | 929  | ARG  | 2.2  |
| 1   | A     | 187  | GLY  | 2.2  |
| 2   | I     | 499  | ALA  | 2.2  |
| 3   | D     | 139  | GLY  | 2.2  |
| 1   | A     | 233  | LEU  | 2.2  |
| 3   | J     | 696  | HIS  | 2.2  |
| 3   | D     | 663  | GLU  | 2.2  |
| 6   | M     | 38   | VAL  | 2.2  |
| 5   | F     | 220  | ARG  | 2.2  |
| 1   | B     | 118  | ALA  | 2.1  |
| 3   | J     | 1343 | ALA  | 2.1  |
| 3   | D     | 1456 | LYS  | 2.1  |
| 3   | J     | 32   | ILE  | 2.1  |
| 4   | E     | 78   | ASN  | 2.1  |
| 2   | I     | 10   | ARG  | 2.1  |
| 2   | I     | 951  | GLY  | 2.1  |
| 6   | N     | 132  | ALA  | 2.1  |
| 2   | C     | 680  | ASP  | 2.1  |
| 3   | J     | 689  | ASP  | 2.1  |
| 1   | H     | 63   | HIS  | 2.1  |
| 1   | G     | 175  | ARG  | 2.1  |
| 3   | D     | 1093 | TYR  | 2.1  |
| 2   | C     | 160  | ALA  | 2.1  |
| 2   | I     | 287  | GLY  | 2.1  |
| 5   | L     | 164  | GLU  | 2.1  |
| 2   | C     | 200  | LEU  | 2.1  |
| 2   | C     | 549  | PHE  | 2.1  |
| 2   | I     | 703  | ILE  | 2.1  |
| 3   | D     | 949  | ILE  | 2.1  |
| 5   | L     | 163  | LYS  | 2.1  |
| 1   | B     | 66   | SER  | 2.1  |
| 3   | D     | 1141 | GLU  | 2.1  |
| 3   | J     | 723  | GLY  | 2.1  |
| 5   | F     | 260  | GLN  | 2.1  |
| 2   | C     | 175  | GLU  | 2.1  |
| 2   | C     | 1116 | ALA  | 2.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 3   | J     | 996  | TRP  | 2.1  |
| 6   | M     | 139  | GLU  | 2.1  |
| 3   | D     | 761  | ILE  | 2.1  |
| 1   | G     | 205  | VAL  | 2.1  |
| 1   | A     | 30   | ARG  | 2.1  |
| 3   | J     | 628  | ARG  | 2.1  |
| 2   | C     | 320  | HIS  | 2.1  |
| 1   | A     | 44   | LEU  | 2.1  |
| 2   | I     | 222  | LEU  | 2.1  |
| 6   | M     | 30   | GLY  | 2.1  |
| 2   | I     | 599  | GLU  | 2.1  |
| 2   | I     | 730  | SER  | 2.1  |
| 2   | I     | 1041 | GLU  | 2.1  |
| 3   | D     | 1342 | GLU  | 2.1  |
| 3   | J     | 30   | GLU  | 2.1  |
| 6   | N     | 155  | PHE  | 2.1  |
| 2   | I     | 155  | PRO  | 2.1  |
| 3   | D     | 355  | VAL  | 2.1  |
| 6   | N     | 26   | ARG  | 2.1  |
| 2   | C     | 180  | GLY  | 2.1  |
| 1   | G     | 154  | GLU  | 2.1  |
| 2   | C     | 1078 | GLU  | 2.1  |
| 6   | N     | 29   | SER  | 2.1  |
| 2   | I     | 176  | VAL  | 2.1  |
| 2   | I     | 468  | ARG  | 2.1  |
| 2   | I     | 842  | ARG  | 2.1  |
| 3   | D     | 1406 | ARG  | 2.1  |
| 6   | M     | 5    | ARG  | 2.1  |
| 1   | A     | 222  | LEU  | 2.1  |
| 2   | I     | 828  | ALA  | 2.1  |
| 1   | H     | 49   | PRO  | 2.1  |
| 3   | D     | 1154 | GLU  | 2.1  |
| 5   | F     | 164  | GLU  | 2.1  |
| 1   | B     | 140  | MET  | 2.0  |
| 2   | I     | 697  | ARG  | 2.0  |
| 4   | K     | 34   | ARG  | 2.0  |
| 1   | B     | 211  | LEU  | 2.0  |
| 2   | C     | 949  | LYS  | 2.0  |
| 3   | D     | 387  | LEU  | 2.0  |
| 2   | C     | 471  | TYR  | 2.0  |
| 2   | I     | 52   | PHE  | 2.0  |
| 2   | I     | 809  | GLY  | 2.0  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 3   | D     | 588  | GLY  | 2.0  |
| 6   | N     | 25   | GLN  | 2.0  |
| 2   | C     | 645  | VAL  | 2.0  |
| 2   | C     | 776  | SER  | 2.0  |
| 5   | F     | 223  | SER  | 2.0  |
| 1   | G     | 88   | ARG  | 2.0  |
| 1   | H     | 218  | LEU  | 2.0  |
| 2   | C     | 508  | ILE  | 2.0  |
| 1   | G     | 230  | ALA  | 2.0  |
| 2   | I     | 349  | ALA  | 2.0  |
| 2   | I     | 362  | GLY  | 2.0  |
| 6   | N     | 128  | ALA  | 2.0  |
| 2   | I     | 728  | HIS  | 2.0  |
| 3   | J     | 1169 | GLU  | 2.0  |
| 2   | I     | 103  | LYS  | 2.0  |
| 2   | I     | 188  | LYS  | 2.0  |
| 2   | I     | 212  | SER  | 2.0  |
| 5   | L     | 183  | LYS  | 2.0  |
| 2   | I     | 68   | PHE  | 2.0  |
| 3   | D     | 50   | PHE  | 2.0  |
| 3   | D     | 936  | TYR  | 2.0  |
| 5   | L     | 309  | ALA  | 2.0  |
| 2   | C     | 784  | ASP  | 2.0  |
| 2   | C     | 461  | VAL  | 2.0  |
| 3   | J     | 1033 | GLN  | 2.0  |
| 2   | I     | 731  | GLU  | 2.0  |
| 3   | J     | 1203 | LYS  | 2.0  |
| 2   | C     | 191  | PHE  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

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 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 10  | MG   | J     | 2003 | 1/1   | 0.65 | 0.13 | 219,219,219,219             | 0     |
| 10  | MG   | D     | 2003 | 1/1   | 0.85 | 0.10 | 198,198,198,198             | 0     |
| 9   | ZN   | J     | 2002 | 1/1   | 0.99 | 0.04 | 242,242,242,242             | 0     |
| 9   | ZN   | D     | 2002 | 1/1   | 0.99 | 0.03 | 203,203,203,203             | 0     |
| 9   | ZN   | J     | 2001 | 1/1   | 0.99 | 0.05 | 200,200,200,200             | 0     |
| 9   | ZN   | D     | 2001 | 1/1   | 1.00 | 0.02 | 96,96,96,96                 | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.