



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:09 PM UTC

PDB ID : 5VI8 / pdb\_00005vi8  
Title : Structure of a mycobacterium smegmatis transcription initiation complex with an upstream-fork promoter fragment  
Authors : Hubin, E.A.; Campbell, E.A.; Darst, S.A.  
Deposited on : 2017-04-14  
Resolution : 2.76 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

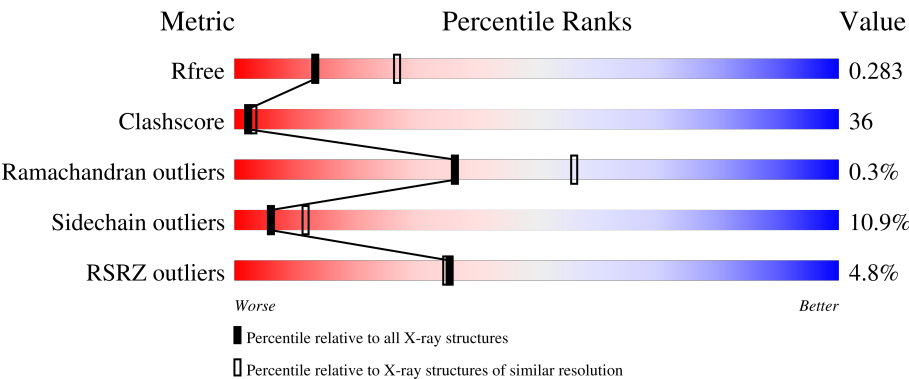
|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                             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

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.76 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 1009 (2.76-2.76)                                      |
| Clashscore            | 190562                      | 1044 (2.76-2.76)                                      |
| Ramachandran outliers | 187476                      | 1024 (2.76-2.76)                                      |
| Sidechain outliers    | 187428                      | 1024 (2.76-2.76)                                      |
| RSRZ outliers         | 180081                      | 1009 (2.76-2.76)                                      |

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   | J     | 114    |                  |
| 2   | A     | 350    |                  |
| 2   | B     | 350    |                  |
| 3   | C     | 1169   |                  |
| 4   | D     | 1317   |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 5   | E     | 107    |                  |
| 6   | F     | 466    |                  |
| 7   | O     | 31     |                  |
| 8   | P     | 26     |                  |
| 9   | T     | 100    |                  |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 10  | SO4  | C     | 1203 | -         | -        | X       | -                |
| 10  | SO4  | D     | 2005 | -         | -        | X       | -                |

## 2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 26631 atoms, of which 36 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 RNA polymerase-binding protein RbpA.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | J     | 83       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 667   | 419 | 118 | 128 | 2 |         |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2   | A     | 218      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1617  | 1020 | 276 | 318 | 3 |         |         |       |
| 2   | B     | 233      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1667  | 1054 | 289 | 322 | 2 |         |         |       |

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

| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 3   | C     | 1099     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 8250  | 5164 | 1448 | 1603 | 35 |         |         |       |

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

| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 4   | D     | 1248     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 9588  | 6016 | 1727 | 1805 | 40 |         |         |       |

- Molecule 5 is a protein called DNA-directed RNA polymerase subunit omega.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 5   | E     | 76       | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 592   | 378 | 100 | 114 |         |         |       |

- Molecule 6 is a protein called RNA polymerase sigma factor SigA.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 6   | F     | 319      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2481  | 1553 | 450 | 471 | 7 |         |         |       |

- Molecule 7 is a DNA chain called DNA (31-MER).

| Mol | Chain | Residues | Atoms |     |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 7   | O     | 31       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 634   | 305 | 114 | 185 | 30 |         |         |       |

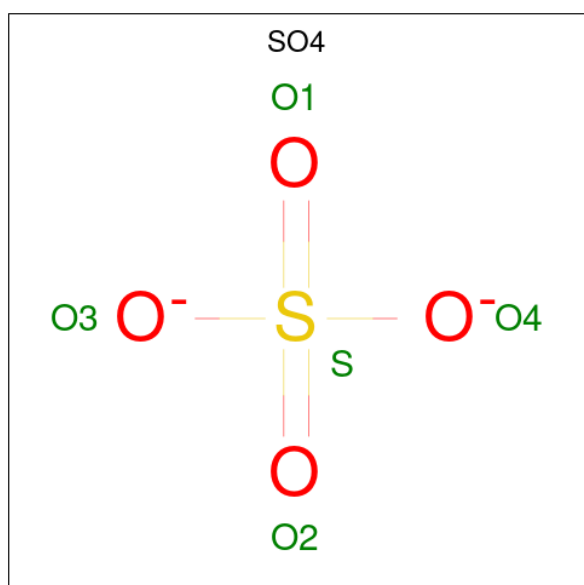
- Molecule 8 is a DNA chain called DNA (26-MER).

| Mol | Chain | Residues | Atoms |     |    |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|---------|-------|
| 8   | P     | 26       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 526   | 254 | 94 | 153 | 25 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 9   | T     | 53       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 377   | 237 | 66 | 73 | 1 |         |         |       |

- Molecule 10 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



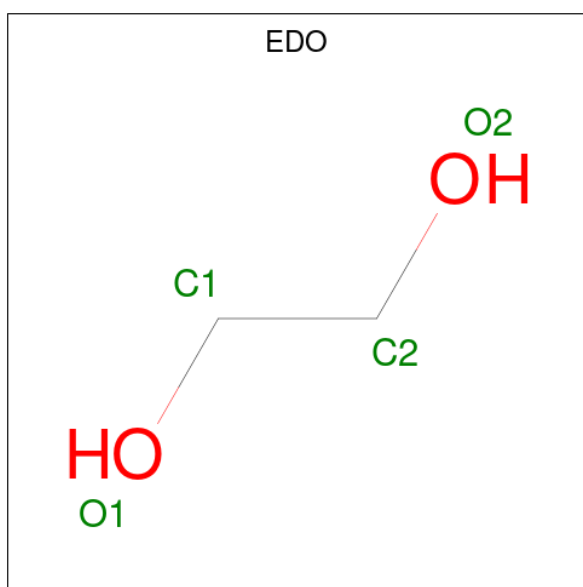
| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 10  | C     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

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| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 10  | C     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 10  | C     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 10  | D     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 10  | D     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 10  | D     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 10  | D     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 10  | F     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 10  | F     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 10  | F     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 10  | F     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

- Molecule 11 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



| Mol | Chain | Residues | Atoms                   | ZeroOcc | AltConf |
|-----|-------|----------|-------------------------|---------|---------|
| 11  | C     | 1        | Total C H O<br>10 2 6 2 | 0       | 0       |
| 11  | C     | 1        | Total C H O<br>10 2 6 2 | 0       | 0       |
| 11  | D     | 1        | Total C H O<br>10 2 6 2 | 0       | 0       |
| 11  | D     | 1        | Total C H O<br>10 2 6 2 | 0       | 0       |
| 11  | D     | 1        | Total C H O<br>10 2 6 2 | 0       | 0       |
| 11  | F     | 1        | Total C H O<br>10 2 6 2 | 0       | 0       |

- Molecule 12 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 12  | D     | 2        | Total Zn<br>2 2 | 0       | 0       |

- Molecule 13 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 13  | D     | 1        | Total Mg<br>1 1 | 0       | 0       |

- Molecule 14 is water.

| Mol | Chain | Residues | Atoms            | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 14  | J     | 1        | Total O<br>1 1   | 0       | 0       |
| 14  | A     | 3        | Total O<br>3 3   | 0       | 0       |
| 14  | B     | 1        | Total O<br>1 1   | 0       | 0       |
| 14  | C     | 17       | Total O<br>17 17 | 0       | 0       |
| 14  | D     | 51       | Total O<br>51 51 | 0       | 0       |
| 14  | E     | 2        | Total O<br>2 2   | 0       | 0       |
| 14  | F     | 16       | Total O<br>16 16 | 0       | 0       |

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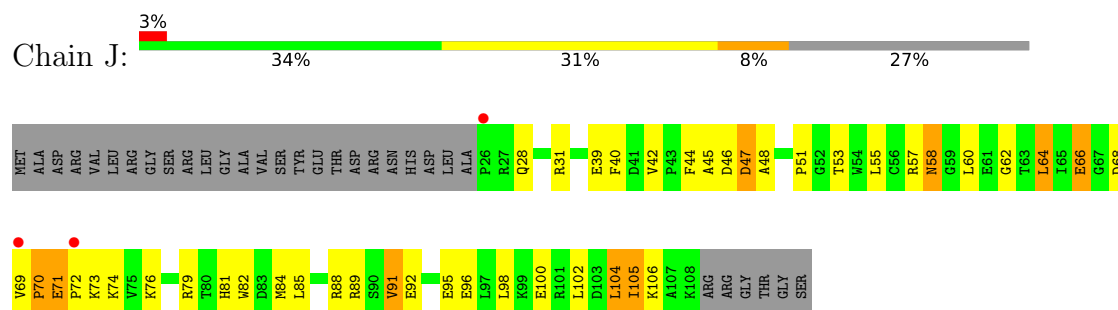
| Mol | Chain | Residues | Atoms       |         | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 14  | O     | 13       | Total<br>13 | O<br>13 | 0       | 0       |
| 14  | P     | 4        | Total<br>4  | O<br>4  | 0       | 0       |
| 14  | T     | 1        | Total<br>1  | O<br>1  | 0       | 0       |



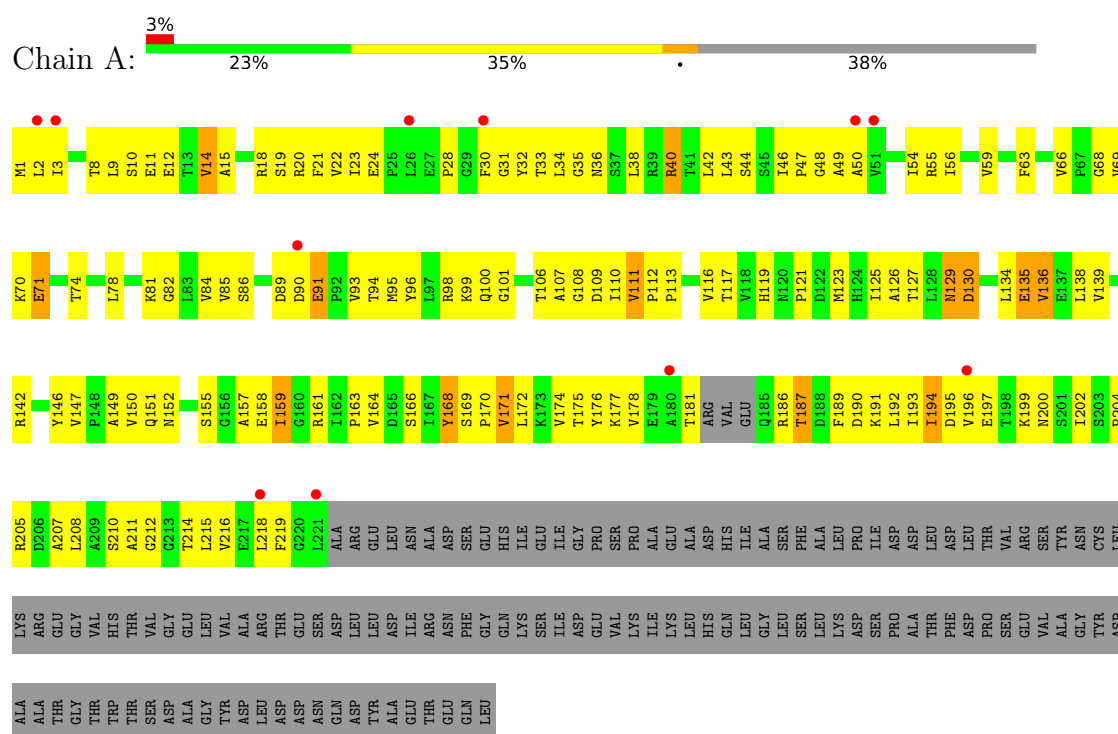
### 3 Residue-property plots [i](#)

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.

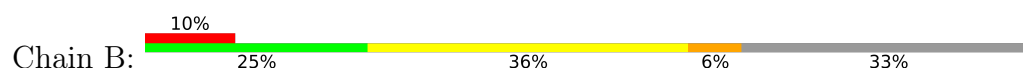
- Molecule 1: RNA polymerase-binding protein RbpA

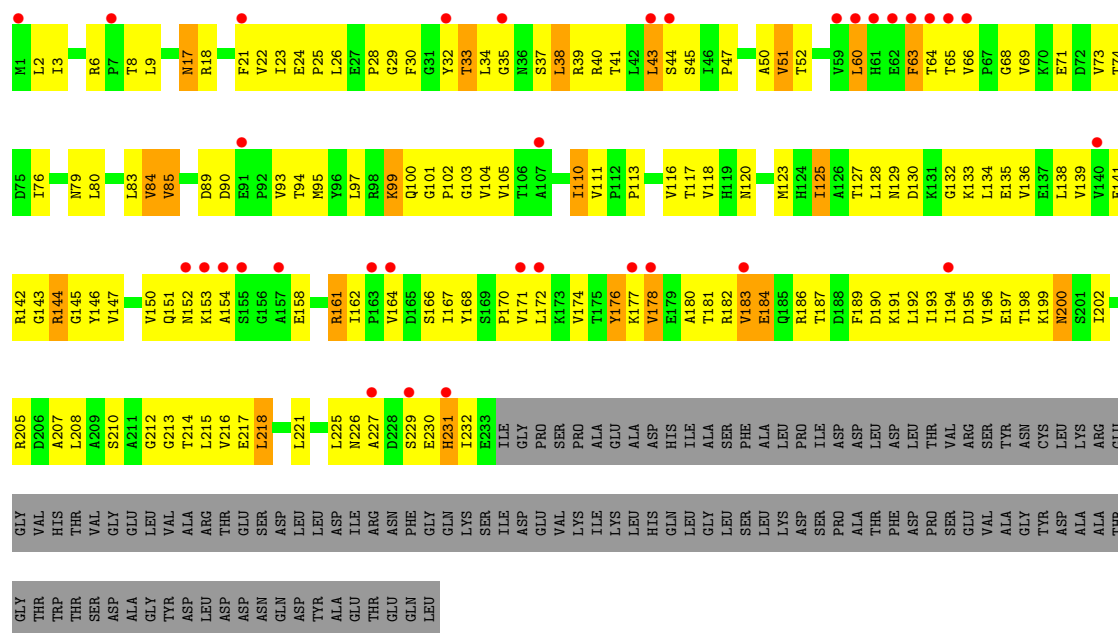


- Molecule 2: DNA-directed RNA polymerase subunit alpha



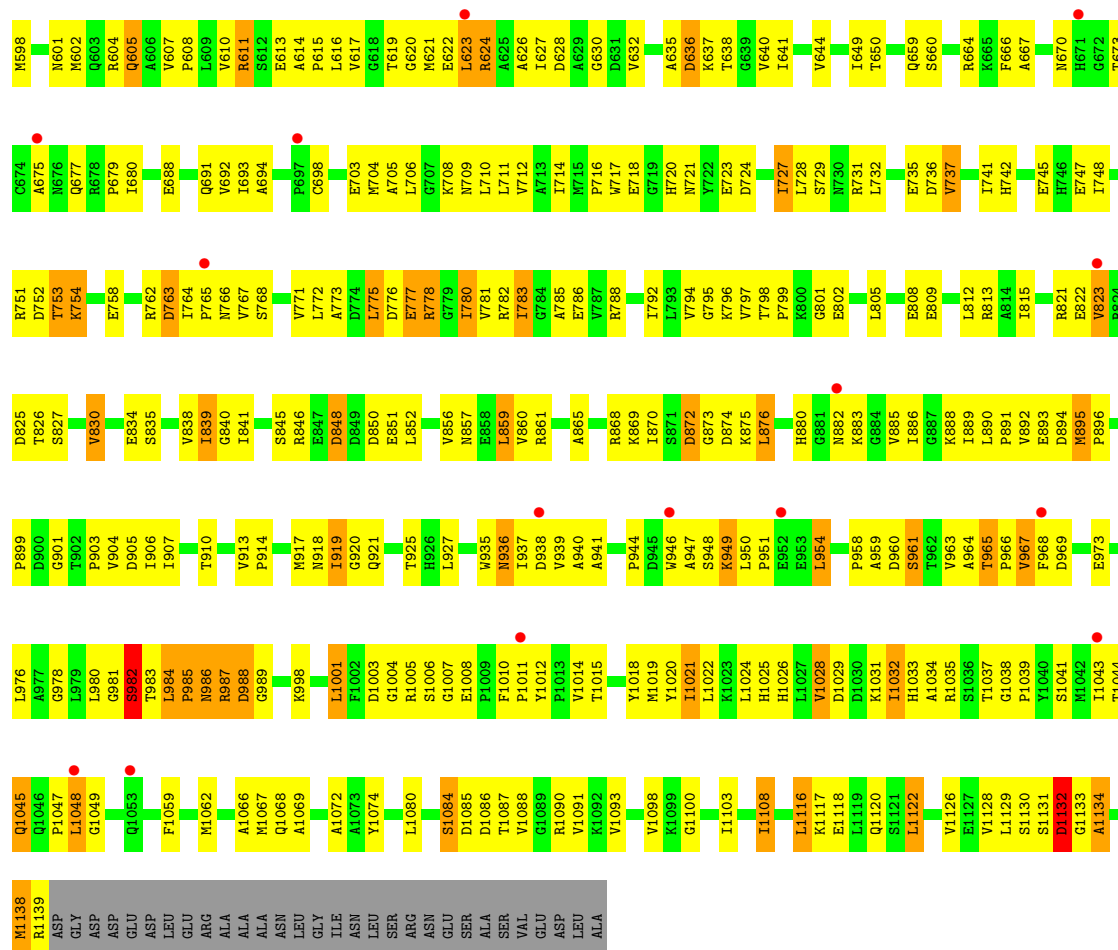
- Molecule 2: DNA-directed RNA polymerase subunit alpha



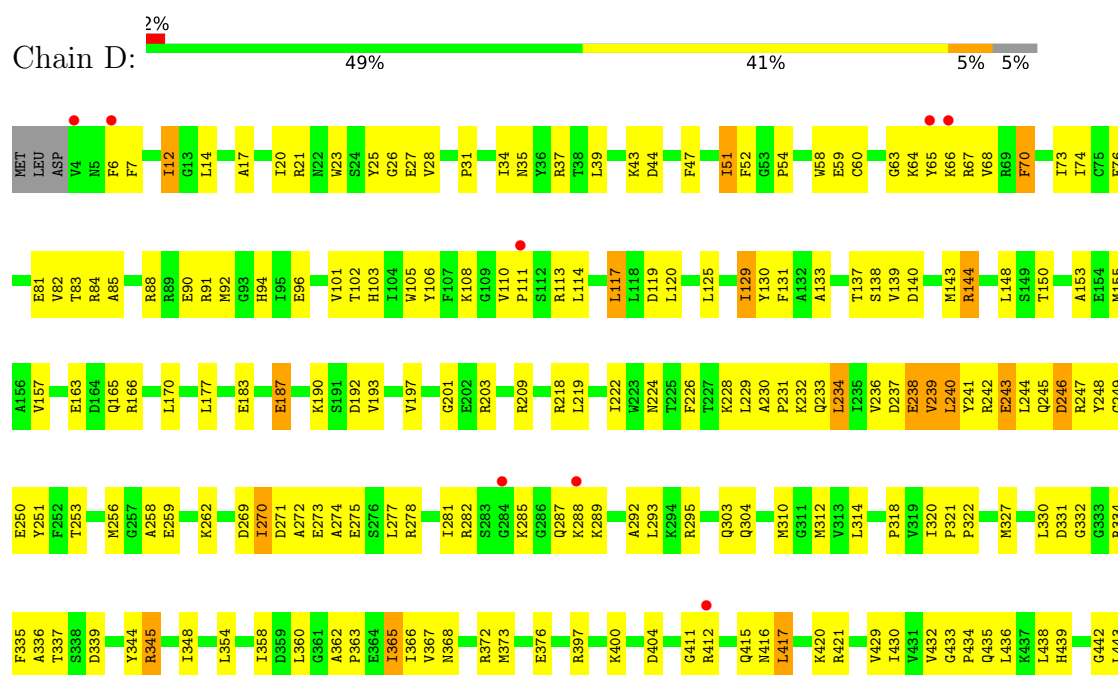


• Molecule 3: DNA-directed RNA polymerase subunit beta





• Molecule 4: DNA-directed RNA polymerase subunit beta'







ASP  
ALA  
ALA  
THR  
GLY  
THR  
TRP  
THR  
SER  
ASP  
ALA  
GLY  
TYR  
ASP  
LEU  
ASP  
ASN  
GLN  
ASP  
TYR  
ALA  
GLU  
THR  
GLU  
GLN  
LEU

## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 1 21 1                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 133.01Å 161.63Å 139.21Å<br>90.00° 107.72° 90.00°            | Depositor        |
| Resolution (Å)                                                          | 51.99 – 2.76<br>51.99 – 2.76                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.5 (51.99-2.76)<br>99.5 (51.99-2.76)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.23                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.16 (at 2.77Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX (1.10.1_2155)                                        | Depositor        |
| R, $R_{free}$                                                           | 0.240 , 0.281<br>0.245 , 0.283                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 1989 reflections (1.37%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 78.4                                                        | Xtriage          |
| Anisotropy                                                              | 0.150                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.30 , 46.9                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$ | Xtriage          |
| Estimated twinning fraction                                             | 0.003 for l,-k,h                                            | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.94                                                        | EDS              |
| Total number of atoms                                                   | 26631                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 86.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, SO4, EDO, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths |         | Bond angles |                |
|-----|-------|--------------|---------|-------------|----------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5        |
| 1   | J     | 0.14         | 0/681   | 0.42        | 0/923          |
| 2   | A     | 0.13         | 0/1641  | 0.39        | 0/2236         |
| 2   | B     | 0.14         | 0/1693  | 0.44        | 0/2316         |
| 3   | C     | 0.13         | 0/8394  | 0.42        | 2/11410 (0.0%) |
| 4   | D     | 0.13         | 0/9742  | 0.39        | 1/13189 (0.0%) |
| 5   | E     | 0.16         | 0/604   | 0.47        | 0/822          |
| 6   | F     | 0.10         | 0/2510  | 0.33        | 1/3389 (0.0%)  |
| 7   | O     | 0.21         | 0/710   | 0.43        | 0/1095         |
| 8   | P     | 0.24         | 0/589   | 0.45        | 0/906          |
| 9   | T     | 0.09         | 0/379   | 0.28        | 0/515          |
| All | All   | 0.13         | 0/26943 | 0.40        | 4/36801 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | J     | 0                   | 1                   |
| 3   | C     | 0                   | 5                   |
| All | All   | 0                   | 6                   |

There are no bond length outliers.

All (4) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | C     | 949  | LYS  | N-CA-C  | 7.22  | 122.27      | 113.17   |
| 3   | C     | 1132 | ASP  | N-CA-C  | -7.18 | 98.94       | 108.34   |
| 4   | D     | 901  | ALA  | CB-CA-C | -6.54 | 108.01      | 115.79   |
| 6   | F     | 144  | PRO  | N-CA-CB | 6.37  | 110.27      | 103.39   |



There are no chirality outliers.

All (6) planarity outliers are listed below:

| Mol | Chain | Res  | Type | Group   |
|-----|-------|------|------|---------|
| 3   | C     | 1131 | SER  | Peptide |
| 3   | C     | 368  | ARG  | Peptide |
| 3   | C     | 433  | GLN  | Peptide |
| 3   | C     | 982  | SER  | Peptide |
| 3   | C     | 985  | PRO  | Peptide |
| 1   | J     | 70   | PRO  | Peptide |

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | J     | 667   | 0        | 649      | 50      | 0            |
| 2   | A     | 1617  | 0        | 1636     | 181     | 0            |
| 2   | B     | 1667  | 0        | 1636     | 202     | 0            |
| 3   | C     | 8250  | 0        | 7989     | 707     | 1            |
| 4   | D     | 9588  | 0        | 9552     | 658     | 1            |
| 5   | E     | 592   | 0        | 583      | 54      | 0            |
| 6   | F     | 2481  | 0        | 2481     | 140     | 0            |
| 7   | O     | 634   | 0        | 350      | 34      | 0            |
| 8   | P     | 526   | 0        | 296      | 16      | 0            |
| 9   | T     | 377   | 0        | 348      | 30      | 0            |
| 10  | C     | 15    | 0        | 0        | 2       | 0            |
| 10  | D     | 20    | 0        | 0        | 2       | 0            |
| 10  | F     | 25    | 0        | 0        | 1       | 0            |
| 11  | C     | 8     | 12       | 12       | 1       | 0            |
| 11  | D     | 12    | 18       | 18       | 3       | 0            |
| 11  | F     | 4     | 6        | 6        | 1       | 0            |
| 12  | D     | 2     | 0        | 0        | 0       | 0            |
| 13  | D     | 1     | 0        | 0        | 0       | 0            |
| 14  | A     | 3     | 0        | 0        | 1       | 0            |
| 14  | B     | 1     | 0        | 0        | 1       | 0            |
| 14  | C     | 17    | 0        | 0        | 8       | 0            |
| 14  | D     | 51    | 0        | 0        | 7       | 0            |
| 14  | E     | 2     | 0        | 0        | 0       | 0            |
| 14  | F     | 16    | 0        | 0        | 2       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 14  | J     | 1     | 0        | 0        | 0       | 0            |
| 14  | O     | 13    | 0        | 0        | 4       | 0            |
| 14  | P     | 4     | 0        | 0        | 0       | 0            |
| 14  | T     | 1     | 0        | 0        | 1       | 0            |
| All | All   | 26595 | 36       | 25556    | 1896    | 1            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 36.

All (1896) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:184:GLU:HA    | 2:B:187:THR:HG22  | 1.28                     | 1.16              |
| 6:F:253:MET:HE3   | 6:F:297:MET:HA    | 1.28                     | 1.14              |
| 3:C:940:ALA:HB1   | 3:C:941:ALA:HA    | 1.27                     | 1.14              |
| 6:F:253:MET:HE2   | 6:F:300:GLN:HB2   | 1.26                     | 1.13              |
| 4:D:527:LEU:HD21  | 4:D:581:MET:HE1   | 1.32                     | 1.11              |
| 3:C:228:LEU:HD21  | 3:C:268:ILE:HG12  | 1.33                     | 1.08              |
| 3:C:540:ASP:HB2   | 3:C:546:THR:HG23  | 1.30                     | 1.08              |
| 3:C:176:VAL:HG12  | 3:C:195:VAL:HG22  | 1.36                     | 1.06              |
| 4:D:106:TYR:HB3   | 4:D:312:MET:HE3   | 1.37                     | 1.06              |
| 4:D:622:MET:HE2   | 4:D:629:VAL:HG22  | 1.36                     | 1.06              |
| 4:D:641:ARG:HA    | 4:D:656:LYS:HE3   | 1.40                     | 1.04              |
| 3:C:982:SER:HB3   | 3:C:983:THR:HG23  | 1.40                     | 1.03              |
| 3:C:799:PRO:HA    | 3:C:823:VAL:HG12  | 1.36                     | 1.03              |
| 4:D:1275:PRO:HG3  | 5:E:76:VAL:HG11   | 1.34                     | 1.03              |
| 3:C:602:MET:HE1   | 3:C:883:LYS:HB3   | 1.37                     | 1.02              |
| 3:C:215:VAL:HG23  | 3:C:225:VAL:HA    | 1.39                     | 1.02              |
| 3:C:710:LEU:HD22  | 3:C:1021:ILE:HD11 | 1.40                     | 1.01              |
| 3:C:635:ALA:HB2   | 3:C:693:ILE:HD11  | 1.40                     | 1.00              |
| 4:D:432:VAL:HG22  | 4:D:434:PRO:HD3   | 1.41                     | 1.00              |
| 3:C:444:ARG:HH21  | 3:C:491:LEU:HD23  | 1.24                     | 1.00              |
| 9:T:289:PHE:HE2   | 9:T:294:ILE:HG13  | 1.26                     | 0.99              |
| 4:D:622:MET:HE3   | 4:D:667:LEU:HD13  | 1.45                     | 0.99              |
| 2:A:31:GLY:HA2    | 2:A:192:LEU:HD23  | 1.46                     | 0.97              |
| 4:D:1174:THR:HG23 | 4:D:1176:PHE:H    | 1.28                     | 0.97              |
| 4:D:603:THR:HG22  | 4:D:604:LYS:HE2   | 1.49                     | 0.95              |
| 3:C:478:GLU:OE2   | 3:C:604:ARG:NH2   | 1.98                     | 0.94              |
| 2:A:1:MET:N       | 2:B:142:ARG:O     | 1.99                     | 0.94              |
| 4:D:815:THR:HG22  | 4:D:820:LYS:HA    | 1.49                     | 0.94              |
| 3:C:150:MET:HA    | 3:C:150:MET:HE2   | 1.50                     | 0.93              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 4:D:951:LEU:HB3   | 4:D:956:ILE:HD11 | 1.50                     | 0.93              |
| 3:C:191:HIS:HA    | 3:C:192:SER:HB3  | 1.47                     | 0.93              |
| 3:C:41:VAL:O      | 3:C:624:ARG:NH2  | 2.01                     | 0.92              |
| 6:F:308:VAL:HG21  | 7:O:23:DT:H71    | 1.49                     | 0.92              |
| 3:C:217:ILE:HD11  | 3:C:272:LEU:HD11 | 1.52                     | 0.92              |
| 6:F:219:MET:HA    | 6:F:219:MET:HE2  | 1.51                     | 0.92              |
| 3:C:338:ARG:HD2   | 3:C:346:MET:HG3  | 1.49                     | 0.92              |
| 3:C:1132:ASP:HB3  | 3:C:1133:GLY:HA2 | 1.51                     | 0.92              |
| 2:B:34:LEU:HD11   | 2:B:192:LEU:HD22 | 1.52                     | 0.91              |
| 3:C:783:ILE:HD12  | 3:C:783:ILE:H    | 1.34                     | 0.91              |
| 4:D:327:MET:HG3   | 4:D:337:THR:HB   | 1.51                     | 0.91              |
| 2:B:63:PHE:CE2    | 4:D:603:THR:HG23 | 2.05                     | 0.90              |
| 3:C:935:TRP:HA    | 3:C:983:THR:HG23 | 1.51                     | 0.90              |
| 2:A:89:ASP:CB     | 2:A:90:ASP:HA    | 2.00                     | 0.90              |
| 2:B:152:ASN:C     | 2:B:154:ALA:HA   | 1.96                     | 0.90              |
| 2:B:84:VAL:HB     | 2:B:199:LYS:HD3  | 1.53                     | 0.90              |
| 3:C:92:GLY:O      | 3:C:133:ASN:ND2  | 2.06                     | 0.89              |
| 5:E:86:GLU:OE2    | 5:E:94:ARG:NH1   | 2.06                     | 0.89              |
| 6:F:211:LEU:HB2   | 6:F:216:ARG:HD2  | 1.54                     | 0.89              |
| 3:C:454:LEU:HD22  | 3:C:459:ALA:HB2  | 1.55                     | 0.89              |
| 3:C:508:ARG:HD3   | 3:C:515:VAL:HG11 | 1.54                     | 0.88              |
| 6:F:324:LEU:HD23  | 6:F:328:LEU:HD13 | 1.54                     | 0.88              |
| 2:A:98:ARG:HG2    | 2:A:135:GLU:HG2  | 1.54                     | 0.88              |
| 2:B:153:LYS:N     | 2:B:154:ALA:HA   | 1.86                     | 0.88              |
| 3:C:77:LEU:HD11   | 3:C:124:LEU:HD11 | 1.54                     | 0.88              |
| 4:D:573:PRO:HG2   | 4:D:576:MET:HE3  | 1.56                     | 0.87              |
| 3:C:159:ILE:HB    | 3:C:164:ARG:HD2  | 1.56                     | 0.87              |
| 4:D:930:ASP:O     | 4:D:933:GLY:HA3  | 1.74                     | 0.87              |
| 3:C:758:GLU:HG2   | 3:C:798:THR:HG22 | 1.54                     | 0.87              |
| 3:C:510:VAL:N     | 3:C:568:ASP:O    | 2.08                     | 0.87              |
| 2:A:152:ASN:HB2   | 2:A:157:ALA:HB3  | 1.57                     | 0.87              |
| 1:J:31:ARG:NH2    | 1:J:39:GLU:OE1   | 2.08                     | 0.86              |
| 3:C:584:MET:HA    | 3:C:619:THR:HG21 | 1.55                     | 0.86              |
| 3:C:649:ILE:HD11  | 3:C:679:PRO:HB3  | 1.57                     | 0.86              |
| 4:D:1174:THR:HG21 | 4:D:1176:PHE:HB2 | 1.58                     | 0.86              |
| 4:D:1071:ASP:HB2  | 4:D:1073:GLY:N   | 1.91                     | 0.86              |
| 4:D:269:ASP:HB3   | 4:D:272:ALA:HB3  | 1.58                     | 0.86              |
| 4:D:442:GLY:HA3   | 4:D:523:GLN:HB2  | 1.56                     | 0.86              |
| 4:D:740:GLN:HE21  | 4:D:740:GLN:H    | 1.22                     | 0.86              |
| 3:C:938:ASP:O     | 3:C:944:PRO:HD3  | 1.76                     | 0.85              |
| 4:D:365:ILE:H     | 4:D:365:ILE:HD12 | 1.40                     | 0.85              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 4:D:655:TRP:HA    | 4:D:655:TRP:CE3  | 2.09                     | 0.85              |
| 2:B:21:PHE:HB2    | 2:B:194:ILE:HG22 | 1.59                     | 0.85              |
| 4:D:1088:ARG:HG2  | 4:D:1089:VAL:H   | 1.42                     | 0.85              |
| 2:B:6:ARG:O       | 2:B:25:PRO:HD2   | 1.77                     | 0.85              |
| 3:C:170:LEU:HA    | 3:C:369:LEU:H    | 1.42                     | 0.84              |
| 6:F:253:MET:CE    | 6:F:300:GLN:HB2  | 2.06                     | 0.84              |
| 2:B:32:TYR:HB3    | 3:C:1005:ARG:HG3 | 1.57                     | 0.84              |
| 2:B:95:MET:HG2    | 2:B:113:PRO:HD2  | 1.60                     | 0.84              |
| 2:A:157:ALA:HB1   | 2:A:161:ARG:HD2  | 1.57                     | 0.84              |
| 6:F:280:LYS:HG2   | 7:O:30:DC:OP2    | 1.76                     | 0.84              |
| 4:D:599:TYR:HB2   | 4:D:610:GLY:HA3  | 1.56                     | 0.84              |
| 3:C:981:GLY:O     | 3:C:982:SER:OG   | 1.95                     | 0.83              |
| 3:C:1048:LEU:HD23 | 3:C:1048:LEU:H   | 1.44                     | 0.83              |
| 2:B:64:THR:O      | 2:B:65:THR:OG1   | 1.95                     | 0.83              |
| 3:C:379:GLN:HG2   | 3:C:421:PHE:HB2  | 1.61                     | 0.83              |
| 4:D:901:ALA:H     | 4:D:912:ASP:HB2  | 1.44                     | 0.83              |
| 9:T:289:PHE:CE2   | 9:T:294:ILE:HG13 | 2.12                     | 0.83              |
| 3:C:574:PRO:O     | 3:C:575:ARG:HG2  | 1.79                     | 0.82              |
| 3:C:940:ALA:HB1   | 3:C:941:ALA:CA   | 2.09                     | 0.82              |
| 4:D:1174:THR:HG23 | 4:D:1176:PHE:N   | 1.94                     | 0.82              |
| 3:C:718:GLU:H     | 4:D:724:THR:HG21 | 1.45                     | 0.82              |
| 4:D:155:MET:HE1   | 4:D:219:LEU:HD22 | 1.61                     | 0.82              |
| 4:D:612:TYR:HB2   | 4:D:635:VAL:HG12 | 1.59                     | 0.82              |
| 4:D:929:VAL:HG12  | 4:D:935:VAL:HG22 | 1.60                     | 0.82              |
| 4:D:818:GLY:O     | 4:D:838:SER:HB3  | 1.79                     | 0.81              |
| 2:B:151:GLN:HG2   | 2:B:154:ALA:HB1  | 1.63                     | 0.81              |
| 4:D:12:ILE:HD11   | 4:D:1221:TRP:CD2 | 2.16                     | 0.81              |
| 4:D:1275:PRO:HB3  | 5:E:79:LEU:HD11  | 1.62                     | 0.81              |
| 2:B:100:GLN:HA    | 2:B:133:LYS:HA   | 1.62                     | 0.81              |
| 7:O:28:DT:H2''    | 7:O:29:DA:H5'    | 1.62                     | 0.81              |
| 5:E:85:GLN:HE21   | 5:E:85:GLN:H     | 1.29                     | 0.81              |
| 2:A:48:GLY:HA2    | 2:A:49:ALA:HB3   | 1.61                     | 0.81              |
| 3:C:540:ASP:CB    | 3:C:546:THR:HG23 | 2.11                     | 0.81              |
| 3:C:445:ARG:NH2   | 14:C:1304:HOH:O  | 2.13                     | 0.80              |
| 4:D:643:PRO:O     | 4:D:647:GLU:HB3  | 1.80                     | 0.80              |
| 4:D:114:LEU:HG    | 4:D:312:MET:HE2  | 1.63                     | 0.80              |
| 4:D:1248:GLY:O    | 4:D:1252:ASN:ND2 | 2.14                     | 0.80              |
| 1:J:102:LEU:O     | 1:J:105:ILE:HG22 | 1.81                     | 0.79              |
| 2:A:181:THR:N     | 2:A:189:PHE:O    | 2.15                     | 0.79              |
| 3:C:148:PHE:HE1   | 3:C:380:ILE:HD11 | 1.46                     | 0.79              |
| 4:D:642:PRO:HD3   | 4:D:656:LYS:HG2  | 1.63                     | 0.79              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:D:1171:SER:CA  | 4:D:1174:THR:HG22 | 2.12                     | 0.79              |
| 3:C:412:ARG:HD2  | 6:F:322:ARG:HE    | 1.47                     | 0.79              |
| 7:O:11:DA:H2"    | 7:O:12:DG:H5"     | 1.64                     | 0.79              |
| 2:B:18:ARG:HG3   | 2:B:197:GLU:HG3   | 1.64                     | 0.79              |
| 4:D:47:PHE:O     | 4:D:88:ARG:NH2    | 2.15                     | 0.79              |
| 2:A:152:ASN:CB   | 2:A:157:ALA:HB3   | 2.13                     | 0.79              |
| 3:C:348:VAL:HB   | 3:C:351:GLY:HA3   | 1.65                     | 0.79              |
| 5:E:84:LEU:H     | 5:E:84:LEU:HD12   | 1.46                     | 0.78              |
| 4:D:599:TYR:CE1  | 4:D:601:ALA:HB2   | 2.18                     | 0.78              |
| 2:A:40:ARG:HD3   | 2:B:33:THR:HG22   | 1.65                     | 0.78              |
| 3:C:891:PRO:HB2  | 3:C:893:GLU:HG2   | 1.64                     | 0.78              |
| 6:F:454:HIS:ND1  | 6:F:455:PRO:HD2   | 1.98                     | 0.78              |
| 2:A:86:SER:OG    | 2:A:119:HIS:NE2   | 2.14                     | 0.78              |
| 3:C:88:GLU:HG2   | 3:C:92:GLY:HA2    | 1.65                     | 0.78              |
| 4:D:641:ARG:CA   | 4:D:656:LYS:HE3   | 2.13                     | 0.78              |
| 3:C:51:SER:OG    | 3:C:373:GLY:N     | 2.14                     | 0.78              |
| 4:D:12:ILE:HD11  | 4:D:1221:TRP:CE3  | 2.19                     | 0.78              |
| 3:C:1138:MET:O   | 3:C:1139:ARG:HG3  | 1.84                     | 0.78              |
| 4:D:937:ILE:HD12 | 4:D:951:LEU:HG    | 1.65                     | 0.77              |
| 4:D:111:PRO:O    | 4:D:113:ARG:NH1   | 2.16                     | 0.77              |
| 4:D:26:GLY:HA3   | 4:D:51:ILE:HG22   | 1.65                     | 0.77              |
| 2:A:56:ILE:HB    | 2:A:59:VAL:HG22   | 1.67                     | 0.77              |
| 6:F:253:MET:HE2  | 6:F:300:GLN:CB    | 2.11                     | 0.77              |
| 2:B:170:PRO:HB2  | 2:B:202:ILE:HD11  | 1.66                     | 0.77              |
| 3:C:593:ALA:HB2  | 4:D:852:THR:HG22  | 1.67                     | 0.77              |
| 3:C:763:ASP:HB3  | 3:C:821:ARG:HH22  | 1.50                     | 0.77              |
| 5:E:30:LEU:O     | 5:E:33:THR:HG22   | 1.85                     | 0.77              |
| 3:C:508:ARG:HD2  | 3:C:570:MET:HE2   | 1.67                     | 0.77              |
| 3:C:637:LYS:HD2  | 3:C:659:GLN:HE22  | 1.49                     | 0.77              |
| 9:T:279:THR:HG23 | 9:T:282:ASP:HB2   | 1.67                     | 0.77              |
| 1:J:68:ASP:HA    | 1:J:69:VAL:HB     | 1.66                     | 0.77              |
| 4:D:962:ARG:NH1  | 4:D:977:CYS:SG    | 2.58                     | 0.77              |
| 3:C:1003:ASP:OD1 | 3:C:1006:SER:N    | 2.17                     | 0.77              |
| 4:D:1165:ARG:HD2 | 4:D:1209:MET:HE1  | 1.66                     | 0.77              |
| 6:F:404:THR:O    | 6:F:457:ARG:NH2   | 2.18                     | 0.77              |
| 4:D:444:PRO:HG3  | 4:D:521:ALA:O     | 1.84                     | 0.76              |
| 3:C:940:ALA:CB   | 3:C:941:ALA:HA    | 2.11                     | 0.76              |
| 4:D:573:PRO:HG2  | 4:D:576:MET:CE    | 2.15                     | 0.76              |
| 4:D:735:VAL:HG12 | 4:D:840:ARG:HD2   | 1.66                     | 0.76              |
| 7:O:14:DG:H2"    | 7:O:15:DT:OP2     | 1.84                     | 0.76              |
| 2:A:86:SER:HG    | 2:A:119:HIS:HE2   | 1.31                     | 0.76              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:D:1168:ILE:HD13 | 4:D:1176:PHE:HB3  | 1.65                     | 0.76              |
| 4:D:901:ALA:HB2   | 4:D:911:ARG:HA    | 1.66                     | 0.76              |
| 4:D:487:LEU:HG    | 4:D:491:ILE:HD12  | 1.67                     | 0.76              |
| 6:F:201:LEU:HD11  | 6:F:219:MET:HB3   | 1.67                     | 0.76              |
| 2:B:32:TYR:HE1    | 2:B:178:VAL:HG21  | 1.50                     | 0.75              |
| 2:B:184:GLU:CA    | 2:B:187:THR:HG22  | 2.14                     | 0.75              |
| 3:C:720:HIS:O     | 4:D:432:VAL:HG11  | 1.86                     | 0.75              |
| 2:B:95:MET:HE3    | 2:B:110:ILE:HD11  | 1.68                     | 0.75              |
| 3:C:773:ALA:O     | 3:C:782:ARG:NH2   | 2.20                     | 0.75              |
| 3:C:935:TRP:HA    | 3:C:983:THR:CG2   | 2.16                     | 0.75              |
| 4:D:772:SER:O     | 4:D:776:ILE:HG13  | 1.87                     | 0.75              |
| 4:D:822:LEU:HD23  | 4:D:834:PRO:HA    | 1.67                     | 0.75              |
| 4:D:1009:LEU:HD12 | 4:D:1146:GLN:HG3  | 1.67                     | 0.75              |
| 4:D:951:LEU:HB3   | 4:D:956:ILE:CD1   | 2.15                     | 0.75              |
| 2:B:26:LEU:HD11   | 2:B:34:LEU:HD21   | 1.69                     | 0.75              |
| 4:D:417:LEU:HG    | 4:D:1254:ILE:HG23 | 1.67                     | 0.75              |
| 2:A:28:PRO:HA     | 2:A:190:ASP:OD2   | 1.87                     | 0.74              |
| 3:C:215:VAL:HG12  | 3:C:217:ILE:CG2   | 2.16                     | 0.74              |
| 4:D:277:LEU:HD11  | 4:D:295:ARG:HG2   | 1.67                     | 0.74              |
| 3:C:509:LYS:O     | 3:C:516:THR:HG22  | 1.87                     | 0.74              |
| 3:C:205:PHE:CE1   | 3:C:215:VAL:HG13  | 2.22                     | 0.74              |
| 4:D:139:VAL:HG12  | 4:D:231:PRO:HD3   | 1.69                     | 0.74              |
| 9:T:264:LEU:HB3   | 9:T:269:VAL:CG2   | 2.18                     | 0.74              |
| 4:D:951:LEU:C     | 4:D:956:ILE:HD11  | 2.13                     | 0.74              |
| 3:C:1059:PHE:HZ   | 3:C:1067:MET:HE3  | 1.53                     | 0.74              |
| 4:D:796:ASN:HD21  | 4:D:798:ILE:HB    | 1.53                     | 0.74              |
| 3:C:204:GLU:OE1   | 3:C:216:ARG:NH1   | 2.19                     | 0.74              |
| 4:D:143:MET:HE1   | 4:D:250:GLU:O     | 1.88                     | 0.74              |
| 4:D:721:TYR:O     | 4:D:725:ARG:HG2   | 1.86                     | 0.74              |
| 4:D:644:THR:HA    | 4:D:647:GLU:OE1   | 1.88                     | 0.74              |
| 7:O:6:DA:H2''     | 7:O:7:DC:H5'      | 1.69                     | 0.74              |
| 3:C:191:HIS:HA    | 3:C:192:SER:CB    | 2.17                     | 0.74              |
| 3:C:720:HIS:CE1   | 3:C:888:LYS:HD3   | 2.23                     | 0.74              |
| 2:A:66:VAL:O      | 2:A:69:VAL:HG22   | 1.87                     | 0.74              |
| 2:B:24:GLU:OE2    | 2:B:191:LYS:HD3   | 1.87                     | 0.74              |
| 3:C:235:THR:N     | 3:C:238:GLN:OE1   | 2.20                     | 0.74              |
| 3:C:361:ILE:H     | 3:C:361:ILE:HD12  | 1.53                     | 0.74              |
| 4:D:590:THR:HG21  | 4:D:630:ARG:HH21  | 1.53                     | 0.74              |
| 4:D:859:LEU:O     | 4:D:862:THR:HG22  | 1.87                     | 0.74              |
| 4:D:237:ASP:HB3   | 4:D:240:LEU:HB3   | 1.70                     | 0.73              |
| 4:D:596:THR:HG22  | 4:D:626:ALA:O     | 1.88                     | 0.73              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 8:P:11:DA:H2''   | 8:P:12:DA:O5'    | 1.88                     | 0.73              |
| 3:C:742:HIS:CD2  | 3:C:868:ARG:HG3  | 2.23                     | 0.73              |
| 4:D:642:PRO:HG3  | 4:D:661:TRP:CE2  | 2.22                     | 0.73              |
| 2:A:14:VAL:HG13  | 2:A:18:ARG:HG3   | 1.68                     | 0.73              |
| 3:C:231:ALA:HB1  | 3:C:265:LEU:CD1  | 2.17                     | 0.73              |
| 3:C:494:TYR:HB3  | 3:C:506:PRO:HG3  | 1.69                     | 0.73              |
| 3:C:132:ASN:HB3  | 3:C:135:THR:HG22 | 1.68                     | 0.73              |
| 2:B:22:VAL:HG12  | 2:B:193:ILE:HD12 | 1.70                     | 0.73              |
| 2:B:158:GLU:HB3  | 2:B:161:ARG:HB2  | 1.70                     | 0.73              |
| 3:C:728:LEU:CD2  | 3:C:906:ILE:HG22 | 2.19                     | 0.73              |
| 2:A:14:VAL:HG12  | 2:A:19:SER:HA    | 1.69                     | 0.73              |
| 2:B:181:THR:O    | 2:B:189:PHE:N    | 2.20                     | 0.73              |
| 3:C:578:VAL:HG13 | 3:C:582:THR:HB   | 1.70                     | 0.73              |
| 3:C:1018:TYR:O   | 14:C:1302:HOH:O  | 2.04                     | 0.73              |
| 4:D:238:GLU:HA   | 4:D:241:TYR:HB3  | 1.69                     | 0.73              |
| 4:D:26:GLY:HA3   | 4:D:51:ILE:CG2   | 2.19                     | 0.73              |
| 4:D:1069:PRO:HG2 | 4:D:1073:GLY:H   | 1.54                     | 0.73              |
| 8:P:13:DC:H2''   | 8:P:14:DA:C8     | 2.24                     | 0.73              |
| 2:A:82:GLY:HA3   | 2:A:123:MET:HE1  | 1.70                     | 0.73              |
| 3:C:249:MET:O    | 3:C:253:LEU:HD23 | 1.89                     | 0.72              |
| 3:C:939:VAL:CG2  | 3:C:940:ALA:HA   | 2.19                     | 0.72              |
| 4:D:655:TRP:HA   | 4:D:655:TRP:HE3  | 1.52                     | 0.72              |
| 3:C:47:VAL:HG23  | 3:C:497:VAL:HG21 | 1.71                     | 0.72              |
| 3:C:637:LYS:HD2  | 3:C:659:GLN:NE2  | 2.03                     | 0.72              |
| 4:D:344:TYR:O    | 4:D:348:ILE:HG22 | 1.89                     | 0.72              |
| 3:C:636:ASP:OD1  | 3:C:636:ASP:N    | 2.21                     | 0.72              |
| 3:C:984:LEU:HB2  | 3:C:985:PRO:HA   | 1.70                     | 0.72              |
| 2:B:2:LEU:CB     | 2:B:231:HIS:HA   | 2.19                     | 0.72              |
| 6:F:251:ARG:HB2  | 6:F:297:MET:HE1  | 1.72                     | 0.72              |
| 2:A:48:GLY:CA    | 2:A:49:ALA:HB3   | 2.19                     | 0.72              |
| 3:C:87:ILE:HD12  | 3:C:388:GLU:HG3  | 1.69                     | 0.72              |
| 4:D:581:MET:HE3  | 4:D:716:LYS:HA   | 1.70                     | 0.72              |
| 4:D:587:TYR:O    | 4:D:590:THR:HG22 | 1.89                     | 0.72              |
| 3:C:426:GLN:HE21 | 3:C:451:PRO:HD3  | 1.55                     | 0.72              |
| 4:D:527:LEU:HD22 | 4:D:575:ALA:O    | 1.89                     | 0.72              |
| 7:O:19:DA:H2''   | 7:O:20:DT:O5'    | 1.88                     | 0.72              |
| 3:C:205:PHE:HE1  | 3:C:215:VAL:HG13 | 1.55                     | 0.72              |
| 3:C:982:SER:OG   | 14:C:1303:HOH:O  | 2.06                     | 0.71              |
| 4:D:488:GLU:HG3  | 4:D:516:LEU:HD12 | 1.71                     | 0.71              |
| 3:C:444:ARG:NH2  | 3:C:492:SER:O    | 2.23                     | 0.71              |
| 3:C:1130:SER:HB3 | 3:C:1132:ASP:O   | 1.90                     | 0.71              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:C:239:ILE:HG21 | 3:C:253:LEU:HD22  | 1.71                     | 0.71              |
| 3:C:496:ARG:NH2  | 3:C:504:GLU:OE1   | 2.23                     | 0.71              |
| 3:C:845:SER:N    | 3:C:850:ASP:OD2   | 2.21                     | 0.71              |
| 7:O:15:DT:OP1    | 9:T:258:VAL:HG21  | 1.89                     | 0.71              |
| 3:C:482:GLY:O    | 3:C:485:ILE:HG13  | 1.90                     | 0.71              |
| 4:D:819:MET:HE2  | 4:D:821:GLY:HA2   | 1.71                     | 0.71              |
| 3:C:936:ASN:HD22 | 3:C:937:ILE:H     | 1.37                     | 0.71              |
| 3:C:1086:ASP:O   | 3:C:1090:ARG:HG2  | 1.90                     | 0.71              |
| 4:D:278:ARG:O    | 4:D:281:ILE:HG13  | 1.90                     | 0.71              |
| 3:C:494:TYR:HD2  | 3:C:572:VAL:HG21  | 1.55                     | 0.71              |
| 2:A:11:GLU:OE1   | 2:A:205:ARG:NE    | 2.22                     | 0.71              |
| 3:C:780:ILE:HD11 | 3:C:841:ILE:HD13  | 1.73                     | 0.71              |
| 3:C:973:GLU:O    | 4:D:732:MET:HE1   | 1.91                     | 0.71              |
| 4:D:138:SER:HB3  | 4:D:253:THR:OG1   | 1.90                     | 0.71              |
| 5:E:45:SER:OG    | 5:E:105:GLU:OE2   | 2.01                     | 0.71              |
| 4:D:155:MET:CE   | 4:D:219:LEU:HB3   | 2.20                     | 0.71              |
| 6:F:308:VAL:HG22 | 14:F:607:HOH:O    | 1.91                     | 0.71              |
| 6:F:320:ILE:HG23 | 6:F:340:GLU:HG2   | 1.72                     | 0.71              |
| 3:C:250:MET:HA   | 3:C:253:LEU:HD21  | 1.73                     | 0.70              |
| 6:F:397:GLN:O    | 6:F:401:VAL:HG23  | 1.90                     | 0.70              |
| 3:C:508:ARG:HD3  | 3:C:515:VAL:CG1   | 2.21                     | 0.70              |
| 3:C:613:GLU:HB3  | 3:C:708:LYS:HD3   | 1.71                     | 0.70              |
| 1:J:91:VAL:HG22  | 1:J:92:GLU:OE1    | 1.92                     | 0.70              |
| 3:C:711:LEU:HD23 | 3:C:904:VAL:HA    | 1.73                     | 0.70              |
| 3:C:44:LEU:HD13  | 3:C:440:LEU:HD21  | 1.72                     | 0.70              |
| 6:F:164:ASP:OD1  | 6:F:166:VAL:HG22  | 1.91                     | 0.70              |
| 3:C:328:ASP:O    | 3:C:332:THR:HG23  | 1.92                     | 0.70              |
| 3:C:1026:HIS:HB3 | 3:C:1031:LYS:HE3  | 1.74                     | 0.70              |
| 1:J:84:MET:HE3   | 6:F:272:LYS:HE2   | 1.73                     | 0.70              |
| 3:C:102:ARG:NH2  | 3:C:127:THR:OG1   | 2.23                     | 0.70              |
| 3:C:1045:GLN:HG2 | 3:C:1087:THR:HG22 | 1.73                     | 0.70              |
| 3:C:1100:GLY:HA3 | 4:D:458:LYS:HE3   | 1.74                     | 0.70              |
| 4:D:238:GLU:OE2  | 4:D:242:ARG:NH2   | 2.23                     | 0.70              |
| 3:C:1068:GLN:NE2 | 4:D:1249:LEU:HD13 | 2.07                     | 0.70              |
| 1:J:79:ARG:NH2   | 7:O:25:DC:OP1     | 2.25                     | 0.70              |
| 3:C:265:LEU:HD11 | 3:C:287:LEU:HD12  | 1.73                     | 0.70              |
| 3:C:728:LEU:HB2  | 3:C:889:ILE:HG12  | 1.73                     | 0.69              |
| 3:C:982:SER:HB3  | 3:C:983:THR:CG2   | 2.21                     | 0.69              |
| 4:D:1166:VAL:HA  | 4:D:1207:VAL:HG23 | 1.74                     | 0.69              |
| 9:T:256:LEU:HD22 | 9:T:297:VAL:HG22  | 1.74                     | 0.69              |
| 2:B:63:PHE:HE2   | 4:D:603:THR:HG23  | 1.53                     | 0.69              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:C:390:VAL:O    | 3:C:394:ARG:HB2   | 1.92                     | 0.69              |
| 3:C:1108:ILE:H   | 3:C:1108:ILE:HD12 | 1.55                     | 0.69              |
| 4:D:1232:ARG:NH1 | 4:D:1236:ASP:OD2  | 2.24                     | 0.69              |
| 2:A:38:LEU:HD13  | 2:A:208:LEU:HD11  | 1.75                     | 0.69              |
| 4:D:444:PRO:HD2  | 4:D:447:MET:HE2   | 1.73                     | 0.69              |
| 2:B:30:PHE:HA    | 2:B:33:THR:HG23   | 1.72                     | 0.69              |
| 5:E:26:TYR:HE1   | 5:E:29:PRO:HD3    | 1.57                     | 0.69              |
| 3:C:299:LEU:HB3  | 3:C:323:THR:HA    | 1.74                     | 0.69              |
| 3:C:531:VAL:HG13 | 3:C:552:VAL:CG2   | 2.22                     | 0.69              |
| 4:D:668:GLY:HA2  | 4:D:671:MET:CE    | 2.22                     | 0.69              |
| 6:F:399:GLN:O    | 6:F:403:GLU:HG2   | 1.92                     | 0.69              |
| 3:C:246:SER:CB   | 3:C:337:VAL:HG11  | 2.22                     | 0.69              |
| 4:D:668:GLY:HA2  | 4:D:671:MET:HE3   | 1.73                     | 0.69              |
| 3:C:575:ARG:HE   | 3:C:967:VAL:HG22  | 1.57                     | 0.69              |
| 3:C:754:LYS:HE2  | 3:C:754:LYS:H     | 1.58                     | 0.69              |
| 2:B:47:PRO:HA    | 2:B:144:ARG:HG3   | 1.74                     | 0.69              |
| 2:B:182:ARG:N    | 2:B:186:ARG:O     | 2.25                     | 0.69              |
| 2:B:32:TYR:CB    | 3:C:1005:ARG:HG3  | 2.23                     | 0.69              |
| 2:B:216:VAL:HG13 | 2:B:217:GLU:H     | 1.58                     | 0.69              |
| 3:C:776:ASP:HB2  | 3:C:777:GLU:OE1   | 1.93                     | 0.69              |
| 7:O:28:DT:OP1    | 14:O:101:HOH:O    | 2.11                     | 0.69              |
| 2:A:94:THR:HG22  | 2:A:139:VAL:HG22  | 1.74                     | 0.68              |
| 3:C:732:LEU:HA   | 3:C:737:VAL:CG1   | 2.23                     | 0.68              |
| 4:D:1174:THR:HA  | 4:D:1175:GLU:CB   | 2.22                     | 0.68              |
| 2:A:24:GLU:CD    | 2:A:191:LYS:HD3   | 2.18                     | 0.68              |
| 2:A:106:THR:HA   | 2:A:125:ILE:HD13  | 1.75                     | 0.68              |
| 3:C:727:ILE:HG22 | 3:C:888:LYS:HB3   | 1.73                     | 0.68              |
| 4:D:230:ALA:N    | 4:D:233:GLN:OE1   | 2.23                     | 0.68              |
| 3:C:507:TYR:OH   | 3:C:527:GLU:OE2   | 2.10                     | 0.68              |
| 3:C:910:THR:HG23 | 4:D:730:VAL:HG23  | 1.75                     | 0.68              |
| 4:D:647:GLU:HB2  | 4:D:655:TRP:CZ3   | 2.29                     | 0.68              |
| 2:B:3:ILE:HA     | 2:B:232:ILE:CB    | 2.24                     | 0.68              |
| 3:C:148:PHE:CE1  | 3:C:380:ILE:HD11  | 2.29                     | 0.68              |
| 3:C:754:LYS:H    | 3:C:754:LYS:CE    | 2.07                     | 0.68              |
| 5:E:35:PRO:HG2   | 5:E:40:LEU:HD11   | 1.76                     | 0.68              |
| 2:A:158:GLU:H    | 2:A:161:ARG:HH11  | 1.42                     | 0.68              |
| 4:D:708:VAL:O    | 4:D:712:VAL:HG23  | 1.93                     | 0.68              |
| 3:C:650:THR:HG22 | 3:C:660:SER:OG    | 1.93                     | 0.68              |
| 4:D:400:LYS:HE3  | 4:D:404:ASP:HB3   | 1.76                     | 0.68              |
| 4:D:931:ALA:HB1  | 4:D:932:ASN:HD22  | 1.59                     | 0.68              |
| 8:P:11:DA:H2''   | 8:P:12:DA:C5'     | 2.24                     | 0.68              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:1098:VAL:HG11 | 4:D:469:ILE:HD12  | 1.75                     | 0.67              |
| 4:D:73:ILE:O      | 4:D:82:VAL:HG12   | 1.94                     | 0.67              |
| 1:J:42:VAL:HG13   | 4:D:74:ILE:HD12   | 1.75                     | 0.67              |
| 3:C:191:HIS:HB2   | 3:C:336:LEU:HD21  | 1.76                     | 0.67              |
| 3:C:239:ILE:CG2   | 3:C:253:LEU:HD22  | 2.24                     | 0.67              |
| 3:C:851:GLU:O     | 3:C:852:LEU:HG    | 1.94                     | 0.67              |
| 6:F:330:ARG:NH2   | 6:F:336:GLU:OE2   | 2.25                     | 0.67              |
| 4:D:599:TYR:CB    | 4:D:610:GLY:HA3   | 2.25                     | 0.67              |
| 4:D:648:ALA:O     | 4:D:652:GLU:HB2   | 1.93                     | 0.67              |
| 3:C:613:GLU:O     | 3:C:705:ALA:HB1   | 1.94                     | 0.67              |
| 4:D:603:THR:CG2   | 4:D:604:LYS:HE2   | 2.23                     | 0.67              |
| 1:J:89:ARG:NH2    | 6:F:276:THR:HG23  | 2.09                     | 0.67              |
| 2:B:74:THR:HG21   | 4:D:611:VAL:HG11  | 1.74                     | 0.67              |
| 2:B:79:ASN:O      | 2:B:123:MET:HE3   | 1.95                     | 0.67              |
| 3:C:45:LEU:HD12   | 3:C:628:ASP:O     | 1.94                     | 0.67              |
| 1:J:64:LEU:HD22   | 1:J:66:GLU:H      | 1.58                     | 0.67              |
| 2:A:33:THR:HG21   | 2:B:37:SER:HA     | 1.76                     | 0.67              |
| 3:C:426:GLN:NE2   | 3:C:450:GLY:HA2   | 2.09                     | 0.67              |
| 3:C:1028:VAL:O    | 3:C:1032:ILE:HG22 | 1.94                     | 0.67              |
| 6:F:254:ALA:HA    | 10:F:502:SO4:O3   | 1.95                     | 0.67              |
| 4:D:588:LEU:HD22  | 4:D:668:GLY:HA3   | 1.77                     | 0.67              |
| 4:D:878:ASP:OD2   | 4:D:1250:LYS:NZ   | 2.28                     | 0.67              |
| 4:D:1165:ARG:CD   | 4:D:1209:MET:HE1  | 2.25                     | 0.67              |
| 6:F:253:MET:HE3   | 6:F:297:MET:CA    | 2.17                     | 0.67              |
| 7:O:27:DA:OP1     | 14:O:102:HOH:O    | 2.13                     | 0.67              |
| 3:C:467:HIS:CG    | 3:C:468:PRO:HD2   | 2.30                     | 0.67              |
| 3:C:250:MET:HA    | 3:C:253:LEU:CD2   | 2.25                     | 0.66              |
| 3:C:667:ALA:N     | 14:C:1301:HOH:O   | 2.03                     | 0.66              |
| 3:C:710:LEU:HD13  | 3:C:1021:ILE:HG12 | 1.76                     | 0.66              |
| 4:D:1168:ILE:O    | 4:D:1178:PRO:HA   | 1.95                     | 0.66              |
| 5:E:57:ARG:NE     | 5:E:95:GLU:OE1    | 2.23                     | 0.66              |
| 4:D:826:PRO:HD3   | 4:D:853:HIS:ND1   | 2.10                     | 0.66              |
| 2:B:79:ASN:OD1    | 4:D:636:ARG:NH2   | 2.24                     | 0.66              |
| 2:B:83:LEU:N      | 2:B:123:MET:HE1   | 2.08                     | 0.66              |
| 3:C:77:LEU:CD1    | 3:C:124:LEU:HD11  | 2.25                     | 0.66              |
| 3:C:533:ALA:HB2   | 3:C:567:VAL:HG11  | 1.77                     | 0.66              |
| 3:C:872:ASP:OD1   | 3:C:872:ASP:N     | 2.17                     | 0.66              |
| 4:D:647:GLU:HG2   | 4:D:648:ALA:N     | 2.11                     | 0.66              |
| 4:D:1174:THR:CG2  | 4:D:1176:PHE:HB2  | 2.25                     | 0.66              |
| 2:B:105:VAL:HB    | 2:B:125:ILE:HG23  | 1.78                     | 0.66              |
| 2:B:120:ASN:ND2   | 2:B:123:MET:SD    | 2.67                     | 0.66              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 4:D:578:ARG:HB2   | 11:D:2008:EDO:C2 | 2.26                     | 0.66              |
| 4:D:599:TYR:CZ    | 4:D:601:ALA:HB2  | 2.30                     | 0.66              |
| 4:D:1087:LEU:HD23 | 4:D:1113:MET:HE2 | 1.76                     | 0.66              |
| 2:B:32:TYR:CG     | 3:C:1005:ARG:HG3 | 2.29                     | 0.66              |
| 3:C:799:PRO:CA    | 3:C:823:VAL:HG12 | 2.21                     | 0.66              |
| 4:D:780:ALA:O     | 4:D:784:VAL:HG22 | 1.95                     | 0.66              |
| 2:B:32:TYR:CE1    | 2:B:178:VAL:HG21 | 2.30                     | 0.66              |
| 3:C:250:MET:O     | 3:C:253:LEU:HG   | 1.96                     | 0.66              |
| 4:D:706:ILE:HD12  | 5:E:36:PRO:HB3   | 1.76                     | 0.66              |
| 3:C:796:LYS:HB3   | 3:C:826:THR:O    | 1.95                     | 0.66              |
| 3:C:454:LEU:HD22  | 3:C:459:ALA:CB   | 2.24                     | 0.66              |
| 4:D:106:TYR:HB3   | 4:D:312:MET:CE   | 2.20                     | 0.66              |
| 4:D:1089:VAL:HG13 | 4:D:1098:GLY:C   | 2.21                     | 0.66              |
| 2:A:177:LYS:HE2   | 2:A:193:ILE:HD11 | 1.77                     | 0.66              |
| 2:B:43:LEU:HD12   | 2:B:171:VAL:HG23 | 1.78                     | 0.66              |
| 3:C:721:ASN:HD22  | 3:C:727:ILE:HD11 | 1.61                     | 0.66              |
| 4:D:889:ASP:OD2   | 4:D:891:GLU:N    | 2.29                     | 0.66              |
| 3:C:712:VAL:HB    | 3:C:906:ILE:HD11 | 1.76                     | 0.65              |
| 3:C:44:LEU:CD1    | 3:C:440:LEU:HD21 | 2.25                     | 0.65              |
| 3:C:1103:ILE:HD12 | 4:D:548:SER:HA   | 1.78                     | 0.65              |
| 4:D:59:GLU:OE2    | 4:D:66:LYS:NZ    | 2.29                     | 0.65              |
| 4:D:139:VAL:CG1   | 4:D:231:PRO:HD3  | 2.26                     | 0.65              |
| 3:C:508:ARG:CD    | 3:C:570:MET:HE2  | 2.26                     | 0.65              |
| 3:C:1059:PHE:CZ   | 3:C:1067:MET:HE3 | 2.31                     | 0.65              |
| 4:D:143:MET:HE3   | 4:D:251:TYR:CD1  | 2.31                     | 0.65              |
| 2:A:66:VAL:HB     | 2:A:69:VAL:HG21  | 1.77                     | 0.65              |
| 2:B:143:GLY:HA3   | 2:B:168:TYR:CD1  | 2.31                     | 0.65              |
| 4:D:881:GLN:HE22  | 4:D:1250:LYS:HE2 | 1.62                     | 0.65              |
| 4:D:1074:GLU:O    | 14:D:2102:HOH:O  | 2.12                     | 0.65              |
| 4:D:1079:ASP:N    | 4:D:1079:ASP:OD1 | 2.28                     | 0.65              |
| 2:A:177:LYS:HE2   | 2:A:193:ILE:CD1  | 2.26                     | 0.65              |
| 2:A:157:ALA:CB    | 2:A:161:ARG:HD2  | 2.25                     | 0.65              |
| 3:C:176:VAL:HG12  | 3:C:195:VAL:CG2  | 2.23                     | 0.65              |
| 4:D:642:PRO:CD    | 4:D:656:LYS:HG2  | 2.27                     | 0.65              |
| 4:D:218:ARG:O     | 4:D:222:ILE:HG13 | 1.96                     | 0.65              |
| 4:D:576:MET:HE2   | 4:D:693:ALA:HA   | 1.79                     | 0.65              |
| 4:D:924:LEU:HD21  | 4:D:943:LEU:HD11 | 1.78                     | 0.65              |
| 5:E:40:LEU:HB3    | 5:E:50:LEU:HD11  | 1.79                     | 0.65              |
| 2:A:89:ASP:CB     | 2:A:90:ASP:CA    | 2.75                     | 0.65              |
| 2:A:99:LYS:HE3    | 2:A:109:ASP:CG   | 2.21                     | 0.65              |
| 3:C:772:LEU:HA    | 3:C:775:LEU:HD22 | 1.79                     | 0.65              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:C:1062:MET:HE3 | 14:C:1308:HOH:O   | 1.94                     | 0.65              |
| 4:D:320:ILE:HG12 | 4:D:321:PRO:HD2   | 1.79                     | 0.65              |
| 3:C:52:PHE:HZ    | 3:C:150:MET:HE2   | 1.62                     | 0.64              |
| 4:D:980:ARG:HD3  | 4:D:985:GLY:O     | 1.98                     | 0.64              |
| 7:O:12:DG:N7     | 14:O:104:HOH:O    | 2.30                     | 0.64              |
| 2:A:33:THR:CG2   | 2:B:37:SER:HA     | 2.28                     | 0.64              |
| 3:C:338:ARG:HD3  | 3:C:343:GLN:NE2   | 2.11                     | 0.64              |
| 3:C:434:ASN:O    | 3:C:608:PRO:HD3   | 1.97                     | 0.64              |
| 3:C:480:PRO:O    | 3:C:485:ILE:HG12  | 1.97                     | 0.64              |
| 3:C:710:LEU:CD2  | 3:C:1021:ILE:HD11 | 2.23                     | 0.64              |
| 4:D:193:VAL:O    | 4:D:197:VAL:HG23  | 1.97                     | 0.64              |
| 3:C:236:ASN:OD1  | 3:C:253:LEU:HD13  | 1.97                     | 0.64              |
| 4:D:155:MET:HE1  | 4:D:219:LEU:CD2   | 2.27                     | 0.64              |
| 7:O:19:DA:H4'    | 7:O:20:DT:OP1     | 1.96                     | 0.64              |
| 3:C:1072:ALA:HB1 | 4:D:554:GLU:OE2   | 1.97                     | 0.64              |
| 4:D:661:TRP:HZ3  | 4:D:663:ALA:HB2   | 1.62                     | 0.64              |
| 4:D:956:ILE:HD12 | 4:D:956:ILE:O     | 1.98                     | 0.64              |
| 4:D:1171:SER:HA  | 4:D:1174:THR:HG22 | 1.78                     | 0.64              |
| 6:F:451:LYS:O    | 6:F:454:HIS:HB3   | 1.98                     | 0.64              |
| 2:A:95:MET:HE2   | 2:A:110:ILE:CG2   | 2.28                     | 0.64              |
| 3:C:531:VAL:HG13 | 3:C:552:VAL:HG23  | 1.80                     | 0.64              |
| 10:C:1203:SO4:O1 | 4:D:540:GLN:NE2   | 2.30                     | 0.64              |
| 4:D:363:PRO:HB2  | 4:D:365:ILE:CD1   | 2.27                     | 0.64              |
| 6:F:345:PRO:O    | 6:F:348:VAL:HG13  | 1.98                     | 0.64              |
| 3:C:215:VAL:HG12 | 3:C:217:ILE:HG23  | 1.80                     | 0.64              |
| 3:C:348:VAL:HB   | 3:C:351:GLY:CA    | 2.27                     | 0.64              |
| 3:C:771:VAL:HG23 | 3:C:772:LEU:CD1   | 2.27                     | 0.64              |
| 4:D:237:ASP:OD1  | 4:D:239:VAL:HG13  | 1.98                     | 0.64              |
| 4:D:438:LEU:HA   | 4:D:525:HIS:CD2   | 2.33                     | 0.64              |
| 4:D:614:SER:HB2  | 4:D:615:PRO:HD2   | 1.78                     | 0.64              |
| 4:D:627:LEU:HD13 | 4:D:667:LEU:HD12  | 1.80                     | 0.64              |
| 2:A:42:LEU:O     | 2:A:171:VAL:HG11  | 1.98                     | 0.64              |
| 2:B:198:THR:HG21 | 2:B:202:ILE:HD12  | 1.80                     | 0.64              |
| 3:C:510:VAL:HG12 | 3:C:568:ASP:C     | 2.23                     | 0.64              |
| 2:A:40:ARG:NH1   | 2:B:33:THR:HG22   | 2.13                     | 0.64              |
| 2:B:85:VAL:HG23  | 2:B:117:THR:C     | 2.23                     | 0.64              |
| 3:C:477:ILE:CD1  | 4:D:852:THR:HG21  | 2.28                     | 0.64              |
| 3:C:846:ARG:N    | 3:C:857:ASN:O     | 2.28                     | 0.64              |
| 2:B:30:PHE:HA    | 2:B:33:THR:CG2    | 2.28                     | 0.63              |
| 3:C:981:GLY:O    | 14:C:1303:HOH:O   | 2.15                     | 0.63              |
| 4:D:21:ARG:NE    | 4:D:96:GLU:OE2    | 2.26                     | 0.63              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 4:D:642:PRO:HG3   | 4:D:661:TRP:CD2  | 2.32                     | 0.63              |
| 4:D:846:LEU:O     | 4:D:850:ILE:HG12 | 1.98                     | 0.63              |
| 4:D:1071:ASP:HB2  | 4:D:1072:GLY:C   | 2.23                     | 0.63              |
| 3:C:729:SER:OG    | 3:C:905:ASP:HA   | 1.99                     | 0.63              |
| 4:D:6:PHE:CD1     | 4:D:1257:LYS:HE3 | 2.34                     | 0.63              |
| 6:F:338:ALA:HB1   | 6:F:343:ILE:O    | 1.98                     | 0.63              |
| 2:A:8:THR:OG1     | 2:A:24:GLU:O     | 2.12                     | 0.63              |
| 3:C:135:THR:HG23  | 3:C:137:GLU:H    | 1.64                     | 0.63              |
| 4:D:190:LYS:HE3   | 4:D:193:VAL:HG23 | 1.81                     | 0.63              |
| 8:P:11:DA:H4'     | 8:P:12:DA:OP1    | 1.98                     | 0.63              |
| 3:C:765:PRO:HD2   | 3:C:825:ASP:HB2  | 1.79                     | 0.63              |
| 6:F:462:ARG:NH1   | 6:F:465:LEU:HD12 | 2.14                     | 0.63              |
| 2:A:14:VAL:CG1    | 2:A:18:ARG:HG3   | 2.29                     | 0.63              |
| 5:E:29:PRO:HG2    | 5:E:34:ASN:HB2   | 1.80                     | 0.63              |
| 3:C:718:GLU:H     | 4:D:724:THR:CG2  | 2.11                     | 0.63              |
| 4:D:31:PRO:HB2    | 4:D:345:ARG:HG2  | 1.81                     | 0.63              |
| 1:J:96:GLU:O      | 1:J:100:GLU:HG3  | 1.99                     | 0.63              |
| 4:D:190:LYS:NZ    | 4:D:192:ASP:HB3  | 2.13                     | 0.63              |
| 2:A:40:ARG:NH2    | 3:C:894:ASP:OD2  | 2.32                     | 0.63              |
| 4:D:1119:PRO:HA   | 4:D:1122:VAL:CG1 | 2.28                     | 0.63              |
| 6:F:181:ALA:O     | 6:F:185:VAL:HG23 | 1.99                     | 0.63              |
| 2:B:95:MET:HG2    | 2:B:113:PRO:CD   | 2.29                     | 0.62              |
| 3:C:203:LEU:HD13  | 3:C:217:ILE:HG22 | 1.80                     | 0.62              |
| 3:C:876:LEU:HD13  | 3:C:886:ILE:HG13 | 1.81                     | 0.62              |
| 4:D:435:GLN:OE1   | 4:D:435:GLN:N    | 2.26                     | 0.62              |
| 2:B:50:ALA:HB3    | 2:B:168:TYR:HD2  | 1.63                     | 0.62              |
| 2:B:85:VAL:HG23   | 2:B:117:THR:O    | 1.98                     | 0.62              |
| 3:C:727:ILE:HG13  | 3:C:907:ILE:HB   | 1.79                     | 0.62              |
| 4:D:527:LEU:CD2   | 4:D:581:MET:HE1  | 2.20                     | 0.62              |
| 4:D:665:THR:HG22  | 4:D:684:ASN:ND2  | 2.15                     | 0.62              |
| 4:D:726:SER:OG    | 4:D:728:VAL:HG23 | 1.98                     | 0.62              |
| 4:D:1168:ILE:HD13 | 4:D:1176:PHE:CB  | 2.29                     | 0.62              |
| 4:D:1275:PRO:HG3  | 5:E:76:VAL:CG1   | 2.20                     | 0.62              |
| 2:A:95:MET:HE2    | 2:A:110:ILE:HG22 | 1.80                     | 0.62              |
| 2:A:158:GLU:H     | 2:A:161:ARG:NH1  | 1.97                     | 0.62              |
| 4:D:177:LEU:HD23  | 4:D:177:LEU:O    | 1.99                     | 0.62              |
| 4:D:594:GLY:HA2   | 4:D:598:GLU:OE1  | 1.99                     | 0.62              |
| 4:D:602:ALA:HB3   | 4:D:607:PRO:O    | 2.00                     | 0.62              |
| 4:D:846:LEU:H     | 4:D:846:LEU:HD12 | 1.62                     | 0.62              |
| 6:F:204:LEU:O     | 6:F:208:GLY:N    | 2.32                     | 0.62              |
| 1:J:89:ARG:NH2    | 6:F:274:ASP:OD1  | 2.21                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:A:177:LYS:HG2   | 2:A:193:ILE:HD11  | 1.82                     | 0.62              |
| 4:D:1100:LEU:HD23 | 4:D:1101:SER:N    | 2.13                     | 0.62              |
| 4:D:1188:GLU:O    | 4:D:1192:ARG:HG3  | 1.99                     | 0.62              |
| 2:A:3:ILE:O       | 2:A:3:ILE:HG13    | 1.98                     | 0.62              |
| 3:C:937:ILE:CB    | 3:C:939:VAL:HG12  | 2.28                     | 0.62              |
| 4:D:453:LYS:HB3   | 4:D:454:PRO:HD3   | 1.82                     | 0.62              |
| 2:A:82:GLY:CA     | 2:A:123:MET:HE1   | 2.29                     | 0.62              |
| 3:C:302:VAL:O     | 3:C:306:LYS:HG2   | 2.00                     | 0.62              |
| 3:C:732:LEU:HD22  | 3:C:737:VAL:HG11  | 1.82                     | 0.62              |
| 3:C:751:ARG:NH1   | 4:D:332:GLY:O     | 2.32                     | 0.62              |
| 4:D:1054:VAL:HG12 | 4:D:1104:ASP:O    | 2.00                     | 0.62              |
| 8:P:17:DT:O5'     | 9:T:290:GLY:HA3   | 1.99                     | 0.62              |
| 4:D:137:THR:HG22  | 4:D:253:THR:C     | 2.25                     | 0.62              |
| 4:D:275:GLU:HA    | 4:D:278:ARG:HB2   | 1.82                     | 0.62              |
| 2:A:113:PRO:HD2   | 2:A:116:VAL:HG21  | 1.82                     | 0.62              |
| 2:B:144:ARG:NH1   | 2:B:144:ARG:HB2   | 2.15                     | 0.62              |
| 3:C:38:PRO:HB3    | 3:C:508:ARG:HH21  | 1.63                     | 0.62              |
| 3:C:1045:GLN:HG3  | 3:C:1090:ARG:HH21 | 1.64                     | 0.61              |
| 1:J:47:ASP:OD1    | 1:J:47:ASP:N      | 2.19                     | 0.61              |
| 2:A:24:GLU:OE1    | 2:A:191:LYS:HD3   | 2.00                     | 0.61              |
| 2:A:36:ASN:HB2    | 2:A:176:TYR:OH    | 2.00                     | 0.61              |
| 2:B:21:PHE:HB2    | 2:B:194:ILE:CG2   | 2.29                     | 0.61              |
| 3:C:302:VAL:HG11  | 3:C:368:ARG:HD3   | 1.82                     | 0.61              |
| 3:C:363:HIS:NE2   | 3:C:528:ASP:OD2   | 2.32                     | 0.61              |
| 3:C:572:VAL:HG22  | 3:C:576:GLN:CD    | 2.25                     | 0.61              |
| 3:C:45:LEU:HD21   | 3:C:443:LYS:HD2   | 1.81                     | 0.61              |
| 3:C:221:ARG:O     | 3:C:223:GLN:NE2   | 2.29                     | 0.61              |
| 3:C:783:ILE:HG13  | 3:C:841:ILE:HD12  | 1.81                     | 0.61              |
| 4:D:436:LEU:O     | 4:D:716:LYS:NZ    | 2.32                     | 0.61              |
| 3:C:584:MET:HA    | 3:C:619:THR:CG2   | 2.27                     | 0.61              |
| 4:D:102:THR:HG23  | 4:D:258:ALA:HB2   | 1.82                     | 0.61              |
| 4:D:137:THR:HG22  | 4:D:253:THR:O     | 1.98                     | 0.61              |
| 3:C:1028:VAL:HG12 | 4:D:429:VAL:HG12  | 1.83                     | 0.61              |
| 6:F:324:LEU:HD22  | 6:F:332:PRO:HB3   | 1.82                     | 0.61              |
| 4:D:58:TRP:CD2    | 4:D:68:VAL:HG22   | 2.36                     | 0.61              |
| 4:D:920:PHE:CE2   | 4:D:948:ILE:HG13  | 2.34                     | 0.61              |
| 4:D:108:LYS:O     | 4:D:108:LYS:HG3   | 2.01                     | 0.61              |
| 2:B:212:GLY:O     | 2:B:216:VAL:HG12  | 2.00                     | 0.61              |
| 4:D:578:ARG:HB2   | 11:D:2008:EDO:H21 | 1.83                     | 0.61              |
| 6:F:176:VAL:HG12  | 6:F:177:ALA:N     | 2.15                     | 0.61              |
| 6:F:444:ILE:O     | 6:F:448:THR:HG23  | 2.01                     | 0.61              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 9:T:279:THR:HG23 | 9:T:282:ASP:CB    | 2.30                     | 0.61              |
| 6:F:321:GLN:O    | 6:F:325:LEU:HB2   | 2.00                     | 0.61              |
| 1:J:98:LEU:O     | 1:J:102:LEU:HD13  | 2.00                     | 0.60              |
| 3:C:148:PHE:HD2  | 3:C:150:MET:HE3   | 1.66                     | 0.60              |
| 3:C:421:PHE:O    | 3:C:425:SER:HB3   | 2.01                     | 0.60              |
| 3:C:805:LEU:HD12 | 3:C:809:GLU:CD    | 2.26                     | 0.60              |
| 3:C:876:LEU:HD11 | 3:C:886:ILE:CD1   | 2.31                     | 0.60              |
| 3:C:966:PRO:HG2  | 3:C:969:ASP:O     | 2.01                     | 0.60              |
| 4:D:745:LEU:O    | 4:D:749:GLU:HG2   | 2.00                     | 0.60              |
| 4:D:1171:SER:CB  | 4:D:1174:THR:HG22 | 2.31                     | 0.60              |
| 6:F:345:PRO:HA   | 6:F:348:VAL:CG1   | 2.31                     | 0.60              |
| 2:A:169:SER:OG   | 14:A:401:HOH:O    | 2.16                     | 0.60              |
| 3:C:299:LEU:C    | 3:C:299:LEU:HD12  | 2.26                     | 0.60              |
| 4:D:785:GLY:O    | 4:D:789:GLU:HG3   | 2.00                     | 0.60              |
| 1:J:74:LYS:HG3   | 1:J:74:LYS:O      | 2.01                     | 0.60              |
| 1:J:82:TRP:CE2   | 6:F:199:GLN:HG2   | 2.36                     | 0.60              |
| 2:A:40:ARG:HD3   | 2:B:33:THR:CG2    | 2.30                     | 0.60              |
| 3:C:394:ARG:HG3  | 3:C:398:GLN:HG3   | 1.83                     | 0.60              |
| 3:C:522:LEU:HB3  | 3:C:526:GLU:HG3   | 1.83                     | 0.60              |
| 3:C:795:GLY:HA2  | 3:C:827:SER:OG    | 2.01                     | 0.60              |
| 2:B:74:THR:CG2   | 4:D:611:VAL:HG11  | 2.31                     | 0.60              |
| 3:C:32:PHE:O     | 3:C:34:LYS:HD2    | 2.02                     | 0.60              |
| 3:C:742:HIS:HD2  | 3:C:868:ARG:HG3   | 1.64                     | 0.60              |
| 3:C:873:GLY:HA3  | 3:C:1028:VAL:HG11 | 1.82                     | 0.60              |
| 4:D:735:VAL:HG22 | 4:D:798:ILE:HD11  | 1.83                     | 0.60              |
| 5:E:85:GLN:H     | 5:E:85:GLN:NE2    | 1.96                     | 0.60              |
| 3:C:751:ARG:HG2  | 3:C:856:VAL:HG22  | 1.84                     | 0.60              |
| 3:C:895:MET:HG3  | 3:C:896:PRO:HD2   | 1.83                     | 0.60              |
| 4:D:673:ASN:HA   | 4:D:676:LEU:HD13  | 1.82                     | 0.60              |
| 6:F:272:LYS:HE3  | 7:O:25:DC:OP1     | 2.01                     | 0.60              |
| 2:A:100:GLN:OE1  | 2:A:101:GLY:N     | 2.30                     | 0.60              |
| 2:B:64:THR:C     | 2:B:65:THR:HG1    | 1.97                     | 0.60              |
| 3:C:1045:GLN:HG3 | 3:C:1090:ARG:NH2  | 2.15                     | 0.60              |
| 2:A:48:GLY:HA2   | 2:A:49:ALA:CB     | 2.32                     | 0.60              |
| 2:B:52:THR:OG1   | 2:B:141:GLU:HG2   | 2.02                     | 0.60              |
| 3:C:768:SER:O    | 3:C:771:VAL:HG22  | 2.02                     | 0.60              |
| 4:D:144:ARG:NH2  | 4:D:229:LEU:O     | 2.35                     | 0.60              |
| 2:A:210:SER:HB3  | 2:B:229:SER:HB2   | 1.83                     | 0.60              |
| 2:B:41:THR:O     | 2:B:45:SER:HB3    | 2.02                     | 0.60              |
| 3:C:712:VAL:HA   | 3:C:906:ILE:HG13  | 1.83                     | 0.60              |
| 3:C:1034:ALA:HB2 | 4:D:447:MET:HG3   | 1.84                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:647:GLU:HB2  | 4:D:655:TRP:CH2  | 2.37                     | 0.60              |
| 7:O:6:DA:C2'     | 7:O:7:DC:H5'     | 2.31                     | 0.60              |
| 3:C:203:LEU:HD22 | 3:C:217:ILE:HG22 | 1.84                     | 0.60              |
| 3:C:680:ILE:HD11 | 3:C:692:VAL:O    | 2.01                     | 0.60              |
| 3:C:32:PHE:HE1   | 3:C:963:VAL:CG1  | 2.15                     | 0.59              |
| 3:C:412:ARG:HD2  | 6:F:322:ARG:NE   | 2.16                     | 0.59              |
| 3:C:1026:HIS:HB3 | 3:C:1031:LYS:CE  | 2.30                     | 0.59              |
| 4:D:755:ILE:HD12 | 4:D:776:ILE:HD11 | 1.83                     | 0.59              |
| 6:F:176:VAL:HG12 | 6:F:177:ALA:H    | 1.65                     | 0.59              |
| 6:F:317:LEU:HD21 | 6:F:337:LEU:HG   | 1.84                     | 0.59              |
| 2:B:101:GLY:N    | 2:B:132:GLY:O    | 2.35                     | 0.59              |
| 2:B:198:THR:CG2  | 2:B:202:ILE:HD12 | 2.32                     | 0.59              |
| 3:C:335:TYR:CE1  | 3:C:356:VAL:HG13 | 2.37                     | 0.59              |
| 3:C:602:MET:HE1  | 3:C:883:LYS:CB   | 2.23                     | 0.59              |
| 3:C:876:LEU:CD1  | 3:C:886:ILE:HG13 | 2.32                     | 0.59              |
| 3:C:1116:LEU:O   | 3:C:1120:GLN:HG3 | 2.02                     | 0.59              |
| 2:A:30:PHE:CE1   | 2:B:40:ARG:HG3   | 2.37                     | 0.59              |
| 3:C:299:LEU:HD12 | 3:C:299:LEU:O    | 2.03                     | 0.59              |
| 3:C:649:ILE:HD13 | 3:C:693:ILE:HG22 | 1.84                     | 0.59              |
| 4:D:17:ALA:O     | 4:D:21:ARG:HG3   | 2.01                     | 0.59              |
| 4:D:901:ALA:HB1  | 4:D:910:ILE:O    | 2.02                     | 0.59              |
| 1:J:68:ASP:HA    | 1:J:69:VAL:CB    | 2.32                     | 0.59              |
| 4:D:275:GLU:O    | 4:D:278:ARG:N    | 2.35                     | 0.59              |
| 4:D:1041:PRO:HB3 | 4:D:1116:ALA:HB3 | 1.82                     | 0.59              |
| 4:D:661:TRP:CZ3  | 4:D:663:ALA:HB2  | 2.36                     | 0.59              |
| 5:E:80:VAL:HG12  | 5:E:81:GLU:N     | 2.17                     | 0.59              |
| 2:B:146:TYR:OH   | 14:B:401:HOH:O   | 2.14                     | 0.59              |
| 3:C:721:ASN:HD22 | 3:C:727:ILE:CD1  | 2.14                     | 0.59              |
| 4:D:240:LEU:HD23 | 4:D:244:LEU:HG   | 1.83                     | 0.59              |
| 3:C:523:THR:HG22 | 3:C:526:GLU:CD   | 2.28                     | 0.59              |
| 3:C:876:LEU:HD11 | 3:C:886:ILE:HD11 | 1.85                     | 0.59              |
| 4:D:924:LEU:HD22 | 4:D:959:VAL:CG1  | 2.33                     | 0.59              |
| 2:A:90:ASP:O     | 2:A:91:GLU:HG2   | 2.03                     | 0.59              |
| 3:C:176:VAL:HG22 | 3:C:307:VAL:HG12 | 1.85                     | 0.59              |
| 3:C:766:ASN:O    | 3:C:767:VAL:HG13 | 2.03                     | 0.59              |
| 3:C:171:VAL:N    | 3:C:368:ARG:O    | 2.35                     | 0.59              |
| 3:C:348:VAL:HG13 | 3:C:349:PRO:HD2  | 1.85                     | 0.59              |
| 3:C:578:VAL:HG12 | 3:C:579:SER:O    | 2.02                     | 0.59              |
| 3:C:745:GLU:OE2  | 3:C:861:ARG:HD2  | 2.03                     | 0.59              |
| 4:D:248:TYR:HA   | 4:D:251:TYR:CD2  | 2.38                     | 0.59              |
| 4:D:982:MET:CE   | 4:D:1153:LYS:HE3 | 2.33                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:F:289:ILE:O     | 6:F:293:ILE:HG13  | 2.02                     | 0.59              |
| 1:J:95:GLU:OE1    | 1:J:95:GLU:HA     | 2.03                     | 0.59              |
| 2:B:76:ILE:HA     | 2:B:79:ASN:HB2    | 1.85                     | 0.59              |
| 6:F:180:ASN:OD1   | 6:F:183:GLU:HG3   | 2.02                     | 0.59              |
| 2:A:197:GLU:OE1   | 3:C:987:ARG:NH1   | 2.35                     | 0.58              |
| 3:C:231:ALA:HB1   | 3:C:265:LEU:HD13  | 1.82                     | 0.58              |
| 3:C:509:LYS:HA    | 3:C:569:TYR:HA    | 1.84                     | 0.58              |
| 3:C:549:ARG:HA    | 3:C:563:SER:HA    | 1.85                     | 0.58              |
| 4:D:850:ILE:O     | 4:D:853:HIS:HB2   | 2.02                     | 0.58              |
| 4:D:957:THR:O     | 4:D:958:THR:HG23  | 2.03                     | 0.58              |
| 4:D:982:MET:HE2   | 4:D:1153:LYS:HE3  | 1.83                     | 0.58              |
| 1:J:44:PHE:HE2    | 4:D:76:GLU:HA     | 1.69                     | 0.58              |
| 2:B:84:VAL:HB     | 2:B:199:LYS:CD    | 2.30                     | 0.58              |
| 2:B:183:VAL:O     | 2:B:183:VAL:HG12  | 2.02                     | 0.58              |
| 3:C:1045:GLN:HG2  | 3:C:1087:THR:CG2  | 2.32                     | 0.58              |
| 6:F:462:ARG:HH12  | 6:F:465:LEU:HD12  | 1.68                     | 0.58              |
| 2:A:85:VAL:HG22   | 2:A:86:SER:H      | 1.68                     | 0.58              |
| 3:C:698:CYS:O     | 3:C:705:ALA:N     | 2.31                     | 0.58              |
| 3:C:792:ILE:HD12  | 3:C:792:ILE:H     | 1.67                     | 0.58              |
| 4:D:622:MET:HE3   | 4:D:667:LEU:CD1   | 2.28                     | 0.58              |
| 6:F:402:LEU:HD23  | 6:F:414:ARG:HE    | 1.67                     | 0.58              |
| 2:B:34:LEU:CD1    | 2:B:192:LEU:HD22  | 2.32                     | 0.58              |
| 2:B:39:ARG:NH2    | 4:D:623:ASP:OD2   | 2.36                     | 0.58              |
| 3:C:649:ILE:HG21  | 3:C:693:ILE:HG21  | 1.85                     | 0.58              |
| 3:C:710:LEU:HD13  | 3:C:1021:ILE:CG1  | 2.33                     | 0.58              |
| 4:D:6:PHE:HD1     | 4:D:1257:LYS:HE3  | 1.68                     | 0.58              |
| 3:C:221:ARG:HG3   | 3:C:222:ARG:HG3   | 1.86                     | 0.58              |
| 9:T:256:LEU:CD2   | 9:T:297:VAL:HG22  | 2.33                     | 0.58              |
| 2:B:200:ASN:H     | 2:B:200:ASN:ND2   | 2.02                     | 0.58              |
| 3:C:498:ASN:OD1   | 3:C:499:PRO:HD2   | 2.03                     | 0.58              |
| 3:C:910:THR:CG2   | 4:D:730:VAL:HG23  | 2.34                     | 0.58              |
| 3:C:998:LYS:NZ    | 4:D:734:ASP:OD2   | 2.32                     | 0.58              |
| 2:B:34:LEU:HD12   | 2:B:35:GLY:N      | 2.18                     | 0.58              |
| 2:B:180:ALA:HA    | 2:B:189:PHE:O     | 2.04                     | 0.58              |
| 3:C:714:ILE:O     | 3:C:714:ILE:HG22  | 2.02                     | 0.58              |
| 3:C:1029:ASP:OD1  | 4:D:520:LYS:HD2   | 2.04                     | 0.58              |
| 4:D:602:ALA:HB3   | 4:D:607:PRO:C     | 2.28                     | 0.58              |
| 4:D:622:MET:CE    | 4:D:629:VAL:HG22  | 2.23                     | 0.58              |
| 4:D:1009:LEU:HB3  | 4:D:1029:LEU:HD13 | 1.86                     | 0.58              |
| 4:D:1132:GLN:HE21 | 4:D:1163:LEU:HD12 | 1.69                     | 0.58              |
| 4:D:1249:LEU:HD12 | 4:D:1250:LYS:N    | 2.19                     | 0.58              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:C:166:VAL:HG11 | 3:C:372:VAL:HG23  | 1.86                     | 0.58              |
| 4:D:1036:PHE:HA  | 4:D:1162:MET:HE1  | 1.85                     | 0.58              |
| 1:J:89:ARG:HH22  | 6:F:274:ASP:CG    | 2.11                     | 0.58              |
| 2:A:93:VAL:HG22  | 2:A:113:PRO:HG3   | 1.86                     | 0.58              |
| 2:A:152:ASN:HA   | 2:A:155:SER:OG    | 2.03                     | 0.58              |
| 3:C:937:ILE:HA   | 3:C:938:ASP:CB    | 2.34                     | 0.58              |
| 2:A:170:PRO:HB3  | 2:A:202:ILE:HG12  | 1.84                     | 0.58              |
| 2:B:22:VAL:CG1   | 2:B:193:ILE:HD12  | 2.34                     | 0.58              |
| 3:C:727:ILE:CG1  | 3:C:907:ILE:HB    | 2.34                     | 0.58              |
| 4:D:262:LYS:HG3  | 4:D:310:MET:HE1   | 1.85                     | 0.58              |
| 2:B:151:GLN:CG   | 2:B:154:ALA:HB1   | 2.34                     | 0.57              |
| 3:C:132:ASN:CB   | 3:C:135:THR:HG22  | 2.33                     | 0.57              |
| 3:C:229:LEU:O    | 3:C:229:LEU:HD12  | 2.04                     | 0.57              |
| 3:C:530:HIS:HB3  | 3:C:568:ASP:CG    | 2.29                     | 0.57              |
| 4:D:273:GLU:O    | 4:D:277:LEU:HB2   | 2.04                     | 0.57              |
| 4:D:924:LEU:CD2  | 4:D:959:VAL:HG11  | 2.34                     | 0.57              |
| 1:J:45:ALA:HB2   | 4:D:73:ILE:HD12   | 1.85                     | 0.57              |
| 2:A:50:ALA:HB3   | 2:A:168:TYR:CD1   | 2.39                     | 0.57              |
| 4:D:155:MET:HE1  | 4:D:219:LEU:HB3   | 1.85                     | 0.57              |
| 4:D:1231:THR:O   | 4:D:1235:THR:HG23 | 2.03                     | 0.57              |
| 5:E:26:TYR:CE1   | 5:E:29:PRO:HD3    | 2.38                     | 0.57              |
| 2:A:2:LEU:HD12   | 2:B:143:GLY:HA2   | 1.85                     | 0.57              |
| 2:A:9:LEU:HD13   | 2:A:23:ILE:CG1    | 2.34                     | 0.57              |
| 2:A:199:LYS:O    | 2:A:200:ASN:HB2   | 2.03                     | 0.57              |
| 2:B:213:GLY:HA2  | 2:B:216:VAL:HG12  | 1.86                     | 0.57              |
| 3:C:338:ARG:HB3  | 3:C:343:GLN:HE21  | 1.70                     | 0.57              |
| 2:A:192:LEU:C    | 2:A:192:LEU:HD12  | 2.30                     | 0.57              |
| 2:B:210:SER:O    | 2:B:214:THR:HG23  | 2.05                     | 0.57              |
| 3:C:575:ARG:NH2  | 3:C:966:PRO:HB2   | 2.19                     | 0.57              |
| 4:D:603:THR:HG22 | 4:D:604:LYS:CE    | 2.30                     | 0.57              |
| 5:E:84:LEU:HB2   | 5:E:85:GLN:HE21   | 1.70                     | 0.57              |
| 8:P:3:DC:H2"     | 8:P:4:DA:C8       | 2.40                     | 0.57              |
| 2:B:167:ILE:HD11 | 4:D:617:GLU:HG3   | 1.85                     | 0.57              |
| 3:C:38:PRO:HB3   | 3:C:508:ARG:NH2   | 2.19                     | 0.57              |
| 3:C:476:PRO:O    | 4:D:856:ARG:NH2   | 2.35                     | 0.57              |
| 3:C:506:PRO:HB2  | 3:C:572:VAL:HG11  | 1.86                     | 0.57              |
| 2:A:112:PRO:HB2  | 2:A:116:VAL:HG23  | 1.86                     | 0.57              |
| 2:B:66:VAL:O     | 2:B:69:VAL:HG22   | 2.04                     | 0.57              |
| 2:B:105:VAL:HG23 | 2:B:128:LEU:CD1   | 2.34                     | 0.57              |
| 3:C:216:ARG:HG2  | 3:C:221:ARG:HA    | 1.85                     | 0.57              |
| 4:D:269:ASP:HB3  | 4:D:272:ALA:CB    | 2.33                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:F:293:ILE:O    | 6:F:297:MET:HG3  | 2.04                     | 0.57              |
| 2:A:14:VAL:HG13  | 2:A:15:ALA:H     | 1.68                     | 0.57              |
| 2:A:31:GLY:HA2   | 2:A:192:LEU:CD2  | 2.28                     | 0.57              |
| 3:C:21:ASN:O     | 3:C:22:SER:OG    | 2.21                     | 0.57              |
| 4:D:743:GLU:O    | 4:D:747:ARG:HG3  | 2.05                     | 0.57              |
| 5:E:76:VAL:HG13  | 5:E:77:GLY:N     | 2.19                     | 0.57              |
| 5:E:80:VAL:HG12  | 5:E:81:GLU:H     | 1.69                     | 0.57              |
| 6:F:324:LEU:HD23 | 6:F:328:LEU:CD1  | 2.30                     | 0.57              |
| 6:F:338:ALA:HB2  | 6:F:348:VAL:HG11 | 1.86                     | 0.57              |
| 7:O:11:DA:C2'    | 7:O:12:DG:H5''   | 2.35                     | 0.57              |
| 2:B:44:SER:HA    | 2:B:145:GLY:HA2  | 1.86                     | 0.57              |
| 3:C:224:PRO:HB2  | 3:C:227:VAL:HG13 | 1.87                     | 0.57              |
| 3:C:721:ASN:ND2  | 3:C:727:ILE:HD11 | 2.20                     | 0.57              |
| 4:D:460:LEU:HD11 | 4:D:472:ALA:HB1  | 1.87                     | 0.57              |
| 4:D:1128:PRO:HG3 | 4:D:1206:PRO:CB  | 2.35                     | 0.57              |
| 1:J:92:GLU:OE1   | 1:J:92:GLU:N     | 2.37                     | 0.56              |
| 3:C:203:LEU:HD22 | 3:C:217:ILE:CB   | 2.35                     | 0.56              |
| 3:C:338:ARG:CD   | 3:C:346:MET:HG3  | 2.31                     | 0.56              |
| 4:D:585:LEU:HD12 | 4:D:692:GLN:NE2  | 2.19                     | 0.56              |
| 2:A:106:THR:CA   | 2:A:125:ILE:HD13 | 2.34                     | 0.56              |
| 2:A:210:SER:CB   | 2:B:229:SER:HB2  | 2.35                     | 0.56              |
| 3:C:202:TRP:C    | 3:C:203:LEU:HD23 | 2.30                     | 0.56              |
| 3:C:540:ASP:O    | 3:C:543:GLY:N    | 2.32                     | 0.56              |
| 2:A:85:VAL:HG22  | 2:A:86:SER:N     | 2.19                     | 0.56              |
| 2:A:89:ASP:CB    | 2:A:142:ARG:HD2  | 2.35                     | 0.56              |
| 2:A:211:ALA:O    | 2:A:215:LEU:N    | 2.36                     | 0.56              |
| 2:B:76:ILE:HG23  | 2:B:125:ILE:CD1  | 2.35                     | 0.56              |
| 2:B:97:LEU:HB3   | 2:B:136:VAL:CG1  | 2.36                     | 0.56              |
| 3:C:763:ASP:CB   | 3:C:821:ARG:HH22 | 2.17                     | 0.56              |
| 3:C:885:VAL:CG1  | 4:D:538:GLY:HA2  | 2.35                     | 0.56              |
| 4:D:468:ASN:ND2  | 6:F:463:ASP:OD2  | 2.33                     | 0.56              |
| 4:D:607:PRO:O    | 4:D:609:GLN:HG2  | 2.04                     | 0.56              |
| 4:D:641:ARG:NE   | 4:D:655:TRP:HZ2  | 2.04                     | 0.56              |
| 4:D:901:ALA:HB2  | 4:D:911:ARG:CA   | 2.35                     | 0.56              |
| 4:D:1087:LEU:CD2 | 4:D:1113:MET:HE2 | 2.36                     | 0.56              |
| 4:D:1088:ARG:HG2 | 4:D:1089:VAL:N   | 2.17                     | 0.56              |
| 5:E:81:GLU:OE1   | 5:E:81:GLU:HA    | 2.06                     | 0.56              |
| 4:D:76:GLU:CD    | 4:D:76:GLU:H     | 2.12                     | 0.56              |
| 6:F:364:THR:O    | 6:F:364:THR:HG23 | 2.05                     | 0.56              |
| 2:A:9:LEU:HD23   | 2:B:221:LEU:O    | 2.05                     | 0.56              |
| 2:A:207:ALA:O    | 2:A:210:SER:OG   | 2.10                     | 0.56              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:C:510:VAL:HG11 | 3:C:567:VAL:HB    | 1.87                     | 0.56              |
| 4:D:203:ARG:NE   | 4:D:203:ARG:HA    | 2.20                     | 0.56              |
| 2:A:43:LEU:HD11  | 2:A:174:VAL:HB    | 1.88                     | 0.56              |
| 3:C:431:MET:O    | 3:C:670:ASN:ND2   | 2.38                     | 0.56              |
| 3:C:939:VAL:HG23 | 3:C:940:ALA:HA    | 1.86                     | 0.56              |
| 4:D:354:LEU:O    | 4:D:358:ILE:HG12  | 2.06                     | 0.56              |
| 4:D:930:ASP:HB3  | 4:D:954:ALA:HB1   | 1.87                     | 0.56              |
| 4:D:1062:PHE:CD2 | 4:D:1080:LYS:HD2  | 2.41                     | 0.56              |
| 4:D:1275:PRO:CG  | 5:E:76:VAL:HG11   | 2.24                     | 0.56              |
| 6:F:449:MET:O    | 6:F:453:ARG:HG3   | 2.06                     | 0.56              |
| 2:A:197:GLU:OE1  | 3:C:987:ARG:NH2   | 2.39                     | 0.56              |
| 3:C:736:ASP:OD1  | 3:C:869:LYS:HE2   | 2.06                     | 0.56              |
| 4:D:890:CYS:SG   | 4:D:892:THR:HG22  | 2.45                     | 0.56              |
| 4:D:1171:SER:C   | 4:D:1174:THR:HG22 | 2.30                     | 0.56              |
| 4:D:622:MET:HE2  | 4:D:629:VAL:CG2   | 2.24                     | 0.56              |
| 4:D:631:ALA:O    | 4:D:666:THR:HA    | 2.05                     | 0.56              |
| 4:D:937:ILE:CD1  | 4:D:951:LEU:HG    | 2.33                     | 0.56              |
| 3:C:641:ILE:HG21 | 3:C:644:VAL:HG13  | 1.87                     | 0.56              |
| 4:D:706:ILE:HD11 | 5:E:36:PRO:HA     | 1.87                     | 0.56              |
| 4:D:753:ASP:O    | 4:D:757:ARG:N     | 2.38                     | 0.56              |
| 4:D:932:ASN:N    | 4:D:933:GLY:HA2   | 2.21                     | 0.56              |
| 6:F:360:SER:HB3  | 6:F:363:GLN:HG3   | 1.87                     | 0.56              |
| 3:C:380:ILE:HG12 | 3:C:418:ILE:HD11  | 1.87                     | 0.56              |
| 3:C:717:TRP:HH2  | 3:C:1005:ARG:NH2  | 2.04                     | 0.56              |
| 3:C:984:LEU:HD13 | 3:C:989:GLY:O     | 2.06                     | 0.56              |
| 3:C:988:ASP:OD1  | 3:C:988:ASP:N     | 2.38                     | 0.56              |
| 3:C:534:GLN:NE2  | 4:D:846:LEU:HD11  | 2.20                     | 0.55              |
| 3:C:556:GLY:N    | 3:C:557:GLY:HA2   | 2.21                     | 0.55              |
| 4:D:653:ASN:HB2  | 4:D:654:GLY:CA    | 2.35                     | 0.55              |
| 4:D:687:MET:HE2  | 4:D:695:ILE:CD1   | 2.36                     | 0.55              |
| 6:F:465:LEU:HD23 | 6:F:466:ASP:N     | 2.21                     | 0.55              |
| 2:A:99:LYS:HE3   | 2:A:109:ASP:OD1   | 2.06                     | 0.55              |
| 2:B:177:LYS:HG3  | 2:B:193:ILE:HB    | 1.89                     | 0.55              |
| 4:D:170:LEU:HD13 | 4:D:209:ARG:NH2   | 2.21                     | 0.55              |
| 4:D:1121:GLU:OE2 | 4:D:1124:ARG:NH2  | 2.31                     | 0.55              |
| 4:D:1168:ILE:CD1 | 4:D:1176:PHE:HB3  | 2.36                     | 0.55              |
| 2:A:82:GLY:HA3   | 2:A:123:MET:CE    | 2.37                     | 0.55              |
| 3:C:269:TYR:CE2  | 3:C:278:PRO:HB3   | 2.40                     | 0.55              |
| 3:C:549:ARG:HB2  | 3:C:561:PHE:CE2   | 2.41                     | 0.55              |
| 3:C:808:GLU:O    | 3:C:812:LEU:HD13  | 2.07                     | 0.55              |
| 4:D:183:GLU:O    | 4:D:187:GLU:HG2   | 2.07                     | 0.55              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:C:62:ARG:O     | 3:C:66:ILE:HG13   | 2.06                     | 0.55              |
| 3:C:921:GLN:HB2  | 3:C:1019:MET:HE3  | 1.88                     | 0.55              |
| 7:O:28:DT:H2''   | 7:O:29:DA:C5'     | 2.33                     | 0.55              |
| 2:A:40:ARG:HD3   | 2:B:33:THR:CB     | 2.37                     | 0.55              |
| 2:B:50:ALA:HB3   | 2:B:168:TYR:CD2   | 2.42                     | 0.55              |
| 3:C:132:ASN:CG   | 3:C:135:THR:HG22  | 2.32                     | 0.55              |
| 3:C:891:PRO:HB2  | 3:C:893:GLU:CG    | 2.35                     | 0.55              |
| 3:C:892:VAL:CG2  | 3:C:903:PRO:HG2   | 2.37                     | 0.55              |
| 3:C:973:GLU:OE1  | 4:D:840:ARG:NH2   | 2.40                     | 0.55              |
| 3:C:986:ASN:OD1  | 3:C:986:ASN:N     | 2.34                     | 0.55              |
| 4:D:39:LEU:HD13  | 4:D:335:PHE:HZ    | 1.71                     | 0.55              |
| 4:D:334:ARG:HD3  | 6:F:356:ARG:HH21  | 1.71                     | 0.55              |
| 4:D:641:ARG:CZ   | 4:D:655:TRP:HZ2   | 2.19                     | 0.55              |
| 4:D:901:ALA:HB2  | 4:D:912:ASP:N     | 2.22                     | 0.55              |
| 2:B:162:ILE:HG23 | 4:D:607:PRO:HG2   | 1.88                     | 0.55              |
| 3:C:346:MET:HB2  | 3:C:356:VAL:HG21  | 1.88                     | 0.55              |
| 3:C:937:ILE:CA   | 3:C:938:ASP:CB    | 2.85                     | 0.55              |
| 4:D:676:LEU:HD12 | 4:D:676:LEU:N     | 2.22                     | 0.55              |
| 4:D:781:THR:HG22 | 4:D:814:ARG:HD2   | 1.89                     | 0.55              |
| 4:D:1229:GLU:O   | 4:D:1233:VAL:HG23 | 2.05                     | 0.55              |
| 6:F:219:MET:HE2  | 6:F:219:MET:CA    | 2.33                     | 0.55              |
| 2:A:192:LEU:HD12 | 2:A:192:LEU:O     | 2.06                     | 0.55              |
| 3:C:268:ILE:O    | 3:C:272:LEU:HD13  | 2.06                     | 0.55              |
| 3:C:578:VAL:HG13 | 3:C:582:THR:CB    | 2.36                     | 0.55              |
| 3:C:771:VAL:HG23 | 3:C:772:LEU:HD12  | 1.87                     | 0.55              |
| 4:D:143:MET:CE   | 4:D:251:TYR:HA    | 2.36                     | 0.55              |
| 4:D:962:ARG:HB3  | 4:D:977:CYS:HA    | 1.88                     | 0.55              |
| 2:A:48:GLY:HA3   | 2:A:168:TYR:HB3   | 1.89                     | 0.55              |
| 3:C:202:TRP:H    | 3:C:202:TRP:CD1   | 2.25                     | 0.55              |
| 3:C:712:VAL:HG11 | 3:C:925:THR:HG23  | 1.89                     | 0.55              |
| 3:C:680:ILE:HG12 | 3:C:693:ILE:O     | 2.07                     | 0.55              |
| 3:C:935:TRP:HB2  | 3:C:982:SER:CB    | 2.37                     | 0.55              |
| 4:D:706:ILE:O    | 4:D:710:GLN:HG3   | 2.07                     | 0.55              |
| 7:O:15:DT:H2''   | 7:O:16:DT:OP2     | 2.07                     | 0.55              |
| 1:J:40:PHE:CZ    | 1:J:58:ASN:HB2    | 2.42                     | 0.55              |
| 4:D:1037:GLU:HG2 | 4:D:1039:ARG:NH1  | 2.22                     | 0.55              |
| 6:F:394:LEU:HB2  | 6:F:464:TYR:CD1   | 2.42                     | 0.55              |
| 2:B:213:GLY:HA2  | 2:B:216:VAL:CG1   | 2.38                     | 0.54              |
| 3:C:635:ALA:CB   | 3:C:693:ILE:HD11  | 2.28                     | 0.54              |
| 5:E:29:PRO:HB2   | 5:E:33:THR:HG23   | 1.88                     | 0.54              |
| 6:F:272:LYS:HE3  | 7:O:25:DC:P       | 2.47                     | 0.54              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 6:F:291:GLN:HG3   | 6:F:292:ALA:N    | 2.21                     | 0.54              |
| 3:C:839:ILE:HG22  | 3:C:840:GLY:N    | 2.21                     | 0.54              |
| 3:C:984:LEU:HB2   | 3:C:985:PRO:CA   | 2.36                     | 0.54              |
| 4:D:951:LEU:CB    | 4:D:956:ILE:HD11 | 2.31                     | 0.54              |
| 4:D:1276:THR:HG22 | 5:E:102:GLU:CG   | 2.37                     | 0.54              |
| 9:T:251:ILE:HG21  | 9:T:270:HIS:O    | 2.06                     | 0.54              |
| 2:A:50:ALA:HB3    | 2:A:168:TYR:CE1  | 2.43                     | 0.54              |
| 4:D:131:PHE:HA    | 4:D:256:MET:HE2  | 1.89                     | 0.54              |
| 4:D:901:ALA:N     | 4:D:912:ASP:HB2  | 2.20                     | 0.54              |
| 6:F:254:ALA:HB3   | 6:F:257:ASP:OD2  | 2.08                     | 0.54              |
| 1:J:82:TRP:CZ2    | 6:F:199:GLN:HG2  | 2.42                     | 0.54              |
| 2:A:106:THR:C     | 2:A:125:ILE:HD13 | 2.32                     | 0.54              |
| 2:B:97:LEU:HB3    | 2:B:136:VAL:HG13 | 1.90                     | 0.54              |
| 2:B:99:LYS:O      | 2:B:133:LYS:HG3  | 2.07                     | 0.54              |
| 3:C:215:VAL:CG2   | 3:C:225:VAL:HA   | 2.27                     | 0.54              |
| 3:C:729:SER:OG    | 3:C:904:VAL:O    | 2.25                     | 0.54              |
| 4:D:988:VAL:HG23  | 4:D:992:GLU:HG3  | 1.88                     | 0.54              |
| 4:D:1056:LEU:HD21 | 4:D:1063:PHE:HD1 | 1.72                     | 0.54              |
| 6:F:438:ARG:NH1   | 8:P:20:DG:N7     | 2.54                     | 0.54              |
| 1:J:64:LEU:HD22   | 1:J:66:GLU:HB2   | 1.89                     | 0.54              |
| 3:C:876:LEU:N     | 3:C:876:LEU:HD12 | 2.23                     | 0.54              |
| 4:D:885:VAL:O     | 4:D:990:ILE:O    | 2.25                     | 0.54              |
| 4:D:1071:ASP:N    | 4:D:1072:GLY:HA2 | 2.22                     | 0.54              |
| 3:C:193:VAL:HG12  | 3:C:205:PHE:HB2  | 1.89                     | 0.54              |
| 2:A:33:THR:HG22   | 2:B:37:SER:OG    | 2.08                     | 0.54              |
| 2:A:129:ASN:H     | 2:A:129:ASN:HD22 | 1.55                     | 0.54              |
| 2:B:143:GLY:HA3   | 2:B:168:TYR:CE1  | 2.43                     | 0.54              |
| 2:B:144:ARG:HB2   | 2:B:144:ARG:HH11 | 1.73                     | 0.54              |
| 3:C:45:LEU:HD21   | 3:C:443:LYS:CD   | 2.38                     | 0.54              |
| 3:C:275:GLY:O     | 6:F:171:LYS:HD2  | 2.07                     | 0.54              |
| 3:C:852:LEU:CD2   | 3:C:856:VAL:HG12 | 2.37                     | 0.54              |
| 4:D:706:ILE:CD1   | 5:E:36:PRO:HB3   | 2.37                     | 0.54              |
| 6:F:335:GLU:OE1   | 6:F:335:GLU:N    | 2.39                     | 0.54              |
| 9:T:251:ILE:O     | 9:T:254:LEU:HG   | 2.07                     | 0.54              |
| 3:C:368:ARG:HA    | 3:C:369:LEU:CB   | 2.38                     | 0.54              |
| 3:C:369:LEU:HB3   | 3:C:501:GLY:O    | 2.07                     | 0.54              |
| 3:C:723:GLU:O     | 3:C:724:ASP:HB2  | 2.08                     | 0.54              |
| 3:C:141:GLN:OE1   | 3:C:404:THR:OG1  | 2.26                     | 0.54              |
| 3:C:568:ASP:OD1   | 3:C:568:ASP:N    | 2.41                     | 0.54              |
| 3:C:967:VAL:HG23  | 3:C:968:PHE:H    | 1.72                     | 0.54              |
| 4:D:248:TYR:HA    | 4:D:251:TYR:HD2  | 1.73                     | 0.54              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:D:460:LEU:HD11 | 4:D:472:ALA:CB    | 2.38                     | 0.54              |
| 4:D:577:PRO:HB3  | 4:D:581:MET:HE2   | 1.90                     | 0.54              |
| 4:D:936:ILE:CG2  | 4:D:951:LEU:HD23  | 2.37                     | 0.54              |
| 2:A:66:VAL:HB    | 2:A:69:VAL:CG2    | 2.38                     | 0.54              |
| 2:B:24:GLU:HG3   | 2:B:191:LYS:HG3   | 1.88                     | 0.54              |
| 3:C:393:GLU:OE2  | 6:F:247:ARG:HD3   | 2.08                     | 0.54              |
| 3:C:479:THR:OG1  | 3:C:480:PRO:HD2   | 2.08                     | 0.54              |
| 3:C:1132:ASP:HB3 | 3:C:1133:GLY:CA   | 2.32                     | 0.54              |
| 4:D:368:ASN:ND2  | 14:D:2111:HOH:O   | 2.41                     | 0.54              |
| 7:O:6:DA:H1'     | 7:O:7:DC:H5'      | 1.90                     | 0.54              |
| 3:C:917:MET:HE2  | 4:D:839:PHE:CD2   | 2.43                     | 0.53              |
| 4:D:363:PRO:HB2  | 4:D:365:ILE:HD12  | 1.90                     | 0.53              |
| 6:F:194:GLY:HA2  | 6:F:222:ILE:HG22  | 1.91                     | 0.53              |
| 3:C:874:ASP:OD1  | 3:C:1028:VAL:HG22 | 2.07                     | 0.53              |
| 4:D:270:ILE:O    | 4:D:274:ALA:N     | 2.39                     | 0.53              |
| 5:E:62:ASN:O     | 5:E:66:ASN:ND2    | 2.41                     | 0.53              |
| 6:F:215:GLN:O    | 6:F:219:MET:HG2   | 2.08                     | 0.53              |
| 6:F:309:HIS:O    | 6:F:313:VAL:HG12  | 2.07                     | 0.53              |
| 4:D:129:ILE:HD11 | 4:D:130:TYR:CZ    | 2.42                     | 0.53              |
| 4:D:443:LEU:HD22 | 4:D:514:PRO:HB3   | 1.91                     | 0.53              |
| 2:A:21:PHE:HB2   | 2:A:194:ILE:HG12  | 1.89                     | 0.53              |
| 2:B:216:VAL:HG13 | 2:B:217:GLU:N     | 2.23                     | 0.53              |
| 3:C:338:ARG:HD3  | 3:C:343:GLN:HE22  | 1.73                     | 0.53              |
| 4:D:231:PRO:O    | 4:D:232:LYS:HB2   | 2.07                     | 0.53              |
| 4:D:285:LYS:HA   | 4:D:289:LYS:HD2   | 1.91                     | 0.53              |
| 4:D:1034:GLU:OE2 | 4:D:1042:ARG:HG2  | 2.09                     | 0.53              |
| 2:A:8:THR:O      | 2:A:23:ILE:HA     | 2.09                     | 0.53              |
| 2:A:36:ASN:CB    | 3:C:1007:GLY:HA3  | 2.39                     | 0.53              |
| 2:A:181:THR:H    | 2:A:189:PHE:C     | 2.13                     | 0.53              |
| 6:F:304:ILE:HB   | 14:F:604:HOH:O    | 2.07                     | 0.53              |
| 2:A:56:ILE:HG12  | 2:A:136:VAL:HB    | 1.91                     | 0.53              |
| 3:C:51:SER:OG    | 3:C:371:THR:HG23  | 2.09                     | 0.53              |
| 3:C:338:ARG:HB3  | 3:C:343:GLN:NE2   | 2.23                     | 0.53              |
| 3:C:590:HIS:O    | 3:C:919:ILE:HD11  | 2.09                     | 0.53              |
| 6:F:219:MET:HA   | 6:F:219:MET:CE    | 2.32                     | 0.53              |
| 2:B:60:LEU:HD22  | 2:B:60:LEU:N      | 2.24                     | 0.53              |
| 3:C:624:ARG:NH1  | 3:C:628:ASP:OD2   | 2.41                     | 0.53              |
| 3:C:939:VAL:HG22 | 3:C:940:ALA:HA    | 1.90                     | 0.53              |
| 4:D:12:ILE:HG12  | 4:D:1221:TRP:CZ2  | 2.44                     | 0.53              |
| 6:F:164:ASP:OD1  | 6:F:166:VAL:N     | 2.41                     | 0.53              |
| 3:C:822:GLU:HG2  | 3:C:823:VAL:HG22  | 1.91                     | 0.53              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:D:844:THR:H    | 4:D:847:GLU:HB2   | 1.73                     | 0.53              |
| 4:D:848:TYR:O    | 4:D:852:THR:HG23  | 2.09                     | 0.53              |
| 4:D:872:LEU:HG   | 4:D:876:LEU:CD2   | 2.39                     | 0.53              |
| 4:D:992:GLU:OE1  | 5:E:48:TYR:OH     | 2.27                     | 0.53              |
| 2:B:205:ARG:CZ   | 2:B:205:ARG:HB2   | 2.38                     | 0.53              |
| 3:C:76:GLY:O     | 3:C:80:VAL:HG23   | 2.08                     | 0.53              |
| 3:C:538:PRO:HB2  | 3:C:546:THR:OG1   | 2.09                     | 0.53              |
| 4:D:602:ALA:HB1  | 4:D:606:ALA:HB3   | 1.90                     | 0.53              |
| 6:F:465:LEU:HD23 | 6:F:465:LEU:C     | 2.34                     | 0.53              |
| 9:T:260:SER:O    | 9:T:264:LEU:HG    | 2.08                     | 0.53              |
| 2:B:198:THR:HG22 | 2:B:199:LYS:O     | 2.08                     | 0.53              |
| 3:C:41:VAL:HG13  | 3:C:493:VAL:HG12  | 1.91                     | 0.53              |
| 3:C:176:VAL:HG13 | 3:C:307:VAL:HG11  | 1.90                     | 0.53              |
| 3:C:444:ARG:NH2  | 3:C:491:LEU:HD23  | 2.08                     | 0.53              |
| 3:C:478:GLU:OE1  | 3:C:579:SER:OG    | 2.20                     | 0.53              |
| 3:C:505:THR:CG2  | 3:C:506:PRO:HD2   | 2.39                     | 0.53              |
| 3:C:1003:ASP:HB2 | 3:C:1010:PHE:CZ   | 2.44                     | 0.53              |
| 4:D:190:LYS:HZ2  | 4:D:192:ASP:HB3   | 1.73                     | 0.53              |
| 4:D:579:LEU:HG   | 11:D:2008:EDO:H22 | 1.90                     | 0.53              |
| 4:D:1123:LEU:HA  | 4:D:1131:VAL:CG2  | 2.39                     | 0.53              |
| 2:A:138:LEU:HD12 | 2:A:138:LEU:N     | 2.24                     | 0.52              |
| 3:C:712:VAL:CG1  | 3:C:925:THR:HG23  | 2.39                     | 0.52              |
| 3:C:1039:PRO:HB2 | 3:C:1048:LEU:HD21 | 1.90                     | 0.52              |
| 3:C:1069:ALA:HB3 | 4:D:506:ARG:HB3   | 1.91                     | 0.52              |
| 3:C:1117:LYS:HD2 | 3:C:1120:GLN:NE2  | 2.24                     | 0.52              |
| 5:E:98:GLY:O     | 5:E:100:LEU:HD12  | 2.09                     | 0.52              |
| 3:C:368:ARG:HB3  | 3:C:501:GLY:O     | 2.09                     | 0.52              |
| 3:C:777:GLU:CD   | 3:C:777:GLU:H     | 2.15                     | 0.52              |
| 4:D:85:ALA:N     | 14:D:2108:HOH:O   | 2.41                     | 0.52              |
| 3:C:106:VAL:HG11 | 3:C:120:TYR:CE1   | 2.44                     | 0.52              |
| 3:C:228:LEU:HD21 | 3:C:268:ILE:CG1   | 2.22                     | 0.52              |
| 3:C:948:SER:C    | 3:C:950:LEU:CB    | 2.83                     | 0.52              |
| 3:C:1084:SER:HB2 | 4:D:421:ARG:O     | 2.09                     | 0.52              |
| 4:D:744:ILE:O    | 4:D:748:HIS:HD2   | 1.93                     | 0.52              |
| 3:C:132:ASN:HB3  | 3:C:135:THR:CG2   | 2.38                     | 0.52              |
| 3:C:171:VAL:HG12 | 3:C:172:ARG:N     | 2.24                     | 0.52              |
| 3:C:493:VAL:HG12 | 3:C:494:TYR:CD1   | 2.44                     | 0.52              |
| 3:C:573:SER:HB2  | 3:C:574:PRO:HD2   | 1.92                     | 0.52              |
| 2:A:11:GLU:CD    | 2:A:205:ARG:HG2   | 2.35                     | 0.52              |
| 2:A:111:VAL:O    | 2:A:111:VAL:HG22  | 2.08                     | 0.52              |
| 3:C:549:ARG:HD3  | 3:C:561:PHE:CE2   | 2.44                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:852:LEU:HD22  | 3:C:856:VAL:HG12  | 1.90                     | 0.52              |
| 4:D:1054:VAL:HG11 | 4:D:1100:LEU:HD21 | 1.92                     | 0.52              |
| 5:E:56:LYS:HA     | 5:E:59:ARG:HG3    | 1.91                     | 0.52              |
| 2:A:113:PRO:HD2   | 2:A:116:VAL:CG2   | 2.39                     | 0.52              |
| 3:C:102:ARG:O     | 3:C:124:LEU:HD23  | 2.09                     | 0.52              |
| 3:C:921:GLN:HB2   | 3:C:1019:MET:CE   | 2.39                     | 0.52              |
| 4:D:1174:THR:CA   | 4:D:1175:GLU:CB   | 2.87                     | 0.52              |
| 6:F:462:ARG:NH1   | 6:F:465:LEU:HB2   | 2.24                     | 0.52              |
| 3:C:1084:SER:OG   | 3:C:1085:ASP:N    | 2.40                     | 0.52              |
| 3:C:1126:VAL:HG12 | 4:D:12:ILE:HG23   | 1.91                     | 0.52              |
| 4:D:932:ASN:N     | 4:D:933:GLY:CA    | 2.73                     | 0.52              |
| 3:C:29:ARG:CD     | 3:C:964:ALA:HB2   | 2.39                     | 0.52              |
| 3:C:33:ALA:HB2    | 3:C:966:PRO:HG3   | 1.90                     | 0.52              |
| 3:C:584:MET:CA    | 3:C:619:THR:HG21  | 2.35                     | 0.52              |
| 4:D:103:HIS:CE1   | 4:D:105:TRP:HB2   | 2.45                     | 0.52              |
| 4:D:362:ALA:HB3   | 4:D:367:VAL:HG23  | 1.91                     | 0.52              |
| 4:D:767:THR:O     | 4:D:771:GLU:HB2   | 2.10                     | 0.52              |
| 4:D:815:THR:HG22  | 4:D:820:LYS:CA    | 2.33                     | 0.52              |
| 8:P:17:DT:P       | 9:T:290:GLY:HA3   | 2.49                     | 0.52              |
| 4:D:1132:GLN:CG   | 4:D:1163:LEU:HD12 | 2.40                     | 0.52              |
| 2:A:78:LEU:O      | 2:A:81:LYS:HB2    | 2.10                     | 0.52              |
| 2:B:183:VAL:O     | 2:B:184:GLU:CB    | 2.58                     | 0.52              |
| 3:C:516:THR:HG21  | 3:C:518:GLN:HB2   | 1.91                     | 0.52              |
| 3:C:614:ALA:HB1   | 3:C:615:PRO:HD2   | 1.90                     | 0.52              |
| 4:D:54:PRO:HG3    | 4:D:81:GLU:O      | 2.10                     | 0.52              |
| 4:D:365:ILE:HD13  | 6:F:235:GLU:HG2   | 1.92                     | 0.52              |
| 3:C:174:PRO:HD2   | 3:C:302:VAL:HB    | 1.91                     | 0.51              |
| 4:D:1088:ARG:HD2  | 4:D:1111:GLN:HB3  | 1.92                     | 0.51              |
| 3:C:329:VAL:O     | 3:C:332:THR:OG1   | 2.27                     | 0.51              |
| 4:D:85:ALA:O      | 4:D:88:ARG:HB2    | 2.11                     | 0.51              |
| 4:D:872:LEU:HG    | 4:D:876:LEU:HD22  | 1.91                     | 0.51              |
| 4:D:878:ASP:OD1   | 14:D:2103:HOH:O   | 2.19                     | 0.51              |
| 4:D:1034:GLU:OE2  | 4:D:1042:ARG:N    | 2.43                     | 0.51              |
| 4:D:1165:ARG:NE   | 4:D:1209:MET:HE1  | 2.25                     | 0.51              |
| 1:J:102:LEU:HA    | 1:J:105:ILE:HG22  | 1.92                     | 0.51              |
| 2:A:70:LYS:HB3    | 2:A:71:GLU:OE1    | 2.11                     | 0.51              |
| 3:C:894:ASP:HA    | 3:C:1004:GLY:HA3  | 1.92                     | 0.51              |
| 4:D:243:GLU:O     | 4:D:247:ARG:HG3   | 2.11                     | 0.51              |
| 4:D:363:PRO:HG2   | 4:D:366:ILE:HD12  | 1.92                     | 0.51              |
| 9:T:286:ILE:HG22  | 9:T:289:PHE:CB    | 2.40                     | 0.51              |
| 1:J:88:ARG:HG3    | 1:J:89:ARG:H      | 1.75                     | 0.51              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:A:9:LEU:HD23    | 2:B:221:LEU:C    | 2.35                     | 0.51              |
| 3:C:96:LEU:HD22   | 3:C:98:PHE:CE1   | 2.46                     | 0.51              |
| 3:C:959:ALA:O     | 3:C:960:ASP:HB2  | 2.09                     | 0.51              |
| 3:C:1043:ILE:HD12 | 3:C:1043:ILE:N   | 2.24                     | 0.51              |
| 2:A:197:GLU:CD    | 3:C:987:ARG:HH22 | 2.17                     | 0.51              |
| 3:C:272:LEU:C     | 3:C:274:PRO:HD3  | 2.35                     | 0.51              |
| 4:D:653:ASN:CB    | 4:D:654:GLY:CA   | 2.89                     | 0.51              |
| 4:D:915:VAL:HG23  | 4:D:920:PHE:CE2  | 2.46                     | 0.51              |
| 6:F:140:ALA:HA    | 6:F:143:ALA:HB3  | 1.91                     | 0.51              |
| 6:F:308:VAL:HG21  | 7:O:23:DT:C7     | 2.31                     | 0.51              |
| 3:C:150:MET:HA    | 3:C:150:MET:CE   | 2.33                     | 0.51              |
| 3:C:446:LEU:N     | 3:C:446:LEU:HD23 | 2.26                     | 0.51              |
| 4:D:924:LEU:CD2   | 4:D:943:LEU:HD11 | 2.40                     | 0.51              |
| 4:D:1164:ARG:NH1  | 10:D:2005:SO4:O1 | 2.44                     | 0.51              |
| 2:A:130:ASP:N     | 2:A:130:ASP:OD1  | 2.42                     | 0.51              |
| 2:A:172:LEU:HD13  | 2:A:197:GLU:OE2  | 2.11                     | 0.51              |
| 3:C:335:TYR:O     | 3:C:335:TYR:HD1  | 1.93                     | 0.51              |
| 3:C:748:ILE:O     | 3:C:859:LEU:HD23 | 2.10                     | 0.51              |
| 4:D:517:VAL:HG12  | 4:D:518:GLU:O    | 2.10                     | 0.51              |
| 4:D:1275:PRO:CB   | 5:E:79:LEU:HD11  | 2.36                     | 0.51              |
| 7:O:12:DG:H2'     | 7:O:13:DT:H71    | 1.92                     | 0.51              |
| 3:C:299:LEU:HD23  | 3:C:323:THR:N    | 2.25                     | 0.51              |
| 3:C:404:THR:CG2   | 3:C:407:THR:HG23 | 2.41                     | 0.51              |
| 3:C:508:ARG:HD2   | 3:C:570:MET:CE   | 2.39                     | 0.51              |
| 3:C:626:ALA:HB2   | 3:C:704:MET:HG2  | 1.93                     | 0.51              |
| 3:C:680:ILE:HD11  | 3:C:692:VAL:HG12 | 1.93                     | 0.51              |
| 4:D:285:LYS:HG3   | 4:D:289:LYS:HD2  | 1.93                     | 0.51              |
| 3:C:94:MET:CE     | 3:C:395:MET:HB3  | 2.40                     | 0.51              |
| 3:C:494:TYR:HB3   | 3:C:506:PRO:CG   | 2.38                     | 0.51              |
| 3:C:727:ILE:HG13  | 3:C:907:ILE:HD12 | 1.93                     | 0.51              |
| 4:D:432:VAL:HG22  | 4:D:434:PRO:CD   | 2.27                     | 0.51              |
| 4:D:936:ILE:HG23  | 4:D:951:LEU:HD23 | 1.93                     | 0.51              |
| 9:T:259:ARG:NH2   | 14:T:401:HOH:O   | 2.44                     | 0.51              |
| 2:B:103:GLY:O     | 2:B:128:LEU:HB2  | 2.10                     | 0.51              |
| 3:C:280:LYS:O     | 3:C:284:GLN:HG2  | 2.11                     | 0.51              |
| 3:C:1014:VAL:HG13 | 4:D:729:THR:HG21 | 1.93                     | 0.51              |
| 4:D:262:LYS:CG    | 4:D:310:MET:HE1  | 2.41                     | 0.51              |
| 4:D:937:ILE:HD12  | 4:D:951:LEU:CG   | 2.37                     | 0.51              |
| 2:B:97:LEU:HD21   | 2:B:105:VAL:HG11 | 1.92                     | 0.50              |
| 2:B:162:ILE:CG2   | 4:D:607:PRO:HG2  | 2.41                     | 0.50              |
| 3:C:370:ARG:HH22  | 3:C:452:GLY:HA3  | 1.76                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:910:THR:O     | 3:C:914:PRO:HD3   | 2.11                     | 0.50              |
| 3:C:1045:GLN:CG   | 3:C:1090:ARG:HH21 | 2.24                     | 0.50              |
| 3:C:1098:VAL:HG11 | 4:D:469:ILE:CD1   | 2.40                     | 0.50              |
| 4:D:612:TYR:HB2   | 4:D:635:VAL:CG1   | 2.34                     | 0.50              |
| 4:D:735:VAL:HG22  | 4:D:798:ILE:CD1   | 2.40                     | 0.50              |
| 4:D:875:ARG:HH22  | 4:D:1033:GLN:CD   | 2.18                     | 0.50              |
| 3:C:936:ASN:HD22  | 3:C:937:ILE:N     | 2.05                     | 0.50              |
| 4:D:67:ARG:HH12   | 6:F:423:GLN:HA    | 1.76                     | 0.50              |
| 4:D:103:HIS:HB3   | 4:D:106:TYR:HD2   | 1.75                     | 0.50              |
| 4:D:781:THR:O     | 4:D:784:VAL:HG23  | 2.11                     | 0.50              |
| 6:F:279:TYR:CE1   | 7:O:28:DT:H5"     | 2.46                     | 0.50              |
| 2:A:31:GLY:O      | 2:A:35:GLY:N      | 2.32                     | 0.50              |
| 2:B:172:LEU:O     | 4:D:616:ALA:HB1   | 2.10                     | 0.50              |
| 4:D:581:MET:HE3   | 4:D:716:LYS:CA    | 2.41                     | 0.50              |
| 4:D:826:PRO:HG3   | 4:D:853:HIS:CE1   | 2.46                     | 0.50              |
| 4:D:1272:GLN:OE1  | 4:D:1272:GLN:HA   | 2.12                     | 0.50              |
| 6:F:317:LEU:CD2   | 6:F:337:LEU:HG    | 2.41                     | 0.50              |
| 6:F:385:ALA:O     | 6:F:389:VAL:HG23  | 2.12                     | 0.50              |
| 2:A:68:GLY:HA3    | 2:A:129:ASN:HD21  | 1.76                     | 0.50              |
| 2:A:147:VAL:HG13  | 2:A:147:VAL:O     | 2.12                     | 0.50              |
| 3:C:148:PHE:HD2   | 3:C:150:MET:CE    | 2.25                     | 0.50              |
| 3:C:586:PRO:O     | 3:C:880:HIS:HE1   | 1.95                     | 0.50              |
| 3:C:946:TRP:CZ2   | 3:C:978:GLY:HA3   | 2.46                     | 0.50              |
| 3:C:1032:ILE:HG21 | 4:D:520:LYS:HD3   | 1.93                     | 0.50              |
| 3:C:1133:GLY:O    | 3:C:1134:ALA:HB3  | 2.11                     | 0.50              |
| 4:D:612:TYR:OH    | 4:D:627:LEU:HG    | 2.12                     | 0.50              |
| 4:D:736:LEU:N     | 4:D:792:TYR:OH    | 2.34                     | 0.50              |
| 4:D:991:GLY:HA2   | 4:D:1265:ILE:HD12 | 1.92                     | 0.50              |
| 1:J:76:LYS:HG3    | 1:J:76:LYS:O      | 2.10                     | 0.50              |
| 2:A:211:ALA:O     | 2:A:215:LEU:HB2   | 2.11                     | 0.50              |
| 3:C:87:ILE:CD1    | 3:C:388:GLU:HG3   | 2.40                     | 0.50              |
| 3:C:762:ARG:HG3   | 3:C:762:ARG:O     | 2.11                     | 0.50              |
| 3:C:797:VAL:CG1   | 3:C:823:VAL:HB    | 2.41                     | 0.50              |
| 3:C:965:THR:O     | 3:C:965:THR:OG1   | 2.24                     | 0.50              |
| 4:D:981:SER:HB3   | 4:D:984:THR:OG1   | 2.10                     | 0.50              |
| 4:D:1056:LEU:HD21 | 4:D:1063:PHE:CD1  | 2.47                     | 0.50              |
| 4:D:1069:PRO:O    | 4:D:1072:GLY:HA2  | 2.12                     | 0.50              |
| 2:A:48:GLY:CA     | 2:A:49:ALA:CB     | 2.88                     | 0.50              |
| 2:A:177:LYS:HG2   | 2:A:193:ILE:CD1   | 2.42                     | 0.50              |
| 2:B:105:VAL:HG23  | 2:B:128:LEU:HD13  | 1.94                     | 0.50              |
| 3:C:44:LEU:HG     | 3:C:628:ASP:OD2   | 2.12                     | 0.50              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:C:126:VAL:HB    | 3:C:145:MET:HE2  | 1.93                     | 0.50              |
| 3:C:426:GLN:CD    | 3:C:450:GLY:HA2  | 2.37                     | 0.50              |
| 3:C:578:VAL:HG13  | 3:C:582:THR:CG2  | 2.42                     | 0.50              |
| 3:C:797:VAL:HG12  | 3:C:823:VAL:HB   | 1.94                     | 0.50              |
| 4:D:935:VAL:O     | 4:D:935:VAL:HG12 | 2.11                     | 0.50              |
| 2:A:193:ILE:HD12  | 2:A:193:ILE:O    | 2.11                     | 0.50              |
| 3:C:180:GLU:HG3   | 3:C:180:GLU:O    | 2.11                     | 0.50              |
| 3:C:404:THR:HG23  | 3:C:407:THR:H    | 1.76                     | 0.50              |
| 4:D:1106:VAL:HG13 | 4:D:1110:ASP:HB2 | 1.93                     | 0.50              |
| 6:F:313:VAL:CG2   | 6:F:351:ILE:HD13 | 2.42                     | 0.50              |
| 3:C:32:PHE:HE1    | 3:C:963:VAL:HG13 | 1.77                     | 0.50              |
| 3:C:123:PRO:HB3   | 3:C:144:PHE:HE1  | 1.76                     | 0.50              |
| 3:C:614:ALA:HA    | 3:C:705:ALA:HB2  | 1.94                     | 0.50              |
| 4:D:585:LEU:HD12  | 4:D:692:GLN:HE21 | 1.75                     | 0.50              |
| 4:D:653:ASN:CB    | 4:D:654:GLY:HA3  | 2.41                     | 0.50              |
| 2:A:9:LEU:HD13    | 2:A:23:ILE:HG13  | 1.94                     | 0.50              |
| 2:B:93:VAL:HG11   | 2:B:116:VAL:HG11 | 1.92                     | 0.50              |
| 3:C:174:PRO:HB2   | 3:C:303:GLY:CA   | 2.42                     | 0.50              |
| 3:C:269:TYR:CD2   | 3:C:278:PRO:HB3  | 2.47                     | 0.50              |
| 4:D:43:LYS:O      | 4:D:44:ASP:HB2   | 2.12                     | 0.50              |
| 4:D:599:TYR:HA    | 4:D:610:GLY:HA3  | 1.94                     | 0.50              |
| 5:E:95:GLU:HB3    | 5:E:101:LEU:CD2  | 2.42                     | 0.50              |
| 6:F:244:LEU:HD12  | 6:F:289:ILE:CG2  | 2.42                     | 0.50              |
| 2:A:78:LEU:HD12   | 3:C:611:ARG:HH11 | 1.77                     | 0.49              |
| 2:B:170:PRO:O     | 2:B:199:LYS:HB2  | 2.12                     | 0.49              |
| 3:C:41:VAL:HG13   | 3:C:493:VAL:CG1  | 2.42                     | 0.49              |
| 3:C:203:LEU:C     | 3:C:204:GLU:HG3  | 2.37                     | 0.49              |
| 3:C:601:ASN:O     | 3:C:604:ARG:HG2  | 2.12                     | 0.49              |
| 3:C:1103:ILE:CD1  | 4:D:547:LEU:HB3  | 2.41                     | 0.49              |
| 4:D:336:ALA:HA    | 6:F:359:ILE:O    | 2.12                     | 0.49              |
| 4:D:432:VAL:CG2   | 4:D:434:PRO:HD3  | 2.28                     | 0.49              |
| 4:D:638:THR:HA    | 4:D:659:ASP:O    | 2.12                     | 0.49              |
| 2:A:107:ALA:HB3   | 2:A:121:PRO:HA   | 1.94                     | 0.49              |
| 2:B:22:VAL:HA     | 2:B:192:LEU:O    | 2.13                     | 0.49              |
| 3:C:284:GLN:HG3   | 3:C:285:THR:N    | 2.27                     | 0.49              |
| 3:C:788:ARG:O     | 3:C:830:VAL:HG11 | 2.11                     | 0.49              |
| 3:C:873:GLY:HA3   | 3:C:1028:VAL:CG1 | 2.42                     | 0.49              |
| 7:O:2:DC:H2''     | 7:O:3:DT:H5'     | 1.94                     | 0.49              |
| 1:J:53:THR:HA     | 1:J:62:GLY:O     | 2.11                     | 0.49              |
| 2:A:159:ILE:HD11  | 3:C:785:ALA:HA   | 1.93                     | 0.49              |
| 3:C:467:HIS:ND1   | 3:C:468:PRO:HD2  | 2.27                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:728:LEU:HD23  | 3:C:906:ILE:HG22  | 1.94                     | 0.49              |
| 3:C:888:LYS:HG2   | 3:C:890:LEU:HD13  | 1.95                     | 0.49              |
| 3:C:1103:ILE:HD13 | 4:D:547:LEU:HB3   | 1.94                     | 0.49              |
| 4:D:58:TRP:CE3    | 4:D:68:VAL:HG22   | 2.47                     | 0.49              |
| 5:E:57:ARG:O      | 5:E:57:ARG:HD3    | 2.12                     | 0.49              |
| 3:C:368:ARG:HA    | 3:C:369:LEU:HB3   | 1.94                     | 0.49              |
| 3:C:984:LEU:HD13  | 3:C:989:GLY:CA    | 2.43                     | 0.49              |
| 3:C:1080:LEU:HD12 | 4:D:1253:VAL:HG13 | 1.95                     | 0.49              |
| 6:F:166:VAL:O     | 6:F:170:LEU:HG    | 2.11                     | 0.49              |
| 6:F:176:VAL:CG1   | 6:F:177:ALA:H     | 2.25                     | 0.49              |
| 3:C:215:VAL:O     | 3:C:223:GLN:HB2   | 2.12                     | 0.49              |
| 3:C:410:ASN:ND2   | 3:C:412:ARG:HG3   | 2.28                     | 0.49              |
| 3:C:1074:TYR:CE1  | 4:D:1258:LEU:HD21 | 2.47                     | 0.49              |
| 3:C:1085:ASP:OD2  | 4:D:420:LYS:NZ    | 2.40                     | 0.49              |
| 4:D:27:GLU:HB2    | 4:D:94:HIS:CE1    | 2.47                     | 0.49              |
| 4:D:1009:LEU:HD23 | 4:D:1029:LEU:HD12 | 1.93                     | 0.49              |
| 6:F:173:ILE:HG22  | 6:F:238:LEU:CD1   | 2.43                     | 0.49              |
| 2:A:18:ARG:NH1    | 2:A:195:ASP:OD2   | 2.45                     | 0.49              |
| 2:A:147:VAL:HG12  | 2:A:168:TYR:HE2   | 1.77                     | 0.49              |
| 2:A:212:GLY:O     | 2:A:216:VAL:N     | 2.34                     | 0.49              |
| 2:B:102:PRO:HB3   | 2:B:130:ASP:HA    | 1.94                     | 0.49              |
| 3:C:71:GLU:C      | 3:C:73:PRO:HD3    | 2.38                     | 0.49              |
| 3:C:602:MET:HE2   | 3:C:1024:LEU:HD21 | 1.93                     | 0.49              |
| 3:C:632:VAL:CG1   | 3:C:692:VAL:HG13  | 2.43                     | 0.49              |
| 4:D:67:ARG:NH1    | 6:F:423:GLN:HA    | 2.27                     | 0.49              |
| 4:D:411:GLY:O     | 4:D:415:GLN:HB3   | 2.13                     | 0.49              |
| 4:D:898:VAL:HG11  | 4:D:919:ALA:HB2   | 1.93                     | 0.49              |
| 4:D:1086:ARG:O    | 4:D:1087:LEU:HD23 | 2.13                     | 0.49              |
| 4:D:1276:THR:HG22 | 5:E:102:GLU:HG3   | 1.95                     | 0.49              |
| 6:F:310:MET:O     | 6:F:313:VAL:HG13  | 2.13                     | 0.49              |
| 3:C:741:ILE:HG22  | 3:C:742:HIS:N     | 2.27                     | 0.49              |
| 4:D:177:LEU:HD12  | 4:D:201:GLY:HA3   | 1.94                     | 0.49              |
| 4:D:602:ALA:CB    | 4:D:607:PRO:O     | 2.60                     | 0.49              |
| 4:D:644:THR:HA    | 4:D:647:GLU:CD    | 2.36                     | 0.49              |
| 4:D:1032:VAL:HG23 | 4:D:1142:VAL:HG11 | 1.95                     | 0.49              |
| 3:C:176:VAL:O     | 3:C:176:VAL:HG23  | 2.11                     | 0.49              |
| 3:C:199:ARG:HG2   | 3:C:200:GLY:N     | 2.27                     | 0.49              |
| 3:C:704:MET:CE    | 3:C:706:LEU:HD21  | 2.43                     | 0.49              |
| 3:C:848:ASP:OD1   | 3:C:848:ASP:N     | 2.46                     | 0.49              |
| 4:D:656:LYS:HD3   | 4:D:656:LYS:H     | 1.77                     | 0.49              |
| 4:D:846:LEU:HD12  | 4:D:846:LEU:N     | 2.27                     | 0.49              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 4:D:1222:LEU:HD23 | 4:D:1244:ASP:OD2 | 2.12                     | 0.49              |
| 5:E:80:VAL:HG12   | 5:E:94:ARG:HH21  | 1.78                     | 0.49              |
| 3:C:36:ARG:O      | 3:C:38:PRO:HD3   | 2.11                     | 0.49              |
| 3:C:196:ILE:HG23  | 3:C:196:ILE:O    | 2.13                     | 0.49              |
| 3:C:203:LEU:HD22  | 3:C:217:ILE:CG2  | 2.43                     | 0.49              |
| 4:D:125:LEU:O     | 4:D:129:ILE:HG23 | 2.13                     | 0.49              |
| 4:D:915:VAL:O     | 4:D:920:PHE:HD2  | 1.96                     | 0.49              |
| 6:F:414:ARG:HG2   | 6:F:419:LEU:HD12 | 1.95                     | 0.49              |
| 1:J:40:PHE:HZ     | 1:J:58:ASN:HB2   | 1.78                     | 0.49              |
| 2:A:1:MET:O       | 2:A:1:MET:HG2    | 2.12                     | 0.49              |
| 2:A:18:ARG:HA     | 2:A:204:PRO:HG3  | 1.95                     | 0.49              |
| 2:A:18:ARG:HB2    | 2:A:196:VAL:O    | 2.12                     | 0.49              |
| 2:B:69:VAL:HG23   | 2:B:71:GLU:O     | 2.12                     | 0.49              |
| 3:C:649:ILE:HG21  | 3:C:693:ILE:CG2  | 2.43                     | 0.49              |
| 4:D:20:ILE:HD13   | 4:D:318:PRO:HD3  | 1.95                     | 0.49              |
| 4:D:363:PRO:HB2   | 4:D:365:ILE:HD13 | 1.95                     | 0.49              |
| 4:D:716:LYS:HE3   | 4:D:717:ASP:OD1  | 2.13                     | 0.49              |
| 9:T:286:ILE:CG2   | 9:T:289:PHE:HB2  | 2.42                     | 0.49              |
| 3:C:55:LEU:HD22   | 3:C:376:ILE:HB   | 1.95                     | 0.48              |
| 3:C:589:GLU:OE1   | 3:C:589:GLU:N    | 2.36                     | 0.48              |
| 4:D:240:LEU:HD23  | 4:D:240:LEU:C    | 2.38                     | 0.48              |
| 4:D:331:ASP:N     | 4:D:331:ASP:OD1  | 2.45                     | 0.48              |
| 7:O:2:DC:H2''     | 7:O:3:DT:C5'     | 2.43                     | 0.48              |
| 2:A:31:GLY:CA     | 2:A:192:LEU:HD23 | 2.32                     | 0.48              |
| 2:B:214:THR:O     | 2:B:218:LEU:HB2  | 2.12                     | 0.48              |
| 3:C:202:TRP:H     | 3:C:202:TRP:HD1  | 1.59                     | 0.48              |
| 3:C:577:MET:HE3   | 4:D:849:PHE:HD1  | 1.77                     | 0.48              |
| 4:D:1171:SER:O    | 4:D:1202:ALA:HB2 | 2.13                     | 0.48              |
| 2:B:26:LEU:CD1    | 2:B:34:LEU:HD21  | 2.40                     | 0.48              |
| 2:B:171:VAL:HG23  | 2:B:171:VAL:O    | 2.12                     | 0.48              |
| 3:C:326:GLU:O     | 3:C:330:VAL:HG23 | 2.14                     | 0.48              |
| 3:C:475:CYS:CB    | 3:C:579:SER:HB3  | 2.43                     | 0.48              |
| 4:D:224:ASN:O     | 4:D:228:LYS:HG3  | 2.12                     | 0.48              |
| 4:D:1069:PRO:HG2  | 4:D:1073:GLY:N   | 2.24                     | 0.48              |
| 5:E:80:VAL:CG1    | 5:E:94:ARG:HH21  | 2.26                     | 0.48              |
| 5:E:92:ALA:O      | 5:E:96:ILE:HG13  | 2.14                     | 0.48              |
| 6:F:306:ILE:CG2   | 6:F:310:MET:HB3  | 2.43                     | 0.48              |
| 2:A:49:ALA:HB1    | 2:A:85:VAL:O     | 2.12                     | 0.48              |
| 2:A:186:ARG:O     | 2:A:187:THR:HG22 | 2.13                     | 0.48              |
| 3:C:35:LEU:N      | 3:C:35:LEU:HD12  | 2.28                     | 0.48              |
| 3:C:510:VAL:HG11  | 3:C:567:VAL:CG1  | 2.44                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:710:LEU:O     | 3:C:1018:TYR:HA   | 2.13                     | 0.48              |
| 3:C:859:LEU:HD22  | 3:C:860:VAL:N     | 2.28                     | 0.48              |
| 4:D:889:ASP:OD2   | 4:D:962:ARG:NH2   | 2.46                     | 0.48              |
| 2:A:32:TYR:CE1    | 2:A:178:VAL:HG22  | 2.48                     | 0.48              |
| 2:A:112:PRO:HB2   | 2:A:116:VAL:CG2   | 2.43                     | 0.48              |
| 2:B:105:VAL:HG12  | 2:B:125:ILE:HG21  | 1.94                     | 0.48              |
| 2:B:152:ASN:O     | 2:B:153:LYS:CB    | 2.62                     | 0.48              |
| 4:D:373:MET:SD    | 6:F:256:LEU:HB3   | 2.54                     | 0.48              |
| 4:D:884:ILE:HD12  | 4:D:885:VAL:O     | 2.13                     | 0.48              |
| 4:D:1005:PRO:HG3  | 4:D:1150:ILE:HD11 | 1.95                     | 0.48              |
| 4:D:1271:ILE:HG12 | 5:E:105:GLU:HA    | 1.95                     | 0.48              |
| 9:T:257:THR:OG1   | 9:T:260:SER:OG    | 2.31                     | 0.48              |
| 2:A:44:SER:HB3    | 3:C:893:GLU:OE1   | 2.13                     | 0.48              |
| 2:A:71:GLU:OE2    | 2:A:126:ALA:HA    | 2.12                     | 0.48              |
| 2:B:172:LEU:HD12  | 4:D:620:MET:SD    | 2.54                     | 0.48              |
| 3:C:268:ILE:HG23  | 3:C:272:LEU:HD22  | 1.96                     | 0.48              |
| 3:C:516:THR:CG2   | 3:C:518:GLN:HB2   | 2.43                     | 0.48              |
| 3:C:958:PRO:O     | 3:C:961:SER:OG    | 2.31                     | 0.48              |
| 4:D:924:LEU:HD22  | 4:D:959:VAL:HG11  | 1.92                     | 0.48              |
| 6:F:251:ARG:CB    | 6:F:297:MET:HE1   | 2.42                     | 0.48              |
| 2:B:52:THR:O      | 2:B:164:VAL:HG22  | 2.13                     | 0.48              |
| 2:B:76:ILE:HG23   | 2:B:125:ILE:HD11  | 1.94                     | 0.48              |
| 3:C:124:LEU:HD23  | 3:C:125:PHE:H     | 1.79                     | 0.48              |
| 3:C:169:GLN:OE1   | 3:C:370:ARG:NH2   | 2.44                     | 0.48              |
| 3:C:729:SER:HA    | 3:C:895:MET:HE1   | 1.95                     | 0.48              |
| 3:C:753:THR:HG21  | 3:C:799:PRO:HD2   | 1.96                     | 0.48              |
| 3:C:754:LYS:HD3   | 4:D:39:LEU:HD12   | 1.94                     | 0.48              |
| 3:C:875:LYS:C     | 3:C:876:LEU:HD12  | 2.37                     | 0.48              |
| 4:D:330:LEU:HD22  | 4:D:330:LEU:H     | 1.77                     | 0.48              |
| 4:D:1062:PHE:CE2  | 4:D:1080:LYS:HD2  | 2.49                     | 0.48              |
| 2:A:40:ARG:HH21   | 2:B:32:TYR:HD2    | 1.62                     | 0.48              |
| 2:A:54:ILE:C      | 2:A:54:ILE:HD12   | 2.38                     | 0.48              |
| 2:A:177:LYS:HE2   | 2:A:193:ILE:HG12  | 1.96                     | 0.48              |
| 3:C:572:VAL:O     | 3:C:573:SER:HB3   | 2.13                     | 0.48              |
| 4:D:70:PHE:O      | 4:D:82:VAL:HG11   | 2.13                     | 0.48              |
| 4:D:129:ILE:HD11  | 4:D:130:TYR:CE2   | 2.49                     | 0.48              |
| 4:D:400:LYS:CE    | 4:D:404:ASP:HB3   | 2.42                     | 0.48              |
| 1:J:81:HIS:CG     | 6:F:195:LEU:HD21  | 2.49                     | 0.48              |
| 2:A:86:SER:CB     | 2:A:119:HIS:HE2   | 2.24                     | 0.48              |
| 3:C:45:LEU:CD2    | 3:C:443:LYS:HD2   | 2.43                     | 0.48              |
| 3:C:794:VAL:HG11  | 3:C:860:VAL:HG11  | 1.95                     | 0.48              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:D:988:VAL:CG2  | 4:D:992:GLU:HG3   | 2.44                     | 0.48              |
| 2:A:152:ASN:HB3  | 2:A:157:ALA:HB3   | 1.93                     | 0.48              |
| 3:C:771:VAL:HG23 | 3:C:772:LEU:HD13  | 1.94                     | 0.48              |
| 3:C:1130:SER:HB3 | 3:C:1132:ASP:C    | 2.39                     | 0.48              |
| 9:T:283:LEU:O    | 9:T:286:ILE:HG22  | 2.14                     | 0.48              |
| 2:B:94:THR:HA    | 2:B:138:LEU:O     | 2.14                     | 0.47              |
| 3:C:29:ARG:HG2   | 3:C:964:ALA:HB2   | 1.96                     | 0.47              |
| 3:C:664:ARG:HB2  | 3:C:677:GLN:OE1   | 2.14                     | 0.47              |
| 3:C:797:VAL:HG11 | 3:C:823:VAL:HG21  | 1.96                     | 0.47              |
| 3:C:882:ASN:ND2  | 3:C:1019:MET:HE1  | 2.28                     | 0.47              |
| 2:B:79:ASN:O     | 2:B:123:MET:CE    | 2.62                     | 0.47              |
| 3:C:38:PRO:CB    | 3:C:508:ARG:HH21  | 2.26                     | 0.47              |
| 3:C:87:ILE:O     | 3:C:95:SER:HA     | 2.13                     | 0.47              |
| 3:C:154:LYS:HE2  | 3:C:630:GLY:O     | 2.14                     | 0.47              |
| 4:D:285:LYS:HA   | 4:D:289:LYS:HB2   | 1.94                     | 0.47              |
| 4:D:633:ILE:C    | 4:D:633:ILE:HD12  | 2.39                     | 0.47              |
| 6:F:316:LYS:HD3  | 6:F:341:MET:HE3   | 1.95                     | 0.47              |
| 9:T:251:ILE:HD12 | 9:T:254:LEU:HD11  | 1.96                     | 0.47              |
| 2:A:193:ILE:HD12 | 2:A:193:ILE:C     | 2.38                     | 0.47              |
| 2:B:9:LEU:HD21   | 2:B:208:LEU:HD21  | 1.96                     | 0.47              |
| 2:B:151:GLN:C    | 2:B:154:ALA:HB1   | 2.39                     | 0.47              |
| 3:C:202:TRP:O    | 3:C:203:LEU:HD23  | 2.13                     | 0.47              |
| 3:C:572:VAL:H    | 3:C:576:GLN:NE2   | 2.12                     | 0.47              |
| 3:C:716:PRO:O    | 4:D:724:THR:HB    | 2.14                     | 0.47              |
| 3:C:792:ILE:HD12 | 3:C:792:ILE:N     | 2.29                     | 0.47              |
| 4:D:1279:ALA:HB1 | 5:E:79:LEU:HD13   | 1.95                     | 0.47              |
| 6:F:416:ARG:HA   | 6:F:430:ILE:HD11  | 1.96                     | 0.47              |
| 3:C:477:ILE:HD11 | 4:D:852:THR:HG21  | 1.96                     | 0.47              |
| 4:D:137:THR:HG23 | 4:D:253:THR:OG1   | 2.15                     | 0.47              |
| 4:D:665:THR:HG21 | 4:D:682:PHE:CE2   | 2.50                     | 0.47              |
| 4:D:723:ALA:O    | 4:D:726:SER:HB3   | 2.14                     | 0.47              |
| 9:T:264:LEU:HB3  | 9:T:269:VAL:HG21  | 1.92                     | 0.47              |
| 1:J:58:ASN:HD21  | 1:J:60:LEU:HD12   | 1.80                     | 0.47              |
| 2:B:198:THR:HG21 | 2:B:202:ILE:O     | 2.15                     | 0.47              |
| 3:C:52:PHE:CZ    | 3:C:150:MET:HE2   | 2.47                     | 0.47              |
| 3:C:752:ASP:OD1  | 3:C:857:ASN:ND2   | 2.47                     | 0.47              |
| 3:C:919:ILE:HD12 | 3:C:920:GLY:N     | 2.30                     | 0.47              |
| 3:C:976:LEU:O    | 3:C:980:LEU:HD23  | 2.14                     | 0.47              |
| 4:D:467:GLN:NE2  | 4:D:467:GLN:HA    | 2.29                     | 0.47              |
| 4:D:1081:LEU:HB3 | 4:D:1113:MET:SD   | 2.54                     | 0.47              |
| 4:D:1153:LYS:O   | 4:D:1157:VAL:HG23 | 2.14                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:A:9:LEU:HB2     | 2:A:23:ILE:HG12   | 1.97                     | 0.47              |
| 2:A:108:GLY:HA2   | 2:A:121:PRO:HB3   | 1.96                     | 0.47              |
| 2:B:85:VAL:HB     | 2:B:118:VAL:HA    | 1.96                     | 0.47              |
| 3:C:174:PRO:HB2   | 3:C:303:GLY:HA3   | 1.97                     | 0.47              |
| 3:C:203:LEU:HD13  | 3:C:217:ILE:CG2   | 2.43                     | 0.47              |
| 3:C:475:CYS:HA    | 3:C:577:MET:O     | 2.15                     | 0.47              |
| 4:D:880:SER:O     | 4:D:995:GLY:HA3   | 2.13                     | 0.47              |
| 4:D:1119:PRO:HA   | 4:D:1122:VAL:HG12 | 1.94                     | 0.47              |
| 6:F:462:ARG:HH11  | 6:F:465:LEU:HB2   | 1.78                     | 0.47              |
| 7:O:15:DT:H1'     | 7:O:16:DT:H5''    | 1.97                     | 0.47              |
| 2:B:18:ARG:HG3    | 2:B:197:GLU:CG    | 2.41                     | 0.47              |
| 2:B:63:PHE:N      | 2:B:63:PHE:CD1    | 2.81                     | 0.47              |
| 2:B:80:LEU:HG     | 2:B:125:ILE:HD13  | 1.96                     | 0.47              |
| 2:B:139:VAL:HG21  | 2:B:161:ARG:HH21  | 1.79                     | 0.47              |
| 2:B:147:VAL:HG13  | 2:B:166:SER:HB2   | 1.95                     | 0.47              |
| 2:B:202:ILE:HD13  | 2:B:207:ALA:HB2   | 1.96                     | 0.47              |
| 3:C:346:MET:HE2   | 3:C:348:VAL:HA    | 1.96                     | 0.47              |
| 3:C:741:ILE:HG22  | 3:C:742:HIS:H     | 1.80                     | 0.47              |
| 3:C:1033:HIS:HB3  | 11:C:1205:EDO:O1  | 2.13                     | 0.47              |
| 3:C:1126:VAL:HG23 | 3:C:1126:VAL:O    | 2.15                     | 0.47              |
| 4:D:91:ARG:O      | 4:D:321:PRO:HG3   | 2.15                     | 0.47              |
| 4:D:105:TRP:CE2   | 4:D:1231:THR:HG23 | 2.49                     | 0.47              |
| 4:D:590:THR:CG2   | 4:D:630:ARG:HE    | 2.27                     | 0.47              |
| 4:D:653:ASN:N     | 4:D:654:GLY:HA3   | 2.30                     | 0.47              |
| 4:D:799:ILE:HD13  | 4:D:799:ILE:HA    | 1.69                     | 0.47              |
| 4:D:869:SER:HB2   | 4:D:1029:LEU:HD21 | 1.97                     | 0.47              |
| 4:D:1247:ASN:O    | 4:D:1260:PRO:HG3  | 2.15                     | 0.47              |
| 4:D:1276:THR:HG22 | 5:E:102:GLU:HG2   | 1.96                     | 0.47              |
| 3:C:896:PRO:HB2   | 3:C:1001:LEU:HD13 | 1.97                     | 0.47              |
| 4:D:52:PHE:O      | 4:D:91:ARG:HD2    | 2.15                     | 0.47              |
| 4:D:430:ILE:HD13  | 4:D:541:MET:HG3   | 1.96                     | 0.47              |
| 1:J:73:LYS:O      | 1:J:74:LYS:HG3    | 2.15                     | 0.47              |
| 3:C:265:LEU:CD1   | 3:C:287:LEU:HD12  | 2.45                     | 0.47              |
| 4:D:1117:ALA:O    | 4:D:1119:PRO:HD3  | 2.15                     | 0.47              |
| 8:P:11:DA:H2'     | 8:P:12:DA:C8      | 2.48                     | 0.47              |
| 9:T:257:THR:O     | 9:T:260:SER:N     | 2.48                     | 0.47              |
| 2:B:43:LEU:HD12   | 2:B:43:LEU:HA     | 1.77                     | 0.47              |
| 3:C:361:ILE:HD12  | 3:C:361:ILE:N     | 2.24                     | 0.47              |
| 3:C:598:MET:O     | 3:C:602:MET:HG3   | 2.15                     | 0.47              |
| 3:C:764:ILE:HB    | 3:C:767:VAL:HG21  | 1.96                     | 0.47              |
| 3:C:1084:SER:OG   | 4:D:420:LYS:HD3   | 2.15                     | 0.47              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:C:1117:LYS:HE2  | 4:D:90:GLU:O     | 2.15                     | 0.47              |
| 4:D:687:MET:CE    | 4:D:695:ILE:HD11 | 2.45                     | 0.47              |
| 3:C:460:GLY:HA3   | 3:C:462:GLU:OE1  | 2.15                     | 0.46              |
| 3:C:731:ARG:NH1   | 3:C:735:GLU:OE1  | 2.48                     | 0.46              |
| 3:C:885:VAL:HG22  | 4:D:536:PHE:O    | 2.14                     | 0.46              |
| 4:D:133:ALA:C     | 4:D:256:MET:HE3  | 2.40                     | 0.46              |
| 4:D:629:VAL:CG1   | 4:D:671:MET:HE1  | 2.45                     | 0.46              |
| 4:D:704:PRO:HD2   | 4:D:707:VAL:HG21 | 1.97                     | 0.46              |
| 2:B:182:ARG:C     | 2:B:184:GLU:H    | 2.21                     | 0.46              |
| 3:C:70:GLU:N      | 3:C:70:GLU:OE1   | 2.48                     | 0.46              |
| 3:C:167:VAL:HG13  | 3:C:445:ARG:O    | 2.16                     | 0.46              |
| 3:C:616:LEU:HB2   | 3:C:709:ASN:CG   | 2.40                     | 0.46              |
| 4:D:113:ARG:HB2   | 4:D:312:MET:CE   | 2.46                     | 0.46              |
| 4:D:236:VAL:O     | 4:D:236:VAL:HG12 | 2.15                     | 0.46              |
| 4:D:285:LYS:HG3   | 4:D:289:LYS:CD   | 2.45                     | 0.46              |
| 4:D:915:VAL:HG23  | 4:D:920:PHE:HE2  | 1.80                     | 0.46              |
| 4:D:1056:LEU:HD23 | 4:D:1057:GLU:H   | 1.79                     | 0.46              |
| 3:C:118:MET:HE2   | 3:C:118:MET:HB3  | 1.82                     | 0.46              |
| 3:C:372:VAL:O     | 3:C:376:ILE:HG12 | 2.15                     | 0.46              |
| 3:C:549:ARG:HB2   | 3:C:561:PHE:CZ   | 2.50                     | 0.46              |
| 3:C:754:LYS:HE2   | 3:C:754:LYS:N    | 2.26                     | 0.46              |
| 3:C:767:VAL:HB    | 3:C:771:VAL:HG21 | 1.96                     | 0.46              |
| 4:D:66:LYS:HG2    | 4:D:66:LYS:O     | 2.14                     | 0.46              |
| 4:D:493:GLU:HA    | 4:D:513:GLU:OE1  | 2.14                     | 0.46              |
| 4:D:920:PHE:CZ    | 4:D:948:ILE:HG13 | 2.50                     | 0.46              |
| 2:A:177:LYS:HE2   | 2:A:193:ILE:CG1  | 2.46                     | 0.46              |
| 2:A:210:SER:HB3   | 2:B:229:SER:CB   | 2.44                     | 0.46              |
| 2:B:22:VAL:HG12   | 2:B:193:ILE:CD1  | 2.42                     | 0.46              |
| 3:C:494:TYR:CD2   | 3:C:572:VAL:HG21 | 2.44                     | 0.46              |
| 3:C:754:LYS:HD3   | 4:D:39:LEU:CD1   | 2.46                     | 0.46              |
| 3:C:797:VAL:HG11  | 3:C:823:VAL:CG2  | 2.45                     | 0.46              |
| 3:C:845:SER:O     | 3:C:850:ASP:HB2  | 2.16                     | 0.46              |
| 3:C:935:TRP:HB2   | 3:C:982:SER:HB2  | 1.97                     | 0.46              |
| 2:A:68:GLY:CA     | 2:A:129:ASN:HD21 | 2.27                     | 0.46              |
| 2:A:151:GLN:HB3   | 3:C:786:GLU:OE2  | 2.15                     | 0.46              |
| 2:B:34:LEU:O      | 2:B:37:SER:N     | 2.49                     | 0.46              |
| 2:B:181:THR:HB    | 2:B:182:ARG:CB   | 2.46                     | 0.46              |
| 3:C:400:VAL:C     | 3:C:402:ALA:H    | 2.22                     | 0.46              |
| 3:C:523:THR:CG2   | 3:C:526:GLU:HG2  | 2.46                     | 0.46              |
| 3:C:560:GLU:HG3   | 3:C:562:VAL:HG23 | 1.98                     | 0.46              |
| 3:C:714:ILE:O     | 3:C:910:THR:OG1  | 2.23                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:981:GLY:C    | 3:C:982:SER:HG   | 2.06                     | 0.46              |
| 6:F:454:HIS:CD2  | 6:F:456:SER:HG   | 2.33                     | 0.46              |
| 8:P:4:DA:H2''    | 8:P:5:DC:C6      | 2.50                     | 0.46              |
| 2:B:63:PHE:N     | 2:B:63:PHE:HD1   | 2.13                     | 0.46              |
| 2:B:105:VAL:HG23 | 2:B:128:LEU:HD11 | 1.96                     | 0.46              |
| 3:C:26:ALA:HB1   | 3:C:623:LEU:HD21 | 1.97                     | 0.46              |
| 3:C:477:ILE:O    | 3:C:477:ILE:HG22 | 2.16                     | 0.46              |
| 3:C:584:MET:O    | 14:C:1305:HOH:O  | 2.21                     | 0.46              |
| 3:C:727:ILE:HA   | 3:C:888:LYS:O    | 2.16                     | 0.46              |
| 3:C:1066:ALA:HB1 | 4:D:506:ARG:HA   | 1.96                     | 0.46              |
| 4:D:102:THR:OG1  | 4:D:129:ILE:HD12 | 2.15                     | 0.46              |
| 4:D:618:ALA:HB1  | 4:D:627:LEU:CD1  | 2.46                     | 0.46              |
| 2:B:65:THR:HG22  | 2:B:66:VAL:N     | 2.31                     | 0.46              |
| 3:C:96:LEU:HD22  | 3:C:98:PHE:HE1   | 1.79                     | 0.46              |
| 3:C:781:VAL:HG21 | 3:C:838:VAL:HG21 | 1.98                     | 0.46              |
| 4:D:226:PHE:CE1  | 4:D:248:TYR:HB3  | 2.50                     | 0.46              |
| 4:D:622:MET:CE   | 4:D:667:LEU:HD13 | 2.31                     | 0.46              |
| 4:D:693:ALA:O    | 4:D:697:ASN:HB2  | 2.16                     | 0.46              |
| 4:D:699:LEU:CD1  | 4:D:711:THR:HG21 | 2.45                     | 0.46              |
| 4:D:1041:PRO:HB3 | 4:D:1116:ALA:CB  | 2.46                     | 0.46              |
| 6:F:234:LEU:HD23 | 6:F:270:VAL:HG21 | 1.97                     | 0.46              |
| 8:P:11:DA:H2'    | 8:P:12:DA:H8     | 1.81                     | 0.46              |
| 2:B:95:MET:HE3   | 2:B:110:ILE:CD1  | 2.41                     | 0.46              |
| 3:C:193:VAL:CG1  | 3:C:205:PHE:HB2  | 2.46                     | 0.46              |
| 3:C:510:VAL:HG12 | 3:C:568:ASP:O    | 2.16                     | 0.46              |
| 4:D:64:LYS:NZ    | 4:D:76:GLU:OE2   | 2.43                     | 0.46              |
| 4:D:500:ARG:HB2  | 4:D:541:MET:HG2  | 1.98                     | 0.46              |
| 4:D:1034:GLU:OE2 | 4:D:1041:PRO:HA  | 2.15                     | 0.46              |
| 6:F:406:SER:HB3  | 6:F:409:GLU:HG3  | 1.98                     | 0.46              |
| 3:C:809:GLU:O    | 3:C:813:ARG:HG2  | 2.15                     | 0.46              |
| 4:D:60:CYS:SG    | 4:D:63:GLY:N     | 2.81                     | 0.46              |
| 4:D:588:LEU:HD22 | 4:D:668:GLY:CA   | 2.44                     | 0.46              |
| 4:D:590:THR:HG23 | 4:D:630:ARG:HE   | 1.81                     | 0.46              |
| 4:D:863:ALA:O    | 4:D:866:THR:HG22 | 2.15                     | 0.46              |
| 4:D:1174:THR:OG1 | 4:D:1175:GLU:CB  | 2.64                     | 0.46              |
| 6:F:394:LEU:HB2  | 6:F:464:TYR:CE1  | 2.51                     | 0.46              |
| 6:F:465:LEU:HD23 | 6:F:466:ASP:HB2  | 1.98                     | 0.46              |
| 7:O:6:DA:C1'     | 7:O:7:DC:H5'     | 2.46                     | 0.46              |
| 2:A:24:GLU:HB3   | 2:A:191:LYS:HB2  | 1.98                     | 0.46              |
| 2:A:63:PHE:HE1   | 3:C:741:ILE:HD13 | 1.81                     | 0.46              |
| 3:C:169:GLN:HB2  | 3:C:427:LEU:HD21 | 1.97                     | 0.46              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:C:178:PHE:CD1  | 3:C:193:VAL:HB    | 2.51                     | 0.46              |
| 3:C:659:GLN:OE1  | 3:C:659:GLN:N     | 2.48                     | 0.46              |
| 3:C:895:MET:HE2  | 3:C:895:MET:HB2   | 1.65                     | 0.46              |
| 3:C:984:LEU:CD1  | 3:C:989:GLY:HA2   | 2.46                     | 0.46              |
| 4:D:140:ASP:OD2  | 4:D:143:MET:HB2   | 2.16                     | 0.46              |
| 4:D:320:ILE:HG12 | 4:D:321:PRO:CD    | 2.46                     | 0.46              |
| 4:D:633:ILE:O    | 4:D:665:THR:O     | 2.34                     | 0.46              |
| 4:D:656:LYS:O    | 4:D:656:LYS:CE    | 2.64                     | 0.46              |
| 4:D:1009:LEU:CD1 | 4:D:1146:GLN:HG3  | 2.44                     | 0.46              |
| 2:A:42:LEU:HD23  | 2:A:211:ALA:HB2   | 1.98                     | 0.45              |
| 2:A:56:ILE:HB    | 2:A:59:VAL:CG2    | 2.43                     | 0.45              |
| 2:A:125:ILE:N    | 2:A:125:ILE:HD12  | 2.30                     | 0.45              |
| 3:C:1118:GLU:OE1 | 4:D:412:ARG:HG3   | 2.17                     | 0.45              |
| 4:D:518:GLU:O    | 14:D:2104:HOH:O   | 2.21                     | 0.45              |
| 4:D:738:PRO:HA   | 4:D:791:PHE:HD2   | 1.81                     | 0.45              |
| 4:D:755:ILE:HD12 | 4:D:776:ILE:CD1   | 2.46                     | 0.45              |
| 4:D:788:LEU:C    | 4:D:788:LEU:HD23  | 2.41                     | 0.45              |
| 4:D:923:THR:OG1  | 4:D:962:ARG:HD2   | 2.16                     | 0.45              |
| 4:D:1162:MET:HE2 | 4:D:1211:ILE:HG23 | 1.98                     | 0.45              |
| 6:F:201:LEU:HD11 | 6:F:219:MET:CB    | 2.42                     | 0.45              |
| 6:F:253:MET:HE1  | 6:F:296:ALA:C     | 2.41                     | 0.45              |
| 7:O:2:DC:H2''    | 7:O:3:DT:O5'      | 2.16                     | 0.45              |
| 7:O:28:DT:P      | 14:O:101:HOH:O    | 2.74                     | 0.45              |
| 1:J:73:LYS:O     | 1:J:74:LYS:CG     | 2.64                     | 0.45              |
| 2:B:66:VAL:HG12  | 2:B:69:VAL:HG22   | 1.98                     | 0.45              |
| 2:B:76:ILE:HG23  | 2:B:125:ILE:HD12  | 1.97                     | 0.45              |
| 3:C:766:ASN:HB3  | 6:F:465:LEU:HD21  | 1.98                     | 0.45              |
| 4:D:765:ASN:ND2  | 4:D:767:THR:HG23  | 2.31                     | 0.45              |
| 4:D:899:THR:O    | 4:D:957:THR:O     | 2.34                     | 0.45              |
| 4:D:1123:LEU:HB2 | 4:D:1131:VAL:HG21 | 1.97                     | 0.45              |
| 7:O:6:DA:H1'     | 7:O:7:DC:C5'      | 2.46                     | 0.45              |
| 2:A:11:GLU:OE2   | 2:B:225:LEU:HD22  | 2.16                     | 0.45              |
| 2:B:28:PRO:HA    | 2:B:190:ASP:OD2   | 2.16                     | 0.45              |
| 2:B:174:VAL:HA   | 2:B:195:ASP:O     | 2.16                     | 0.45              |
| 3:C:62:ARG:HG3   | 3:C:66:ILE:HD11   | 1.98                     | 0.45              |
| 4:D:271:ASP:HA   | 4:D:303:GLN:NE2   | 2.31                     | 0.45              |
| 4:D:956:ILE:CD1  | 4:D:956:ILE:O     | 2.64                     | 0.45              |
| 2:A:95:MET:HE2   | 2:A:110:ILE:HG21  | 1.99                     | 0.45              |
| 3:C:747:GLU:HG3  | 3:C:859:LEU:HD21  | 1.98                     | 0.45              |
| 3:C:767:VAL:HB   | 3:C:771:VAL:CG2   | 2.46                     | 0.45              |
| 3:C:1035:ARG:CZ  | 3:C:1047:PRO:HB3  | 2.45                     | 0.45              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:C:1103:ILE:HD12 | 4:D:548:SER:CA   | 2.46                     | 0.45              |
| 4:D:931:ALA:HA    | 4:D:932:ASN:HA   | 1.64                     | 0.45              |
| 4:D:952:LEU:HD12  | 4:D:952:LEU:HA   | 1.85                     | 0.45              |
| 6:F:176:VAL:CG1   | 6:F:177:ALA:N    | 2.79                     | 0.45              |
| 6:F:408:ARG:HH21  | 11:F:506:EDO:H22 | 1.82                     | 0.45              |
| 7:O:27:DA:H4'     | 7:O:28:DT:OP1    | 2.17                     | 0.45              |
| 2:A:55:ARG:HH12   | 2:A:161:ARG:CZ   | 2.28                     | 0.45              |
| 2:A:63:PHE:O      | 3:C:666:PHE:CD2  | 2.70                     | 0.45              |
| 2:B:213:GLY:CA    | 2:B:216:VAL:HG12 | 2.45                     | 0.45              |
| 3:C:130:PHE:CZ    | 3:C:403:ILE:HG13 | 2.52                     | 0.45              |
| 3:C:523:THR:HG22  | 3:C:526:GLU:OE2  | 2.16                     | 0.45              |
| 3:C:638:THR:HG23  | 3:C:688:GLU:HA   | 1.98                     | 0.45              |
| 3:C:918:ASN:O     | 3:C:920:GLY:N    | 2.50                     | 0.45              |
| 4:D:277:LEU:HD21  | 4:D:292:ALA:O    | 2.17                     | 0.45              |
| 4:D:287:GLN:HG3   | 4:D:288:LYS:HZ2  | 1.82                     | 0.45              |
| 4:D:376:GLU:OE2   | 6:F:165:SER:OG   | 2.24                     | 0.45              |
| 4:D:948:ILE:O     | 4:D:952:LEU:HB2  | 2.16                     | 0.45              |
| 5:E:28:THR:HG23   | 5:E:28:THR:O     | 2.17                     | 0.45              |
| 5:E:76:VAL:CG1    | 5:E:77:GLY:N     | 2.80                     | 0.45              |
| 5:E:80:VAL:CG2    | 5:E:100:LEU:HD22 | 2.47                     | 0.45              |
| 3:C:29:ARG:HD3    | 3:C:964:ALA:HB2  | 1.98                     | 0.45              |
| 3:C:94:MET:HE3    | 3:C:395:MET:HB3  | 1.99                     | 0.45              |
| 3:C:203:LEU:HD22  | 3:C:217:ILE:HB   | 1.99                     | 0.45              |
| 3:C:231:ALA:HB1   | 3:C:265:LEU:HD12 | 1.97                     | 0.45              |
| 3:C:780:ILE:HD12  | 3:C:781:VAL:O    | 2.16                     | 0.45              |
| 3:C:1048:LEU:HD23 | 3:C:1048:LEU:N   | 2.21                     | 0.45              |
| 4:D:448:ALA:HB1   | 4:D:491:ILE:HD11 | 1.98                     | 0.45              |
| 6:F:170:LEU:HA    | 6:F:173:ILE:HG12 | 1.98                     | 0.45              |
| 8:P:17:DT:H5''    | 9:T:290:GLY:N    | 2.31                     | 0.45              |
| 2:A:108:GLY:CA    | 2:A:121:PRO:HB3  | 2.47                     | 0.45              |
| 2:B:153:LYS:N     | 2:B:154:ALA:CA   | 2.70                     | 0.45              |
| 3:C:77:LEU:HD23   | 3:C:77:LEU:HA    | 1.74                     | 0.45              |
| 3:C:575:ARG:HE    | 3:C:967:VAL:CG2  | 2.25                     | 0.45              |
| 3:C:850:ASP:HB3   | 3:C:851:GLU:H    | 1.55                     | 0.45              |
| 4:D:475:MET:HE3   | 4:D:475:MET:HB2  | 1.79                     | 0.45              |
| 4:D:910:ILE:O     | 4:D:910:ILE:HG12 | 2.17                     | 0.45              |
| 6:F:186:GLU:OE1   | 6:F:186:GLU:HA   | 2.17                     | 0.45              |
| 1:J:51:PRO:O      | 1:J:64:LEU:HD12  | 2.16                     | 0.45              |
| 3:C:346:MET:HB2   | 3:C:356:VAL:CG2  | 2.47                     | 0.45              |
| 3:C:913:VAL:HB    | 3:C:914:PRO:HD3  | 1.97                     | 0.45              |
| 3:C:1037:THR:HG22 | 3:C:1038:GLY:N   | 2.32                     | 0.45              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 8:P:11:DA:H2''    | 8:P:12:DA:H5'    | 1.96                     | 0.45              |
| 2:B:74:THR:OG1    | 4:D:608:GLU:OE1  | 2.35                     | 0.45              |
| 2:B:99:LYS:HE2    | 2:B:99:LYS:HB3   | 1.65                     | 0.45              |
| 3:C:394:ARG:HG3   | 3:C:398:GLN:CG   | 2.47                     | 0.45              |
| 3:C:1043:ILE:HD12 | 3:C:1043:ILE:H   | 1.81                     | 0.45              |
| 4:D:102:THR:HG23  | 4:D:258:ALA:CB   | 2.47                     | 0.45              |
| 4:D:608:GLU:O     | 4:D:609:GLN:HB2  | 2.17                     | 0.45              |
| 4:D:972:GLY:HA2   | 10:D:2005:SO4:O2 | 2.17                     | 0.45              |
| 1:J:88:ARG:HG3    | 1:J:89:ARG:N     | 2.32                     | 0.45              |
| 2:B:147:VAL:HG13  | 2:B:147:VAL:O    | 2.17                     | 0.45              |
| 2:B:196:VAL:HG13  | 2:B:196:VAL:O    | 2.17                     | 0.45              |
| 3:C:523:THR:HG23  | 3:C:526:GLU:HG2  | 1.99                     | 0.45              |
| 3:C:614:ALA:HA    | 3:C:705:ALA:CB   | 2.47                     | 0.45              |
| 4:D:1110:ASP:N    | 4:D:1110:ASP:OD1 | 2.50                     | 0.45              |
| 4:D:1165:ARG:HE   | 4:D:1209:MET:HE1 | 1.81                     | 0.45              |
| 2:B:28:PRO:HD3    | 2:B:189:PHE:CD1  | 2.52                     | 0.44              |
| 3:C:193:VAL:HG22  | 3:C:194:LYS:N    | 2.32                     | 0.44              |
| 3:C:577:MET:CE    | 4:D:849:PHE:HD1  | 2.30                     | 0.44              |
| 3:C:632:VAL:HG13  | 3:C:694:ALA:O    | 2.17                     | 0.44              |
| 3:C:1003:ASP:OD1  | 3:C:1005:ARG:HB3 | 2.17                     | 0.44              |
| 4:D:720:PHE:O     | 4:D:724:THR:HG23 | 2.17                     | 0.44              |
| 1:J:57:ARG:HG3    | 4:D:25:TYR:HA    | 1.98                     | 0.44              |
| 3:C:53:GLU:OE2    | 3:C:60:ARG:NH1   | 2.35                     | 0.44              |
| 3:C:197:PRO:HB3   | 3:C:297:TYR:OH   | 2.16                     | 0.44              |
| 4:D:243:GLU:HG2   | 4:D:247:ARG:HH21 | 1.81                     | 0.44              |
| 4:D:823:VAL:HG12  | 4:D:824:THR:N    | 2.31                     | 0.44              |
| 8:P:3:DC:H2''     | 8:P:4:DA:H8      | 1.81                     | 0.44              |
| 2:A:216:VAL:HG13  | 2:B:216:VAL:HG23 | 1.99                     | 0.44              |
| 2:A:219:PHE:CE1   | 2:B:38:LEU:HD21  | 2.52                     | 0.44              |
| 3:C:291:PHE:O     | 3:C:297:TYR:HB3  | 2.17                     | 0.44              |
| 3:C:404:THR:HG23  | 3:C:407:THR:HG23 | 1.98                     | 0.44              |
| 3:C:615:PRO:HB3   | 3:C:1020:TYR:CE2 | 2.51                     | 0.44              |
| 3:C:723:GLU:HA    | 3:C:723:GLU:OE1  | 2.18                     | 0.44              |
| 4:D:536:PHE:C     | 4:D:538:GLY:H    | 2.25                     | 0.44              |
| 4:D:591:LEU:HD23  | 4:D:630:ARG:O    | 2.18                     | 0.44              |
| 5:E:53:TYR:CE1    | 5:E:101:LEU:HD12 | 2.53                     | 0.44              |
| 6:F:394:LEU:HD13  | 6:F:464:TYR:CG   | 2.52                     | 0.44              |
| 2:A:18:ARG:HA     | 2:A:204:PRO:CG   | 2.47                     | 0.44              |
| 3:C:80:VAL:CG2    | 3:C:377:GLN:HG3  | 2.47                     | 0.44              |
| 3:C:1015:THR:OG1  | 4:D:731:SER:OG   | 2.36                     | 0.44              |
| 4:D:58:TRP:HH2    | 4:D:84:ARG:NH2   | 2.16                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:911:ARG:HG2  | 4:D:952:LEU:HD21 | 2.00                     | 0.44              |
| 4:D:929:VAL:HG23 | 4:D:929:VAL:O    | 2.17                     | 0.44              |
| 5:E:57:ARG:NH2   | 5:E:77:GLY:HA3   | 2.31                     | 0.44              |
| 6:F:462:ARG:HA   | 6:F:462:ARG:HD3  | 1.79                     | 0.44              |
| 1:J:58:ASN:HD21  | 1:J:60:LEU:CG    | 2.31                     | 0.44              |
| 3:C:154:LYS:O    | 3:C:443:LYS:HE3  | 2.17                     | 0.44              |
| 3:C:538:PRO:C    | 3:C:546:THR:OG1  | 2.61                     | 0.44              |
| 2:A:90:ASP:O     | 2:A:91:GLU:CG    | 2.66                     | 0.44              |
| 2:A:174:VAL:O    | 3:C:901:GLY:HA3  | 2.18                     | 0.44              |
| 2:A:187:THR:O    | 2:A:187:THR:HG23 | 2.17                     | 0.44              |
| 2:B:150:VAL:HG13 | 2:B:150:VAL:O    | 2.17                     | 0.44              |
| 4:D:130:TYR:O    | 4:D:372:ARG:HD3  | 2.17                     | 0.44              |
| 4:D:814:ARG:O    | 4:D:817:ALA:O    | 2.36                     | 0.44              |
| 4:D:884:ILE:HD11 | 4:D:886:ARG:CD   | 2.48                     | 0.44              |
| 4:D:1165:ARG:HG2 | 4:D:1183:GLU:HA  | 1.99                     | 0.44              |
| 4:D:1174:THR:CG2 | 4:D:1176:PHE:N   | 2.74                     | 0.44              |
| 6:F:337:LEU:HD12 | 6:F:337:LEU:HA   | 1.78                     | 0.44              |
| 1:J:28:GLN:CD    | 1:J:46:ASP:HA    | 2.42                     | 0.44              |
| 1:J:28:GLN:N     | 1:J:44:PHE:O     | 2.50                     | 0.44              |
| 1:J:69:VAL:N     | 1:J:70:PRO:HD3   | 2.33                     | 0.44              |
| 2:A:48:GLY:O     | 2:A:142:ARG:HG2  | 2.16                     | 0.44              |
| 2:A:78:LEU:CD1   | 3:C:611:ARG:HH11 | 2.31                     | 0.44              |
| 3:C:41:VAL:HG22  | 3:C:494:TYR:HE1  | 1.83                     | 0.44              |
| 3:C:291:PHE:HA   | 3:C:297:TYR:HB2  | 1.99                     | 0.44              |
| 4:D:58:TRP:HA    | 4:D:82:VAL:HG23  | 2.00                     | 0.44              |
| 4:D:129:ILE:HG12 | 4:D:130:TYR:CD2  | 2.53                     | 0.44              |
| 4:D:439:HIS:O    | 4:D:513:GLU:N    | 2.48                     | 0.44              |
| 4:D:525:HIS:O    | 4:D:528:VAL:HG22 | 2.18                     | 0.44              |
| 4:D:600:GLN:CB   | 4:D:601:ALA:HA   | 2.48                     | 0.44              |
| 4:D:633:ILE:HD13 | 4:D:635:VAL:HG13 | 1.99                     | 0.44              |
| 4:D:739:PRO:HD3  | 4:D:791:PHE:CE2  | 2.53                     | 0.44              |
| 9:T:280:GLU:HG3  | 9:T:294:ILE:HD13 | 2.00                     | 0.44              |
| 1:J:104:LEU:HD23 | 1:J:104:LEU:O    | 2.18                     | 0.44              |
| 2:A:10:SER:OG    | 2:A:22:VAL:HG13  | 2.18                     | 0.44              |
| 2:A:96:TYR:O     | 2:A:111:VAL:HG13 | 2.17                     | 0.44              |
| 3:C:62:ARG:HG3   | 3:C:66:ILE:CD1   | 2.47                     | 0.44              |
| 3:C:619:THR:OG1  | 3:C:620:GLY:N    | 2.50                     | 0.44              |
| 3:C:1066:ALA:CB  | 4:D:506:ARG:HA   | 2.48                     | 0.44              |
| 4:D:12:ILE:HD11  | 4:D:1221:TRP:CE2 | 2.53                     | 0.44              |
| 4:D:23:TRP:HB3   | 4:D:92:MET:HE3   | 2.00                     | 0.44              |
| 4:D:796:ASN:ND2  | 4:D:798:ILE:HB   | 2.28                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:E:29:PRO:CG     | 5:E:34:ASN:HB2    | 2.47                     | 0.44              |
| 2:B:170:PRO:CB    | 2:B:202:ILE:HD11  | 2.43                     | 0.44              |
| 2:B:191:LYS:HG2   | 2:B:193:ILE:HD11  | 1.99                     | 0.44              |
| 4:D:735:VAL:CG1   | 4:D:816:LEU:HD22  | 2.48                     | 0.44              |
| 4:D:735:VAL:CG1   | 4:D:840:ARG:HD2   | 2.42                     | 0.44              |
| 6:F:320:ILE:HG22  | 6:F:337:LEU:HD12  | 2.00                     | 0.44              |
| 3:C:498:ASN:HB2   | 3:C:502:PHE:O     | 2.18                     | 0.43              |
| 4:D:397:ARG:HG3   | 4:D:397:ARG:O     | 2.18                     | 0.43              |
| 4:D:1152:ASP:O    | 4:D:1156:GLU:HG3  | 2.18                     | 0.43              |
| 9:T:269:VAL:O     | 9:T:269:VAL:HG23  | 2.17                     | 0.43              |
| 2:B:17:ASN:OD1    | 2:B:17:ASN:N      | 2.36                     | 0.43              |
| 2:B:111:VAL:O     | 2:B:111:VAL:HG13  | 2.17                     | 0.43              |
| 3:C:166:VAL:CG1   | 3:C:372:VAL:HG23  | 2.48                     | 0.43              |
| 3:C:228:LEU:HD23  | 3:C:228:LEU:HA    | 1.70                     | 0.43              |
| 3:C:595:ARG:HA    | 3:C:595:ARG:HD2   | 1.90                     | 0.43              |
| 3:C:706:LEU:N     | 14:C:1306:HOH:O   | 2.25                     | 0.43              |
| 3:C:788:ARG:O     | 3:C:830:VAL:CG1   | 2.67                     | 0.43              |
| 4:D:799:ILE:CG2   | 4:D:803:LYS:HE2   | 2.48                     | 0.43              |
| 4:D:1123:LEU:HA   | 4:D:1131:VAL:HG22 | 2.01                     | 0.43              |
| 6:F:244:LEU:HD12  | 6:F:289:ILE:HG21  | 2.00                     | 0.43              |
| 8:P:4:DA:H2"      | 8:P:5:DC:H6       | 1.82                     | 0.43              |
| 2:A:40:ARG:CZ     | 2:B:33:THR:HG22   | 2.48                     | 0.43              |
| 2:B:104:VAL:O     | 2:B:104:VAL:HG13  | 2.18                     | 0.43              |
| 2:B:151:GLN:HG2   | 2:B:151:GLN:O     | 2.17                     | 0.43              |
| 3:C:947:ALA:O     | 3:C:951:PRO:HD2   | 2.19                     | 0.43              |
| 3:C:1028:VAL:HG12 | 4:D:429:VAL:CG1   | 2.47                     | 0.43              |
| 4:D:47:PHE:CD1    | 4:D:322:PRO:HB3   | 2.52                     | 0.43              |
| 4:D:119:ASP:C     | 4:D:120:LEU:HD12  | 2.43                     | 0.43              |
| 4:D:339:ASP:CG    | 4:D:397:ARG:HH22  | 2.26                     | 0.43              |
| 4:D:813:THR:O     | 4:D:813:THR:HG22  | 2.18                     | 0.43              |
| 4:D:884:ILE:HD12  | 4:D:885:VAL:C     | 2.44                     | 0.43              |
| 4:D:1181:LEU:HD22 | 4:D:1207:VAL:HG11 | 2.01                     | 0.43              |
| 2:B:71:GLU:OE2    | 2:B:127:THR:HG23  | 2.18                     | 0.43              |
| 3:C:780:ILE:O     | 3:C:780:ILE:HG13  | 2.16                     | 0.43              |
| 4:D:281:ILE:HD12  | 4:D:281:ILE:C     | 2.43                     | 0.43              |
| 4:D:901:ALA:HB2   | 4:D:912:ASP:H     | 1.82                     | 0.43              |
| 6:F:345:PRO:HA    | 6:F:348:VAL:HG13  | 1.99                     | 0.43              |
| 3:C:174:PRO:O     | 3:C:303:GLY:HA2   | 2.18                     | 0.43              |
| 3:C:344:THR:O     | 3:C:344:THR:HG22  | 2.19                     | 0.43              |
| 3:C:505:THR:HG22  | 3:C:506:PRO:HD2   | 2.00                     | 0.43              |
| 3:C:587:PHE:HB3   | 3:C:590:HIS:HD2   | 1.84                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 6:F:321:GLN:NE2  | 6:F:331:GLU:OE2   | 2.52                     | 0.43              |
| 6:F:349:LEU:HD12 | 6:F:349:LEU:HA    | 1.80                     | 0.43              |
| 9:T:254:LEU:HB2  | 9:T:256:LEU:HG    | 2.01                     | 0.43              |
| 1:J:69:VAL:N     | 1:J:70:PRO:CD     | 2.82                     | 0.43              |
| 2:B:152:ASN:CA   | 2:B:154:ALA:HA    | 2.47                     | 0.43              |
| 3:C:265:LEU:HD21 | 3:C:284:GLN:HA    | 2.00                     | 0.43              |
| 3:C:390:VAL:HG11 | 3:C:394:ARG:HH21  | 1.84                     | 0.43              |
| 3:C:597:LEU:HD23 | 3:C:597:LEU:C     | 2.43                     | 0.43              |
| 3:C:667:ALA:HB3  | 3:C:675:ALA:HB3   | 2.01                     | 0.43              |
| 3:C:1025:HIS:CD2 | 3:C:1025:HIS:O    | 2.72                     | 0.43              |
| 4:D:163:GLU:HG2  | 4:D:166:ARG:HH21  | 1.83                     | 0.43              |
| 6:F:171:LYS:HB3  | 6:F:171:LYS:HE2   | 1.78                     | 0.43              |
| 6:F:465:LEU:O    | 6:F:466:ASP:HB2   | 2.17                     | 0.43              |
| 1:J:57:ARG:HG3   | 4:D:25:TYR:C      | 2.43                     | 0.43              |
| 1:J:106:LYS:HE2  | 1:J:106:LYS:HB3   | 1.77                     | 0.43              |
| 2:B:74:THR:HG21  | 4:D:608:GLU:OE1   | 2.18                     | 0.43              |
| 3:C:43:GLY:O     | 3:C:46:ASP:HB2    | 2.18                     | 0.43              |
| 4:D:246:ASP:OD1  | 4:D:246:ASP:N     | 2.50                     | 0.43              |
| 4:D:269:ASP:OD2  | 4:D:272:ALA:N     | 2.52                     | 0.43              |
| 4:D:629:VAL:HG13 | 4:D:671:MET:HE1   | 1.99                     | 0.43              |
| 4:D:1119:PRO:O   | 4:D:1122:VAL:HG13 | 2.19                     | 0.43              |
| 2:A:210:SER:CB   | 2:B:229:SER:CB    | 2.96                     | 0.43              |
| 2:B:33:THR:OG1   | 2:B:34:LEU:N      | 2.51                     | 0.43              |
| 3:C:361:ILE:H    | 3:C:361:ILE:CD1   | 2.28                     | 0.43              |
| 3:C:447:SER:HB2  | 3:C:449:LEU:HD11  | 2.00                     | 0.43              |
| 3:C:728:LEU:HD22 | 3:C:906:ILE:HG22  | 1.96                     | 0.43              |
| 3:C:1100:GLY:CA  | 4:D:458:LYS:HE3   | 2.43                     | 0.43              |
| 5:E:37:ILE:H     | 5:E:37:ILE:HG13   | 1.27                     | 0.43              |
| 2:B:28:PRO:HA    | 2:B:29:GLY:HA2    | 1.80                     | 0.43              |
| 2:B:134:LEU:HD23 | 2:B:134:LEU:C     | 2.44                     | 0.43              |
| 3:C:51:SER:HB2   | 3:C:371:THR:OG1   | 2.19                     | 0.43              |
| 3:C:365:GLY:HA3  | 3:C:525:ASP:OD1   | 2.19                     | 0.43              |
| 3:C:369:LEU:HD12 | 3:C:369:LEU:HA    | 1.61                     | 0.43              |
| 3:C:405:PRO:O    | 3:C:409:ILE:HG13  | 2.19                     | 0.43              |
| 3:C:479:THR:OG1  | 3:C:480:PRO:CD    | 2.67                     | 0.43              |
| 3:C:1001:LEU:HB2 | 3:C:1010:PHE:HD2  | 1.83                     | 0.43              |
| 4:D:818:GLY:C    | 4:D:838:SER:HB3   | 2.44                     | 0.43              |
| 4:D:982:MET:HE3  | 4:D:1151:HIS:CG   | 2.54                     | 0.43              |
| 4:D:1140:GLN:NE2 | 4:D:1155:ILE:HD12 | 2.34                     | 0.43              |
| 2:A:175:THR:OG1  | 3:C:899:PRO:O     | 2.31                     | 0.43              |
| 2:B:68:GLY:O     | 2:B:129:ASN:N     | 2.41                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:197:PRO:HB3   | 3:C:297:TYR:CZ    | 2.54                     | 0.43              |
| 3:C:427:LEU:HD12  | 3:C:427:LEU:N     | 2.34                     | 0.43              |
| 3:C:851:GLU:C     | 3:C:852:LEU:HD12  | 2.44                     | 0.43              |
| 3:C:895:MET:HG3   | 3:C:896:PRO:CD    | 2.49                     | 0.43              |
| 3:C:1049:GLY:HA3  | 4:D:421:ARG:CZ    | 2.49                     | 0.43              |
| 4:D:656:LYS:O     | 4:D:656:LYS:HE2   | 2.19                     | 0.43              |
| 5:E:53:TYR:HE1    | 5:E:101:LEU:HD12  | 1.84                     | 0.43              |
| 2:A:40:ARG:CD     | 2:B:33:THR:HG22   | 2.41                     | 0.42              |
| 2:B:192:LEU:C     | 2:B:193:ILE:HD13  | 2.43                     | 0.42              |
| 3:C:113:CYS:HA    | 3:C:118:MET:HG3   | 2.01                     | 0.42              |
| 3:C:128:ALA:CB    | 3:C:405:PRO:HB3   | 2.49                     | 0.42              |
| 3:C:466:VAL:HG12  | 4:D:856:ARG:CZ    | 2.49                     | 0.42              |
| 3:C:584:MET:HE3   | 3:C:622:GLU:HG3   | 2.01                     | 0.42              |
| 3:C:815:ILE:HG13  | 6:F:449:MET:HE1   | 2.01                     | 0.42              |
| 3:C:839:ILE:HD12  | 3:C:865:ALA:HB2   | 2.01                     | 0.42              |
| 3:C:949:LYS:HG3   | 3:C:949:LYS:O     | 2.19                     | 0.42              |
| 4:D:397:ARG:NH2   | 6:F:360:SER:OG    | 2.52                     | 0.42              |
| 4:D:938:GLU:OE1   | 4:D:938:GLU:N     | 2.35                     | 0.42              |
| 4:D:1056:LEU:HD23 | 4:D:1057:GLU:N    | 2.34                     | 0.42              |
| 2:A:24:GLU:HB3    | 2:A:191:LYS:CG    | 2.49                     | 0.42              |
| 2:A:147:VAL:CG1   | 2:A:166:SER:HB2   | 2.48                     | 0.42              |
| 2:B:22:VAL:HG12   | 2:B:193:ILE:HG23  | 2.00                     | 0.42              |
| 2:B:64:THR:HA     | 2:B:73:VAL:HG21   | 2.00                     | 0.42              |
| 3:C:114:LYS:HG2   | 3:C:161:GLY:O     | 2.19                     | 0.42              |
| 3:C:310:LYS:O     | 3:C:354:VAL:HG21  | 2.19                     | 0.42              |
| 3:C:475:CYS:HB2   | 3:C:579:SER:HB3   | 2.00                     | 0.42              |
| 3:C:834:GLU:O     | 3:C:835:SER:OG    | 2.31                     | 0.42              |
| 3:C:1090:ARG:O    | 3:C:1093:VAL:HG12 | 2.19                     | 0.42              |
| 4:D:599:TYR:CA    | 4:D:610:GLY:HA3   | 2.48                     | 0.42              |
| 4:D:831:ILE:HA    | 4:D:831:ILE:HD12  | 1.72                     | 0.42              |
| 6:F:263:ASN:O     | 6:F:267:ILE:HG13  | 2.19                     | 0.42              |
| 6:F:440:ARG:O     | 6:F:444:ILE:HG13  | 2.19                     | 0.42              |
| 1:J:58:ASN:HD21   | 1:J:60:LEU:HG     | 1.83                     | 0.42              |
| 2:A:34:LEU:HD23   | 2:A:34:LEU:HA     | 1.77                     | 0.42              |
| 2:A:84:VAL:HG13   | 2:A:84:VAL:O      | 2.19                     | 0.42              |
| 3:C:31:SER:HA     | 3:C:964:ALA:O     | 2.19                     | 0.42              |
| 3:C:562:VAL:HG12  | 3:C:563:SER:N     | 2.34                     | 0.42              |
| 3:C:1001:LEU:N    | 3:C:1001:LEU:HD23 | 2.34                     | 0.42              |
| 4:D:647:GLU:OE1   | 4:D:655:TRP:HH2   | 2.02                     | 0.42              |
| 4:D:1034:GLU:O    | 14:D:2105:HOH:O   | 2.21                     | 0.42              |
| 4:D:1163:LEU:HA   | 4:D:1163:LEU:HD23 | 1.79                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:E:81:GLU:O      | 5:E:94:ARG:NH2    | 2.48                     | 0.42              |
| 6:F:452:LEU:HD12  | 6:F:452:LEU:HA    | 1.83                     | 0.42              |
| 2:A:98:ARG:O      | 2:A:99:LYS:HD2    | 2.19                     | 0.42              |
| 2:A:161:ARG:O     | 2:A:163:PRO:HD3   | 2.19                     | 0.42              |
| 3:C:169:GLN:HB2   | 3:C:427:LEU:CD2   | 2.50                     | 0.42              |
| 3:C:529:ARG:HB3   | 3:C:529:ARG:CZ    | 2.49                     | 0.42              |
| 3:C:602:MET:HA    | 3:C:605:GLN:HB2   | 2.02                     | 0.42              |
| 4:D:35:ASN:OD1    | 4:D:37:ARG:N      | 2.47                     | 0.42              |
| 4:D:568:PRO:HB3   | 4:D:983:ALA:HB2   | 2.02                     | 0.42              |
| 4:D:686:GLN:O     | 4:D:686:GLN:HG3   | 2.19                     | 0.42              |
| 2:A:146:TYR:OH    | 3:C:869:LYS:NZ    | 2.53                     | 0.42              |
| 3:C:454:LEU:HD12  | 3:C:454:LEU:O     | 2.19                     | 0.42              |
| 3:C:1003:ASP:HB2  | 3:C:1010:PHE:CE1  | 2.54                     | 0.42              |
| 3:C:1074:TYR:CZ   | 4:D:1258:LEU:HD21 | 2.55                     | 0.42              |
| 4:D:51:ILE:H      | 4:D:51:ILE:HG12   | 1.67                     | 0.42              |
| 4:D:83:THR:OG1    | 4:D:84:ARG:N      | 2.53                     | 0.42              |
| 4:D:452:PHE:CE1   | 4:D:491:ILE:HG12  | 2.55                     | 0.42              |
| 4:D:584:GLY:HA3   | 4:D:719:GLY:O     | 2.19                     | 0.42              |
| 4:D:641:ARG:CZ    | 4:D:655:TRP:CZ2   | 3.02                     | 0.42              |
| 4:D:781:THR:CG2   | 4:D:814:ARG:HD2   | 2.49                     | 0.42              |
| 4:D:900:LEU:HD11  | 4:D:948:ILE:HD12  | 2.02                     | 0.42              |
| 4:D:1044:LYS:HE3  | 4:D:1118:ASP:HB2  | 2.01                     | 0.42              |
| 4:D:1170:ASP:O    | 4:D:1202:ALA:HA   | 2.19                     | 0.42              |
| 5:E:60:GLN:HG3    | 5:E:74:GLU:CB     | 2.49                     | 0.42              |
| 6:F:325:LEU:HD23  | 6:F:330:ARG:O     | 2.18                     | 0.42              |
| 2:A:175:THR:HG22  | 2:A:195:ASP:HB3   | 2.01                     | 0.42              |
| 2:B:26:LEU:HD13   | 2:B:30:PHE:HB3    | 2.02                     | 0.42              |
| 3:C:691:GLN:HG2   | 3:C:692:VAL:H     | 1.84                     | 0.42              |
| 3:C:751:ARG:CD    | 3:C:856:VAL:HG22  | 2.50                     | 0.42              |
| 4:D:117:LEU:O     | 4:D:117:LEU:HD22  | 2.19                     | 0.42              |
| 4:D:334:ARG:HD3   | 6:F:356:ARG:NH2   | 2.35                     | 0.42              |
| 4:D:735:VAL:HG11  | 4:D:816:LEU:CD2   | 2.50                     | 0.42              |
| 4:D:934:ASN:OD1   | 4:D:934:ASN:N     | 2.53                     | 0.42              |
| 4:D:1171:SER:HA   | 4:D:1174:THR:CG2  | 2.48                     | 0.42              |
| 4:D:1208:LEU:HD23 | 4:D:1208:LEU:HA   | 1.85                     | 0.42              |
| 3:C:985:PRO:HB3   | 3:C:989:GLY:HA2   | 2.01                     | 0.42              |
| 4:D:653:ASN:HB2   | 4:D:654:GLY:HA2   | 1.99                     | 0.42              |
| 2:A:149:ALA:HB2   | 2:A:164:VAL:C     | 2.45                     | 0.42              |
| 2:B:50:ALA:HB2    | 2:B:167:ILE:O     | 2.19                     | 0.42              |
| 3:C:203:LEU:HD22  | 3:C:217:ILE:HA    | 2.02                     | 0.42              |
| 3:C:627:ILE:HD12  | 3:C:628:ASP:N     | 2.35                     | 0.42              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:C:963:VAL:HG12  | 3:C:964:ALA:N    | 2.35                     | 0.42              |
| 4:D:245:GLN:O     | 4:D:249:GLY:HA3  | 2.19                     | 0.42              |
| 6:F:310:MET:O     | 6:F:314:ILE:HG13 | 2.20                     | 0.42              |
| 2:A:40:ARG:NH2    | 2:B:32:TYR:HD2   | 2.18                     | 0.42              |
| 3:C:885:VAL:HG11  | 4:D:538:GLY:HA2  | 2.02                     | 0.42              |
| 3:C:1122:LEU:HD12 | 3:C:1122:LEU:HA  | 1.83                     | 0.42              |
| 4:D:250:GLU:HG3   | 4:D:251:TYR:CE2  | 2.55                     | 0.42              |
| 4:D:640:LEU:O     | 4:D:656:LYS:HE3  | 2.19                     | 0.42              |
| 4:D:991:GLY:HA2   | 4:D:1265:ILE:CD1 | 2.50                     | 0.42              |
| 1:J:48:ALA:HB2    | 4:D:65:TYR:OH    | 2.19                     | 0.42              |
| 2:A:93:VAL:CG2    | 2:A:113:PRO:HG3  | 2.49                     | 0.42              |
| 2:B:226:ASN:O     | 2:B:227:ALA:HB3  | 2.19                     | 0.42              |
| 3:C:89:ASP:OD1    | 3:C:89:ASP:N     | 2.51                     | 0.42              |
| 3:C:178:PHE:CE1   | 3:C:193:VAL:HG21 | 2.55                     | 0.42              |
| 3:C:263:GLU:HA    | 3:C:266:LEU:HD12 | 2.01                     | 0.42              |
| 3:C:467:HIS:HD2   | 3:C:469:SER:OG   | 2.02                     | 0.42              |
| 3:C:510:VAL:HG11  | 3:C:567:VAL:CB   | 2.50                     | 0.42              |
| 3:C:870:ILE:HD12  | 3:C:870:ILE:HA   | 1.91                     | 0.42              |
| 3:C:982:SER:CB    | 3:C:983:THR:HG23 | 2.29                     | 0.42              |
| 4:D:555:ALA:HA    | 4:D:559:MET:HE3  | 2.01                     | 0.42              |
| 4:D:556:ARG:O     | 4:D:560:LEU:HB2  | 2.19                     | 0.42              |
| 4:D:579:LEU:HD23  | 4:D:807:THR:HB   | 2.02                     | 0.42              |
| 4:D:742:GLN:O     | 4:D:746:GLU:HG2  | 2.19                     | 0.42              |
| 4:D:951:LEU:HD22  | 4:D:956:ILE:HG12 | 2.01                     | 0.42              |
| 6:F:320:ILE:O     | 6:F:324:LEU:HB2  | 2.19                     | 0.42              |
| 2:A:95:MET:N      | 2:A:138:LEU:O    | 2.32                     | 0.41              |
| 2:B:65:THR:N      | 2:B:73:VAL:HG23  | 2.35                     | 0.41              |
| 2:B:147:VAL:CG1   | 2:B:166:SER:HB2  | 2.50                     | 0.41              |
| 3:C:85:SER:HA     | 3:C:86:PRO:HA    | 1.68                     | 0.41              |
| 3:C:939:VAL:HG22  | 3:C:940:ALA:CA   | 2.50                     | 0.41              |
| 4:D:113:ARG:HB2   | 4:D:312:MET:HE1  | 2.01                     | 0.41              |
| 4:D:527:LEU:CD1   | 4:D:712:VAL:HG12 | 2.49                     | 0.41              |
| 4:D:1036:PHE:HD2  | 4:D:1162:MET:HE1 | 1.84                     | 0.41              |
| 2:B:97:LEU:HD23   | 2:B:136:VAL:CG1  | 2.50                     | 0.41              |
| 3:C:71:GLU:OE2    | 3:C:71:GLU:HA    | 2.17                     | 0.41              |
| 3:C:393:GLU:CD    | 6:F:247:ARG:HD3  | 2.46                     | 0.41              |
| 3:C:583:ALA:HB3   | 3:C:621:MET:HG3  | 2.01                     | 0.41              |
| 3:C:584:MET:HE2   | 3:C:584:MET:HB3  | 1.93                     | 0.41              |
| 4:D:110:VAL:O     | 4:D:110:VAL:HG13 | 2.20                     | 0.41              |
| 4:D:687:MET:HE2   | 4:D:695:ILE:HD11 | 2.00                     | 0.41              |
| 4:D:740:GLN:H     | 4:D:740:GLN:NE2  | 2.04                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:D:1036:PHE:O    | 4:D:1211:ILE:HG23 | 2.20                     | 0.41              |
| 4:D:1100:LEU:HD23 | 4:D:1100:LEU:C    | 2.45                     | 0.41              |
| 4:D:1258:LEU:HD12 | 4:D:1258:LEU:HA   | 1.90                     | 0.41              |
| 5:E:80:VAL:CG1    | 5:E:81:GLU:H      | 2.34                     | 0.41              |
| 9:T:256:LEU:HB3   | 9:T:260:SER:HB2   | 2.00                     | 0.41              |
| 1:J:71:GLU:HG2    | 1:J:72:PRO:HD2    | 2.02                     | 0.41              |
| 2:A:2:LEU:HD12    | 2:B:143:GLY:CA    | 2.50                     | 0.41              |
| 2:A:214:THR:HG23  | 2:B:231:HIS:CG    | 2.55                     | 0.41              |
| 2:B:176:TYR:H     | 2:B:176:TYR:HD1   | 1.68                     | 0.41              |
| 3:C:723:GLU:HB3   | 4:D:536:PHE:HD1   | 1.85                     | 0.41              |
| 3:C:973:GLU:CB    | 4:D:732:MET:HE3   | 2.50                     | 0.41              |
| 3:C:1014:VAL:HA   | 4:D:729:THR:HG21  | 2.02                     | 0.41              |
| 4:D:82:VAL:HG13   | 4:D:82:VAL:O      | 2.21                     | 0.41              |
| 4:D:433:GLY:HA3   | 4:D:436:LEU:HD12  | 2.01                     | 0.41              |
| 6:F:246:LYS:HE2   | 6:F:246:LYS:HB3   | 1.96                     | 0.41              |
| 2:B:8:THR:O       | 2:B:23:ILE:HA     | 2.21                     | 0.41              |
| 2:B:47:PRO:HA     | 2:B:144:ARG:CG    | 2.45                     | 0.41              |
| 3:C:370:ARG:HG2   | 3:C:374:GLU:CD    | 2.45                     | 0.41              |
| 3:C:445:ARG:C     | 3:C:446:LEU:HD23  | 2.45                     | 0.41              |
| 3:C:493:VAL:HG23  | 3:C:578:VAL:O     | 2.20                     | 0.41              |
| 3:C:851:GLU:O     | 3:C:852:LEU:CG    | 2.64                     | 0.41              |
| 3:C:1031:LYS:NZ   | 10:C:1203:SO4:S   | 2.93                     | 0.41              |
| 4:D:133:ALA:HB3   | 4:D:234:LEU:HD21  | 2.01                     | 0.41              |
| 4:D:924:LEU:HD21  | 4:D:959:VAL:HG11  | 2.01                     | 0.41              |
| 4:D:1249:LEU:HB3  | 4:D:1260:PRO:HD2  | 2.02                     | 0.41              |
| 2:A:106:THR:HB    | 2:A:123:MET:O     | 2.20                     | 0.41              |
| 2:B:161:ARG:HA    | 2:B:161:ARG:HD3   | 1.53                     | 0.41              |
| 3:C:103:PHE:CE2   | 3:C:124:LEU:HG    | 2.56                     | 0.41              |
| 3:C:186:THR:HG23  | 3:C:188:LYS:H     | 1.84                     | 0.41              |
| 3:C:610:VAL:HG23  | 3:C:611:ARG:N     | 2.36                     | 0.41              |
| 4:D:92:MET:N      | 14:D:2109:HOH:O   | 2.32                     | 0.41              |
| 4:D:699:LEU:HD11  | 4:D:711:THR:HG21  | 2.02                     | 0.41              |
| 4:D:1191:ASN:OD1  | 4:D:1202:ALA:HB3  | 2.20                     | 0.41              |
| 5:E:29:PRO:CB     | 5:E:33:THR:HG23   | 2.50                     | 0.41              |
| 1:J:84:MET:CE     | 6:F:272:LYS:HB2   | 2.51                     | 0.41              |
| 3:C:180:GLU:HB3   | 3:C:191:HIS:CD2   | 2.56                     | 0.41              |
| 3:C:781:VAL:CG2   | 3:C:838:VAL:HG21  | 2.50                     | 0.41              |
| 3:C:870:ILE:HG13  | 3:C:886:ILE:CD1   | 2.50                     | 0.41              |
| 3:C:946:TRP:CE2   | 3:C:978:GLY:HA3   | 2.56                     | 0.41              |
| 4:D:740:GLN:O     | 4:D:744:ILE:HG13  | 2.19                     | 0.41              |
| 4:D:884:ILE:HD11  | 4:D:886:ARG:HD3   | 2.03                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:T:297:VAL:O     | 9:T:301:LEU:HG    | 2.20                     | 0.41              |
| 2:A:12:GLU:HB2    | 2:A:20:ARG:O      | 2.20                     | 0.41              |
| 2:A:42:LEU:O      | 2:A:46:ILE:HG12   | 2.21                     | 0.41              |
| 3:C:400:VAL:O     | 3:C:401:GLU:HB3   | 2.20                     | 0.41              |
| 3:C:506:PRO:O     | 3:C:572:VAL:HG13  | 2.20                     | 0.41              |
| 3:C:727:ILE:O     | 3:C:728:LEU:HD23  | 2.21                     | 0.41              |
| 3:C:967:VAL:HG23  | 3:C:968:PHE:N     | 2.33                     | 0.41              |
| 4:D:293:LEU:HD23  | 4:D:293:LEU:C     | 2.46                     | 0.41              |
| 4:D:755:ILE:HD13  | 4:D:772:SER:OG    | 2.20                     | 0.41              |
| 4:D:791:PHE:O     | 4:D:791:PHE:HD1   | 2.04                     | 0.41              |
| 4:D:877:VAL:O     | 4:D:881:GLN:HB3   | 2.21                     | 0.41              |
| 4:D:1122:VAL:HG23 | 4:D:1126:GLN:HE21 | 1.84                     | 0.41              |
| 4:D:1168:ILE:HD13 | 4:D:1176:PHE:CG   | 2.55                     | 0.41              |
| 4:D:1181:LEU:CD1  | 4:D:1213:LYS:HE2  | 2.51                     | 0.41              |
| 1:J:85:LEU:O      | 1:J:85:LEU:HD12   | 2.20                     | 0.41              |
| 2:B:158:GLU:CB    | 2:B:161:ARG:HB2   | 2.46                     | 0.41              |
| 3:C:189:THR:O     | 3:C:190:LEU:HG    | 2.20                     | 0.41              |
| 3:C:783:ILE:H     | 3:C:783:ILE:CD1   | 2.07                     | 0.41              |
| 2:A:46:ILE:HA     | 2:A:47:PRO:HD3    | 1.91                     | 0.41              |
| 2:B:30:PHE:CA     | 2:B:33:THR:HG23   | 2.47                     | 0.41              |
| 2:B:151:GLN:CG    | 2:B:151:GLN:O     | 2.68                     | 0.41              |
| 2:B:191:LYS:HE2   | 2:B:191:LYS:HB3   | 1.90                     | 0.41              |
| 3:C:165:VAL:HG23  | 3:C:431:MET:HB2   | 2.02                     | 0.41              |
| 3:C:434:ASN:HA    | 3:C:673:THR:OG1   | 2.21                     | 0.41              |
| 3:C:494:TYR:HD2   | 3:C:572:VAL:CG2   | 2.28                     | 0.41              |
| 3:C:538:PRO:O     | 3:C:546:THR:OG1   | 2.38                     | 0.41              |
| 3:C:644:VAL:O     | 3:C:644:VAL:HG23  | 2.21                     | 0.41              |
| 3:C:708:LYS:HG3   | 3:C:737:VAL:HG23  | 2.03                     | 0.41              |
| 3:C:1011:PRO:HB2  | 3:C:1012:TYR:CD2  | 2.56                     | 0.41              |
| 4:D:155:MET:HE1   | 4:D:219:LEU:CB    | 2.51                     | 0.41              |
| 4:D:177:LEU:HD23  | 4:D:177:LEU:C     | 2.46                     | 0.41              |
| 4:D:229:LEU:HA    | 4:D:233:GLN:OE1   | 2.21                     | 0.41              |
| 4:D:365:ILE:HD11  | 6:F:235:GLU:OE2   | 2.21                     | 0.41              |
| 4:D:500:ARG:HH21  | 4:D:539:ASP:CG    | 2.29                     | 0.41              |
| 4:D:680:TYR:HA    | 4:D:681:PRO:HD3   | 1.94                     | 0.41              |
| 4:D:797:PRO:O     | 4:D:801:ILE:HG13  | 2.21                     | 0.41              |
| 4:D:815:THR:CG2   | 4:D:820:LYS:HA    | 2.35                     | 0.41              |
| 4:D:1004:GLU:HB3  | 4:D:1005:PRO:HD3  | 2.03                     | 0.41              |
| 4:D:1069:PRO:HB2  | 4:D:1071:ASP:OD1  | 2.21                     | 0.41              |
| 5:E:78:PRO:O      | 5:E:80:VAL:O      | 2.39                     | 0.41              |
| 5:E:80:VAL:CG1    | 5:E:81:GLU:N      | 2.83                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 6:F:306:ILE:HG22 | 6:F:310:MET:HB3   | 2.03                     | 0.41              |
| 7:O:31:DT:H5'    | 7:O:31:DT:C6      | 2.56                     | 0.41              |
| 9:T:279:THR:CG2  | 9:T:282:ASP:HB2   | 2.44                     | 0.41              |
| 9:T:283:LEU:HD23 | 9:T:283:LEU:HA    | 1.87                     | 0.41              |
| 2:B:134:LEU:HD23 | 2:B:135:GLU:N     | 2.36                     | 0.41              |
| 3:C:31:SER:O     | 3:C:954:LEU:HD11  | 2.21                     | 0.41              |
| 3:C:574:PRO:HB2  | 3:C:968:PHE:HB2   | 2.03                     | 0.41              |
| 3:C:758:GLU:CG   | 3:C:798:THR:HG22  | 2.38                     | 0.41              |
| 3:C:1041:SER:HB3 | 3:C:1044:THR:O    | 2.21                     | 0.41              |
| 4:D:31:PRO:HB3   | 4:D:348:ILE:HG23  | 2.03                     | 0.41              |
| 4:D:412:ARG:HA   | 4:D:416:ASN:HD22  | 1.86                     | 0.41              |
| 4:D:831:ILE:O    | 4:D:831:ILE:HG22  | 2.19                     | 0.41              |
| 6:F:324:LEU:CD2  | 6:F:328:LEU:HD22  | 2.51                     | 0.41              |
| 6:F:359:ILE:HG22 | 6:F:360:SER:N     | 2.35                     | 0.41              |
| 7:O:6:DA:H2''    | 7:O:7:DC:OP2      | 2.20                     | 0.41              |
| 2:B:105:VAL:HB   | 2:B:125:ILE:CG2   | 2.47                     | 0.40              |
| 3:C:33:ALA:HB2   | 3:C:966:PRO:CG    | 2.50                     | 0.40              |
| 3:C:270:ARG:O    | 3:C:274:PRO:HG3   | 2.21                     | 0.40              |
| 3:C:808:GLU:H    | 3:C:808:GLU:CD    | 2.25                     | 0.40              |
| 4:D:243:GLU:HA   | 4:D:246:ASP:OD1   | 2.21                     | 0.40              |
| 4:D:281:ILE:HD12 | 4:D:282:ARG:N     | 2.36                     | 0.40              |
| 4:D:1181:LEU:CD2 | 4:D:1207:VAL:HG11 | 2.51                     | 0.40              |
| 6:F:332:PRO:HA   | 6:F:336:GLU:OE1   | 2.21                     | 0.40              |
| 1:J:58:ASN:HD21  | 1:J:60:LEU:CD1    | 2.33                     | 0.40              |
| 2:A:218:LEU:HD12 | 2:A:218:LEU:HA    | 1.84                     | 0.40              |
| 2:B:183:VAL:O    | 2:B:183:VAL:CG1   | 2.70                     | 0.40              |
| 3:C:44:LEU:HD11  | 3:C:628:ASP:HB2   | 2.03                     | 0.40              |
| 3:C:169:GLN:O    | 3:C:369:LEU:HA    | 2.20                     | 0.40              |
| 3:C:273:ARG:N    | 3:C:274:PRO:HD3   | 2.35                     | 0.40              |
| 3:C:778:ARG:H    | 3:C:778:ARG:HG3   | 1.63                     | 0.40              |
| 4:D:592:VAL:HG23 | 4:D:630:ARG:HB3   | 2.03                     | 0.40              |
| 4:D:600:GLN:CB   | 4:D:601:ALA:CA    | 2.98                     | 0.40              |
| 4:D:873:THR:O    | 4:D:877:VAL:HG23  | 2.22                     | 0.40              |
| 4:D:1129:ARG:O   | 4:D:1133:ILE:HG12 | 2.20                     | 0.40              |
| 4:D:1171:SER:CB  | 4:D:1172:GLY:CA   | 2.99                     | 0.40              |
| 9:T:279:THR:O    | 9:T:282:ASP:N     | 2.50                     | 0.40              |
| 2:A:36:ASN:HB2   | 3:C:1007:GLY:HA3  | 2.03                     | 0.40              |
| 2:B:89:ASP:O     | 2:B:90:ASP:HB2    | 2.21                     | 0.40              |
| 2:B:230:GLU:OE1  | 2:B:230:GLU:HA    | 2.21                     | 0.40              |
| 3:C:196:ILE:HD12 | 3:C:196:ILE:HA    | 1.94                     | 0.40              |
| 3:C:412:ARG:NH1  | 6:F:322:ARG:HH11  | 2.19                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:508:ARG:HH11 | 3:C:570:MET:CE   | 2.34                     | 0.40              |
| 3:C:571:ASP:HB3  | 3:C:576:GLN:HE21 | 1.86                     | 0.40              |
| 3:C:621:MET:HA   | 3:C:621:MET:HE3  | 2.03                     | 0.40              |
| 4:D:656:LYS:HA   | 4:D:659:ASP:HB2  | 2.03                     | 0.40              |
| 4:D:859:LEU:HD12 | 4:D:862:THR:HG21 | 2.03                     | 0.40              |
| 6:F:437:THR:OG1  | 7:O:3:DT:OP2     | 2.39                     | 0.40              |
| 6:F:439:GLU:OE1  | 8:P:22:DC:H5     | 2.04                     | 0.40              |
| 2:B:51:VAL:CG1   | 2:B:164:VAL:HG21 | 2.50                     | 0.40              |
| 3:C:228:LEU:O    | 3:C:231:ALA:N    | 2.55                     | 0.40              |
| 3:C:444:ARG:O    | 3:C:446:LEU:HD23 | 2.22                     | 0.40              |
| 3:C:523:THR:OG1  | 3:C:524:ALA:N    | 2.54                     | 0.40              |
| 4:D:34:ILE:O     | 6:F:304:ILE:HG23 | 2.21                     | 0.40              |
| 4:D:153:ALA:O    | 4:D:157:VAL:HG23 | 2.21                     | 0.40              |
| 4:D:277:LEU:O    | 4:D:277:LEU:HD23 | 2.21                     | 0.40              |
| 4:D:644:THR:O    | 4:D:647:GLU:HG2  | 2.21                     | 0.40              |
| 4:D:666:THR:HG23 | 4:D:669:ARG:HD2  | 2.04                     | 0.40              |
| 4:D:1004:GLU:N   | 4:D:1005:PRO:HD2 | 2.35                     | 0.40              |
| 2:B:198:THR:HG22 | 2:B:199:LYS:N    | 2.37                     | 0.40              |
| 3:C:698:CYS:O    | 3:C:705:ALA:O    | 2.38                     | 0.40              |
| 3:C:754:LYS:H    | 3:C:754:LYS:NZ   | 2.20                     | 0.40              |
| 3:C:801:GLY:HA2  | 3:C:802:GLU:C    | 2.47                     | 0.40              |
| 4:D:640:LEU:O    | 4:D:656:LYS:CE   | 2.70                     | 0.40              |

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

| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 3:C:777:GLU:OE2 | 4:D:209:ARG:NH1[2_356] | 2.19                     | 0.01              |

## 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   | J     | 81/114 (71%)    | 75 (93%)   | 6 (7%)   | 0        | 100         | 100 |
| 2   | A     | 214/350 (61%)   | 201 (94%)  | 13 (6%)  | 0        | 100         | 100 |
| 2   | B     | 231/350 (66%)   | 216 (94%)  | 13 (6%)  | 2 (1%)   | 14          | 28  |
| 3   | C     | 1093/1169 (94%) | 1039 (95%) | 50 (5%)  | 4 (0%)   | 30          | 50  |
| 4   | D     | 1238/1317 (94%) | 1190 (96%) | 45 (4%)  | 3 (0%)   | 43          | 64  |
| 5   | E     | 72/107 (67%)    | 65 (90%)   | 5 (7%)   | 2 (3%)   | 4           | 6   |
| 6   | F     | 313/466 (67%)   | 307 (98%)  | 6 (2%)   | 0        | 100         | 100 |
| 9   | T     | 51/100 (51%)    | 51 (100%)  | 0        | 0        | 100         | 100 |
| All | All   | 3293/3973 (83%) | 3144 (96%) | 138 (4%) | 11 (0%)  | 36          | 56  |

All (11) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 5   | E     | 76   | VAL  |
| 3   | C     | 982  | SER  |
| 3   | C     | 544  | ARG  |
| 3   | C     | 1134 | ALA  |
| 4   | D     | 902  | GLU  |
| 4   | D     | 1194 | VAL  |
| 2   | B     | 184  | GLU  |
| 5   | E     | 78   | PRO  |
| 2   | B     | 183  | VAL  |
| 3   | C     | 967  | VAL  |
| 4   | D     | 935  | VAL  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|-------------|----|
| 1   | J     | 71/98 (72%)   | 62 (87%)  | 9 (13%)  | 4           | 8  |
| 2   | A     | 178/297 (60%) | 159 (89%) | 19 (11%) | 6           | 12 |
| 2   | B     | 171/297 (58%) | 151 (88%) | 20 (12%) | 5           | 9  |
| 3   | C     | 857/984 (87%) | 762 (89%) | 95 (11%) | 6           | 11 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers  | Percentiles |    |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 4   | D     | 994/1095 (91%)  | 894 (90%)  | 100 (10%) | 7           | 14 |
| 5   | E     | 62/86 (72%)     | 52 (84%)   | 10 (16%)  | 2           | 4  |
| 6   | F     | 252/379 (66%)   | 227 (90%)  | 25 (10%)  | 7           | 15 |
| 9   | T     | 36/86 (42%)     | 29 (81%)   | 7 (19%)   | 1           | 2  |
| All | All   | 2621/3322 (79%) | 2336 (89%) | 285 (11%) | 6           | 12 |

All (285) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | J     | 47  | ASP  |
| 1   | J     | 55  | LEU  |
| 1   | J     | 58  | ASN  |
| 1   | J     | 64  | LEU  |
| 1   | J     | 66  | GLU  |
| 1   | J     | 71  | GLU  |
| 1   | J     | 91  | VAL  |
| 1   | J     | 104 | LEU  |
| 1   | J     | 105 | ILE  |
| 2   | A     | 14  | VAL  |
| 2   | A     | 40  | ARG  |
| 2   | A     | 71  | GLU  |
| 2   | A     | 74  | THR  |
| 2   | A     | 91  | GLU  |
| 2   | A     | 111 | VAL  |
| 2   | A     | 117 | THR  |
| 2   | A     | 127 | THR  |
| 2   | A     | 129 | ASN  |
| 2   | A     | 130 | ASP  |
| 2   | A     | 134 | LEU  |
| 2   | A     | 135 | GLU  |
| 2   | A     | 136 | VAL  |
| 2   | A     | 150 | VAL  |
| 2   | A     | 159 | ILE  |
| 2   | A     | 168 | TYR  |
| 2   | A     | 171 | VAL  |
| 2   | A     | 187 | THR  |
| 2   | A     | 194 | ILE  |
| 2   | B     | 17  | ASN  |
| 2   | B     | 33  | THR  |
| 2   | B     | 38  | LEU  |
| 2   | B     | 43  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 51  | VAL  |
| 2   | B     | 60  | LEU  |
| 2   | B     | 63  | PHE  |
| 2   | B     | 84  | VAL  |
| 2   | B     | 85  | VAL  |
| 2   | B     | 99  | LYS  |
| 2   | B     | 110 | ILE  |
| 2   | B     | 125 | ILE  |
| 2   | B     | 144 | ARG  |
| 2   | B     | 161 | ARG  |
| 2   | B     | 176 | TYR  |
| 2   | B     | 178 | VAL  |
| 2   | B     | 200 | ASN  |
| 2   | B     | 215 | LEU  |
| 2   | B     | 218 | LEU  |
| 2   | B     | 231 | HIS  |
| 3   | C     | 44  | LEU  |
| 3   | C     | 45  | LEU  |
| 3   | C     | 46  | ASP  |
| 3   | C     | 58  | SER  |
| 3   | C     | 70  | GLU  |
| 3   | C     | 71  | GLU  |
| 3   | C     | 77  | LEU  |
| 3   | C     | 81  | LEU  |
| 3   | C     | 94  | MET  |
| 3   | C     | 96  | LEU  |
| 3   | C     | 119 | THR  |
| 3   | C     | 124 | LEU  |
| 3   | C     | 202 | TRP  |
| 3   | C     | 204 | GLU  |
| 3   | C     | 227 | VAL  |
| 3   | C     | 241 | GLU  |
| 3   | C     | 248 | ILE  |
| 3   | C     | 253 | LEU  |
| 3   | C     | 268 | ILE  |
| 3   | C     | 280 | LYS  |
| 3   | C     | 299 | LEU  |
| 3   | C     | 301 | ARG  |
| 3   | C     | 336 | LEU  |
| 3   | C     | 347 | THR  |
| 3   | C     | 364 | PHE  |
| 3   | C     | 404 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 434 | ASN  |
| 3   | C     | 437 | LEU  |
| 3   | C     | 441 | THR  |
| 3   | C     | 443 | LYS  |
| 3   | C     | 446 | LEU  |
| 3   | C     | 449 | LEU  |
| 3   | C     | 454 | LEU  |
| 3   | C     | 462 | GLU  |
| 3   | C     | 466 | VAL  |
| 3   | C     | 491 | LEU  |
| 3   | C     | 531 | VAL  |
| 3   | C     | 546 | THR  |
| 3   | C     | 552 | VAL  |
| 3   | C     | 568 | ASP  |
| 3   | C     | 605 | GLN  |
| 3   | C     | 607 | VAL  |
| 3   | C     | 611 | ARG  |
| 3   | C     | 617 | VAL  |
| 3   | C     | 623 | LEU  |
| 3   | C     | 624 | ARG  |
| 3   | C     | 636 | ASP  |
| 3   | C     | 640 | VAL  |
| 3   | C     | 703 | GLU  |
| 3   | C     | 727 | ILE  |
| 3   | C     | 737 | VAL  |
| 3   | C     | 753 | THR  |
| 3   | C     | 754 | LYS  |
| 3   | C     | 763 | ASP  |
| 3   | C     | 775 | LEU  |
| 3   | C     | 777 | GLU  |
| 3   | C     | 778 | ARG  |
| 3   | C     | 780 | ILE  |
| 3   | C     | 783 | ILE  |
| 3   | C     | 823 | VAL  |
| 3   | C     | 830 | VAL  |
| 3   | C     | 839 | ILE  |
| 3   | C     | 848 | ASP  |
| 3   | C     | 859 | LEU  |
| 3   | C     | 872 | ASP  |
| 3   | C     | 876 | LEU  |
| 3   | C     | 895 | MET  |
| 3   | C     | 919 | ILE  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | C     | 927  | LEU  |
| 3   | C     | 936  | ASN  |
| 3   | C     | 954  | LEU  |
| 3   | C     | 961  | SER  |
| 3   | C     | 965  | THR  |
| 3   | C     | 984  | LEU  |
| 3   | C     | 986  | ASN  |
| 3   | C     | 987  | ARG  |
| 3   | C     | 988  | ASP  |
| 3   | C     | 1001 | LEU  |
| 3   | C     | 1008 | GLU  |
| 3   | C     | 1021 | ILE  |
| 3   | C     | 1022 | LEU  |
| 3   | C     | 1028 | VAL  |
| 3   | C     | 1032 | ILE  |
| 3   | C     | 1045 | GLN  |
| 3   | C     | 1048 | LEU  |
| 3   | C     | 1084 | SER  |
| 3   | C     | 1088 | VAL  |
| 3   | C     | 1091 | VAL  |
| 3   | C     | 1108 | ILE  |
| 3   | C     | 1116 | LEU  |
| 3   | C     | 1122 | LEU  |
| 3   | C     | 1128 | VAL  |
| 3   | C     | 1129 | LEU  |
| 3   | C     | 1132 | ASP  |
| 3   | C     | 1138 | MET  |
| 4   | D     | 7    | PHE  |
| 4   | D     | 12   | ILE  |
| 4   | D     | 14   | LEU  |
| 4   | D     | 28   | VAL  |
| 4   | D     | 51   | ILE  |
| 4   | D     | 70   | PHE  |
| 4   | D     | 101  | VAL  |
| 4   | D     | 117  | LEU  |
| 4   | D     | 129  | ILE  |
| 4   | D     | 144  | ARG  |
| 4   | D     | 148  | LEU  |
| 4   | D     | 150  | THR  |
| 4   | D     | 165  | GLN  |
| 4   | D     | 187  | GLU  |
| 4   | D     | 234  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | D     | 238 | GLU  |
| 4   | D     | 239 | VAL  |
| 4   | D     | 240 | LEU  |
| 4   | D     | 243 | GLU  |
| 4   | D     | 246 | ASP  |
| 4   | D     | 259 | GLU  |
| 4   | D     | 270 | ILE  |
| 4   | D     | 304 | GLN  |
| 4   | D     | 314 | LEU  |
| 4   | D     | 345 | ARG  |
| 4   | D     | 360 | LEU  |
| 4   | D     | 365 | ILE  |
| 4   | D     | 417 | LEU  |
| 4   | D     | 449 | LEU  |
| 4   | D     | 451 | LEU  |
| 4   | D     | 456 | VAL  |
| 4   | D     | 467 | GLN  |
| 4   | D     | 489 | GLU  |
| 4   | D     | 504 | LEU  |
| 4   | D     | 507 | LEU  |
| 4   | D     | 513 | GLU  |
| 4   | D     | 518 | GLU  |
| 4   | D     | 558 | LEU  |
| 4   | D     | 562 | SER  |
| 4   | D     | 566 | LEU  |
| 4   | D     | 567 | SER  |
| 4   | D     | 574 | LEU  |
| 4   | D     | 576 | MET  |
| 4   | D     | 588 | LEU  |
| 4   | D     | 591 | LEU  |
| 4   | D     | 599 | TYR  |
| 4   | D     | 600 | GLN  |
| 4   | D     | 603 | THR  |
| 4   | D     | 627 | LEU  |
| 4   | D     | 629 | VAL  |
| 4   | D     | 635 | VAL  |
| 4   | D     | 647 | GLU  |
| 4   | D     | 653 | ASN  |
| 4   | D     | 655 | TRP  |
| 4   | D     | 656 | LYS  |
| 4   | D     | 666 | THR  |
| 4   | D     | 667 | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 4   | D     | 675  | LEU  |
| 4   | D     | 687  | MET  |
| 4   | D     | 706  | ILE  |
| 4   | D     | 713  | ASP  |
| 4   | D     | 724  | THR  |
| 4   | D     | 740  | GLN  |
| 4   | D     | 741  | LYS  |
| 4   | D     | 743  | GLU  |
| 4   | D     | 746  | GLU  |
| 4   | D     | 767  | THR  |
| 4   | D     | 769  | ARG  |
| 4   | D     | 784  | VAL  |
| 4   | D     | 799  | ILE  |
| 4   | D     | 831  | ILE  |
| 4   | D     | 853  | HIS  |
| 4   | D     | 876  | LEU  |
| 4   | D     | 900  | LEU  |
| 4   | D     | 914  | HIS  |
| 4   | D     | 923  | THR  |
| 4   | D     | 939  | ARG  |
| 4   | D     | 945  | ASP  |
| 4   | D     | 952  | LEU  |
| 4   | D     | 956  | ILE  |
| 4   | D     | 961  | VAL  |
| 4   | D     | 1009 | LEU  |
| 4   | D     | 1039 | ARG  |
| 4   | D     | 1042 | ARG  |
| 4   | D     | 1056 | LEU  |
| 4   | D     | 1079 | ASP  |
| 4   | D     | 1086 | ARG  |
| 4   | D     | 1087 | LEU  |
| 4   | D     | 1112 | LEU  |
| 4   | D     | 1122 | VAL  |
| 4   | D     | 1150 | ILE  |
| 4   | D     | 1183 | GLU  |
| 4   | D     | 1186 | GLU  |
| 4   | D     | 1208 | LEU  |
| 4   | D     | 1215 | SER  |
| 4   | D     | 1222 | LEU  |
| 4   | D     | 1234 | LEU  |
| 4   | D     | 1241 | CYS  |
| 4   | D     | 1258 | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 4   | D     | 1278 | GLU  |
| 5   | E     | 37   | ILE  |
| 5   | E     | 50   | LEU  |
| 5   | E     | 59   | ARG  |
| 5   | E     | 76   | VAL  |
| 5   | E     | 84   | LEU  |
| 5   | E     | 85   | GLN  |
| 5   | E     | 89   | LEU  |
| 5   | E     | 101  | LEU  |
| 5   | E     | 102  | GLU  |
| 5   | E     | 104  | THR  |
| 6   | F     | 166  | VAL  |
| 6   | F     | 172  | GLN  |
| 6   | F     | 182  | GLU  |
| 6   | F     | 216  | ARG  |
| 6   | F     | 268  | ARG  |
| 6   | F     | 291  | GLN  |
| 6   | F     | 310  | MET  |
| 6   | F     | 313  | VAL  |
| 6   | F     | 317  | LEU  |
| 6   | F     | 324  | LEU  |
| 6   | F     | 325  | LEU  |
| 6   | F     | 337  | LEU  |
| 6   | F     | 348  | VAL  |
| 6   | F     | 349  | LEU  |
| 6   | F     | 373  | LEU  |
| 6   | F     | 383  | VAL  |
| 6   | F     | 402  | LEU  |
| 6   | F     | 412  | VAL  |
| 6   | F     | 420  | THR  |
| 6   | F     | 433  | VAL  |
| 6   | F     | 437  | THR  |
| 6   | F     | 452  | LEU  |
| 6   | F     | 462  | ARG  |
| 6   | F     | 465  | LEU  |
| 6   | F     | 466  | ASP  |
| 9   | T     | 254  | LEU  |
| 9   | T     | 255  | ASP  |
| 9   | T     | 260  | SER  |
| 9   | T     | 275  | LEU  |
| 9   | T     | 279  | THR  |
| 9   | T     | 284  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | T     | 288 | ASN  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | J     | 58   | ASN  |
| 2   | A     | 129  | ASN  |
| 3   | C     | 48   | GLN  |
| 3   | C     | 160  | ASN  |
| 3   | C     | 343  | GLN  |
| 3   | C     | 410  | ASN  |
| 3   | C     | 426  | GLN  |
| 3   | C     | 433  | GLN  |
| 3   | C     | 434  | ASN  |
| 3   | C     | 467  | HIS  |
| 3   | C     | 534  | GLN  |
| 3   | C     | 576  | GLN  |
| 3   | C     | 590  | HIS  |
| 3   | C     | 603  | GLN  |
| 3   | C     | 685  | GLN  |
| 3   | C     | 700  | GLN  |
| 3   | C     | 720  | HIS  |
| 3   | C     | 742  | HIS  |
| 3   | C     | 936  | ASN  |
| 3   | C     | 1046 | GLN  |
| 3   | C     | 1057 | GLN  |
| 3   | C     | 1068 | GLN  |
| 3   | C     | 1120 | GLN  |
| 4   | D     | 165  | GLN  |
| 4   | D     | 287  | GLN  |
| 4   | D     | 303  | GLN  |
| 4   | D     | 368  | ASN  |
| 4   | D     | 416  | ASN  |
| 4   | D     | 467  | GLN  |
| 4   | D     | 494  | HIS  |
| 4   | D     | 515  | GLN  |
| 4   | D     | 552  | GLN  |
| 4   | D     | 564  | ASN  |
| 4   | D     | 600  | GLN  |
| 4   | D     | 740  | GLN  |
| 4   | D     | 748  | HIS  |
| 4   | D     | 765  | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 4   | D     | 778  | GLN  |
| 4   | D     | 796  | ASN  |
| 4   | D     | 881  | GLN  |
| 4   | D     | 932  | ASN  |
| 4   | D     | 1126 | GLN  |
| 4   | D     | 1146 | GLN  |
| 5   | E     | 34   | ASN  |
| 5   | E     | 85   | GLN  |
| 5   | E     | 103  | HIS  |
| 6   | F     | 172  | GLN  |
| 6   | F     | 199  | GLN  |
| 6   | F     | 214  | GLN  |
| 6   | F     | 309  | HIS  |
| 6   | F     | 321  | GLN  |

### 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 21 ligands modelled in this entry, 3 are monoatomic - leaving 18 for Mogul analysis.

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 11  | EDO  | C     | 1204 | -    | 3,3,3        | 0.42 | 0        | 2,2,2       | 0.38 | 0        |
| 11  | EDO  | D     | 2009 | -    | 3,3,3        | 0.42 | 0        | 2,2,2       | 0.35 | 0        |
| 11  | EDO  | F     | 506  | -    | 3,3,3        | 0.43 | 0        | 2,2,2       | 0.31 | 0        |
| 10  | SO4  | D     | 2004 | -    | 4,4,4        | 0.24 | 0        | 6,6,6       | 0.10 | 0        |
| 10  | SO4  | C     | 1202 | -    | 4,4,4        | 0.24 | 0        | 6,6,6       | 0.11 | 0        |
| 10  | SO4  | C     | 1203 | -    | 4,4,4        | 0.23 | 0        | 6,6,6       | 0.05 | 0        |
| 10  | SO4  | D     | 2007 | -    | 4,4,4        | 0.24 | 0        | 6,6,6       | 0.09 | 0        |
| 10  | SO4  | F     | 501  | -    | 4,4,4        | 0.23 | 0        | 6,6,6       | 0.09 | 0        |
| 10  | SO4  | F     | 502  | -    | 4,4,4        | 0.23 | 0        | 6,6,6       | 0.10 | 0        |
| 10  | SO4  | F     | 503  | -    | 4,4,4        | 0.24 | 0        | 6,6,6       | 0.09 | 0        |
| 11  | EDO  | D     | 2008 | -    | 3,3,3        | 0.43 | 0        | 2,2,2       | 0.33 | 0        |
| 11  | EDO  | D     | 2010 | -    | 3,3,3        | 0.43 | 0        | 2,2,2       | 0.23 | 0        |
| 10  | SO4  | F     | 504  | -    | 4,4,4        | 0.24 | 0        | 6,6,6       | 0.08 | 0        |
| 10  | SO4  | F     | 505  | -    | 4,4,4        | 0.23 | 0        | 6,6,6       | 0.07 | 0        |
| 11  | EDO  | C     | 1205 | -    | 3,3,3        | 0.43 | 0        | 2,2,2       | 0.33 | 0        |
| 10  | SO4  | D     | 2006 | -    | 4,4,4        | 0.24 | 0        | 6,6,6       | 0.07 | 0        |
| 10  | SO4  | D     | 2005 | -    | 4,4,4        | 0.23 | 0        | 6,6,6       | 0.07 | 0        |
| 10  | SO4  | C     | 1201 | -    | 4,4,4        | 0.23 | 0        | 6,6,6       | 0.07 | 0        |

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

| Mol | Type | Chain | Res  | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|----------|-------|
| 11  | EDO  | C     | 1204 | -    | -       | 1/1/1/1  | -     |
| 11  | EDO  | D     | 2009 | -    | -       | 0/1/1/1  | -     |
| 11  | EDO  | F     | 506  | -    | -       | 1/1/1/1  | -     |
| 11  | EDO  | D     | 2008 | -    | -       | 1/1/1/1  | -     |
| 11  | EDO  | D     | 2010 | -    | -       | 0/1/1/1  | -     |
| 11  | EDO  | C     | 1205 | -    | -       | 1/1/1/1  | -     |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       |
|-----|-------|------|------|-------------|
| 11  | C     | 1204 | EDO  | O1-C1-C2-O2 |
| 11  | D     | 2008 | EDO  | O1-C1-C2-O2 |
| 11  | C     | 1205 | EDO  | O1-C1-C2-O2 |

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| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 11  | F     | 506 | EDO  | O1-C1-C2-O2 |

There are no ring outliers.

6 monomers are involved in 10 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 11  | F     | 506  | EDO  | 1       | 0            |
| 10  | C     | 1203 | SO4  | 2       | 0            |
| 10  | F     | 502  | SO4  | 1       | 0            |
| 11  | D     | 2008 | EDO  | 3       | 0            |
| 11  | C     | 1205 | EDO  | 1       | 0            |
| 10  | D     | 2005 | SO4  | 2       | 0            |

## 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   | J     | 83/114 (72%)    | 0.50   | 3 (3%) 46 44   | 65, 98, 141, 159      | 0     |
| 2   | A     | 218/350 (62%)   | 0.57   | 11 (5%) 34 34  | 60, 88, 120, 139      | 0     |
| 2   | B     | 233/350 (66%)   | 1.05   | 34 (14%) 6 5   | 82, 112, 136, 148     | 0     |
| 3   | C     | 1099/1169 (94%) | 0.51   | 58 (5%) 32 31  | 43, 86, 149, 168      | 0     |
| 4   | D     | 1248/1317 (94%) | 0.25   | 31 (2%) 58 56  | 39, 74, 127, 157      | 0     |
| 5   | E     | 76/107 (71%)    | 0.33   | 2 (2%) 57 55   | 52, 79, 113, 118      | 0     |
| 6   | F     | 319/466 (68%)   | 0.13   | 9 (2%) 55 53   | 40, 74, 136, 159      | 0     |
| 7   | O     | 31/31 (100%)    | -0.48  | 0 100 100      | 52, 65, 85, 90        | 0     |
| 8   | P     | 26/26 (100%)    | -0.41  | 0 100 100      | 60, 70, 84, 94        | 0     |
| 9   | T     | 53/100 (53%)    | 1.34   | 14 (26%) 1 1   | 115, 149, 167, 170    | 0     |
| All | All   | 3386/4030 (84%) | 0.41   | 162 (4%) 35 35 | 39, 83, 143, 170      | 0     |

All (162) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | B     | 155 | SER  | 6.0  |
| 9   | T     | 275 | LEU  | 5.9  |
| 3   | C     | 228 | LEU  | 5.0  |
| 3   | C     | 229 | LEU  | 4.4  |
| 2   | B     | 157 | ALA  | 4.2  |
| 2   | A     | 2   | LEU  | 4.0  |
| 2   | A     | 218 | LEU  | 4.0  |
| 3   | C     | 562 | VAL  | 4.0  |
| 3   | C     | 277 | PRO  | 3.8  |
| 6   | F     | 154 | ALA  | 3.8  |
| 1   | J     | 26  | PRO  | 3.8  |
| 2   | B     | 1   | MET  | 3.7  |
| 6   | F     | 156 | ALA  | 3.7  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 2   | B     | 229  | SER  | 3.5  |
| 4   | D     | 663  | ALA  | 3.4  |
| 2   | B     | 171  | VAL  | 3.4  |
| 3   | C     | 311  | LEU  | 3.4  |
| 3   | C     | 299  | LEU  | 3.4  |
| 3   | C     | 330  | VAL  | 3.3  |
| 2   | B     | 64   | THR  | 3.3  |
| 3   | C     | 481  | GLU  | 3.3  |
| 2   | B     | 43   | LEU  | 3.2  |
| 4   | D     | 901  | ALA  | 3.2  |
| 2   | A     | 90   | ASP  | 3.2  |
| 3   | C     | 201  | ALA  | 3.2  |
| 3   | C     | 968  | PHE  | 3.2  |
| 3   | C     | 248  | ILE  | 3.1  |
| 3   | C     | 287  | LEU  | 3.1  |
| 2   | B     | 183  | VAL  | 3.1  |
| 4   | D     | 111  | PRO  | 3.1  |
| 9   | T     | 283  | LEU  | 3.1  |
| 3   | C     | 252  | THR  | 3.0  |
| 6   | F     | 151  | SER  | 3.0  |
| 3   | C     | 324  | LEU  | 3.0  |
| 2   | B     | 152  | ASN  | 3.0  |
| 9   | T     | 269  | VAL  | 3.0  |
| 2   | B     | 107  | ALA  | 3.0  |
| 4   | D     | 611  | VAL  | 3.0  |
| 3   | C     | 455  | SER  | 2.9  |
| 2   | B     | 140  | VAL  | 2.9  |
| 4   | D     | 4    | VAL  | 2.9  |
| 3   | C     | 227  | VAL  | 2.9  |
| 4   | D     | 817  | ALA  | 2.9  |
| 2   | B     | 61   | HIS  | 2.9  |
| 4   | D     | 633  | ILE  | 2.9  |
| 9   | T     | 251  | ILE  | 2.9  |
| 4   | D     | 1179 | GLY  | 2.9  |
| 4   | D     | 1009 | LEU  | 2.9  |
| 4   | D     | 991  | GLY  | 2.8  |
| 3   | C     | 323  | THR  | 2.8  |
| 3   | C     | 240  | VAL  | 2.8  |
| 3   | C     | 329  | VAL  | 2.8  |
| 4   | D     | 728  | VAL  | 2.8  |
| 2   | B     | 177  | LYS  | 2.8  |
| 1   | J     | 69   | VAL  | 2.8  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 3   | C     | 361  | ILE  | 2.7  |
| 2   | B     | 44   | SER  | 2.7  |
| 3   | C     | 675  | ALA  | 2.7  |
| 1   | J     | 72   | PRO  | 2.7  |
| 3   | C     | 21   | ASN  | 2.7  |
| 4   | D     | 65   | TYR  | 2.7  |
| 4   | D     | 903  | ARG  | 2.6  |
| 2   | B     | 21   | PHE  | 2.6  |
| 4   | D     | 607  | PRO  | 2.6  |
| 3   | C     | 218  | ASP  | 2.6  |
| 3   | C     | 190  | LEU  | 2.6  |
| 9   | T     | 272  | VAL  | 2.5  |
| 3   | C     | 938  | ASP  | 2.5  |
| 4   | D     | 924  | LEU  | 2.5  |
| 3   | C     | 254  | GLU  | 2.5  |
| 9   | T     | 276  | VAL  | 2.5  |
| 4   | D     | 849  | PHE  | 2.5  |
| 3   | C     | 145  | MET  | 2.5  |
| 2   | B     | 65   | THR  | 2.5  |
| 5   | E     | 24   | SER  | 2.5  |
| 2   | B     | 7    | PRO  | 2.5  |
| 3   | C     | 1053 | GLN  | 2.5  |
| 3   | C     | 459  | ALA  | 2.5  |
| 9   | T     | 294  | ILE  | 2.4  |
| 2   | B     | 178  | VAL  | 2.4  |
| 2   | B     | 63   | PHE  | 2.4  |
| 2   | B     | 154  | ALA  | 2.4  |
| 3   | C     | 535  | ALA  | 2.4  |
| 2   | A     | 3    | ILE  | 2.4  |
| 2   | A     | 221  | LEU  | 2.4  |
| 2   | B     | 163  | PRO  | 2.4  |
| 4   | D     | 1178 | PRO  | 2.4  |
| 2   | B     | 32   | TYR  | 2.4  |
| 6   | F     | 144  | PRO  | 2.4  |
| 2   | B     | 164  | VAL  | 2.4  |
| 3   | C     | 225  | VAL  | 2.4  |
| 3   | C     | 671  | HIS  | 2.4  |
| 3   | C     | 203  | LEU  | 2.3  |
| 9   | T     | 270  | HIS  | 2.3  |
| 2   | B     | 227  | ALA  | 2.3  |
| 9   | T     | 264  | LEU  | 2.3  |
| 6   | F     | 147  | ARG  | 2.3  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 3   | C     | 1048 | LEU  | 2.3  |
| 4   | D     | 1283 | ALA  | 2.3  |
| 9   | T     | 301  | LEU  | 2.3  |
| 2   | B     | 231  | HIS  | 2.3  |
| 4   | D     | 813  | THR  | 2.3  |
| 3   | C     | 594  | ASN  | 2.3  |
| 4   | D     | 1173 | SER  | 2.3  |
| 3   | C     | 765  | PRO  | 2.3  |
| 3   | C     | 1011 | PRO  | 2.3  |
| 3   | C     | 205  | PHE  | 2.3  |
| 4   | D     | 1169 | ILE  | 2.3  |
| 4   | D     | 66   | LYS  | 2.3  |
| 2   | B     | 35   | GLY  | 2.3  |
| 2   | A     | 51   | VAL  | 2.3  |
| 2   | B     | 172  | LEU  | 2.3  |
| 3   | C     | 823  | VAL  | 2.3  |
| 9   | T     | 297  | VAL  | 2.3  |
| 2   | A     | 30   | PHE  | 2.3  |
| 3   | C     | 196  | ILE  | 2.2  |
| 3   | C     | 267  | ASP  | 2.2  |
| 2   | B     | 60   | LEU  | 2.2  |
| 2   | B     | 153  | LYS  | 2.2  |
| 5   | E     | 26   | TYR  | 2.2  |
| 2   | A     | 26   | LEU  | 2.2  |
| 9   | T     | 254  | LEU  | 2.2  |
| 3   | C     | 1043 | ILE  | 2.2  |
| 4   | D     | 729  | THR  | 2.2  |
| 4   | D     | 599  | TYR  | 2.2  |
| 3   | C     | 463  | VAL  | 2.2  |
| 3   | C     | 572  | VAL  | 2.2  |
| 3   | C     | 234  | TRP  | 2.2  |
| 4   | D     | 6    | PHE  | 2.2  |
| 3   | C     | 331  | ALA  | 2.2  |
| 6   | F     | 149  | ALA  | 2.2  |
| 2   | B     | 62   | GLU  | 2.2  |
| 9   | T     | 271  | THR  | 2.2  |
| 3   | C     | 623  | LEU  | 2.2  |
| 3   | C     | 573  | SER  | 2.2  |
| 4   | D     | 733  | ALA  | 2.1  |
| 4   | D     | 284  | GLY  | 2.1  |
| 2   | B     | 194  | ILE  | 2.1  |
| 6   | F     | 145  | ALA  | 2.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 3   | C     | 946 | TRP  | 2.1  |
| 3   | C     | 952 | GLU  | 2.1  |
| 3   | C     | 266 | LEU  | 2.1  |
| 3   | C     | 550 | VAL  | 2.1  |
| 4   | D     | 605 | ASP  | 2.1  |
| 2   | A     | 180 | ALA  | 2.1  |
| 4   | D     | 412 | ARG  | 2.1  |
| 3   | C     | 279 | THR  | 2.1  |
| 3   | C     | 697 | PRO  | 2.1  |
| 3   | C     | 882 | ASN  | 2.1  |
| 6   | F     | 140 | ALA  | 2.1  |
| 6   | F     | 143 | ALA  | 2.1  |
| 3   | C     | 268 | ILE  | 2.1  |
| 4   | D     | 635 | VAL  | 2.1  |
| 2   | A     | 50  | ALA  | 2.0  |
| 3   | C     | 558 | GLU  | 2.0  |
| 4   | D     | 288 | LYS  | 2.0  |
| 2   | A     | 196 | VAL  | 2.0  |
| 2   | B     | 91  | GLU  | 2.0  |
| 3   | C     | 22  | SER  | 2.0  |
| 9   | T     | 256 | LEU  | 2.0  |
| 2   | B     | 59  | VAL  | 2.0  |
| 2   | B     | 66  | VAL  | 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.

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 10  | SO4  | D     | 2007 | 5/5   | 0.71 | 0.08 | 95,100,113,141              | 0     |
| 10  | SO4  | F     | 504  | 5/5   | 0.72 | 0.07 | 115,115,118,128             | 0     |
| 10  | SO4  | C     | 1203 | 5/5   | 0.73 | 0.08 | 106,115,140,197             | 0     |
| 10  | SO4  | C     | 1202 | 5/5   | 0.75 | 0.08 | 108,111,116,178             | 0     |
| 13  | MG   | D     | 2003 | 1/1   | 0.78 | 0.29 | 79,79,79,79                 | 0     |
| 10  | SO4  | C     | 1201 | 5/5   | 0.79 | 0.07 | 113,115,126,138             | 0     |
| 11  | EDO  | D     | 2009 | 4/4   | 0.80 | 0.12 | 74,89,104,104               | 0     |
| 11  | EDO  | C     | 1205 | 4/4   | 0.80 | 0.15 | 74,94,102,113               | 0     |
| 11  | EDO  | F     | 506  | 4/4   | 0.83 | 0.12 | 74,88,95,95                 | 0     |
| 11  | EDO  | C     | 1204 | 4/4   | 0.85 | 0.11 | 52,66,79,80                 | 0     |
| 11  | EDO  | D     | 2008 | 4/4   | 0.87 | 0.10 | 73,90,108,108               | 0     |
| 10  | SO4  | D     | 2006 | 5/5   | 0.87 | 0.10 | 85,104,119,125              | 0     |
| 10  | SO4  | F     | 501  | 5/5   | 0.87 | 0.06 | 100,100,118,124             | 0     |
| 10  | SO4  | F     | 502  | 5/5   | 0.87 | 0.09 | 88,88,104,107               | 0     |
| 10  | SO4  | D     | 2004 | 5/5   | 0.89 | 0.11 | 70,77,85,88                 | 0     |
| 10  | SO4  | F     | 505  | 5/5   | 0.90 | 0.10 | 79,86,117,167               | 0     |
| 10  | SO4  | F     | 503  | 5/5   | 0.91 | 0.10 | 86,95,99,116                | 0     |
| 11  | EDO  | D     | 2010 | 4/4   | 0.92 | 0.21 | 63,76,77,90                 | 0     |
| 10  | SO4  | D     | 2005 | 5/5   | 0.93 | 0.14 | 86,87,98,125                | 0     |
| 12  | ZN   | D     | 2002 | 1/1   | 0.95 | 0.16 | 222,222,222,222             | 0     |
| 12  | ZN   | D     | 2001 | 1/1   | 1.00 | 0.08 | 78,78,78,78                 | 0     |

## 6.5 Other polymers

There are no such residues in this entry.